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SPECTRRAD

Spectrometer Software System

Version 16

2025

Special thanks to Evgenii Nikolaevich Kurnikov. Evgenii perform translation of the programs packet first version from FORTRAN to C++, made a great contribution to father development of the packet, write a main part of the program code for controlling the spectrometric devices.

General remarks

The software package, united by the name "SPECTRRAD", is designed to control alpha, beta and gamma radiation spectrometers with any type of detectors.

The Windows version of the package runs on Windows 95, 98, NT, 2000, XP, 7, 8, 10.

It provides control of spectrometric ADC units and autonomous spectrometers from "Aspect" and "Parsek" companies, spectrometers from "Canberra", "GreenStar", "GBS ELEKTRONIK", "ORTEC", "Amplituda", "Dose", "RADEK", "CB RADAR", "Expertcenter".

When a spectrometer operating under the control of the SPECTRRAD package is put into operation, its calibration and initial verification (metrological certification) must be carried out.

Since the program, as a rule, is delivered already installed and configured for a specific spectrometric complex, the package description is structured in such a way that for routine work with the package it is enough to familiarize yourself with the section "Working with the package" placed at the beginning of the description. Those users who want to independently form the spectrometric complexes and processing procedures they need will need to read the package description to the end. The description does not include procedures for file operations common to all programs running on Windows: "Create", "Open", "Save", "Save as...", etc., and data: "Cut", "Copy", "Paste", etc.

Brief description

Full automation of the measurements and results processing.

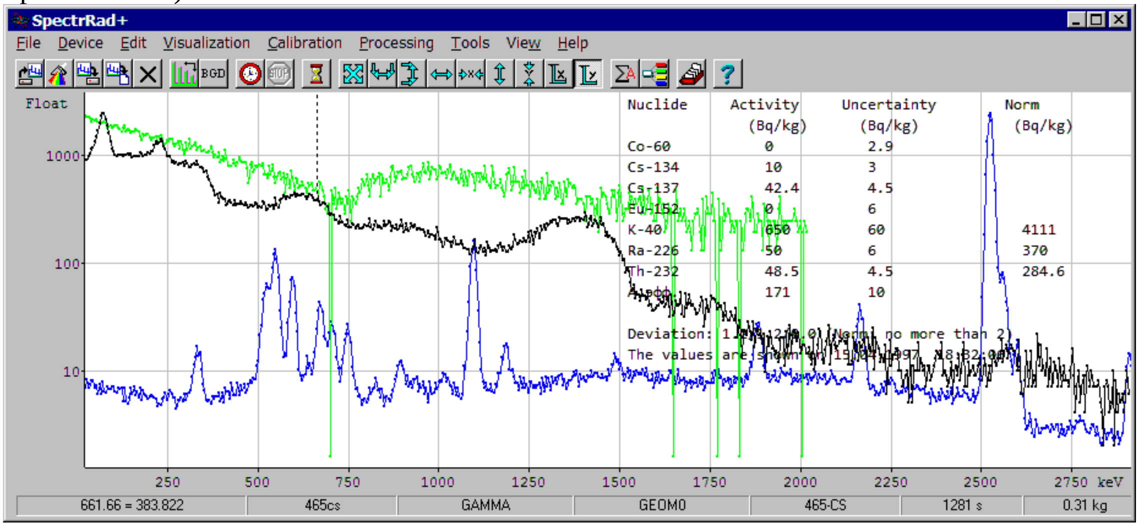
- The openness of the software provides the user with the opportunity to connect new detectors, form measurement geometries and libraries of nuclides - create spectrometric systems that meet their requirements.
- Processing of alpha, beta and gamma spectra measured on all types of detectors, joint processing of spectra allows creating the most effective spectrometric systems operating under the control of the “SPECTRRAD” package.
- The most modern methods of data processing (robust estimation, use of the full response function of the spectrometer, accounting true coincidences and escape lines), special methods for poorly resolved spectra, allow us to obtain the most effective estimates and determine up to 100 radionuclides at one measurement of the sample, detect the presence of radionuclides in the sample, that were not taken into account when processing the spectrum.
- A unique algorithm for accounting for deformations of spectra associated with energy scale drift (correction of gain, zero scale and nonlinear distortion of energy calibration, correction of spectrometer resolution) when processing spectra.
- Accounting for radiation absorption in the sample substance, media and shield materials in accordance with the chemical composition of the sample, automatic determination of the effective charge of the nuclei of the sample substance during spectrum processing.
- Accounting changes in the shape of peaks, elementary spectra, registration efficiency from physical ones (density of the counting sample, effective atomic number and effective atomic mass of the elements of the sample substance) and geometric parameters of the counting sample and geometry of measurements, loading of the spectrometer ensures high accuracy of estimates of nuclide activity.
- The cyclic measurement mode and the joint group processing of the spectra implement an amplitude–time analysis technique that is most effective in processing the spectra of samples containing short-lived nuclides. This takes into account the processes of decay and accumulation of nuclides during measurements. When processing the spectra in groups, a common system of equations is formed for all the spectra of the selected group. The group can include up to 100 spectra that are the results of measurements of the same counting sample carried out at different dates.

- The combined processing of beta and gamma spectra ensures reliable and effective determination of pure beta emitters (Sr-90, Y-90) in samples contaminated with other radionuclides.
- Automatic correction of spectrometer drift during measurements allows for multi-hour and multi-day measurements and, as a result, significantly reduces the lower limits of activity detection.
- Automatic energy calibration of spectrometers based on the results of processing the samples under study free the consumer from spectrometer calibration procedures significantly increases the accuracy of sample analysis.
- A convenient program for forming and editing nuclide tables, which allows you to form the necessary equilibrium chains of nuclides with just two mouse clicks. The basic library of nuclides includes more than 500 of the most common radionuclides.
- The programmable calculator allows the consumer to calculate the necessary additional radiation parameters based on the results of spectrum processing, control the measurement process and external processes, and create their own report forms.
- The built-in database automates the creation of a measurement archive, provides convenient access to the archive, allows statistical processing of an arbitrary sample of measurement results, and creates graphs of changes in spectrometer parameters over time (Shewhart control charts).
- The tables of sanitary rules and regulations and Radiation Protection and the Safety of Radiation Source standards allow you to automatically form conclusions about the results of sample studies.
- A flexible scheme for generating a report on measurement results allows you to generate reports of any required form, including in accordance with the requirements of MI 2453-2000.
- A multi-level control scheme for changing the parameters of the spectrometer provides reliable measurement quality control. The package provides the ability to automatically track and archive the parameters of the spectrometer's energy scale drift over time (resolution drift, gain factor and scale zero), peak shape, registration efficiency and background changes. The measurement quality control system prohibits operational measurements when the critical parameters of the spectrometer exceed the specified limits.
- Additional functions of precision radiometry and dosimetry expand the area of the spectrometer applies.
- Two modes of access to the programs setup and management procedures: limited and full (password protected) provides an effective protection scheme against unauthorized or low-skilled access to programs management. A user with full access rights has the ability to configure a restricted access system.

Working with the package

Application start. The main window

To launch the package from the Windows operating shell, click on the "Start" key of the Windows desktop taskbar, find the "SPECTRRAD" program shortcut in the "Programs" group and click on it with the left mouse button. Or, if the program shortcut is placed on the Windows desktop, double-click the package icon with the left mouse button. After launching, the main window of the "SPECTRRAD" program will appear on the screen (executable file SpectrRad.exe).



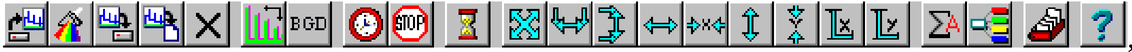
Nuclide	Activity (Bq/kg)	Uncertainty (Bq/kg)	Norm (Bq/kg)
Co-60	0	2.9	
Cs-134	10	3	
Cs-137	42.4	4.5	
Eu-152	0	6	
K-40	650	60	4111
Ra-226	50	6	370
Th-232	48.5	4.5	284.6
Aэфф	171	10	

Deviation: 1.[illegible] (Norm) no more than 2)

The values are shown on 15.04.1997 18:32:00

661.66 = 383.822 | 465cs | GAMMA | GEOM0 | 465-CS | 1281 s | 0.31 kg

In the upper part of the window there is a menu bar ("File", "Device", "Edit",...), "buttons" of the toolbar,



, providing more convenient access to the main menu items.

On the left is the ordinate scale (Y) for the spectrum being viewed. The dimension depends on the type of object being visualized. For the usual spectrum, it is the number of registered impulses. "**Float/Fixed**" - pointer: "floating/fixed" Y scale.

At the bottom is the abscissa scale (X). The dimension is also determined by the type of spectrum or function table. For a conventional spectrum, the channels of the spectrometer, if the energy calibration of the X scale is missing or disabled, or the energy in the units that were used during calibration of the spectrometer (usually in kiloelectronvolts), if calibration is enabled.

Below is a line of information about the spectrum:

- Information about the position of the "marker" - a movable pointer moving along the spectrum:
  - the position of the marker on the energy / channel scale (661.66),
  - the number of registered pulses in the corresponding channel of the spectrometer (383.822).
- The name of the spectrum files (465cs).
- The name of the spectrometer (GAMMA).
- The geometry of measurements (GEOM0).
- The code of the sample (465-CS).
- Sample measurement time in seconds (1281 s).
- The mass of the counting sample (0.31 kg).

The main parameters of the main window can be changed using the group of menu items "**View**" (see "Main Menu").

The program allows simultaneous visualization of up to 12 spectra. The maximum number of visualized spectra and the colors of the spectra, markers, grid, window background, etc. are set by calling the menu item "**View / Number and colors of spectra...**".

There are three main types of scaling of spectra along the ordinate axis in the program:

Scale	**Designation**	**Description**
Normal		A single scale for all visualized spectra. The scale parameters are determined by the range of changes in the values of the selected (working) spectrum in the visualization area.
Float	***Float***	Individual scale for each visualized spectrum. The scale parameters are determined by the range of variation in the values of each spectrum in the visualization area. The grid of the ordinate axis changes when switching from the one spectrum to another.
Fixed	***Fixed***	A single scale for all visualized spectra. The scale parameters are set by the operator.

The operator can switch from one type of zoom to another by double-clicking the mouse in the area of the ordinate axis of the main program window. Double-clicking in the area of the abscissa axis switches the abscissa axis from the channel scale to the energy scale and back.

The operator can change the type of spectrum visualization, parameters and scale type using the **Visualization** group of the main menu or the corresponding toolbar buttons .

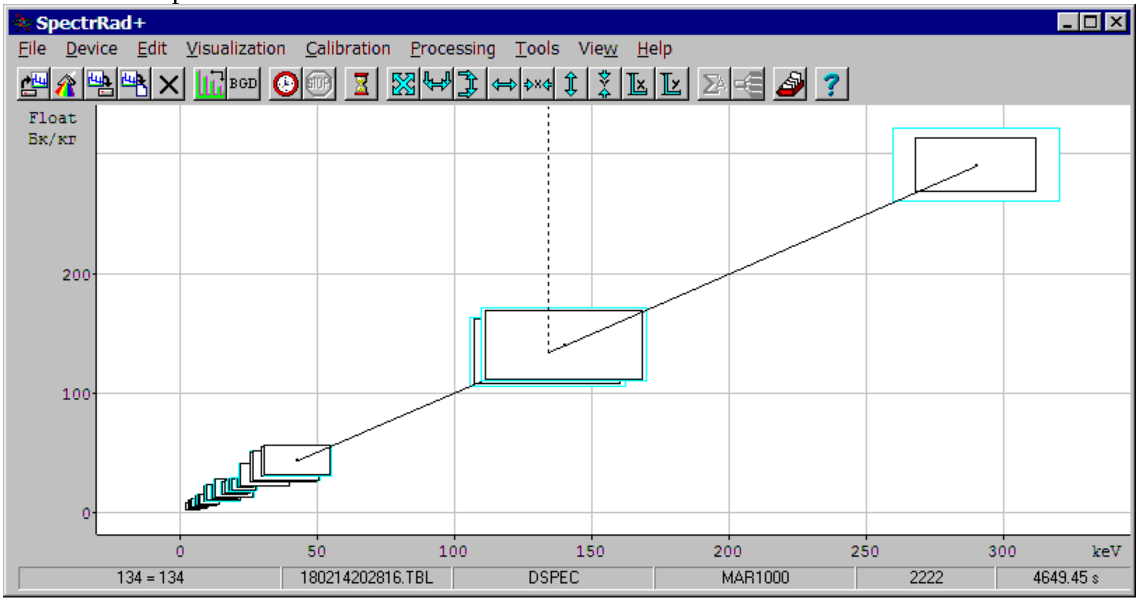
Moving the mouse in the X or Y axes area with the left button pressed changes the scale of the corresponding axis.

Moving the mouse to the right and down in the spectrum area highlights a rectangle, clicking inside which with the left mouse button stretches it over the entire window, respectively changing the scaling of the spectrum along the abscissa and ordinate axes.

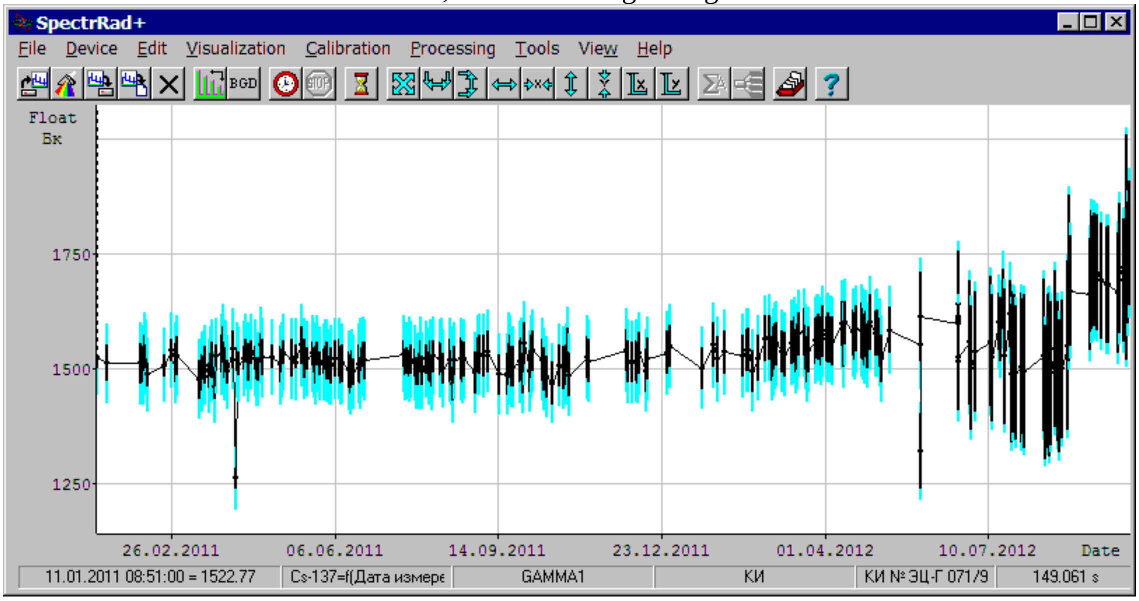
Right-clicking in the area of the abscissa or ordinate scale opens a pop-up menu duplicating some of the main menu items related to controlling the scaling of the abscissa or ordinate axis.

The "SPECTRRAD" package has two types of objects that can be visualized in the main window of the main program: spectra and function tables. **Spectrum** is a table of numbers displaying a function given with a uniform step along the abscissa axis. Therefore, the abscissa axis is not given in the spectrum, only the ordinate values are given, and the abscissa values are calculated by calibrating the abscissa scale. The uncertainty value of the ordinate in the spectrum is also missing and is calculated, if necessary, based on the assumed nature of the spectrum. Depending on the selected visualization type, the spectrum in the main window is displayed either by dots corresponding to the ordinate values (**Dots** mode), or by vertical lines (**Histogram** mode), or by lines connecting the points (**Contour** mode). A **table of numbers** is a table of numbers displaying a function set in arbitrary increments along the abscissa axis. Therefore, the point of the table of numbers is not one number, but four: the abscissa, the ordinate, the uncertainty of the abscissa and the uncertainty of the ordinate. The abscissa and ordinate values are displayed in the same mode as in the spectrum, and the uncertainty values are displayed by a rectangle {x-dx, y-dy, x+dx, y+dy}. And since uncertainties can be total and statistical, and statistical uncertainty is part of total uncertainty, if an additional error is indicated in the table of numbers, two squares are drawn for each point of the table: total and statistical uncertainty.

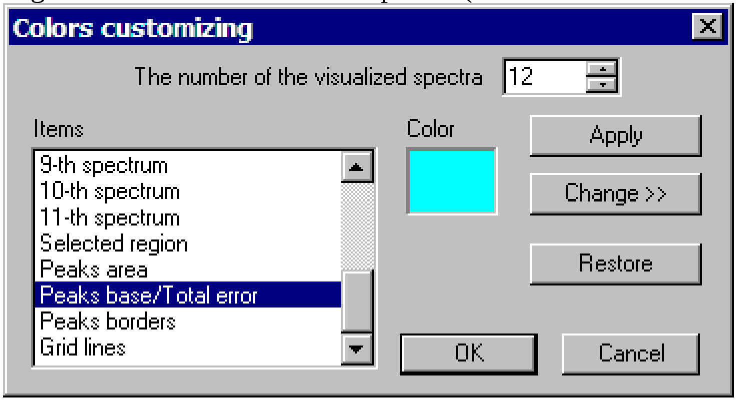
For example:



Often there is no error of the abscissa, and the rectangles degenerate into columns:



Statistical uncertainty is drawn in the same color as the spectrum, and total uncertainty is drawn in a different color (in the examples, blue). The color of total uncertainty is set by the procedure for determining the number and colors of spectra (menu item "**View/ Number and colors of spectra...**"): .



Colors customizing

The number of the visualized spectra 12

Items:
9-th spectrum
10-th spectrum
11-th spectrum
Selected region
Peaks area
Peaks base/Total error
Peaks borders
Grid lines

Main menu

Windows program operation is controlled through a menu that provides the user with convenient access to all commands or program parameters. The menu bar is located at the top of the program window under the program title bar. To work with the menu, you need to left-click the desired item in the menu or press the "Alt" key, and use the cursor keys to select the desired menu item, press the "Enter" key. You can also hold down the "Alt" key and press the underlined letter in the name of the menu item on the keyboard. As a result, a rectangle with a group of subordinate menu items will open under the menu item. By clicking on the desired item (or selecting it using the cursor keys), we will either open a new group of subordinate menu items, or perform an action related to this menu item.

Menu item		***Action***
File:		
Open:		
File…	***F3***	Open (read from a file) the spectrum for visualization and processing. Next to the name of the menu item (***File...***), can be indicated the button of the toolbar and the hotkey (***F3***), attached to this menu item, clicking on which activates this menu item.
Spectrometer…	***Ctrl+F3***	Select a spectrometer, read the spectrum from the spectrometer. Edit, if necessary, information about the spectrum.
Save	**F2**	Save the spectrum in the same file.
Save as…		Save the spectrum in a new file.
Close	**Ctrl+C**	Delete the previously opened spectrum from the program window.
Print…		Create a document for printing the spectrum.
Exit	**Alt+F4**	Exit the program.

The last section of the "***File...***" menu displays the names of all open spectrum files. The selected (working) spectrum file is marked with a "tick". The operator can switch to any other spectrum, making it operational, using the left mouse button. Pressing the "TAB" key switches the selected spectrum to the next one, "Shift+TAB" switches the selected spectrum to the previous one.

Device:

Spectrometer:[1]

Install…	Connecting a formed spectrometer (a spectrometer with certain pack of parameters, libraries of elementary spectra and nuclides) to a specific ADC input or installing a new one. Editing the parameters of the spectrometer.
Save as…	Saving all settings and calibrations of the selected spectrometer under a new name.
Delete…	Deletes all settings and calibrations of the selected spectrometer.

Geometry:

Install…	Changing geometry parameters, setting new measurement geometry.
Save as…	Saving all settings and calibrations of the selected measurement geometry under a new name.
Delete…	Deletes all settings and calibrations of the selected measurement geometry.

Configuration:

Common parameters…	Creation of a common group of spectrometers, installation of parameters common to all spectrometers, geometries and processing templates used in the formation of spectrum processing reports.
Cyclic measurements…	Setting the parameters of cyclic measurements.
Loading monitoring…	Setting the parameters of the procedure for monitoring the intensity of the radiation recorded by the spectrometer.
Watch mode… ***Ctrl+W***	Switching on/off the spectrum watch mode, setting the watching period.

Acquire:

Start… ***F5*** ⏲	Starting measurements.
Stop… ***Ctrl+F5*** STOP	Stopping measurements.
Clear… ***F4***	Clearing the spectrometer memory.

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[1] Some functions of the spectrometer installation and calibration are available only in the "full access" mode (see the menu item "Access mode").

State	**F8**	Enabling/disabling the additional "**Spectrometers State**" window, this contains information about the parameters of the current measurements.

Edit:

Filtrate…	**Ctrl+F**	Smoothing of the spectrum by averaging over a given number of channels or with a given weight function, reverse smoothing filtering (resolution improvement), correction of outliers.
Approximate…		Approximation of a spectrum or table by a spline.
Erase…	**Ctrl+Z**	Zeroing of a given section of the spectrum.
Normalize X scale…	**Ctrl+N**	Bringing the energy scale of the spectrum to a given form.
Add	**Ctrl+A**	The channel-by-channel addition of two spectra or a spectrum with a constant. Combining two tables into one.
Multiply	**Ctrl+M**	Channel-by-channel multiplication or division of two spectra or multiplication (division) of a spectrum by a constant.
Convolute…		Convolution of the selected section of the current spectrum with the spectrum or function table selected from the list of open spectra and function tables. Convolution expands the possibilities of filtering spectra.
Set mark	**Ins**	Marking of the spectrum channel selected using a movable marker.
Delete mark	**Del**	Removing the spectrum mark closest to the movable marker.
Mark all points	**Ctrl+Ins**	Marking all points of the spectrum.
Delete all marks	**Ctrl+Del**	Deleting all spectrum marks.
Edit data…		Editing spectrum or table data in numerical representation.

Visualization:

Logarithmic scale Y	**Ctrl+L**	Switching the ordinate scale (Y) from linear to logarithmic and back.
Logarithmic scale X	**Alt+L**	Switching the abscissa scale (X) from linear to logarithmic and back.
Select a sector X	**Ctrl+X**	Set the left and right boundaries of the abscissa scale according to the channels of the spectrum marked with a marker. The marked channels closest to the left and right of the movable marker are selected as boundaries, and if they are missing, then the boundaries of the spectrum.

Set the scale Y by spectrum **Ctrl+Y**	Setting the Y scale according to the range of values of the visualized part of the spectrum.
Extend scale X **Shift+Right**	Set a more detailed scale of the abscissa scale. At the same time, the X scale will have a scroll bar, with which you can view various sections of the spectrum.
Shrink scale X **Shift+Left**	Set a smaller scale of the abscissa scale.
Extend scale Y **Shift+Up**	Set a more detailed scale of the ordinate scale. The Y scale will also have a scroll bar.
Shrink scale Y **Shift+Down**	Set a smaller scale of the ordinate scale.

Setting the scale:

By spectra\spectrum ***Home***	Setting the X and Y scales. The first call to the procedure sets the scales according to the length and range of values of all the visualized spectra. The repeated call sets the scales according to the length and range of values of the selected spectrum.
Fixed scale Y ***Ctrl+R***	Fixing the current value of the Y scale. In this case, the Y scale will not change when switching from the one spectrum to another.
Float scale Y ***Ctrl+Q***	All open spectra are visualized on the scale of the Y scale "by spectrum".
Custom scale ***Ctrl+S***	Setting the X and Y scales by the operator.

Scale X units:

Energy – eV	The X scale in electronvolts.
Energy – keV ***Ctrl+E***	The X scale is in kiloelectronvolts.
Energy – MeV	The X scale is in megaelectronvolts.
Date ***Ctrl+E***	The X scale is the date.
Time – sec.	The menu item is available if the X scale is the date. When selecting **Scale X units / Time – sec**. - the abscissa axis will be the deviation of the current date from the measurement start date in seconds.
Time –min. ***Time – hour*** ***Time – day*** ***Time – year***	The X scale is the time from the beginning of measurements in minutes, hours, days or years.

Dots	**Ctrl-D**	Visualization of the spectrum by dots.
Contour		Visualization of the spectrum by lines connecting the points of the spectrum.
Histogram	**Ctrl+H**	Visualization of the spectrum in the form of a histogram.
Show peaks		Visualization of spectra with a linear structure showing the peaks of the spectrum found using the peak search procedure.
Show decomposition results		The output in the upper right corner of the main form of the program of the results of spectrum processing, if they exist.

Gridlines:

Ordinate	***Ctrl+G***	Drawing of the scale grid of the ordinate scale.
Abscissa	***Alt+G***	Drawing the scale grid of the abscissa scale.
Level line…	**Ctrl+B**	Drawing up to 5 lines of the required style and color with the specified values of the ordinate scale. The procedure is useful when creating Shewhart control charts.

Calibration:

Scale X (Energy):

By entered data…	***Ctrl+K***	Calibration of the spectrometer channel scale. The operator must first mark the points of the spectrum with markers with known energies (abscissa values) and enter the energy values (abscissa) into the fields of the plate corresponding to the marked channels.
By peak models…		Energy calibration of the spectrometer based on calculated peak models for linear spectra.
Visualization	***Ctrl+V***	Visualization of the graph of the energy calibration function.

Peaks width:

By entered data …	Calibration of peak widths as a function of the energy of gamma or alpha lines. The operator must first mark with markers the points of the spectrum corresponding to half the height of the peaks to the left and right of the tops of the single peaks.
By peak models…	Calibration of peak widths based on calculated peak models for linear spectra.
Visualization	Drawing the graph of the peak width calibration function. When the "Energy" visualization mode is set for X scale, the width of the peaks is displayed in energy values, otherwise in channels.

Quanta registration efficiency	Calculation of quanta registration efficiency tables for spectra with a linear structure.
In full energy peaks...	Calculation of the table of the efficiency of quanta registration in the peaks of total absorption and the table of the total efficiency of quanta registration in the detector.
In single escape peaks...	Calculation of the quanta registration efficiency table for single escape peaks.
In double escape peaks...	Calculation of the quanta registration efficiency table for double escape peaks.
Autocalibration:	
Start… ***F6***	Automatic energy scale calibration and verification of the spectrometer by reference source.
Configure…	Setting parameters for the auto-calibration procedure.
Setup…	Setting the spectrum of the reference source for auto-calibration procedures.
Reset drift …	Setting the initial (zero) values of the spectrometer drift parameters.
Background:	
Start ***F7*** BGD	Checking and installing the background spectrum in the processing program.
Configure…	Setting parameters for the spectrometer background spectrum check procedure.
Elementary spectrum:	
Calculate by acquired spectra…	Calculation of the elementary spectrum of a nuclide (the response of the spectrometer to radiation from 1 decay of a nuclide) from the spectra of standards (referenced measures of activity).
Generate by nuclides table	
By lines models…	Calculation of the elementary spectra of nuclides from the library of nuclides and the spectra of the spectrometer's responses to a quantum of radiation of a given energy (line spectra).
By peaks models …	Calculation of elementary peak spectra (without continuous scattering spectrum) of gamma radiation of nuclides from the nuclide library, registration efficiency tables and peak models of a given energy.
Calculate lines spectra…	Calculation of the spectrometer response to a quantum of radiation of a given energy.

Calculate peaks spectra…	Calculation of peak models for various types of gamma and X-ray radiation lines. The peak model determines the shape of the peak, and the area of the peak model is set to one.
List of elementary spectra…	Viewing and editing the list of calculated elementary spectra.
List of lines spectra…	Viewing and editing the list of calculated line models.
List of peaks spectra…	Viewing and editing the list of calculated peak models.
List of efficiency tables….	Viewing and editing the list of calculated registration efficiency tables.

Processing:

Integral:	
Spectrum area… ***Ctrl+I***	Calculation of the sum of channels of the marked portion of the spectrum - "total area". The area of the trapezoid formed by the left and right markers and the straight line connecting them is also calculated - the "background area" and the difference between the total and background area - the "net area".
Spectrum energy… ***Alt+I***	Calculation of the registered energy and power of the spectrum within the boundaries set by markers.
Radiometry:	
Start ***Ctrl+J***	Determination of the integral characteristics of the sample radiation: radiation power, "total activity", "total effective activity"[2].
Configure…	Setting the parameters of the procedure for calculating the "total activity" of the sample.
Decomposition… **Ctrl+P**	Decomposition of the spectrum into components of elementary spectra of nuclides, calculation of the activity of nuclides.
Peak search:	
Search ***Alt+P***	Search and determination of peak parameters in the linear spectrum, calculation of the Compton scattering spectrum.
Configure …	Setting parameters of the procedure for searching and determining peak parameters.

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[2] **Total activity** is the conditional activity of the sample equal to the intensity of the radioactive radiation from the sample. The total gamma activity is the number of gamma quanta emitted by the breakdown in 1 second, the total alpha and beta, respectively, is the number of alpha and beta particles per unit time. The **total effective activity** is the conditional activity of the sample, assumed to be equal to the radiation activity of a given nuclide with equal radiation energy power. For gamma radiation, Ra-226 is used as a reference nuclide in equilibrium with daughter nuclides.

Add peaks… ***Alt+Ins***	The last three menu items in the Peak Search group are used to manually edit the list of peaks found. The "Add peaks..." item adds the peaks of the marked area of the spectrum to the list. The operator must first mark the left and right borders of the peak area and place a movable marker inside the marked area. The procedure calculates the Compton scattering spectrum for the selected region and highlights the regions of individual peaks, if it is a multiplet. The peaks of the selected area will be added to the list of peaks if the error in estimating their area does not exceed 100%.
Delete peak ***Alt+Del***	Remove the peak indicated by the movable marker from the list of peaks found in the spectrum.
Delete group of peaks… ***Shift+Del***	Remove the peaks of the marked spectrum area from the list of peaks.
Unite peaks	Combine the two peaks closest to the marker in the multiplet into one peak.

Tools:

Archive of measurements…	Calling the program that manages the archive of measurement results. .
Nuclides table…	Calling the program for creating and editing nuclide libraries.
Norms and materials…	Calling the program for creating and editing tables of safety standards (SanPiN, NRB, etc.), physical constants related to the chemical composition of the sample substance.
Upgrade files structure…	Calling the procedure for converting outdated file formats generated by the program "SPECTR" (spectra, processing results) or "SPECTRRAD" to the current version of the program "SPECTRRAD".
Open the spectrum in the "Spectrad-V" window	Opening the current spectrum in the application window "**SpectrRad-V**" for visualization and editing.
Spectrum parameters…	Calling the program for viewing and editing the spectrum header.
Spectrum decomposition report…	Output of a report on the results of spectrum processing. If the report was included in a Word document, both report forms are displayed.
Peaks report…	Output of the search results report for peaks in the linear spectrum.
Selected peak parameters…	Output of the parameters of the peak indicated by the marker in the linear spectrum.
Calculate function…	Calculation of the function table according to the formula

	specified by the operator. The resulting table can be used to form a line model or as a wavelet for filtering spectra.
License…	View the current license, download a new one.
Access mode…	Installation of limited or full access to the procedures and data of the "SPECTRRAD" package. Limited access prevents certain types of spectrometer calibrations and changes to spectrometer parameters and processing templates. Setting full access requires entering the password requested at the first start of the program.

View:

Tool bar	Enabling or disabling the "tool bar" - a set of "buttons" under the menu bar, providing a more convenient way to access some menu items.
Full	The full tool bar.
Short	A short tool bar.
Scale Y	Enabling or disabling the ordinate scale for the spectrum.
Number and colors of spectra…	Setting the value of the maximum possible number of simultaneously visualized spectra in the program window and setting the colors for the visualized spectra, the background color of the window, the colors of auxiliary graphic elements (area boundaries, markers).
Decomposition report font…	Selecting a font for displaying a report on the results of spectrum processing in the observation mode in the main window of the program.
Hint mode	Enable or disable the tool tip mode for the buttons of the tool bar.

Help:

Content **F1** ?	Description of the program.
About…	Brief information about the program.

Keyboard and mouse

In addition to the functions standard for the Windows keyboard (switching between windows, writing a copy of the screen or active window to the clipboard, switching between menu items, etc.), the keyboard in the SPECTRRAD program is used for the following functions:

- In the main window, the cursor keys to the left or right are used to move a movable marker.
- A number of keyboard shortcuts are reserved as "hotkeys" for some menu items (indicated in the menu description).

- In the main window, simultaneously pressing the cursor keys and one of the register switching keys: "Shift", "Ctrl" or "Alt" causes a change in the scale of the spectrum visualization.
- Simultaneous pressing of the "F9"-"F12" keys and the "Alt" key for the main window causes the spectrum shift in the window to the left, right, down or up.
- Pressing the "Esc" key, as a rule, causes a return to the previous state: if any procedure was started, it is interrupted, if there is no active procedure associated with the active window, the active window closes.
- "F1" is used to call help for the active window.

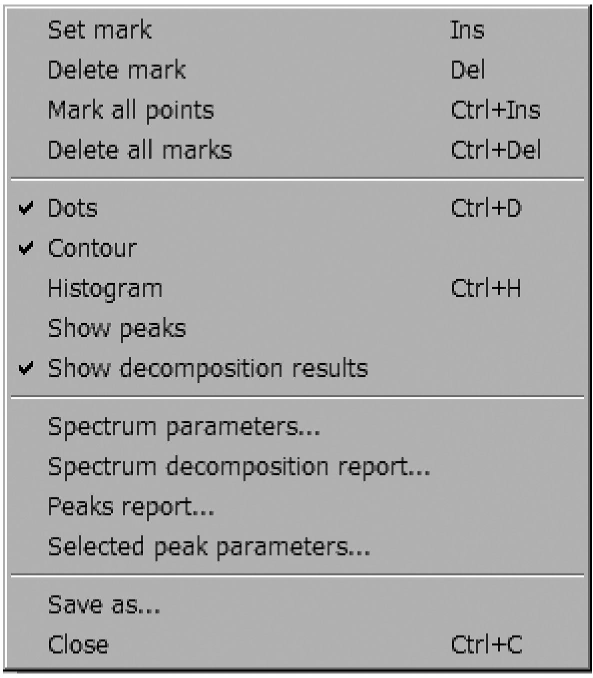
In addition to standard functions (activating a menu item, resizing a window, operations with scroll bars, displaying hints, etc.), the mouse can also perform a number of special operations in the SPECTRRAD program:

- Using the left mouse button, the operator, pointing to a movable marker, can drag it to the desired location. You can move the marker by double-clicking the left button in the desired location of the window.
- Moving the mouse in the direction to the right and down with the left button pressed in the spectrum area highlights a rectangle, clicking inside which with the left mouse button stretches it over the entire window, thus changing the scaling of the spectrum.
- By pointing to any of the open spectra and clicking the left mouse button, the operator switches to the selected spectrum.
- Moving the mouse in the X or Y axes area with the left button pressed changes the scale of the corresponding axis.
- Double-clicking the mouse in the area of the X or Y scale changes the type of the corresponding scale (floating or fixed for the Y scale, channel scale or energy scale for the X scale).
- The right mouse button activates a small menu ("pop-up" menu), the contents of which change depending on the position of the mouse pointer and the moment of the call.

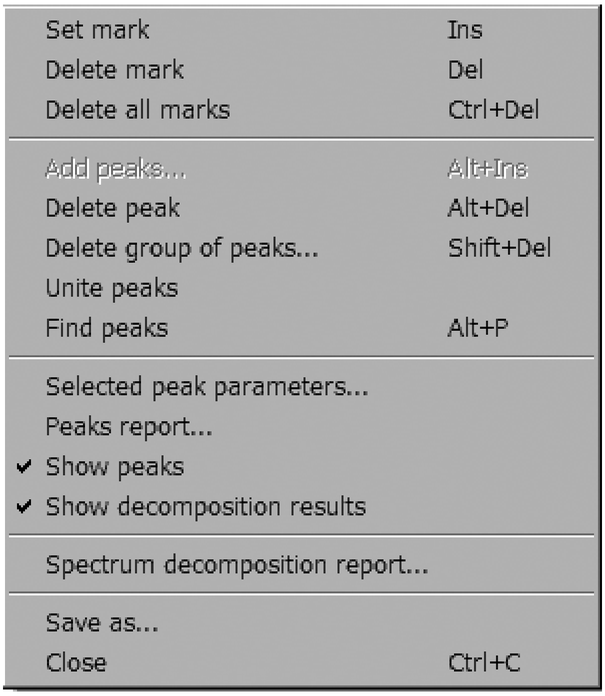
With a large spectrum stretch, the scroll area may be less than the length of the spectrum. In this case, the scroll area is shifted to the left or right by pressing the left mouse button on the border squares of the scroll bar: ◄, ►.

Popup menu

Right-clicking causes a "pop-up" menu to appear. The contents of the menu depend on the position of the mouse pointer in the program window and the status of the program. Clicking on the spectrum visualization window opens two options for the "pop-up" menu, depending on whether the peak visualization mode is set or not (menu item "**Visualization / Show peaks**"). If the peak visualization mode is not set, the following menu is called:

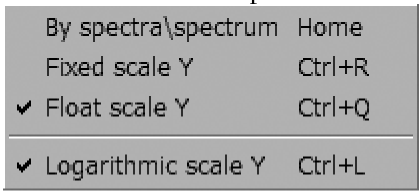


, and when the peak visualization mode is set, a menu that allows you to edit the list of peaks found by the program:

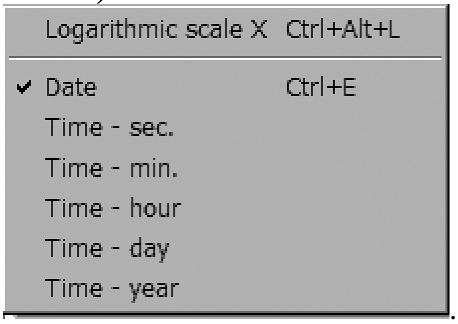


The permission or prohibition of the menu items "**Add peaks...**", "**Delete peak**", "**Delete group of peaks...**" and "**Unite peaks**" depends on the position of the marker and the selected area of the spectrum. If there are no peaks found by the program in the selected area, the operation of adding peaks is allowed and, accordingly, if peaks are present in the selected area, peak removal operations are allowed.

Right-clicking in the ordinate axis area opens a menu that allows you to change the scale type of the ordinate scale , and clicking on the abscissa axis - a menu that allows you to switch the scale from the energy scale (or another dimension of the



abscissa scale) to the channel scale and back, from the linear scale to the logarithmic scale and back: .



"Spectrometers state" window»

The "**Device / State**" menu item (toolbar button) is used to turn on and off an additional window - "**Spectrometers state**", informing the operator about the status and measurement time of the connected spectrometers. The "**Spectrometers state**" window is automatically turned on when measurements are started in any of the connected spectrometers. If, for example, three spectrometers are enabled in the system: "ALPHA", "BETA" and "GAMMA", the window may look like this:

Spectrometers state

		Load		Acquisition time				Total
	Spectrometer	Imp./sec.	%	Real	Live	Time left	Cycle	Cycles
✗	ALPHA	0.00	● 0	0:00:00	**0:00:00**	0:00:00		
🔈	BETA	2.00	● 0	0:00:35	**0:00:35**	**0:59:25**	1	3
🔈	● GAMMA	3.00	● 0	0:00:13	**0:00:13**	0:59:47		

On the left there are buttons for turning on/off the sound scheme for accompanying certain events (completion of measurements, overload or sudden change in load) in the spectrometer - 🔈. The pressed state of the button corresponds to the sound being turned on.

A spectrometer whose spectrum is selected (information about the spectrum is displayed in the status bar) is marked by pressing the state of the key with the name of the spectrometer and a blue indicator ●.

"**Load**" is the number of pulses recorded by the spectrometer per unit of time (Imp./sec) and the ratio as a percentage of the "dead" time of the spectrometer to the real one (%). Loading is usually associated with the activity of the sample, but it may also indicate a malfunction of the spectrometer - registration of a large number of pulses of the spectrometer's own noise. The loading indicator has four states:

● - measurements in the spectrometer stopped,
● - measurements started, loading does not exceed the established norm,
● - measurements started, loading slightly exceeds the established norm,
● - measurements started, loading significantly exceeds the established norm.

The time is displayed in the format: hours:minutes:seconds. The "**live**" measurement time is less than the "**Real**" time that the spectrometer spends on pulse processing - the "**dead**" time of the spectrometer.

The "**Time left**" column is the time ("real" or "**live**" - depending on what is set when starting measurements, it is displayed in regular or bold font) that remains until the end of measurements with normal measurements and until the end of the current cycle with cyclic ones. If the pause or delay mode for the start of measurements is enabled, the time remaining before the start of measurements is displayed in the column.

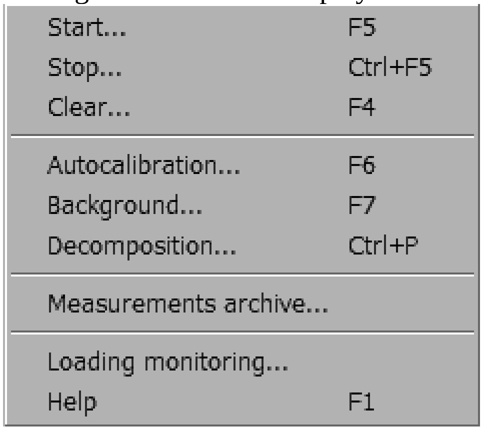
"**Cycle**" is the number of the current cycle for cyclic measurements.

"**Total cycles**" – is the total number of cycles in cyclic measurements.

Left-clicking on the name of the spectrometer displays the spectrum of this spectrometer in the main program window and makes it active.

Double-clicking displays a window for starting (if measurements are not started) or stopping (if measurements are already being performed) measurements.

The right mouse button displays a small menu,



that duplicates part of the main menu items of the program (the "**Loading monitoring...**" item duplicates the main menu item "**Device / Configuration / Loading monitoring...**"). This duplication allows you to perform routine measurements by minimizing the main program window and thus freeing up the Windows Desktop.

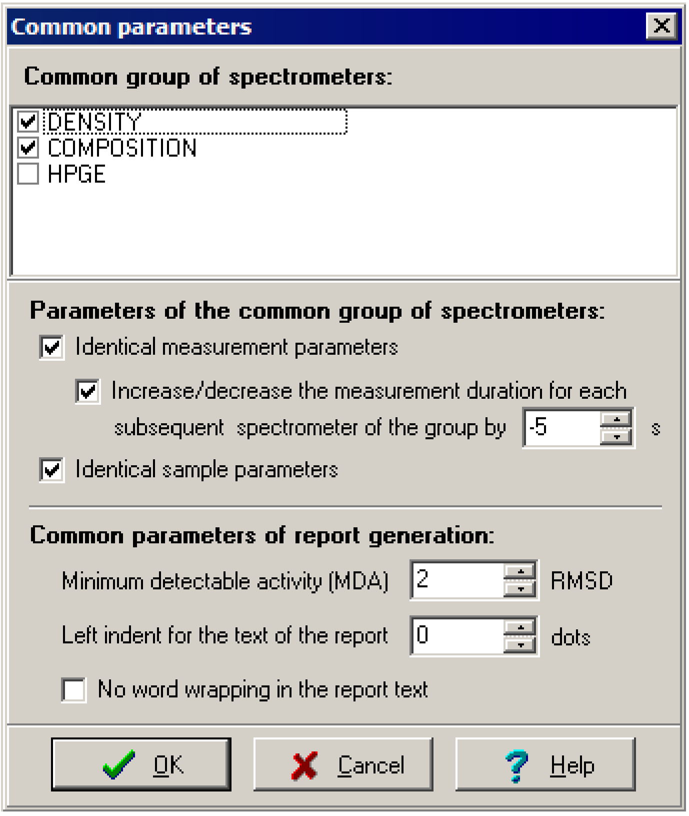
Carrying out measurements

Creating a common group of spectrometers

Often, to increase the efficiency of radiation detection by the spectrometer, to implement the functions of coincidence, anti-coincidence, 2d and 3d spectrometry, to determine the density of the sample, several detectors are connected to the spectrometer, which must work simultaneously: measurements in all detectors must be started at one operator's command, and sometimes they must stop simultaneously.

In the "SPECTRRAD" package, the procedure for creating a common group of spectrometers is used for these purposes, which is included in the general parameters setting function (the main menu item "**Device / Configuration / Common parameters...**").

When calling the procedure, a window appears on the screen with a list of connected spectrometers and a number of common parameters used for generating reports:



Common group of spectrometers:

☑ DENSITY
☑ COMPOSITION
☐ HPGE

Parameters of the common group of spectrometers:

☑ Identical measurement parameters
☑ Increase/decrease the measurement duration for each subsequent spectrometer of the group by -5 s
☑ Identical sample parameters

Common parameters of report generation:

Minimum detectable activity (MDA) 2 RMSD
Left indent for the text of the report 0 dots
☐ No word wrapping in the report text

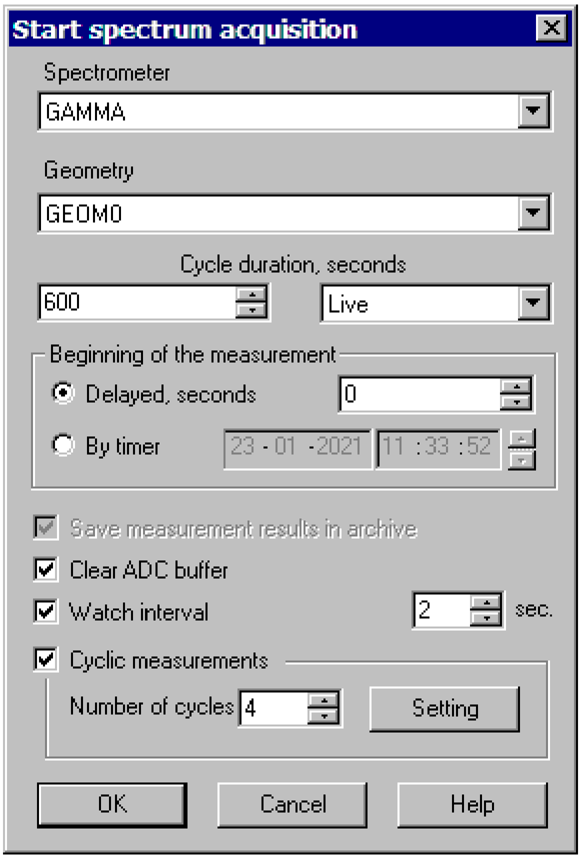
Common group of spectrometers is a group in which all operations related to the launch of measurements are synchronized – performed simultaneously. The measurement stop by the operator will also be synchronous. The measurements will be completed simultaneously if the "**Identical measurement parameters**" checkbox is selected. In this case, all measurement parameters in the group will be identical. If the "**Increase/decrease the measurement duration for each subordinate spectrometer of the group by n s**" checkbox is selected (**n** is the set value, a negative value of **n** reduces the duration of measurements), the measurement parameters in the spectrometers of the group will differ in the duration of the acquisition. This allows you to organize the streamline processing of spectra, which is important when implementing sequential processing of spectra in a group of spectrometers. For example, in Bayesian estimation, when the measurement results in the previous spectrometer is used as a priori data for spectrum processing in the current spectrometer.

If the "**Identical sample parameters**" checkbox is selected, the sample parameters will be entered only for one spectrometer from the group. The data collected will be used for other spectrometers of the group.

To create a common group of spectrometers, the operator must tick the appropriate spectrometers. Creating and editing a group is only available in **Full access** mode.

Starting measurements

The main menu item "**Device / Acquire / Start...**", clicking on the button, or pressing the "**F5**" key triggers the measurement startup program. At the same time, the following window appears on the screen:



Start spectrum acquisition

Spectrometer: GAMMA

Geometry: GEOM0

Cycle duration, seconds: 600 Live

Beginning of the measurement

● Delayed, seconds 0

○ By timer 23 - 01 -2021 11 :33 :52

☑ Save measurement results in archive

☑ Clear ADC buffer

☑ Watch interval 2 sec.

☑ Cyclic measurements

Number of cycles 4

The operator has the opportunity to select the spectrometer and measurement geometry by clicking on the button of the corresponding drop down list "**Spectrometer**", "**Geometry**" and selecting the necessary line in the list that opens with the mouse.

You can set the measurement time by directly entering its value, or modify the preset value using the scroll buttons. The panel to the right of the time input field allows you to select the normalization mode: live - **Live** or real -**Real** time. Normalization by "live" time increases the measurement time relative to "real" (astronomical) time by the time during which the spectrometer was busy processing pulses (the "dead" time of the spectrometer). When the time value is set to zero, the time-unlimited mode will be enabled.

In the "**Beginning of the measurement**" group, the operator can set either the delay time before the start of measurements (select "**Delayed, seconds**"), or the date and time of the start of measurements (select "**By timer**"). This can be convenient if a delay is required from the start of measurements to the start of data acquisition in order to end any transient or technological processes (heating of equipment, decay of short-lived nuclides, sample change, etc.) or to start measurements simultaneously in all spectrometers.

The operator can set, or reset a number of checkboxes defining the measurement mode:

- **Save measurements results in archive** - when the checkbox is selected, the measured spectrum, at the end of the measurements, will be recorded in the archive of measurement results. The corresponding background spectrum at the time of measurement will also be saved in the archive. If the spectrum is processed immediately after the measurement, the measured spectrum can be saved after processing. In this case, the check box is not required.

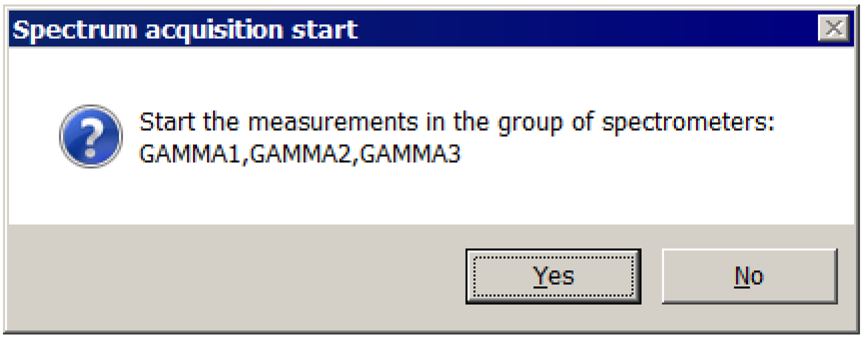
- **Clear ADC buffer** - the requirement to clear the spectrometer memory before starting measurements (old data is destroyed, new measurements will begin). If the checkbox is cleared, the memory will not be reset - the measurements will be continued (the new measurements will be summed with the old ones). Obviously, the summation mode is acceptable if measurements of the same sample continue.
- **Watch interval n sec.** - when the check box is selected, the spectrum during measurements will be read regularly, after a specified time, for visualization.
- **Cyclic measurements** - selecting the checkbox sets the cyclic measurement mode, in which the sample measurements will be repeated for a specified **number of cycles**, and the resulting (total) spectrum or spectra of each cycle will be saved in the measurement archive. In this case, the spectrometer drift can be automatically corrected for each measurement cycle. The parameters of cyclic measurements can be changed by clicking on the [Setting] button (pre-setting the parameters is performed by calling the menu item "**Device / Configuration / Cyclic measurements...**"). The action of the "**Clear ADC buffer**" checkbox in cyclic measurement mode is slightly different from the usual one. If the checkbox is cleared, the accumulated data will be recorded (added) to the accumulation spectrum, the spectrometer memory is cleared and the second measurement cycle will begin. If it is installed, the memory will be reset, the first measurement cycle will begin and at the end of the cycle the accumulated spectrum will be written to a file for accumulation.

It is necessary to take into account some features of the measurement start procedure in order to minimize the cost of entering the parameters of the measured sample. When starting measurements normally (from the main program window), the program inserts the values of the last measured sample for the current spectrometer into the table for entering parameters. Choosing a different spectrometer in the measurement start plate does not change these values, so if we are going to measure samples from the same material on different spectrometers, it is more convenient to switch to another spectrometer after pressing the measurement start button. For example: after starting measurements in the beta spectrometer, to start measurements of a sample from the same material in the gamma spectrometer, without switching to the gamma spectrometer, click on the measurement start key 🕓 and only switch to the gamma spectrometer in the "**Start spectrum acquisition**" form - in this case you will have to adjust only the weight of the sample and the geometry of the measurements (the other values substituted by the program will be the same).

You can also start measurements from the "**Spectrometers state**" window by calling the "**Start...**" pop-up menu item and from the "**Archive of measurements**" window (menu item "**Commands / Start acquisition..**", button 🕓). Running measurements from the archive of results substitutes all values of the selected sample. The operator can either continue measuring it (by checking the cyclic measurement checkbox), or, after correcting the data, start measuring a new sample.

Pressing the "**OK**" key closes the first window and displays a new one.

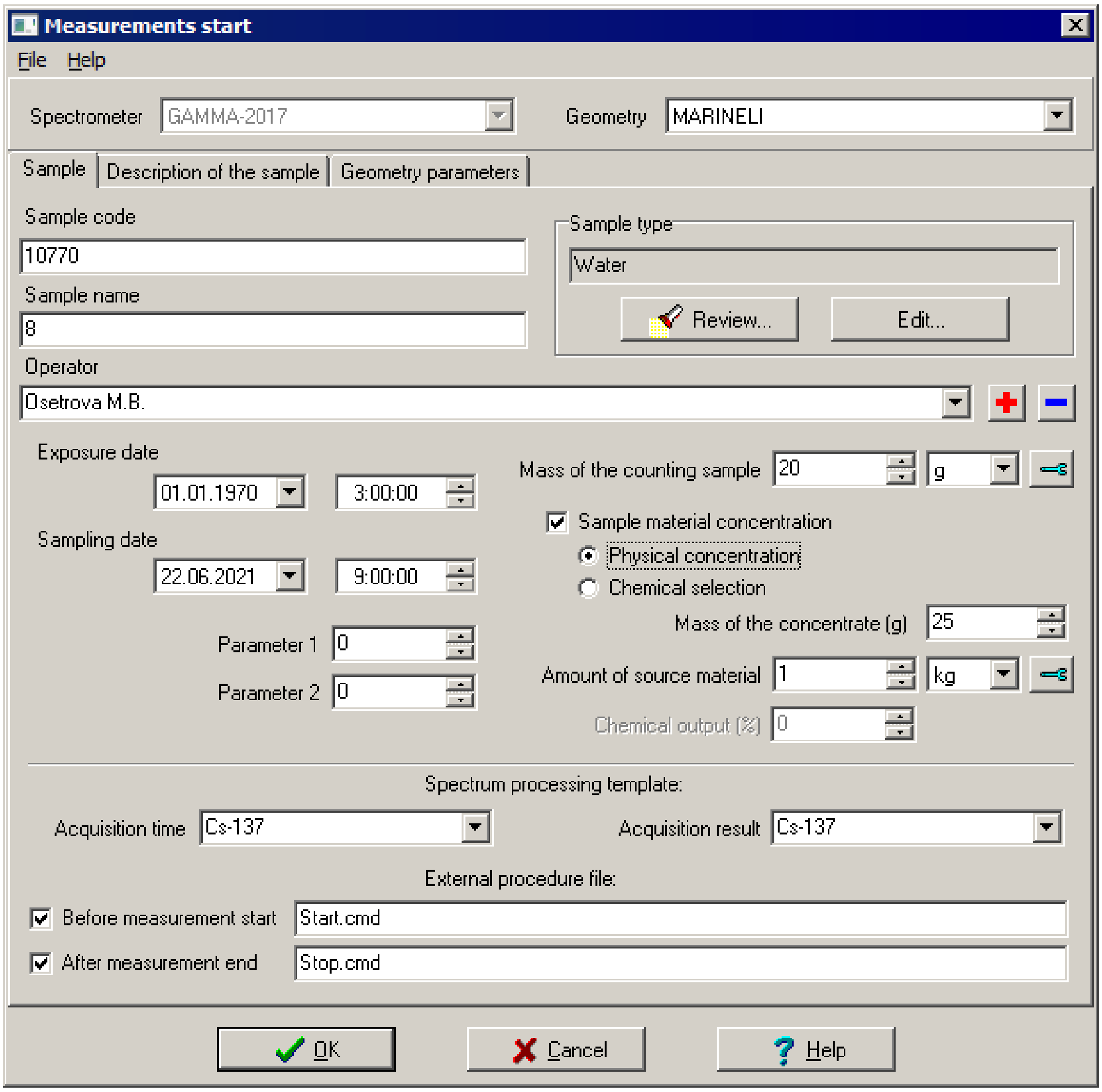
If a common spectrometer group is defined, a window will appear to confirm the start of measurements in the spectrometer group. For example:



Start the measurements in the group of spectrometers:
GAMMA1,GAMMA2,GAMMA3

If the answer is "**Yes**", measurements will be started in all spectrometers of the group, if the answer is "**No**" - only in the selected spectrometer.

After that, a window will appear on the screen to enter the sample parameters:



Spectrometer: GAMMA-2017
Geometry: MARINELI

Sample code: 10770
Sample name: 8
Sample type: Water
Operator: Osetrova M.B.

Exposure date: 01.01.1970 3:00:00
Sampling date: 22.06.2021 9:00:00
Parameter 1: 0
Parameter 2: 0

Mass of the counting sample: 20 g
☑ Sample material concentration
● Physical concentration
○ Chemical selection
Mass of the concentrate (g): 25
Amount of source material: 1 kg
Chemical output (%): 0

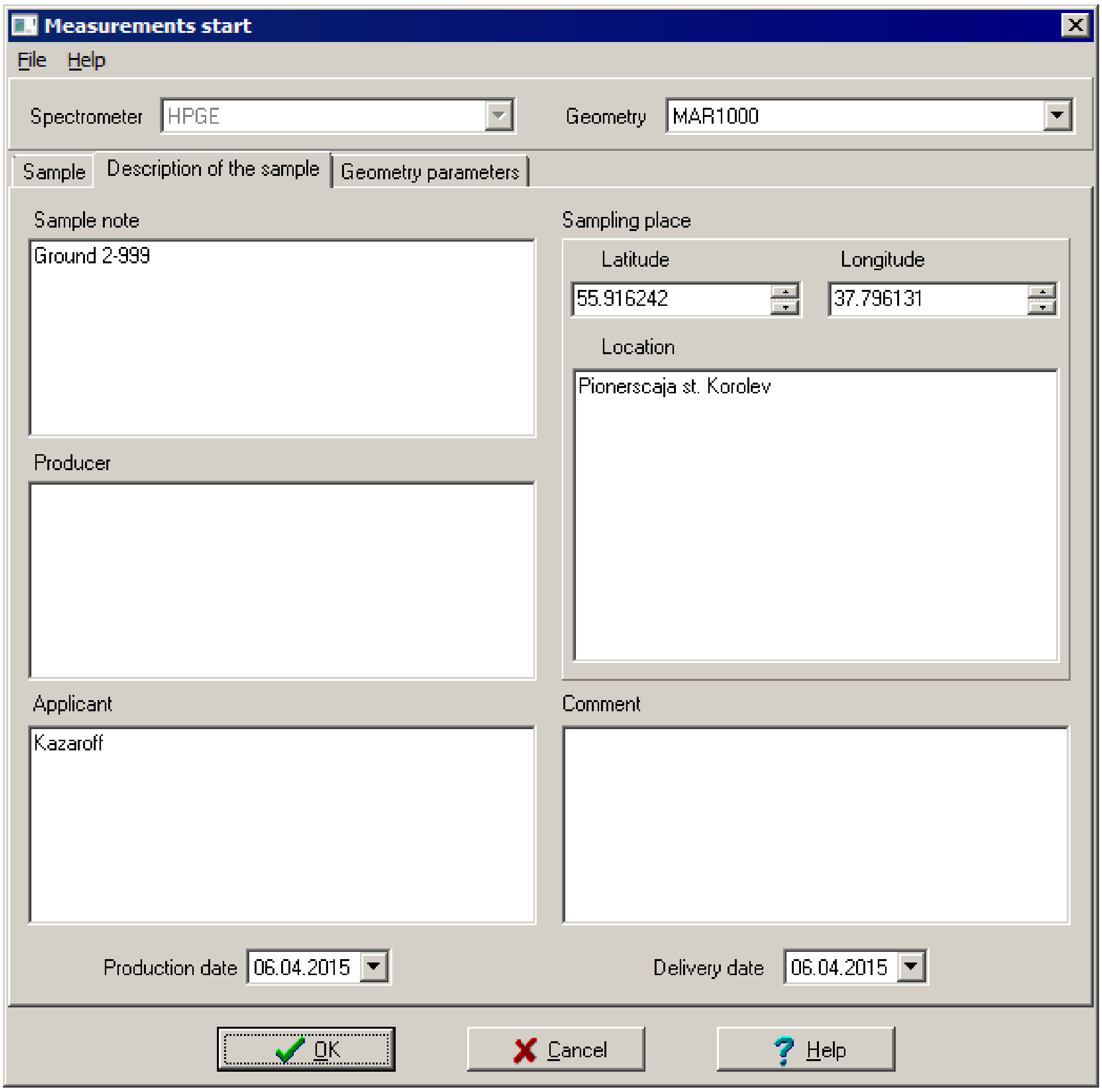
Spectrum processing template:
Acquisition time: Cs-137
Acquisition result: Cs-137

External procedure file:
☑ Before measurement start: Start.cmd
☑ After measurement end: Stop.cmd

The operator can fill in, if necessary, the fields of the form with information about the sample, adjust, if necessary, the geometry of the measurements.

The form contains two pages of sample parameters "**Sample**" and "**Description of the sample**". The first page contains the main fields of the sample description, the "**Operator**" field for entering data about the laboratory technician conducting measurements and two lists with spectrum processing templates.

The second page contains fields for entering additional information about the sample and looks like this:



Spectrometer: HPGE

Geometry: MAR1000

Sample note: Ground 2-999

Latitude: 55.916242

Longitude: 37.796131

Location: Pionerscaja st. Korolev

Applicant: Kazaroff

Production date: 06.04.2015

Delivery date: 06.04.2015

The fields "**Sample code**", "**Sample name**", "**Sample note**", "**Producer**", "**Applicant**", "**Sampling place**", "**Comment**", "**Parameter 1**" and "**Parameter 2**" can contain arbitrary information about the sample, which will be included in the archive of measurement and in the results report. The names of the fields and their very presence on the form are set when setting up the archive of measurement results assigned to this spectrometer and measurement geometry. Therefore, the field "**Parameter 1**" can be, for example, the field "**Well depth (m)**" or be absent on the form.

If the operator left the first field ("**Sample code**") of the "**Sample**" page empty, the program will write the measurement start date in it as a number, for example **170702195311**.

The field "**Sample type**" is associated with information about the safety standards of SanPiN, NRB, etc. and the chemical composition of the sample substance and must contain the full path to the file of the corresponding standard, starting with the folder "**Sample types**" (but not including it) and, accordingly, should not include characters prohibited in file names and have a path structure to the file. For example: **Food products\Vegetable oil (all types)**. Direct input of the sample type is not allowed. It is recommended to use the Review... button to select a sample type from existing sample types, and create new sample types using the "**Standards**" procedure (menu item "**Tools / Norms and materials...**"). If desired, you can also use direct input of the sample type - to do this, double-click on the "**Sample type**" field or press the "**F4**" key. In the event that this type of sample is not in the "**Sample types**" folder, the program will call the procedure for creating a standard for a new type of sample. The program for creating and editing standards and constants can be called by pressing the Edit... key.

The field "**Mass of the counting sample**" should contain information about the mass (kg, g or mg) of the counting sample - the sample that will be measured on this spectrometer, in a given geometry.

In the event that pre-concentration or dilution of the sample material was used to prepare the counting sample, the operator must tick the "**Sample material concentration**" item and enter the data in the fields "**Mass of the concentrate**" and "**Amount of source material**", which determine the concentration coefficient (dilution) of the material under study. The mass of the concentrate is entered in the same units as the mass of the counting sample, and the amount of the starting material can be either mass or volume (set in cubic meters, liters, ml) or sample area (sq.m, sq.cm, sq.km). In this case, the calculated activity will be normalized per unit of weight, volume or area. If the mass of the counting sample is not set or is equal to zero, the normalization will not be performed. If the mass of the counting sample is not set and the sample is concentrated, normalization will be performed for the amount of the source material. In this case, the entire amount of concentrate must be placed in the counting sample.

The type of concentration "**Physical concentration**" (i.e. drying, evaporation, incineration, etc.) and "**Chemical selection**" determines the elemental composition of the counting sample specified in the file of standards and materials related to this type of sample and is required for correct accounting of radiation absorption in the sample substance. During the **chemical separation** of the sample, the operator must enter the **chemical output (%)** of the released substance as a percentage necessary for the correct calculation of the concentration coefficient (during **physical concentration**, it is assumed that the entire substance passes into the concentrate).

To tick the item "**Sample material concentration**", "**Physical concentration**" and enter the necessary data on the mass of the concentrate and the amount of the starting material is necessary even if there was no concentration or dilution of the material, but the calculation of specific activity is required not per mass, but per the volume or area of the sample, which corresponds to the specified mass of the counting sample or the calculation of the total activity of the sample, of which the counting sample is a part, is required.

The "**Sampling date**" field is used to recalculate activity for a given date - the sampling date. At the same time, the program takes into account both the number of years and the situation with the transfer the clock to summer or winter mode. The name of the field is customizable (it can be called, for example, "**Date of sampling**"), but the purpose is unchanged.

The purpose and name of the "**Exposure date**" field is also customizable. The value of the field, in addition to the report, is available in a programmable calculator and its purpose is determined in the calculator program.

The "**Sampling place**" field can also contain the geographical coordinates of the sampling location – **Latitude** and **Longitude**, set in degrees. The "**Location**" field is the address or description of the selection location.

The operator can also set spectrum processing programs during the monitoring of the data acquisition and at the end of the data acquisition by selecting the necessary templates from two **Spectrum processing template** lists: "**Acquisition time**" and "**Acquisition result**". Automatic spectrum processing has a number of limitations and features:

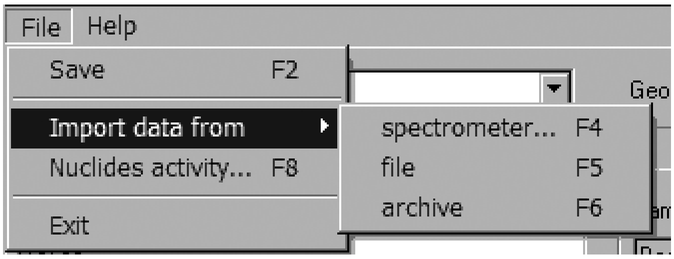
- It is impossible to set processing templates that require the operator to specify a priori data in measurement archives.
- Patterns requiring operator intervention may suspend spectrum acquisition.
- It is not recommended to adjust the energy drift of the spectrometer based on the results of spectrum processing during the acquisition, since small statistics at the beginning of measurements do not allow to correctly estimating the energy drift.
- The output of the processing results in the "**Acquisition time**" mode occurs in the upper-right corner of the main window of the "SPECTRRAD" program, regardless of whether the "**Display the report on the screen**" checkbox of the decomposition template is selected.
- The **measurement result** is processed in cyclic measurement mode after each cycle and the results are stored in the archive without being displayed on the screen, regardless of the checkboxes "**Display the report on the screen**" and "**Save the report in the archive**" of the decomposition template.

The number of characters entered in some fields cannot exceed a certain number of characters:

Field	**Maximum number of characters**
Sample code	***63***
Sample name	***63***
Operator	***63***
Sample type	***255***
Sample note	***127***
Producer	***127***
Applicant	***127***
Sampling place	***255***
Comment	***127***

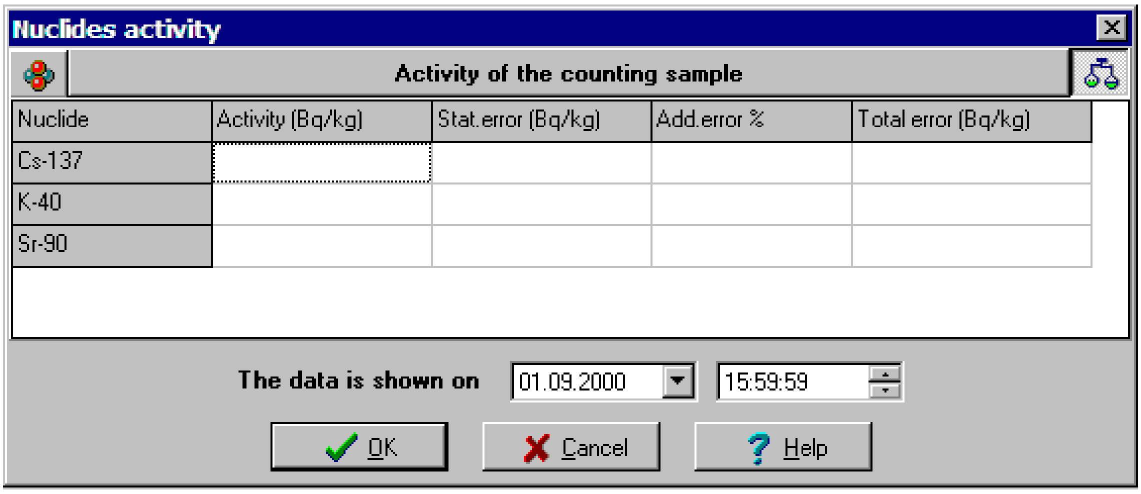
A number of fields of the description of the sample can be combined (see "**Archive setup**"). In this case, the combined field will have a total capacity. You can combine "**Sample code**" and "**Sample name**" - the total capacity of the "**Sample code**" column will be 127 characters. You can combine "**Sample note**" and "**Producer**" - the length of the "**Sample note**" field will be 255 characters. You can combine "**Sample note**", "**Producer**" and "**Applicant**" - the length of the "**Sample note**" field will be 383 characters. You can combine "**Producer**" and "**Applicant**" - the length of the "Producer" field will be 255 characters. You can combine "**Sampling place**" and "**Comment"** - the length of the "**Sampling place**" field will be 383 characters.

The form has a small menu:



The menu item "**File / Import data from**" allows you to import data into the form from another spectrometer, a spectrum file, or from a selected archive entry, which saves time filling in the form fields.

The menu item "**Nuclides activity...**" allows you to enter a priori data on the activities of nuclides, which will be used in the processing of spectra according to the template for processing the measurement result specified in the sample parameters, if this template requires the input of such data. Or this data will be used as comparison data in the formation of verification protocols or the construction of Shewhart maps. At the same time, a form for entering such data will appear on the screen, such as the following:



Nuclide	Activity (Bq/kg)	Stat.error (Bq/kg)	Add.error %	Total error (Bq/kg)
Cs-137				
K-40				
Sr-90				

The data is shown on 01.09.2000 15:59:59

The operator must enter data on the activities of nuclides and the errors in their determination. The error (uncertainty) includes two components: statistical uncertainty and additional uncertainty, defined as a percentage of activity. The total uncertainty is not entered by the operator, but is calculated by the program from the values of statistical and additional uncertainty. A 95% confidence interval of activity estimation is used as a random component of the total uncertainty (statistical uncertainty). The absence of data in the activity and statistical uncertainty columns means that there is no a priori data on the activity of this nuclide.

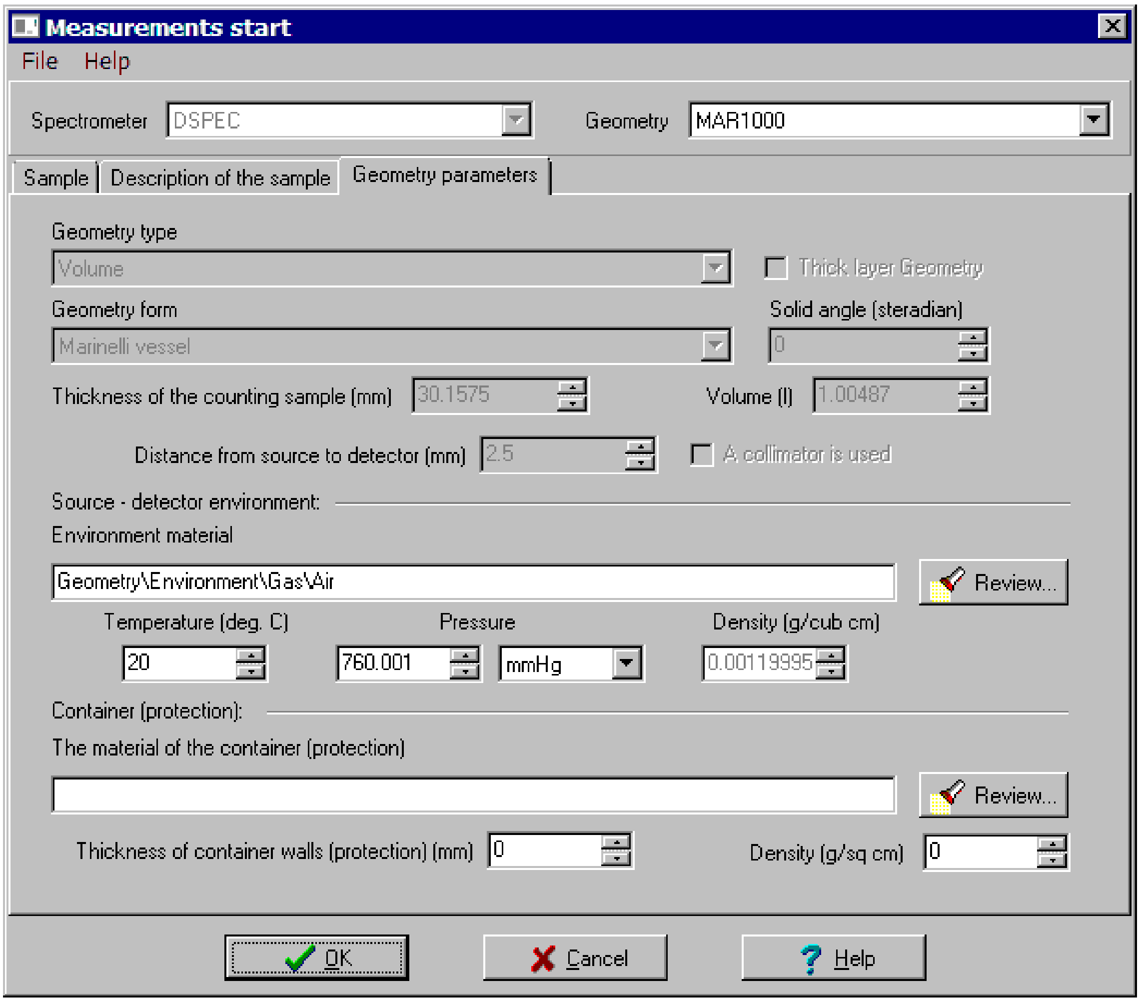
The values of statistical uncertainty and values of nuclide activities averaged over the time of sample measurement are used as a priori data during spectrum processing, therefore, the values entered by the operator will be recalculated at the start date of measurements of the processed sample and from these values the average values for the time of measurement of the activity sample according to the table of nuclides and processing parameters specified in the processing template will be calculated. Since, when recalculating activities on the required date and calculating the average during the measurement of activities, the processes of accumulation and decay of nuclides in the decay chains are taken into account, it is necessary to indicate the activities of all nuclides of the decay chains used.

The **Activity of the counting sample** key in the value entry plate allows you to enter data either on the activities of nuclides in the substance of the counting sample (when the key is not pressed), or in the source material (when the key is pressed **Activity of the source material**). At the same time, it should be borne in mind that the program recalculates the activity values by the value of the initial sample material. This makes it possible to use the measurement results of native samples when processing counting samples from a concentrated substance.

The ⚖ key allows you to enter data either in the values of the total activity of the counting sample or the entire starting substance used to concentrate the sample (when the key is not pressed), or in the values of the specific activity of the counting sample or the starting material (when the ⚖ key is pressed).

The key allows you to add data on additional nuclides or information on the total alpha, beta or gamma activity of the sample to the final report that is not included in the decomposition template used.

The third page of the Geometry parameters form allows you to edit the variable parameters of the measurement geometry.



Spectrometer: DSPEC
Geometry: MAR1000

Geometry type: Volume
☐ Thick layer Geometry
Geometry form: Marinelli vessel
Solid angle (steradian): 0
Thickness of the counting sample (mm): 30.1575
Volume (l): 1.00487
Distance from source to detector (mm): 2.5
☐ A collimator is used

Environment material: Geometry\Environment\Gas\Air
Temperature (deg. C): 20
Pressure: 760.001 mmHg
Density (g/cub cm): 0.00119995

The material of the container (protection):
Thickness of container walls (protection) (mm): 0
Density (g/sq cm): 0

The operator can change the parameters of the environment in which the detector and the radiation source are located: the material of the medium, the temperature and pressure of the medium, the parameters of the container (protection) in which the source is located. If geometry with a variable source distance from the detector is set, the operator must set the current value of the distance from the source to the detector in mm. The distance includes the thickness of the protection (container).

By pressing the "**OK**" key, measurements in the selected spectrometer will be started. In order to save time, you can click "**OK**" without entering sample data, and enter all the necessary data already when measurements are running by calling the menu item "**File / Open / Spectrometer...**" or by clicking on the button.

Running measurements can be stopped at any time by calling the menu item "**Device / Acquire / Stop...**" (button) or start over by clearing the spectrometer memory (menu item "**Device / Acquire / Clear...**").

Cyclic measurement mode

If the estimated measurement time is several times higher than the average measurement time of the sample, the drift of the spectrometer parameters during the measurement time of the sample can significantly distort the spectrum. In this case, it is recommended to use the cyclic measurement procedure with correction of energy drift (check the box "**Cyclic measurements**" in the plate "**Start spectrum acquisition**").

Cyclic measurements are also recommended if there is a possibility of a spectrometer accident, since they allow in the event of an accident (power is lost, the computer freezes hopelessly, etc.) to save the accumulated spectrum, since all cycles accumulated by the time of the accident are already stored in the measurement archive and only the last cycle will be lost. After the accident has been eliminated (in principle, at any time, if there was no accident), the operator can continue the measurement in cyclic mode.

The cyclic measurement mode is necessary when measuring a group of samples with an automatic sample changer. The sample changer is controlled from the spectrum processing procedure of the current cycle.

The cyclic measurement mode is also necessary when organizing the control (monitoring) mode of technological processes.

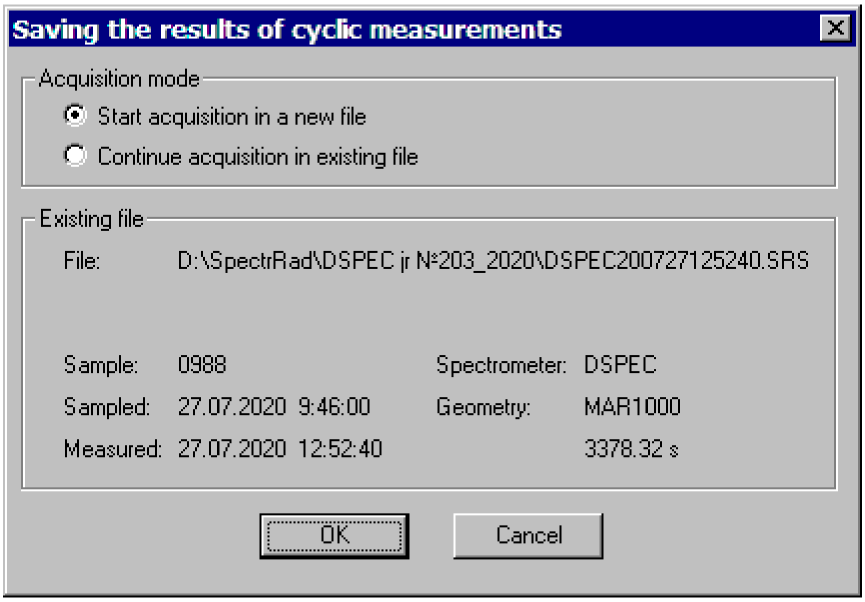
In addition, cyclic measurements with an established mode of preserving all spectra make it possible to implement an amplitude-time analysis scheme for measuring samples containing short-lived nuclides.

It is possible to process the spectrum after each cycle (when setting a processing template in the sample parameters), which can be useful for rapid analysis of the nuclide composition, analysis of changes in the nuclide composition, working with an automatic sample changer or process monitoring mode. In the event that drift correction according to the procedure for comparing the accumulated spectrum and the spectrum of the last cycle is impossible due to the variability of the spectrum, correction of the drift of the spectrometer during cyclic measurements can be carried out after each cycle based on the results of processing the accumulated spectrum.

The cyclic measurement program requires setting the cycle duration and the number of cycles.

If cyclic measurements are used to correct the drift of the spectrometer, the cycle duration should be a compromise between the requirement to accumulate sufficient statistics for the drift correction procedure and the requirement to be shorter in order to minimize drift during the cycle.

If measurements are started from the measurement archive window, the operator can continue accumulating information in the spectrum file of the selected archive entry, which allows additional measurements of the sample. In this case, the measurement startup procedure displays an additional window:



Saving the results of cyclic measurements

Acquisition mode

● Start acquisition in a new file

○ Continue acquisition in existing file

Existing file

File: D:\SpectrRad\DSPEC jr №203_2020\DSPEC200727125240.SRS

Sample: 0988

Sampled: 27.07.2020 9:46:00

Measured: 27.07.2020 12:52:40

Spectrometer: DSPEC

Geometry: MAR1000

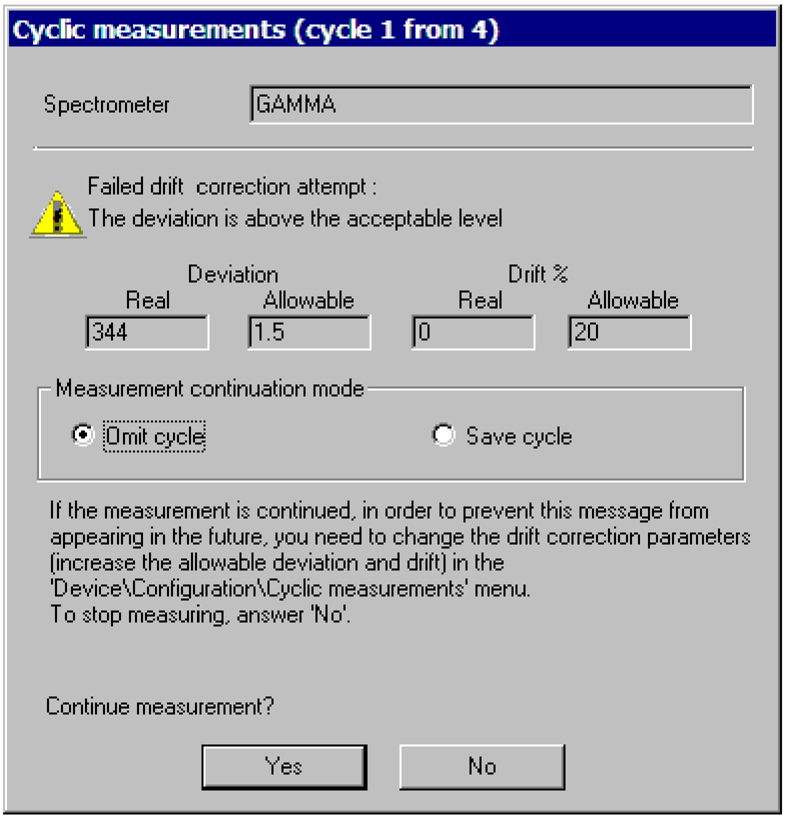
3378.32 s

The operator can choose the accumulation mode - **Acquisition mode**: start accumulation of information in a new file (**Start acquisition in a new file**) - start new measurements, or continue accumulation in an existing file (**Continue acquisition in existing file**) **-** continue measurements.

The parameters of cyclic measurements are preset by calling the menu item "**Device / Configuration / Cyclic measurements...**".

Before starting cyclic measurements, it is recommended to perform an energy auto-calibration procedure of the spectrometer.

During cyclic measurements with the spectrum comparison mode enabled (the accumulated spectrum and the spectrum of the last cycle), if the comparison does not meet the specified parameters, the measurements are suspended, and a window of the following type is displayed on the screen, for example:



Cyclic measurements (cycle 1 from 4)

Spectrometer: GAMMA

Failed drift correction attempt :
The deviation is above the acceptable level

Deviation		Drift %	
Real	Allowable	Real	Allowable
344	1.5	0	20

Measurement continuation mode

● Omit cycle ○ Save cycle

If the measurement is continued, in order to prevent this message from appearing in the future, you need to change the drift correction parameters (increase the allowable deviation and drift) in the 'Device\Configuration\Cyclic measurements' menu.
To stop measuring, answer 'No'.

Continue measurement?

The operator can continue the measurements by pressing the "**Yes**" button and selecting the **Measurement continuation mode**. When the "**Save cycle**" mode is selected, the spectrum of the last cycle will be combined with the already accumulated spectrum, despite poor comparison results, and measurements will continue. When the "**Omit cycle**" mode is selected, the cycle spectrum will not be combined with the accumulated spectrum.

If you refuse to continue the measurements, the spectrum of the cycle that has not been compared will be archived as a separate file and the measurements will be stopped.

Automatic energy scale calibration & spectrometer verification

The parameters of the spectrometric tracts can change over time (drifting); therefore they require **periodic monitoring and calibration** with the use of reference (calibration) source according to the automatic calibration procedure (menu item "**Calibration / Autocalibration / Start...**", button). The autocalibration procedure starts the measurement of the calibration source for a specified time and, upon completion of the measurements, processes the accumulated spectrum. The following frequency of autocalibration is recommended:

- Alpha radiometers require energy calibration before each sample measurement. The recommended reference source is the Pu-239 thin source (10-50 Bq.).
- The beta tract requires energy calibration before each sample measurement. The recommended reference source is the Sr-90 point source (500-3000 Bq).
- Gamma tracts and scintillation (with NaI(Tl), CsI(Tl) detector), and semiconductor (with HPGe or Ge(Li) detector) require daily energy calibration after switching on and warming up the equipment. The recommended control source is Th-232 or Eu-152 (500 - 5000 Bq.).

To assess the long-term stability of the tract parameters during spectrometer verification, it is recommended to carry out auto-calibration at the end of the working day, after measurements are completed.

All tracts, except for periodic calibration, require adjustment and recalibration of the spectrometer with significant changes in the parameters of the general drift and resolution drift. (For scintillation gamma tracts - at values of the total energy drift of more than 100%). In this case, you can adjust the changed gain and (or) the zero of the scale by reconfiguring the ADC parameters (menu item "**Device/ Spectrometer/ Install...**"), or use the adjustment devices provided in the equipment.

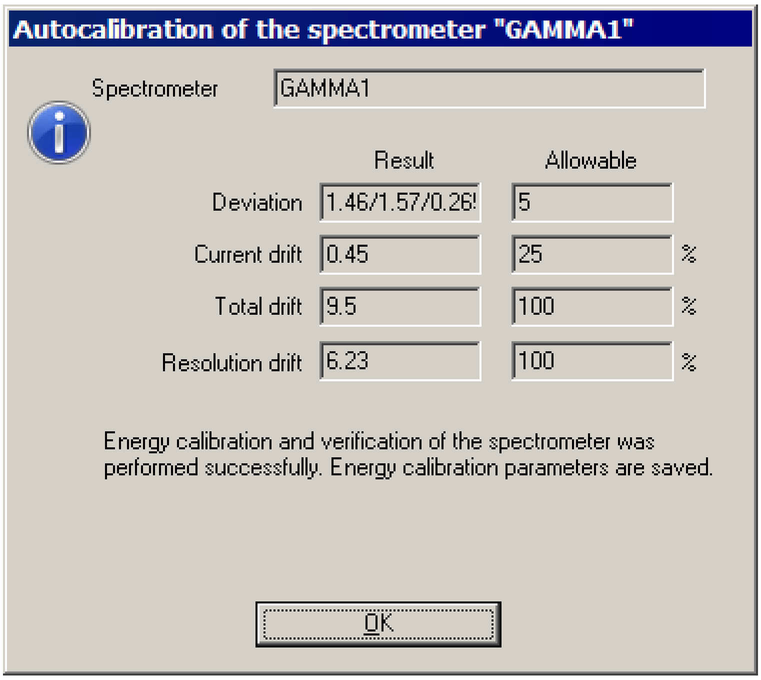
To perform **autocalibration**, it is required to measure the reference (calibration) source in a fixed geometry with duration sufficient to accumulate an average of at least 20 pulses per channel in the operating range of the spectrum. The measurement time of the calibration source and the parameters for monitoring the results of autocalibration is pre-set by the setup procedure - menu item "**Calibration / Autocalibration / Configure...**".

Based on the results of processing the accumulated spectrum, the energy calibration and resolution calibration of the spectrometer are corrected, and the following parameters are calculated:

- **Current drift** – the energy drift of the spectrometer, expressed as a percentage, over time since the previous calibration/autocalibration procedure.
- **Total drift** – the energy drift of the spectrometer since the initial calibration of the spectrometer.
- **Resolution drift** – the drift of the spectrometer resolution over time since the initial calibration of the spectrometer.

Then, depending on the setting of the autocalibration procedure, either the general shape of the measured spectrum and its intensity are compared with the shape and intensity of the spectrum of the calibration source stored during the initial calibration of the spectrometer, or the shape of the measured spectrum with the shape of the spectrum of the calibration source and the estimated activities of the calibration source with passport data. The comparison procedure calculates the parameter of the difference between the measured and reference (calibration) spectra – **Deviation** and compares it with a given threshold value. In this way, the parameters of the spectrometer are adjusted and verified.

At the end of the spectrum processing procedure, a form of the following type is displayed on the screen:



Autocalibration of the spectrometer "GAMMA1"

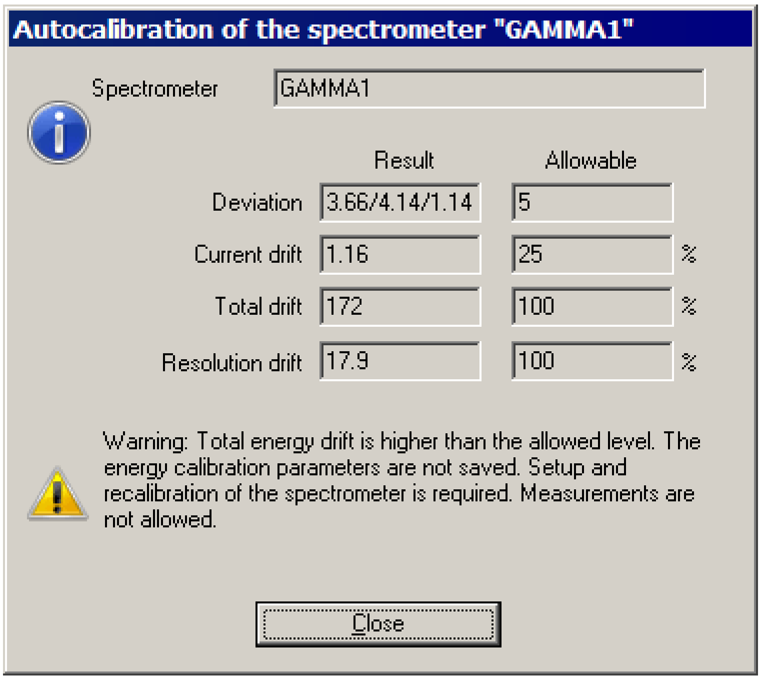
Spectrometer: GAMMA1

	Result	Allowable	
Deviation	1.46/1.57/0.26	5	
Current drift	0.45	25	%
Total drift	9.5	100	%
Resolution drift	6.23	100	%

Energy calibration and verification of the spectrometer was performed successfully. Energy calibration parameters are saved.

The "**Deviation**" parameter includes three values: the total spectrum discrepancy (deviation of the model spectrum from the measured spectrum), the maximum value of the discrepancy for each nuclide and the activity discrepancy (deviation of the activities of the reference source calculated from the measured spectrum from the certified values). The activity discrepancy is calculated if the autocalibration procedure compares not only the spectra, but also the activities. The maximum value of the three deviations is used as the final discrepancy.

The results of calibration and verification of the spectrometer will be accepted if "**Deviation**", "**Current drift**", "**Total drift**" and "**Resolution drif**t" are less than the corresponding permissible values set when setting up the auto-calibration procedure. Otherwise, the window may look like this:



Autocalibration of the spectrometer "GAMMA1"

Spectrometer: GAMMA1

	Result	Allowable	
Deviation	3.66/4.14/1.14	5	
Current drift	1.16	25	%
Total drift	172	100	%
Resolution drift	17.9	100	%

Warning: Total energy drift is higher than the allowed level. The energy calibration parameters are not saved. Setup and recalibration of the spectrometer is required. Measurements are not allowed.

In case of failure of auto-calibration, measurements are allowed only in full access mode. If the auto-calibration parameters specify a reminder mode for the need for autocalibration after a certain time, it is allowed to ignore the autocalibration procedure only in full access mode or in limited access mode, but with the allowed measurement start mode without pre-autocalibration set in the settings of the limited access mode**.**

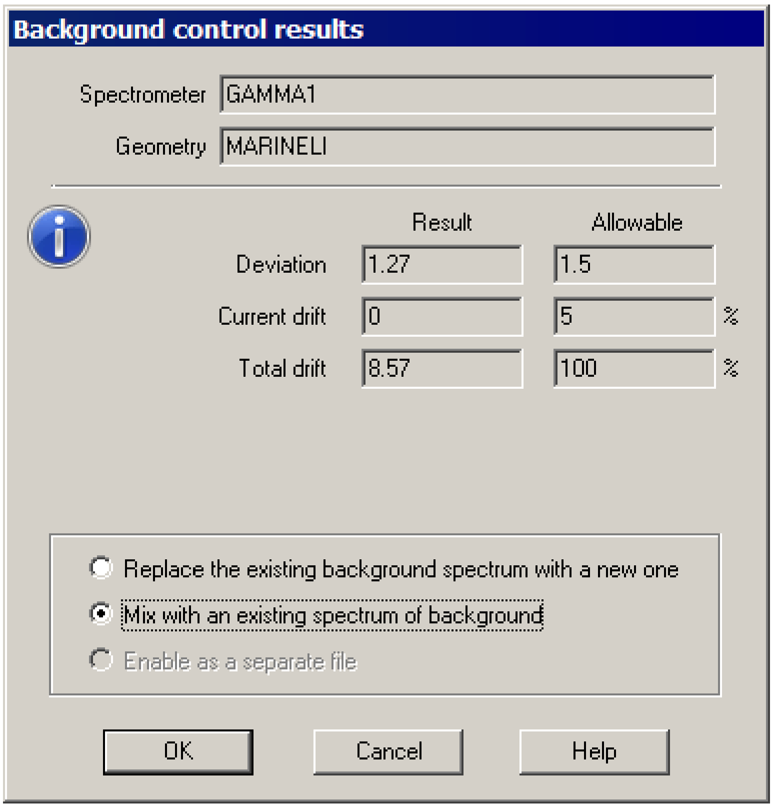
Background radiation control

Both gamma and beta tracts require daily background monitoring (menu item "**Calibration / Background / Start...**", button BGD).

To control the background in the spectrometer, it is required to measure the background sample in a **certified geometry** with duration not less than the average measurement time of the working samples. The measurement time of the background sample and the parameters for monitoring the measurement results is pre-set by the setup procedure - the menu item "**Calibration / Background / Configure...**". If the background control procedure parameters specify a reminder mode to monitor the background after a certain time, it is allowed to ignore the background control procedure only in full access mode or in restricted access mode, but with the allowed measurement start mode without prior background control set in the settings of the restricted access mode.

Distilled water in a vessel designed for sample measurement can be used as a background sample.

After the background measurements are completed, the processing procedure is started (the procedure for comparing the measured background spectrum and the background spectrum installed in the program). The procedure is started either automatically or by the operator, depending on the settings. At the end of it, a form of the following type is displayed on the screen



Background control results

Spectrometer: GAMMA1

Geometry: MARINELI

	Result	Allowable	
Deviation	1.27	1.5	
Current drift	0	5	%
Total drift	8.57	100	%

○ Replace the existing background spectrum with a new one
● Mix with an existing spectrum of background
○ Enable as a separate file

In the event that the background control parameters do not exceed the established norms, it is recommended to mix the measured spectrum with the existing background spectrum ("**Mix with existing spectrum of background**"). In this case, the previously measured background spectrum, before reaching the maximum background accumulation time set in the background control parameters (menu item "**Calibration / Background / Configure...**"), will be summed with the newly measured one, and when exceeded, it will be mixed in proportion determined by the ratio of the measurement time to the maximum background accumulation time. This mode allows you to accumulate the necessary background measurement time (the background measurement time should be at least twice the maximum time for measuring working samples) and gradually update the background spectrum, tracking its changes.

If the norm is exceeded, mixing with the existing background spectrum is prohibited, since, for some reason, an unacceptably sharp change in the background in the spectrometer occurred. In this case, it is recommended to find out the reason for the background change (contamination of the detector, damage of the detector packaging, etc.), eliminate it if possible, and repeat the background control procedure. If it is impossible to achieve the existing parameters of the spectrometer background, the background must be reset - "**Replace the existing background with a new one**". The background spectrum replacement operation is available only in full access mode, or in restricted access mode, but with the allowed background spectrum replacement mode set in the Restricted access mode settings.

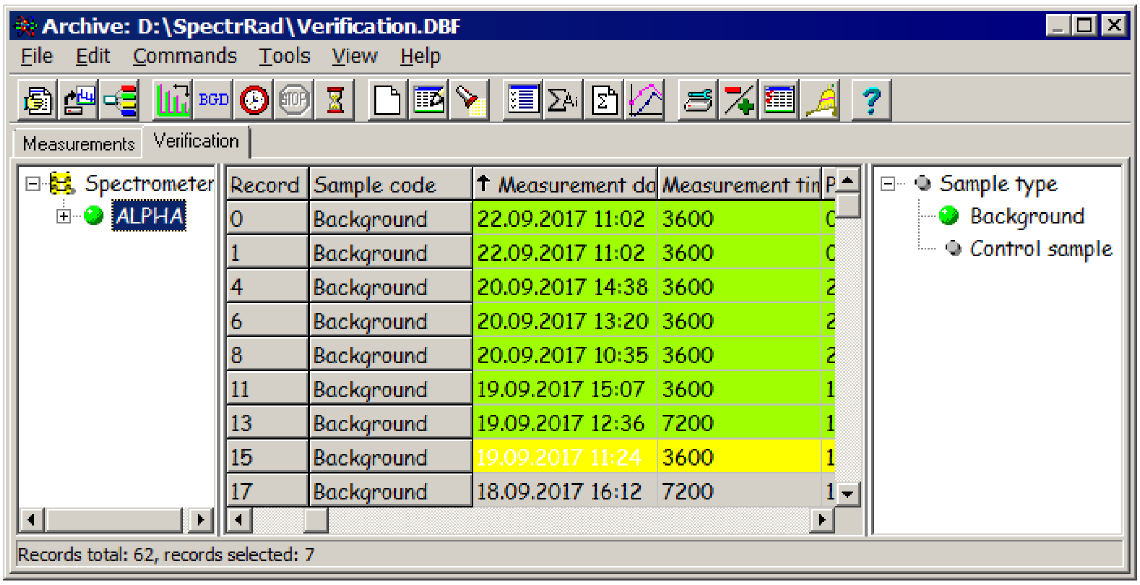
If recalculation to the density of the background sample is allowed in the background control parameters, the operator can select the "**Enable as separate file**" mode. In this case, the measured spectrum will be included as one of the basic background files with a certain background sample density to bring the background spectrum to the density of the measured sample when processing the working spectra.

The background control procedure can also be started from the measurement archive. If we are going to carry out a routine procedure for daily background monitoring, then running the procedure from the archive gives only the advantage that we can pre-select the spectrometer and measurement geometry. But calling the background control procedure from the archive is intended for other purposes – for the purpose of implementing measurement techniques on spectrometers with high background variability.

These are, first of all, alpha radiometers with registration of alpha radiation in normal atmospheric conditions (without pumping air, without displacing air with non-radioactive gases), and ordinary air contains radioactive gases (radon, thoron and, perhaps, not natural radioactive gases).

In this case, the background is not stable and we cannot be sure that the background accumulated in the past days corresponds to the background of today and the hour of measurements. In such conditions, it is more reasonable to carry out sample measurements alternating them with background measurements. Moreover, you need to start by measuring the background (of course, all measurements should be preceded by auto-calibration) and finish by measuring the background. Then set the background spectrum to the program, which is the sum of the background spectra measured during this time, calculate the background variability, set the resulting value to the processing program (menu item "**Calibration/ Background / Configure...**") and only then process the spectra of the samples. In this case, we can be sure that the values of the activities and measurement errors will be calculated correctly.

The launch of the background control procedure from the measurement archive is intended primarily for the implementation of this technique. The operator must select in the measurement log entries related to background measurements for the required group of sample and background measurement records. For example:



Record	Sample code	Measurement da	Measurement tin	P
0	Background	22.09.2017 11:02	3600	C
1	Background	22.09.2017 11:02	3600	C
4	Background	20.09.2017 14:38	3600	2
6	Background	20.09.2017 13:20	3600	2
8	Background	20.09.2017 10:35	3600	2
11	Background	19.09.2017 15:07	3600	1
13	Background	19.09.2017 12:36	7200	1
15	Background	19.09.2017 11:24	3600	1
17	Background	18.09.2017 16:12	7200	1

Records total: 62, records selected: 7

Then press the BGD key, thus starting the procedure for monitoring and setting the background spectrum. The background control procedure will be performed for all selected measurement log entries, starting from the earliest. For each entry, a form of background control results will be displayed on the screen. The operator must choose: mix the background with the background spectrum of the current recording, replace the background spectrum or skip the recording. It is recommended to replace the background for the first recording, and mix it for subsequent recordings.

Starting the background control procedure from the measurement archive can be used to restore the current background spectrum that has been corrupted for some reason. The operator must select several (2, 3, ...,10 or more) recent unspoiled background measurement records for the required spectrometer and geometry in the measurement log and start the procedure for monitoring and setting the background spectrum. Replace the background for the first record, and mix it for the subsequent ones.

Spectrum processing. Decomposition

"Decomposition" is the decomposition of a spectrum into components with an assessment of the contribution of components to the spectrum. Elementary spectra[3] are usually used as components. At this case, the estimates of contributions are the activities of nuclides.

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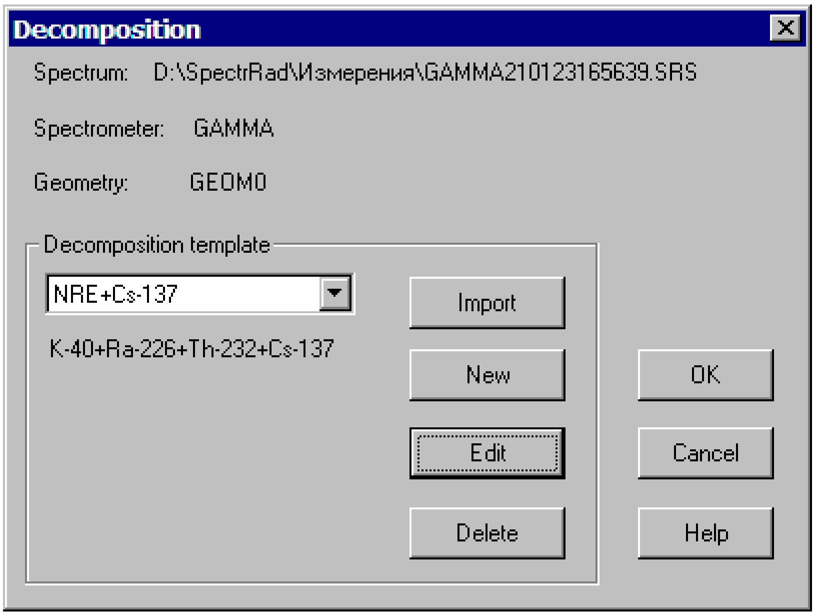
[3] The **elementary spectrum** is the response of the spectrometer normalized for nuclide decay to radiation from a nuclide or a chain of nuclides in a state of radioactive equilibrium (the probability distribution density of recording pulses through the channels of the spectrometer at a single nuclide decay).

When clicking on the button (selecting the "**Processing / Decomposition...**" menu item), the following window is displayed:



Spectrum: D:\SpectrRad\Измерения\GAMMA210123165639.SRS

Spectrometer: GAMMA

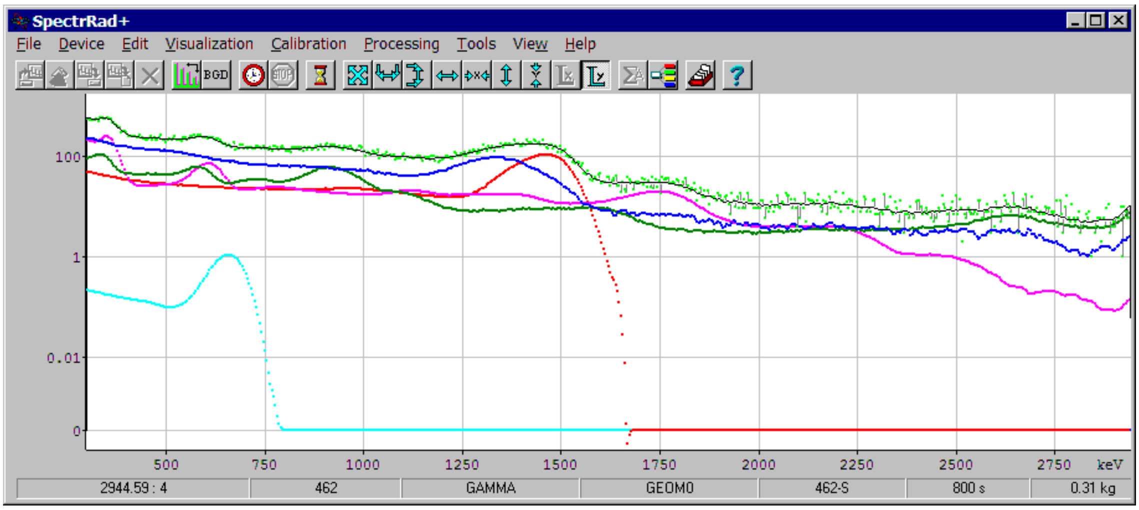
Geometry: GEOM0

Decomposition template

NRE+Cs-137

K-40+Ra-226+Th-232+Cs-137

The operator can select one of the existing decomposition templates (**Decomposition template**) or create the necessary template himself[4] (see “Creating a decomposition template”) and, by clicking on the "**OK**" key, start the processing program. In this case, the main window of the program is converted into a decomposition window, which may look like this, for example:



The window displays the procedure for decomposing the spectrum into components. The color setting for the processed spectrum, component spectra, window background, etc. is performed using the menu item "**View / Number and colors of spectra...**". The status bar displays the same data as in the main window.

The type of spectrum visualization is set by selecting the menu item "**Visualization / Histogram**". When visualized as histograms, the window may look like this:
The window displays the procedure for decomposing the spectrum into components. The color setting for the processed spectrum, component spectra, window background, etc. is performed

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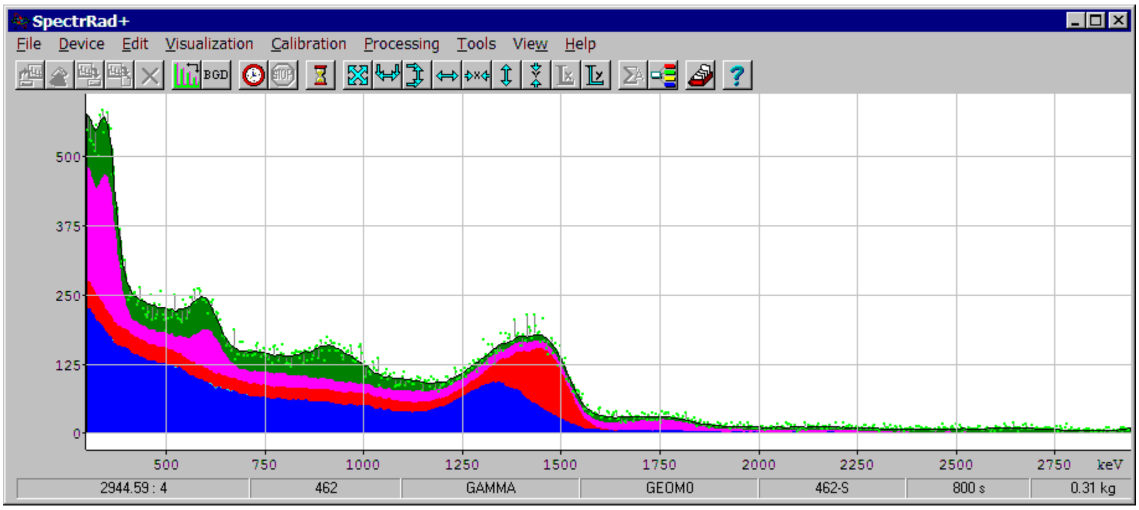
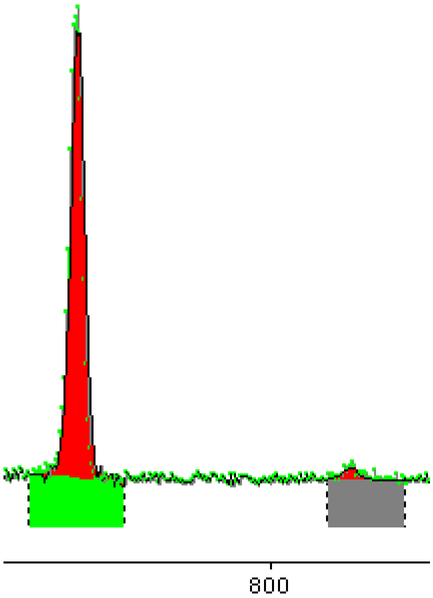
[4] The "**Import**", "**New**", "**Edit**" and "**Delete**" buttons are available only in full access mode (menu item “**Tools / Access mode...**”)

using the menu item "**View / Number and colors of spectra...**". The status bar displays the same data as in the main window.

The type of spectrum visualization is set by selecting the menu item "**Visualization / Histogram**". When visualized as histograms, the window may look like this:



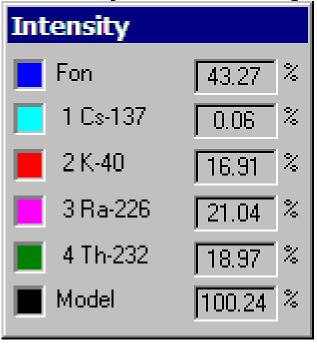
The "windows" method of processing poorly resolved spectra uses the energy windows specified when setting up the processing procedure, and when processing linear spectra with peak search, energy windows corresponding to the peaks found in the spectrum and the windows of the lines of the determined nuclides are used. When the visualization mode of energy windows is set (see the pop-up menu "**Energy windows/Peak boundaries**") the position of the windows is displayed on the screen, for example, as in the figure:



Windows are divided into two types: "**significant**" - windows used to assess the activity of nuclides (windows corresponding to "significant" nuclide lines) and "**insignificant**" - not used to calculate the activity of nuclides, but participating in the overall assessment of the success of the decomposition procedure. "**Significant**" windows are drawn in the color specified when setting up the decomposition procedure (in the example - green), "**insignificant**" - in the color matching the color of the residual spectrum (in the example - gray),

Additionally, two more windows are formed:

The "**Intensity**" window displays the contribution of components (in %) to the sample spectrum. (**Model** is the sum of the contribution of all components.)



Intensity

Fon 43.27 %

1 Cs-137 0.06 %

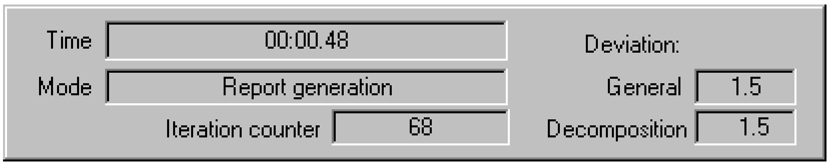
2 K-40 16.91 %

3 Ra-226 21.04 %

4 Th-232 18.97 %

Model 100.24 %

And the "**State**" window.



Time 00:00.48

Mode Report generation

Iteration counter 68

Deviation:

General 1.5

Decomposition 1.5

The window displays:

- **Time** – the time elapsed since the beginning of spectrum processing in the clock format: hours:min:sec.
- **Mode** – short description of the spectrum processing mode:

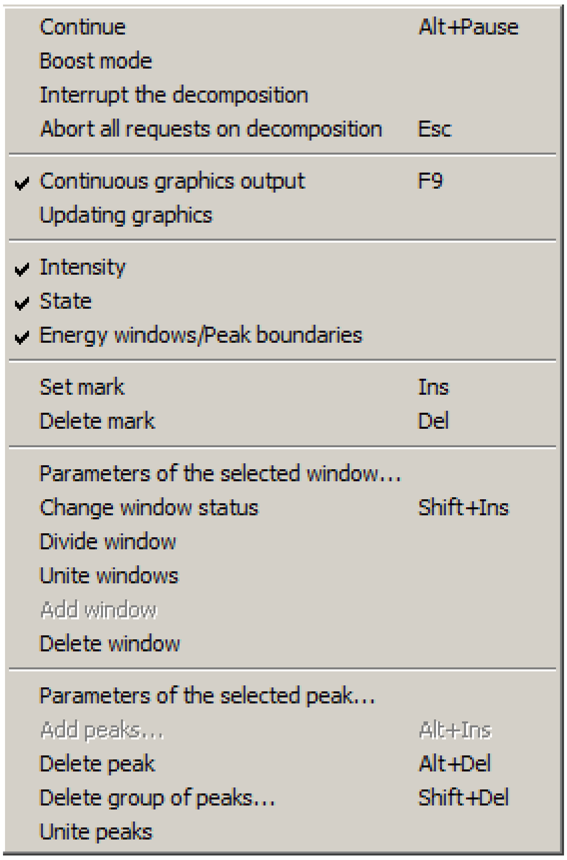
Mode	Description
Linear estimation	Linear assessment of the contribution of the components.
Spline construction	Evaluation of unknown components. The model is complemented by a spline.
Drift variation: Ax; Bx; W	Global search for the best values of the energy drift parameters of the spectrum (**Ax** is the gain factor, **Bx** is the zero of the channel scale, **W** is the resolution of the spectrometer) by varying the parameter values in a given range with a given step.
Drift estimation: Ax; Bx; Cx; W	Correction of the energy drift of the spectrum by the Gauss-Newton method. **Ax** is the gain factor, **Bx** is the zero of the channel scale, **Cx** is the coefficient of nonlinear distortion, **W** is the resolution (peak width).
Drift estimation: Axi; Bxi; Cxi;	Correction of the energy drifts of components by the Gauss-Newton method.
Absorption variation	Search for the best value of the averaged atomic number of the substance of the counting sample (Z effective) and/or the thickness of the counting sample.
Zero components removal	Removal of insignificant components from the decomposition procedure.
Report generation	Completion of processing, report generation.

- **Iteration counter** - the number of cycles of refinement of estimates.
- **Deviation (General and Decomposition)** is the deviation of the calculated model from the measured spectrum normalized by the estimated value of the standard deviation $G = \sqrt{\sum((X_i - X_m)^2 / G_i^2)/(n-m)}$. **General deviation** is a discrepancy across the entire spectrum within the processing boundaries. **Decomposition deviation** - discrepancy of the solution of a system of equations.

With the windowed processing method, the decomposition residual can be zero; the total residual cannot be zero.

Menu

The main menu of the decomposition window duplicates the menu of the main program window, but only a part of the items remain available. Right-clicking on the decomposition window activates the following pop-up menu:



	Continue	Alt+Pause
	Boost mode	
	Interrupt the decomposition	
	Abort all requests on decomposition	Esc
✓	Continuous graphics output	F9
	Updating graphics	
✓	Intensity	
✓	State	
✓	Energy windows/Peak boundaries	
	Set mark	Ins
	Delete mark	Del
	Parameters of the selected window…	
	Change window status	Shift+Ins
	Divide window	
	Unite windows	
	Add window	
	Delete window	
	Parameters of the selected peak…	
	Add peaks…	Alt+Ins
	Delete peak	Alt+Del
	Delete group of peaks…	Shift+Del
	Unite peaks	

Some of the pop-up menu items also duplicate the contents of the main menu, but also have additional items related directly to the decomposition:

Pause (Continue) Alt+Pause	Stop (or continue, if stopped) the decomposition process.
Boost mode	The decomposition process has a multi-level and iterative nature. Forcing the mode interrupts iterations in the current level and causes a transition to the next one.
Interrupt the decomposition	Complete the decomposition at the current iteration.
Interrupt all request on decomposition Esc	If there is a queue of processing requests (decomposition when observing the acquisition of spectrum, processing a group of spectra from the archive), executing this menu item cancels all decomposition requests, the current processing is not interrupted.
Continuous graphics output F9	A menu item with a status lock. With continuous graphics output, the decomposition process is constantly displayed on the screen. This may slow down spectrum processing. When the output is disabled, only the final solution is visualized.

Updating graphics		One-time graphics update when continuous graphics output is disabled.
Intensity		Turning on/off the "Intensity" window.
State		Turning on/off the "State" window
Energy windows / Peaks boundaries		Enabling/disabling visualization of energy windows or peak boundaries, with the "windows" method of spectrum processing, spectrum processing with peak search or spectrum decomposition into peak spectra.
Set mark	**Ins**	Mark the spectrum channel selected using a movable marker.
Delete mark	**Del**	Removing the spectrum mark closest to the movable marker.
Parameters of the selected window…		Displays the parameters of the window specified by the marker.
Change window status	**Shift+Ins**	Change the status of the decomposition window: "significant"-> "excluded"-> "not significant"-> "significant"-> .... Excluded windows are not used in any way in the decomposition procedure. "Significant" and "not-significant" windows are used according to the mode specified in the decomposition template (see "Settings" / "Creating decomposition templates" / "Decomposition Options" / "Windows settings").
Divide window		The procedure divides the selected decomposition window into two according to the position of the movable marker.
Unite windows		Two windows (the selected window and the one closest to the movable marker) are combined into one.
Add window		A window limited by preset marks (menu item "Set mark"), or the borders of neighboring windows are added to the decomposition procedure.
Delete window		The decomposition window selected using a movable marker is removed from the spectrum processing procedure.
Parameters of the selected peak…		Output of the parameters of the peak indicated by the marker when processing linear spectra.
Add peaks	**Alt+Ins**	The procedure adds to the list of found peaks of the spectrum, the peak missed by the search procedure, the boundaries of which the operator previously indicated by marking them with a marker (menu item "Set mark").
Delete peak	**Alt+Del**	The peak indicated by the movable marker is removed from the list of found peaks of the spectrum.
Delete group of peaks	**Shift+Del**	All peaks located in the selected spectral region are removed from the list of found peaks.

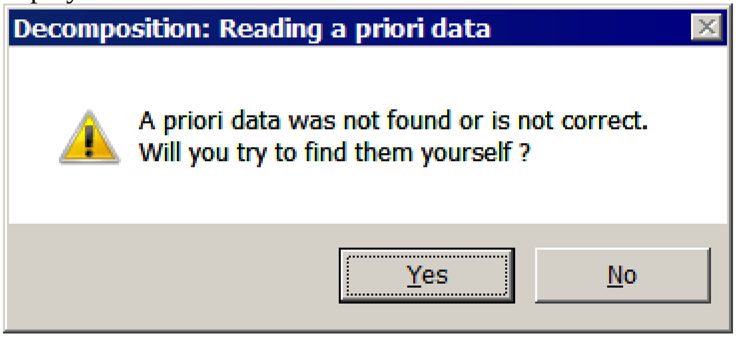
Unite peaks	The peak indicated by the movable marker is combined with the peak closest to the marker in the multiplet into one peak.

The group of menu items associated with windows is available only when processing spectra using energy windows, and the group of items associated with peaks is available only when processing spectra in peak search mode. Some of the menu items may be missing depending on the processing mode.

Entering a priori data

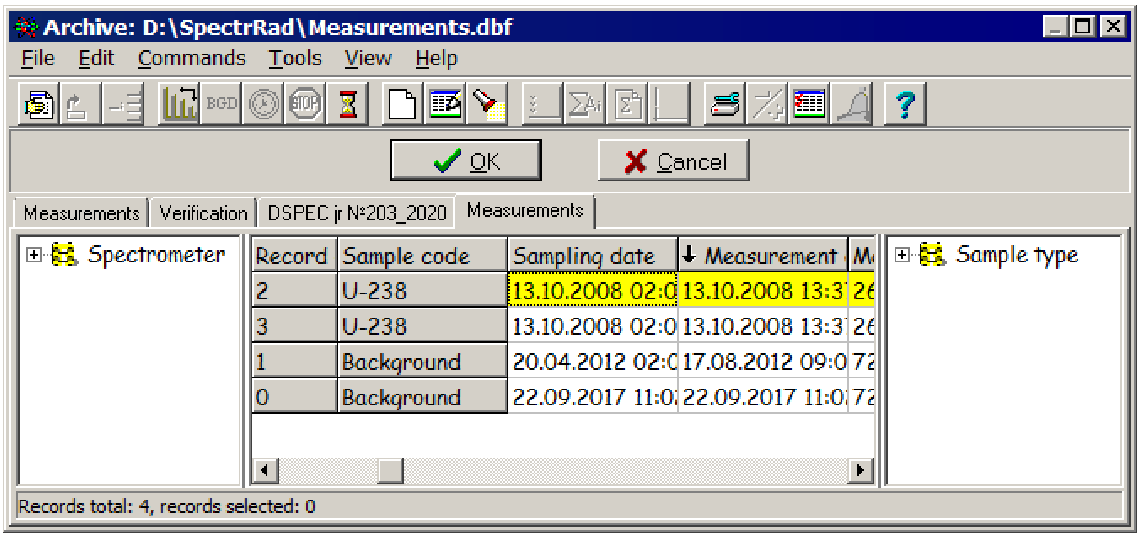
If it is necessary to take into account the results of processing the spectrum of this sample (samples from the same material) measured earlier or on another detector (results of processing the gamma spectrum of the sample during processing the beta spectrum), depending on the a priori data search mode set in the processing template, the program can either search for the necessary data by itself, or will offer the operator to select from the database the data of the measurement results is the necessary record.

If the a priori data search mode was set in the processing procedure and the program did not find the required data, the operator will be asked to find them independently. A window is displayed on the screen:



A priori data was not found or is not correct.
Will you try to find them yourself ?

The answer "No" means refusal of processing. When the answer is "Yes", a window of the archive of measurement results of the following type is displayed on the screen, for example:

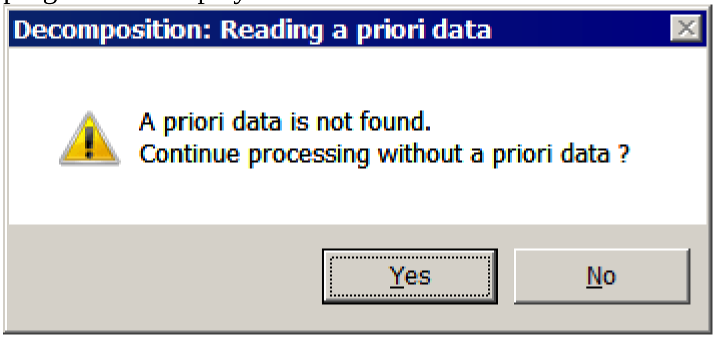


Record	Sample code	Sampling date	Measurement	M
2	U-238	13.10.2008 02:0	13.10.2008 13:3	2
3	U-238	13.10.2008 02:0	13.10.2008 13:3	2
1	Background	20.04.2012 02:0	17.08.2012 09:0	7
0	Background	22.09.2017 11:0	22.09.2017 11:0	7

Records total: 4, records selected: 0

The operator needs to open the measurement archive containing the necessary record (or select the desired one from the already open ones), select the necessary record in the archive as a working one (highlighted in yellow when selecting from regular records or blue when selecting from a group selection) by clicking on it with the left mouse button, and press the "**OK**" key. Previously, you can make sure that we have selected exactly the record we need by clicking on the "button" or by selecting the menu item "**Commands / Report**".

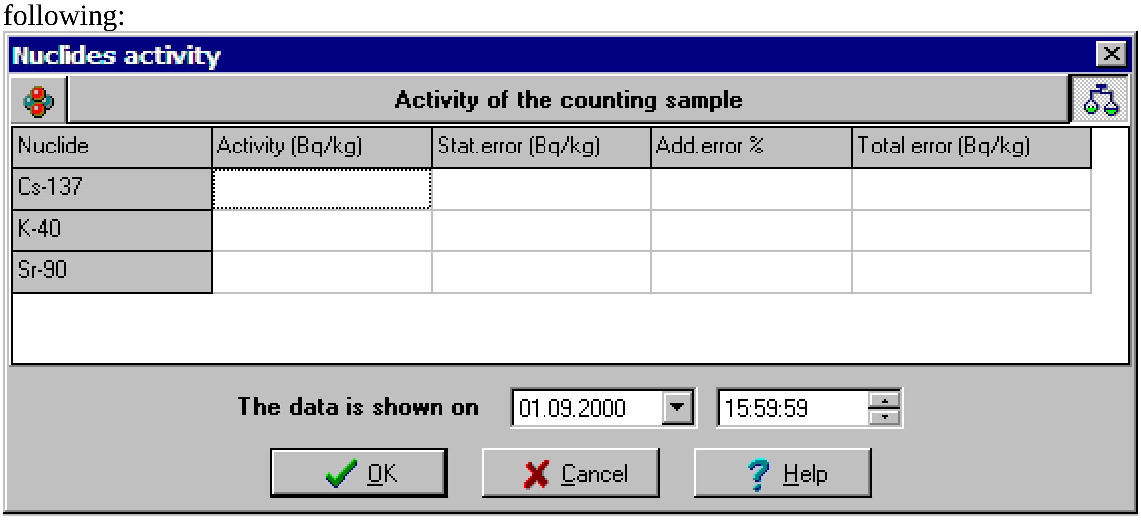
In the event that a priori data is not available in the measurement archive, the operator can refuse to select a priori data in the archive by clicking on the "**Cancel**" button. In this case, the program will display a form:



Decomposition: Reading a priori data

A priori data is not found.
Continue processing without a priori data ?

. If the answer is "Yes", the program will process the spectrum without a priori data. When the answer is "No", a form is displayed on the screen, depending on the list of nuclides to be determined, such as the following:



Nuclides activity

Activity of the counting sample

Nuclide	Activity (Bq/kg)	Stat.error (Bq/kg)	Add.error %	Total error (Bq/kg)
Cs-137				
K-40				
Sr-90				

The data is shown on 01.09.2000 15:59:59

The operator must enter data on the activities of nuclides and the errors in their determination. The error (uncertainty) includes two components: statistical uncertainty and additional uncertainty, defined as a percentage of activity. The total uncertainty is not entered by the operator, but is calculated by the program from the values of statistical and additional uncertainty. A 95% confidence interval of activity estimation is used as a random component of the overall uncertainty (statistical uncertainty). The absence of data in the activity and statistical uncertainty columns means that there is no a priori data on the activity of this nuclide.

The **Activity of the counting sample** key in the value entry panel allows you to enter data either on the activities of nuclides in the substance of the counting sample (when the key is not pressed), or in the source material (when the key is pressed **Activity of the source material**). At the same time, **it should be borne in mind** that the program recalculates the activity values by the value of the initial sample material. This allows you to use the measurement results of native samples when processing counting samples from a concentrated substance, but it can serve as a source of errors if the operator forgot to indicate that one of the samples is concentrated or the nuclide composition of the sample has changed as a result of concentration.

The ⚖ key allows you to enter data either in the values of the total activity of the counting sample or the entire starting substance used to concentrate the sample (when the key is not pressed), or in the values of the specific activity of the counting sample or the starting material (when the ⚖ key is pressed).

As correct a priori data for processing, it is necessary to use the results of processing samples of the same source material measured on another spectrometer or at another time. It is allowed to use the results of processing concentrated or diluted samples when processing native samples (and the reverse option) if we are sure that during the concentration of the substance there were no loss of any nuclides that are components of the decomposition of the spectrum.

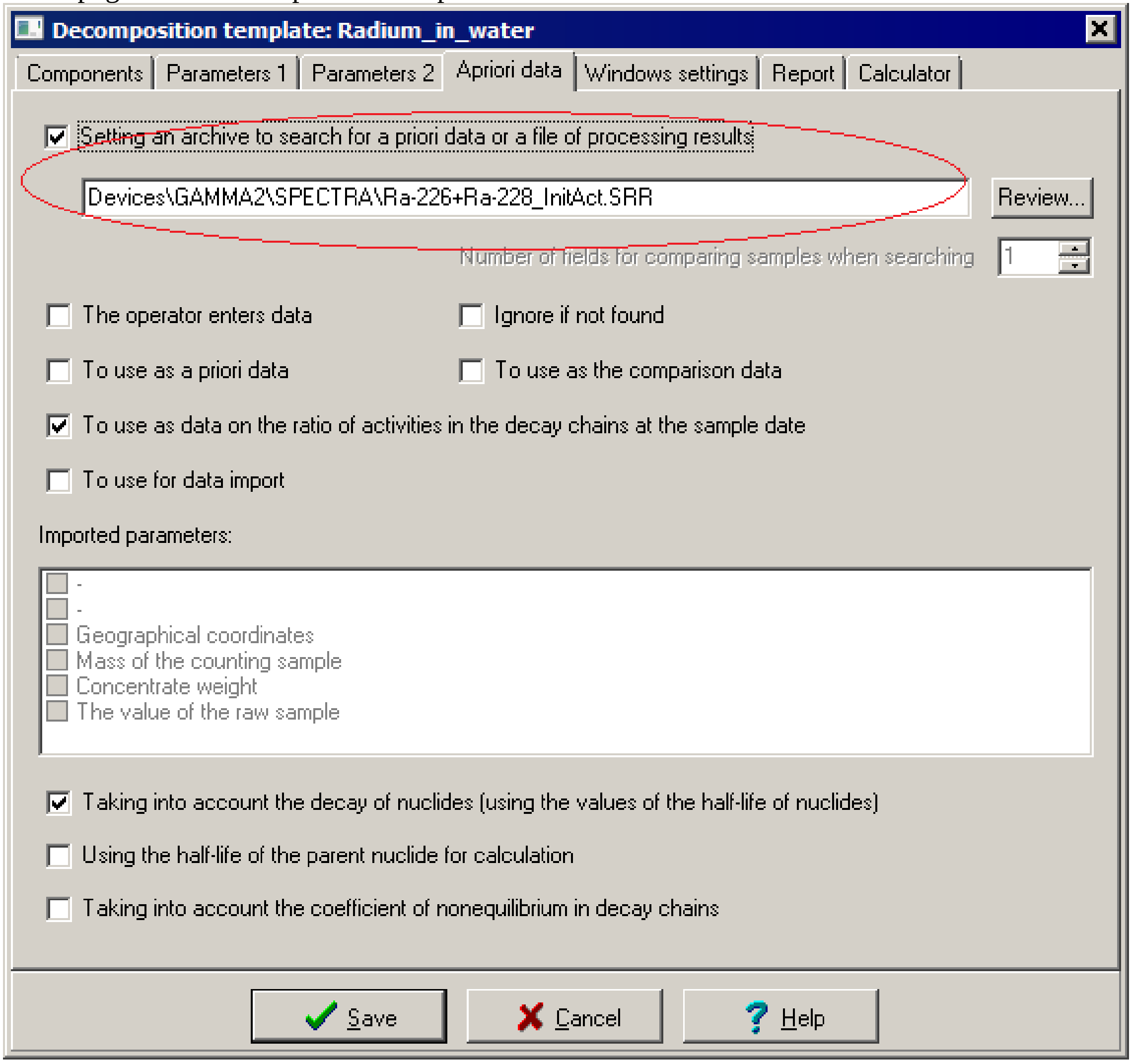
The values of statistical uncertainty and the values of nuclide activities averaged over the time of sample measurement are used as a priori data for spectrum processing. Therefore, the values entered by the operator will be recalculated on the date of the start of measurements of the processed sample and from these values the average activity during the measurement of the sample will be calculated according to the nuclide table and processing parameters specified in the processing template. Since, when recalculating activities on the required date and calculating the average during the measurement of activities, the processes of accumulation and decay of nuclides in the decay chains are taken into account, it is necessary to indicate the activities of all nuclides of the decay chains used.

The key allows you to add data on additional nuclides or information on the total alpha, beta or gamma activity of the sample to the final report that is not included in the decomposition template used.

The mode of entering a priori data by the operator without searching for data in the archive can be set in the processing program (template).

A priori data can also be data on the initial ratio of activities in the decay chains of nuclides at the sample date. The date of sampling may be the date of chemical separation of the element from the sample, the end date of air passage through the filter when analyzing air for radioactive aerosols, etc. In principle, any date for which the ratio of nuclide activities in the decay chain is known.

If the data on this ratio is not provided in the specified a priori data file on the "**Apriori data**" page of the decomposition template



Decomposition template: Radium_in_water

☑ Setting an archive to search for a priori data or a file of processing results

Devices\GAMMA2\SPECTRA\Ra-226+Ra-228_InitAct.SRR

Number of fields for comparing samples when searching 1

☐ The operator enters data

☐ Ignore if not found

☐ To use as a priori data

☐ To use as the comparison data

☑ To use as data on the ratio of activities in the decay chains at the sample date

☐ To use for data import

Imported parameters:

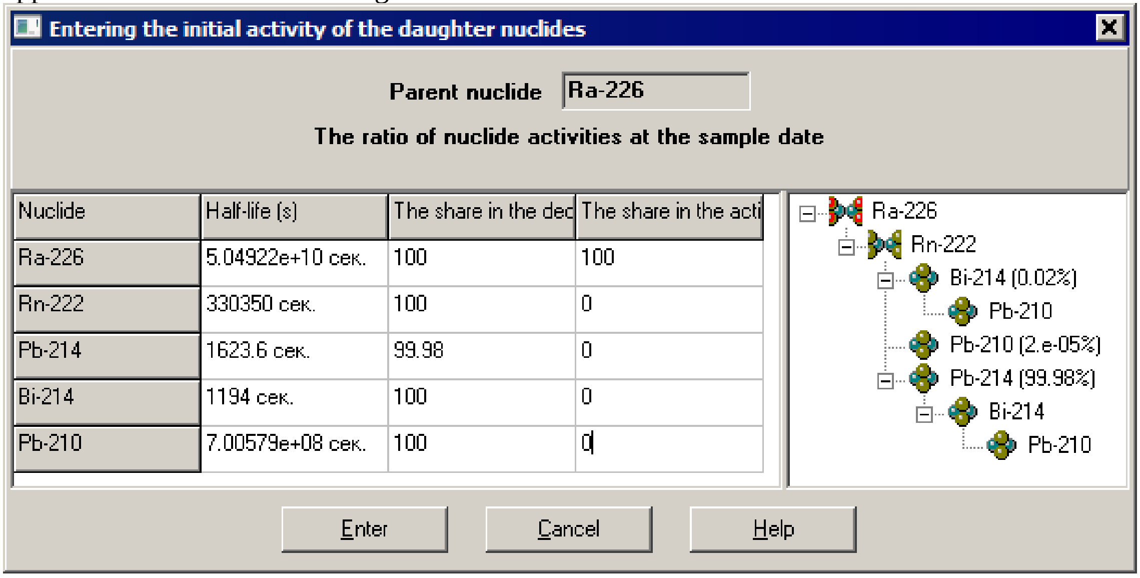
☐ -
☐ -
☐ Geographical coordinates
☐ Mass of the counting sample
☐ Concentrate weight
☐ The value of the raw sample

☑ Taking into account the decay of nuclides (using the values of the half-life of nuclides)

☐ Using the half-life of the parent nuclide for calculation

☐ Taking into account the coefficient of nonequilibrium in decay chains

, The processing procedure will prompt the operator to enter them. In this case, a window will appear on the screen for entering such data:



Entering the initial activity of the daughter nuclides

Parent nuclide Ra-226

The ratio of nuclide activities at the sample date

Nuclide	Half-life (s)	The share in the dec	The share in the acti
Ra-226	5.04922e+10 сек.	100	100
Rn-222	330350 сек.	100	0
Pb-214	1623.6 сек.	99.98	0
Bi-214	1194 сек.	100	0
Pb-210	7.00579e+08 сек.	100	0

The operator must enter the activity for the daughter nuclides as a percentage relative to the parent nuclide at the date of sampling. In the example, the date of sampling should be the date of radium separation. Accordingly, the activity of the daughters of Ra-226 on this date will be zero (in the example, this data has already been entered). When air is drawn through the filter, an equilibrium occurs after a while between the rate of accumulation of nuclide on the filter and the rate of its decay. And this ratio is proportional to the half-lives of nuclides. The state of radioactive equilibrium at the sampling date may also be a possible option. In this case, the activity ratio must be pre-calculated using the "**Tools / Nuclide table / Tools / Nuclides equilibrium chain / Construct…**" procedure.

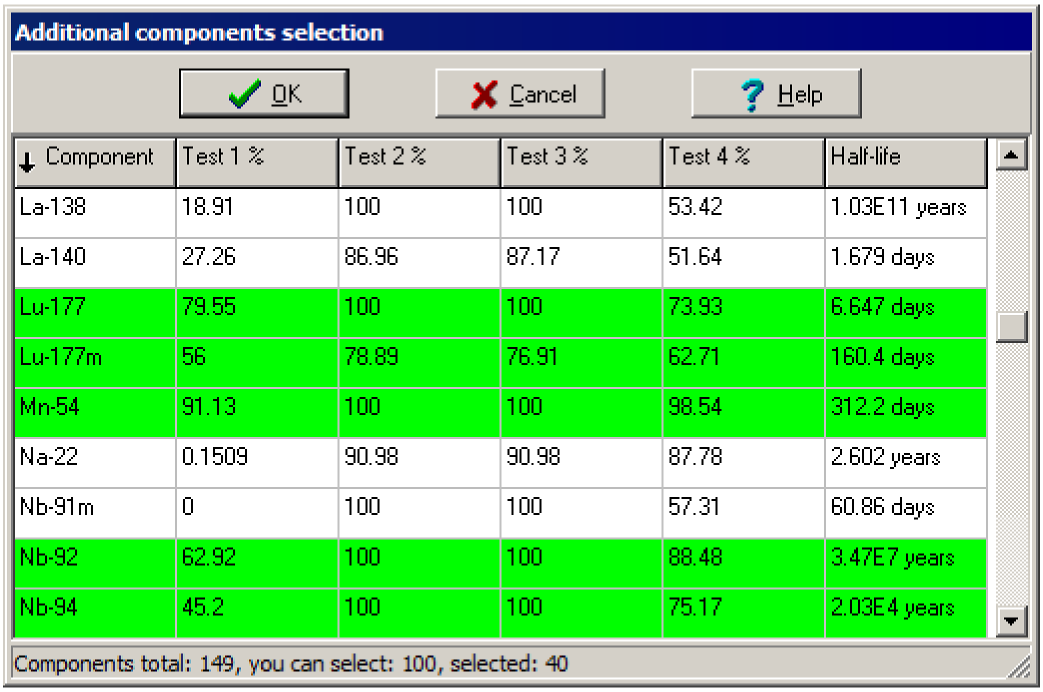
These data are necessary for the correct calculation of the processes of accumulation and decay of nuclides in the chain. Pressing the "**Cancel**" key by the operator cancels the decomposition procedure, since correct calculation is impossible without such information.

Double-clicking on the nuclide icon in the decay tree triggers the tree editing procedure. The procedure will prompt the operator to either break the link with the parent nuclide, or to break all links for all nuclides of the tree, if the parent nuclide of the decay tree is selected. When the bond between two nuclides is broken, the chain is divided into two parts, and when the bonds between all nuclides are broken, all nuclides will be considered independent, which corresponds to the rejection of the use of a priori information. Without breaking ties, all data on daughter lines will be included in the maternal nuclide line table, and instead of five unknowns, the program will determine only the activity of one maternal nuclide, which will significantly increase the efficiency (accuracy) of the assessment. If we break one connection, we will get a pair of unknowns instead of one unknown activity. Which, of course, is better than five, but worse than one. Breaking the connection is justified if we are sure that the activity of the parent nuclide is zero or negligible.

In order not to enter data on the activity ratios in the decay chains every time the decomposition procedure is started, the program will suggest saving the entered data as a priori data. After saving, the operator must specify the saved information in the decomposition template for use as information about the ratio of activities in the decay chains at the date of sampling (see."**Creating decomposition templates / Decomposition parameters**").

Selection of additional components

If the "**Add components that have lines near the marker to the components list**" or "**Automatic analysis of the composition**" checkbox is selected in the processing template parameters, but the "**without operator intervention**" checkbox is not selected, the program will display a table containing a list of "suspected" additional components of the following type, for example:



Component	Test 1 %	Test 2 %	Test 3 %	Test 4 %	Half-life
La-138	18.91	100	100	53.42	1.03E11 years
La-140	27.26	86.96	87.17	51.64	1.679 days
Lu-177	79.55	100	100	73.93	6.647 days
Lu-177m	56	78.89	76.91	62.71	160.4 days
Mn-54	91.13	100	100	98.54	312.2 days
Na-22	0.1509	90.98	90.98	87.78	2.602 years
Nb-91m	0	100	100	57.31	60.86 days
Nb-92	62.92	100	100	88.48	3.47E7 years
Nb-94	45.2	100	100	75.17	2.03E4 years

Components total: 149, you can select: 100, selected: 40

The total number of decomposition components cannot exceed one hundred, so the analysis program removes all unnecessary components from the list of additional components (you can remove any component from the list of main components only by changing the decomposition template). The remaining enabled components are marked in green.

One of the components is the selected (or active) component. It is highlighted in yellow for non-enabled components and blue for enabled components. The cursor keys move the position of the selected component, left-clicking on the line of the component makes it active

To select the components, the program calculates four test values:

- **Test1** is the correlation coefficient of the component spectrum with the analyzed spectrum in the processing area. The program removes components from the list of enabled components that have Test1 values less than the level specified by the operator.
- **Test2** is the probability of the component's presence in the spectrum calculated for the usual energy range (+/- 3 peak widths) for all nuclide lines included in the component.
- **Test3** is the probability of the component's presence in the spectrum (as a percentage) calculated for an extended energy range (+/- 6 peak widths) for all nuclide lines included in the component.
- **Test4** - the proximity of the energies of the component lines to the positions of the peaks of the spectrum, normalized by double the width of the peaks (if the positions of the peaks coincide with the energies of the lines, Test4 is equal to 100%).

For reference, the table also shows the values of the half-lives of the nuclides forming the components.

The values of the **Test2-Test4** test values are calculated either for all nuclide lines with the exception of lines with unreliable quantum yield, or only for "significant" ones (see "Tables of nuclides" / "Tables structure"), depending on the set spectrum processing mode: "use only significant lines", or use all lines (see "Creating decomposition templates" / "Decomposition parameters". The correlation coefficient (**Test1**) is always calculated only for lines marked as "significant" or "calibration" in the nuclide table used.

When processing spectra without searching for peaks (scintillation spectra), the values of the two test quantities **Test2** and **Test3** are almost always equal to 100%, since Compton scattering is also included in the peak region.

The operator can independently include or remove any component. First, you need to select the component by clicking on it with the left mouse button and press the "**Insert**" key or open a pop-up menu by right-clicking and select the appropriate menu item "**Select**" or "**Unselect all**". A double-click with the left mouse button or a single click, with the "**Ctrl**" key pressed on the computer keyboard, switches the component on the selected line.

If desired, the operator can open the spectrum of the selected component for visual analysis of the component's presence in the spectrum by right-clicking and selecting the "**Open spectrum**" pop-up menu item.

The list can be sorted by the values of any column by left-clicking on the column name. The sorting order is indicated by an arrow in front of the column name.

Entering data into the calculator program

If the decomposition template contains a calculator program, the processing procedure may request additional data. The type of the input window depends on the calculator program.

Calculation of total activity

If the "**Calculate the total nuclides activity based on nuclide**" checkbox is selected in the processing template parameters, the processing procedure will calculate the "total activity"[5] of the sample.

The correct calculation of the total activity for poorly resolved spectra (processing without peaks) is possible only with knowledge of the chemical and radionuclide composition of the substance of the counting sample, since the efficiency of radiation registration depends on the chemical composition of the substance of the counting sample and the radiation energy. If these data are unknown, we must be sure that the standard used in calibration of the radiation detection efficiency is similar in chemical and radionuclide composition to the counting sample.

In the "SPECTRRAD" package, the chemical composition of samples is set when forming the "**Sample types**" list by the "Standards and Materials" procedure (menu item "**Tools / Norms and materials**").

Correct accounting of the absorption of radiation quanta on the path from birth to registration in the detector is possible only with knowledge of the energy spectrum of radiation. With this knowledge, there is no need for such a rough estimate as "total activity" - it is possible to calculate the specific activity of all nuclides of the sample. Therefore, the "total activity" is calculated from the average radiation energy of the nuclides of the reference and sample.

When calibrating the registration efficiency, we know both the chemical and radionuclide composition of the standard. The elementary spectrum calculation procedure calculates the average line energy (for alpha and gamma radiation) and the average energy of beta particles and electrons of internal conversion and stores its value in the "**Line energy**" parameter of the elementary spectrum. For the sample spectrum, the "total activity" calculation procedure calculates the average energy of the spectrum, but for alpha spectra, the operator can set the average initial alpha radiation energy of the sample in the "**Line energy**" parameter of the "**Spectrum heading**" form:

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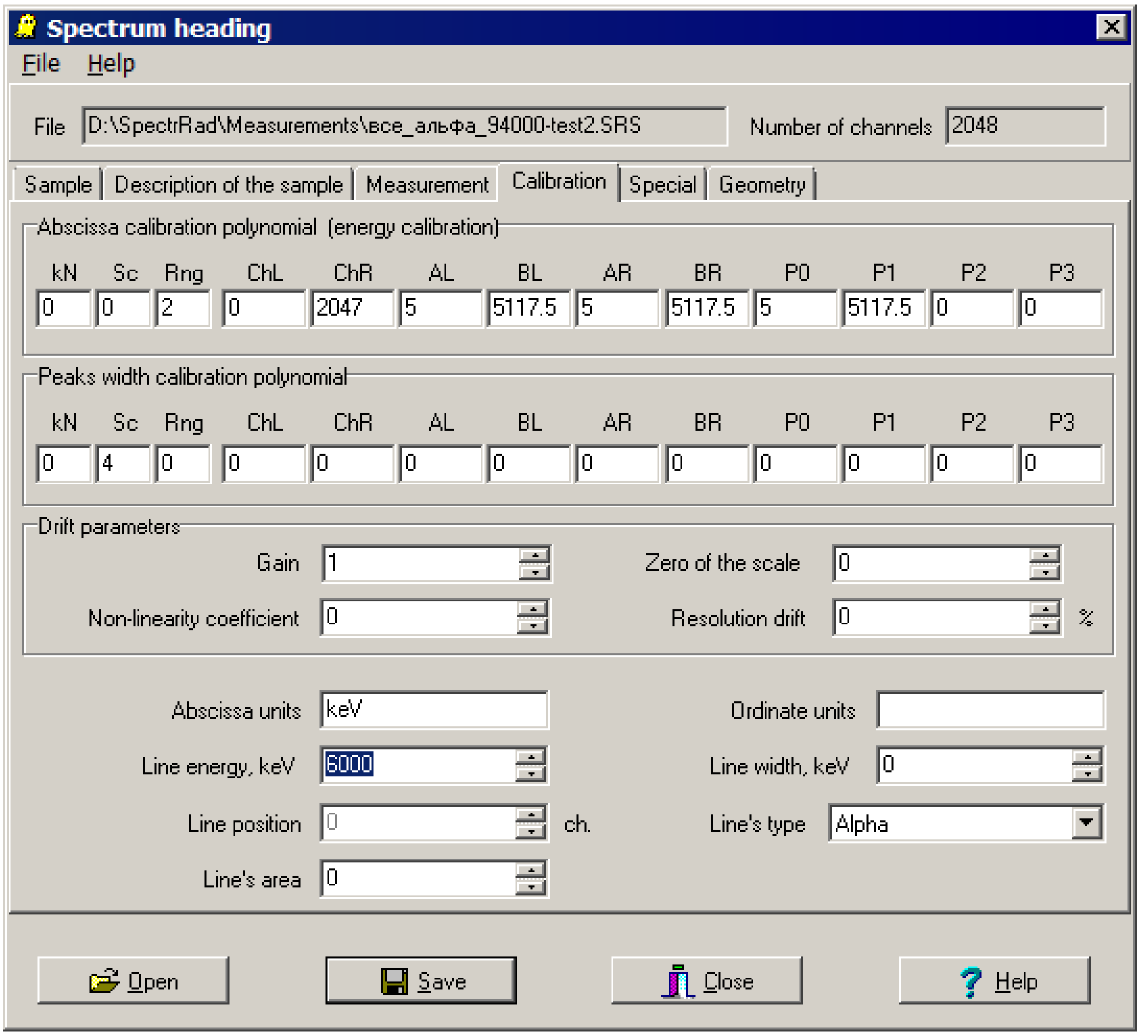
[5] **Total activity** is the conditional activity of the sample equal to the intensity of the radioactive radiation from the sample. The total gamma activity is the number of gamma quanta emitted in 1 second, the total alpha and beta, respectively, is the number of alpha and beta particles per unit time.



File D:\SpectrRad\Measurements\все_альфа_94000-test2.SRS

Number of channels 2048

Abscissa calibration polynomial (energy calibration)

kN	Sc	Rng	ChL	ChR	AL	BL	AR	BR	P0	P1	P2	P3
0	0	2	0	2047	5	5117.5	5	5117.5	5	5117.5	0	0

Peaks width calibration polynomial

kN	Sc	Rng	ChL	ChR	AL	BL	AR	BR	P0	P1	P2	P3
0	4	0	0	0	0	0	0	0	0	0	0	0

Drift parameters

Gain 1

Zero of the scale 0

Non-linearity coefficient 0

Resolution drift 0 %

Abscissa units keV

Ordinate units

Line energy, keV 6000

Line width, keV 0

Line position 0 ch.

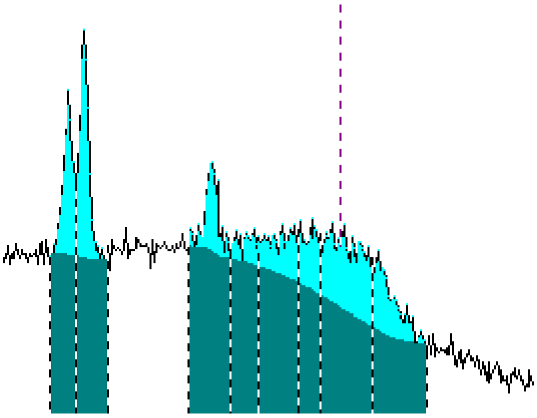
Line's type Alpha

Line's area 0

In the example, the average energy of the sample spectrum is set to 6000 keV. In the event that the spectrum is the spectrum of the spectrometer, the set value will be valid for all spectra subsequently measured on this spectrometer.

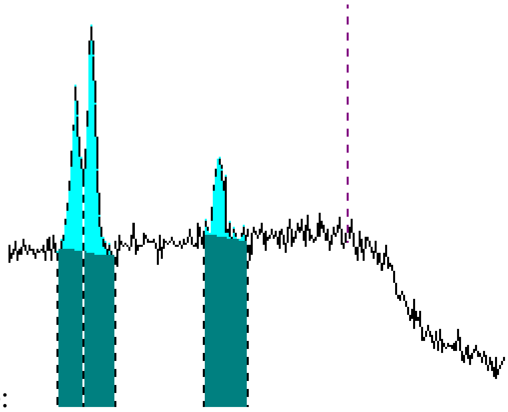
Spectrum processing. Peaks search

When processing linear spectra, the decomposition procedure searches for peaks in the spectrum, evaluates their parameters, calculates the Compton scattering spectrum and then decomposes the spectrum into components of the peaks spectra. The operator has the opportunity to search for peaks in advance – before starting the decomposition procedure. In this case, the decomposition program will use these results, and the operator has the opportunity to manually edit the list of peaks and the shape of the continuous scattering spectrum.

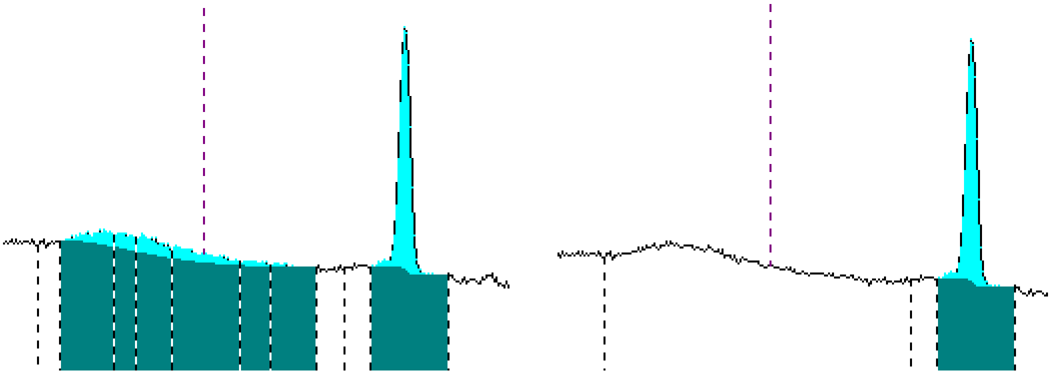


For example, if the parameters of the peak search procedure are not correctly configured, the program may take the edges of Compton scattering from high-power lines as peaks:

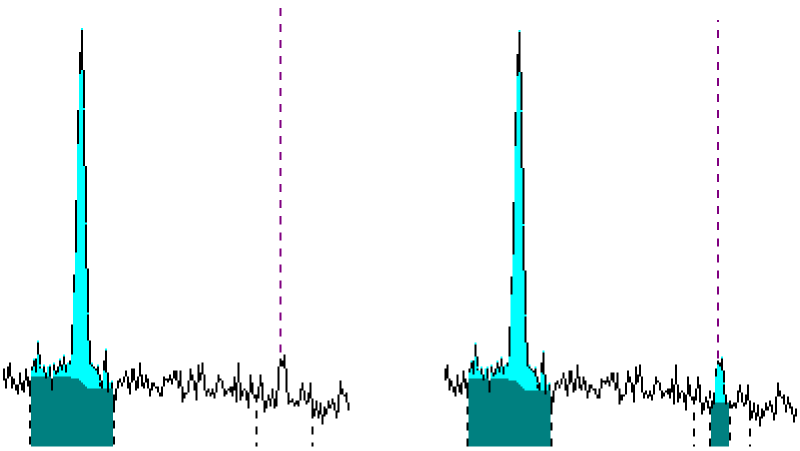
The operator can correct the miss. To do this, by setting the marker to a false peak, you need to call the peak removal procedure (the main or pop-up menu item "**Delete peak**"). As a result, we will get a completely acceptable picture:



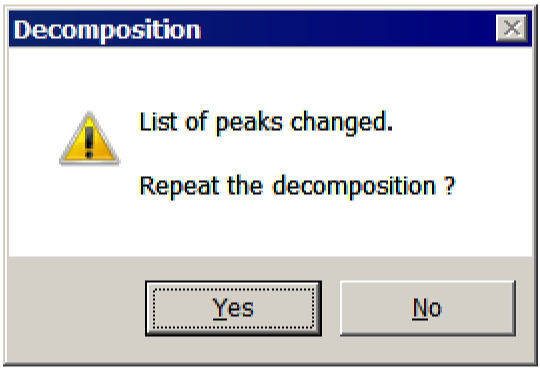
By calling the menu item "**Delete group of peaks...**", the operator can delete all peaks in the previously marked area of the spectrum.



Peaks missed by the automatic search procedure can be added to the list of peaks by calling the menu item "**Add peaks**". The region of the spectrum with missing peaks should be marked with markers and contain no detected peaks:



Manual correction of the list of peaks and, accordingly, the Compton scattering spectrum can also be performed directly in the decomposition procedure. In this case, the procedure for correcting the list of peaks is available either in the "**Pause**" mode, or after the decomposition is completed in the decomposition results viewing mode. If the correction of the list of peaks was carried out in the decomposition results viewing mode, when closing the processing results


Decomposition

List of peaks changed.

Repeat the decomposition ?

report form, the program displays a message . If the answer is "**Yes**", the decomposition will continue with a new list of peaks and a new Compton scattering spectrum.

Spectrum processing. Radiometry

Clicking on the ΣA button (selecting the "**Processing / Radiometry / Start**" menu item) starts the procedure for calculating the "total activity"[6], the total effective activity[7] and radiation power of the sample according to the preset parameters of the boundaries of the energy window and the efficiency of radiation registration in this window.

In this case, the main window of the program takes the same form as when decomposing the spectrum (see Spectrum processing. Decomposition), but two additional windows are not formed. The parameters of the radiometry procedure are set using the menu item "**Processing / Radiometry / Configure...**".

Processing results report

In the "SpectrRad" package, the operator has the ability to create any form of measurement results reports. The principle of forming a report is that data on the results of processing, sample, measuring instrument, regulatory documentation, etc. can be included in a pre-generated document (**report template**). The report template is an arbitrary MSWord document in which special labels are included in the text. A label is a specific word from a given set of words enclosed in curly brackets, for example **{Sample}** (see the section "Report template labels"). When forming the report, the labels are replaced with data about the spectrometer, the test sample and the processing results. As a result, a report of the required form is generated in the form of an MSWord document. The selection of the desired report template can be made by the calculator program, depending on the group to which the sample type belongs (for example, for the "Products" group one form of the template, and for the "Soils" group another) and on the result of spectrum processing (compliance or non-compliance with any standards).

If there is no need to use a report template, a report in the form of an MSWord document is not generated, but in any case, the program generates a mandatory "internal" report in accordance with the parameters set in the decomposition template for configuring the form of such a report.

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[6] **Total activity** is the conditional activity of the sample equal to the intensity of the radioactive radiation from the sample. The total gamma activity is the number of gamma quanta emitted in 1 second, the total alpha and beta, respectively, is the number of alpha and beta particles per unit time.

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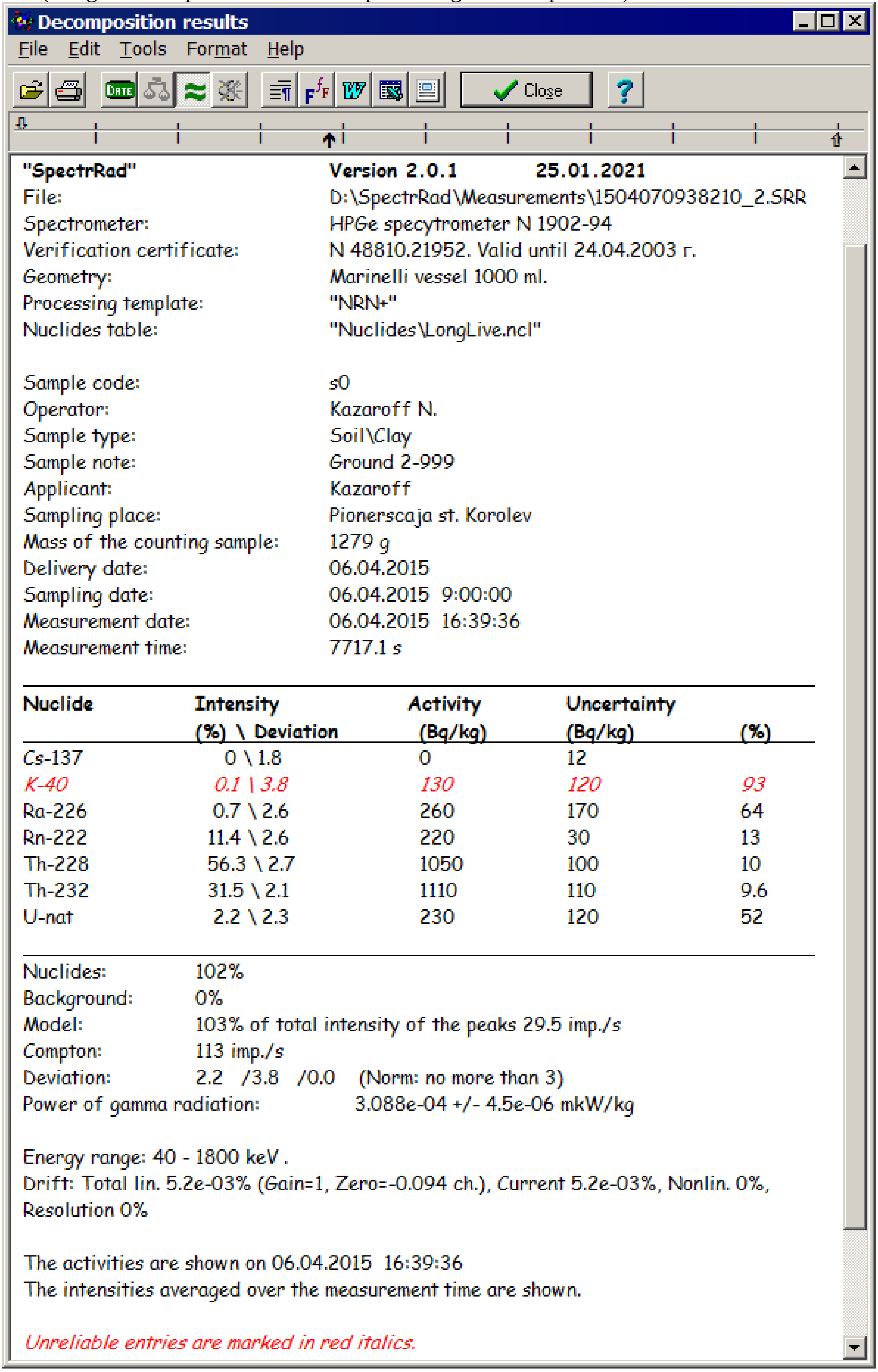
[7] **The total effective activity** is the activity of the sample equal to the activity of the selected nuclide (for gamma radiation – Ra–226) with equal energy power of radiation.

A sufficiently detailed form of the “internal” spectrum decomposition report may look like this (using the example of the results of processing the real spectrum):



"SpectrRad" **Version 2.0.1** **25.01.2021**

File: D:\SpectrRad\Measurements\1504070938210_2.SRR
Spectrometer: HPGe specytrometer N 1902-94
Verification certificate: N 48810.21952. Valid until 24.04.2003 г.
Geometry: Marinelli vessel 1000 ml.
Processing template: "NRN+"
Nuclides table: "Nuclides\LongLive.ncl"

Sample code: s0
Operator: Kazaroff N.
Sample type: Soil\Clay
Sample note: Ground 2-999
Applicant: Kazaroff
Sampling place: Pionerscaja st. Korolev
Mass of the counting sample: 1279 g
Delivery date: 06.04.2015
Sampling date: 06.04.2015 9:00:00
Measurement date: 06.04.2015 16:39:36
Measurement time: 7717.1 s

Nuclide	**Intensity** **(%) \ Deviation**	**Activity** **(Bq/kg)**	**Uncertainty** **(Bq/kg)**	 **(%)**
Cs-137	0 \ 1.8	0	12	
K-40	*0.1 \ 3.8*	*130*	*120*	*93*
Ra-226	0.7 \ 2.6	260	170	64
Rn-222	11.4 \ 2.6	220	30	13
Th-228	56.3 \ 2.7	1050	100	10
Th-232	31.5 \ 2.1	1110	110	9.6
U-nat	2.2 \ 2.3	230	120	52

Nuclides: 102%
Background: 0%
Model: 103% of total intensity of the peaks 29.5 imp./s
Compton: 113 imp./s
Deviation: 2.2 /3.8 /0.0 (Norm: no more than 3)
Power of gamma radiation: 3.088e-04 +/- 4.5e-06 mkW/kg

Energy range: 40 - 1800 keV .
Drift: Total lin. 5.2e-03% (Gain=1, Zero=-0.094 ch.), Current 5.2e-03%, Nonlin. 0%, Resolution 0%

The activities are shown on 06.04.2015 16:39:36
The intensities averaged over the measurement time are shown.

Unreliable entries are marked in red italics.

Here:

- **File -** the name of the file with the processing results.
- **Spectrometer, verification certificate** – description of the spectrometer.
- **Geometry** – geometry of measurements.
- **Processing template -** the used spectrum processing script.
- **Nuclides table** – the table of nuclides used in the processing.
- **Sample code**[8] is the cipher of the sample.
- **Operator** – the operator who performed the measurement.
- **Sample type** is the name in the group of sample types registered in the program. The type of sample is related to the safety standards of the NRB, SanPiN and includes a description of the chemical composition of the sample substance that affects the absorption of radiation in the substance of the counting sample.
- **Sample note, Applicant, Sampling place -** text fields describing the sample.
- **Intensity (%) \ Deviation - Intensity** is the contribution to the spectrum in the studied energy range (as a percentage) of the recorded pulses from a given nuclide. **Deviation -** the decomposition deviation for a given nuclide is the partial deviation. When processing spectra without peaks, the spectra of all nuclides are correlated with each other due to the Compton scattering spectrum, therefore all partial deviations are equal to the total decomposition deviation.
- **Activity (Bq/kg)** is the activity of a nuclide in Becquerel per kilogram.
- **Uncertainty (Bq/kg)** is the uncertainty (error) of measurements in Becquerel per kilogram. The error corresponds to a 95% confidence probability.
- **Uncertainty (%) -** uncertainty as a percentage of the nuclide activity.
- **Nuclides** is the total estimated intensity of radiation from nuclides in the specified energy range.
- **Background -** the intensity of the background radiation.
- **Model** is the sum of the background radiation and the estimated contribution of nuclides, normalized by the registered radiation intensity from the sample.
- **Deviation** is the standard deviation of the calculated model from the measured spectrum $G = \sqrt{\sum((X_i - X_m)^2 / G_i^2)/(n-m)}$. Three values are given: **General deviation / Decomposition deviation / Comparison deviation**. **General deviation** is the deviation of the spectrum from the model in the entire energy range used in the processing. **Decomposition deviation** – the maximum value from the list of partial deviations (partial deviation is the deviation for a given nuclide) and the deviation of the solution of the system of equations. If the partial deviation exceeds the permissible level, the data for this nuclide are highlighted in red and italics. **Comparison deviation** – deviation of the obtained activity values from the values of a priori data (comparison data). The comparison deviation is different from zero if a priori data was used in the spectrum processing. It is used when checking the spectrometer.
- **Energy range -** the left and right boundaries of the energy range of the spectrum used in processing.
- **Drift -** estimated drift of the energy scale of the spectrometer, based on the results of processing.

A 95% confidence interval is used as an uncertainty (error) and either the complete uncertainty of activity estimates $\Delta_x = \sqrt{(2\sigma_x)^2 + (E_0 \cdot x)^2 + (E_i \cdot x)^2}$ or a random component

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[8] The names of terms and parameters: "Spectrometer", "Geometry", "Sample code", "Sample name", "Sample note", "Producer", "Applicant", "Sampling place", "Comment", "Parameter 1", "Parameter 2" when generating the report, copy the column names an archive of measurements that can be set by the operator (see "Archive of measurement results". "Configuring the archive").

of the complete uncertainty $\Delta_x = 2\sigma_x$ can be shown in the report. Here: σ_x is the value of the standard deviation estimate for the activity of the nuclide *x*. E_0 is the relative error specified in the decomposition parameters and is associated with violations of the measurement geometry, the error in estimating the sample quantity, etc. E_i is the relative error calculated during calibration of the spectrometer and is associated with the error of the certified activity values in the standards (when using mono standards, it is equal to the error of the certification of standards). For clarity, the table of nuclide activities in the report, if a random component of the total error is given, is displayed in blue.

The values of the discrepancy and intensity of the model determine the reliability of the decomposition of the spectrum. It is clear that the best values are: 1.0 for the discrepancy and 100% for the model calculated at the date of measurement. Deviations in the geometry of measurements, non-compliance of the sample density with the standard densities, overload of the spectrometer, uncompensated energy drift, the presence of unaccounted nuclides in the sample or a violation of the radioactive equilibrium in the chains of nuclides assumed to be equilibrium, lead to an increase in the discrepancy. **A significant increase in the discrepancy above the experimentally selected and established level (usually 2.0) indicates the unreliability of decomposition and the likely presence of unaccounted nuclides**.

Other standard forms of the report differ from the given degree of detail, and do not require additional comments.

If the decomposition template contains a calculator program, the report may contain additional data. The content and form of the data output depending on the calculator program.

Upon completion of processing, the computer displays a table of results in the selected form on the display screen. The results can be inserted into the report template, recalculated by the date of sampling, by the amount of the sample source material, customize the report form, change the font used and print by clicking on the corresponding "key" of the button panel or opening the corresponding menu item:

open the report template (menu item "**File / Open...**"),

print (menu item "**File / Print...**"),

recalculation by the sampling date (menu item "**Tools / Recalculate on the sampling date**"),

recalculation by the amount of the sample source material (menu item "**Tools /Recalculate on amount of source material**").

The "button" (menu item "**Tools / Round up values**") is used to turn on/off the rounding mode of the results. In the event that the list of nuclides to be determined was formed by automatic composition determination procedures, turning on/off the rounding results mode also affects the list of nuclides given in the report. When the rounding mode is turned off, the entire list of nuclides is shown, when turned on, only those nuclides added by the automatic composition determination procedures, the relative error in determining the activity of which is less than a certain level associated with the rounding accuracy.

The "button" (menu item "**Format / Font...**") - sets the font for the selected text or, if there is no selected text, sets the font for the text of the processing results. If the font is set for the entire report, then the font attributes "italics" and "bold" are not work, since the report generation procedure independently sets the required attributes. The "*italics*" and "**bold**" attributes are set only for the selected text.

"Button" (menu item "**Tools / Export to Word**") - transfer the contents of the report window to Microsoft Word.

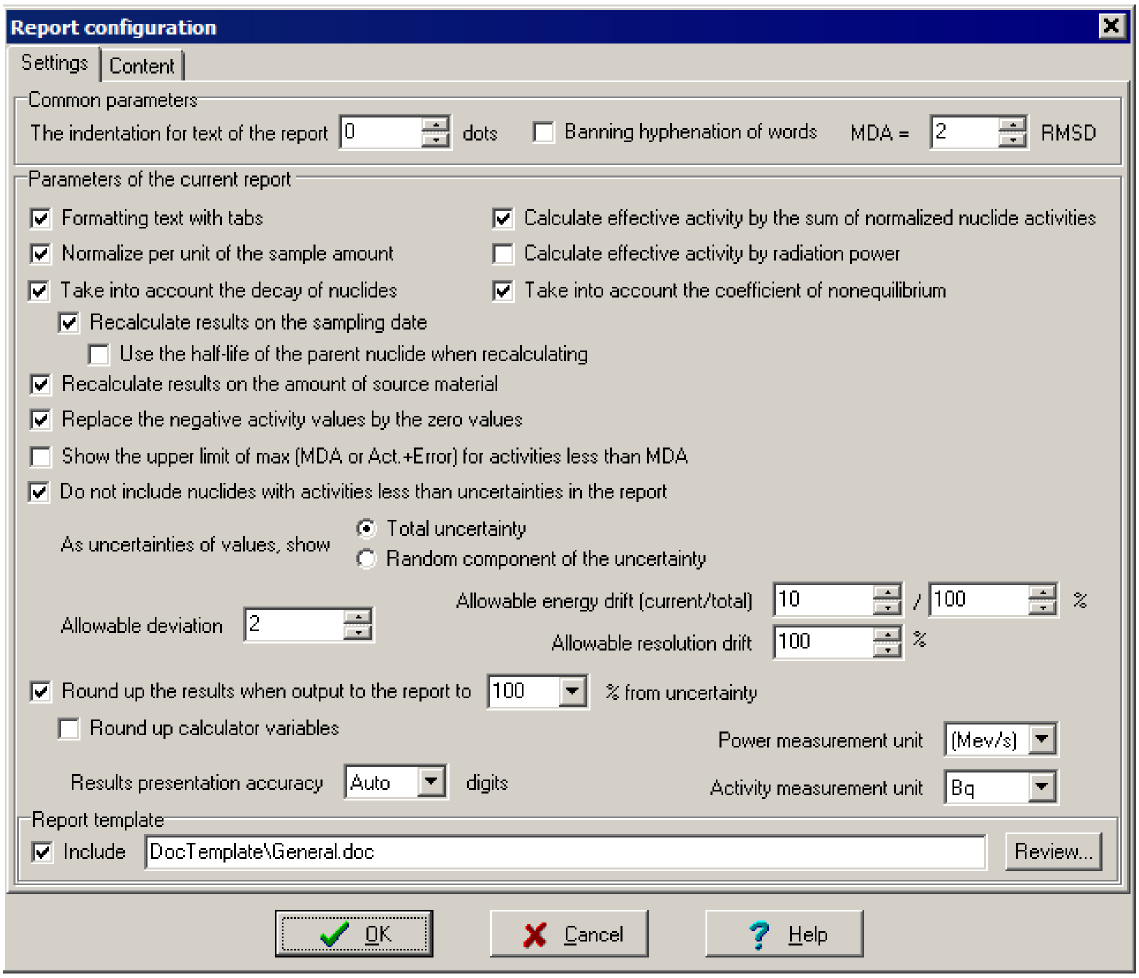
"Button" (menu item "**Tools / Export to Excel**") - transfer the contents of the report window to Microsoft Excel.

Clicking on the "button" (menu item "**Tools / Insert picture**") inserts an image of the main window of the program with a picture of the spectrum decomposition into the text of the report. The position of the image insertion into the report is determined by the cursor position.

The text formatting ruler allows you to set the left (⇩) and right (⇧) fields for the selected text or for the current line if there is no selected text. The pointer ↑ sets the indentation for the text moved to a new line when words are automatically transferred.

Configuring the report form

"Button" (menu item "**Format / Report form...**") - customize the content and form of the report. At the same time, the report form settings window is displayed:



Common parameters

The indentation for text of the report: 0 dots

☐ Banning hyphenation of words

MDA = 2 RMSD

Parameters of the current report

☑ Formatting text with tabs

☑ Calculate effective activity by the sum of normalized nuclide activities

☑ Normalize per unit of the sample amount

☐ Calculate effective activity by radiation power

☑ Take into account the decay of nuclides

☑ Take into account the coefficient of nonequilibrium

☑ Recalculate results on the sampling date

☐ Use the half-life of the parent nuclide when recalculating

☑ Recalculate results on the amount of source material

☑ Replace the negative activity values by the zero values

☐ Show the upper limit of max (MDA or Act.+Error) for activities less than MDA

☑ Do not include nuclides with activities less than uncertainties in the report

As uncertainties of values, show:
● Total uncertainty
○ Random component of the uncertainty

Allowable deviation: 2

Allowable energy drift (current/total): 10 / 100 %

Allowable resolution drift: 100 %

☑ Round up the results when output to the report to 100 % from uncertainty

☐ Round up calculator variables

Power measurement unit: (Mev/s)

Results presentation accuracy: Auto digits

Activity measurement unit: Bq

Report template

☑ Include DocTemplate\General.doc

The form has two pages: "**Settings**" and "**Content**". There are two groups on the **Settings** page:

Common parameters- parameters used in the formation of all reports:

- **The indentation for left of the report**- indentation from the left border of the form to the text of the report. The value is set in points. This parameter is used if the report is not included in the report template (in this case, its position is determined by the position of the **{Report}** or **{Table}** label).
- **Banning hyphenation of words** - setting or disabling the automatic word wrapping mode in a paragraph.
- **MDA =** - setting the value of the minimum detectable activity in terms of standard deviations.

Parameters of the current report:

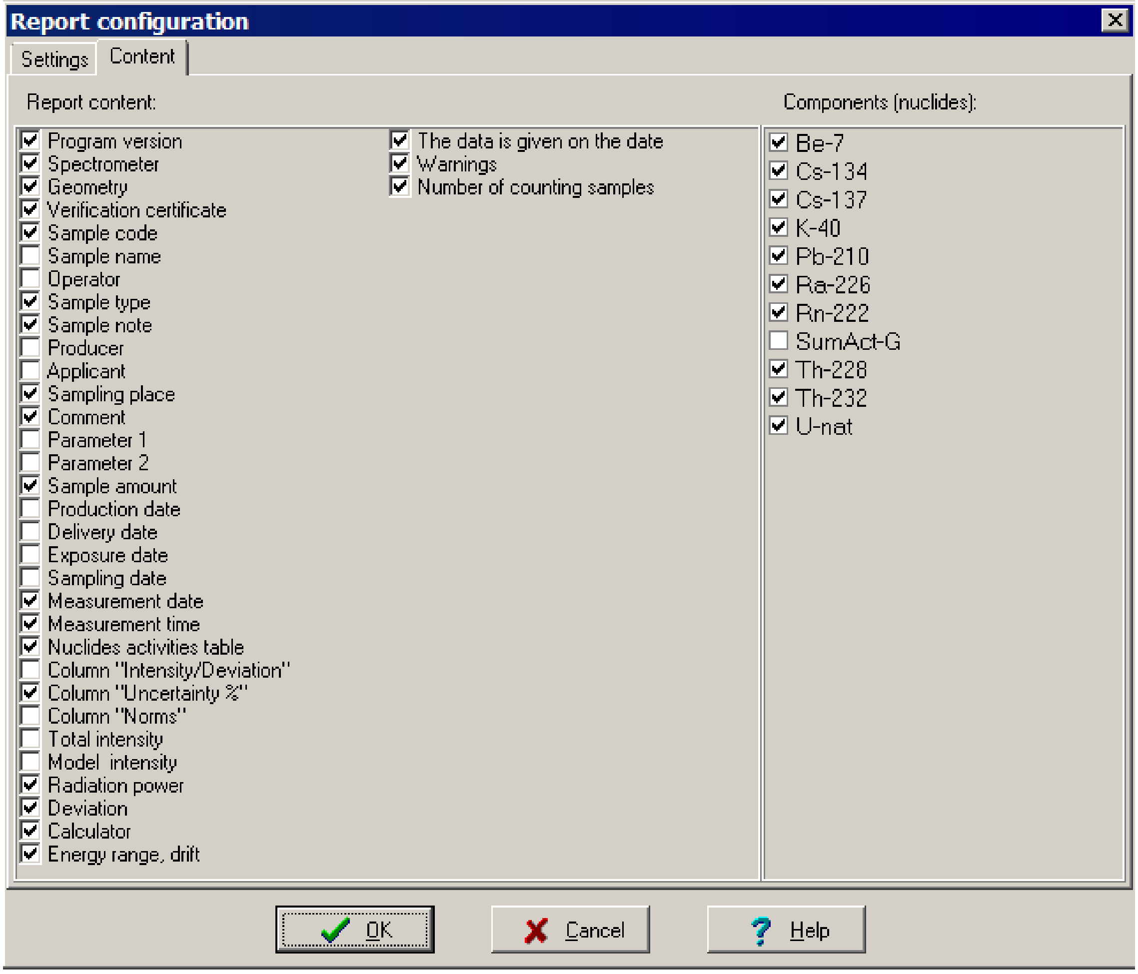
- **Formatting text with tabs** – when the checkbox is selected, the procedure for generating a report before each new paragraph of text containing descriptions of the sample, spectrometer, and measurement conditions will include a tab character to align the text with the first tab position (the position of the "red" line).
- **Normalize per unit of the sample amount -** output values of the specific or total activity of the sample. Normalization by sample mass means dividing the estimated activity of the counting sample by the mass of the counting sample – that is, calculating the specific activity of the counting sample. When the "**Normalize per unit of the sample amount**" and "**Recalculate results on the amount of source material**" checkboxes are checked simultaneously, the estimated specific activity of the sample source material is displayed in the report.
- **Calculate effective activity by the sum of normalized nuclide activities**. When you check the box, the report will show the total effective gamma activity of the sample. The activity of nuclides equivalent to the activity of Ra-226 is considered to be effective. The calculation program takes data on equivalence coefficients for nuclides from the working library of nuclides and, if the gamma coefficient of the Ra-226 equivalent for a nuclide is different from zero, the contribution of the nuclide to the total effective activity of the sample will be taken into account. It should be borne in mind that such a calculation of effective activity for a standard set of coefficients (three coefficients: 1 for Ra–226, 1.3 for Th-232 and 0.09 for K–40) will be correct only if only K-40, Ra–226 and Th-232 are present in the sample. in a state of radioactive equilibrium with daughter nuclides.
- **Calculate effective activity by radiation power** – when the "tick" is set, the program calculates the total effective activity by the power of alpha, beta or gamma radiation in comparison with the power of the selected type of radiation of 1 Bq of the specified comparison nuclide.
- **Take into account the decay of nuclides** – when the "tick" is set, the activity of nuclides will be recalculated on the specified date (the date of the beginning of measurements or the date of sampling), and otherwise the averaged activity during the measurement will be given. By default, the activities are recalculated at the start date of measurements, taking into account the processes of decay and accumulation of nuclides in the decay chains. Correct recalculation is generally impossible – in a chain of nuclides that is not an equilibrium chain, there may be nuclides that are not determined by this type of spectrometry. And the correct calculation of the activities of any nuclide on a given date, taking into account the processes of accumulation and decay of nuclides in the chain, is possible only with knowledge of the activities of all preceding nuclides in the chain. In this case, it is recommended not to take into account the decay of nuclides, and the final calculation of activities should be carried out using the **SpectrRadNuc**l program after evaluating the activities of all nuclides in the chain.
- **Recalculate results on the sampling date** – if the "tick" is set, the nuclide activity will be recalculated on the date of sampling, otherwise – on the date of the beginning of measurements.
- **Use the half-life of the parent nuclide when recalculating** – when the checkbox is selected, the half-life of the maternal nuclide will be used to recalculate activity at the beginning of measurements or on another date, if it is present in the list of nuclides to be determined and the half-life of the maternal nuclide is greater than the half-life of the recalculated nuclide (radioactive equilibrium with the maternal is assumed). In addition, if the checkbox is selected, only the processes of nuclide decay will be taken into account when calculating activities, the accumulation processes in the decay chains will not be taken into account.
- Selecting the "**Take into account the coefficient of nonequilibrium**" checkbox allows you to take into account the imbalance in the decay chain that is not taken into account when calculating equilibrium chains (emanation, leaking of nuclides, etc.), if the activity of a nuclide is determined by the radiation of another nuclide of the equilibrium

chain. In this case, the activity of the nuclide is calculated taking into account the coefficient of nonequilibrium. The nonequilibrium coefficient is related to the type of sample and is given as "**Kneq.(Norm 5)**" when forming safety standards and constants for the selected sample type and a specific nuclide (the menu item "**Tools/Norms and materials...**").

- **Recalculate results on the amount of source material** – output of the nuclide activities of the source sample material (if the item is marked) or the nuclide activities in the counting sample.
- **Replace the negative activity values by the zero** – in the event that negative activity values are allowed during spectrum processing, when the "check mark" is set, the negative activity values in the report will be replaced with zero.
- **Show the upper limit of max (MDA or Act+Error) for activities less then MDA**. When the "check mark" is set, the upper limit of values for values with activity estimates less than the minimum detectable in accordance with ISO and IEC recommendations will be given in the report. For such values, the report shows MDA or Activity+Error with a "<" sign or the word "less", depending on which value is greater. The MDA value in units of standard deviations is set in the archive settings.
- If the "**Do not include nuclides with activities less than uncertainties in the report**" checkbox is selected, the report will contain entries only for nuclides with a relative error of determining activity of less than 100%.
- **As uncertainties of values, show "Total uncertainty" or "Random component of the uncertainty"** - the operator is given the choice of one of two options for presenting the error in the report: complete or random. If you select a random component of the uncertainty, the activity table in the report will be displayed in blue font.
- **Allowable deviation, Allowable drift**. The spectrum decomposition procedure calculates the total decomposition discrepancy and the change in the parameters of the energy calibration and resolution of the spectrometer - the drift of the spectrum. In the event that the calculated values exceed the permissible values, the corresponding message is displayed in the report: if the permissible discrepancy is exceeded, "**Significant unaccounted components may be present**", if the permissible energy drift is exceeded, "**Drift is higher than permissible, it is necessary to auto calibrate the spectrometer tract**", if the permissible resolution drift is exceeded, "**Resolution drift is higher than permissible, it is necessary to make calibration of the spectrometer tract**". The operator has the ability to change these parameters of the decomposition procedure and thus edit the report.
- **Round up the results when output to the report to nn % from uncertainty** – setting the mode and form of rounding estimates of nuclide activities in the report. When 100% rounding is set, the values of activities and errors in the report will be given in accordance with the requirements of MI 2453-2000. If the list of nuclides to be determined was formed by automatic composition determination procedures, turning on/off the rounding results mode and rounding accuracy also affect the list of nuclides given in the report. When the rounding mode is turned off, the entire list of nuclides is shown, when turned on, only those nuclides added by the automatic composition determination procedures, the relative error in determining the activity of which is less than a certain level associated with the rounding accuracy.
- **Round up calculator variables** – when the checkbox is selected, the variables of the programmable calculator will also be rounded when output to the report. Since the rounding procedure in this case has no information about the error of the rounded value, the value of the value will be rounded with a relative accuracy of 10% of the specified rounding accuracy. For example, if 100% rounding is set and the value of the value is 353.265, and then this value will be rounded to 10% accuracy in the report and presented as 350. For correct rounding of the values calculated in the calculator, it is necessary to use the rounding functions existing in the calculator.

- **Results presentation accuracy** – select the number of digits to represent the results in the report. The value "**Auto**" corresponds to the automatic determination of the required accuracy of the presentation of the results. In this case, insignificant zeros are not output.
- **Activity measurement unit** – select the unit of measurement (Becquerel or Curie) in which the activity of nuclides in the report will be shown.
- **Power measurement unit** – select the unit of measurement of the radiation power from the sample calculated by the procedure (keV/s, MeV/s, mcW or W) in which the power will be shown in the report. The radiation power is calculated within the selected energy range.
- **Report template -** the operator, if desired, can specify the report template file. The file must contain the template text saved in RTF format or as a Word document (DOC, DOCX). An example of a report template is provided in the appendix. The Review... button provides an overview of existing report templates.

The second page contains two tables:



Report content:

- ☑ Program version
- ☑ Spectrometer
- ☑ Geometry
- ☑ Verification certificate
- ☑ Sample code
- ☐ Sample name
- ☐ Operator
- ☑ Sample type
- ☑ Sample note
- ☐ Producer
- ☐ Applicant
- ☑ Sampling place
- ☑ Comment
- ☐ Parameter 1
- ☐ Parameter 2
- ☑ Sample amount
- ☐ Production date
- ☐ Delivery date
- ☐ Exposure date
- ☐ Sampling date
- ☑ Measurement date
- ☑ Measurement time
- ☑ Nuclides activities table
- ☐ Column "Intensity/Deviation"
- ☑ Column "Uncertainty %"
- ☐ Column "Norms"
- ☐ Total intensity
- ☐ Model intensity
- ☑ Radiation power
- ☑ Deviation
- ☑ Calculator
- ☑ Energy range, drift
- ☑ The data is given on the date
- ☑ Warnings
- ☑ Number of counting samples

Components (nuclides):

- ☑ Be-7
- ☑ Cs-134
- ☑ Cs-137
- ☑ K-40
- ☑ Pb-210
- ☑ Ra-226
- ☑ Rn-222
- ☐ SumAct-G
- ☑ Th-228
- ☑ Th-232
- ☑ U-nat

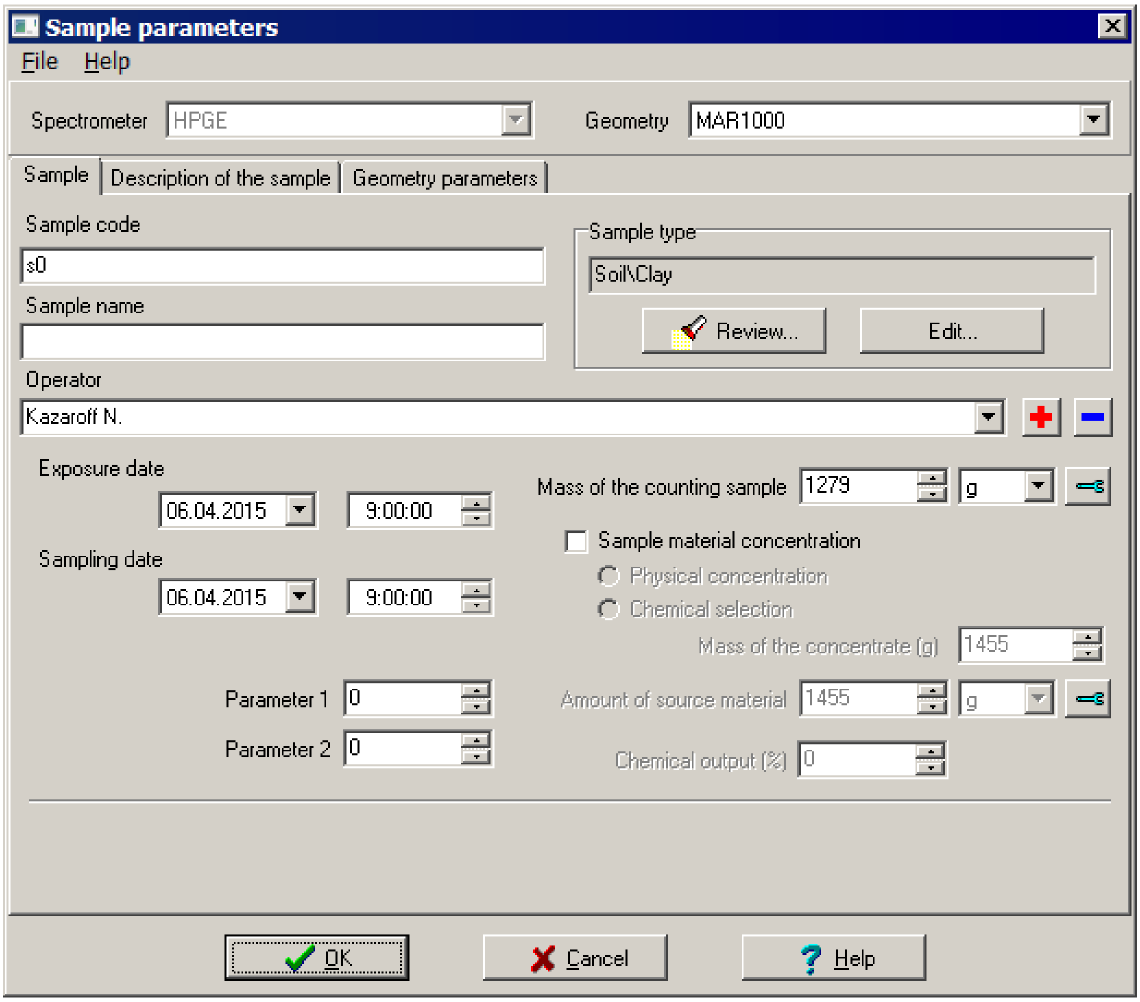
- The "**Report content**" table allows you to set the rows and columns of the output form for the results of spectrum processing, which will be shown in the report.
- The "**Components (nuclides)**" table allows you to select from the general list of certain nuclides those nuclides that will be shown in the report. All determined nuclides of the decomposition procedure are divided into two grades: nuclides specified by the operator and nuclides included in the automatic composition determination procedures. For those nuclides that are specified by the operator, only the operator can specify

whether to include them in the report or not. For nuclides included in the list by automatic composition determination procedures, the decision to include them in the report at the stage of report generation is made by the processing procedure depending on the rounding parameters. When rounding is disabled, the entire list of nuclides is included in the report, when enabled, only those nuclides from the list whose activity estimation error is less than a certain level associated with rounding accuracy. The general list of nuclides, to account for the total alpha, beta and gamma activity of the sample, is supplemented by three conditional nuclides: **SumAct-A**, **SumAct-B** and **SumAct-G** (the example shows the form for configuring the gamma spectrum processing report and, accordingly, the conditional nuclide **SumAct-G** is indicated – the total gamma activity of the sample).

Editing a report

The "**Edit**" menu item allows you to edit the contents of the report. The entire list of operations of this menu item ("**Cut**", "**Copy**", "**Paste**", etc.) except the last line of the list are intended for editing the text of the report. Changes in the text of the report will not affect the main binary file of processing results and will not change the content of the line about recording processing results in the measurement log.

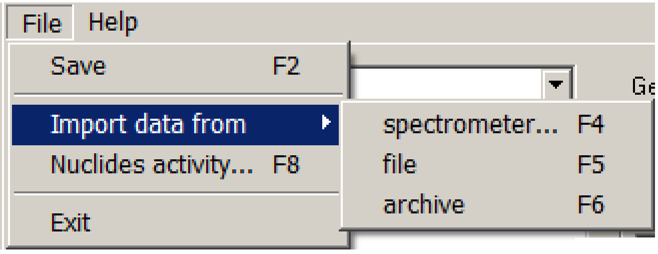
The last line is "**Edit results binary file (.SRR)...**" allows you to edit the binary file of spectrum processing results generated by the decomposition procedure. When you call the procedure for editing the results file, a form for editing the sample parameters will appear on the screen:



Spectrometer HPGE
Geometry MAR1000
Sample code s0
Sample name
Sample type Soil\Clay
Operator Kazaroff N.
Exposure date 06.04.2015 9:00:00
Sampling date 06.04.2015 9:00:00
Parameter 1 0
Parameter 2 0
Mass of the counting sample 1279 g
☐ Sample material concentration
○ Physical concentration
○ Chemical selection
Mass of the concentrate (g) 1455
Amount of source material 1455 g
Chemical output (%) 0

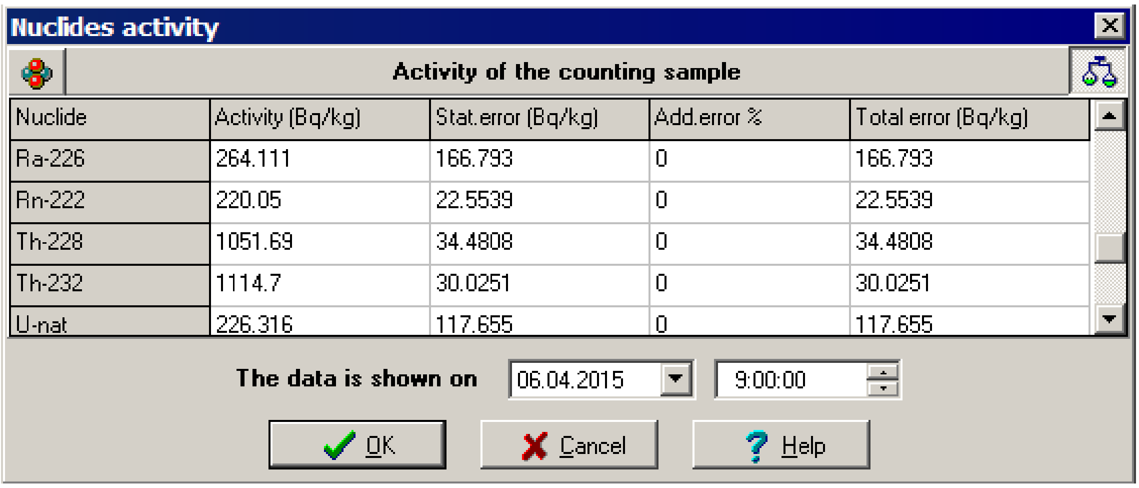
It is forbidden to change the parameters of the sample, which may affect the efficiency of radiation detection in the detector (mass of the counting sample, type of sample, parameters of the geometry of measurements). To do this, you can use the procedure for editing the sample parameters called from the main menu of the SPECTRRAD program "**Tools / Spectrum parameters...**". In this case, the decomposition procedure will be repeated to account for such changes. If, for example, changing the sample type changes only the safety standards and does not change the chemical composition of the counting sample, which means it does not change the radiation absorption (in the SPECTRRAD package the database on standards and chemical composition of counting samples is combined), you can use the editing procedure of the processing results file, since repeated decomposition in this case does not required, and the editing procedure will recalculate the compliance of nuclides activities with the standards.

The form has a small menu:



The menu item "**File / Import data from**" allows you to import sample parameters from another spectrometer, a spectrum file, or from a selected archive entry, which saves time filling in the form fields.

The menu item "**File / Nuclides activity...**" of the "**Sample parameters**" form allows you to edit the list of nuclides and calculated activity values, add data on nuclide activities obtained on other devices to the processing results file, or enter data on certified values of nuclide activities. At this case, a form for entering a priori data on the activities of nuclides will appear on the screen:



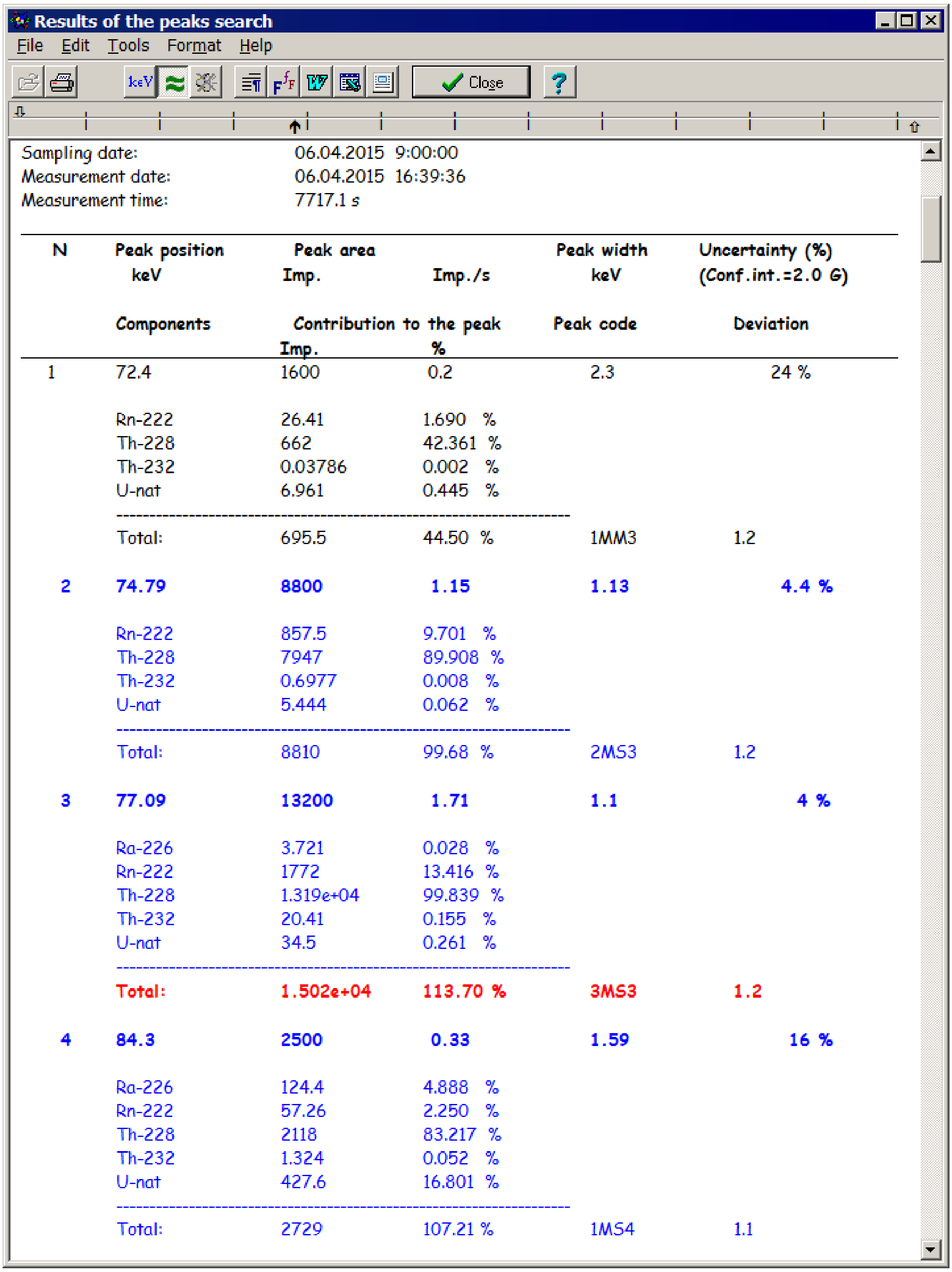
Nuclide	Activity (Bq/kg)	Stat.error (Bq/kg)	Add.error %	Total error (Bq/kg)
Ra-226	264.111	166.793	0	166.793
Rn-222	220.05	22.5539	0	22.5539
Th-228	1051.69	34.4808	0	34.4808
Th-232	1114.7	30.0251	0	30.0251
U-nat	226.316	117.655	0	117.655

The data is shown on 06.04.2015 9:00:00

The operator has the opportunity to edit data on the activities and uncertainties of the sample, change the list of nuclides (button). Data can be entered either in the form of total sample activity (counting sample) or in the form of specific activity. The button switches the input form. The random component of the total uncertainty in absolute values and additional uncertainty as a percentage of activity should be indicated, the procedure calculates the full uncertainty itself.

List of peaks found

When processing linear spectra with peak search, the operator can display a list of peaks found by clicking on the menu item "**Tools / List of peaks...**". At the same time, a window with a list of peaks found in the energy range of the spectrum specified for processing is displayed on the screen. For example:



```
Sampling date:          06.04.2015  9:00:00
Measurement date:       06.04.2015  16:39:36
Measurement time:       7717.1 s

   N     Peak position     Peak area                     Peak width     Uncertainty (%)
            keV            Imp.            Imp./s           keV         (Conf.int.=2.0 G)

         Components        Contribution to the peak      Peak code          Deviation
                           Imp.             %
  1      72.4              1600            0.2           2.3                  24 %

         Rn-222            26.41           1.690  %
         Th-228            662             42.361  %
         Th-232            0.03786         0.002  %
         U-nat             6.961           0.445  %
         ------------------------------------------------------
         Total:            695.5           44.50  %      1MM3           1.2

  2      74.79             8800             1.15         1.13                 4.4 %

         Rn-222            857.5           9.701  %
         Th-228            7947            89.908  %
         Th-232            0.6977          0.008  %
         U-nat             5.444           0.062  %
         ------------------------------------------------------
         Total:            8810            99.68  %      2MS3           1.2

  3      77.09             13200            1.71         1.1                    4 %

         Ra-226            3.721           0.028  %
         Rn-222            1772            13.416  %
         Th-228            1.319e+04       99.839  %
         Th-232            20.41           0.155  %
         U-nat             34.5            0.261  %
         ------------------------------------------------------
         Total:            1.502e+04       113.70 %      3MS3           1.2

  4      84.3              2500             0.33         1.59                  16 %

         Ra-226            124.4           4.888  %
         Rn-222            57.26           2.250  %
         Th-228            2118            83.217  %
         Th-232            1.324           0.052  %
         U-nat             427.6           16.801  %
         ------------------------------------------------------
         Total:            2729            107.21 %      1MS4           1.1
```

The form contains a numbered list of peaks with an explanation of the contribution of the components (background, nuclides) forming the spectrum to each peak. The peaks used to calculate the activity of nuclides are highlighted in blue. In the event that the total contribution of the component does not match (within the margin of error) one hundred percent, it is marked in red.

The line "**Total:**", in addition to the contribution to the peak of the lines of the components forming the peak, contains the peak code and the modulus of the residues of the peak decomposition into line models and the Compton scattering spectrum. The peak code is a cipher of five or four digits and letters describing the peak:

The 1st character is the number of the peak in the multiplet.

The 2nd character – the letter **W** may be missing. If the letter **W** is present in the peak code, it means that the peak parameters are not reliably determined.

The 3rd character is the letter **S** – the peak is defined as a singlet, the **M** – peak is defined as a multiplet.

The 4th character is the letter **S** – the multiplet is revealed, **M** – the multiplet is not revealed.

The 5th symbol is the number of resolved peaks in the multiplet.

The keV button (menu item ("**Tools / Energy scale / channels scale**") switches the energy scale to the channel scale and back.

Additional features

Clicking on the "button" ▤ (menu item "**Tools / Insert picture**") inserts an image of the main window of the program with a picture of the spectrum decomposition into the text of the report. The position of the image insertion into the report is determined by the cursor position.

The operator can view the nuclide table used in processing by calling the menu item "**Tools / Nuclides table...**".

The menu item "**Tools / A priory data...**" is a view of a priori data (comparison data) used in spectrum processing.

The operator can edit the output text and, if desired, copy it into the window of any word processor or save it as a file using the main menu or the menu called when clicking on the right mouse button (the mouse pointer should be in the window of the "Decomposition Results" form). You can select the necessary text using the left mouse button (moving the mouse when the button is pressed) or using the cursor keys when the "Shift" key is pressed. By moving the mouse with the left button pressed, the selected text can be dragged both within the document window and between windows.

The reverse operation is also possible - to insert text in character or RTF format into the report window from another document window or another report window.

Saving the report

Pressing the ✓ Save key (menu item "**File / Save**") saves the processing results in the archive of measurement results. At the same time, in case of successful spectrum processing (the discrepancy and drift do not exceed the permissible values) and when the drift correction is allowed in the processing parameters, the energy calibration of the processed spectrum (spectrometer) will also be changed - data updated by the results of spectrum processing will be recorded as new calibration data. In this way, the process of automatic energy calibration of the spectrometer is carried out during the processing of working samples.

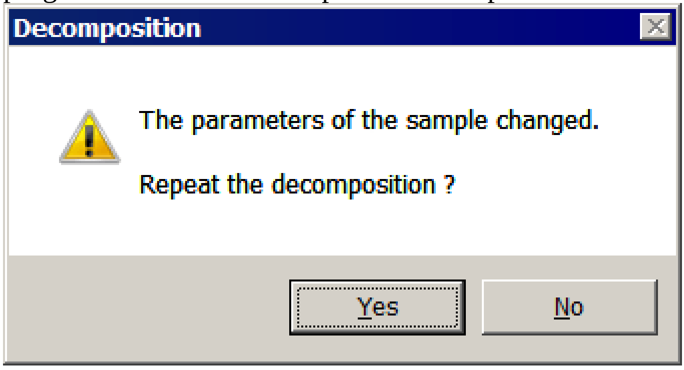
If you need to save a report or a binary file of processing results (SRR file) not in the measurement archive but in another folder (for example, after editing a report or a file of processing results, save its edited version in a separate folder), you can use the menu item "**File / Save as…**".

Radiometry results report

The radiometry report has a similar form and differs only in that there is only one line in the nuclide table: "**Total**" - the total activity of the sample.

Editing decomposition parameters

In case of unsatisfactory processing results, the operator has the opportunity to change the processing parameters, geometry parameters or sample parameters and repeat the decomposition. To do this, it is necessary to change the required parameters without closing the report, and in this case, after changing the parameters, when trying to close the report, the program will offer to re-process the spectrum with the changed parameters, for example:



The parameters of the sample changed.

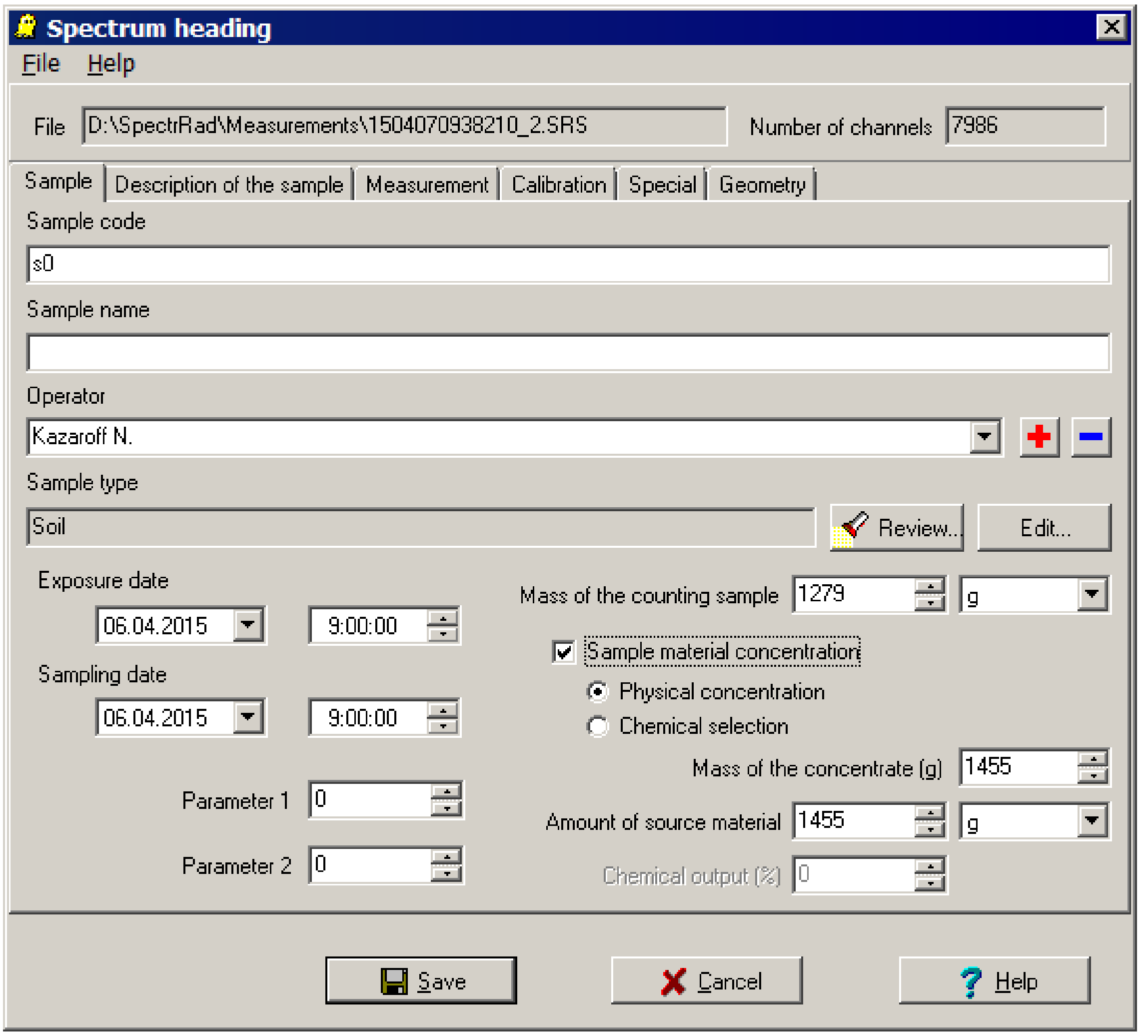
Repeat the decomposition ?

.

Geometry parameters can be changed by calling the geometry installation procedure (menu item "**Device / Geometry / Install...**"). Geometry parameters such as "**Volume**", "**Average thickness of the counting sample**" and "**Interpolation**", which determine the calculation of radiation absorption in the sample, can influence the processing results.

The decomposition parameters are edited by calling the procedure for creating and editing decomposition templates (menu item "**Processing / Decomposition parameters...**", button). The operator can change the list of nuclides, processing parameters and the calculator program.

The sample parameters can be changed by calling the menu item "**Tools / Spectrum Parameters...**". At the same time, a form for editing the spectrum header will appear on the screen, for example:



File D:\SpectrRad\Measurements\1504070938210_2.SRS
Number of channels 7986

Sample code
s0

Sample name

Operator
Kazaroff N.

Sample type
Soil

Exposure date
06.04.2015 9:00:00

Sampling date
06.04.2015 9:00:00

Parameter 1 0
Parameter 2 0

Mass of the counting sample 1279 g
☑ Sample material concentration
● Physical concentration
○ Chemical selection
Mass of the concentrate (g) 1455
Amount of source material 1455 g
Chemical output (%) 0

The operator has the ability to change the data on the "**Sample**", "**Description of the sample**" and "**Geometry**" pages. The data on the other pages is not allowed to be edited in this mode. The decomposition results are influenced by the values associated with the dates of sampling and changes in the efficiency of radiation registration: the geometry of measurements, the mass of the counting sample, the distance from the detector and the type of sample associated with the standards and constants of the substance of the counting sample, which determine the absorption of radiation in the substance of the counting sample.

Brief instructions

When carrying out routine measurements on a spectrometer configured for a specific set of spectrometric tracts and certified geometries, operating under the control of the software package "SPECTRRAD", it is quite sufficient to follow the instructions of the "army" type given below punctually:

1. Warm up the equipment for 30 minutes.
2. After launching, the spectra that were opened in the last session of working with the package are visualized in the program window. Unnecessary spectra can be closed. To do this, by selecting the spectrum to close with the mouse, click on the ✕ toolbar button (menu item "**File / Close**").
3. To monitor the connected spectrometers, click on the button (select the menu item "**File / Open / Spectrometer...**" or press **Ctrl-F3**), and in the opened plate, selecting the required spectrometer, click on the "**OK**" button. The spectrum of the spectrometer appears in the window (after switching on it can have arbitrary values). You can open the spectrum of the spectrometer by clicking on the name of the spectrometer in the "**Spectrometers state**" window.
4. Perform auto-calibration of the spectrometer tract. To do this, install a reference source designed for auto-calibration on the detector and, by clicking on the key (menu item "**Calibration / Autocalibration / Start...**"), start the auto-calibration process including measuring the control source for a set time and processing the measured spectrum with the determination of drift parameters. In case of "bad" auto-calibration results (exceeding the set values for drift or discrepancy parameters), it is necessary to find out the cause (change in the parameters of the spectrometric tract, background change, contamination of the shield house and crystal surface, malfunction of the equipment) and eliminate it.
5. Carry out the background radiation check procedure in the spectrometer: a) install a background sample on the detector (for routine measurements, a "naked" detector without any sample is allowed for gamma detectors, an empty cell for beta and alpha detectors), b) start the background check procedure by clicking on the BGD key (menu item "**Calibration / Background / Start...**"). In case of "bad" background check results (exceeding the set values for the deviations or drift parameters), the procedure prohibits the operation of mixing the measured background with the one set in the program. In this case, it is necessary to find out the cause (a change in the parameters of the spectrometric tract, a change in the background radiation, contamination of the shield house and the crystal surface, malfunction of the equipment) and eliminate it. If the reason is a change in the background radiation of the spectrometer, the measured background must be installed as a working background, replacing the old one.
6. Repeat the auto-calibration procedure.
7. Prepare a working sample: a) pour into a vessel of certified geometry in such a way that the sample substance evenly fills the volume of the vessel, b) install the sample on the detector of the appropriate spectrometer. **It is unacceptable to carry out measurements using non-certified geometries**.
8. Start the measurements by clicking on the ⏲ button (menu item "**Device / Acquire / Start**"), or press the "**F5**" key. In the table that opens, select, if necessary: spectrometer, measurement geometry, acquisition mode (live or real time). Set the necessary checkboxes for the following modes: saving measurement results in the archive, pre-clearing the spectrometer memory, cyclic measurements and set the required measurement time in seconds (the duration of measurements determines the accuracy of measurements). Press the "**OK**" key.
9. In the additional form that opens, fill in the pages the necessary information about the sample.

10. After starting measurements, if the spectrometer status window is enabled (the "**Device / State**" menu item), messages about the measurement time, the spectrometer load, and the remaining time until the end of measurements appear in the status window. If the load exceeds the set level, the yellow or red overload indicator of the spectrometer lights up. In this case, it is necessary either to use the geometry of measurements of a smaller volume, or to dilute the working sample with inactive filler and repeat the measurements in accordance with paragraphs 6-17.

11. The operator can interrupt measurements at any time by clicking on the STOP button or pressing the "**Ctrl-F5**" keys (menu item "**Device / Acquire / Stop...**").

12. The operator can, if necessary, enter new values of the sample parameters by clicking on the key (menu item "**File / Open / Spectrometer...**"). Accordingly, it is possible, if time is expensive, to enter sample data after starting measurements.

13. At the end of the measurement, the message "**Measurements are completed in the spectrometer "NAME"**" will appear on the screen (NAME is the name of a specific spectrometer) and, if there is a sound card, the melody recorded in the audio file associated with the completion of measurements will be played.

14. To process the spectrum, select the menu item "**Processing / Decomposition...**" (button, "**Ctrl-P**" keys).

15. In the window that appears, select the desired one from the generated decomposition templates or, if necessary, create the processing template yourself by clicking on the "**New**" key and setting the necessary processing parameters in the form "**Decomposition template**".

16. If it is necessary to take into account the results of processing the spectrum of this sample (samples from the same material) measured earlier or on another detector (results of processing the gamma spectrum of the sample during processing the beta spectrum), depending on the a priori data search mode set in the processing template, the program can either search for the necessary data itself, or will offer the operator to choose from databases of measurement results the necessary record. In the event that a priori data is not available in the measurement archive, the program may require you to enter them manually.

17. Upon completion of processing, the computer displays a table of results on the display screen. The results can be recalculated on the date of sampling, by the value of the raw sample and printed by clicking on the corresponding "key" of the plate. If desired, you can create the desired report form by clicking on the "**Report form**" key , or select another version of the report template by clicking on the "**Report template**" key .

18. To start measuring a new sample, go to step 6 for the beta spectrometer or step 7 for the gamma and alpha spectrometer.

19. Upon completion of all measurements and processing of the spectrum of the last sample, perform the spectrometer auto-calibration procedure and upon completion exit the program by clicking on the ☒ button in the upper right corner of the program window or by pressing the "**Alt-F4**" keys (menu item "**File / Exit**").

Archive of measurement results

The key (menu item "**Tools / Archive of measurements...**") of the main program window opens the measurement archive management program. The spectra of the samples are automatically saved in the archive at the end of the measurements (if the save mode is set). When processing the spectrum, the operator can also archive the processing results. In this case, the background spectrum used in the processing procedure is also stored in the archive.

The archive management program allows you to statistically process the accumulated results, make any samples based on spectrometers, geometries, sample types, sampling or measurement times, nuclide activities or errors, create graphs, and sort data. It allows the operator to re-process any spectrum stored in the archive with other processing parameters, edit the record or generate a new report, transfer data to more powerful word processors ("Microsoft Word" or "Microsoft Excel"), etc., etc.

The program allows simultaneous shared access to the archive of other users, which allows you to create network archives, optimize work with archives.

Archive editing operations to protect against unqualified access may be prohibited in restricted access mode.

Archive structure

The archive of measurement results is a folder with an arbitrary name specified by the operator when creating the archive and two files with the same name: a table of contents (measurement log) files with the **.dbf** extension and a configuration file with the **.ini** extension. The archive folder stores files of measured spectra and contains two folders: the **ISO** folder for storing processing results and the **Backgr** folder for storing background spectra. The main archive folder, the table of contents file and the settings file must be in the same directory. For example, an archive named "**Archive**" consists of the **Archive** folder and two files **Archive.dbf** and **Archive.ini** located in the same directory.

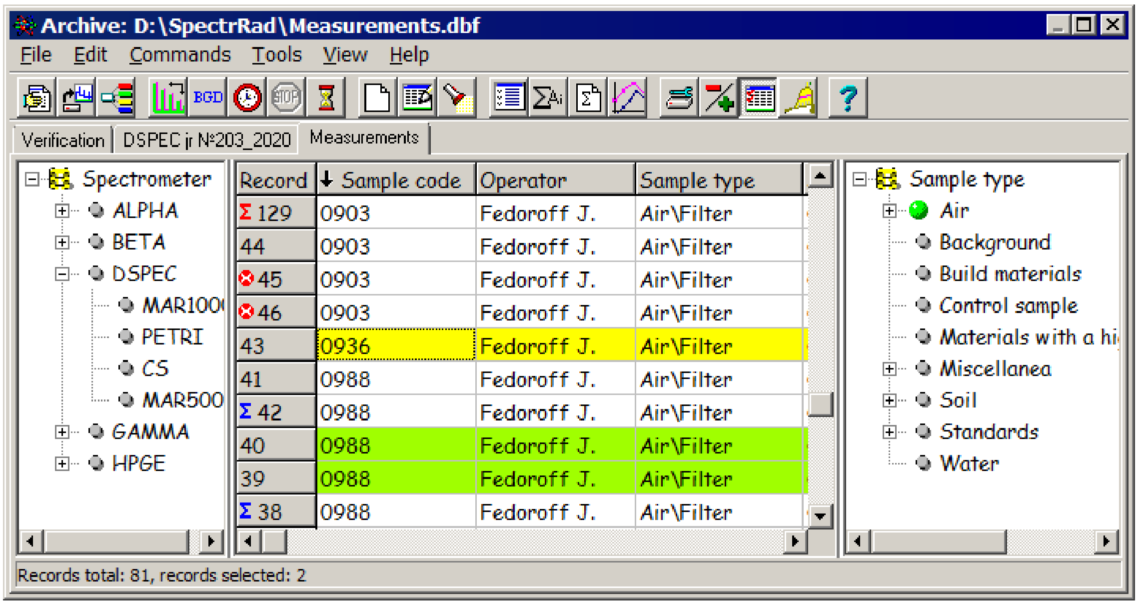
The measurement log is a file in **DBF** format (a long–used and widely used data storage format) that contains information about stored spectra, sample parameters, measurement procedure parameters and the results of spectrum processing. The measurement log is updated when saving the measurement results in the archive and is formed anew each time when the archive parameters are changed by scanning the spectra and processing results.

Each line of the log contains information about one measurement performed. The contents of the journal columns are partially fixed partially configured by the operator and are given in the chapter "**Archive setup**".

The number, size and location of archives are limited only by the computer's capabilities. When configuring the system, the necessary archives are formed and connections are established between spectrometric tracts, measurement geometries and archives. But since the lists of nuclides recorded in the measurement log (table of contents file) will be different for different spectrometers that can register different types of radiation or have different types of detectors, it is recommended to create separate archives for each spectrometric tract. The quality control system for spectrometric measurements in the "SpectrRad" software package provides for the installation of a special geometry "CS" ("Check Source") for each spectrometric tract to measure the check (reference) source. It is recommended to create a separate archive for the "CS" geometry and link it with such geometries of all spectrometric tracts in order to save the results of autocalibration and background radiation check procedures.

Main window

The archive management program window may look like this, for example:



Record	↓ Sample code	Operator	Sample type
Σ 129	0903	Fedoroff J.	Air\Filter
44	0903	Fedoroff J.	Air\Filter
⊗ 45	0903	Fedoroff J.	Air\Filter
⊗ 46	0903	Fedoroff J.	Air\Filter
43	0936	Fedoroff J.	Air\Filter
41	0988	Fedoroff J.	Air\Filter
Σ 42	0988	Fedoroff J.	Air\Filter
40	0988	Fedoroff J.	Air\Filter
39	0988	Fedoroff J.	Air\Filter
Σ 38	0988	Fedoroff J.	Air\Filter

Records total: 81, records selected: 2

In the upper part of the window there are menus and toolbar buttons. Below are the pages of open archives ("Verification", "Measurements", ...). The name of the program window indicates the archive to be visualized ("**D:\SpectrRad\Measurements.dbf** ").

In the left window of the archive page there is a tree of connected spectrometers and installed measurement geometries. The operator can view either records for all spectrometers by selecting the top line of the tree - "**Spectrometer**", or records related to a specific spectrometer or specific measurement geometry by selecting the desired branch of the spectrometer tree. The ⊞ sign in front of the tree node indicates that the node is not open. To open it, click on the ⊞ icon. Double-clicking on the icon of a tree node either expands it if it is collapsed, or collapses it if the node is expanded.

In the right window there is a tree of sample types. The type of sample is one of the parameters of the spectrum. The type of sample is associated with information about the norms of SanPiN, NRB, etc. and the chemical composition of the material of the counting sample. The operator can view either records for all types of samples by selecting the top row of the tree - "**Sample type**", or records related to a specific type of sample by selecting the desired branch of the tree of sample types.

In the main window of the page there is a table of records of the measurement archive. The current (or active) record is marked in yellow (if the current record is one of a group of selected records, its color changes to blue). The current record participates in all operations with single records: report output, spectrum processing, starting measurements, etc. The keys "**up**" and "**down**" of the computer keyboard move the current record accordingly. Pressing the "**Home**" and "**End**" keys makes the first or last table entry active, respectively. Clicking on an entry makes it active.

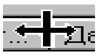
The first column of the record table is the number of the record in the measurement log (file **name.dbf**, where **name** is the name of the archive) and the symbol of the record type:

- ⊗ The entry is marked for deletion. Records marked for deletion are rendered only when the visualization mode of such records is enabled. When cleaning the archive, they can be deleted.
- Σ Recording for a spectrum that is the sum of the spectra measured in the cyclic measurement mode.
- Σ The entry is a result of the statistical processing of a number of spectrum processing results, calculated by the "**Summary Report**" procedure).

Depending on the archive setting, either complete errors or random error components can be given in the error columns for nuclide activities. When displaying a random component, the error columns in the archive will be colored blue

The operator can select a group of records (one record is a special case of a group), marking them with the mouse when the "**Ctrl**" key is pressed, you can mark the group by clicking on the last record in the group when the "**Shift**" key is pressed - the group from the current record to the last one will be marked. Moving the cursor up or down the table, while pressing the "**Shift**" key or pressing the "**Insert**" key, changes the selection of records. The selected entries are marked in green and participate in group operations: "Selection", "Statistics", copying or clipping to the clipboard, "Archive cleaning".

The columns of the table can be fixed (marked in gray) and regular. Fixed columns do not participate in the horizontal scrolling operation and have a fixed width.

The width of the usual columns (fields) of the table  can be adjusted by the operator. To do this, place the mouse pointer on the border between the fields, while the mouse pointer will take the form  and, holding down the left mouse button, drag the border to the desired position.

The table entries can be sorted by the values of any column in the table - just click on the button with the column name. The sorting direction is indicated by an arrow to the left of the column name.

At the bottom of the page there is a line of information about the number of records in the table and the number of selected records.

The right mouse button opens a menu, the contents of which change depending on the position of the mouse pointer and the moment of the call. Some of the menu items duplicate the functions of the main menu.

Double-clicking on any archive entry displays a report on the results of spectrum processing.

Menu

Menu item	*Action*
File:	
Create archive…	Create a new archive.
Open archive…	Open one of the existing archives.
Close archive	Close the opened (visualized) archive.
Save as…	Save the archive under a new name.
Copy to archive…[9]	Copy the contents of the open archive to the archive specified by the operator. Records that are either missing at the receiver archive or do not match the records of the receiver archive are copied. At the end of the operation, a receiver archive will open containing the sum of the two archives

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[9] Since the operations of copying, moving and deleting the entire archive or part of it move and delete files and folders, all programs that can access files and folders of the archive must first be closed, since the operating system does not allow moving or deleting files and folders that other programs have access to, including viewer programs (explorer, Norton commander, Windows commander, etc.).

Move to archive…	The operation is similar to the "Copy to archive" operation, but at the end of the operation, the source archive will be deleted.
Rename archive…	Rename the archive.
Delete archive…	Delete the archive. During this operation, all files and folders of the archive are deleted to the trash, so be careful when deleting the archive.
Exit	Close the "Measurement archive" window.

Edit:

New record… ***Ctrl+N***	Creating a new record. The operator can enter the values of the first 9 sample parameters used when starting measurements. Creating new records allows you to reduce the total time spent during measurements, since the operator can enter data on samples before they start measuring, for example, during the measurement of the current sample. Then, using the launch of measurements from the archive window, use the information already entered. When starting measurements, the information will be supplemented with the values of the sample value, the date of the start of measurements, etc.
Edit record… ***Ctrl+M***	Editing an entry. The operator can change the values of the sample parameters entered when starting measurements.
Data import…	Importing the contents of the columns specified by the operator of the current record into the selected records. The importing data replaces the existing ones. The procedure allows group editing of records. First, edit the current record and import the data of the selected columns of the current record into a pre-selected group of records.
Data transfer…	Transferring the contents of the columns specified by the operator to other columns, the "basket" or from the "basket" to the columns. Clearing the selected columns. The operation is performed for all selected archive records.
Find record… ***Ctrl+F***	Search for records in the archive containing the text specified by the operator and satisfying the specified conditions.
Cut	Move the selected part of the archive entries to the clipboard[10].
Copy	Copy the selected part of the archive entries to the clipboard.
Paste	Paste records from the clipboard into an open archive.

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[10] Clipboard is a temporarily created archive named "~ClipBoard". It cannot store more than one portion of the data placed in it (each time records are moved to the clipboard, its contents are overwritten), so you need to be careful when using the "**Cut**" operation.

Select all	***Ctrl+A***	Select all open entries.
Unselect all	***Del***	Deselect all open archive entries.
Invert selection	***Ctrl+I***	Invert the selection of records. .
Hide (restore)		Deleting selected records from the archive. During this operation, the records are not deleted immediately, but are marked for deletion and deletion can be canceled by marking the necessary records in the "Show hidden records" mode and clicking the "Hide (restore)" button again.

Commands:

Report	***Ctrl+R***	Generate a report for the current (active) archive entry. The operation is available if the spectrum corresponding to the record has been processed.
Open spectrum	***Ctrl+O***	Open the spectrum of the current record.
Decompose spectrum…	***Ctrl+P***	Process the spectra of a group of selected records or the spectrum of the current record if there are no selected records. When processing the spectrum from the archive, if it exists, the background spectrum is also used from the archive corresponding to the time of spectrum measurement.
Start acquisition…	***F5***	Starting measurements. The advantage of starting measurements from the archive is that in this case all the fields of the plates that need to be filled in when starting measurements are filled with the values of the pre-selected record and the operator has the opportunity not to enter them completely, but only to correct them. In addition, when starting measurements from the archive, the operator has the opportunity to continue measuring the sample in cyclic mode.
Stop acquisition…	***Ctrl+F5***	Stopping measurements. The menu item and the toolbar button of the main window are duplicated in the measurement log toolbar for convenience - the operator can take measurements by minimizing the main window if it is not necessary.
Autocalibration…	***F6***	Automatic calibration of the spectrometer by the reference source. In full access mode, the procedure for auto-calibration (verification) by the spectrum stored in the measurement archive is available.
Background control…	***F7***	Background check or installing the background spectrum in the processing program. If a group of background spectrum records is selected, the background installing procedure will be repeated for all records of the selected group, starting with

the background spectrum with the earliest measurement date. Starting the background check procedure for a single recording from the archive window is convenient because the operator can pre-select the spectrometer and measurement geometry.

Spectrometers state	***F8***	Turning on/off the additional "**Spectrometers state**" window, which contains information about the parameters of the current measurements.
Heap…		Formation of a table of measurement results for a given sample. The form of presentation of the results is set in the archive parameters.
Statistics…		Calculation of a number of statistical parameters for a given sample of measurement results.
Summary report	***Ctrl+S***	Combining and averaging the processing results for selected records. Generating a summary report.
Graph…		Forming a graph of the dependence Y=f(X) for the values of the selected records of any numeric columns of the measurement log. The measurement date column can additionally be used for the abscissa (X) axis.

Tools:

Configure…	***Ctrl+T***	Configuring archive settings.
Import configuration…		Import archive parameters from the settings file of another archive.
Archive cleaning…		Cleaning the archive. During this operation, the entries marked for deletion and the corresponding files of spectra and processing results are physically deleted from the header file and from the archive folder.

View:

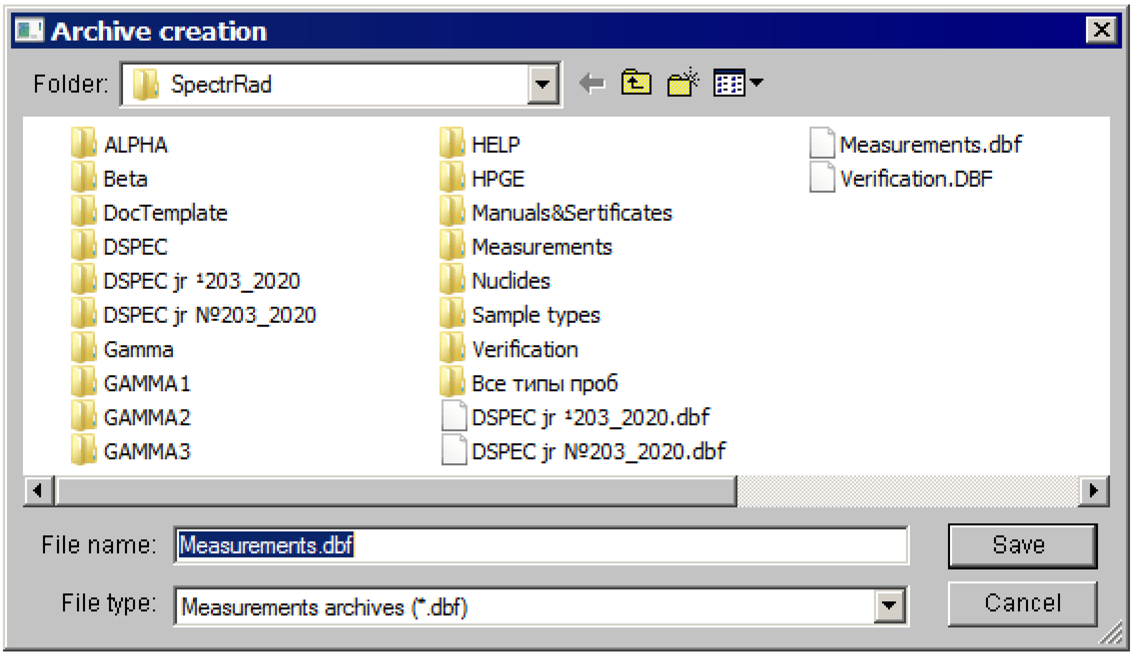
Show hidden	***Ctrl+D***	Enabling or disabling the output mode of records marked as "hidden". When the "hidden" mode is enabled, entries are displayed with the ⊗ icon to the left of the entry.
Grid lines	***Ctrl+G***	The grid output mode for the record table.
Toolbar		Turning on/off the "button bar" under the menu bar, which provides a more convenient way to access some menu items.
«Spectrometers» window		Turning on/off the "Spectrometers" window.
«Sample type» window		Turning on/off the "Sample type" window

Help	**F1**	Description of the program.

Creating an archive

The archive can be created by calling the menu item "**File / Create archive...**" either based on an existing folder with spectrum files, or by creating new folders. In the first case, the archive creation procedure generates a measurement log (archive header file) by scanning all spectrum files and processing results files in the specified folder. In this case, the files of the processing results, if they are in the spectra folder, are moved to the "**ISO**" folder created by the procedure, if it did not exist. In the second case, all the necessary files and folders are created. The measurement log, of course, will not contain any records.

The archive creation procedure forms a dialog box of the following type, for example:


Archive creation

Folder: SpectrRad

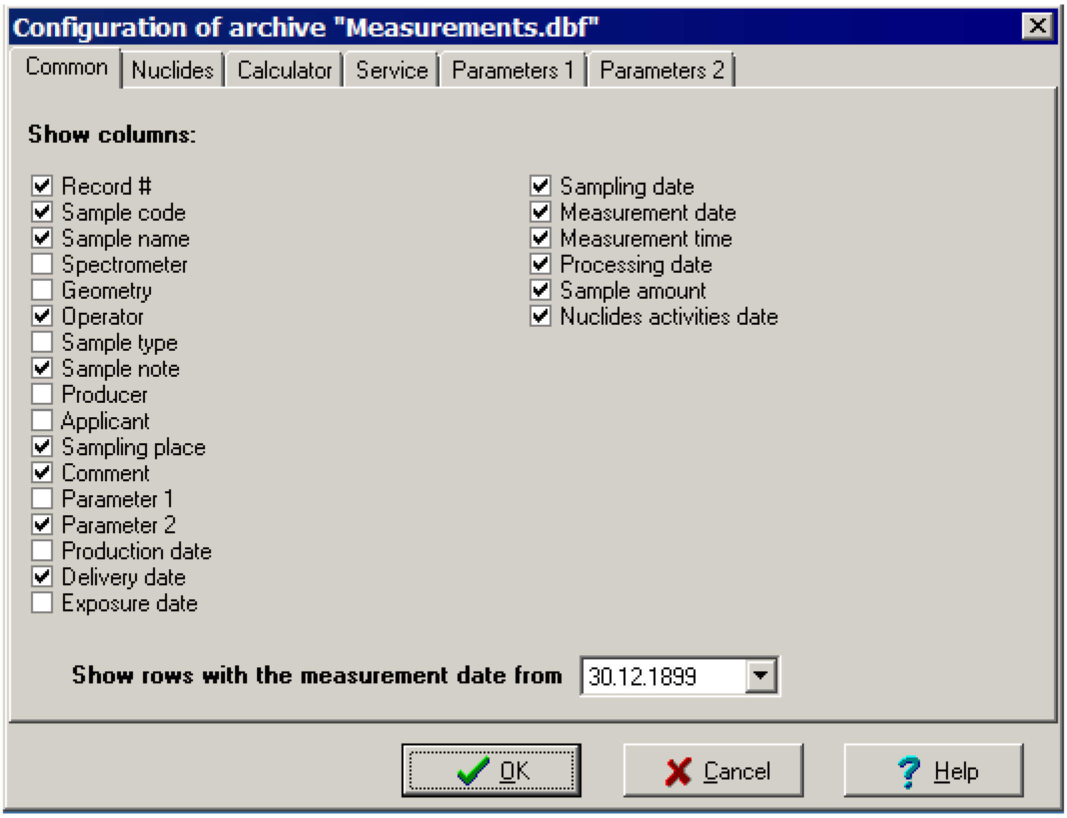
File name: Measurements.dbf

File type: Measurements archives (*.dbf)

When creating an archive based on an existing folder, the operator must enter the folder name in the "**File name**" column with the ".dbf" extension (for example, "**Measurements.dbf**") or, when creating a new archive, enter an arbitrary name that is not in the list of files and folders given in this form (for example, "**Archive.dbf**") and click on the "**Save**" button. If the entered name already exists, the archive creation procedure will warn you about it and suggest replacing the file. If there is also an old archive settings file, it can be used when creating an archive.

Configuring the archive

The number of visualized archive log columns, rows, data logging mode, sorting mode and other parameters are set when configuring the archive - the button (menu item "**Tools / Configure...**"). At the same time, a form is displayed on the screen:



Show columns:

☑ Record #
☑ Sample code
☑ Sample name
☐ Spectrometer
☐ Geometry
☑ Operator
☐ Sample type
☑ Sample note
☐ Producer
☐ Applicant
☑ Sampling place
☑ Comment
☐ Parameter 1
☑ Parameter 2
☐ Production date
☑ Delivery date
☐ Exposure date
☑ Sampling date
☑ Measurement date
☑ Measurement time
☑ Processing date
☑ Sample amount
☑ Nuclides activities date

Show rows with the measurement date from 30.12.1899

The table contains six pages: "**Common**", "**Nuclides**", "**Calculator**", "**Service**", "**Parameters 1**" and "**Parameters 2**".

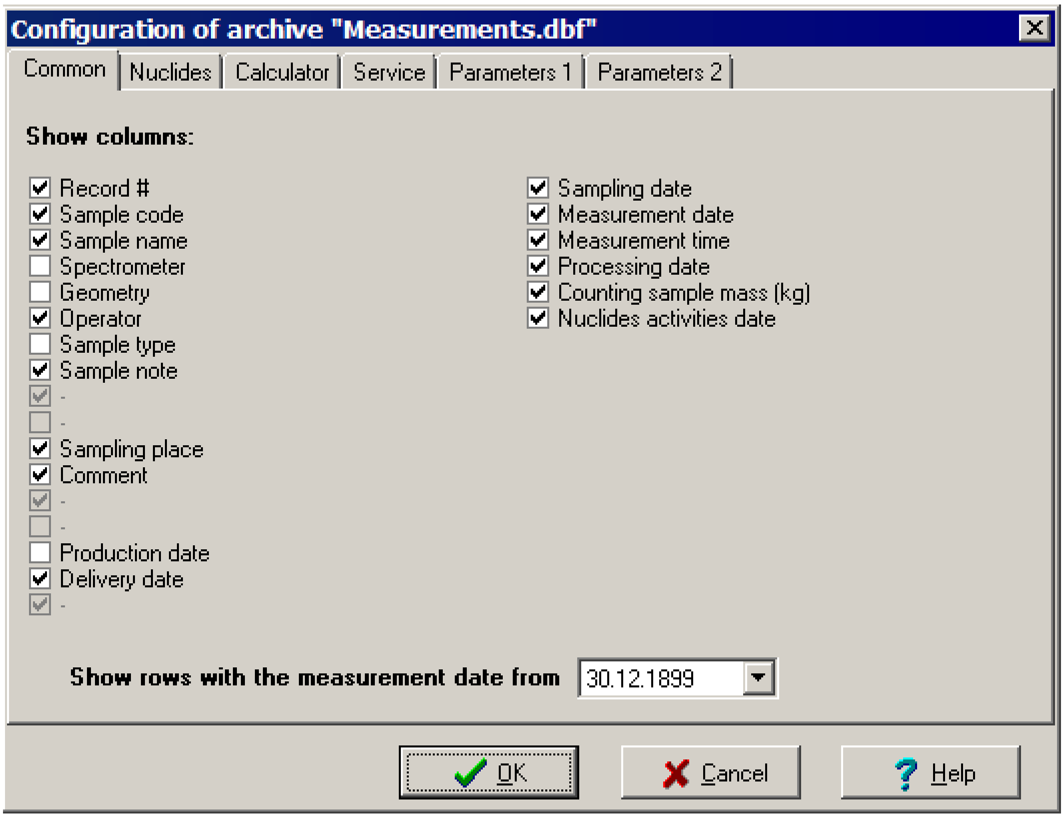
The first four pages contain a list of fields (columns) of the log entry. The operator can mark the columns that will be displayed in the table (marked with "ticks" in the square box before the column name). Changes are made by clicking the left mouse button on the selected item or using the cursor keys (moving inside a table section), tabs symbols (moving between sections) and the space bar (setting or deleting a checkbox).

On the first page of "**Common**", a list of column names for recording information about the sample and measurement parameters. In addition to the list of columns, there is a form for entering the date **-** "**Show rows with the measurements date from**", which allows you to limit the number of lines displayed in the measurement log. The measurement log will contain lines (records of measurement results) with the measurement date not earlier than specified.

The operator has the ability to change the names of the first seventeen columns (from the "**Sample code**" column to the "**Sampling date**" column) of the "**Common**" page - to do this, simply select the desired column in the settings table and, by pressing the "**Enter**" key or double-clicking, enter a new column name, completing the input by pressing the "**Enter**" key. The initial column names are restored when you enter an “empty” name.

The "**Sample amount**" column can change its name to "**Counting sample mass (kg)**" or be deleted from the log depending on the setting of activity normalization for the amount of source material or for the mass of the counting sample on the "**Parameters 1**" page of the archive settings.

If the column name does not contain letters or numbers, the program will delete all columns with such a "meaningless" name from all forms (measurement log, report forms, measurement launch and spectrum saving forms, etc.) associated with this measurement archive. In this case, the measurement log configuration form may look like this, for example.



Show columns:

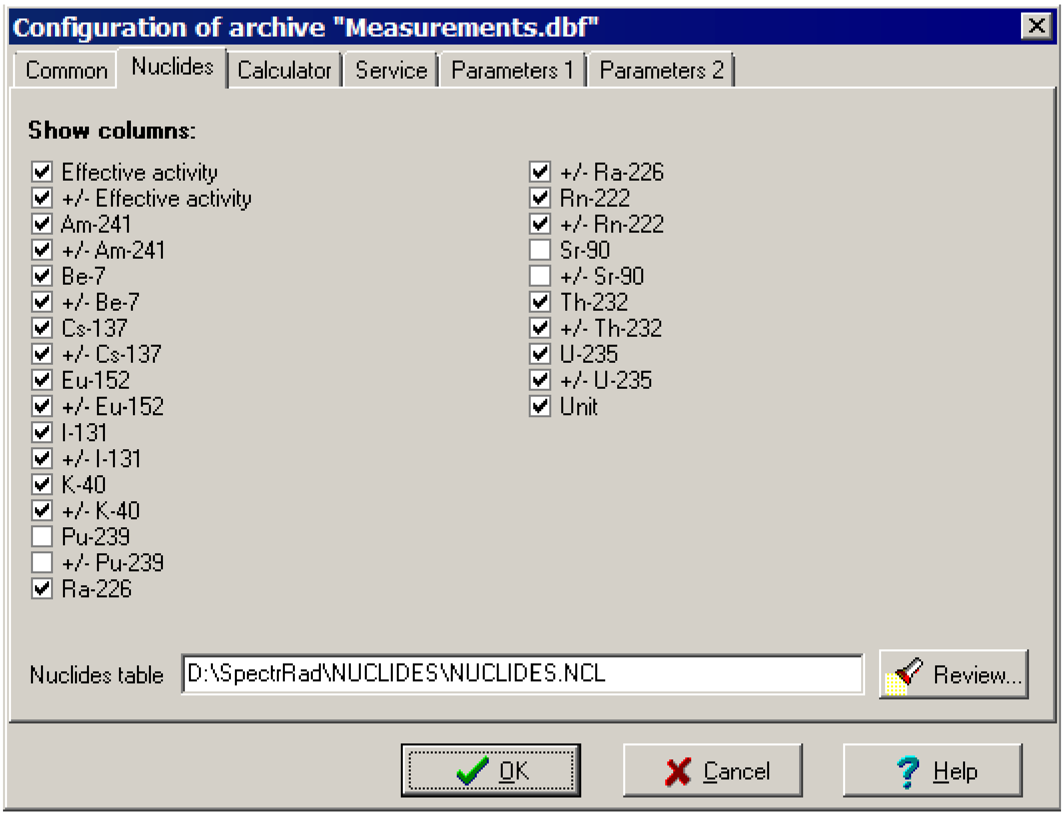
☑ Record #
☑ Sample code
☑ Sample name
☐ Spectrometer
☐ Geometry
☑ Operator
☐ Sample type
☑ Sample note
☑ -
☐ -
☑ Sampling place
☑ Comment
☑ -
☐ -
☐ Production date
☑ Delivery date
☑ -

☑ Sampling date
☑ Measurement date
☑ Measurement time
☑ Processing date
☑ Counting sample mass (kg)
☑ Nuclides activities date

Show rows with the measurement date from 30.12.1899

When deleting the column associated with the sample description, its field in the measurement log is combined with the field of the sample description lying in the sample record to the left. In this case, the combined field will have a total capacity. In this way, you can combine the fields: "**Sample code**" and "**Sample name**", "**Sample note**" and "**Producer**", "**Sample note**", "**Producer**" and "**Applicant**", "**Producer**" and "**Applicant**", and "**Sampling place**" and "**Comment**".

The second page contains a list of nuclides, the activity estimates of which, obtained during the processing of the sample spectrum, will be presented in the measurement log:



Show columns:

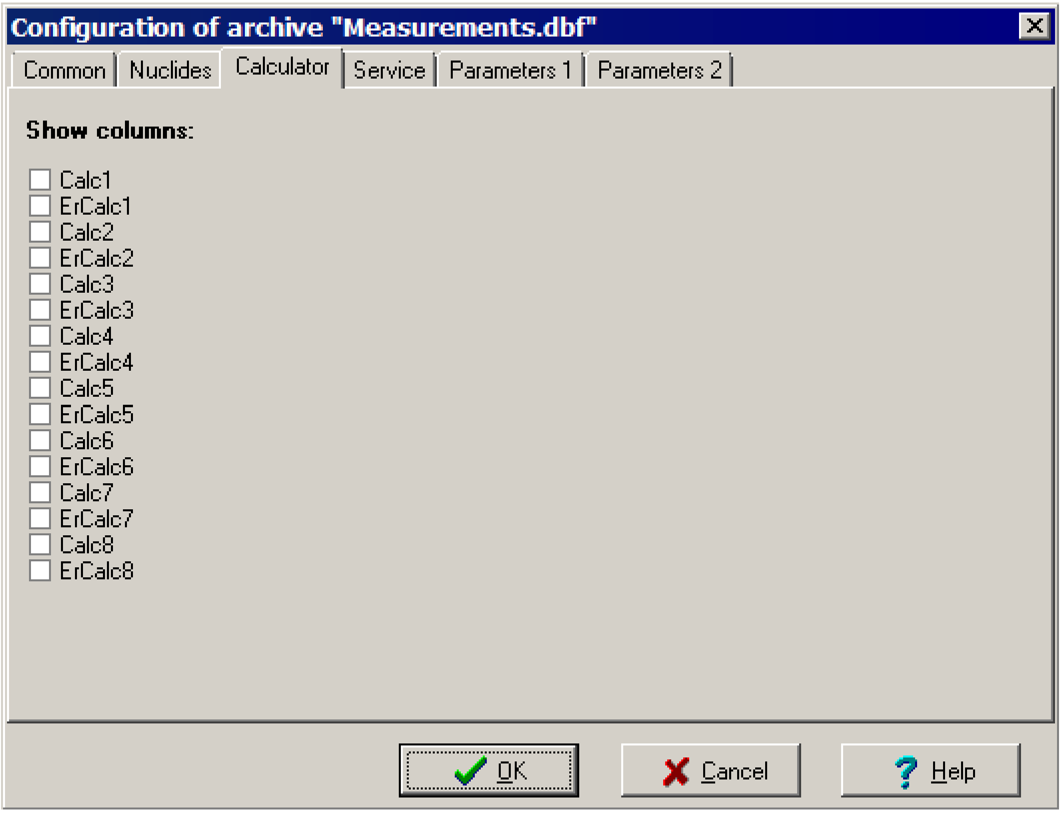
- ☑ Effective activity
- ☑ +/- Effective activity
- ☑ Am-241
- ☑ +/- Am-241
- ☑ Be-7
- ☑ +/- Be-7
- ☑ Cs-137
- ☑ +/- Cs-137
- ☑ Eu-152
- ☑ +/- Eu-152
- ☑ I-131
- ☑ +/- I-131
- ☑ K-40
- ☑ +/- K-40
- ☐ Pu-239
- ☐ +/- Pu-239
- ☑ Ra-226
- ☑ +/- Ra-226
- ☑ Rn-222
- ☑ +/- Rn-222
- ☐ Sr-90
- ☐ +/- Sr-90
- ☑ Th-232
- ☑ +/- Th-232
- ☑ U-235
- ☑ +/- U-235
- ☑ Unit

Nuclides table D:\SpectrRad\NUCLIDES\NUCLIDES.NCL

At the beginning of the list "**Effective activity**" and "**+/- Effective activity**" are estimates of the magnitude and error of the conditional total activity of all nuclides determined in the sample summed with the coefficient "gamma radium equivalent", which the calculation program takes from the table of nuclides used in spectrum processing. The last column ("**Unit**") is the name of the unit of measurement of activities and errors.

The list contains a limited number of nuclides, but this does not mean that the archive does not save estimates of the activities of all nuclides determined during the processing of the spectrum. Everything is saved in the archive. To form the required list of nuclides, the operator must double-click on the name of a nuclide (or, selecting the desired line in the list, press the "Enter" key) and select the desired nuclide from the list proposed by the program. The list of available nuclides is set in the "**Nuclides table**" line. The required nuclide table can be selected by pressing the Review... key. When changing the list of nuclides of an existing measurement log, the program will reformat the log to include the specified nuclides in it.

If it is necessary to display in the measurement log estimates of the activities of nuclides not included in this list, they can be given in the columns of the calculator.


Configuration of archive "Measurements.dbf"

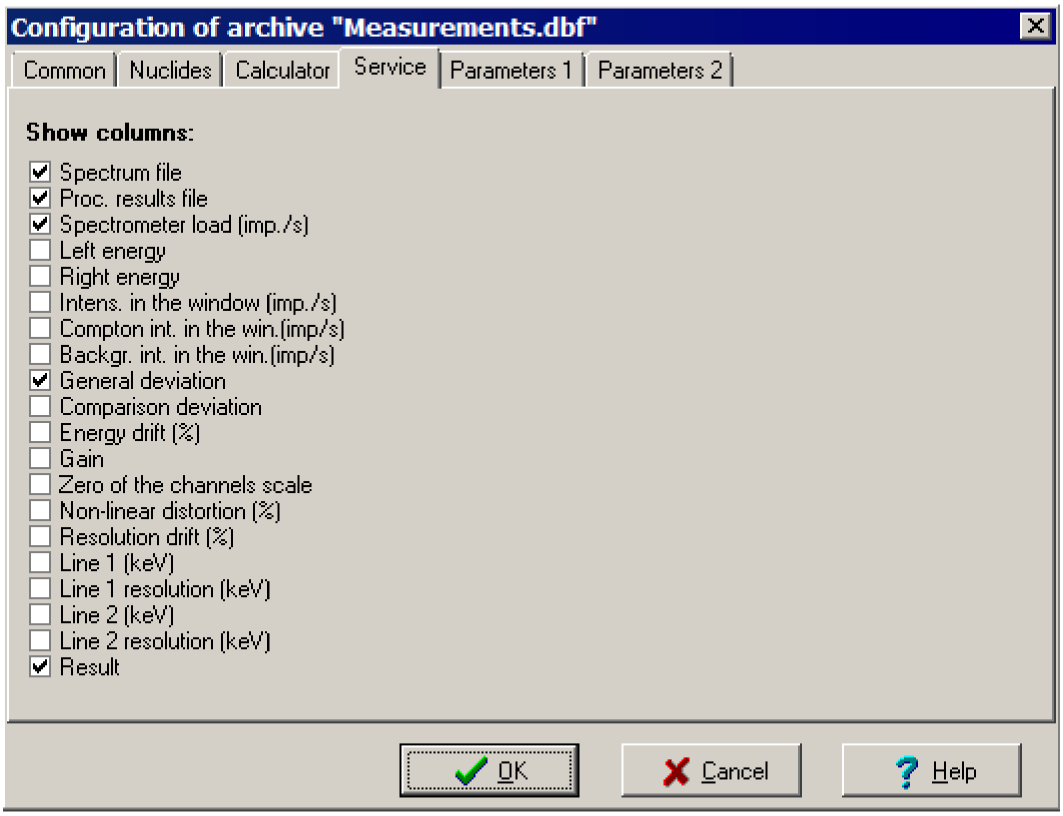
Show columns:

☐ Calc1
☐ ErCalc1
☐ Calc2
☐ ErCalc2
☐ Calc3
☐ ErCalc3
☐ Calc4
☐ ErCalc4
☐ Calc5
☐ ErCalc5
☐ Calc6
☐ ErCalc6
☐ Calc7
☐ ErCalc7
☐ Calc8
☐ ErCalc8

The "**Calculator**" page contains a list of sixteen variables "**Calc1**" - "**ErCalc8**" of the programmable calculator, which the user of the "SpectrRad" package can record in the log.

The operator has the ability to change the names of **Calc1 - ErCalc8** columns, the purpose of which is set by the program user. The initial column names are restored when you enter an “empty” name.

The "**Service**" page contains a list of additional parameters calculated by the spectrum processing program and necessary for monitoring the parameters of the spectrometer and the quality of spectrum processing:



Show columns:

- ☑ Spectrum file
- ☑ Proc. results file
- ☑ Spectrometer load (imp./s)
- ☐ Left energy
- ☐ Right energy
- ☐ Intens. in the window (imp./s)
- ☐ Compton int. in the win.(imp/s)
- ☐ Backgr. int. in the win.(imp/s)
- ☑ General deviation
- ☐ Comparison deviation
- ☐ Energy drift (%)
- ☐ Gain
- ☐ Zero of the channels scale
- ☐ Non-linear distortion (%)
- ☐ Resolution drift (%)
- ☐ Line 1 (keV)
- ☐ Line 1 resolution (keV)
- ☐ Line 2 (keV)
- ☐ Line 2 resolution (keV)
- ☑ Result

- The first two lines: "**Spectrum file**" and "**Proc. results file**" are the names of the columns containing the names of the spectrum files and the results of its processing in the archive.
- "**Spectrometer load (imp./s)**" - the total intensity of the pulses recorded in the spectrum.
- "**Left energy**" and "**Right energy**" are the boundaries of the energy range of the spectrum used in processing.
- "**Intensities in the window (imp./s)**" is the intensity recorded in the energy range of the spectrum used in the processing. If the output mode of error is set as the random component of the error (the column is highlighted in blue), the column shows the intensity of pulses registered not in the general integral window, but in the energy windows used to assess the activity of nuclides, determined by the processing program or set by the operator. This mode of recording in the column is due to the use of the data given in the column when calculating the minimum measured activity of nuclides in the statistical processing procedure. In the event that a full error output mode is set for the log, or if a single integral energy window is used in the processing procedure (a background spectrum check procedure or a standard scintillation spectrum processing mode), the full intensity of the spectrum in the specified energy boundaries will be recorded in the column.
- "**Compton int. in the win. (imp./s)**" - when processing spectra with peak separation, the intensity of pulses registered in the Compton scattering spectrum in the processing window. In the output mode of error is set as the random component of the error (the column is highlighted in blue) is the intensity of the pulses of the Compton scattering spectrum recorded in the energy windows used in assessing activity.
- "**Backgr. int. in the win. (imp./s)**"- the intensity of background radiation in the same windows.

- "**General deviation**"[11] is the deviation of the model spectrum from the sample spectrum over the entire spectrum processing range, expressed in standard deviations.
- "**Comparison deviation**" – deviation of activity estimates from a priori data. It is used in daily spectrometer verification procedures.
- "**Energy drift (%)**" - the total drift of the gain factor and zero of the scale of the spectrometric tract (in percent) - an estimate of the change in the gain factor and zero of the scale relative to the initial values (1 for the gain factor and 0 for zero of the scale) established during the initial energy calibration of the spectrometer.
- "**Gain**" is the value of the conditional gain of the tract. During the initial calibration, the "gain factor" is equal to one, it changes over time - it drifts.
- "**Zero of the channels scale**" - the value of the conditional zero of the channel scale. At the initial calibration, the "zero of the channel scale" is zero. Its change corresponds to the zero drift of the energy scale in the channels.
- "**Non-linear distortion (%)**" is the maximum deviation from the linear drift model normalized by the length of the spectrum.
- "**Resolution drift (%)**" – change the resolution of the spectrometer as a percentage. Negative values correspond to improved resolution.
- "**Line 1 (keV)**" is the energy of the left boundary line used in the energy calibration of the spectrometer.
- "**Line 1 resolution (keV)**" is the resolution of the spectrometer (peak width at half height) for line 1.
- "**Line 2 (keV)**" is the energy of the right boundary line used in the energy calibration of the spectrometer.
- "**Line 2 resolution (keV)**" is the resolution of the spectrometer for line 2.
- "**Results**" - the value of the "Result" column can consist of one "+" or "-" sign, or three - the first sign is supplemented with two characters: "/+", "/-" or "/R". The first sign is the result of a spectrum processing operation (decomposition or calibration of the spectrometer). The "+" sign corresponds to successful processing, the "-" sign to unsuccessful processing. The letter "R" means the replacement of the working spectrum of the background. An unsuccessful processing operation is considered to be in case of exceeding of the specified thresholds by the discrepancy or the parameters of the energy drift and the resolution drift , or the failure of processing a priori information transmitted "by inheritance" when using the Bayesian method of spectrum processing (for example, joint processing of beta and gamma spectra).
  The second sign "+" or "-" is the operator's decision during the operation of auto-calibration and background control: "+" is the result of the operation of auto-calibration or background control accepted by the operator, "-" is not accepted, "R" is the background spectrum replaced.

The service columns of the log table allow you to track changes in the parameters of the spectrometer over time. It is recommended to create a separate archive to save the results of the spectrometers auto-calibration and background radiation control procedures and install visualization of "service columns" for it.

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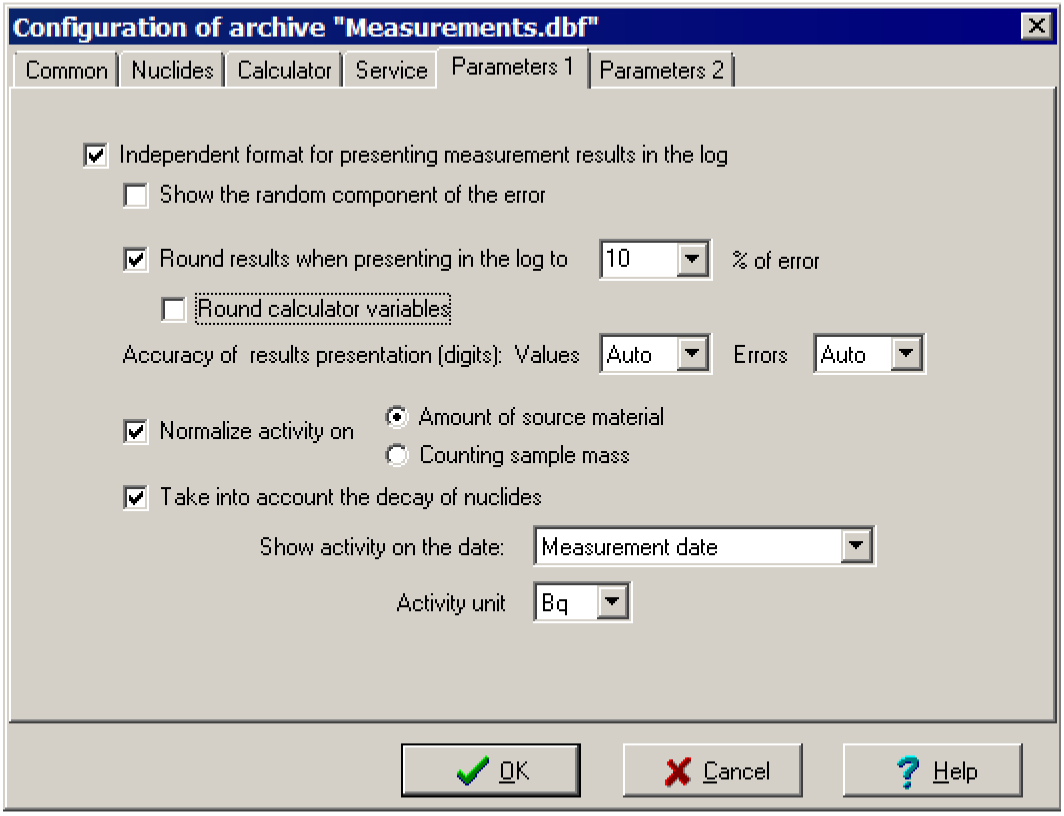
[11] **Deviation** of the calculated model from the object normed on the estimated value of the standard deviation $G = \sqrt{\sum((X_i - X_m)^2 / G_i^2)/(n-m)}$. For the general deviation, the object is the measured spectrum, the model is the sum of the decomposition components. For the comparison deviation, the object is the nuclides activity estimates, the model is the certified nuclides activity.

The "**Parameters 1**" page looks like:



☑ Independent format for presenting measurement results in the log

☐ Show the random component of the error

☑ Round results when presenting in the log to 10 % of error

☐ Round calculator variables

Accuracy of results presentation (digits): Values Auto Errors Auto

☑ Normalize activity on ● Amount of source material ○ Counting sample mass

☑ Take into account the decay of nuclides

Show activity on the date: Measurement date

Activity unit Bq

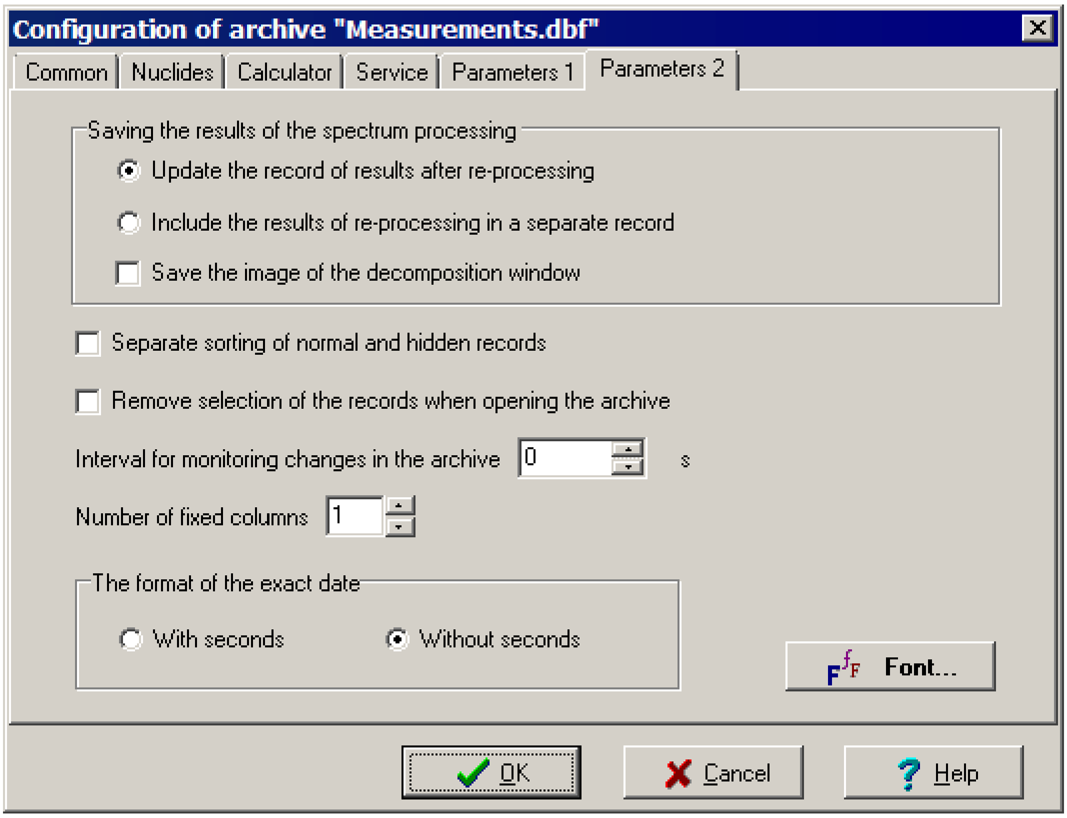
The measurement log is used not only for convenient access to the measured spectra and processing results, but also for group processing of measurement results: sample reports, statistical processing of samples, and creation of graphs. For correct statistical processing, the form of presentation of the results (for example, data rounding) recommended for reports of individual measurements is not suitable. Therefore, the form of displaying the results in the measurement log can be set independently of the form of presenting the results in the report for an individual measurement. To do this, you need to check the "**Independent format for presenting measurements results in the log**" box and set the parameters of such a presentation:

- **Show the random component of the error** – when a check mark is set in the error columns for nuclide activities, a random component of the total error will be presented. In the normal mode, the total error is given. When displaying a random component, the error columns in the archive will be colored blue. The random component of the error is necessary to calculate a number of parameters during statistical processing of the results.
- **Round results when presenting in the log to nn % of error -** the mode and type of rounding for the values of nuclide activities when presenting the results in the measurement log and the "Statistics" and "Heap" reports.
- **Accuracy of result presentation (digits)** – select the number of digits to represent the results in the report. The value "**Auto**" corresponds to the automatic determination of the required accuracy of the presentation of the results. In this case, insignificant zeros are not output. The accuracy of the representation is set separately for **Values** and **Errors**.
- The values of the activities shown in the columns of the measurement log can correspond either to the specific activity of the source material or to the specific activity of the counting sample when the "**Normalize activities on:**" checkmark is set and the appropriate normalization item is selected: "**Amount of source material**" or "**Counting sample mass**", or they are given without normalization (total activity of the counting sample).

- **Take into account the decay of nuclides** – when the "tick" is set, the activity of nuclides will be recalculated on the specified date (the date of the beginning of measurements or the date of sampling), and otherwise the averaged activity during the measurement will be given.
- The operator has the opportunity to select the date on which the activities in the measurement log will be shown from the list "**Show activity on the date:**" measurement date, start or end date of sampling, date of production or delivery of the sample. When choosing the date of values for activities, it must be borne in mind that for short-lived nuclides, for example, Rn-222, there may be an overflow of the bit grid and incorrect data display.
- **Activity unit** – selecting the unit of measurement of the nuclide activity (Becquerel or Curie) or the nuclide content in the sample (gram) in which the activity or content of nuclides in the journal will be shown.

If the "**Independent format for presenting measurements results in the log**" checkbox is unchecked, the form of presentation of measurement results in the log will correspond to the presentation of measurement results in the report for each specific measurement and, in general, may have a different format for each row.

The "**Parameters 2**" page looks like:



Saving the results of the spectrum processing

● Update the record of results after re-processing

○ Include the results of re-processing in a separate record

☐ Save the image of the decomposition window

☐ Separate sorting of normal and hidden records

☐ Remove selection of the records when opening the archive

Interval for monitoring changes in the archive 0 s

Number of fixed columns 1

The format of the exact date

○ With seconds ● Without seconds

By marking the corresponding point with a dot at the top of the **Parameters 2** page (section "**Saving the results of the spectrum processing**"), the operator has the opportunity to choose one of two possible modes for saving the results of spectrum processing:

• **Update the record of results after re-processing**	In this mode, the log line is overwritten - the old values are lost and new data is written in their place.
• **Include the results of re-processing in a separate record**	In this case, the new processing results are included as an additional record.

When the "**Save the image of the decomposition window**" checkmark is set, the program saves the image of the decomposition window in the archive at the end of spectrum processing, which allows you to include such images in reports when they are created, at any time after the end of the decomposition procedure.

A new record is created during re-processing in any mode if the sample parameters change. The mode of saving the results of repeated spectrum processing by a separate record forms a separate record even if no sample parameters have been changed.

Setting the "check mark" in the items listed below enables the corresponding archive operation mode:

- **Separate sorting of normal and hidden records -** allows you to display records marked for deletion (if the "**Show hidden records**" mode is set) not in the general list, but separately at the beginning or end of the table, depending on the sorting order.
- **Remove selection of the records when opening the archive**. If the check box is selected, the archive entries selected by the operator in the previous session of working with the archive will not be highlighted; otherwise the old selections are saved.

Setting a non-zero value of the "**Interval for monitoring changes in the archive**" parameter is necessary if access to the archive is allowed to more than one program (for example, when saving measurement results in a shared network archive for several spectrometers). In this case, the program will monitor the date of the last modification of the archive file after a specified interval and update the measurement log if necessary. A zero time value disables the procedure for monitoring the date of modification of the archive file.

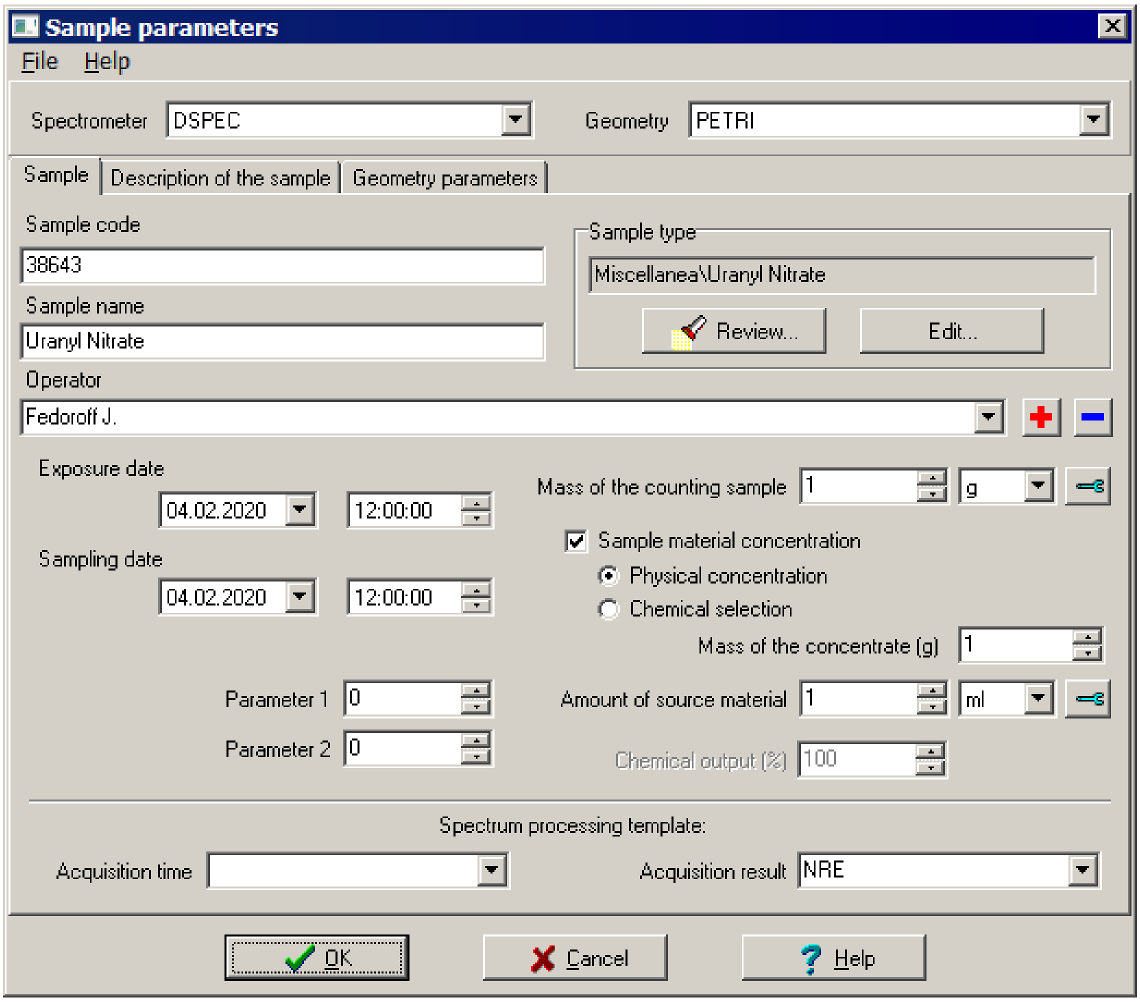
The "**Number of fixed columns**" parameter determines the number of the first columns that will not participate in the horizontal scrolling of the contents of the table of records window. These columns are highlighted in the background color.

The "**The format of the exact date**" group of two items: "**With seconds**" and "**Without seconds**" allow you to choose the format for representing a date including time (selection date, measurement date, etc.).

The Font... button allows you to set the font for displaying entries in the measurement log.

Editing the archive

The button (menu item "**Edit / Edit record...**") allows you to edit the selected measurement log entry, the corresponding spectrum and the file of spectrum processing results, if they exist. The window of the editing procedure looks like:



Spectrometer: DSPEC
Geometry: PETRI

Sample code: 38643
Sample name: Uranyl Nitrate
Sample type: Miscellanea\Uranyl Nitrate
Operator: Fedoroff J.

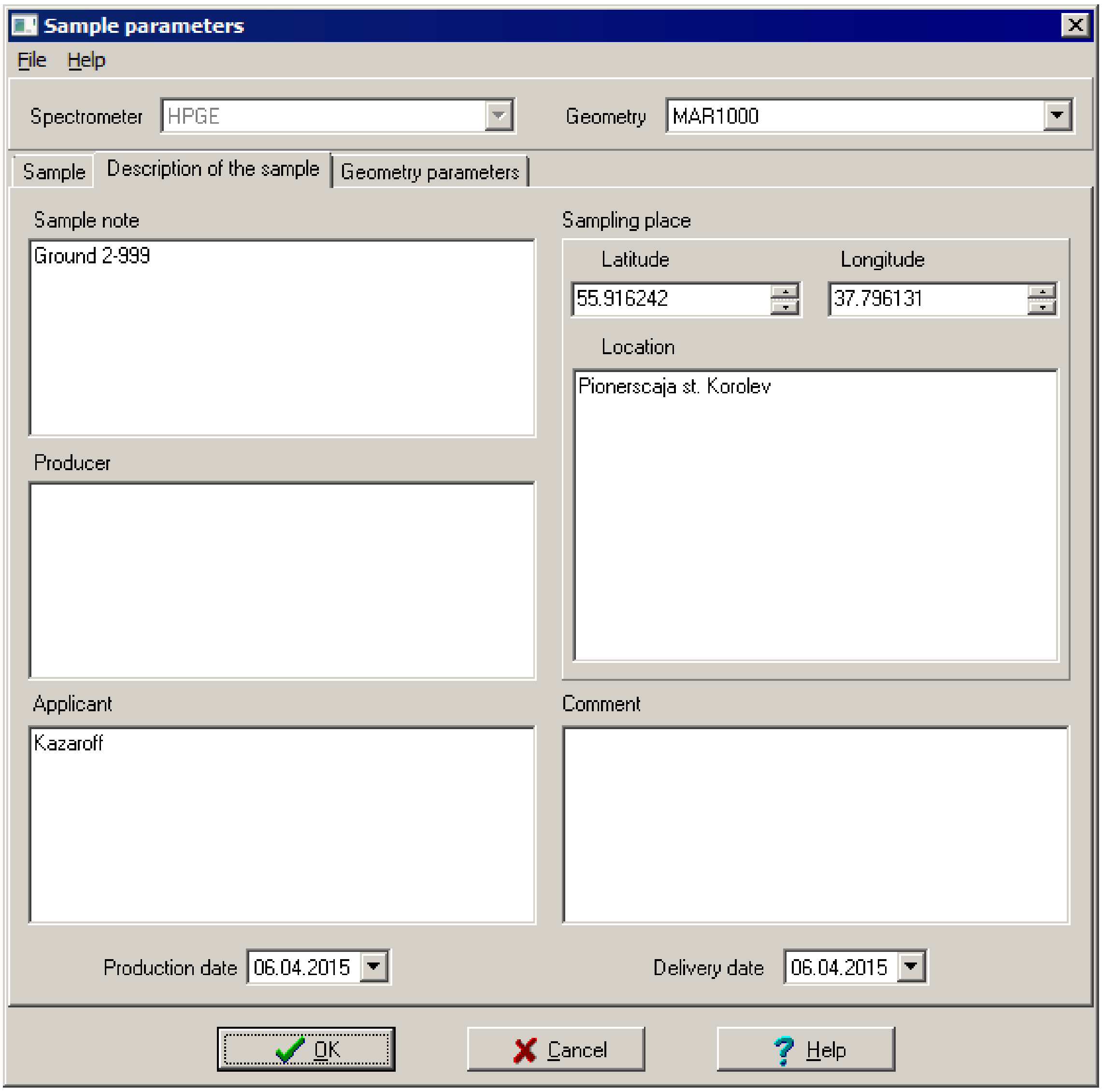
Exposure date: 04.02.2020 12:00:00
Sampling date: 04.02.2020 12:00:00
Parameter 1: 0
Parameter 2: 0

Mass of the counting sample: 1 g
☑ Sample material concentration
● Physical concentration
○ Chemical selection
Mass of the concentrate (g): 1
Amount of source material: 1 ml
Chemical output (%): 100

Spectrum processing template:
Acquisition time:
Acquisition result: NRE

The form contains three pages of sample parameters "**Sample**", "**Description of the sample**" and "**Geometry parameters**". The first page contains the main fields of the sample description, the "Operator" field for entering data about the laboratory technician conducting measurements and two lists with spectrum processing templates

The second page contains fields for entering additional information about the sample and looks like:

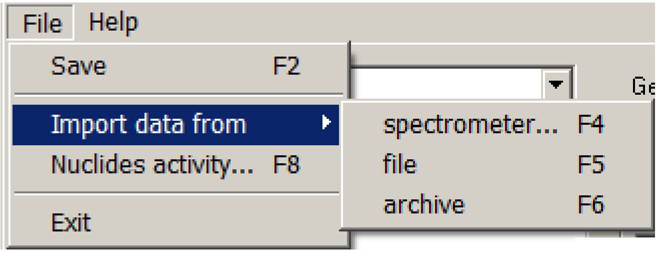


Spectrometer: HPGE
Geometry: MAR1000
Sample note: Ground 2-999
Latitude: 55.916242
Longitude: 37.796131
Location: Pionerscaja st. Korolev
Applicant: Kazaroff
Production date: 06.04.2015
Delivery date: 06.04.2015

On the third page, the operator can also change some parameters of the measurement geometry. Geometry parameters are not displayed in the log, but are an integral part of the spectra and processing results of measurements stored in the archive.

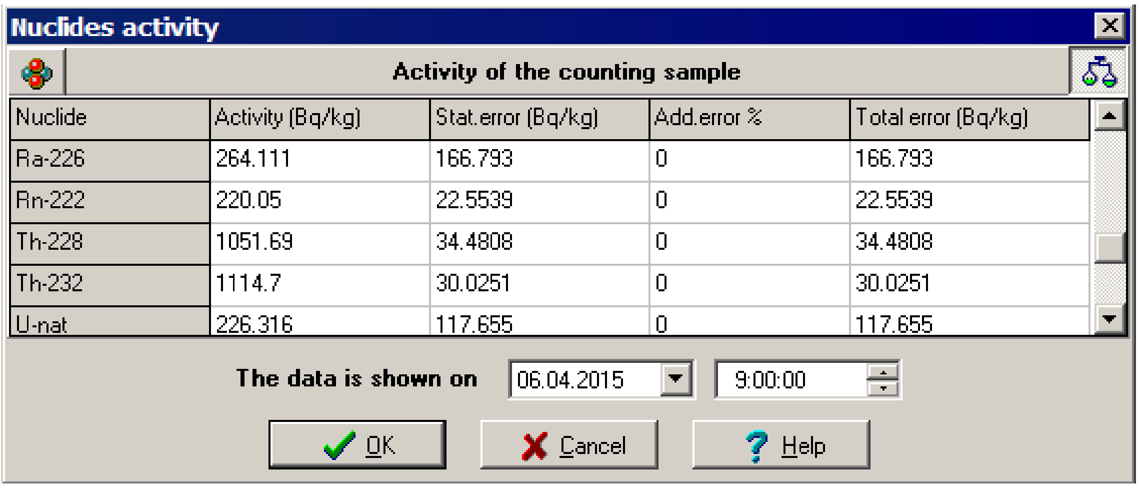
Pressing the "**OK**" key will save the changes in the measurement log and in the files of the spectrum and processing results. In the event that the data on the sample size (the mass of the counting sample, the mass of the concentrate and/or the amount of the starting material) have been changed, the data on specific activities in the processing results will also change accordingly. Such recalculation will be correct if the mass of the counting sample has not changed. And it will be relatively correct if the mass of the counting sample was adjusted, but only if the results are related to the processing of a high-energy gamma spectrum. In the case of alpha, beta radiation, and low-energy gamma radiation, it is necessary to take into account the change in radiation absorption when the mass of the counting sample changes, and in this case it is necessary to re-process the spectrum after correcting the data.

The form also has a small menu:



The menu item "**File / Import data from**" allows you to import sample parameters from another spectrometer, a spectrum file, or from a selected archive entry, which saves time filling in the form fields.

The menu item "**File / Nuclides activity...**" of the "**Sample parameters**" form allows you to edit the list of nuclides and calculated activity values, add data on nuclide activities obtained on other devices to the processing results file, or enter data on certified values of nuclide activities. At this case, a form for entering a priori data on the activities of nuclides will appear on the screen:

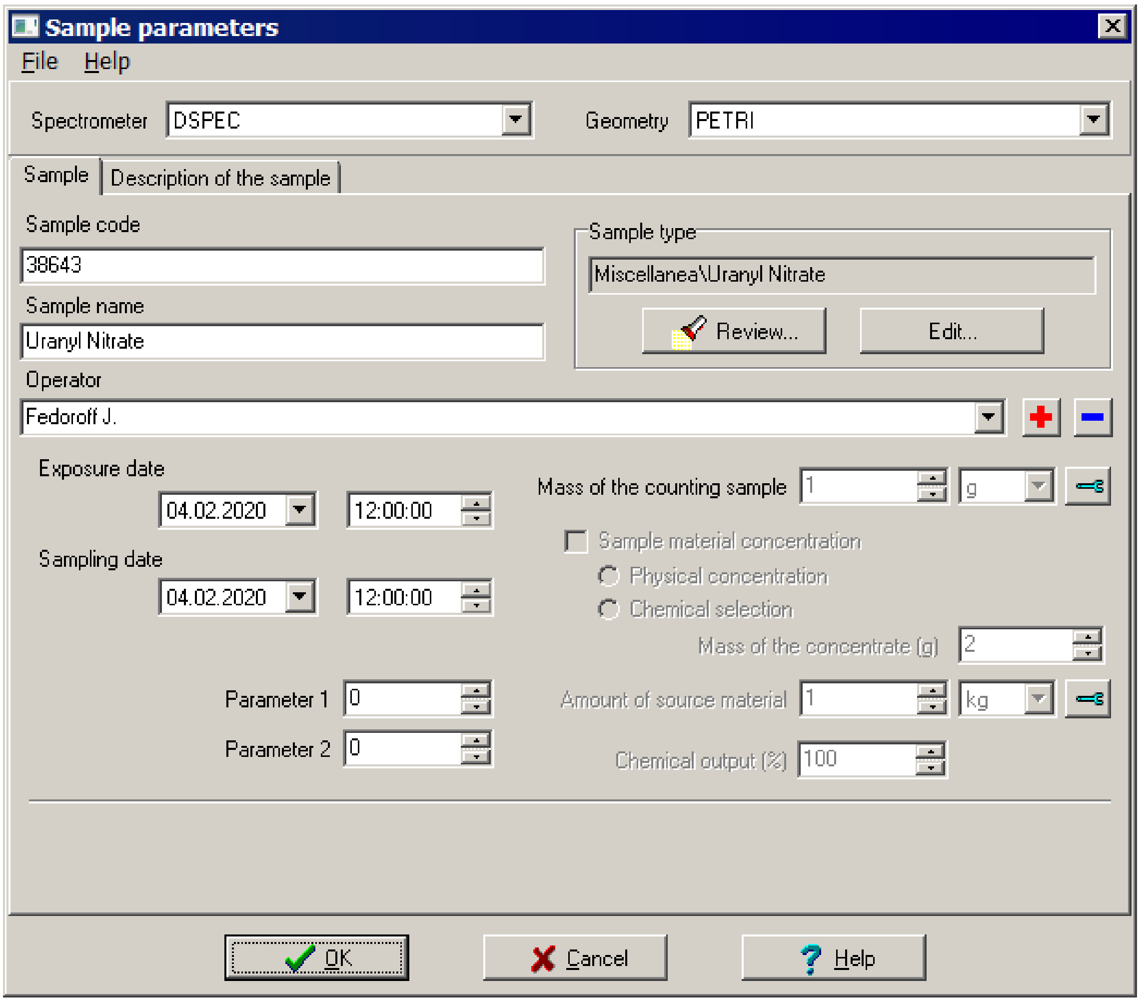


Nuclide	Activity (Bq/kg)	Stat.error (Bq/kg)	Add.error %	Total error (Bq/kg)
Ra-226	264.111	166.793	0	166.793
Rn-222	220.05	22.5539	0	22.5539
Th-228	1051.69	34.4808	0	34.4808
Th-232	1114.7	30.0251	0	30.0251
U-nat	226.316	117.655	0	117.655

The data is shown on 06.04.2015 9:00:00

The operator has the opportunity to edit data on the activities and uncertainties of the sample, change the list of nuclides (button). Data can be entered either in the form of total sample activity (counting sample) or in the form of specific activity. The button switches the input form. The random component of the total uncertainty in absolute values and additional uncertainty as a percentage of activity should be indicated, the procedure calculates the full uncertainty itself.

The button (menu item "**Edit / New record...**") allows you to create a new record in the measurement log based on the selected record. The window of the record creation procedure looks like:



Spectrometer: DSPEC
Geometry: PETRI
Sample code: 38643
Sample name: Uranyl Nitrate
Sample type: Miscellanea\Uranyl Nitrate
Operator: Fedoroff J.
Exposure date: 04.02.2020 12:00:00
Sampling date: 04.02.2020 12:00:00
Mass of the counting sample: 1 g
☐ Sample material concentration
○ Physical concentration
○ Chemical selection
Mass of the concentrate (g): 2
Parameter 1: 0
Parameter 2: 0
Amount of source material: 1 kg
Chemical output (%): 100

The form is identical to the record editing form, except that the fields for entering the sample size (mass of the counting sample, mass of concentrate and amount of source material) and fields for setting spectrum processing patterns are not available. The measurement geometry parameters page is also unavailable.

The procedure for creating a new record allows you to register samples in the measurement log that will be measured in the future. When starting measurements of a sample registered in this way, the operator will need to supplement the sample information only with sample size parameters and processing templates. In this case, measurements should be started from the measurement archive window with the desired selected record.

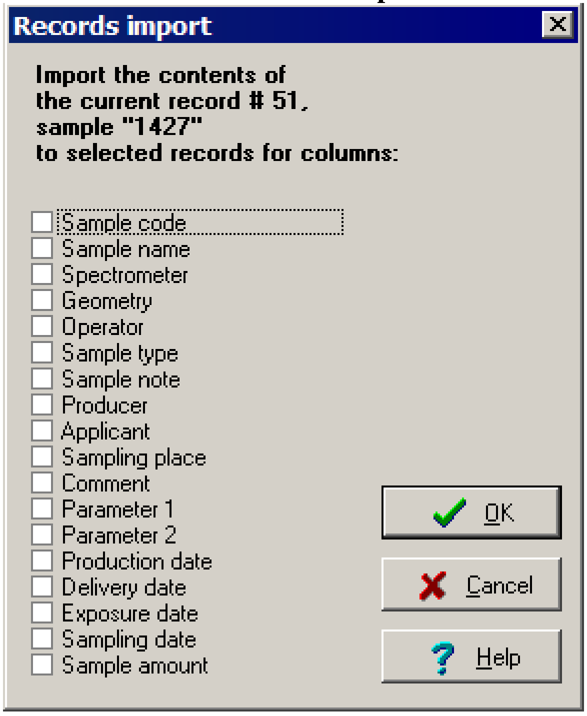
The "**Data import**" and "**Data transfer**" procedures are designed for group editing of records. In this case, the operator must first select the records for group editing. There are several ways to highlight records:

- pressing the "**Insert**" key on the computer keyboard highlights the current line and makes the next line current;
- clicking with the left mouse button while pressing the "**Ctrl**" key on the computer keyboard highlights the entry that was clicked;
- left-clicking on the first entry with the "**Shift**" key pressed highlights the first entry in the group, and the second click on another entry with the "**Shift**" key pressed highlights the entire group from the first to the last entry.

Selected entries are marked in green.

The "**Data import**" procedure imports the contents of the columns of the current record specified by the operator (highlighted in yellow or blue) into the corresponding columns of the selected records and fields of descriptions and parameters of the sample for the spectrum and the processing results file. Thus, group editing is performed as follows: one record is pre–edited, then the required group of records is selected and the data of the edited record is imported into the selected records.

The menu item "**Edit / Data import...**" calls the form of the procedure "**Data import**":



Records import

Import the contents of
the current record # 51,
sample "1427"
to selected records for columns:

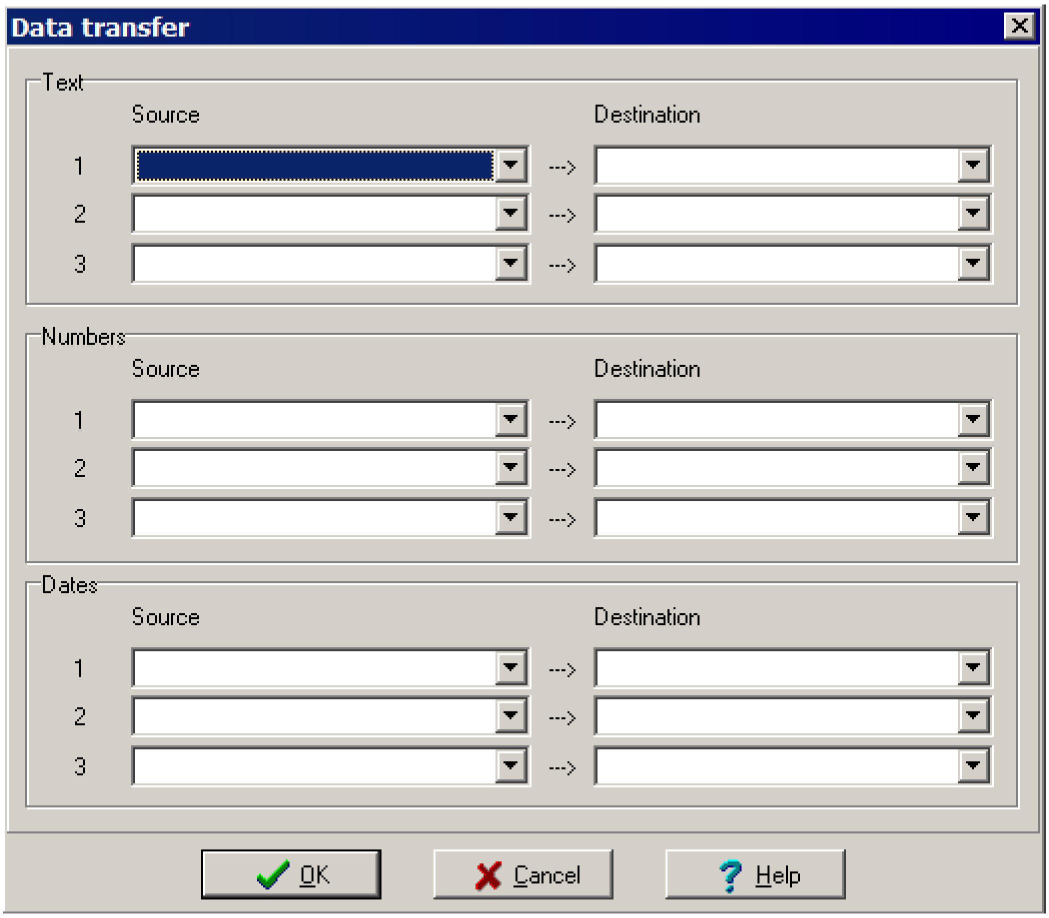
☐ Sample code
☐ Sample name
☐ Spectrometer
☐ Geometry
☐ Operator
☐ Sample type
☐ Sample note
☐ Producer
☐ Applicant
☐ Sampling place
☐ Comment
☐ Parameter 1
☐ Parameter 2
☐ Production date
☐ Delivery date
☐ Exposure date
☐ Sampling date
☐ Sample amount

The operator must check the boxes for those columns whose contents will be imported.

The purpose and name of many columns of the measurement log in the "SpectrRad" package is not strictly regulated, but is determined by the user. Therefore, it may be necessary to transfer their contents when renaming the journal columns. For a single recording, this can be done manually by editing the recording. For a large number of records, manual editing is not the best way. In this case, the "**Data transfer**" operation will help.

The procedure allows you to clear the selected columns or transfer the contents of the columns specified by the operator to other columns, the "basket" or from the "basket" to the specified columns. The operation is performed for all selected archive records.

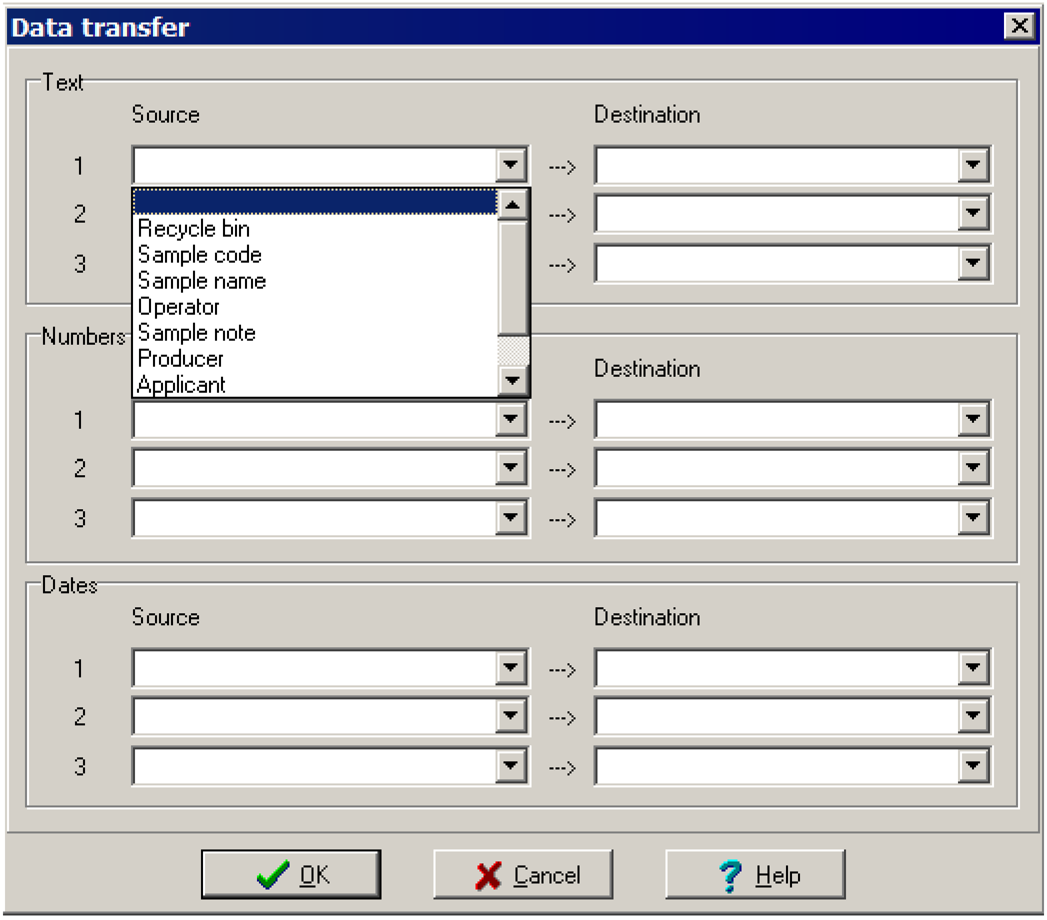
The procedure form has three groups: "**Text**", "**Numbers**" and "**Dates**".



In each group, three transfer operations can be defined - the minimum required for data exchange between the **Source** and **Destination**. For example, three operations are required to exchange data between the "**Sampling place**" and "**Comment**" columns:

1. **Sampling place → Recycle bin**
2. **Comment → Sampling place**
3. **Recycle bin → Comment**

The source and recipient for each group are selected from a drop-down list containing a set of columns of this type in the measurement log supplemented with a "**Recycle bin**" (buffer for saving data) and an empty line. For example, for text data:

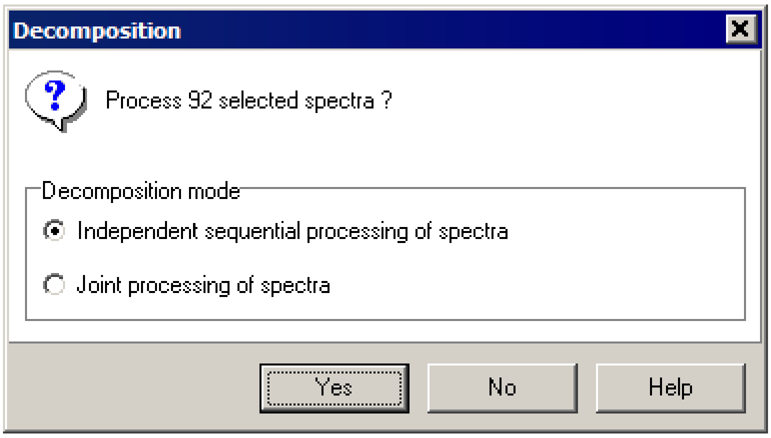


Setting an empty string as the source resets the receiver.

Standard editing procedures for many programs: "**Cut**", "**Copy**" and "**Paste**" in the measurement archive perform operations on selected records and their corresponding files of spectra and processing results. The "**Cut**" and "**Copy**" procedure places the marked entries to the clipboard, and the "**Paste**" procedure copies the entries from the clipboard to the archive. When inserting records, their presence in the archive is not checked, so it is possible to duplicate records.

Group processing of spectra

The button (menu item "***Commands / Decompose spectrum...***"), in the event that the operator has selected several measurement log entries, calls the procedure for the group decomposition of spectra. At the same time, a form appears on the screen:



Process 92 selected spectra ?

Decomposition mode

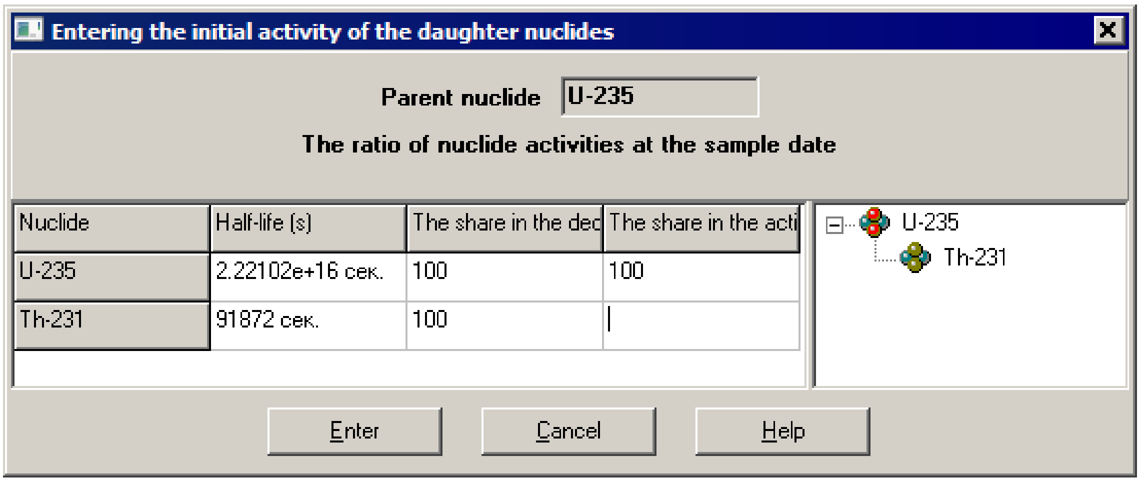
● Independent sequential processing of spectra

○ Joint processing of spectra

The operator must select one of two processing modes: "**Independent sequential processing of spectra**" or "**Joint processing of spectra**". When the **independent sequential processing** mode is selected, the spectra are sequentially processed for all selected records. At the same time, there is no limit on the number of selected records, and records can relate to spectra from various counting samples.

When choosing the **joint processing of spectra** mode, all the spectra should be radiation spectra from the same sample measured at different times. No more than 100 spectra can be included in the joint processing. In this mode, a common system of equations is formed for all spectra, and since this takes into account the rate of decay of nuclides, the general system of equations allows us to separate nuclides with identical or similar radiation spectra and obtain the most effective activity estimates. Thus, the technique of amplitude-time analysis is implemented.

In the event that the list of nuclides to be determined in the processing template contains nuclides included in the decay chain, the program will request information about the initial ratio of nuclide activities in the decay chain. The form for entering values may look like this, for example:



Parent nuclide U-235

The ratio of nuclide activities at the sample date

Nuclide	Half-life (s)	The share in the dec	The share in the acti
U-235	2.22102e+16 сек.	100	100
Th-231	91872 сек.	100	

The operator must enter the activity for the daughter nuclides as a percentage relative to the parent nuclide at the date of sampling. The sampling date may be the date of chemical release of the element or the end date of air passage through the filter. In the example, the selection date should be the date of the uranium release. Accordingly, the activity of Th-231 on this date will be zero. When air is drawn through the filter, an equilibrium occurs after a while between the rate of accumulation of nuclide on the filter and the rate of its decay. And this ratio is proportional to the half-lives of nuclides. The state of radioactive equilibrium at the sampling date may also be a possible option. In this case, the activity ratio must be pre-calculated using the “**Tools / Nuclide table / Tools / Nuclides equilibrium chain / Construct**” procedure.

These data are necessary for the correct calculation of the processes of accumulation and decay of nuclides in the chain. Pressing the "**Cancel**" key by the operator cancels the decomposition procedure, since correct calculation is impossible without such information.

Double-clicking on the nuclide icon in the decay tree triggers the tree editing procedure. The procedure will prompt the operator to either break the link with the parent nuclide, or to break all links for all nuclides of the tree, if the parent nuclide of the decay tree is selected. Breaking the connection is justified if we are sure that the activity of the parent nuclide is zero or negligible.

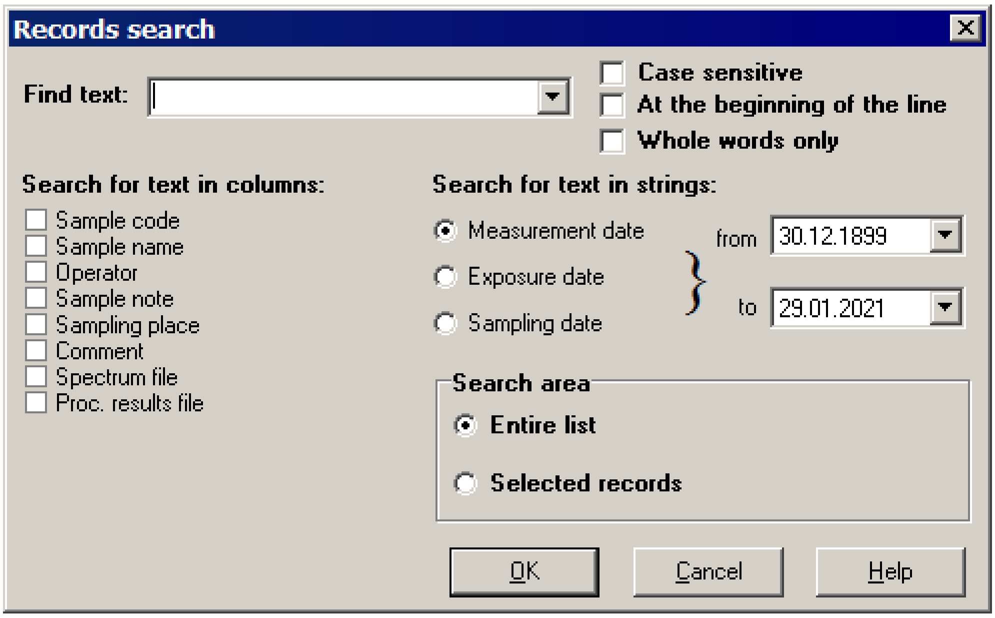
In order not to enter data on the activity ratios in the decay chains each time the decomposition procedure is started, the program will suggest saving the entered data as a priori data. After saving, the operator must specify the saved information in the decomposition template for use as information about the ratio of activities in the decay chains at the date of sampling (see."**Creating decomposition templates / Decomposition parameters**").

The results of the joint processing are saved in the first record of the selected group of records in the measurement log, and this record is marked with Σ. For all other records, the processing results are erased (if they existed) and the processing date for all group records is set to the same.

In any processing mode, all spectra must be obtained by measuring samples on the same spectrometer in the same measurement geometry.

Search for records

The button (menu item "**Edit / Find record...**") calls the procedure for searching and selecting records containing the text specified by the operator in the ticked columns of the archive of measurement results. The search procedure window looks like:



Records search

Find text:

☐ Case sensitive
☐ At the beginning of the line
☐ Whole words only

Search for text in columns:
☐ Sample code
☐ Sample name
☐ Operator
☐ Sample note
☐ Sampling place
☐ Comment
☐ Spectrum file
☐ Proc. results file

Search for text in strings:
● Measurement date
○ Exposure date
○ Sampling date
from 30.12.1899
to 29.01.2021

Search area
● Entire list
○ Selected records

The search is carried out either case-sensitive (uppercase and lowercase letters are considered different), or without taking into account such differences, in accordance with the "**Case sensitive**" mark. The search area for text in a column (at the beginning of a line or across the entire line) is set by the "**At the beginning of the line**" checkbox. The search for whole words or phrases is performed when the "**Whole words only**" checkbox is selected.

Setting the search area by measurement date (item "**Measurement date**") or sampling date (item "**Exposure date**" or "**Sampling date**") is set in the field of the "**Search for text in strings:**". Since the "empty" text is present in all records, searching for records without specifying the text to search for will find all records with the measurement date or selection date falling within the specified interval (at least one column for the search must be specified).

The search area for the list of records is set in the field of the "**Search area**" with the "**Entire list**" or "**Selected records**" radio buttons. Searching the entire list adds additional entries to the already selected entries that meet the search conditions. A search in the selected fragment allows you to find records in already selected records that meet additional conditions.

Statistical processing of measurement results

The ΣΔi button (menu item "**Commands / Statistics...**") calls a procedure that calculates a number of statistical parameters for a group of records of spectrum processing results selected by the operator:

Number of records	n - the number of non-empty cells in the column.
Minimum	The minimum value in the column $X_{\min}$.
Maximum	The maximum value in the column $X_{\max}$.
Arithmetic mean	The arithmetic mean $X_0 = (\sum X_i)/n$ for activity values and calculated parameters Calc 1 - Calc8 and an estimate of the error of the arithmetic mean $\Delta_0 = (\sqrt{\sum \Delta_i^2})/n$ for error values and parameters ErCalc1 - ErCalc8.
Root mean square (RMS)	RMS for error values and calculated parameters ErCalc1 - ErCalc8 $\Delta_S = \sqrt{(\sum \Delta_i^2)/n}$.
Root Mean Square Deviation (RMSD)	RMSD for activity values and calculated parameters Calc 1 - Calc8 $S_x = \sqrt{\sum (X_i - X_0)^2 /(n-1)}$.
Statistical uncertainty	Statistical uncertainty (confidence interval corresponding to 95% confidence probability) for activity values and calculated parameters Calc1 – Calc8 $US_x = t_{95}(n-1) \cdot S_x$.
Total uncertainty	Averaged total uncertainty for activity values. $UT_x = \sqrt{US_x^2 + U_\delta^2}$. Total uncertainty includes statistical uncertainty US_x and the error of the measuring instrument and measurement method $U_\delta = X_0 \cdot \sqrt{\delta_{си}^2 + \delta_{м}^2}$.
Weighted arithmetic mean	Weighted average LSM assessment of activities $X_m = \sum (X_i /\Delta_i^2) / \sum (1/\Delta_i^2)$ and errors $\Delta_m = \sqrt{1/\sum (1/\Delta_i^2)}$.
Bias	$Bias = abs(X_{Norm} - X_0)$ - the deviation of the average estimate from the set value.
Normalized RMSD	RMSD normed per error estimation $S_{norm} = 2 \cdot \sqrt{\sum ((X_i - X_m)^2 / \Delta_i^2) / \chi^2 (n-1)}$ A factor of 2 to account for the fact that as Δ_i a 95% confidence interval is used. The expected value of the

	normalized sum of squared deviations is either the mathematical expectation of the χ^2 distribution, if the normal distribution is selected in the settings, or the median of the χ^2 distribution, if the Student's distributions are selected (the median is considered a more noise-resistant assessment).
Relative accuracy	The ratio of the actual statistical accuracy of the assessment to the declared (calculated by the program): $RAcc = 1/S_{norm}$.
Stat. accuracy surplus (%)	Percentage accuracy surplus $AccSpls = 100 \cdot (RAcc - 1)$.
Coefficient of variation	$K_{\mathrm{var}} = \sqrt{\sum (X_i - X_0)^2 /(n-1)} \,/\, X_0$.
RMSD of mean	$S_{x0} = \sqrt{\sum (X_i - X_0)^2 /(n \cdot (n-1))}$.
Stat. uncertainty of mean	Statistical uncertainty (confidence interval corresponding to 95% confidence probability) of the mean $US_{x0} = t_{95}(n-1) \cdot S_{x0}$.
Total uncertainty of mean	$UT_{x0} = \sqrt{US_{x0}^2 + U_\delta^2}$. Total uncertainty includes statistical uncertainty US_{x0} and the error of the measuring instrument and measurement method U_δ.
Rel. total uncert. of mean	The relative total uncertainty of the mean $\mathrm{Re}\,lUT_{x0} = UT_{x0} / X_0$.
Min. detectable activity	Minimum measurable activity $LOD = k_{lod} \cdot \Delta_S^0 \cdot \sqrt{I_B^0 / I_S^0})/2$.
Coeff. of variability (%)	The coefficient of variability α in the formula of composite Poisson statistics $D_N = N + (\alpha \cdot N)^2$ $\alpha = \sqrt{(S_x)^2 - (I_S^0 \cdot T_m)} /(I_S^0 \cdot T_m)$ is calculated for the column "Intensity in the window (imp./s)" .

X_i - is the value in the column of activities or parameters Calc1 - Calc8.

Δ_i - is the value in the column of errors or parameters ErCalc1 - ErCalc8.

δ_{cu}, $\delta_{м}$ - is relative errors of the measuring instrument and the measuring method.

k_{lod} - is the number of standard deviations used in the calculation of LOD (set in the archive settings).

Δ_S^0 - is the random component of the standard error.

I_B^0 - is the intensity of the background in the energy window used in the processing.

I_S^0 - is the intensity of the sample spectrum in the same energy window.

T_m - is the time of the sample measurement.

$t_{95}(n)$ - is the length of the confidence interval for 95% probability and n degrees of freedom corresponds to the selected statistical distribution (normal or Student distribution).

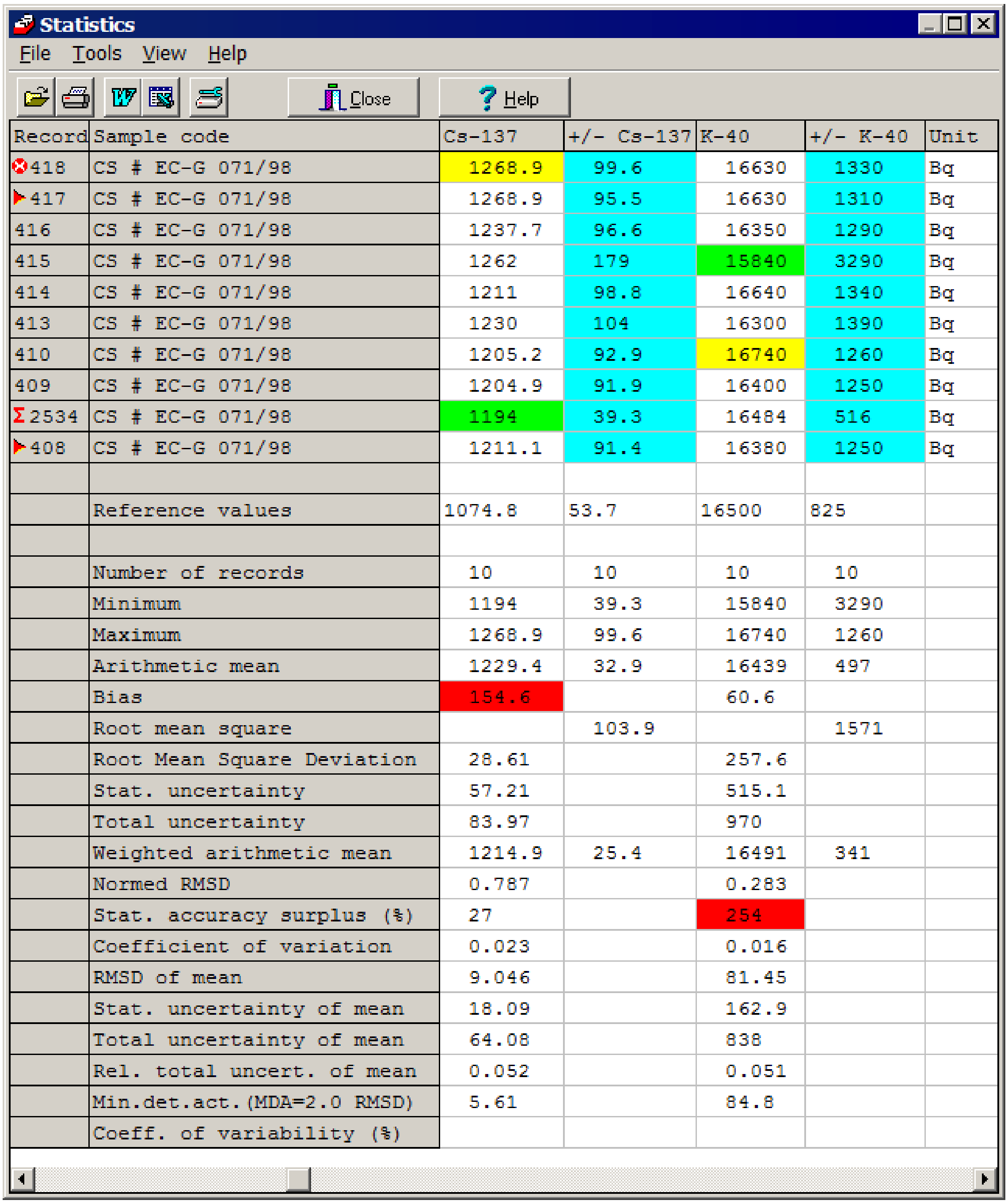
Since the form of presentation of measurement results in the measurement log is configurable (the degree of rounding of measurement results is also configurable), it is recommended to reformulate the measurement log for correct statistical processing, eliminating the requirement of rounding results (see "Configuring the archive").

Statistical parameters can be calculated for two variants of error representation: for the total error and for the random component of the total error. The superscript "^{0}" in the formula for calculating the minimum measured activity indicates that the statistical parameters are calculated for the random component of the error. In this case, the columns of errors and intensities of the registered pulses in the Statistics window will be colored blue, and the intensity columns in this case will contain the intensity of the registered pulses in the energy windows used in calculating the activities. The number and width of windows are determined by the processing procedure, and the values of the left and right energy boundaries only indicate that all windows are within the specified boundaries.

The minimum measured activity is calculated only if the Statistics table contains all the columns necessary for calculation: "**Intens. in the window**", "**Backgr. int. in the win.**", "**General deviation**" and the random error output mode is set.

The normalized standard deviation is calculated for the columns of the "**Spectrometer load**" and "**Intensity in the window**" archive, although there are no error columns for these values. Nevertheless, the calculation is carried out, since the formula for calculating errors for the values of the spectrometer load and the integral intensity in the window is known: $\Delta_x = 2 \cdot \sqrt{X \cdot t + (\alpha \cdot X \cdot t)^2}$. Here X is the value in the column,·t is the measurement time, and α is the coefficient of the linear component for composite Poisson statistics. If the values of loading and intensity in the window relate to the background spectrum $\alpha = K_{var.back} / 100$ ($K_{var.back}$ – the coefficient of background variability is set in the settings of the background control procedure as a percentage). For any other spectrum $\alpha = K_{diff.nonline}$ /100 ($K_{diff.nonline}$- the coefficient of differential nonlinearity of the ADC is set in the settings of the ADC spectrometer). A spectrum is considered a background spectrum if the type of sample registered for the background spectrum is specified for it.

The Statistics program window duplicates the form of the table of records in the archive of results (number and width of columns) and may have the following, for example, form:



Record	Sample code	Cs-137	+/- Cs-137	K-40	+/- K-40	Unit
☒418	CS # EC-G 071/98	1268.9	99.6	16630	1330	Bq
▶417	CS # EC-G 071/98	1268.9	95.5	16630	1310	Bq
416	CS # EC-G 071/98	1237.7	96.6	16350	1290	Bq
415	CS # EC-G 071/98	1262	179	15840	3290	Bq
414	CS # EC-G 071/98	1211	98.8	16640	1340	Bq
413	CS # EC-G 071/98	1230	104	16300	1390	Bq
410	CS # EC-G 071/98	1205.2	92.9	16740	1260	Bq
409	CS # EC-G 071/98	1204.9	91.9	16400	1250	Bq
Σ2534	CS # EC-G 071/98	1194	39.3	16484	516	Bq
▶408	CS # EC-G 071/98	1211.1	91.4	16380	1250	Bq
	Reference values	1074.8	53.7	16500	825	
	Number of records	10	10	10	10	
	Minimum	1194	39.3	15840	3290	
	Maximum	1268.9	99.6	16740	1260	
	Arithmetic mean	1229.4	32.9	16439	497	
	Bias	154.6		60.6		
	Root mean square		103.9		1571	
	Root Mean Square Deviation	28.61		257.6		
	Stat. uncertainty	57.21		515.1		
	Total uncertainty	83.97		970		
	Weighted arithmetic mean	1214.9	25.4	16491	341	
	Normed RMSD	0.787		0.283		
	Stat. accuracy surplus (%)	27		254		
	Coefficient of variation	0.023		0.016		
	RMSD of mean	9.046		81.45		
	Stat. uncertainty of mean	18.09		162.9		
	Total uncertainty of mean	64.08		838		
	Rel. total uncert. of mean	0.052		0.051		
	Min.det.act.(MDA=2.0 RMSD)	5.61		84.8		
	Coeff. of variability (%)					

Cells with a random component of uncertainty are highlighted in blue, cells with statistical parameters that exceed acceptable limits are highlighted in red, a cell with a maximum value in a column is highlighted in yellow, and a cell with a minimum value in a column is highlighted in olive.

The lines included in the list with a warning about the undesirability of their inclusion are highlighted in red characters at the beginning of the line:

Symbol	**Meaning**
☒	The record is marked by the operator for deletion.
Σ	A row with a summary report generated for a group of records. It is impossible to trace correlations.

◀	A record with processing results correlated with processing results in other rows of the sample, since these processing results belong to the same spectrum.
▶	A record with processing results correlated with processing results in other rows of the sample, since common a priori data was used during processing.
N	There is no information about the activities of nuclides in the record.
R	There is no processing results file for recording.
E	Different types of uncertainties (total/statistical) for this record and for the rest of the records in the sample.
U	Different units of measurement for this record and for the rest of the records in the sample.

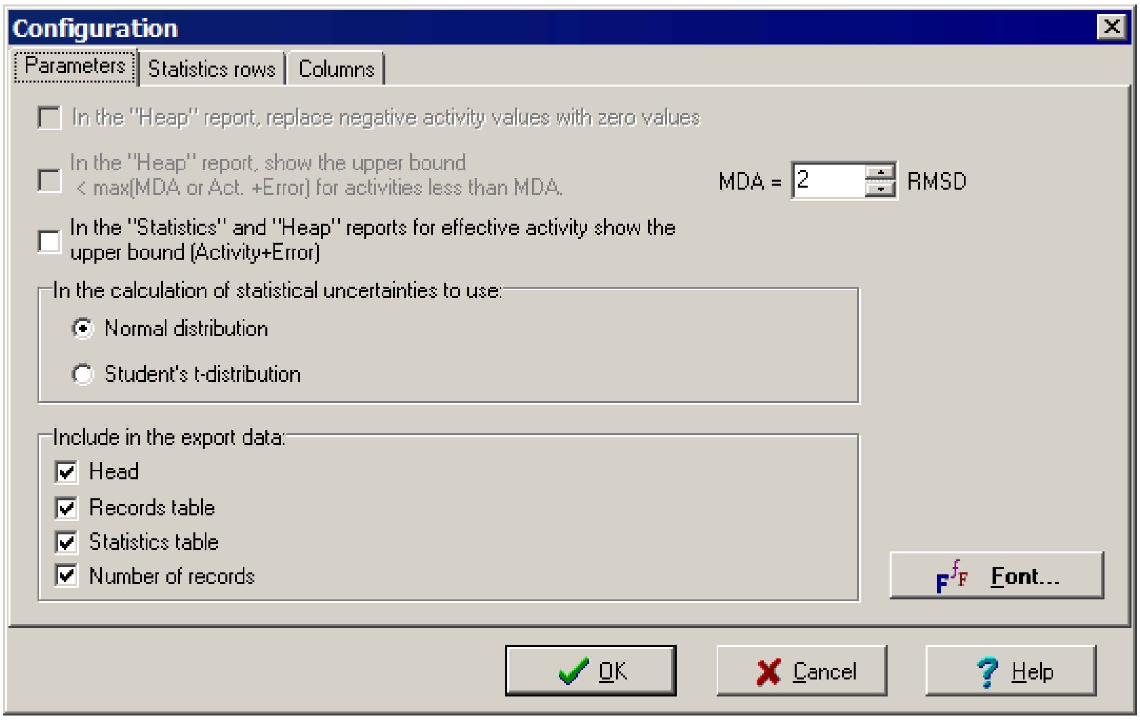
The width of the columns, except for fixed ones (they are highlighted in gray), is also adjustable. The width of fixed columns can be set beforehand in the main archive window, but it is possible to change it directly in the Statistics window. To do this, click on the name of the first column – "**Record #**", while its color will become the same as the rest of the columns, and without moving the mouse pointer outside the column names line, edit their width.

The operator has the ability to edit the values of the comparison data and the processing results in the cells of the table (the values in the archive of the results do not change); the statistical parameters are recalculated accordingly. You can delete an unnecessary row or column by right-clicking on the row or column header.

It should be borne in mind that the estimation of errors of the average or weighted average for a group of measurements cannot generally serve as an estimate of errors in the activity of nuclides (or the values of any parameters calculated from them), since the formulas for calculating statistical parameters do not take into account the correlation of values (the measurement log does not contain complete data on the correlation of values). The correlation of the values occurs due to the presence of non-random values in the error values (systematic error associated, for example, with errors of standards, etc.), the use of identical a priori data in processing. The log may contain several records about the same measurement, but this kind of correlation is monitored and corrected by the procedure at the stage of report generation. If the output mode is set in the archive settings as the error of the random component of the total error, the correlation of values will disappear due to systematic error and the estimation of the random component of the errors of the average or weighted average will be correct, but only if correlated a priori data were not used in the processing of spectra and all measurements are independent.

The total uncertainty of the mean can be used as the error of the mean. At the same time, it should be borne in mind that the complete uncertainty of the average will be correct only when negative activity values are enabled in the parameters of the decomposition template used in spectrum processing (a priori information about the positive certainty of activity estimates makes the estimates correlated).

The button (menu item "**Tools/Configure...**") allow you to configure the parameters for generating and calculating statistical data. At the same time, the form is displayed on the screen:



Configuration

Parameters | Statistics rows | Columns

☐ In the "Heap" report, replace negative activity values with zero values

☐ In the "Heap" report, show the upper bound < max(MDA or Act. +Error) for activities less than MDA. MDA = 2 RMSD

☐ In the "Statistics" and "Heap" reports for effective activity show the upper bound (Activity+Error)

In the calculation of statistical uncertainties to use:
● Normal distribution
○ Student's t-distribution

Include in the export data:
☑ Head
☑ Records table
☑ Statistics table
☑ Number of records

The form contains three pages: "**Parameters**", "**Statistics rows**" and "**Column**s".

On the first page "**Parameters**", the operator can set several checkboxes and values that determine the content, form and values of statistical data:

The value of the minimum detectable (measured) activity (MDA) in units of standard deviations (RMSD) is set in the "**MDA =**" field. This value is used to calculate the minimum measured activity in units of activity. The specified **MDA** value is also used when generating a report for single measurements.

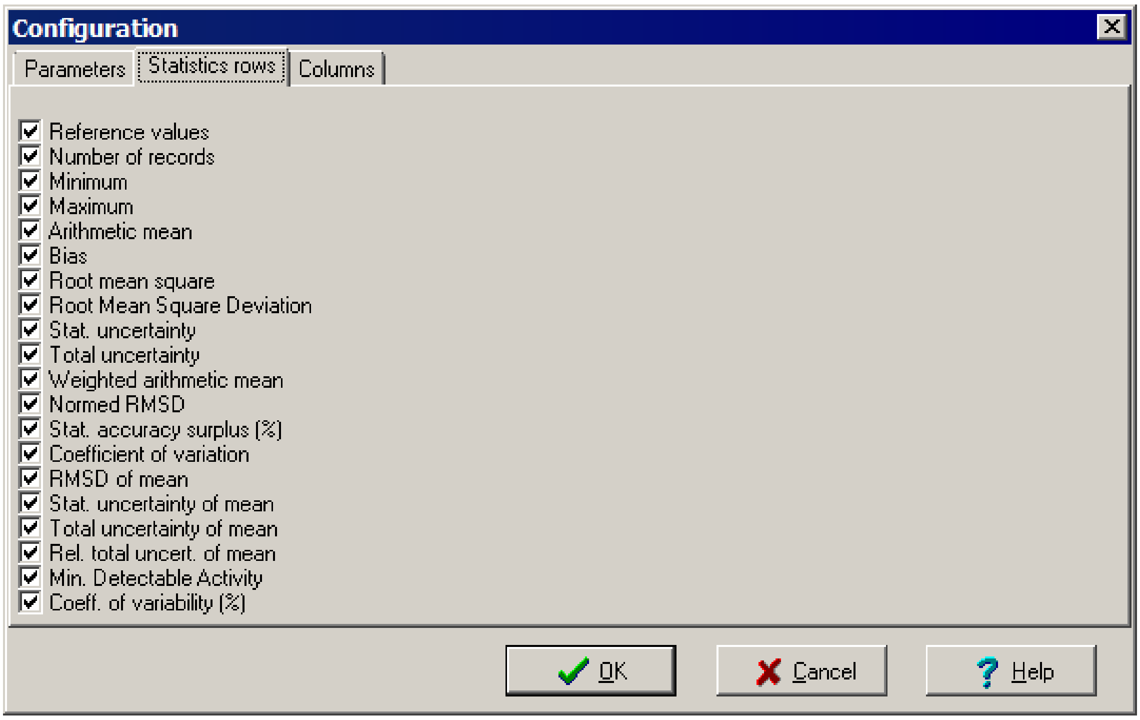
The checkbox "**In the "Statistics" and "Heap" reports for effective activity show the upper bound (Activity + Error)**" defines the mode for displaying the values of effective activity in the "Statistics" and "Heap" windows. When the check box is selected in the column of effective activity values, the upper estimate of the effective activity value is given (A.eff.m=A.eff+$\Delta_{A.eff}$.), the error column does not change.

The choice of the probability density distribution function in the group "**In the calculation of statistical uncertainties to use: Normal distribution, Student's distribution**" determines the calculation of the total and statistical uncertainty of the estimates of the mean. By default, the normal distribution is used.

The group of checkboxes "**Include in the export data**:" defines the content of data transferred to Word or Excel, as well as to print or to an external file.

The Font... button sets the font for the form data.

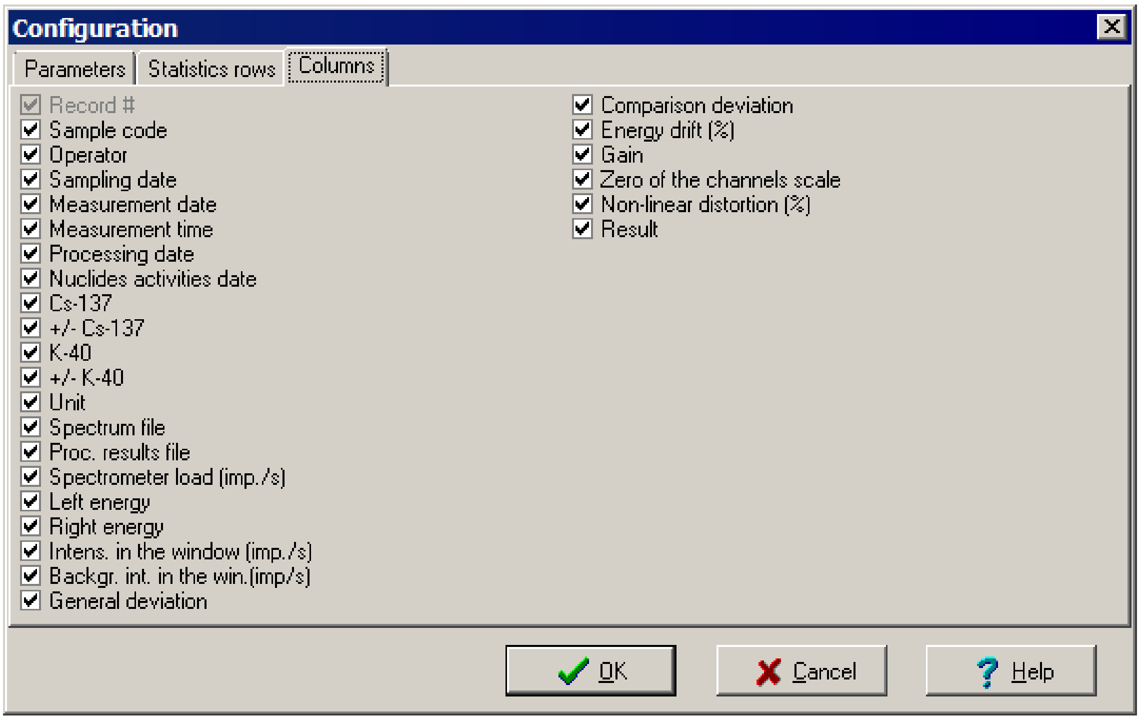
On the second page "**Statistics rows**", the operator can select the rows of calculated statistical parameters of the Statistics table, which will be shown on the form:



☑ Reference values
☑ Number of records
☑ Minimum
☑ Maximum
☑ Arithmetic mean
☑ Bias
☑ Root mean square
☑ Root Mean Square Deviation
☑ Stat. uncertainty
☑ Total uncertainty
☑ Weighted arithmetic mean
☑ Normed RMSD
☑ Stat. accuracy surplus (%)
☑ Coefficient of variation
☑ RMSD of mean
☑ Stat. uncertainty of mean
☑ Total uncertainty of mean
☑ Rel. total uncert. of mean
☑ Min. Detectable Activity
☑ Coeff. of variability (%)

The first line of the list - "**Reference values**" does not belong to the number of calculated statistical parameters, but is used to enter certified parameter values that will be used to calculate the offset of the mean relative to the set value.

The third page "**Columns**" allows you to select the columns of the measurement log, which will be shown in the Statistics table:



☑ Record #
☑ Sample code
☑ Operator
☑ Sampling date
☑ Measurement date
☑ Measurement time
☑ Processing date
☑ Nuclides activities date
☑ Cs-137
☑ +/- Cs-137
☑ K-40
☑ +/- K-40
☑ Unit
☑ Spectrum file
☑ Proc. results file
☑ Spectrometer load (imp./s)
☑ Left energy
☑ Right energy
☑ Intens. in the window (imp./s)
☑ Backgr. int. in the win.(imp/s)
☑ General deviation
☑ Comparison deviation
☑ Energy drift (%)
☑ Gain
☑ Zero of the channels scale
☑ Non-linear distortion (%)
☑ Result

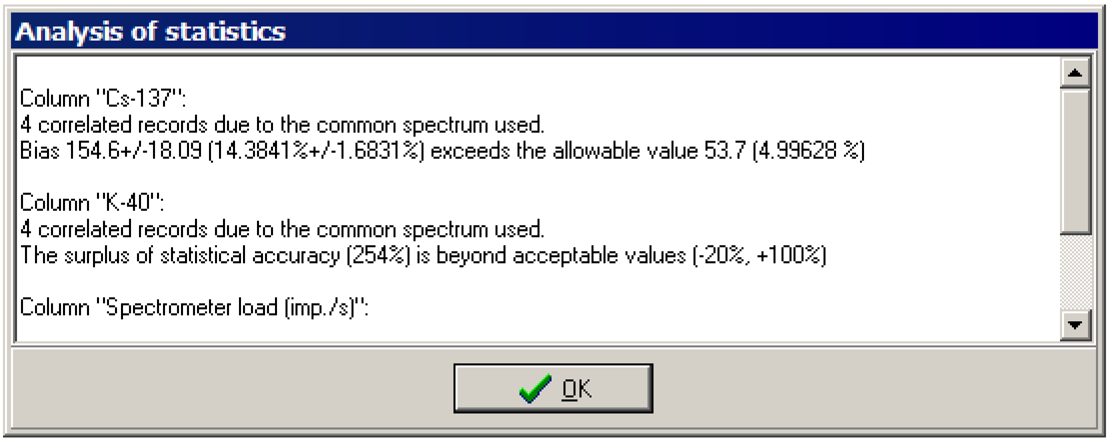
The "button" (menu item "**File / Open...**") allow you to insert form data into a report template (any text in the form of a Microsoft Word document or in RTF format). In this case, the data values replace the set of labels in the report template. If the report template is a Word document, then the report itself is generated as a Word document.

"Button" - print the report (menu item "**File / Print...**").

"Button" (menu item "**File / Export to Word**") - transfer the content to "Microsoft Word".

"Button" (menu item "**File / Export to Excel**") - transfer the content to Microsoft Excel.

The menu item "**Tools / Analysis of statistics...**" calls the procedure for analyzing a number of statistical parameters, and displays the results in the following window:

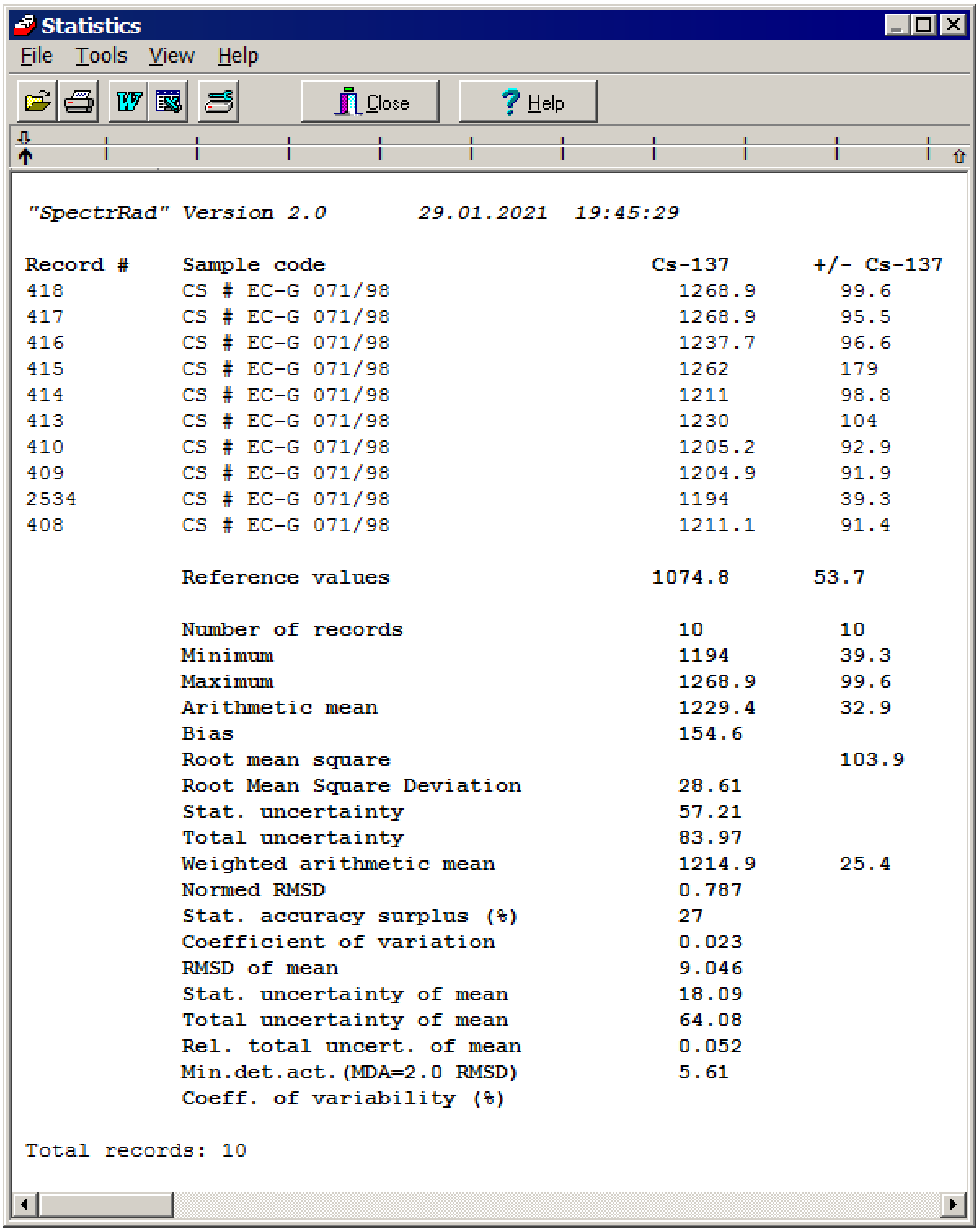


```
Column "Cs-137":
4 correlated records due to the common spectrum used.
Bias 154.6+/-18.09 (14.3841%+/-1.6831%) exceeds the allowable value 53.7 (4.99628 %)

Column "K-40":
4 correlated records due to the common spectrum used.
The surplus of statistical accuracy (254%) is beyond acceptable values (-20%, +100%)

Column "Spectrometer load (imp./s)":
```

The menu item "**View / Text**" allows you to view a table of statistical data in the form of text. The form of statistics in this case may look like this:



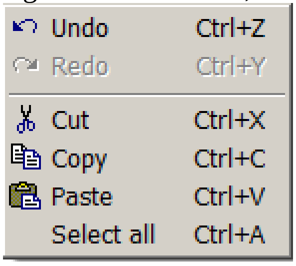
```
"SpectrRad" Version 2.0       29.01.2021  19:45:29

Record #    Sample code                         Cs-137      +/- Cs-137
418         CS # EC-G 071/98                      1268.9      99.6
417         CS # EC-G 071/98                      1268.9      95.5
416         CS # EC-G 071/98                      1237.7      96.6
415         CS # EC-G 071/98                      1262        179
414         CS # EC-G 071/98                      1211        98.8
413         CS # EC-G 071/98                      1230        104
410         CS # EC-G 071/98                      1205.2      92.9
409         CS # EC-G 071/98                      1204.9      91.9
2534        CS # EC-G 071/98                      1194        39.3
408         CS # EC-G 071/98                      1211.1      91.4

            Reference values                    1074.8      53.7

            Number of records                     10          10
            Minimum                               1194        39.3
            Maximum                               1268.9      99.6
            Arithmetic mean                       1229.4      32.9
            Bias                                  154.6
            Root mean square                                  103.9
            Root Mean Square Deviation            28.61
            Stat. uncertainty                     57.21
            Total uncertainty                     83.97
            Weighted arithmetic mean              1214.9      25.4
            Normed RMSD                           0.787
            Stat. accuracy surplus (%)            27
            Coefficient of variation              0.023
            RMSD of mean                          9.046
            Stat. uncertainty of mean             18.09
            Total uncertainty of mean             64.08
            Rel. total uncert. of mean            0.052
            Min.det.act.(MDA=2.0 RMSD)            5.61
            Coeff. of variability (%)

Total records: 10
```

When displaying data in this form, the operator has the opportunity to edit it as text using the pop-up menu: 

and transfer not all the text to Word or Excel, but only the selected fragment.

Generating a report

The formation of any report, including a statistical report and a sample report, in the "SpectrRad" package is based on the fact that in a pre-prepared MSWord document, the report template, part of the text is replaced with a specific text. Such a replaceable text is:

- Certain words enclosed in curly brackets are labels of the report template, for example {**Act[Cs–137]**}. The report template labels are used to insert sample parameters, measurement conditions, and spectrum processing results into the template text
- An arithmetic expression consisting of numbers and labels replaced by numerical values associated with symbols of arithmetic operations and functions in accordance with the syntax and spelling of the built-in programmable calculator, enclosed in operator brackets "~<" and ">~", for example **~<2*({Act[Cs-137]}+{Err[Cs-137]})+100>~**

The report template includes two parts: the general part and the repeatable part (the repeatable part of the template may be missing). The repeatable part of the report template is enclosed in double angle brackets, for example <<**{Report}**>>. Both the common and repeatable parts of the report template can contain arbitrary text, including labels.

The final report is generated as follows:

- All labels of the report template are replaced with data from the first record of the selection.
- The repeated part is copied, and the labels of the repeated part are replaced with data from the second record of the selection.
- The process is repeated until the end of the records in the selection.
- Arithmetic expressions are replaced by calculated values.
- Labels containing spelling errors are removed from the text.

Statistical report labels

A set of labels for a statistical report allows you to insert information into the report that is missing at the statistical report table, but saved in the archive. In this case, the information is taken not from the cells of the table, but directly from the processing results.

Label	***Description***
{Date}	The date the report was created.
{Program}	The version of the program.
{DecTemplate}	The name of the processing template used.
{NuclidesTable}	The table of nuclides used in the processing.
{Analyser}	Name and description of the spectrometer. The text is copied from the description of the spectrometer entered during installation.

{AnalNick}	The short name of the spectrometer.
{Geometry}	Name and description of the measurement geometry. The text is copied from the geometry description entered when installing the geometry.
{GeomNick}	The short name of the measurement geometry.
{Info}	Information about the verification of the spectrometer. The text is copied from the field "Verification certificate" of the description of the spectrometer entered during its installation.
{AddNote}	Additional information about the spectrometer. The text is copied from the "Additional information" field of the description of the spectrometer entered during its installation.
{SampleCode}	The sample code.
{Sample}	The name of the sample.
{Operator}	The data of the operator (laboratory assistant) who carried out the measurements.
{SampleType}	The type of sample and information about the standards associated with this type of sample. Information about the standard is copied from the "Comment" column of the corresponding standard.
{SampleNote}	Description of the sample.
{Producer}	Manufacturer.
{ProductionDate}	Date of production.
{Declarant}	The "**Declarant"** is an organization or individual who has submitted an application for a sample study.
{DeliveryDate}	Delivery date.
{SampleArea}	The place of sampling.
{Comment}	Note.
{Size}	Parameter 1.
{SParam}	Parameter 2.
{RawValue}	The amount of the starting material used in the concentration of the sample.
{ConcMass}	The mass of the concentrate obtained by concentrating the starting material.
{ChemYield}	The yield of the selecting substance (%) during chemical concentration.

{SampleMass}	The mass of the counting sample.
{Weight}	The mass of the counting sample or the amount of the starting material used in the concentration of the sample, depending on how the specific activity values are presented in the processing results.
{ExposeDate}	The date of the beginning of sampling (exposure).
{SampleDate}	The end date of sampling (exposure).
{DecompDate}	Date of spectrum processing.
{MeasDate}	The measurement start date.
{MeasEndDate}	The end date of the measurement.
{ActualDate}	The date on which the values of nuclide activities and radiation intensities are given. The date of the activity value can coincide either with the date of the beginning of measurements or with the date of sampling (SampleDate**)**.
{MeasTime}	The duration of the measurement in seconds.
{Calculator}	The results of the calculator program execution.
{Calc1}, {ErCalc1}... **{Calc8}, {ErCalc8}**	The values of the stored variables of the calculator program.
{Calc&Err1},… **{Calc&Err8}**	The values of the stored variables of the calculator program in the form: Calc±ErCalc (for example 125±15).
{AUnit}	The units of the activity of nuclides.
{Act[Name]} **{Activ[Name]}**	The activity of the nuclide **Name** (for example **{Act[Cs-137]}**). The names of conditional nuclides are reserved for the total activity: **SumAct-A**, **SumAct-B** and **SumAct-G** – total for alpha, beta and gamma radiation..
{SAct[Name]}	The activity of the nuclide. The difference from the **{Activ[]}** label is that in the report, the **{Activ[]}** label can be replaced either by the nuclide activity or by the **Act value+Act error**, depending on the report setting, and the **{Sact[]}** label is always replaced by the nuclide activity.
{StErr[Name]}	The statistical uncertainty of estimating the activity of a given nuclide in units of activity.
{TotErr[Name]}	The total error in estimating the activity of a given nuclide in units of activity. The total error includes statistical uncertainty, the error of the measuring instrument and the measurement method.
{Err[Name]} **{AbsErr[Name]}**	The error (uncertainty) of estimating the activity of a nuclide in units of activity. The error is either complete, statistical, or

	absent, depending on the settings of the report form.
{SErr[Name]}	The error in estimating the activity of a given nuclide in units of activity. The difference from the {Err[]} label is the same as for the {Sact[]} label.
{Act&Err[Name]}	The activity and error of estimating the activity of a nuclide in the form: Act±Err (for example 125±15).
{RelErr[Name]}	The relative error in estimating the nuclide activity as a percentage.
{Mass[Name]}	The mass of the nuclide **Name** (for example {**Mass[Cs-137]**}). For the geometry of the "thin" layer, the mass is given in kilograms, for the geometry of the "thick" layer in relative fractions of the mass of the counting sample.
{MassErr[Name]}	The error in estimating the mass of a given nuclide in units of mass.
{Norm1[Name]}- -{Norm5[Name]}	Five standards for a given nuclide.
{AEff}	The total effective activity of nuclides in the sample is calculated in accordance with the values of the gamma equivalent of nuclide radiation according to Ra-226 set in the table of nuclides used in processing. Either the AEff value itself or the upper threshold (AEff+AeffErr) can be used as AEff, depending on the setting of the report parameters.
{SAEff}	The total effective activity of nuclides in the sample. The AEff value is always used directly as SAEff.
{AEffErr} **{AEffAbsErr}**	The error in estimating AEff in units of activity.
{SAEffErr}	The error in estimating AEff in units of activity. The AEff error value is always used directly as the SAEffErr.
{AEff&Err}	The activity and error of estimating the total effective activity of nuclides in the form: Act±Err (for example 125±15).
{AEffRelErr}	The relative error of the AEff estimate as a percentage.
{InputRate}	The total intensity of the radiation registered by the spectrometer in the imp./c.
{SumIntens}	The total intensity of the recorded radiation from the counting sample and the background in a given energy range in imp./c.
{BgdIntens}	The intensity of background radiation in a given energy range.
{ModelIntens}	The intensity of radiation from the nuclides of the formed model in a given energy range.

{ComptonIntens}	The intensity of the Compton scattering spectrum in a given energy range.
{Residuals}	Decomposition discrepancy.
{GlbResiduals}	The general discrepancy.
{EnergyPar}	The energy range used in the processing and energy drift parameters.
{LEnergy}	The left boundary of the energy range.
{REnergy}	The right boundary of the energy range.
{Drift }	The energy drift of the spectrometer as a percentage.
{ADrift}	The gain drift relative to the initial calibration.
{BDrift}	Zero drift of the energy scale in channels.
{CDrift}	The change in the nonlinear component of the energy drift.
{WDrift}	The resolution drift of the spectrometer as a percentage.
{Line1En}	The energy of the left boundary line used in the energy calibration of the spectrometer.
{Line1Width}	The resolution of the spectrometer (peak width at half height) for line 1 in units of energy.
{Line2En}	The energy of the right boundary line used in the energy calibration of the spectrometer.
{Line2Width}	The resolution of the spectrometer for line 2.
{Result}	The result of a spectrum processing operation (decomposition or calibration of the spectrometer). The "+" sign corresponds to successful processing, the "-" sign to unsuccessful processing.
{NumberOfSamples}	The number of counting samples, the measurement results of which were used to generate the report.
{Spectrum}	The name of the spectrum file in the archive for this entry.
{IsoFile}	The file name of the spectrum processing results in the archive for this record.
{SN}	The sequential number of the record in the selection.
{RN}	The number of the record in the measurement log.
{NumberOfLines}	The number of records in the selection
{Table}	A table of nuclide activities for a single sample record. The activity table includes, in addition to the activities themselves,

	the results of the calculator program and additional information: the intensity of the model, background, discrepancy, energy range, number of samples, warnings about exceeding the specified control parameters.
{Report}	Processing results for a single sample record. The {Report} label is replaced by the full text of the report for the sample, which includes both a table of nuclide activities, and information about the sample, measuring instruments, etc.
{GrossReport}	The report table for the entire sample. The {GrossReport} label is replaced by the report table for the entire selection of records. At the same time, if the number of columns in the statistical report does not exceed 16, the text of the statistical report is converted into a table.
{CmpVal[Par]} **{CmpErr[Par]}**	Comparison data (certified or assigned values): the magnitude and uncertainty for the specified numerical parameter (for example, {CmpVal[Cs-137]} certified activity value Cs-137, {CmpErr[Cs-137]} certified uncertainty value Cs-137). **Par** is the column code of the measurement log (the list of name codes is given below).
{N[Par]}	The number of entries in the column for the specified numeric parameter (for example, {N[Cs-137]} for Cs-137 activity values). **Par** is the column code of the measurement log.
{Xmin[Par]}	The minimum value of the parameter.
{Xmax[Par]}	The maximum value of the parameter.
{Gmin[Par]}	The uncertainty value for the minimum parameter value.
{Gmax[Par]}	The uncertainty value for the maximum value of the parameter.
{X0[Par]}	The arithmetic mean for activity values and calculated parameters Calc 1 - Calc8 $X_0 = (\sum X_i)/n$.
{G0[Par]}	Error of the arithmetic mean for error values and parameters ErCalc1 - ErCalc8 $\Delta_0 = (\sqrt{\sum \Delta_i^2})/n$.
{GS[Par]}	Root Mean Square (RMS) for error values and calculated parameters ErCalc1 - ErCalc8 $\Delta_S = \sqrt{(\sum \Delta_i^2)/n}$.
{Sx[Par]}	Root Mean Square Deviation (RMSD) for activity values and calculated parameters Calc 1 - Calc8 $S_x = \sqrt{\sum (X_i - X_0)^2/(n-1)}$.
{USx[Par]}	Statistical uncertainty (confidence interval corresponding to 95% confidence probability) for activity values and calculated parameters Calc1 – Calc8 $US_x = t_{95}(n-1) \cdot S_x$.

{UTx[Par]}	Averaged total uncertainty for activity values. $UT_x = \sqrt{US_x^2 + U_\delta^2}$. Total uncertainty includes statistical uncertainty US_x and the error of the measuring instrument and measurement method $U_\delta = X_0 \cdot \sqrt{\delta_{си}^2 + \delta_{м}^2}$.
{Xm[Par]}	Weighted average LSM assessment of activities $X_m = \sum(X_i/\Delta_i^2)/\sum(1/\Delta_i^2)$.
{Gm[Par]}	Weighted average LSM assessment of errors $G_m = \sqrt{1/\sum(1/\Delta_i^2)}$.
{Snorm[Par]}	RMSD normed per error estimation $S_{norm} = 2 \cdot \sqrt{\sum((X_i - X_m)^2/\Delta_i^2)/(n-1)}$ A factor of 2 to account for the fact that as Δ_i a 95% confidence interval is used.
{Bias[Par]}	The offset of the mean value from the comparison data {CmpVal[Par]} in the dimension of the parameter Par
{BiasPercent[Par]}	The offset of the average value from the comparison data as a percentage.
{RAccuracy[Par]}	Relative accuracy $RAcc = 1/S_{norm}$.
{AccurSurplus[Par]}	Percentage accuracy surplus $AccSpls = 100 \cdot (RAcc - 1)$.
{Kvar[Par]}	Coefficient of variation $K_{var} = \sqrt{\sum(X_i - X_0)^2/(n-1)}/X_0$.
{Sx0[Par]}	RMSD of mean $S_{x0} = \sqrt{\sum(X_i - X_0)^2/(n \cdot (n-1))}$.
{USx0[Par]}	Statistical uncertainty (confidence interval corresponding to 95% confidence probability) of the mean$US_{x0} = t_{95}(n-1) \cdot S_{x0}$.
{UTx0[Par]}	Total uncertainty of mean $UT_{x0} = \sqrt{US_{x0}^2 + U_\delta^2}$. Total uncertainty includes statistical uncertainty US_{x0} and the error of the measuring instrument and measurement method U_δ .
{RelUTx0[Par]}	The relative total uncertainty of the mean $\mathrm{Re}lUT_{x0} = UT_{x0}/X_0$.

{RelUSx0[Par]}	The relative statistical uncertainty of the mean $\mathrm{Re}lUS_{x0} = US_{x0} / X_0$.
{LOD[Par]}	Minimum measurable activity $LOD = k_{lod} \cdot \Delta_S^0 \cdot \sqrt{I_B^0 / I_S^0})/(2 \cdot Rs)$.
{KDx[Par]}	The coefficient of variability α in the formula of composite Poisson statistics $D_N = N + (\alpha \cdot N)^2$ is calculated for the column "Intensity in the window (imp./s)" $\alpha = \sqrt{(S_x)^2 - (I_S^0 \cdot T_m)} / (I_S^0 \cdot T_m)$.
{Warnings}	The text of the messages generated by the statistics analysis procedure when the specified permissible levels of statistical parameters are exceeded.

The text associated with the corresponding label replaces the label text when generating the report, inheriting the style and font of the label text. Since the names of fields ("Spectrometer", "Geometry", "Sample code", etc.) in the "SpectrRad" software package can change, for labels, from the **{Analyser}** label to the **{MeasTime}** label, there are additional labels of the form **{lbxxxx}**, which are replaced by the current name of the corresponding field. For example: the label **{lbAnalyser}** will be replaced with the text "Spectrometer" or "Analyzer", and the label **{lbSize}** with the text "Sample size", "Well depth" or "Number of adsorbers", depending on the settings of the measurement archive. The case in the label name does not matter – the **{Analyser}** label and the **{analyser}** label are identical labels.

Column codes

The names of the columns of the measurement log are set when setting up the archive and can be changed. At the same time, each column, with the exception of the nuclide columns, is assigned an internal immutable name – the column code. The column code is used in the formation of statistical report labels: **{KDx[Par]}**, **{LOD[Par]}**, etc., where **Par** is the column code (case does not matter). The labels of the statistical report are meaningful only for the numeric columns of the measurement log. Column codes for nuclides coincide with the designation of nuclides adopted in the "SpectrRad" package - the accepted abbreviation of a chemical element followed by a dash by the atomic weight of the isotope and the letter of the isomer, for example: **Cs-137, Ba-137m**, etc.

Column name	**Column code**	**Column type**
Sample code	SampleCode	Text
Sample name	Sample	Text
Spectrometer	Analyser	Text
Geometry	Geometry	Text
Operator	Operator	Text
Sample type	SampleType	Text
Sample note	SampleNote	Text
Producer	Producer	Text

Applicant	Declarant	Text
Sampling place	SampleArea	Text
Comment	Comment	Text
Parameter 1	Size	Number
Parameter 2	SParam	Number
Production date	ProductionDate	Date
Delivery date	DeliveryDate	Date
Exposure date	ExposeDate	Date
Sampling date	SampleDate	Date
Measurement date	MeasDate	Date
Measurement time	MeasTime	Number
Processing date	DecompDate	Date
Sample amount	Weight	Number
Nuclides activities date	ActualDate	Date
Effective activity	AEff	Number
+/- Effective activity	AEffErr	Number
Unit	AUnit	Text
Calc1	Calc1	Number
ErCalc1	ErCalc1	Number
Calc2	Calc2	Number
ErCalc2	ErCalc2	Number
Calc3	Calc3	Number
ErCalc3	ErCalc3	Number
Calc4	Calc4	Number
ErCalc4	ErCalc4	Number
Calc5	Calc5	Number
ErCalc5	ErCalc5	Number
Calc6	Calc6	Number
ErCalc6	ErCalc6	Number
Calc7	Calc7	Number
ErCalc7	ErCalc7	Number
Calc8	Calc8	Number
ErCalc8	ErCalc8	Number
Spectrum file	Spectrum	Text
Proc. results file	IsoFile	Text
Spectrometer load (imp./s)	InputRate	Number
Left energy	LEnergy	Number

Right energy	REnergy	Number
Intens. in the window (imp./s)	SumIntens	Number
Compton int. in the win. (imp./s)	ComptonIntens	Number
Compton int. in the win. (imp./s)	BgdIntens	Number
General deviation	GlbResiduals	Number
Comparison deviation	Residuals	Number
Energy drift (%)	Drift	Number
Gain	ADrift	Number
Zero of channels scale	BDrift	Number
Non-linear distortion (%)	CDrift	Number
Resolution drift (%)	WDrift	Number
Line 1 (keV)	Line1En	Number
Line 1 resolution (keV)	Line1Width	Number
Line 2 (keV)	Line2En	Number
Line 2 resolution (keV)	Line2Width	Number
Result	Result	Text

The codes of nuclides and calculated parameters **Calc1-Calc 8** define two values: the magnitude and the error (uncertainty) of the magnitude. What exactly will be used as the **Par** value in the calculated statistical parameter is determined by the calculated statistical parameter:

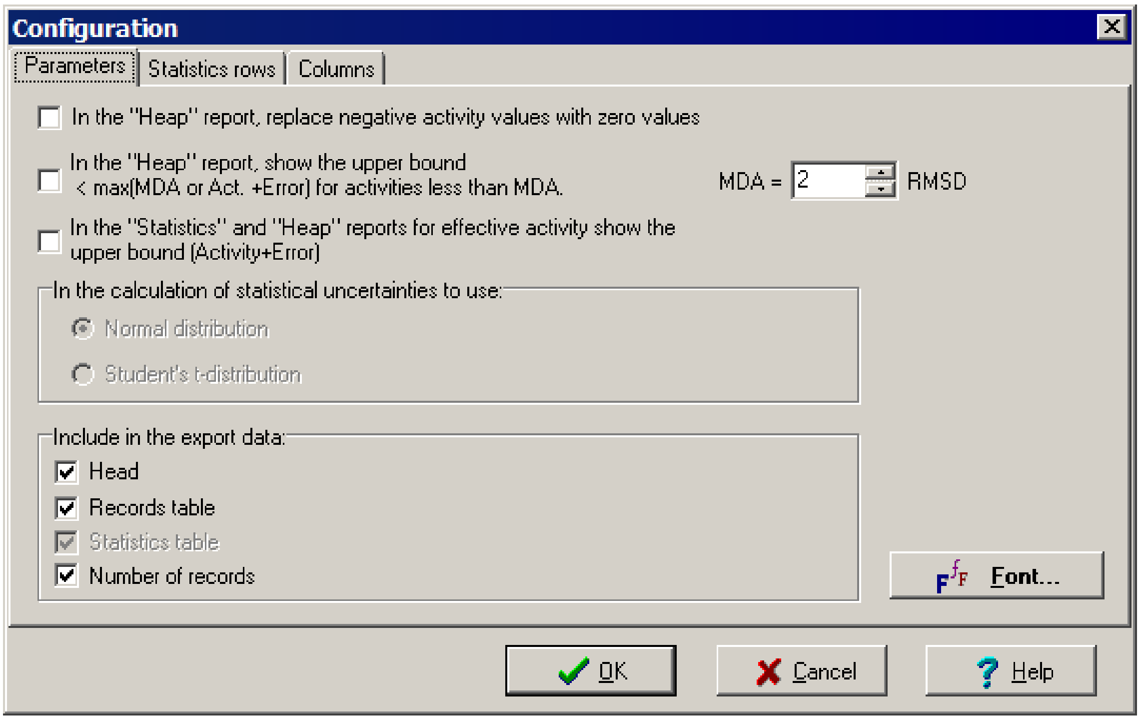
- **{N[Par]}, {Xmin[Par]}, {Xmax[Par]}, {X0[Par]}, {Sx[Par]}, {USx[Par]}, {UTx[Par]}, {Kvar[Par]}, {Sx0[Par]}, {USx0[Par]}, {UTx0[Par]}, {RelUTx0[Par]}, {RelUSx0[Par]}, {KDx[Par]} –** the value of the parameter is used;
- **{Gmin[Par]}, {Gmax[Par]}, {G0[Par]}, {GS[Par]}, {Gm[Par]}** – the parameter error is used;
- **{Xm[Par]}, {Snorm[Par]}** и **{LOD[Par]} –** both parameter values are used.

Heap

The button (menu item "**Commands / Heap...**") calls a program that generates a table for a group of records selected by the operator for the results of spectrum processing.

The window of the "Selection" program is identical to the "Statistics" window, except that there are no rows of statistical parameters and the data in the columns of activities and errors can be given in the usual form or in the form of an upper bound of values (<Act.+Border) depending on the setting of the archive parameters.

The button allows you to configure the parameters for generating data by sample. At the same time, the "**Configuration**" form is displayed on the screen:



Configuration

Parameters | Statistics rows | Columns

☐ In the "Heap" report, replace negative activity values with zero values

☐ In the "Heap" report, show the upper bound < max(MDA or Act. +Error) for activities less than MDA.

MDA = 2 RMSD

☐ In the "Statistics" and "Heap" reports for effective activity show the upper bound (Activity+Error)

In the calculation of statistical uncertainties to use:

● Normal distribution

○ Student's t-distribution

Include in the export data:

☑ Head

☑ Records table

☑ Statistics table

☑ Number of records

The form contains three pages: "**Parameters**", "**Statistics rows**" and "**Column**s".

On the first page "**Parameters"**, the operator can set several checkboxes and values that determine the content, form and values of statistical data:

The value of the minimum detectable (measured) activity (MDA) in units of standard deviations (RMSD) is set in the "**MDA =**" field. This value is used to calculate the minimum measured activity in units of activity. The specified **MDA** value is also used when generating a report for single measurements.

The checkbox "**In the "Heap" report, replace negative activity with zero values**" allows you to generate reports on a group of measurements that do not contain negative values.

The checkbox "**In the "Heap" report, show the upper bound < max(MDA or Act.+Error) for activities less than MDA**" is the mode for displaying results in the "**Heap**" report. When the check box is selected, if the value of the activity or calculated parameter is less than the minimum detectable (MDA) error is not displayed, and the column of activity (calculated parameter) indicates a value equal to the maximum of the MDA or the sum of activity (parameter value) and error with the preceding sign "less" (<). The set value of **MDA** in units of standard deviations (**RMSD**) is also used when generating a report for single measurements.

The checkbox "**In the "Statistics" and "Heap" reports for effective activity show the upper bound (Activity + Error)**" defines the mode for displaying the values of effective activity in the "Statistics" and "Heap" windows. When the check box is selected in the column of effective activity values, the upper estimate of the effective activity value is given (A.eff.m=A.eff+$\Delta_{A.eff}$.), the error column does not change.

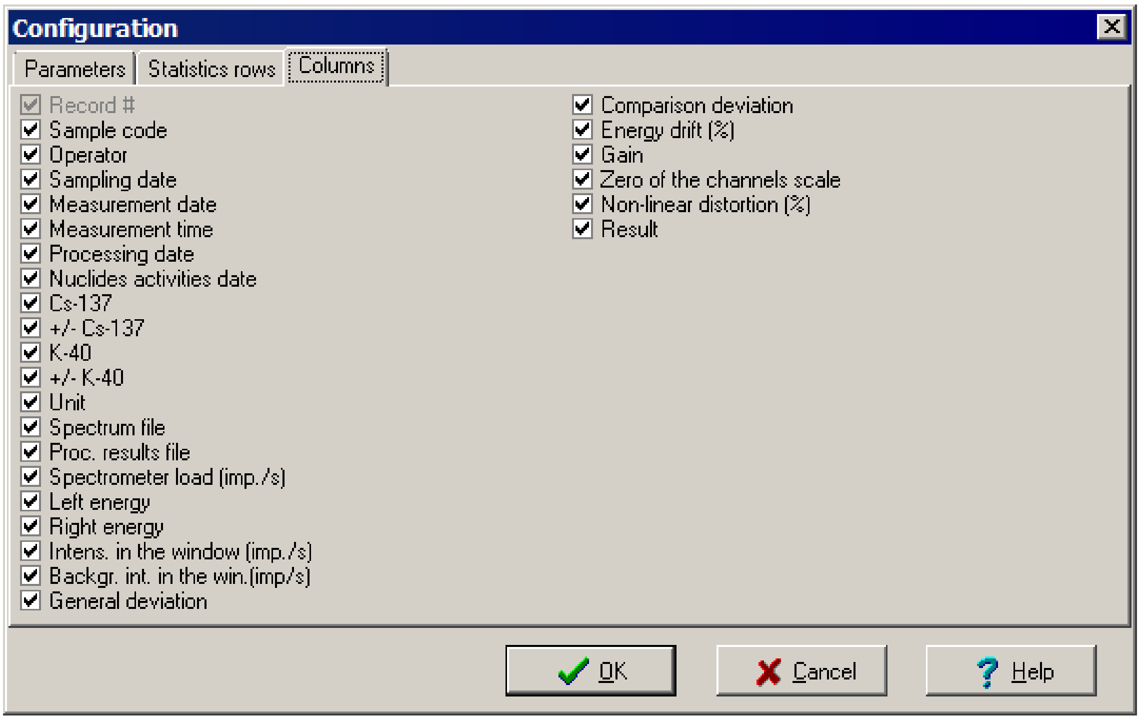
The choice of the probability density distribution function in the group "**In the calculation of statistical uncertainties to use: Normal distribution, Student's distribution**" determines the calculation of the total and statistical uncertainty of the estimates of the mean. By default, the normal distribution is used.

The group of checkboxes "**Include in the export data**:" defines the content of data transferred to Word or Excel, as well as to print or to an external file.

The Font... button sets the font for the form data.

The second page "**Statistics rows**" is not available for "Heap" procedure.

The third page "**Columns**" allows you to select the columns of the measurement log, which will be shown in the "Heap" table:



☑ Record #
☑ Sample code
☑ Operator
☑ Sampling date
☑ Measurement date
☑ Measurement time
☑ Processing date
☑ Nuclides activities date
☑ Cs-137
☑ +/- Cs-137
☑ K-40
☑ +/- K-40
☑ Unit
☑ Spectrum file
☑ Proc. results file
☑ Spectrometer load (imp./s)
☑ Left energy
☑ Right energy
☑ Intens. in the window (imp./s)
☑ Backgr. int. in the win.(imp/s)
☑ General deviation
☑ Comparison deviation
☑ Energy drift (%)
☑ Gain
☑ Zero of the channels scale
☑ Non-linear distortion (%)
☑ Result

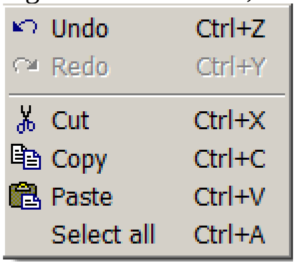
The "button" (menu item "**File / Open...**") allows you to insert form data into a report template (any text in the form of a Microsoft Word document or in RTF format). In this case, the data values replace the set of labels in the report template. If the report template is a Word document, then the report itself is generated as a Word document.

"Button" - print the report (menu item "**File / Print...**").

"Button" (menu item "**File / Export to Word**") - transfer the content to "Microsoft Word".

"Button" (menu item "**File / Export to Excel**") - transfer the content to Microsoft Excel.

The menu item "**View / Text**" allows you to view a table in the form of text. When displaying data in this form, the operator has the opportunity to edit it as text using the pop-up menu: and transfer not all the text to Word or Excel, but only the selected fragment.



The set of labels in the "**Heap**" report template is identical to the set of labels in the statistical report, except that the set of labels for the "**Heap**" does not contain labels for inserting statistical processing results. A number of labels for statistical report templates make sense only in "**Heap**" reports. For example, the label <<**{Report}**>> will generate a Word document that includes all reports on the selected records.

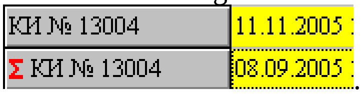
Combined report

The Σ button (menu item "**Commands / Summary report**") calls a procedure that generates a combined report for a group of records selected by the operator for the results of spectrum processing. Such a report, as a rule, can be generated only for the results of processing the same specimen – the procedure checks the identity of the sample in one, two or three columns of the measurement log: "**Sample code**", "**Sample name**" and "**Sample type**" for all selected records and excludes records with the name, code and the type of sample that differs from the name, code, and type of sample for the first record. The "**Sample type**" column is always involved in the comparison. The first two columns of the log "**Sample code**" and "**Sample name**" participate in the comparison if they are present (visualized) in the measurement log. If both "**Sample code**" and "**Sample name**" columns are excluded from the list of visualized columns, a summary report can be generated for different specimens. At the same time, the report can include measurements performed on different spectrometers and in different geometries.

The sample data (sample description, sampling location, etc.) that will be included in the summary report are taken from the first record of the sample. The measurement time is summed up.

The activity of nuclides is recalculated by the mass, date and time of measurement of the spectrum of the first sample record by the measurement date. The measurement time is summed up. The activity of identical nuclides in the sample is averaged with weights corresponding to their covariance matrix (errors and correlations of values are taken into account). The errors for the averaged activity values are also calculated taking into account the full covariance matrix (the correlation of values due to the systematic error of the spectrometer and the use of correlated a priori data is taken into account). Data on the values and their errors in the formation of the summary report are taken not from the measurement log, but from the results of spectrum processing, which contain information about the correlation of the values, therefore all data are calculated correctly.

When saving the summary report in the measurement archive, the record in the measurement log is marked with an Σ in the first position of the record:



КИ № 13004	11.11.2005
Σ КИ № 13004	08.09.2005

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Creation of charts, control charts of Shewhart

A visual representation of the dependence of the spectrometer parameters (resolution, gain, background intensity, etc.) on the operating time of the spectrometer is very useful when analyzing the state of the spectrometer, checking the spectrometer. Graphs of the correlation of nuclide activity (for example, the correlation of Sr-90 content with Cs-137 content) are useful in the analysis of radioactive contamination.

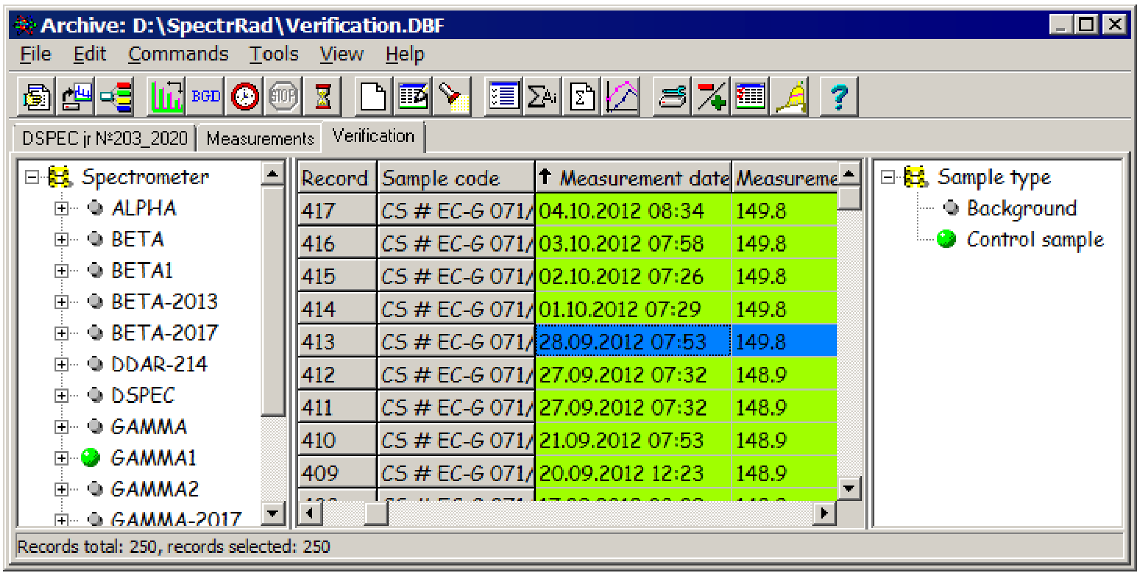
In the 30s of the last century, the American scientist Walter Shewhart, who was engaged in improving the quality of industrial products, proposed using graphs of changes in the parameters of a process or product parameters supplemented with lines of specified control levels to make decisions about process management. The graph is much more informative than the table, since it correctly displays the time axis and allows you to predict the development of the process. Such graphs have since been called Shewhart control charts.

The parameters of a process or product are the results of measurements, and therefore random variables. Therefore, in addition to the graph of the values of a single measurement, we may also be interested in the characteristics of a random variable (mean, span, standard deviation, margin of accuracy, offset) and their dependence on time or other parameters. Accordingly, control charts come in several types:

- The *X*-graph is the dependence of the value of a single measurement on a parameter.

- $\overline{X}$ is a graph of the dependence of the sample mean value on the parameter. $\overline{X} = (\sum_{i=1}^{n} x_i)/n$, n is the sample size.
- R is a graph of the sample range. $R=Xmax-Xmin$.
- s is a graph of the standard deviation. $s = \sqrt{((\sum_{i=1}^{n} (x_i - \overline{X})^2 /(n-1)}$ [12], n is the sample size.
- *AccSps* is the percentage surplus of accuracy for the random component of uncertainty. $AccSpls = 100 \cdot (1/S_{norm} - 1)$, $S_{norm} = 2 \cdot \sqrt{\sum((X_i - \overline{X})^2/\Delta_i^2)/\chi_{50}^2(n-1)}$, Δ_i is the "passport" (calculated by the spectrum processing procedure) value of the random component of uncertainty X_i , $\chi_{50}^2(n-1)$ is the median χ^2 distribution.
- *Bias* is the percentage offset for the systematic error. $Bias = 100 \cdot (X_{real} - \overline{X})/X_{real}$, X_{real} is the passport value of the measured value.

To create a graph, the operator must first enable visualization of the required columns of the measurement log (see "Configuring the archive"), if these columns are not in the log, and select the desired group of records. For example:



Record	Sample code	Measurement date	Measureme
417	CS # EC-G 071/	04.10.2012 08:34	149.8
416	CS # EC-G 071/	03.10.2012 07:58	149.8
415	CS # EC-G 071/	02.10.2012 07:26	149.8
414	CS # EC-G 071/	01.10.2012 07:29	149.8
413	CS # EC-G 071/	28.09.2012 07:53	149.8
412	CS # EC-G 071/	27.09.2012 07:32	148.9
411	CS # EC-G 071/	27.09.2012 07:32	148.9
410	CS # EC-G 071/	21.09.2012 07:53	148.9
409	CS # EC-G 071/	20.09.2012 12:23	148.9

Records total: 250, records selected: 250

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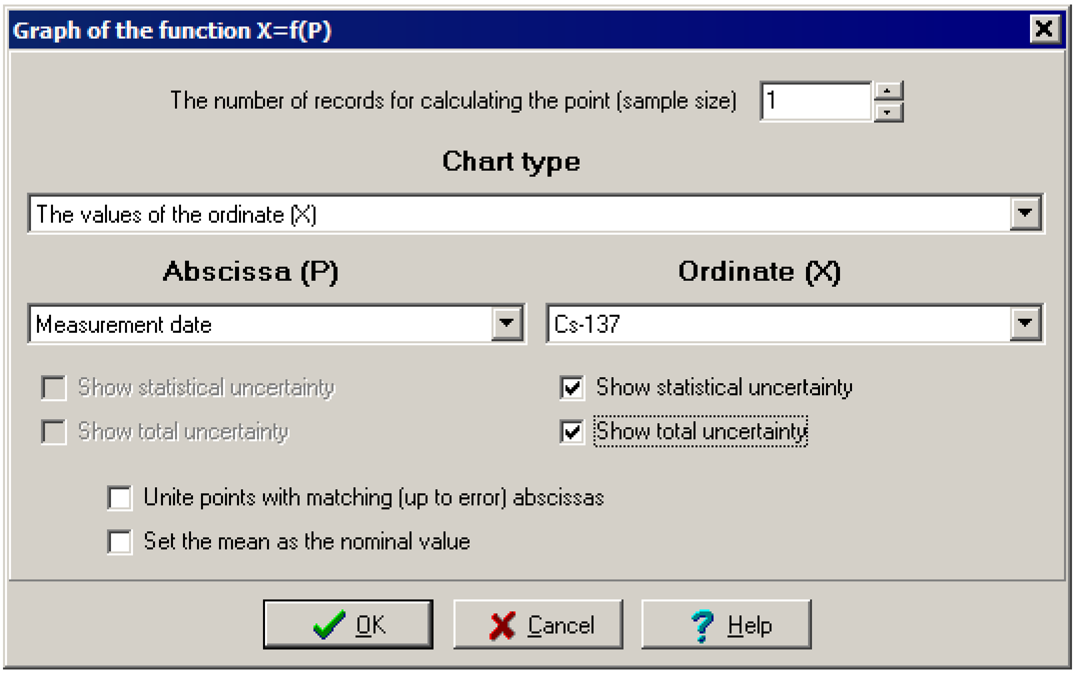
[12] Walter Shewhart worked as a quality engineer at a Bell Telephone company , which produced a large number of similar products. A large number of parts were produced per day. Therefore, a random sample of a certain number of parts was made daily from the manufactured parts, and the average size and size range were calculated from this sample. These data were used to construct two graphs: $\overline{x}$ - the average and R- the range of the spreads. The specimen number in this case was an adequate representation of the time axis. In our case, it is impossible to use measurements of working samples to build a control chart or graph – they are all different. It is possible and necessary to use the measurement results of the reference sample. There may be less than one such measurement per day. In this case, a map of one–time parameter values will be more informative and the time axis cannot be replaced with the specimen number - this will be a complete profanity of displaying the process in time.

Then, by clicking on the button (menu item "**Commands / Graph...**"), call the graph creation procedure. At the same time, a form will appear on the screen:



Graph of the function X=f(P)

The number of records for calculating the point (sample size) 1

Chart type

The values of the ordinate (X)

Abscissa (P)

Measurement date

☐ Show statistical uncertainty

☐ Show total uncertainty

Ordinate (X)

Cs-137

☑ Show statistical uncertainty

☑ Show total uncertainty

☐ Unite points with matching (up to error) abscissas

☐ Set the mean as the nominal value

In statistics, it is customary to designate a random variable with the Latin letter X, therefore the form is called "**Graph of the function X=f(P)**".

If you want to plot the characteristics of a random variable (**Xmean -** mean, **R** – range, **s** – standard deviation, **AccSpls** – surplus of accuracy, **Bias** – offset) or a combined graph - **Xmean±ErX**, you must specify the number of records for calculating the point (**sample size**). To plot the characteristics of a random variable, at least two points are required for the span graph or three points for the remaining parameters. If the sample size is equal to one point, an **X** graph will be constructed – the dependence of the unit values of **X** on **P**. If the sample size is set to be greater than one, all selected log entries are divided into samples according to the specified number of records. And the calculation of the graph points is based on these samples. For the **Xmean**, **R** graphs, the uncertainties calculated from the estimates of the uncertainties of single measurements are given as uncertainties. For all other graphs, the random component of uncertainty is calculated from the standard deviations calculated from the samples and recalculated by the 95% confidence interval. $ErX_{par} = s * t_{95}(n-1)$. *t95(n-1)* is the 95% confidence interval of the Student's distribution for the *n-1* number of degrees of freedom (*n* is the sample size). If the "**Show total uncertainty**" checkbox is not checked, the value of the additional systematic error is set to zero.

Then select the **chart type** from the drop-down list and select from the drop-down lists the **columns of the measurement log** for the **abscissa axis (P)** and the **ordinate axis (X)** of the calculated function **X=f(P)**. In the event that the columns "**Intensity in the window (imp/s)**", "**Compton int. in the win (imp/s)**" or "**Background int. in the win. (imp/s)**" are used as the abscissa or ordinate axis, it must be borne in mind that the values in the columns depend not only on the established energy boundaries, but in the output mode of the random component of the error, and on the processing procedure.

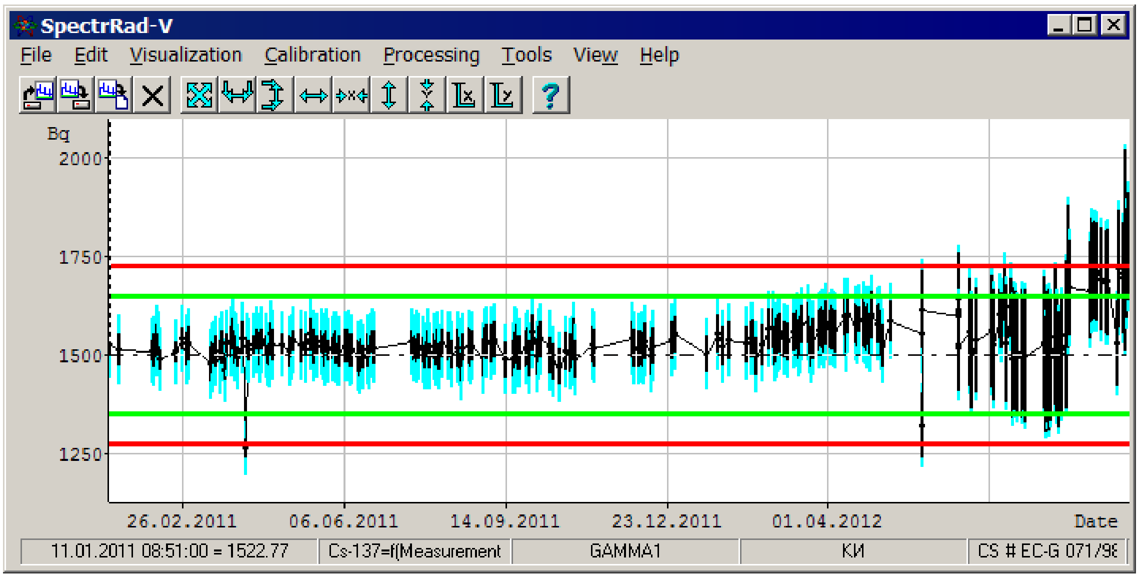
If the abscissas or ordinates of the points contain uncertainty values, the plotting procedure will calculate the uncertainty of the output value and include it in the resulting table when the operator sets the "ticks" in the "**Show statistical uncertainty**" and "**Show total uncertainty**" points.

When you check the "**Unite point with matching (up to the errors) abscissas**" box, the procedure for forming a graph for points with closely spaced abscissas (Pi+ΔPi <= Pj–ΔPj) will form a point with averaged coordinates.

Setting the "tick" in the "**Set the mean as the nominal value**" item allows you to set the mean for all sample values as the nominal value line of the Shewhart chart.

After pressing the "**OK**" key, the program generates a function table, saves it in the "SPECTRA" folder in a file with a unique name including the creation date and visualizes it in the "SPECTRRAD-V" program window.

In the event that an **X** or **Xmean** graph was formed and the measurement date was used as the abscissa, and the nuclide activity was used as the ordinate, the graph formation procedure complements the graph with control levels lines. The nominal level will be the specified nuclide activity, if it is specified. If the nuclide activity is not set or the "**Set the mean as the nominal value**" checkbox is selected, the nominal value will be the mean value for all records. The warning levels will be lines of deviation from the nominal value for the uncertainty of activity. If the uncertainty is not specified by the operator, the averaged uncertainty is used. Warning levels increased 1.5 times (99% confidence interval) is used as action levels. As a result, the graph may look like this:

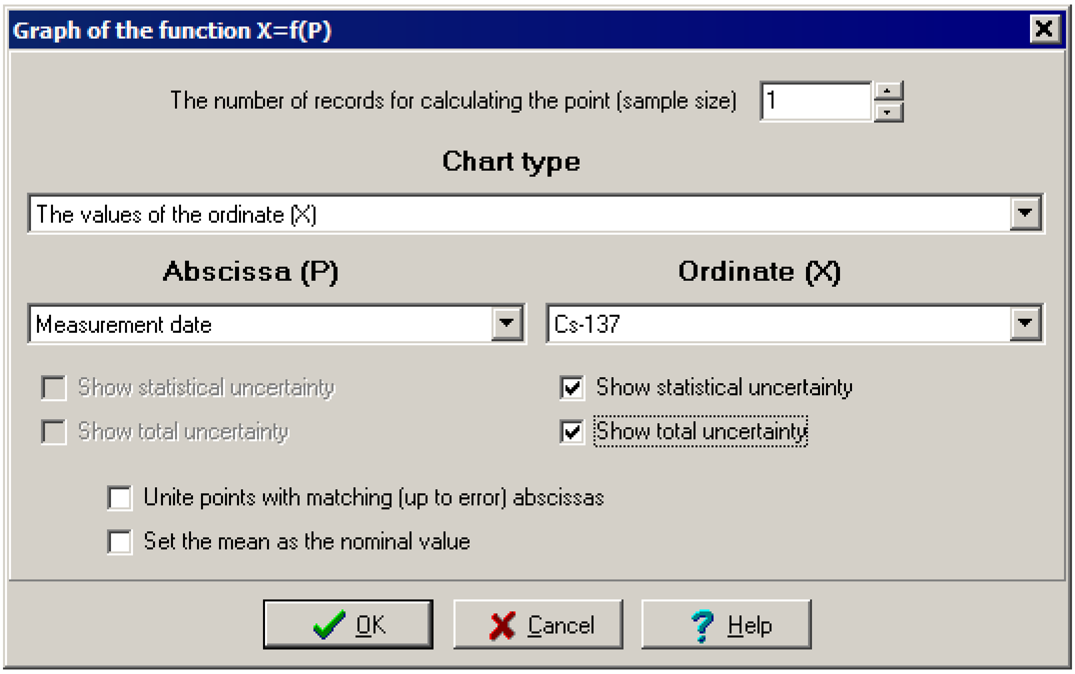


11.01.2011 08:51:00 = 1522.77 | Cs-137=f(Measurement | GAMMA1 | KИ | CS # EC-G 071/9€

The SPECTRRAD package stores in the measurement (verification) log, in addition to estimates of the nuclide activities of the control source (which is recommended to be measured daily), eleven more service parameters indicating the state of the spectrometer (gain drift, zero scale drift, resolution drift, nonlinear distortion, intensity of recorded pulses from the background and the control source, etc.). It is available, if desired, to build Shewhart charts for all these parameters. It is recommended to build Shewhart charts for the values of the activities of the control sources (including the control background sample) used in the daily verification of the spectrometer and for the spectrum decomposition discrepancy, since this parameter is an integral indicator of a change in the shape of the spectrum that is not compensated by the prescribed procedures for configuring the spectrometer.

Let's consider the creation of a Shewhart map using the example of the Cs-137 activity graph contained in the reference specimen from the measurement date:

1. Select the required entries in the measurement log and create a graph, as described in the previous paragraph. We select the measurement date as the abscissa, and the Cs–137 activity as the ordinate.



Graph of the function X=f(P)

The number of records for calculating the point (sample size): 1

Chart type: The values of the ordinate (X)

Abscissa (P): Measurement date

Ordinate (X): Cs-137

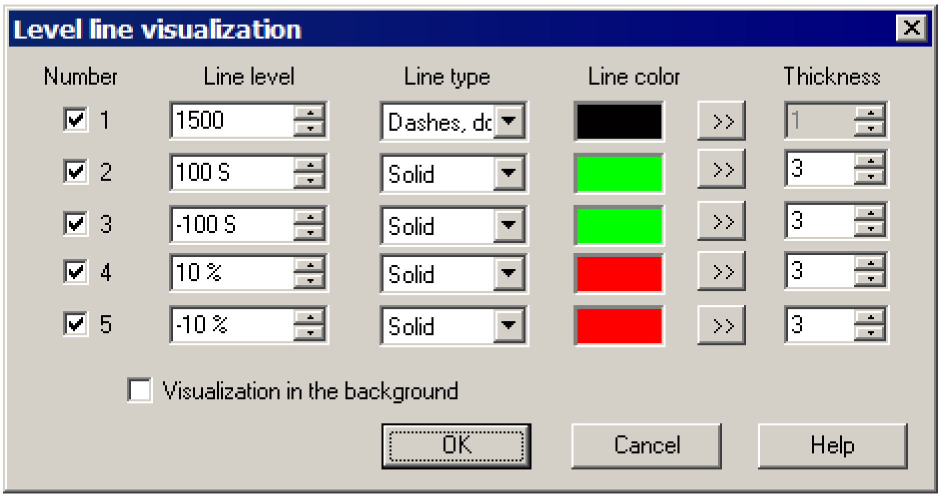
☐ Show statistical uncertainty ☑ Show statistical uncertainty

☐ Show total uncertainty ☑ Show total uncertainty

☐ Unite points with matching (up to error) abscissas

☐ Set the mean as the nominal value

2. Add control levels lines to the graph or edit existing ones. To do this, use the "**Visualization / Level line...**" item in the main menu. In the form that opens, we will set the necessary parameters for five levels: the nominal value (number 1), the boundaries of the warning level (number 2, number 3) and the boundaries of the action level (number 4, number 5). Lines with numbers greater than the first one can be set either in absolute value, or as a deviation in absolute values or as a percentage of the value of the first line. The letter **S** after the number indicates that the value is an offset (Shift) from the first line in absolute numbers, the percentage sign (**%**) indicates that the offset is set as a percentage.



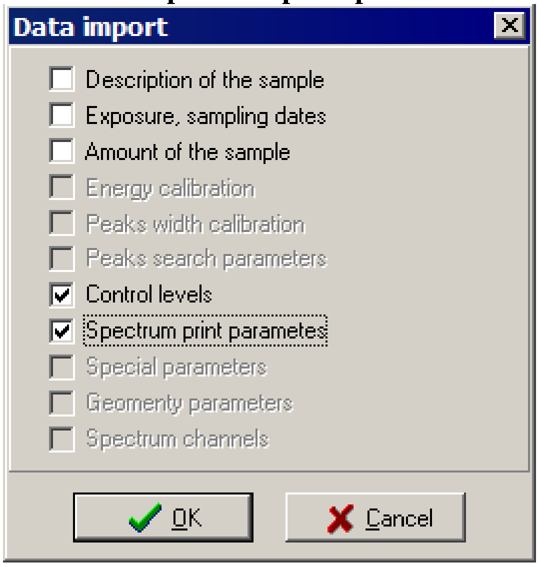
Level line visualization

Number	Line level	Line type	Line color	Thickness
☑ 1	1500	Dashes, dc	■	1
☑ 2	100 S	Solid	🟩	3
☑ 3	-100 S	Solid	🟩	3
☑ 4	10 %	Solid	🟥	3
☑ 5	-10 %	Solid	🟥	3

☐ Visualization in the background

In our case, 1500 is the certified value of Cs-137 activity in Becquerel, 100 S and -100 S are the boundaries of warning levels, 10% and -10% are the boundaries of action levels.

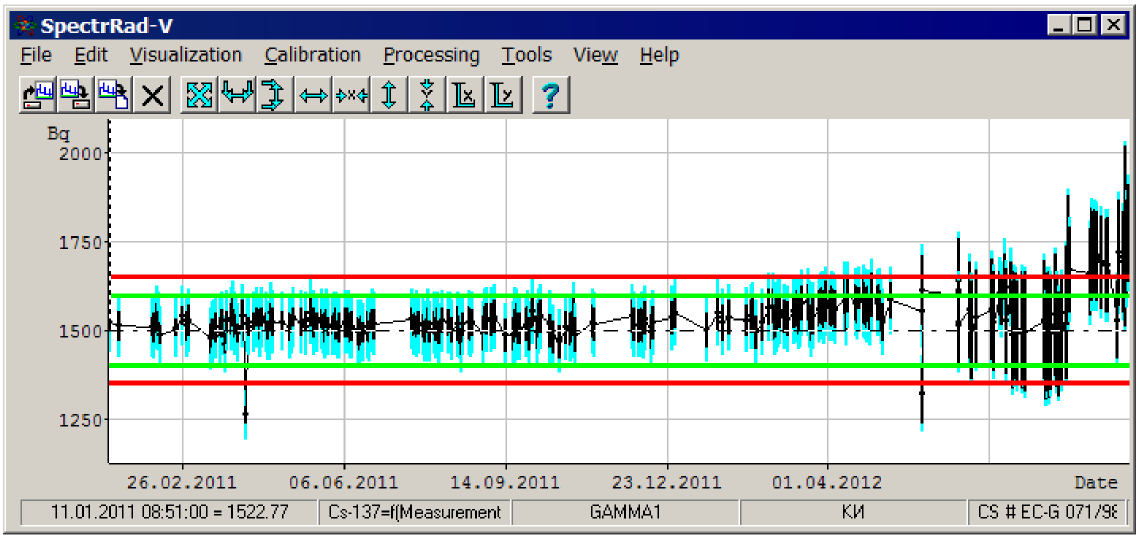
If this is not the first time such a chart has been created, you can import line parameters from a graph file generated earlier. To do this, we call the procedure for editing the spectrum parameters (menu item "**Tools / Spectrum parameters...**"). In the form that opens, click on the menu item "**File / Import data from / file...**", select the table file of the previously generated graph and mark "**Control levels**" and "**Spectrum print parameters**" in the import parameters selection form that appears



Data import

☐ Description of the sample
☐ Exposure, sampling dates
☐ Amount of the sample
☐ Energy calibration
☐ Peaks width calibration
☐ Peaks search parameters
☑ Control levels
☑ Spectrum print parametes
☐ Special parameters
☐ Geomenty parameters
☐ Spectrum channels

As a result, we get a picture of a graph with control levels:



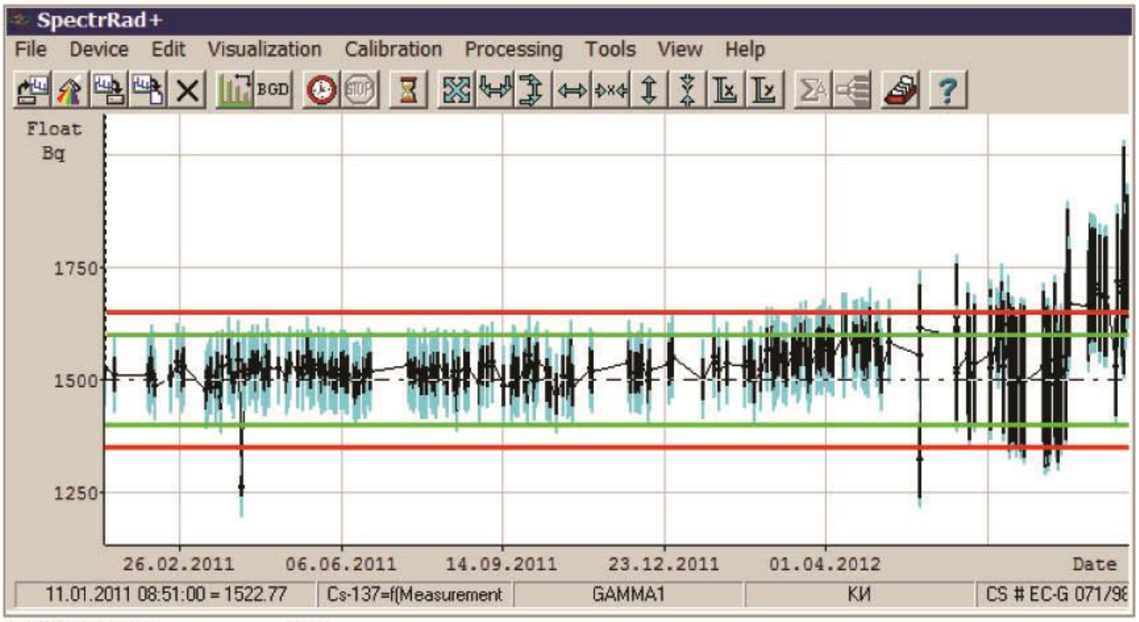
11.01.2011 08:51:00 = 1522.77 | Cs-137=f(Measurement | GAMMA1 | КИ | CS # EC-G 071/98

3. Let's add text information to the picture. To do this, select the main menu item "**File / Print...**". The procedure called by this menu item, generates a report on the spectrum (or graph table), including several basic statistical parameters. The report can be printed or exported to MS WORD. Select export to MS WORD using the prepared template for exporting "Control chart". As a result, we get an MS WORD document:

CONTROL SAMPLE MEASUREMENTS CHART

Sample code:**CS # EC-G 071/98**
Sample name:**Act. Cs-137 = 1500 Bq.,Act. K-40 = 16500 Bq.**
Sample note: **Control sample Cs-137+K-40 № EC-G 071/98 Act. Cs-137 = 1500 Bq. Act. K-40 = 16500 Bq.**
Sample type: **Control sample**
Comment: **Cs-137=f(Measurement date)**
Sampling date: **06.04.1998 12:00:00**

Measuring instrument	
The name of measuring instrument	Verification certificate
0781-Ar-B-G	3004845



Additional error:	5 %
Minimum:	1261±66.2 Bq
Maximum:	1770±160 Bq
Mean:	1540±105 Bq
Bias:	36.2742 Bq (2.41828 %)
Root mean square deviation:	58.5 Bq
Statistical uncertainty:	117 Bq
Total uncertainty:	140Bq
Statistical accuracy surplus:	-59 %

Control levels:

Norm:	1500 Bq
Upper warning level:	1600 (+100) Bq
Lower warning level:	1400 (-100) Bq
Upper action level:	1650 (+10 %) Bq
Lower action level:	1350 (-10 %) Bq

Time range: 11.01.2011 - 04.10.2012 (5.46044e+07 c)
All activities are recalculated on 06.04.1998 12:00:00

25 (10.2 %) values outside the warning level.
17 (6.97 %) values outside the action level.
The surplus of accuracy is outside of acceptable values (-20%, +100%).

Nuclides activities shown on the date of certification of the control sample.

Operator Vasilieva V. ________________

Additional labels are used to create control charts templates:

Label	***Description***
{AddError}	Error, additional to statistical uncertainty, associated with calibration errors, radiation absorption, geometry violations, etc. is set as a percentage when setting up the spectrometer.
{Ymin}	The minimum value of the ordinate of the spectrum, tables..
{YminErr}	The uncertainty of the minimum value.
{YminStatErr}	The statistical part of the uncertainty of the minimum value.
{Ymax}	The maximum value of the ordinate of the spectrum, tables.
{YmaxErr}	The uncertainty of the maximum value.
{YmaxStatErr}	The statistical part of the uncertainty of the maximum value.
{Ymid}	The mean for the given values is $Y_{mid} = (\sum y_i)/n$.
{YErrmid}	Averaged uncertainty $YErr_{mid} = \sqrt{(\sum \Delta_i^2)/n}$. This value is given as the averaged uncertainty for the mean, and not the uncertainty of the mean.
{StatYErrmid}	When calculating $StatYErr_{mid}$ the statistical part of the uncertainty is used.
{YmidStatErr}	Statistical uncertainty of the mean $Y_{mid}StatErr = \sqrt{(\sum (\Delta_i^o)^2)}/n,\ \Delta_i^0$ - statistical uncertainty of the value y_i.
{YmidErr}	Uncertainty of the mean $Y_{mid}Err = \sqrt{(\sum (\Delta_i^0)^2)/n^2 + (Ymid \cdot AddError/100)^2}$.
{StDvn}	The mean square deviation for ordinates $StDvn = \sqrt{\sum (y_i - Y_{mid})^2 /(n-1)}$.
{ExStDvn}	Extended statistical uncertainty (confidence interval corresponding to 95% confidence probability) for ordinate values $ExStDvn = t_{95}(n-1) \cdot StDvn$. Student's distribution is used.
{ExTotDvn}	Extended total uncertainty for ordinate values $ExTotDvn = \sqrt{ExStDvn^2 + U_\delta^2}$. Total uncertainty includes statistical uncertainty $ExStDvn$ and additional error (error of the measuring instrument and measurement method) $U_\delta = Y_{mid} \cdot \sqrt{\delta_{си}^2 + \delta_{м}^2}$.

{RAccuracy[Par]}	Relative accuracy $RAcc = 0.5/\sqrt{\sum((X_i - X_m)^2/(\Delta_i^0)^2)/(n-1)}$. The coefficient is 0.5 to take into account that as Δ_i^0 a 95% confidence interval is used.
{AccurSurplus[Par]}	Percentage accuracy surplus $AccSpls = 100 \cdot (RAcc - 1)$.
{Bias}	The offset of the average value from the certified value in the unit of the ordinate.
{BiasPercent}	The offset of the average value from the certified value as a percentage.
{Level1} – {Level5}	The values of the control levels 1-5.
{Yunit}	The ordinate unit.

Cleaning the archive

The button (menu item "**Tools / Archive cleaning...**") triggers the archive cleaning procedure. The window of the cleaning procedure looks like:

Archive cleaning

Clean

☑ Hidden records

☐ Selected records

Remove for chosen records

☑ Decomposition window picture

☑ RTF and DOC reports

☑ Processing results

☑ Background spectrum

☑ Sample spectrum

☑ Log record

The operator must check the boxes for the type of records to be deleted from the archive: "**Hidden records**" and (or) "**Selected records**" records and the data type for the selected records to be deleted from the archive: "**Decomposition window picture**", "**RTF and DOC reports**", "**Processing results**", "**Background spectrum**", "**Sample spectrum**" and/or "**Log record**". If no records are specified for cleaning, the archive will be cleared of erroneous records (unreadable records, records with corrupted data) and their corresponding files.

By clicking on the "**OK**" button, the archive cleaning operation will begin, which may take a considerable time. It is not recommended to interrupt the cleaning operation, as this may lead to data loss.

During the cleaning operation, the archive entries that should remain in the archive and their corresponding files are overwritten to the temporary archive **~tmp.dbf**. Upon completion of the procedure, the old archive is deleted and the temporary archive is renamed to the old one.

Since the cleaning operation moves and deletes files and folders, all programs that can access files and folders of the archive must first be closed, since the operating system does not allow you to move or delete files and folders that other programs have access to, including viewing programs (Explorer, Norton commander, Windows commander, etc.).

If the operation fails, you can restore the archive as follows: The program creates a copy of the archive file with the same name and extension **~db**. You need to rename it to the name of the old archive and copy all files from the **~tmp** folder to the archive folder.

Files and programs

Structure and placement

The package installation program writes the immutable part of the package (programs and dynamic libraries) to the folder "**Program Files\Dremin\SpectrRad**", the changeable part of the package (nuclide libraries, standards and constants of measured samples, auxiliary files) to the folder specified by the user. In the AD version (ApplicationDir), all files are installed in the folder specified by the user. You can find out the version of the program by calling the menu item "**Help / About...**".

The folder structure in which the modifiable part of the package is written (for the AD version, the entire package) is a tree, in the root folder of which there are common files (general settings files, license file) and a number of folders:

- The "**Devices**" folder containing folders of spectrometers included in the system.
- The "**Sample types**" folder is for storing folders and files containing descriptions, standards (SanPiN, NRB, etc.), radiation absorption cross sections and chemical composition for various types of samples.
- The "**Manuals&Methods**" folder containing the package documentation.
- The "**Help**" folder containing the help system files.
- The "**DocTemplate**" folder, which contains templates for reports generated in MSWord.

Archives of measurement results and libraries of nuclides can be located anywhere (including on the disks of other computers, if they are connected to a network). By default, archives are created in the "**Archives**" folder located in the root folder of the package. By default, nuclide tables are stored in the "**Nuclides**" folder located in the root folder of the package.

The spectrometer folders, in turn, contain common files related to them, the "**SPECTRA**" folder and folders of measurement geometries installed for this spectrometer. Each geometry contains a folder "**ELEMENTS**" for storing calibration data related to this spectrometer and this geometry, a folder "**COMP**" for temporary storage of spectra of decomposition components and two files "**decomp.ini**" and "**decomp.par**" containing information about files and parameters of the spectrum processing procedure.

Programs:

SpectrRad.exe	The main program of the package. Provides measurements management and spectrum processing.
SpectrRadDemo.exe	A demo version of the main program of the package. The control of spectrometers is disabled in the demo version of the program.
SpectrRadView.exe	A version of the program intended only for the purposes of visualizing spectra and data tables.
SpectrRadNucl.exe	A program for creating and editing nuclides libraries.
Radbgd.exe	A program for calculating the background when measuring radon using coal adsorbers.

Files:

***.srs, *.srp, *.clb,** Spectra files. The asterisk "*" corresponds to an arbitrary set of characters

*.mdl, *.cpt, *.spt	allowed for file names.
Backgr.srs	The reserved name for the temporary storage file of the background spectrum.
Autoclbr.clb	The spectrum file of the reference source for automatic calibration.
*.mdl	Files of line spectra models of certain energies.
*.spt	Spectrum files saved in text format.
*.tbl	Files of spectra or functions in a tabular view.
Peakeff.tbl	The reserved name for the quantum registration efficiency files in the peaks of total absorption.
Totaleff.tbl	The reserved name for the file of the full efficiency of registration of quanta in the spectrum.
Effesc1.tbl	The reserved name for the gamma quantum registration efficiency file in the single escape peaks.
Effesc2.tbl	The reserved name for the gamma quantum registration efficiency file in the double escape peaks.
*.srr	Files of spectrum processing results.
*.pkr	Files of search results for peaks in the spectrum.
*.cpt	Files of gamma spectra of continuous scattering (Compton scattering, bremsstrahlung X-ray emission of beta particles) generated by the peak search procedure.
*.srp	The files of gamma spectra with the subtracted spectrum of continuous scattering - peak's spectra.
*.ncl	Nuclides table files.
*.aln	Alpha lines table files corresponding to nuclides tables.
*.btl	Beta lines table files.
*.gml	Files of gamma lines tables.
*.dbf	Header files of measurement results archives.
*.ini	Files of settings and saved parameters.
Saspar.ini	The file of saved parameters for the program "SpectrRad".
NuclBase.ini	The file of saved parameters for the program "SpectrRadNucl".
Analyser.ini	The spectrometer settings file.
Decomp.ini	A text file containing settings for spectrum processing procedures for a given spectrometer and a given geometry.
*.hlp, *.chm	Help and hint files.
*.wav	Audio files to accompany events.
*.rtf	Report files, report templates.
*.doc	Files of descriptions and report templates.
*.dll	Dynamic library files.
Analyser.par	Files of information about connected spectrometers.
Analyser.hd	Files of information about the last measured sample.

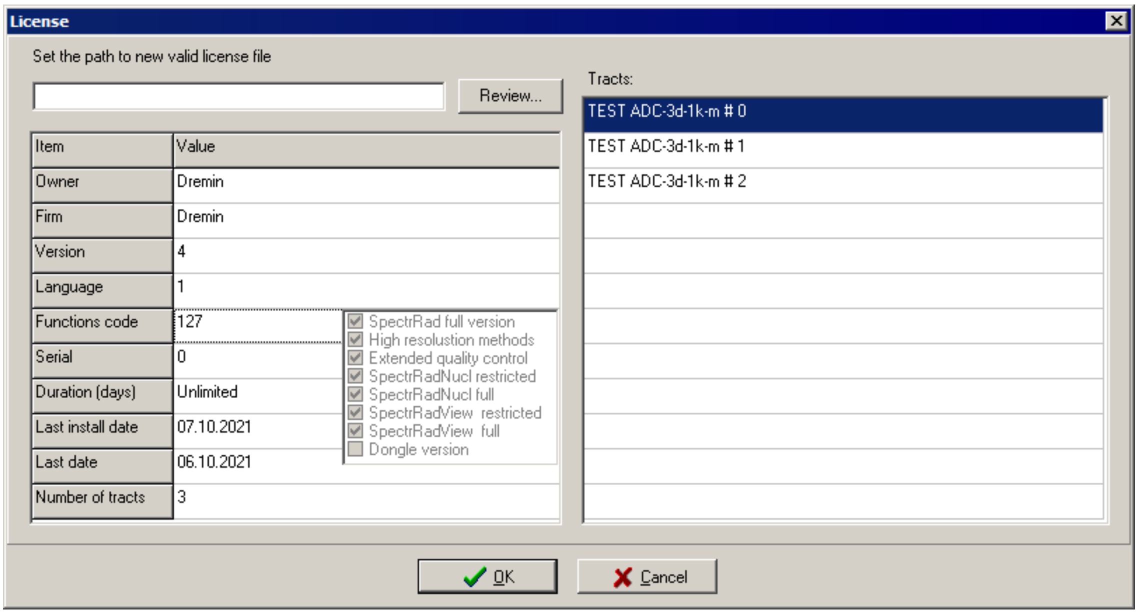
Decomp.par	Decomposition template files.
Norms.nrm	Files of standards and constants for various types of samples.
Norms.txt	Files of notes and comments for standards and constants.
RsAlpha.obj	The object module of the procedure for calculating the average path of alpha particles in the substance of a counting sample.
RsAlpha.h	A file describing the variables of the procedure for calculating the average path of alpha particles in the substance of the counting sample.
RsAlpha.c	A file describing the procedure for calculating the average path of alpha particles in the substance of the counting sample.
RsBeta.obj	The object module of the procedure for calculating the extrapolated path of beta particles in the substance of the counting sample.
RsBeta.h	A file describing the variables of the procedure for calculating the extrapolated path of beta particles in the substance of the counting sample.
RsBeta.c	A file describing the procedure for calculating the extrapolated path of beta particles in the substance of the counting sample.
RsPhoto.obj	The object module of the procedure for calculating the cross section of the photoabsorption reaction of gamma quanta in the substance of the counting sample.
RsPhoto.h	A file describing the variables of the procedure for calculating the cross section of the photoabsorption reaction of gamma quanta in the substance of the counting sample.
RsPhoto.c	A file describing the procedure for calculating the cross section of the gamma quantum photoabsorption reaction in the substance of the counting sample.
RsCompton.obj	The object module of the procedure for calculating the cross section of the reaction of Compton scattering of gamma quanta in a substance of a counting sample.
RsCompton.h	A file describing the variables of the procedure for calculating the cross section of the reaction of Compton scattering of gamma quanta in a substance of a counting sample.
RsCompton.c	A file describing the procedure for calculating the cross section of the reaction of Compton scattering of gamma quanta in a substance of a counting sample.
RsPair.obj	The object module of the procedure for calculating the cross section of the reaction of the formation of electron-positron pairs by gamma quanta in the substance of the counting sample.
RsPair.h	A file describing the variables of the procedure for calculating the cross section of the reaction of the formation of electron-positron pairs by gamma quanta in the substance of the counting sample.
RsPair.c	A file describing the procedure for calculating the cross section of the reaction of the formation of electron-positron pairs by gamma quanta in the substance of the counting sample.
SetupLicense.key	The installation license file.
License.key	The license prolongation file.

Installation and configuration

License

Permission to use the programs of the "SPECTRRAD" package is given by a **license** purchased from the author – a small file **SetupLicense.key** (installation license) or **License.key** (license agreement prolongation file). The file contains information about the license holder, the manufacturer of the spectrometer, package options (permissions to use certain features of the package) and the validity period of the license (the license may be indefinite).

After installing the package, all the information recorded in the license file can be viewed by selecting "**Tools / License...**" in the main menu of the program. The form of the license review procedure may look like:



Item	Value
Owner	Dremin
Firm	Dremin
Version	4
Language	1
Functions code	127
Serial	0
Duration (days)	Unlimited
Last install date	07.10.2021
Last date	06.10.2021
Number of tracts	3

☑ SpectrRad full version
☑ High resolution methods
☑ Extended quality control
☑ SpectrRadNucl restricted
☑ SpectrRadNucl full
☑ SpectrRadView restricted
☑ SpectrRadView full
☐ Dongle version

TEST ADC-3d-1k-m # 0
TEST ADC-3d-1k-m # 1
TEST ADC-3d-1k-m # 2

The **duration** of the license is the number of days the license is valid after installing the software package. **Last install date** is the last allowed date for installing the package programs. **Last date** – the license expiration date is calculated from the actual date of installation of the package on the computer and the duration of the license.

The license may specify the requirement for the software to have an electronic key package – a small device inserted into the USB port of the computer (**Dongle version** option for the **Functions code** string). The "SPECTRRAD" package uses the electronic keys of the company "Activ" - "**Guardant Sign**".

If a limited number of supported spectrometric tracts (**Number of tracts**) are specified, then the allowed spectrometric tracts are listed on the right side of the license.

Installing the security key

The electronic key is connected to the USB port of the computer. This method of protection allows you to create an unlimited number of copies of the software package, change computers during the operation of the package, but the package will only work on a computer with the "**Guardant Sign**" key installed.

For the package to work, you need to install the **Guardant driver** on your computer. During driver installation, all applications must be closed to avoid file splitting errors. The user must have system administrator rights; otherwise driver installation will not be possible. When installing the USB key driver, first disconnect all USB keys from the computer ports.

To install the driver, install the "**Drivers**" disk in the computer's disk drive, which is part of the supplied set of floppy disks, and run the **GrdDriversRU.msi** program (or **Setup.exe** or **Instdrv.exe**) located in the "**Guardant**" folder and follow the instructions of the installation program.

After installing the driver, connect the electronic key to the port.

An indication that the USB key has been successfully initialized by the operating system is the light indication of the key. In addition, the key should appear in the Windows Hardware Manager Device list.

To remove the driver downloaded to the system, click the "**Remove driver**" button in the main window of the driver installation program. In driver removal mode, the utility deletes the driver files and restores the system registry file.

Since the electronic key is a conventional electronic device, it can be disabled as a result of improper operation. To avoid this, follow the following instructions:

- Protect the electronic key from mechanical influences (falls, concussions, vibrations, etc.), as well as from exposure to high and low temperatures and aggressive environments; all this can lead to damage to the housing, printed circuit board elements and connectors of the electronic key.
- Do not make excessive efforts when connecting the electronic key to your computer. The connection of the connectors must be tight and without distortion.
- Do not allow dust, dirt, moisture, etc. to get on the electronic key (and especially on its connectors).
- Do not disassemble the electronic key! This can lead to damage to its housing, as well as to damage or breakage of the printed circuit board elements and, as a result, to unreliable operation or failure of the key itself.

Installing programs package

To install the package on your computer, run the program "**SpectrRad_setup.exe**", located on the installation disk, after closing all programs running on the computer. The installation process is accompanied by the necessary prompts and does not require additional explanations.

Installing the spectrometer drivers

The package provides control of spectrometric boards (installed in "ISA" or "PCI" IBM PC slots) and stand-alone (connected to a parallel, serial or USB port) spectrometers from "Canberra", "GBS ELEKTRONIK", "GreenStar", "ORTEC", "Amplitude", "Aspect", "Dose", "Parsek", "Radek" and "CB RADAR".

The "SpectrRad" package is an add-on to the standard spectrometer control package, which is supplied by the equipment manufacturer: For the company "CANBERRA" - the package "GENIE2K". For the company "ORTEC" - the package "MAESTRO" or "GammaVision". For the company "AMPLITUDE" is the "Progress" program (part of the package that provides control and data exchange with the equipment). For the ASPECT company, there is a SCAR software package (hardware drivers are sufficient for a part of the ASPECT company's equipment). For the company "GreenStar" - a management package for single-board spectrometers of the company. For other companies, there are enough hardware drivers.

To connect the board or stand-alone spectrometer to a computer and connect the detectors, use the appropriate instructions that must be supplied with the equipment you purchased.

The package provides control of ADC boards and autonomous spectrometers of the company "PARSEK" for which the authors of the software package "SpectrRad" have written the necessary hardware drivers. To install the drivers of the connected PARSEK equipment, you must use the standard Windows procedure "**Control Panel / Hardware Installation**". For "ISA" boards, the operator must select the manual installation mode (the answer is "**No**" to the offer of automatic search for new devices) and select "**Spectrometric ADCs**" or "**Other devices**" in the list of connected equipment (device types) if the spectrometers are installed for the first time (at the same time, the operator must indicate the manufacturer and model of the device on the offer select "**Unknown devices**"). Next, you need to install the "**Drivers**" disk into the drive supplied with the package, select the installation mode from the disk and select, according to the working version of Windows, the Win9x (Windows 95, 98) or Win2k folder (Windows NT, 2000, XP, 7. 8, 10), select the desired one from the suggested list of supported hardware type of ADC board or stand-alone spectrometer.

When running the "SpectrRad" program, it searches for ADCs connected to the computer or stand-alone spectrometers from supported equipment manufacturers. For some companies ("CANBERRA", "Amplitude" and "ASPECT"), automatic equipment search does not work and requires the device to be connected to the program by the operator in the spectrometer installation procedure.

To connect the equipment of the company "Amplitude" (distributed by the companies "Amplitude", "Dose" and "Expert Center") to the package "SPECTRRAD", it is necessary, after installing the packages "Progress" and "SPECTRRAD", manually edit the sections [SPHOME0]- [SPHOME11] of the **Saspar.ini** file of the package "SPECTRRAD", adding their information about the connected equipment in accordance with the rules for connecting equipment to the Progress package. For example:

```
[SPHOME0]
Name=Gamma
DllName=serialdrv.hmd
Connection=TypeOfDevice=Unknown Port=COM1 ID=0 DCB={baud=19200 parity=N
data=8 stop=2} SpLen=1024 LLD=0 HLD=16 Active=true Buffer=0
```

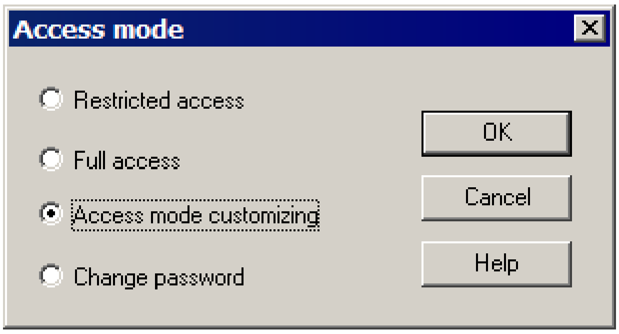
Another option for connecting the Amplitude equipment is also possible - to run the installed and configured Progress program, and then the SPECTRRAD program. In this case, the SPECTRRAD program imports the connection settings from the Progress program and saves them in its settings file when exiting the program.

Access mode

There are two modes of access to the functions and procedures of the package in the "SPECTRRAD" package: **Full access** mode, which allows the user access to all functions and procedures, and **Restricted access** mode, which prohibits access to a number of procedures and functions. The restricted access mode is designed to protect the parameter settings of spectrometric tracts, processing parameters, measurement archive, nuclide tables and standard tables from unqualified access.

The transition to full access mode is protected by a password that the program requests when the package is first launched. The operator may not set a password (enter an empty password), in which case the program will not ask for a password when it is required to switch to full access mode.

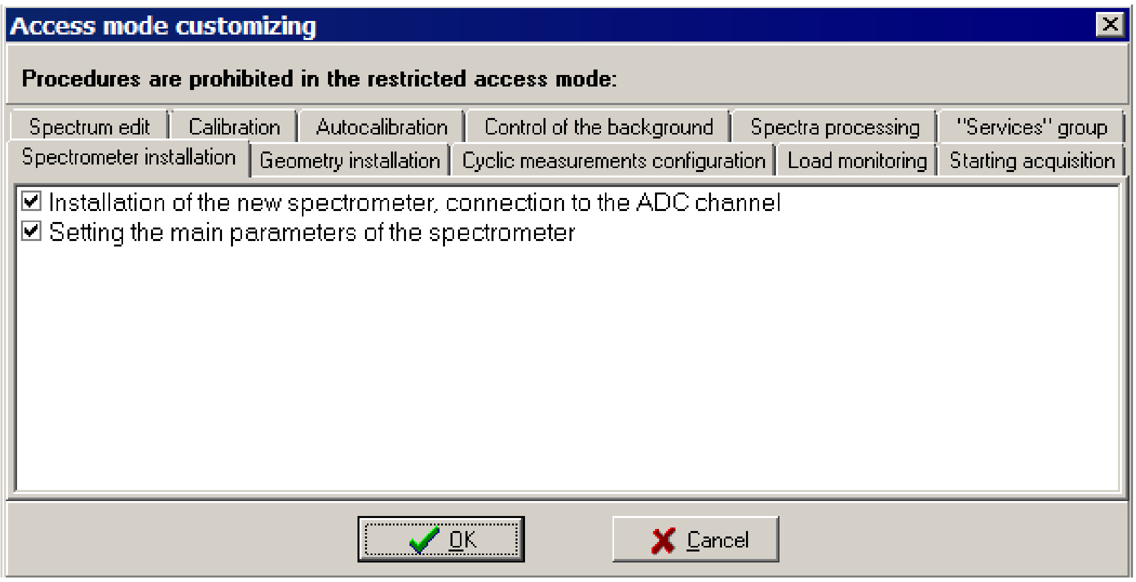
Changing the access mode, changing the password and setting the restricted access mode is performed by calling the menu item "**Tools / Access mode...**". At this, a small form is displayed on the screen to select the necessary procedure:



○ Restricted access
○ Full access
● Access mode customizing
○ Change password

The choice of procedures: switching to full access, setting the access mode and changing the password will require entering the access password.

The "**Access mode customization**" procedure allows the operator to create a list of operations prohibited in the restricted access mode. At the same time, a form is displayed on the screen containing a list of operations that can either be prohibited or allowed in restricted access mode, combined into functionally similar groups:



Procedures are prohibited in the restricted access mode:

☑ Installation of the new spectrometer, connection to the ADC channel
☑ Setting the main parameters of the spectrometer

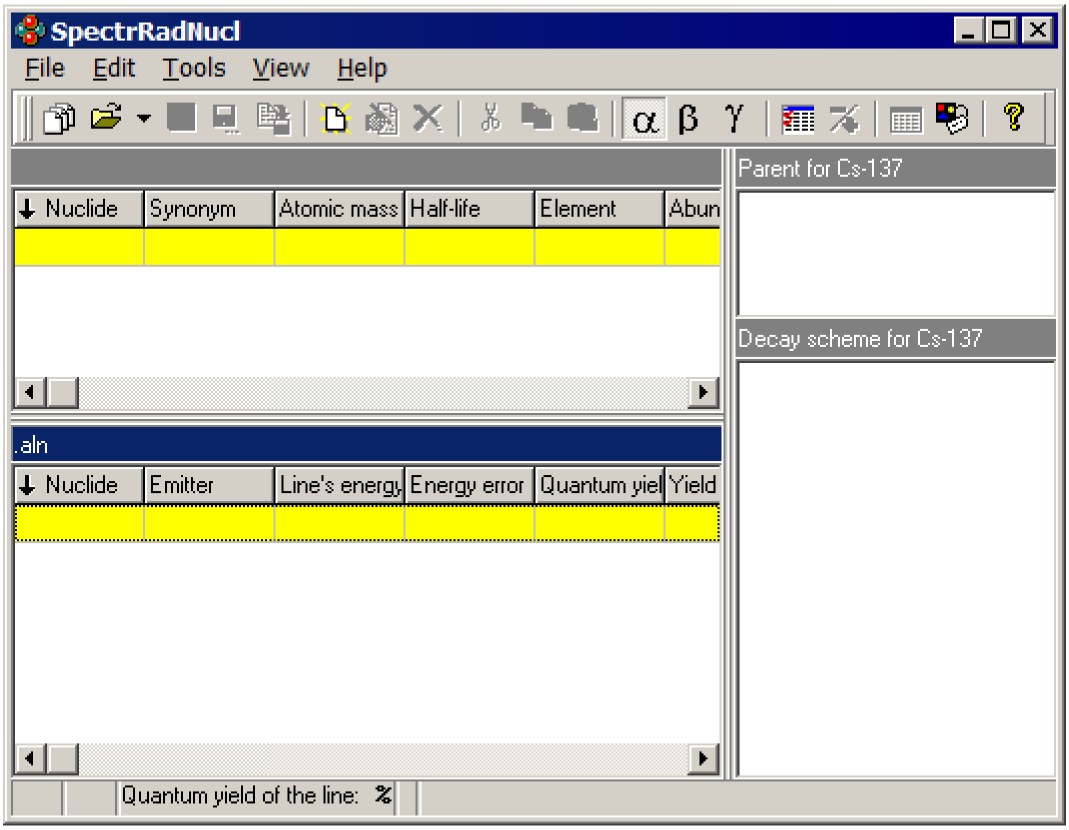
A check mark placed before the name of the operation means that this operation is prohibited in restricted access mode.

Creating nuclide tables[13]

The nuclide tables in the SPECTRRAD software package are used in spectrum processing, spectrometer calibration, when creating and editing safety standards files (SanPiN, NRB, etc.). Energy calibration of the spectrometer, peak width calibration, registration efficiency calibration, calculation of elementary spectra – all these procedures, which the user will have to access more than once, require preformed tables of nuclides.

The procedures for creating and editing nuclide tables are described in detail in the section "**Tables of nuclides**". Here, as an example, we will consider the process of forming a table of nuclides, which will be used in the calibration of a gamma spectrometer with a cooled HPGe detector operating in the range of 30-1500 keV. The good energy resolution of the detector allows the processing of spectra with preliminary subtraction of the continuous scattering spectrum.

First, you need to set the full access mode to the package procedures (menu item "**Tools / Access mode...**"), then call the program for generating and editing nuclide tables (menu item "**Tools / Nuclides table...**"). The window of the program for editing nuclide tables before connecting spectrometers and creating measurement geometries will look like this:



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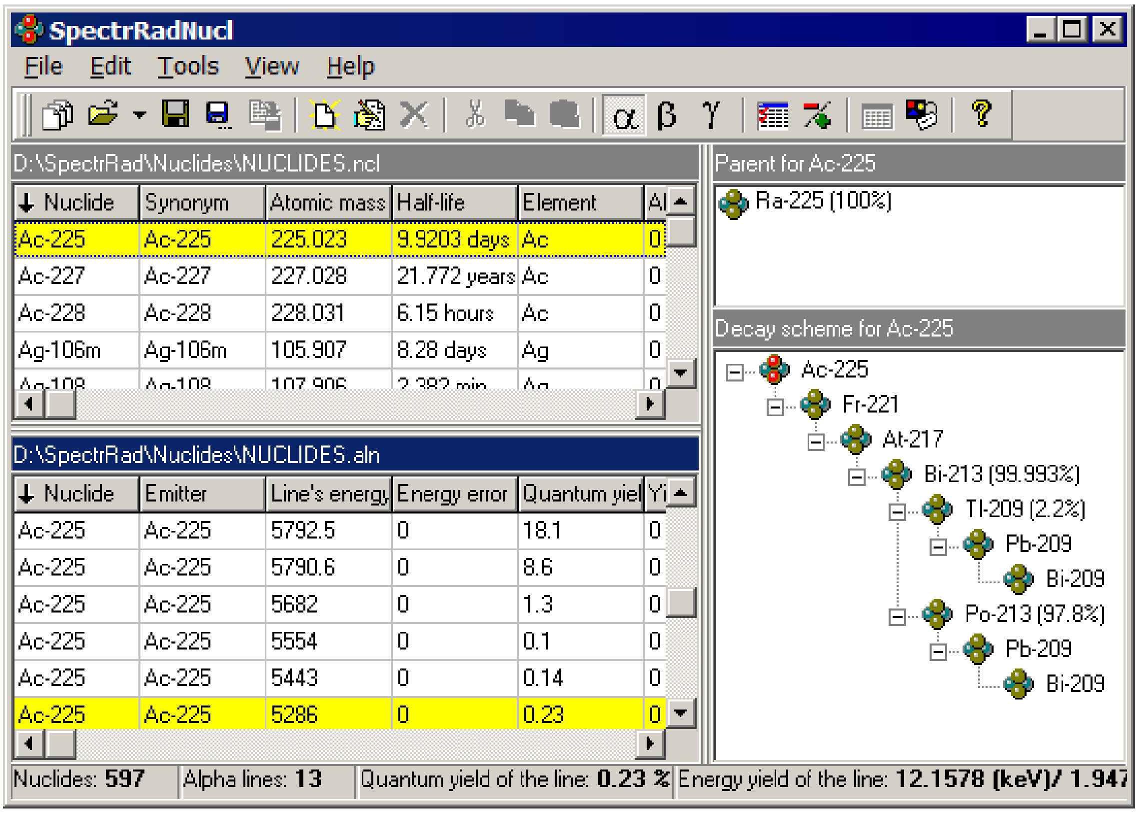
[13] The procedures for creating nuclide tables, installing, configuring, and calibrating the spectrometer are available only in full access mode (menu item "**Tools / Access mode...**")

The delivery package of the "SPECTRRAD" software package includes a number of pre-formed nuclide tables and a basic table "**Nuclides.ncl**", which is located in the "**Nuclides**" folder. Let's open it (menu item "**File / Open...**" of the program "**SpectrRadNucl**"). The program window will look like:



D:\SpectrRad\Nuclides\NUCLIDES.ncl

Nuclide	Synonym	Atomic mass	Half-life	Element	Al
Ac-225	Ac-225	225.023	9.9203 days	Ac	0
Ac-227	Ac-227	227.028	21.772 years	Ac	0
Ac-228	Ac-228	228.031	6.15 hours	Ac	0
Ag-106m	Ag-106m	105.907	8.28 days	Ag	0
Ag-108	Ag-108	107.906	2.382 min	Ag	0

D:\SpectrRad\Nuclides\NUCLIDES.aln

Nuclide	Emitter	Line's energy	Energy error	Quantum yiel	Yi
Ac-225	Ac-225	5792.5	0	18.1	0
Ac-225	Ac-225	5790.6	0	8.6	0
Ac-225	Ac-225	5682	0	1.3	0
Ac-225	Ac-225	5554	0	0.1	0
Ac-225	Ac-225	5443	0	0.14	0
Ac-225	Ac-225	5286	0	0.23	0

Parent for Ac-225

Ra-225 (100%)

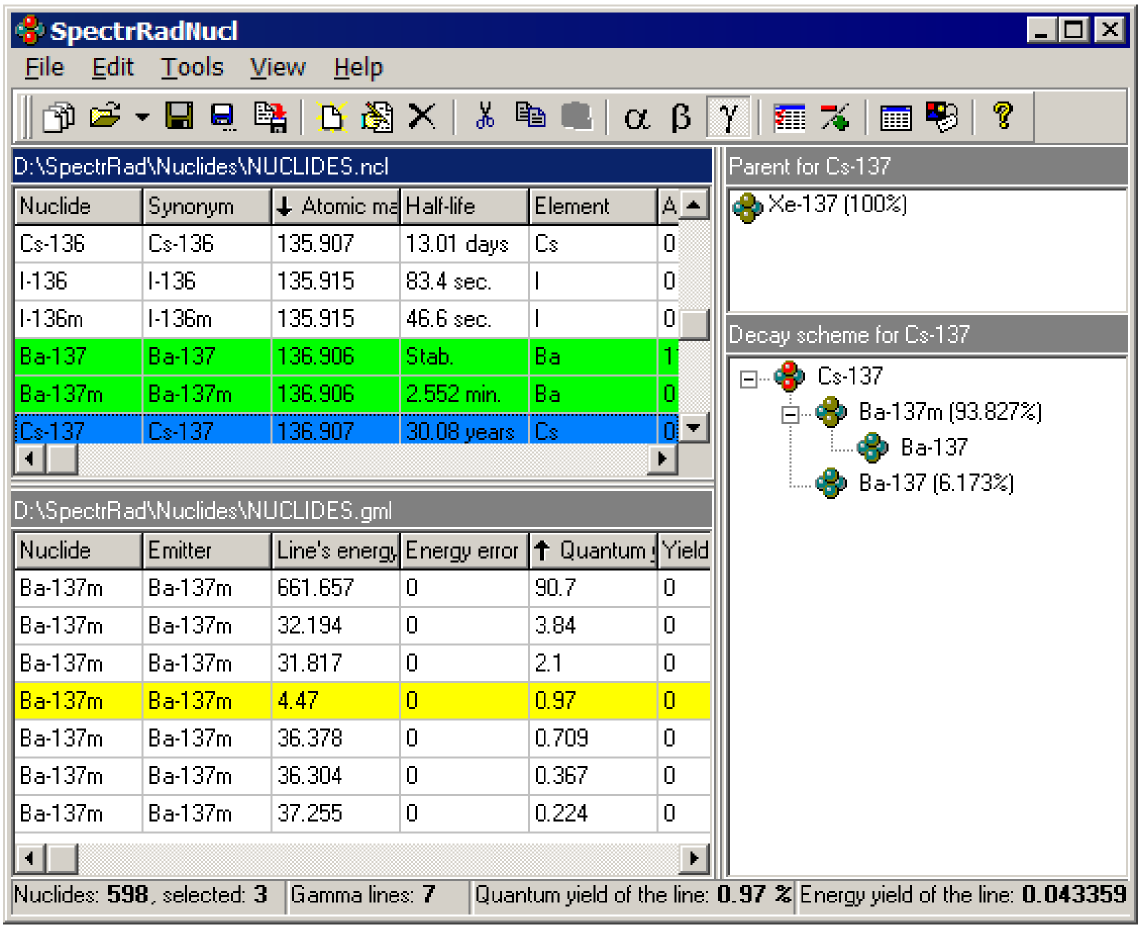
Decay scheme for Ac-225

- Ac-225
  - Fr-221
    - At-217
      - Bi-213 (99.993%)
        - Tl-209 (2.2%)
          - Pb-209
            - Bi-209
        - Po-213 (97.8%)
          - Pb-209
            - Bi-209

Nuclides: **597** | Alpha lines: **13** | Quantum yield of the line: **0.23 %** | Energy yield of the line: **12.1578 (keV)/ 1.947**

Let's assume that we have a set of reference samples at our disposal for calibrating the spectrometer, including the nuclides Am-241, Eu-152, Ba-133, Cs-137. Using the cursor keys or the scroll bar for the mouse, select the required nuclides (selection can be made by clicking the left mouse button on the required entry while pressing the "Ctrl" key of the keyboard). Then we will select the daughter nuclides for the selected nuclides. In this case, we need a single child for Cs-137 – Ba-137m (it is Ba-137m that is the gamma emitter in the Cs-137-Ba-137 chain). It can be selected in the same way as other nuclides. But you can use the pop-up menu (menu item "**Select / Decay chain**") - in this case, all nuclides that are children of the selected nuclides will be added to the nuclides selected by the operator. The pop-up menu is opened by right-clicking on the list of nuclides.

As a result, we get (when selecting the Cs-137 decay chain) the following picture:



D:\SpectrRad\Nuclides\NUCLIDES.ncl

Nuclide	Synonym	↓ Atomic ma	Half-life	Element	A
Cs-136	Cs-136	135.907	13.01 days	Cs	0
I-136	I-136	135.915	83.4 sec.	I	0
I-136m	I-136m	135.915	46.6 sec.	I	0
Ba-137	Ba-137	136.906	Stab.	Ba	1
Ba-137m	Ba-137m	136.906	2.552 min.	Ba	0
Cs-137	Cs-137	136.907	30.08 years	Cs	0

D:\SpectrRad\Nuclides\NUCLIDES.gml

Nuclide	Emitter	Line's energy	Energy error	↑ Quantum y	Yield
Ba-137m	Ba-137m	661.657	0	90.7	0
Ba-137m	Ba-137m	32.194	0	3.84	0
Ba-137m	Ba-137m	31.817	0	2.1	0
Ba-137m	Ba-137m	4.47	0	0.97	0
Ba-137m	Ba-137m	36.378	0	0.709	0
Ba-137m	Ba-137m	36.304	0	0.367	0
Ba-137m	Ba-137m	37.255	0	0.224	0

Parent for Cs-137

Xe-137 (100%)

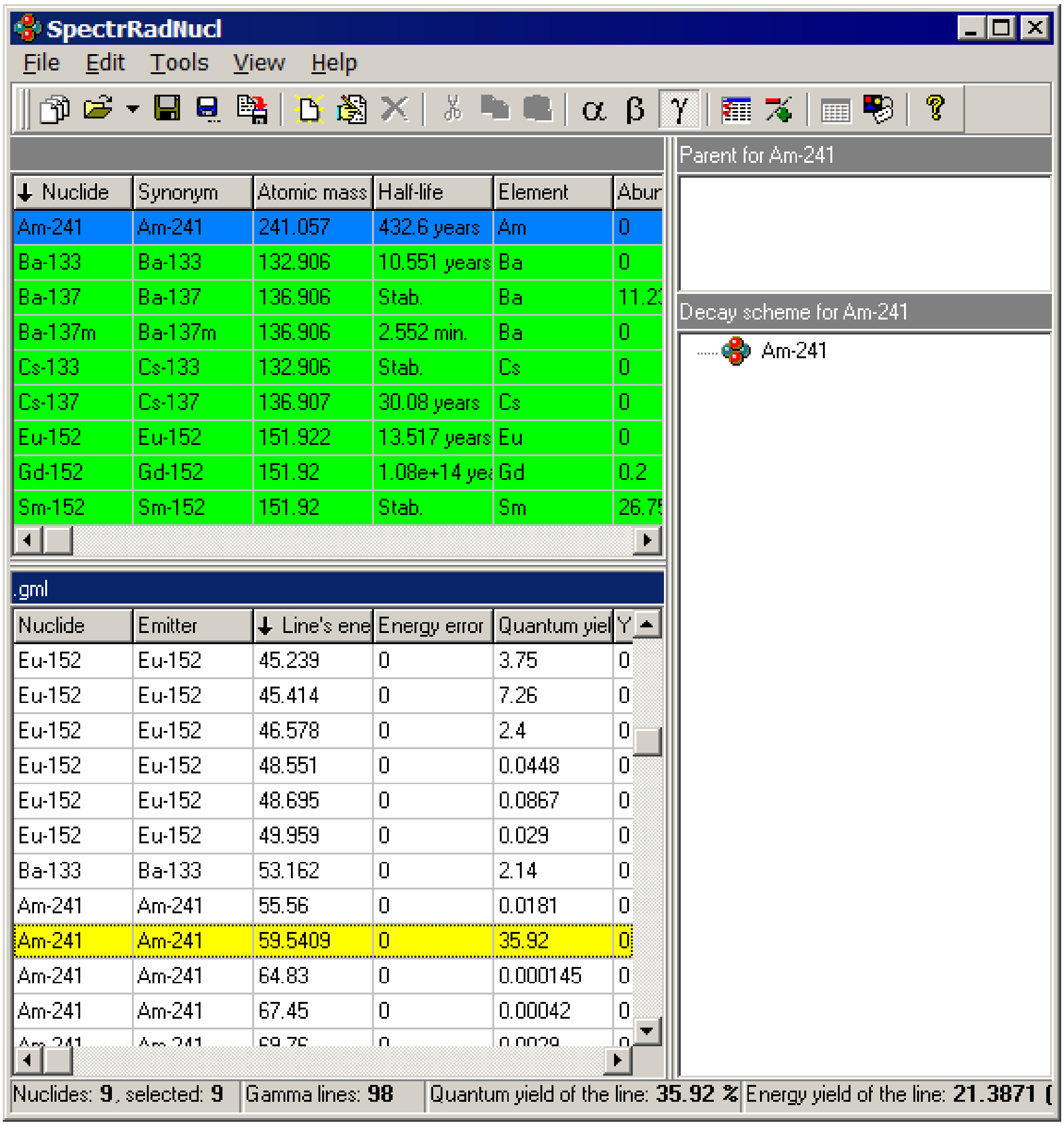
Decay scheme for Cs-137

- Cs-137
  - Ba-137m (93.827%)
    - Ba-137
  - Ba-137 (6.173%)

Nuclides: **598**, selected: **3** | Gamma lines: **7** | Quantum yield of the line: **0.97 %** | Energy yield of the line: **0.043359**

In the same way, we will select the remaining nuclides Am-241, Eu-152 and Ba-133 from the required ones. We are not interested in the chain of decay of Am-241 (radioactive equilibrium in this chain after the release of Am-241 will not occur in a million years), therefore, we select not the chain, but the nuclide.

Copy the selected entries to the clipboard using the menu item "**Edit / Copy**", create a new nuclide table (menu item "**File / New**") and paste the copied entries into a new table (menu item "**Edit / Paste**"). As a result, we will get a picture:



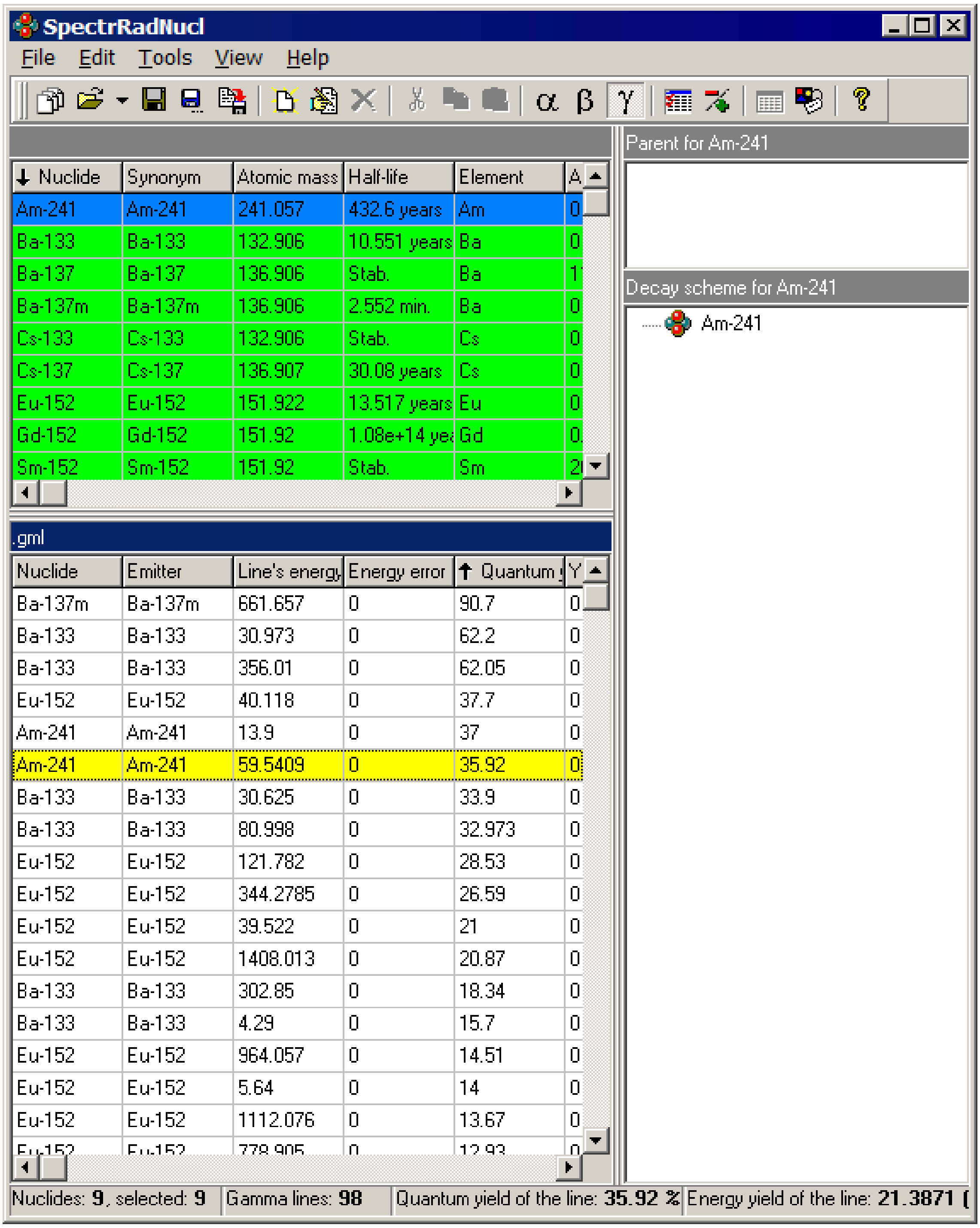
Nuclide	Synonym	Atomic mass	Half-life	Element	Abur
Am-241	Am-241	241.057	432.6 years	Am	0
Ba-133	Ba-133	132.906	10.551 years	Ba	0
Ba-137	Ba-137	136.906	Stab.	Ba	11.2
Ba-137m	Ba-137m	136.906	2.552 min.	Ba	0
Cs-133	Cs-133	132.906	Stab.	Cs	0
Cs-137	Cs-137	136.907	30.08 years	Cs	0
Eu-152	Eu-152	151.922	13.517 years	Eu	0
Gd-152	Gd-152	151.92	1.08e+14 ye	Gd	0.2
Sm-152	Sm-152	151.92	Stab.	Sm	26.7

.gml

Nuclide	Emitter	Line's ene	Energy error	Quantum yiel	Y
Eu-152	Eu-152	45.239	0	3.75	0
Eu-152	Eu-152	45.414	0	7.26	0
Eu-152	Eu-152	46.578	0	2.4	0
Eu-152	Eu-152	48.551	0	0.0448	0
Eu-152	Eu-152	48.695	0	0.0867	0
Eu-152	Eu-152	49.959	0	0.029	0
Ba-133	Ba-133	53.162	0	2.14	0
Am-241	Am-241	55.56	0	0.0181	0
Am-241	Am-241	59.5409	0	35.92	0
Am-241	Am-241	64.83	0	0.000145	0
Am-241	Am-241	67.45	0	0.00042	0

Nuclides: **9**, selected: **9** | Gamma lines: **98** | Quantum yield of the line: **35.92 %** | Energy yield of the line: **21.3871 (**

Let's sort the list of gamma lines by quantum output by clicking on the column name "**Quantum yield**". We will get:



Nuclide	Synonym	Atomic mass	Half-life	Element	A
Am-241	Am-241	241.057	432.6 years	Am	0
Ba-133	Ba-133	132.906	10.551 years	Ba	0
Ba-137	Ba-137	136.906	Stab.	Ba	1
Ba-137m	Ba-137m	136.906	2.552 min.	Ba	0
Cs-133	Cs-133	132.906	Stab.	Cs	0
Cs-137	Cs-137	136.907	30.08 years	Cs	0
Eu-152	Eu-152	151.922	13.517 years	Eu	0
Gd-152	Gd-152	151.92	1.08e+14 yea	Gd	0.
Sm-152	Sm-152	151.92	Stab.	Sm	2

Nuclide	Emitter	Line's energy	Energy error	Quantum	Y
Ba-137m	Ba-137m	661.657	0	90.7	0
Ba-133	Ba-133	30.973	0	62.2	0
Ba-133	Ba-133	356.01	0	62.05	0
Eu-152	Eu-152	40.118	0	37.7	0
Am-241	Am-241	13.9	0	37	0
Am-241	Am-241	59.5409	0	35.92	0
Ba-133	Ba-133	30.625	0	33.9	0
Ba-133	Ba-133	80.998	0	32.973	0
Eu-152	Eu-152	121.782	0	28.53	0
Eu-152	Eu-152	344.2785	0	26.59	0
Eu-152	Eu-152	39.522	0	21	0
Eu-152	Eu-152	1408.013	0	20.87	0
Ba-133	Ba-133	302.85	0	18.34	0
Ba-133	Ba-133	4.29	0	15.7	0
Eu-152	Eu-152	964.057	0	14.51	0
Eu-152	Eu-152	5.64	0	14	0
Eu-152	Eu-152	1112.076	0	13.67	0
Eu-152	Eu-152	778.905	0	12.93	0

Nuclides: **9**, selected: **9** | Gamma lines: **98** | Quantum yield of the line: **35.92 %** | Energy yield of the line: **21.3871 (**

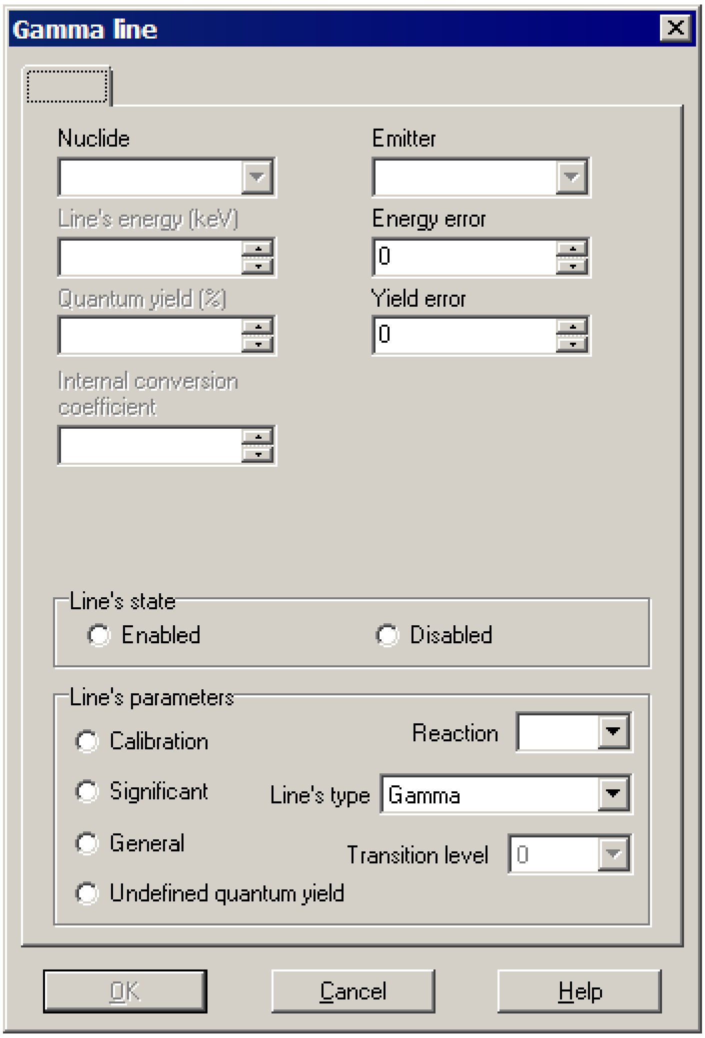
Let's highlight powerful single lines that we will use during calibration. For example:

Nuclide	Synonym	Atomic mass	Half-life	Element	A
Am-241	Am-241	241.057	432.6 years	Am	0
Ba-133	Ba-133	132.906	10.551 years	Ba	0
Ba-137	Ba-137	136.906	Stab.	Ba	1
Ba-137m	Ba-137m	136.906	2.552 min.	Ba	0
Cs-133	Cs-133	132.906	Stab.	Cs	0
Cs-137	Cs-137	136.907	30.08 years	Cs	0
Eu-152	Eu-152	151.922	13.517 years	Eu	0
Gd-152	Gd-152	151.92	1.08e+14 ye	Gd	0
Sm-152	Sm-152	151.92	Stab.	Sm	2

Nuclide	Emitter	Line's energy	Energy error	Quantum	Y
Ba-137m	Ba-137m	661.657	0	90.7	0
Ba-133	Ba-133	30.973	0	62.2	0
Ba-133	Ba-133	356.01	0	62.05	0
Eu-152	Eu-152	40.118	0	37.7	0
Am-241	Am-241	13.9	0	37	0
Am-241	Am-241	59.5409	0	35.92	0
Ba-133	Ba-133	30.625	0	33.9	0
Ba-133	Ba-133	80.998	0	32.973	0
Eu-152	Eu-152	121.782	0	28.53	0
Eu-152	Eu-152	344.2785	0	26.59	0
Eu-152	Eu-152	39.522	0	21	0
Eu-152	Eu-152	1408.013	0	20.87	0
Ba-133	Ba-133	302.85	0	18.34	0
Ba-133	Ba-133	4.29	0	15.7	0
Eu-152	Eu-152	964.057	0	14.51	0
Eu-152	Eu-152	5.64	0	14	0
Eu-152	Eu-152	1112.076	0	13.67	0
Eu-152	Eu-152	778.905	0	12.93	0
Ba-133	Ba-133	34.987	0	11.4	0
Eu-152	Eu-152	1085.837	0	10.11	0

Nuclides: **9**, selected: **9** | Gamma lines: **98**, selected: **10** | Total quantum yield: **335.923 %** | Total energy yield: **1690**

The program "**SpectrRadNucl**" has the ability to edit records in groups. Let's take advantage of this opportunity and edit the selected group of entries in the list of gamma lines by right-clicking on the list of lines in the pop-up menu item "**Edit**". The line editing procedure form will appear on the screen:



Energy error: 0
Yield error: 0
Line's type: Gamma
Transition level: 0

Only a few fields are available for group editing, but in this case we only need the "**Energy error**" field and the "**Line's parameters**" group. In "**Line's parameters**" we must select the "**Calibration**" item, thus setting the status of calibration lines for the gamma lines of the edited group. For calibration lines, calibration procedures will look for the most powerful peak of the spectrum in the energy range from **E-ΔE** to **E+ΔE** to bind it to this line. Here **E** is the energy of the line, and **ΔE** is the specified energy error. By setting the value in the "**Energy error**" field, for example 10 keV, and pressing the "**OK**" key, we get the following view of program "**SpectrRadNucl**":

↓ Nuclide	Synonym	Atomic mass	Half-life	Element	Abundance(	Ga
Am-241	Am-241	241.057	432.6 years	Am	0	0
Ba-133	Ba-133	132.906	10.551 years	Ba	0	0
Ba-137	Ba-137	136.906	Stab.	Ba	11.232	0
Ba-137m	Ba-137m	136.906	2.552 min.	Ba	0	0
Cs-133	Cs-133	132.906	Stab.	Cs	0	0
Cs-137	Cs-137	136.907	30.08 years	Cs	0	0
Eu-152	Eu-152	151.922	13.517 years	Eu	0	0
Gd-152	Gd-152	151.92	1.08e+14 yea	Gd	0.2	0
Sm-152	Sm-152	151.92	Stab.	Sm	26.75	0

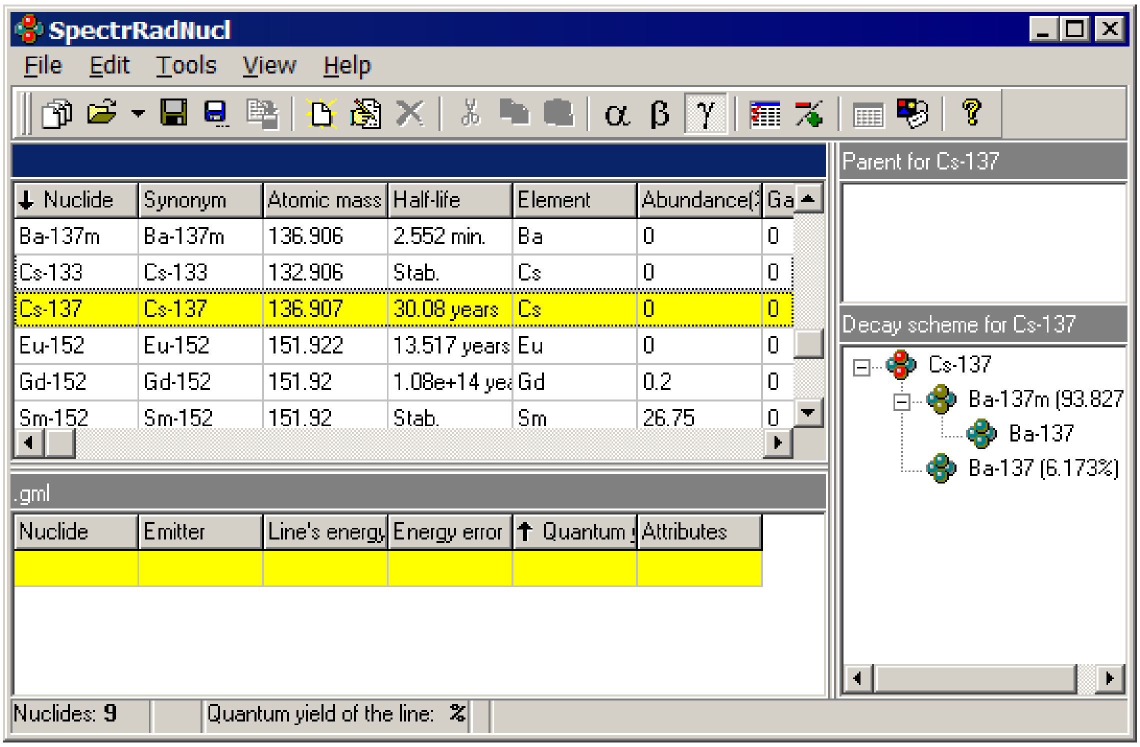
Nuclide	Emitter	Line's energy	Energy error	↑ Quantum	Attributes
Ba-137m	Ba-137m	661.657	10	90.7	5!
Ba-133	Ba-133	30.973	0	62.2	3✕
Ba-133	Ba-133	356.01	10	62.05	3!
Eu-152	Eu-152	40.118	0	37.7	4✕
Am-241	Am-241	13.9	0	37	0✕
Am-241	Am-241	59.5409	10	35.92	0!
Ba-133	Ba-133	30.625	0	33.9	3✕
Ba-133	Ba-133	80.998	10	32.973	3!
Eu-152	Eu-152	121.782	10	28.53	4!
Eu-152	Eu-152	344.2785	10	26.59	1!
Eu-152	Eu-152	39.522	0	21	4✕
Eu-152	Eu-152	1408.013	10	20.87	4!
Ba-133	Ba-133	302.85	0	18.34	3%
Ba-133	Ba-133	4.29	0	15.7	3✕
Eu-152	Eu-152	964.057	10	14.51	4!
Eu-152	Eu-152	5.64	0	14	4✕
Eu-152	Eu-152	1112.076	10	13.67	4!
Eu-152	Eu-152	778.905	0	12.93	1!
Ba-133	Ba-133	34.987	0	11.4	3✕
Eu-152	Eu-152	1085.837	10	10.11	4!
Ba-133	Ba-133	383.85	0	8.94	3

Nuclides: **9**, selected: **9** | Gamma lines: **98**, selected: **10** | Total quantum yield: **335.923 %** | Total energy yield: **1690**

We see that the selected lines have an **energy error** of 10 keV and an **exclamation mark** in the "**Attributes**" column indicating that the line has a calibration status.

It remains for us to form the required equilibrium chains, supplement the table with a list of cascade transition summation lines, and create a certificate of the standard and save the generated nuclide table under some acceptable name.

Let's start with the formation of equilibrium chains. Radioactive equilibrium in the decay chain occurs if the lifetime of the daughter nuclides is more than an order of magnitude shorter than the lifetime of the parent nuclide. In this case, we need to form a single Cs-137-Ba-137m chain. Deselect all nuclides (menu item "**Edit / Select / Unselect all**", "**Del**" key) and select Cs-137 as the current entry in the list of nuclides:



Nuclide	Synonym	Atomic mass	Half-life	Element	Abundance(	Ga
Ba-137m	Ba-137m	136.906	2.552 min.	Ba	0	0
Cs-133	Cs-133	132.906	Stab.	Cs	0	0
Cs-137	Cs-137	136.907	30.08 years	Cs	0	0
Eu-152	Eu-152	151.922	13.517 years	Eu	0	0
Gd-152	Gd-152	151.92	1.08e+14 ye	Gd	0.2	0
Sm-152	Sm-152	151.92	Stab.	Sm	26.75	0

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Nuclide	Emitter	Line's energ	Energy error	Quantum	Attributes

Parent for Cs-137

Decay scheme for Cs-137

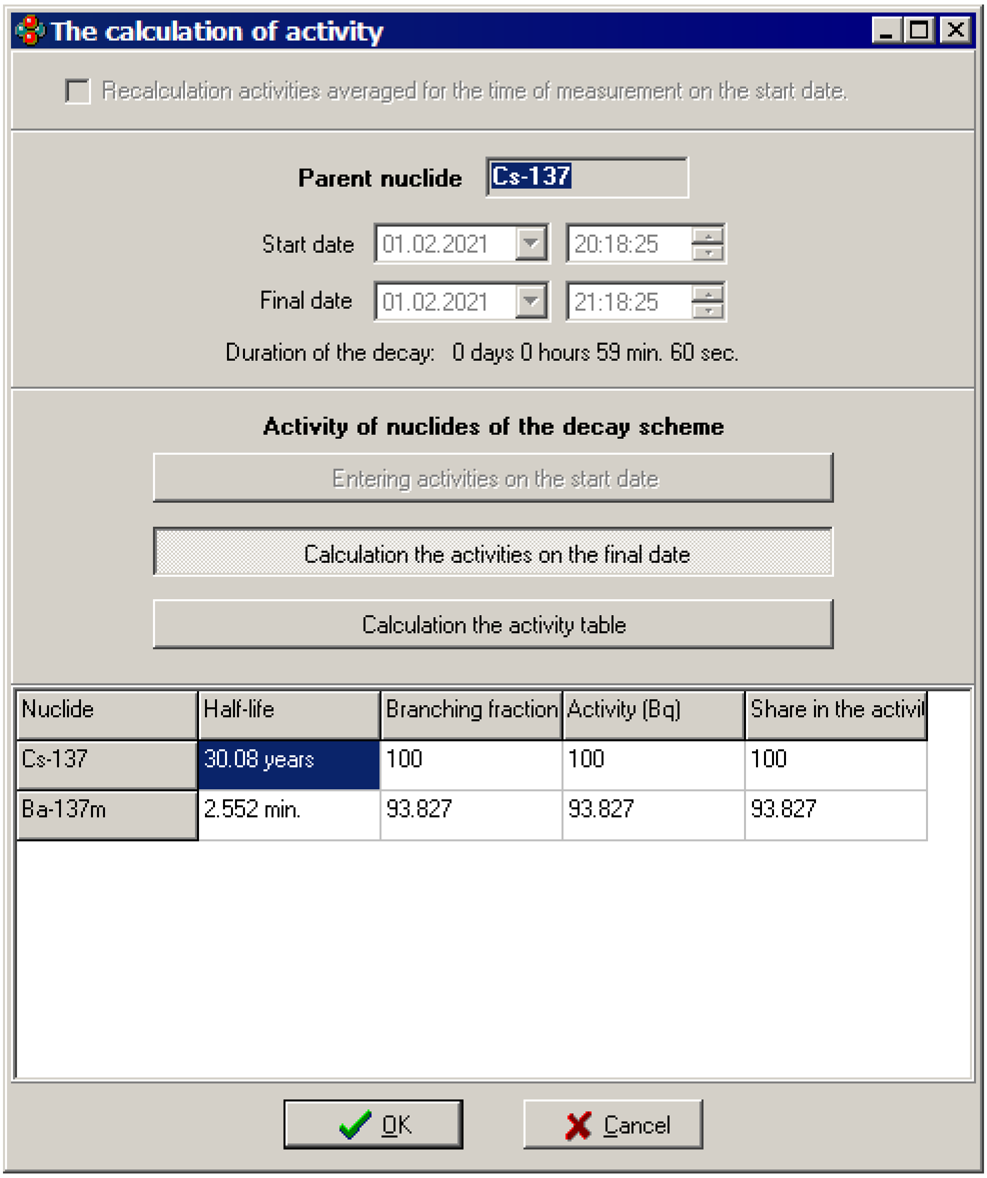
- Cs-137
  - Ba-137m (93.827
    - Ba-137
  - Ba-137 (6.173%)

Nuclides: **9**

Quantum yield of the line: %

The decay scheme of Cs-137 is very simple. If it were more complicated, we would have to specify in the decay scheme ("**Decay scheme**" on the right side of the program window) which specific sections of the branches of the scheme we are going to turn into an equilibrium chain. The chain formation procedure is called by the menu item "**Tools / Nuclides equilibrium chain / Construct..**".

In this case, the program calculates the activity of the nuclides of the chain on the date of formation of radioactive equilibrium in accordance with the processes of accumulation and decay of nuclides in the chain:



☐ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide: Cs-137

Start date: 01.02.2021 20:18:25

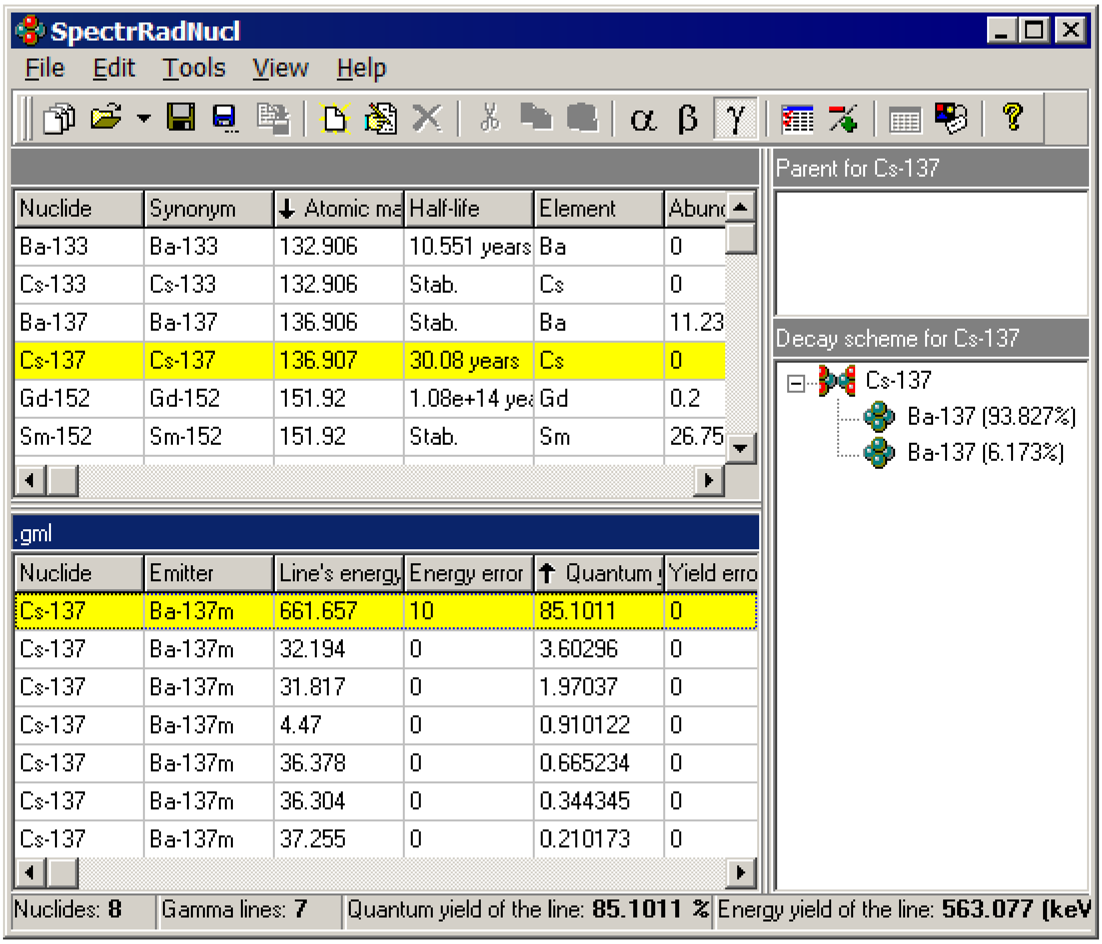
Final date: 01.02.2021 21:18:25

Duration of the decay: 0 days 0 hours 59 min. 60 sec.

Nuclide	Half-life	Branching fraction	Activity (Bq)	Share in the activi
Cs-137	30.08 years	100	100	100
Ba-137m	2.552 min.	93.827	93.827	93.827

In the event that incomplete equilibrium conditions need to be set, the operator can correct the data on the initial activity of nuclides.

In our case, this is not required. Clicking on "**OK**" forms an equilibrium chain:



Nuclide	Synonym	Atomic ma	Half-life	Element	Abun
Ba-133	Ba-133	132.906	10.551 years	Ba	0
Cs-133	Cs-133	132.906	Stab.	Cs	0
Ba-137	Ba-137	136.906	Stab.	Ba	11.23
Cs-137	Cs-137	136.907	30.08 years	Cs	0
Gd-152	Gd-152	151.92	1.08e+14 yea	Gd	0.2
Sm-152	Sm-152	151.92	Stab.	Sm	26.75

Parent for Cs-137

Decay scheme for Cs-137

Cs-137
- Ba-137 (93.827%)
- Ba-137 (6.173%)

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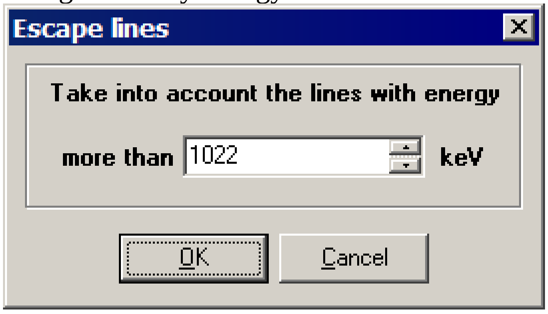
Nuclide	Emitter	Line's energy	Energy error	Quantum	Yield erro
Cs-137	Ba-137m	661.657	10	85.1011	0
Cs-137	Ba-137m	32.194	0	3.60296	0
Cs-137	Ba-137m	31.817	0	1.97037	0
Cs-137	Ba-137m	4.47	0	0.910122	0
Cs-137	Ba-137m	36.378	0	0.665234	0
Cs-137	Ba-137m	36.304	0	0.344345	0
Cs-137	Ba-137m	37.255	0	0.210173	0

Nuclides: **8** | Gamma lines: **7** | Quantum yield of the line: **85.1011 %** | Energy yield of the line: **563.077 (keV**

In the list of nuclides of our reference sample, there are two nuclides with a branched cascade scheme of gamma transitions during decay: Ba-133 and Eu-152. The processes of summation peaks formation during cascade transitions and the corresponding overflow of recorded pulses from photo peaks into summation peaks and into the Compton scattering spectrum can be neglected if the relative efficiency of our detector does not exceed 10%. If we care about accuracy, after the formation of equilibrium chains, it is necessary to supplement the table of nuclides with addition lines of cascade transitions. Selecting the menu item "**Tools / Addition lines of cascading transitions / Include in the table**" causes the required procedure, which calculates the quantum outputs of cascading transitions normalized not for decay, but for the probability of the previous transition for the addition gamma lines of two and three cascading transitions.

The menu item "**Tools / Escape lines / Include in the table...**" calls the program that complements the table of gamma lines of nuclides with lines of single and double escape. At the same time, the program suggests introducing boundary energy for the lines that will be taken into account when forming escape lines



Take into account the lines with energy

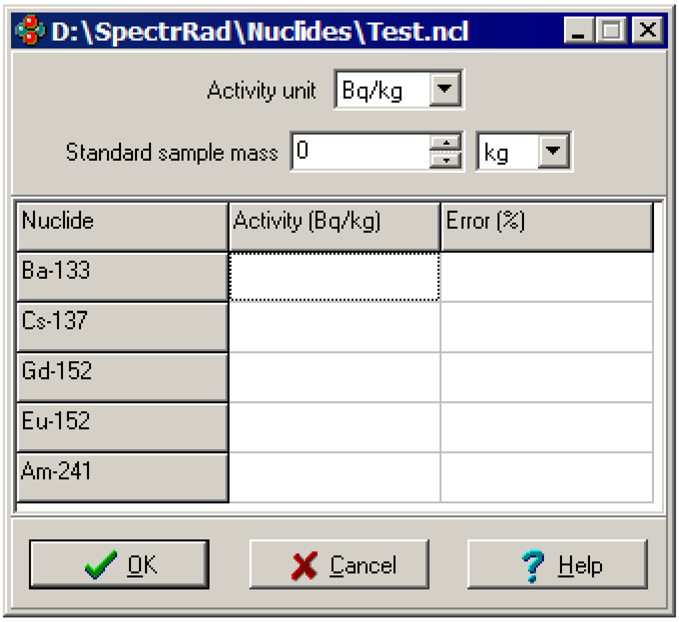
more than 1022 keV

Escape lines are formed due to the effect of the formation of electron-positron pairs in the sample substance and detector by gamma quanta with energies exceeding 1022 keV. 1022 keV for gamma quanta corresponds to zero energy for escape lines, therefore, if we use a range of 30 keV for processing, then it is recommended to set the boundary energy for the procedure for calculating escape lines equal to 1022+30 = 1052 keV.

To correctly calculate the full registration efficiency function, it is necessary to remove from the line table all lines that will not be registered in the spectrum in accordance with the installation of a lower-level discriminator in the recording device (ADC). To do this, you must first select lines with energies less than the threshold, and by calling the line editing procedure, mark the selected lines as excluded.

The generated table needs to be saved. There is a "**Nuclides**" folder in the head folder of the package, where the nuclide tables supplied as part of the package are stored and it is recommended to store newly created tables as well. To save the table, you need to open the menu item "**File /Save as...**".

Since we will have to use the calibration procedure using this reference sample more than once, it is reasonable to record data on the activities of nuclides in the standard somewhere, so that the calibration procedures do not request this data from the operator, but take it from the file where this data is recorded. For these purposes, the program "**SpectrRadNucl**" has a procedure for the formation of a certificate of reference (menu item "**Service / Certificate of standard source ...**"). The procedure window in this case will look like (assuming that we have saved the nuclide table in the "**Test**" file):



Activity unit: Bq/kg

Standard sample mass: 0 kg

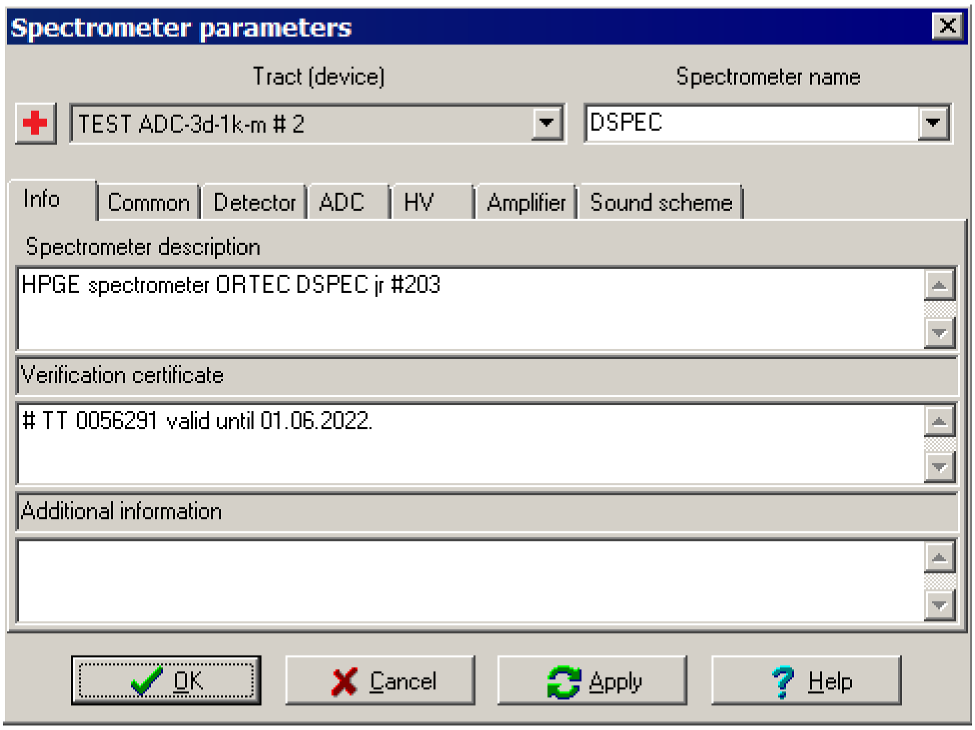
Nuclide	Activity (Bq/kg)	Error (%)
Ba-133		
Cs-137		
Gd-152		
Eu-152		
Am-241		

The operator must specify the nuclide activity in "**Bq**" or "**Bq/kg**" and the errors (uncertainties) as the percentage of activities. The values of the activities must be indicated on the date of certification of the standard(s). The date of certification is not set when forming the certificate, but is indicated when starting the measurements of the standard. Setting the mass of the reference is required if the activity is set to "**Bq**".

Installing the spectrometer

The parameters of the spectrometer in the software package "SPECTRRAD" are stored in a folder with a name corresponding to the name of the spectrometer. Such a folder is formed by the spectrometer installation procedure.

To install and connect the spectrometric tract (spectrometer) to the program, open the menu item in the "SPECTRRAD" window: "**Device / Spectrometer / Install...**".



Tract (device): TEST ADC-3d-1k-m # 2

Spectrometer name: DSPEC

Spectrometer description: HPGE spectrometer ORTEC DSPEC jr #203

Verification certificate: # TT 0056291 valid until 01.06.2022.

Additional information:

The upper part of the form for setting the parameters of the spectrometer contains the button ✚ and two columns:

- **Tract (device)** is the name of the connected tract, which is determined by the name and number of the ADC board and the position of the connector for connecting the detector on the board, or the address value, or the tract identifier.
- **Spectrometer name** - the name of the folder associated with a specific spectrometer (tract). Several names with different tract characteristics can be associated with the same detector, which can be useful in analyzing different energy ranges of the spectrum (low-energy range with a high gain, high-energy range with a lower gain).

The spectrometric tracts found by the program at its launch, the program "SPECTRRAD" includes in the list "**Tract (device)**". For some spectrometric systems, automatic search does not work and the operator must independently specify the spectrometric tracts (devices) connected to the computer. To do this, use the ✚ button. For CANBERRA spectrometers, after pressing the ✚ button, the operator must enter the name of the connected spectrometer – for example: "DET01".

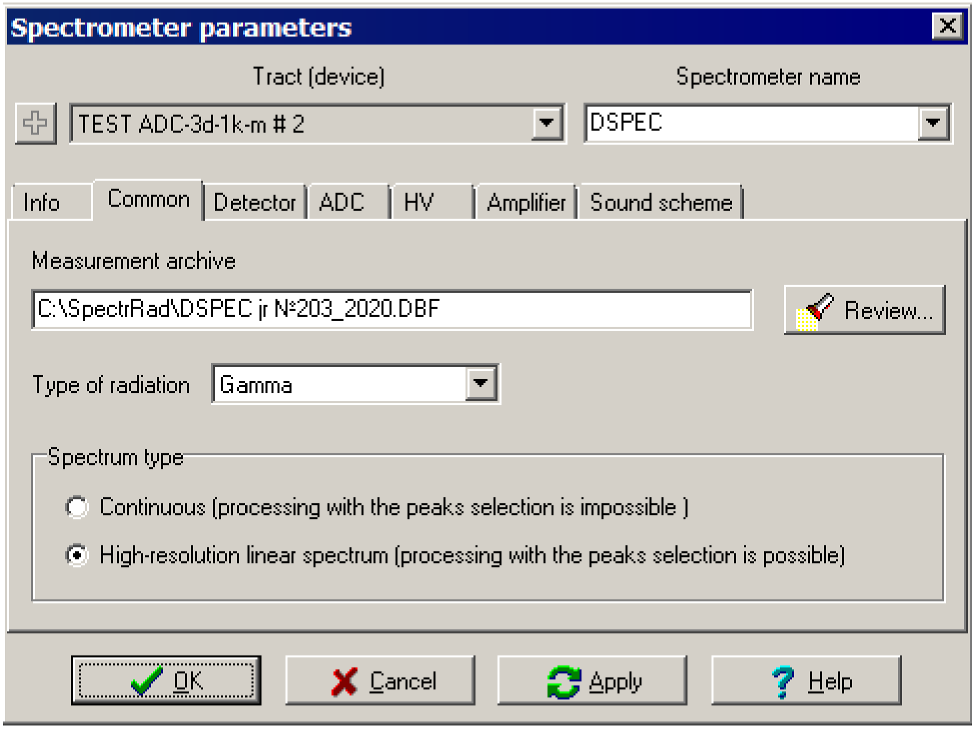
For ASPECT spectrometers operating under the control of the SCAR system, select the connected tract using the SCAR system.

The tracts found by the program or specified by the operator are included in the list of connected tracts (devices) and stored in the settings file of the package "**SASPar.ini**".

The operator must select a **tract** and either select the **name of the spectrometer** from the list of existing spectrometers (when connecting the spectrometer for which the parameters folder was formed earlier to the selected tract), or enter the name of the new spectrometer (when installing the spectrometer) and fill in the fields of the seven pages of the spectrometer parameters:

On the first page "**Info**" of the tabs control: description of the spectrometer, data of the verification certificate and additional information - arbitrary information included in the report on the results of spectrum processing. The contents of this page can be edited in restricted access mode and during measurements. The names of the second and third fields (in the example "**Verification certificate**" and "**Additional information**") are set by the operator. To edit the name, just double-click on the name of the field or press the "**F4**" key on the keyboard.

On the second page "**Common**", the general parameters of the spectrometer:



Tract (device): TEST ADC-3d-1k-m # 2

Spectrometer name: DSPEC

Measurement archive: C:\SpectrRad\DSPEC jr №203_2020.DBF

Type of radiation: Gamma

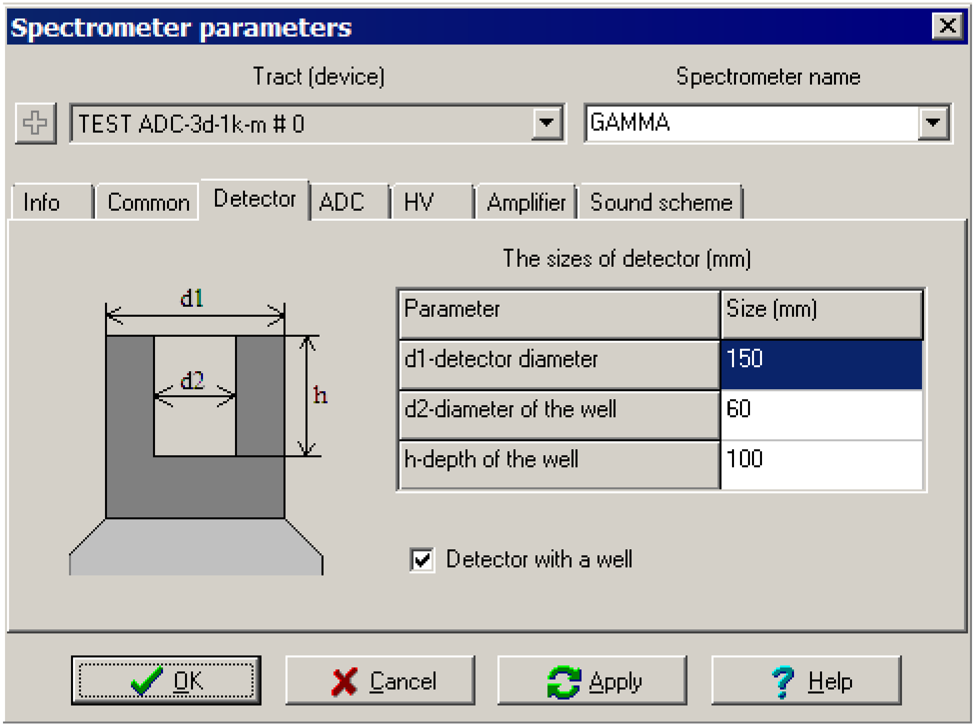
Spectrum type

○ Continuous (processing with the peaks selection is impossible)

● High-resolution linear spectrum (processing with the peaks selection is possible)

- **Measurement archive -** the address of the archive file (path and file name) in which the measurement results on this spectrometer will be stored. The Review... button provides an overview of existing archives.
- **Type of radiation -** select from a list of four possible types of radiation: alpha, beta, gamma and alpha+beta, recorded by this spectrometer.
- **Spectrum type -** the choice of two possible spectrum processing options: **continuous** - processing without peak selection (the recorded spectrum may be linear, but the poor resolution of the detector does not allow you to select the peaks of the spectrum), **high-resolution linear spectrum -** processing with peak selection is possible.

On the third page "**Detector**", the operator must specify the basic parameters and dimensions of the spectrometer detector:



Tract (device): TEST ADC-3d-1k-m # 0

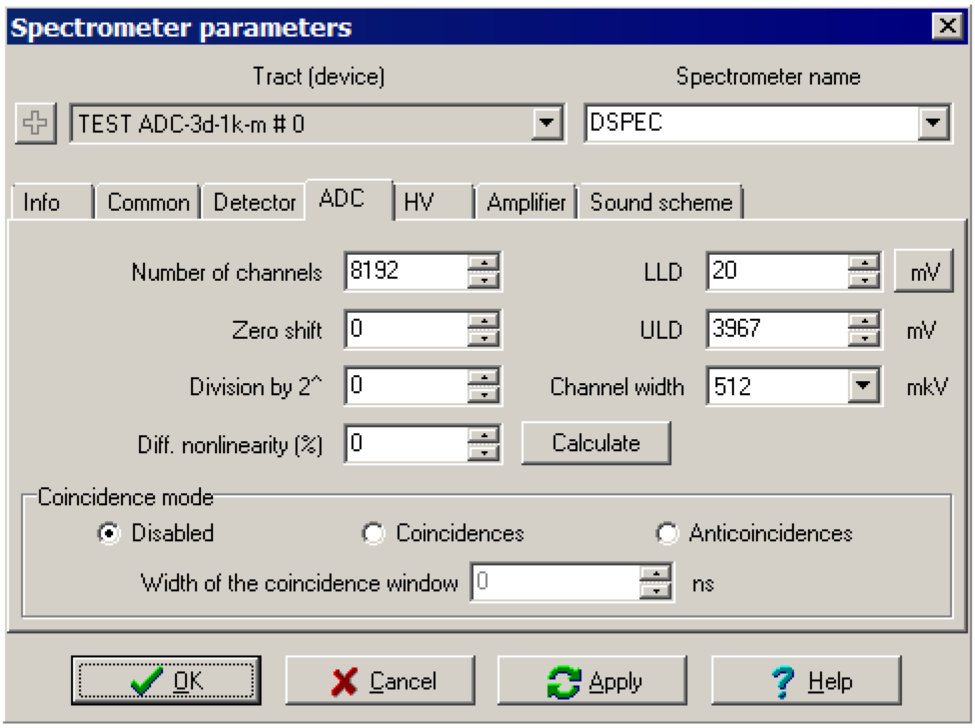
Spectrometer name: GAMMA

The sizes of detector (mm)

Parameter	Size (mm)
d1-detector diameter	150
d2-diameter of the well	60
h-depth of the well	100

☑ Detector with a well

On the fourth page there are parameters configurable for this **ADC** (analog-to-digital converter):



Tract (device): TEST ADC-3d-1k-m # 0

Spectrometer name: DSPEC

Number of channels: 8192

Zero shift: 0

Division by 2^: 0

Diff. nonlinearity (%): 0

LLD: 20 mV

ULD: 3967 mV

Channel width: 512 mkV

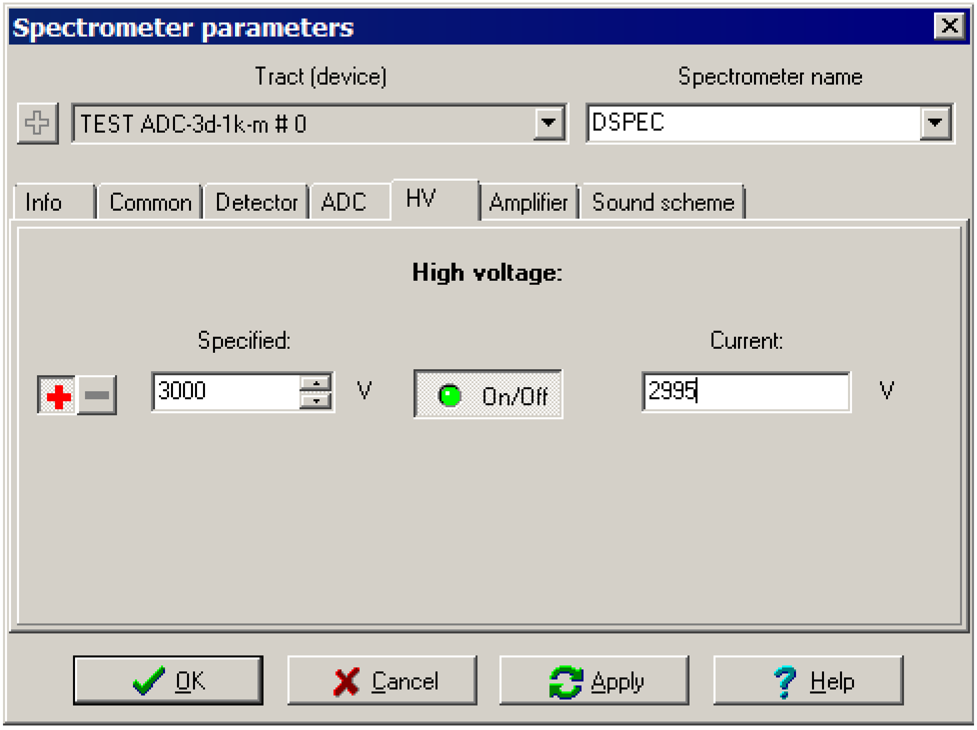
Coincidence mode

● Disabled ○ Coincidences ○ Anticoincidences

Width of the coincidence window: 0 ns

- **Number of channels** – the number of quantization levels of the pulse amplitude.
- **Zero shift** – shift the spectrum in the channels to the left for a positive offset value and to the right for a negative one. In practice, a left shift is used to cut off low-energy noise in the spectrum.

- **LLD** – Lower level discriminator (LLD) - the signal level below which the signal is not processed.
- Button mV (**mV/Ch**) – select units of measurement for the values of the LLD and ULD. The not pressed state of the button is the signal level in millivolts (**mV**), the pressed state of the button is the LLD and the ULD are set in channels (**Ch**). The choice of units of measurement is determined by the type of ADC and is given in the technical description of the ADC.
- **ULD** - Upper Level Discriminator - the signal level, above which the signal is not processed.
- **Channel width** – the quantization step of the pulse amplitude in microvolts. For example, the maximum signal amplitude of 1 volt and the number of channels of 1000 corresponds to a channel width value of 1000 mkV.
- **Division by 2^** - dividing the signal into two to a given degree: shifting the binary value of the pulse amplitude to the right by a given number of digits. It is used in an ADC with digitization of the pulse area to eliminate overflow of the ADC bit grid.
- **Dif. nonlinearity (%)** – the value of the differential nonlinearity of the spectrometer as a percentage. Differential nonlinearity is a component of the statistical uncertainty of the values in the spectrometer channels and is necessary for the correct estimation of errors in the results of spectrum processing. Key Calculate - calculation of differential nonlinearity for a given section of the selected spectrum. The spectrum measured on this spectrometer with good statistics should be used for calculation. The section of the spectrum specified for calculation should not contain peaks and other resonant sections.
- **Coincidence mode** – prohibition or resolution of the spectrum acquisition depending on the external control signal or pulse at the second input of the ADC. It is used to reduce the background level or intensity of the Compton scattering spectrum in some types of ADCs.
- **Width of the coincidence window** – the time interval in nanoseconds, starting from the moment of pulse detection, during which the coincidence/anti-coincidence scheme detects the second pulse.



Spectrometer parameters

Tract (device): TEST ADC-3d-1k-m # 0

Spectrometer name: DSPEC

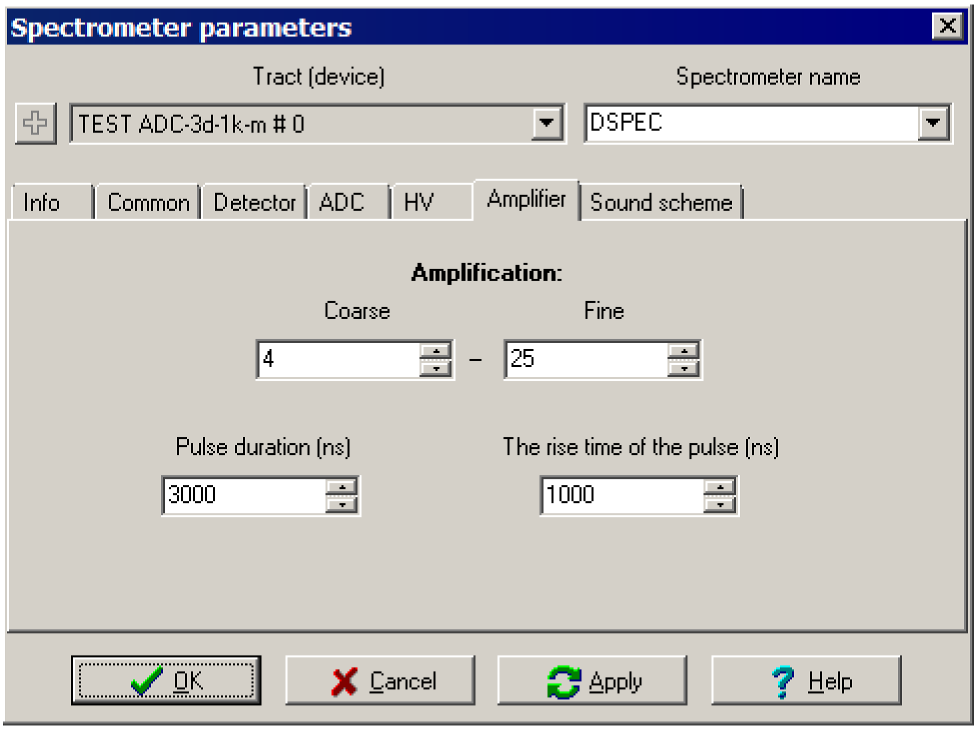
High voltage:

Specified: 3000 V

Current: 2995 V

On the fifth page "**HV**" are the parameters of the high voltage unit for powering the detector:

- **Specified** – the value of the set high voltage level in volts. The + − buttons determine the voltage polarity.
- ● On/Off **button** – determines the state of the high voltage detector power supply and allows you to control this state. The pressed state of the ● On/Off button corresponds to the switched-on state of the power supply circuit. Pressing the button switches the state of the power supply (to prevent accidental pressing of the button, the state of the power supply changes only after pressing the button Apply).
- **Current** – the value of the high voltage level on the detector in volts. Since a sharp change in the value of the high voltage at the detector is unacceptable for some types of detectors, the detector power supply circuit, as a rule, provides a smooth change in the value of the supply voltage. The setpoint value differs from the current value during a high voltage set or drop.



Tract (device): TEST ADC-3d-1k-m # 0

Spectrometer name: DSPEC

Coarse: 4

Fine: 25

Pulse duration (ns): 3000

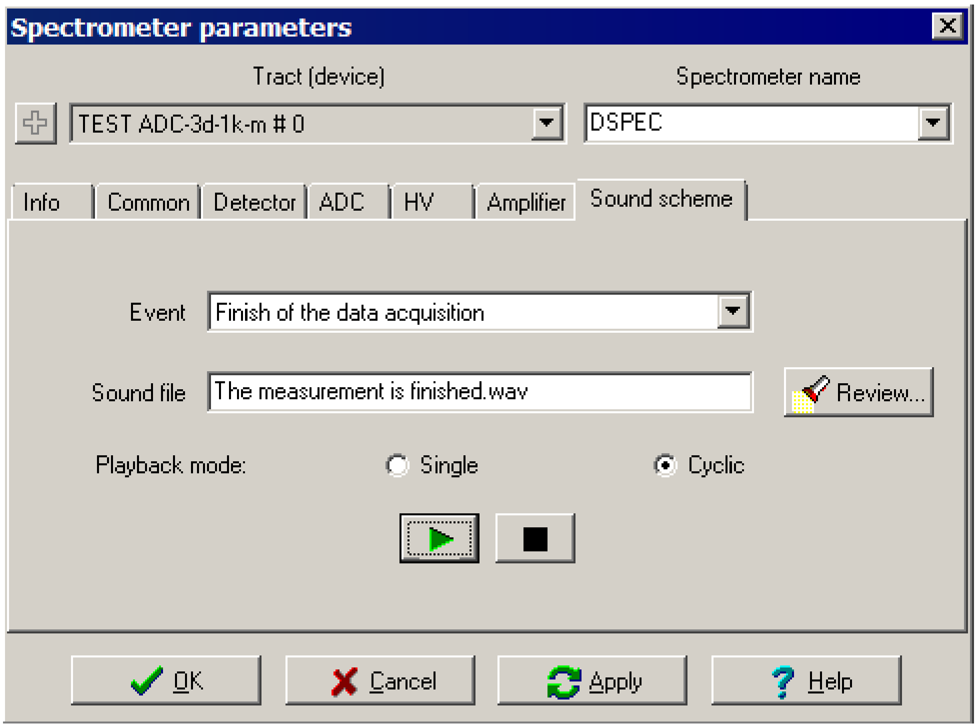
The rise time of the pulse (ns): 1000

The sixth page of the "**Amplifier**" allows you to set the parameters of the signal generation and amplification unit from the detector:

- **Amplification: Coarse, Fine** – setting the amplifier gain. In the "**Fine**" field, the fractional part of the gain is set.
- **Pulse duration (ns)** – sets the pulse duration at the output of the amplifier in nanoseconds.
- **The rise time of the pulse (ns)** – sets the duration of the leading edge of the pulse at the amplifier output in nanoseconds.

The number of configurable parameters for the "**ADC**", "**HV**" and "**Amplifier**" pages depends on the type of equipment being connected.

Setting the values of the adjustable parameters of the ADC, HV and amplifier should ensure the measurement of spectra in the required energy range with a resolution of at least 5 channels for the width of peaks at half the height for the lower boundary energy of the selected range. Therefore, the operator may have to return to setting the parameters of the ADC, NV and amplifier after energy calibration of the spectrometer.



Tract (device): TEST ADC-3d-1k-m # 0

Spectrometer name: DSPEC

Event: Finish of the data acquisition

Sound file: The measurement is finished.wav

Playback mode: ○ Single ● Cyclic

The seventh page is intended for setting up a sound scheme to accompany **events** possible during measurements. In addition to the standard Windows sound scheme, the "SPECTRRAD" program, if there is a sound card, plays several sound files at certain events during measurements:

Event	Sound file	Comment
Finish of the data acquisition.	DATA ACQUISITION IS FINISHED.WAV	The sound signal is played after the measurements are completed.
Finish of the data acquisition cycle.	DATA ACQUISITION CYCLE IS FINISHED.WAV	The sound signal is played once after the end of the cycle in the cyclic measurement mode.
Error in cyclic measurements.	ERROR IN CYCLIC MEASUREMENTS.WAV	An error occurred when performing cyclic measurements: an unacceptably high value of the discrepancy or drift parameters when comparing spectra.
Load exceeds the norm.	LOAD EXCEEDS THE NORM.WAV	The load of the spectrometer exceeds the normal level. The yellow overload indicator in the "Spectrometers" window is lit.
Overload exceeds the allowed limit.	OVERLOAD EXCEEDS THE ALLOWED LIMIT.WAV	The load of the spectrometer exceeds the permissible level. The red overload indicator in the "Spectrometers" window is on.

Abrupt change in loading.	ABRUPT CHANGE IN LOADING.WAV	The change in the load of the spectrometer exceeds the threshold set when setting the load control levels.
No data acquisition in the spectrometer.	NO DATA ACQUISITION IN THE SPECTROMETER.WAV	Measurements are being made in the spectrometer, but no pulses are being recorded.
Autocalibration error.	AUTOCALIBRATION ERROR.WAV	An error occurred during autocalibration: an unacceptably high value of the discrepancy or drift parameters of the spectrometric tract.
Background control error.	BACKGROUND CONTROL ERROR.WAV	An error occurred during the background spectrum control procedure: an unacceptably high value of the discrepancy or drift parameters of the spectrometric tract.

The program searches for the necessary audio file primarily in the folder of the spectrometer in which the event occurred, but if it is not in this folder, the program searches in the main folder of the program. In this way, you can create either individual sound schemes for each (or any) spectrometer, or a general scheme for all.

The Review... key allows you to find and set the required audio file for the selected event other than the default audio file.

The group of switches "**Playback mode: Single, Cyclic**" allows you to set the desired audio signal playback mode for all events except the completion of one measurement cycle, for which only a single playback mode is possible. In cyclic mode, the playback of the audio file will be repeated until the operator intervenes.

The ▶ and ■ keys allow you to start and stop listening to the selected audio file.

Installing the measurement geometry

The proportion of radiation from the counting sample recorded in the detector depends on the size of the detector and the counting sample and their relative position – the geometry of the measurements. As a rule, measurements are carried out in a fixed geometry, which is associated with a certain efficiency of recording radiation from the sample. Several such measurement geometries are required for different sample volumes.

The software package "SPECTRRAD" allows the installation of geometries with one variable geometric parameter (for example: the distance from the detector or the height of the sample filling). In this case, calibration of the spectrometer for several values of the variable geometric parameter is required and the calculation of the registration efficiency for a specific parameter value at which measurements were made is performed by interpolation from the measured values.

Recalculation of the registration efficiency depending on the density[14] of the counting sample is also carried out by interpolation according to several pre-performed calibrations. But if there is only one calibration, such recalculation will be carried out according to the cross sections of the reactions of the interaction of radiation with the substance of the counting sample. The calculation of photo absorption for gamma radiation is carried out according to the cross section of the photo absorption reaction in any case.

In the "SPECTRRAD" package, all parameters related to specific measurement geometry are stored in a folder, the name of which is the name of the measurement geometry. The geometry of the measurements is set by calling the menu item "**Device / Geometry / Install...**".

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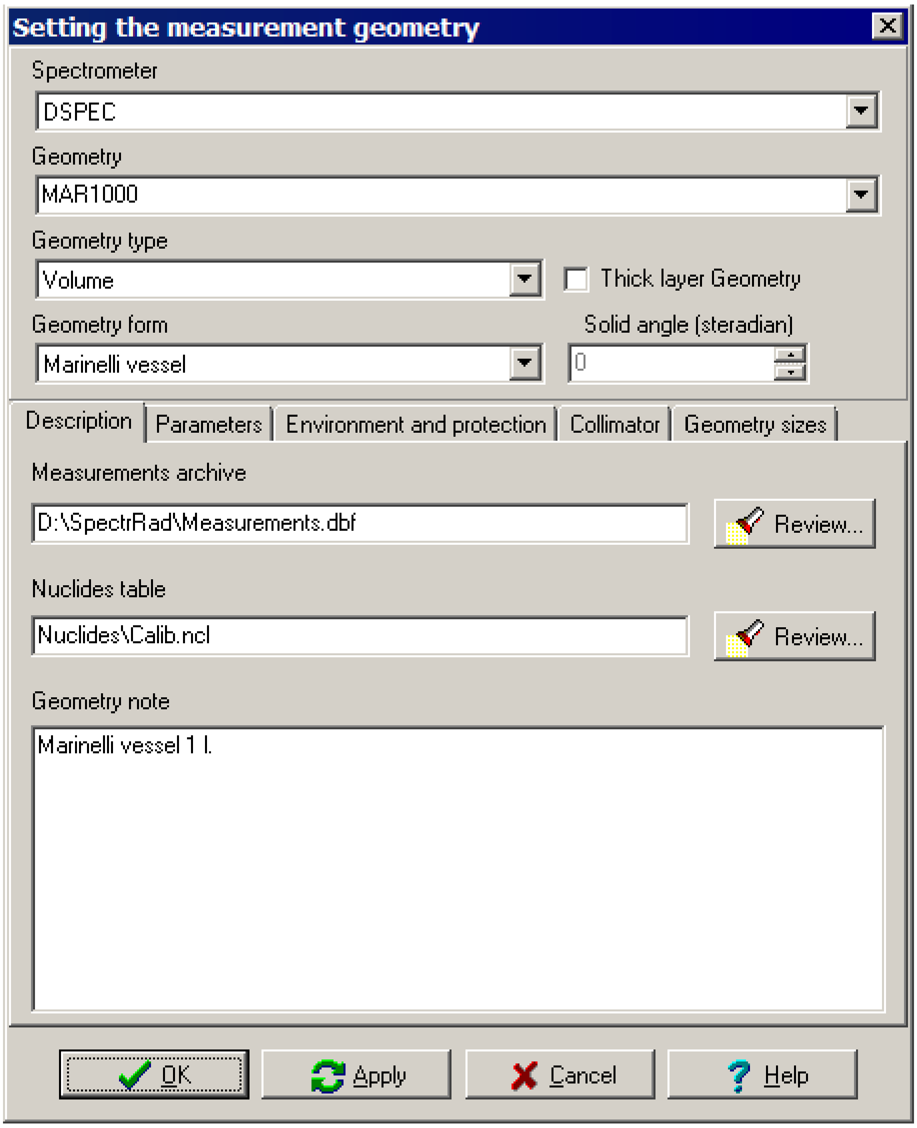
[14] With a constant volume of fixed geometry, the mass of the counting sample corresponds to the density. In the event that the values of the effective charge and effective atomic mass of the substance of the counting sample and the substance of the standards are set, or chemical formulas are set, the calculation of the scattering of alpha and beta particles and Compton scattering of gamma quanta is based on electron density, if these data are not available, physical density is used.

The form for entering geometry parameters looks like this:



Spectrometer: DSPEC

Geometry: MAR1000

Geometry type: Volume

☐ Thick layer Geometry

Geometry form: Marinelli vessel

Solid angle (steradian): 0

Measurements archive: D:\SpectrRad\Measurements.dbf

Nuclides table: Nuclides\Calib.ncl

Geometry note: Marinelli vessel 1 l.

On the first page of the form "Description" , the name, type and description of the geometry and two files related to the geometry: the **Measurement archive** file and the **Nuclides table** file.

The operator needs to:

- Enter the name and description of the geometry. The geometry name must not contain spaces or special characters.
- Select the **geometry type**: **Point**, flat (**Surface**) or volumetric (**Volume**). The type of geometry determines the nature of radiation absorption in the counting sample and the corresponding set of parameters. In point geometry, there is no radiation absorption in the counting sample. In flat geometry, absorption is related to the surface density of the counting sample. In volumetric geometry, absorption is determined by the volumetric density of the counting sample and the effective thickness of the counting sample.
- For a flat geometry type[15], specify the nature of the geometry (check box "**Thick layer geometry**"). The thickness of the radiation source material in the "**thick layer**" must

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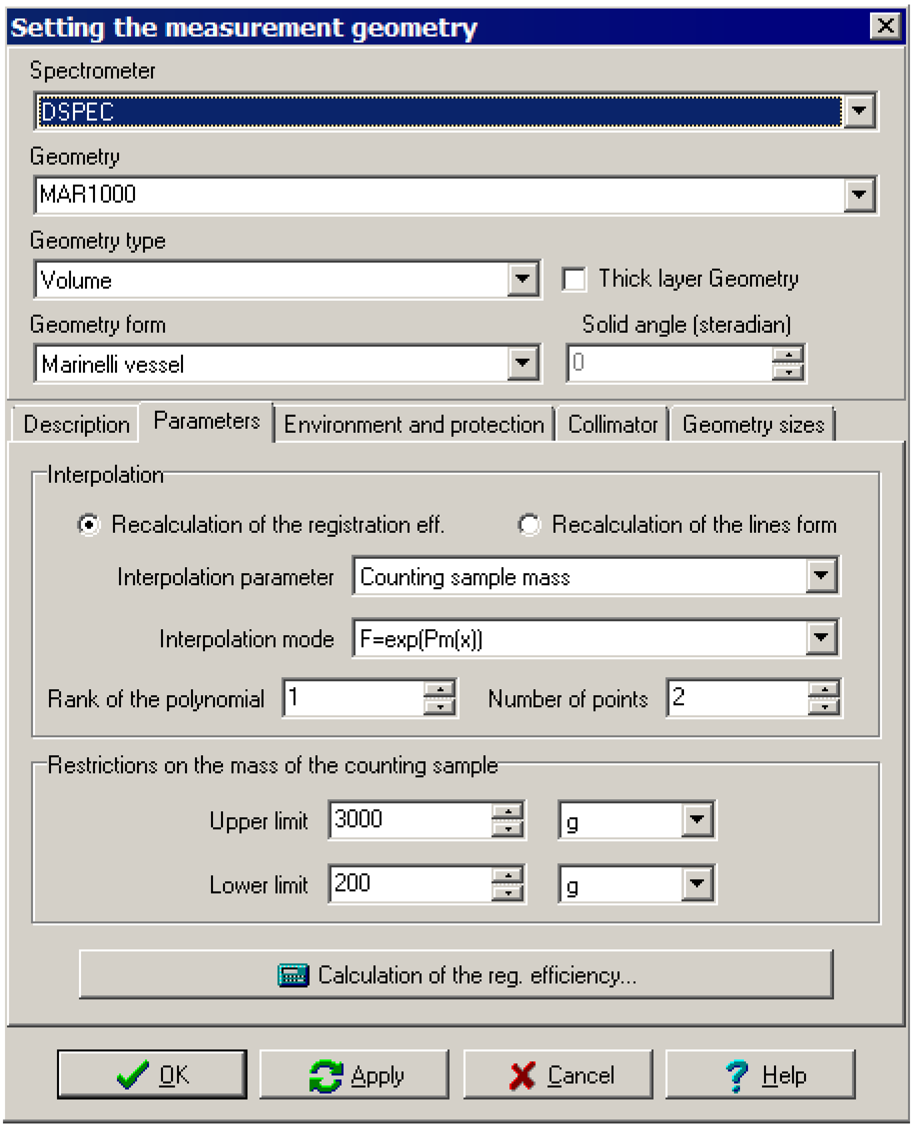
[15] The geometry is considered to be the geometry of a "thick" layer if the average path of the particles detected by the detector in the substance of the counting sample is significantly less than the thickness of the counting sample. For alpha particles with an energy of 4-6 MeV, a layer with a surface density of more than 20 mg/sq.cm will be "thick".

exceed the mean free path of radiation quanta in this material. For the geometry of the thick layer, the response of the spectrometer is proportional not to the total activity, but to the specific activity of the counting sample.

- Select the **geometry form.** For three-dimensional geometry, choose one of the forms of geometry related to the shape and dimensions of the geometry: **Marinelli vessel**, **cylinder (Petri dish)**, **truncated cone**, **cylinder in a well** (for detectors with a well), etc. For the flat geometry of a thick layer, when measuring gamma activity, select the type of flat geometry from the list: **hemisphere (2π)**, **sphere (4π)** or a **given solid angle**. The geometry of the **hemisphere** corresponds to measurements on a plane (the detector is above the earth's surface). The "**Sphere**" geometry is a detector inside a material (in a mine, in a well, etc.). The "**Specified solid angle**" geometry is a geometry in which the solid angle of quantum radiation is structurally limited. For the flat geometry of a thin layer, select the type of flat geometry from the suggested list: **round cuvette**, **rectangular cuvette** or **disk**.
- Select one of the existing archives to save the results of sample measurements in this geometry or enter the name of a new archive. If the archive is not specified, the program will use the archive specified in the parameters of the spectrometer.
- Select a working library of nuclides - a **table of nuclides** used in some spectrometer calibration procedures (calculation of elementary spectra, line spectra and registration efficiency functions) for a given geometry.

On the second page "**Parameters**"



Spectrometer: DSPEC

Geometry: MAR1000

Geometry type: Volume ☐ Thick layer Geometry

Geometry form: Marinelli vessel

Solid angle (steradian): 0

Interpolation

● Recalculation of the registration eff. ○ Recalculation of the lines form

Interpolation parameter: Counting sample mass

Interpolation mode: F=exp(Pm(x))

Rank of the polynomial: 1 Number of points: 2

Restrictions on the mass of the counting sample

Upper limit: 3000 g

Lower limit: 200 g

the operator needs to:

- Set the parameters of the interpolation mode.
- Set the boundary values for the mass of the counting sample. If a zero value is specified for the lower or upper limit of the mass or units of measurement are not specified, the mass of the counting sample will not be controlled by the program.

Explanations are required only the "**Interpolation**" parameter group, which defines the method for calculating the spectra of the decomposition components, the spectra of models and registration efficiency functions corresponding to the **Interpolation parameter**.

The "SPECTRRAD" package uses four types of interpolation parameters:

- **Counting sample mass** – the mass of the counting sample (for a fixed geometry, the mass is directly related to the density of the counting sample) and affects, first of all, the absorption of radiation and, accordingly, the recording efficiency.
- **Distance from detector (mm)** – the distance from the detector to the radiation source along the axis of the detector center - the center of the source. The distance includes the thickness of the source container, but does not include the thickness of the detector package.

- **Spectrometer load** - the intensity of the pulses recorded by the spectrometer in the entire energy range used. The loading of the spectrometer affects, first of all, the shape of the spectral lines
- Selected geometric parameter of the sample or measurement geometry (**Parameter 1**). The name of the parameter is set when setting up the archive associated with this spectrometer and the geometry of measurements, and can be, for example, the height of the fill, etc.

For gamma ray spectrometers with good resolution (peak extraction processing), interpolation is possible by two parameters: for registration efficiency tables by one parameter (item "**Recalculation of the registration eff.**", for example, the mass of the counting sample), and for line tables by another parameter (item "**Recalculation of the lines form**" for example, loading a spectrometer). At the same time, each type of interpolation retains its own set of interpolation parameters.

If we are processing spectra without searching for peaks, a single type of interpolation parameter is used both in the calculation of elementary spectra and in the calculation of spectra of line models.

Interpolation mode defines a piecewise polynomial interpolation (extrapolation) method of the form **F=F([EXP](Pm[LOG](X)))** and can be selected from the following list:

F=Pm(x)	
F=Pm(log(x))	
F=exp(Pm(x))	The recommended interpolation mode for gamma spectrometers with»thin layer" geometry, if the interpolation parameter is the mass of the counting sample.
F=exp(Pm(log(x)))	
F=1/Pm(x)	The recommended type of interpolation is if the interpolation parameter is the distance of the counting sample from the detector. If the **number of points** = 2 and the **rank of the polynomial** = 1, then **F=1/(ax+b)**^{2}.
F=1/Pm(log(x))	
F=1/exp(Pm(x))	
F=1/exp(Pm(log(x)))	
F=F0·(1-exp(-k·x))	The type of interpolation is most suitable for "thick layer" geometries, if the interpolation parameter is the mass of the counting sample.
F=F0·(1-exp(-k·x))/(k·x)	The interpolation mode recommended for alpha and beta spectrometers with»thin layer" geometry.

Here:

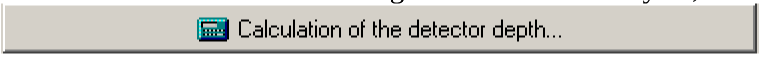
F	The function of the interpolated values:
X	The interpolation parameter.
Pm	A polynomial of a given rank.

The choice of a specific type of interpolation depends on the interpolation parameter. If the interpolation parameter is the distance of the sample from the detector, reverse polynomial interpolation **F=1/Pm(x)** is recommended. Before choosing the type of interpolation, it is necessary to find out the theoretical dependence of the attenuation of the radiation intensity on the selected interpolation parameter and, accordingly, choose the closest type of interpolation.

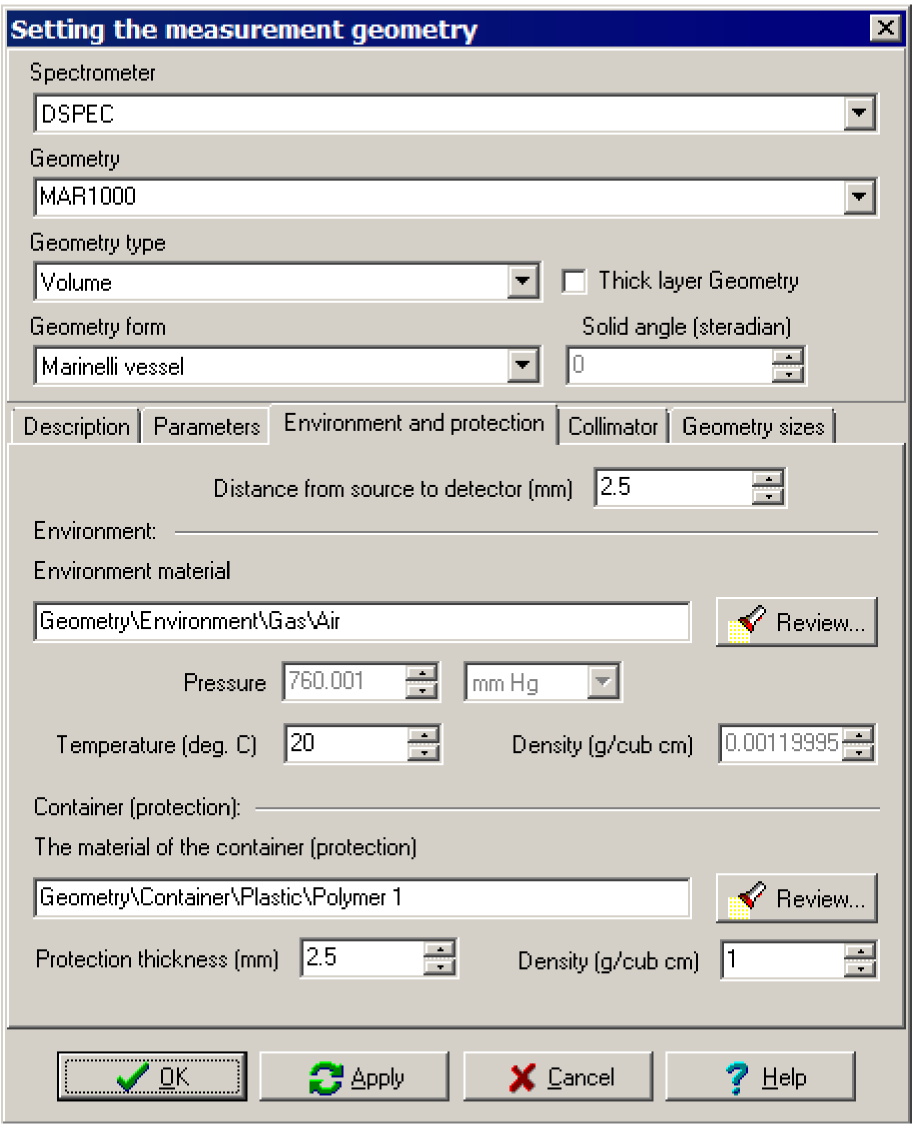
Theoretically, the last two formulas are best suited for the dependence of the radiation intensity on the mass (or density) of the sample: **F=F0·(1-exp(-k·x))** for "thick layer" geometries and **F=F0·(1-exp(-k·x))/(k·x)** for thin layer geometries. And this is true for all types of radiation in the geometries of the "thick layer" and for alpha and beta spectrometers when measuring in the geometry of the "thin layer". For scintillation gamma spectrometers (processing spectra without separating the Compton scattering spectrum), due to the complex nature of the redistribution of pulses from photo peaks into the Compton scattering spectrum with a change in the density of the counting sample, a more free interpolation of the form **F=exp(Pm(x))** or **F=exp(Pm(log(x))** is better suited. For gamma-ray spectrometry with the separation of the continuous scattering spectrum of the formula **F=F0·(1-exp(-k·x))** and **F=F0·(1-exp(-k·x))/(k·x)** are suitable. But due to the fact that the parameters of the formulas are determined by a nonlinear procedure and it is more sensitive to statistical noise of the approximated spectra and functions, their application requires caution.

The **rank of the polynomial** and the **number of points** are related parameters. The number of points is the number of spectra or tables involved in the calculation, which are used for interpolation. The rank of the polynomial must be at least one less than the number of points (if we use three spectra, then we can use parabolic interpolation, with two - only linear). To increase the calculation speed, it is recommended to use piecewise linear interpolation.

The calculation is performed for each channel of the spectrum by interpolation of the selected type according to a given number of spectra having interpolation parameter values closest to the same parameter of the counting sample from a set of elementary spectra, line models spectra or efficiency tables. The user can use up to 6 input spectra or efficiency tables.

The  button calls the procedure for calculating the gamma quantum registration efficiency functions for a number of types and forms of geometries according to the registration efficiency functions for point geometry. Previously, the calculation of the "effective depth of the detector" (calculation of the geometric parameters of the recording area of the detector) should be carried out according to the functions of the gamma quantum registration efficiency for at least two positions of the point radiation source relative to the detector. For the point geometry of measurements, the button "Calculation of registration efficiency...", changes its appearance to . Click on this button triggers the procedure for calculating the "effective depth of the detector".

On the third page "**Environment and protection**", the operator must specify the parameters of the environment in which the radiation source and detector are located, the container in which the radiation source is located, or additional protection.



Setting the measurement geometry

Spectrometer: DSPEC

Geometry: MAR1000

Geometry type: Volume

☐ Thick layer Geometry

Geometry form: Marinelli vessel

Solid angle (steradian): 0

Description | Parameters | Environment and protection | Collimator | Geometry sizes

Distance from source to detector (mm): 2.5

Environment:

Environment material: Geometry\Environment\Gas\Air

Pressure: 760.001 mm Hg

Temperature (deg. C): 20

Density (g/cub cm): 0.00119995

Container (protection):

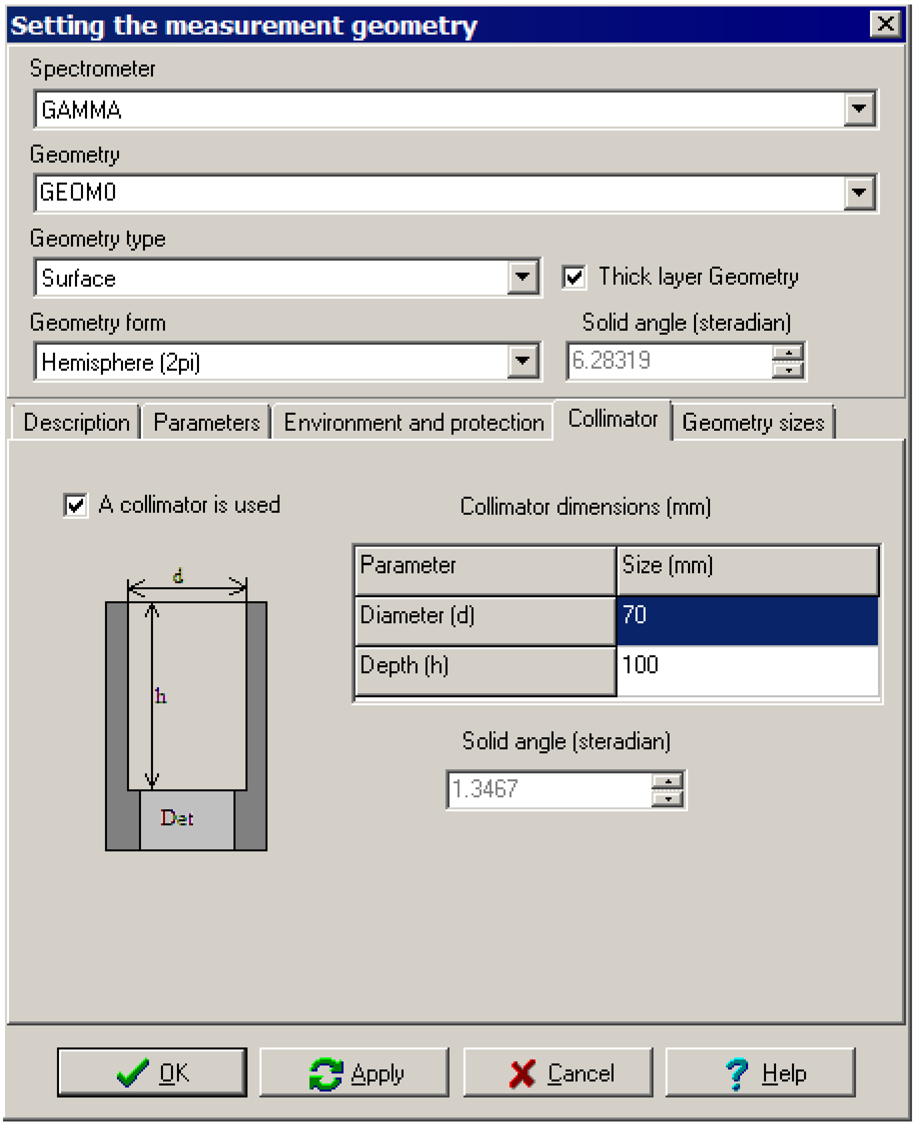
The material of the container (protection): Geometry\Container\Plastic\Polymer 1

Protection thickness (mm): 2.5

Density (g/cub cm): 1

The thickness of the container (protection) should not exceed the distance from the source to the detector. If the thickness of the container is equal to the distance from the source to the detector, it means that all the material of the medium has been displaced by the material of the container, and the calculation of radiation attenuation in the medium will not be performed, the parameters of the medium will not be editable. If the medium is a gas, then the density of the gas is not set directly, but is calculated using the chemical formula of the gas, temperature and pressure values.

On the fourth page "**Collimator**", the operator must specify the dimensions of the collimator if a radiation collimator is used for measurements.


Setting the measurement geometry

Spectrometer: GAMMA

Geometry: GEOM0

Geometry type: Surface

☑ Thick layer Geometry

Geometry form: Hemisphere (2pi)

Solid angle (steradian): 6.28319

☑ A collimator is used

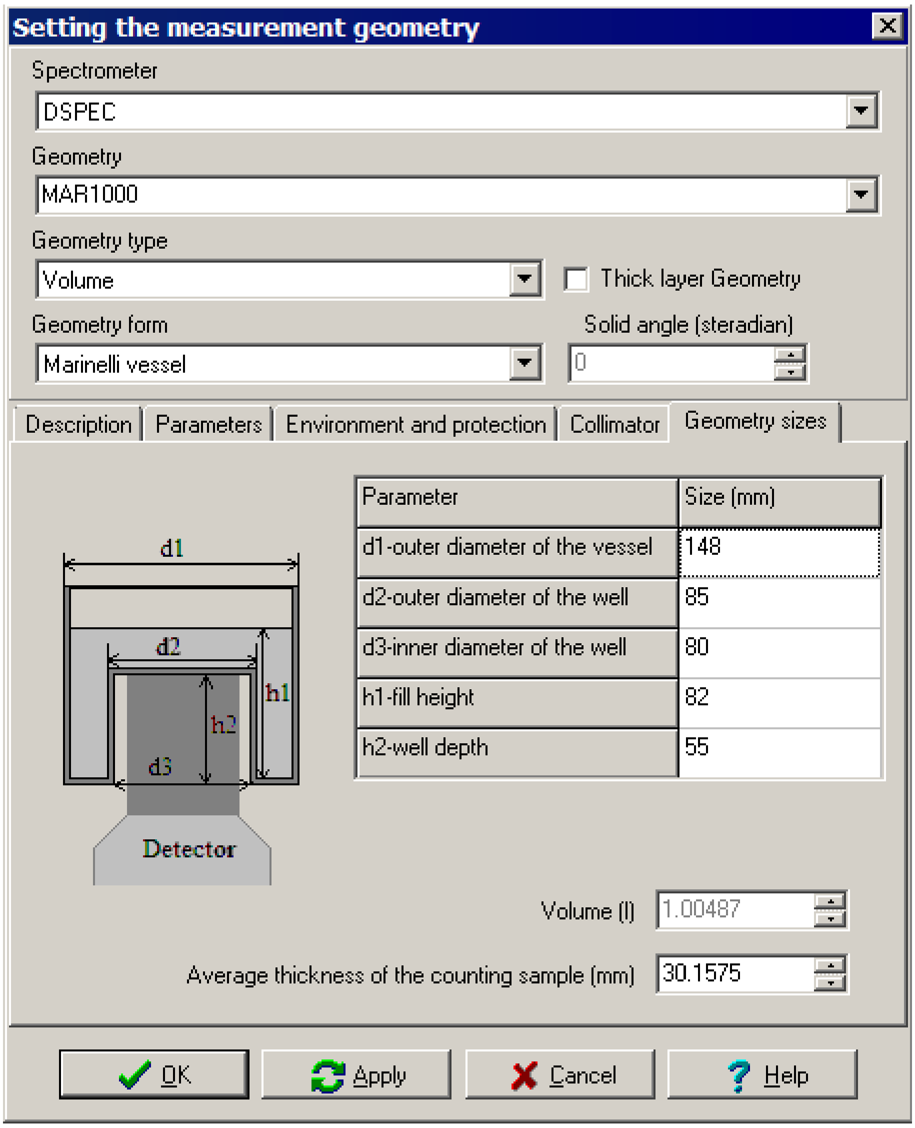
Collimator dimensions (mm)

Parameter	Size (mm)
Diameter (d)	70
Depth (h)	100

Solid angle (steradian): 1.3467

The dimensions of the collimator and the calculated "effective depth of the detector" determine the solid angle of quantum registration for the collimator. The solid angle of quantum registration used to calculate the registration efficiency will be the minimum value from the solid angle of the emitter and the solid angle of the collimator.

On the last page of "**Geometry sizes**", the operator must specify the dimensions of the vessel (container) used for measurements in this geometry. According to the specified dimensions, the program calculates the volume of geometry and the effective thickness of the counting sample - the parameters necessary to calculate the absorption of radiation in the substance of the counting sample.



Setting the measurement geometry

Spectrometer: DSPEC

Geometry: MAR1000

Geometry type: Volume

☐ Thick layer Geometry

Geometry form: Marinelli vessel

Solid angle (steradian): 0

Parameter	Size (mm)
d1-outer diameter of the vessel	148
d2-outer diameter of the well	85
d3-inner diameter of the well	80
h1-fill height	82
h2-well depth	55

Volume (l): 1.00487

Average thickness of the counting sample (mm): 30.1575

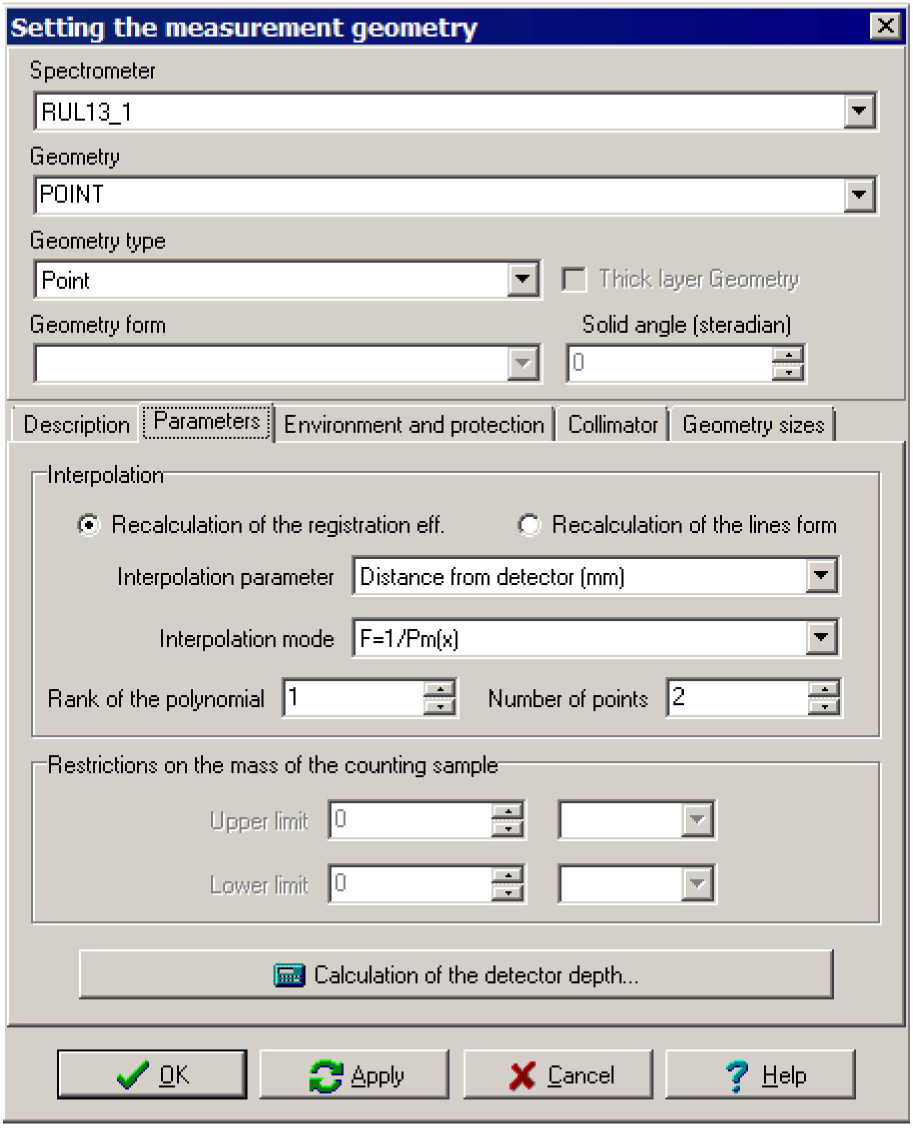
It is recommended to set the geometry of the check source as a separate geometry, even if the geometry of the check source coincides with one of the working geometries. In this case, it is possible to set a separate measurement archive for the geometry of the check source, in which all measurements related to monitoring the performance of the spectrometer will be stored: measurements of the check source and background radiation, which will make it more convenient to form the samples necessary for procedure of the spectrometer verification from this archive.

After installing the geometry of the check source, it is required to measure the check source in this geometry, then perform an energy calibration of the spectrometer, set up working measurement geometries, set up procedures for auto-calibration, background control and cyclic measurements, measure the background and standards in the established geometries, calculate and install elementary nuclide spectra in the program. For radiation spectrometers with a pronounced linear character, calibrate the width of the peaks, calibrate the efficiency of radiation registration in the peaks of total absorption and escape peaks, calculate and install line models in the program.

For a number of geometries, it is impossible to calculate the efficiency of registration by standards due to the lack of standards for this geometry (measuring the activity of soil on the ground, in the well); in this case, the efficiency of quantum registration for such geometries is calculated by the efficiency of quantum registration in point geometry. To do this, it is necessary to establish the point geometry of measurements, calibrate the efficiency of registration of point sources for several positions of sources relative to the detector to evaluate the geometric parameters of the recording volume of the detector – calculate the "**depth of the detector**" and after calculating the "depth of the detector" calculate the efficiency of registration in the required geometry.

Calculation of the "detector depth"

After calibration of the point geometry according to the registration efficiency, the procedure for calculating the "detector depth" becomes available - calculating the effective quantum registration center in a given direction. The change in the efficiency of registering a point source relative to such a center in a given direction has the character of a quadratic attenuation by distance from the center. The shape of the geometry installation in this case has the following form:



Spectrometer: RUL13_1

Geometry: POINT

Geometry type: Point

☐ Thick layer Geometry

Geometry form:

Solid angle (steradian): 0

● Recalculation of the registration eff.
○ Recalculation of the lines form

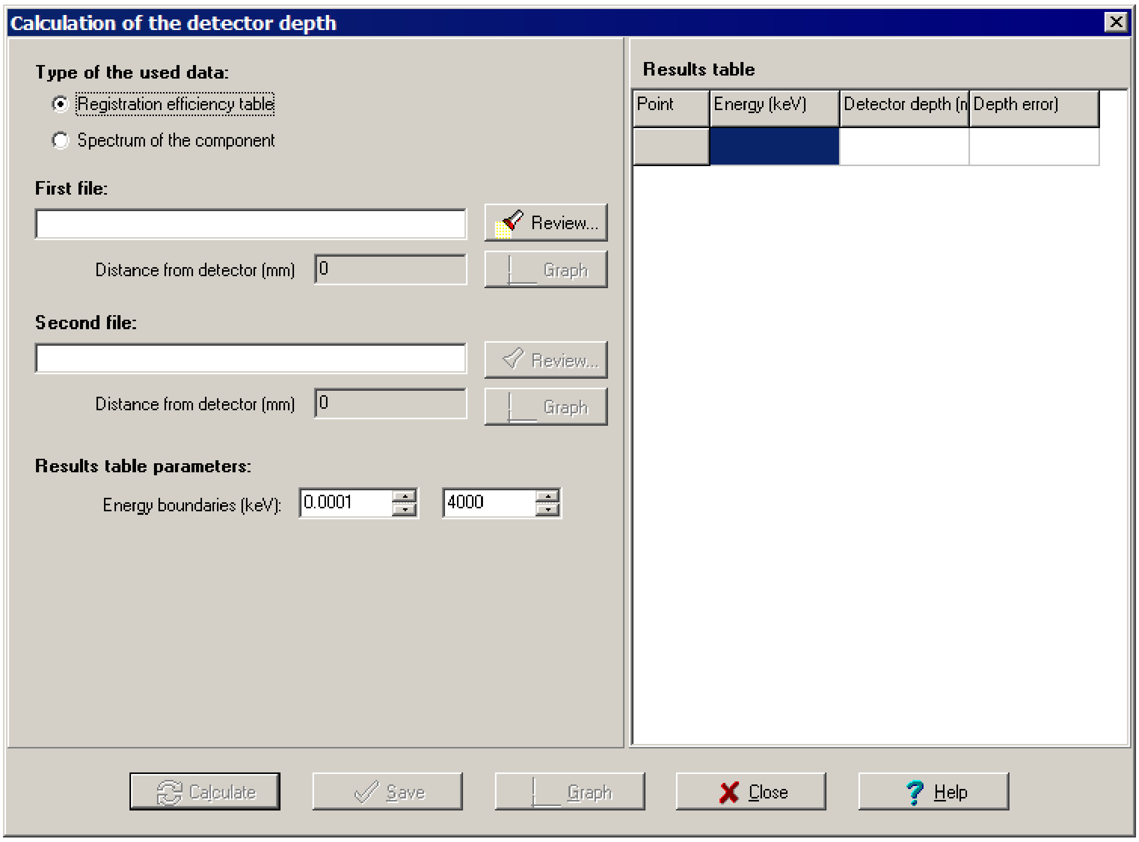
Interpolation parameter: Distance from detector (mm)

Interpolation mode: F=1/Pm(x)

Rank of the polynomial: 1
Number of points: 2

Upper limit: 0
Lower limit: 0

Clicking on the button "**Calculation of the detector depth...**" brings up the form of the calculation procedure:



Type of the used data:
● Registration efficiency table
○ Spectrum of the component

First file:
Distance from detector (mm) 0

Second file:
Distance from detector (mm) 0

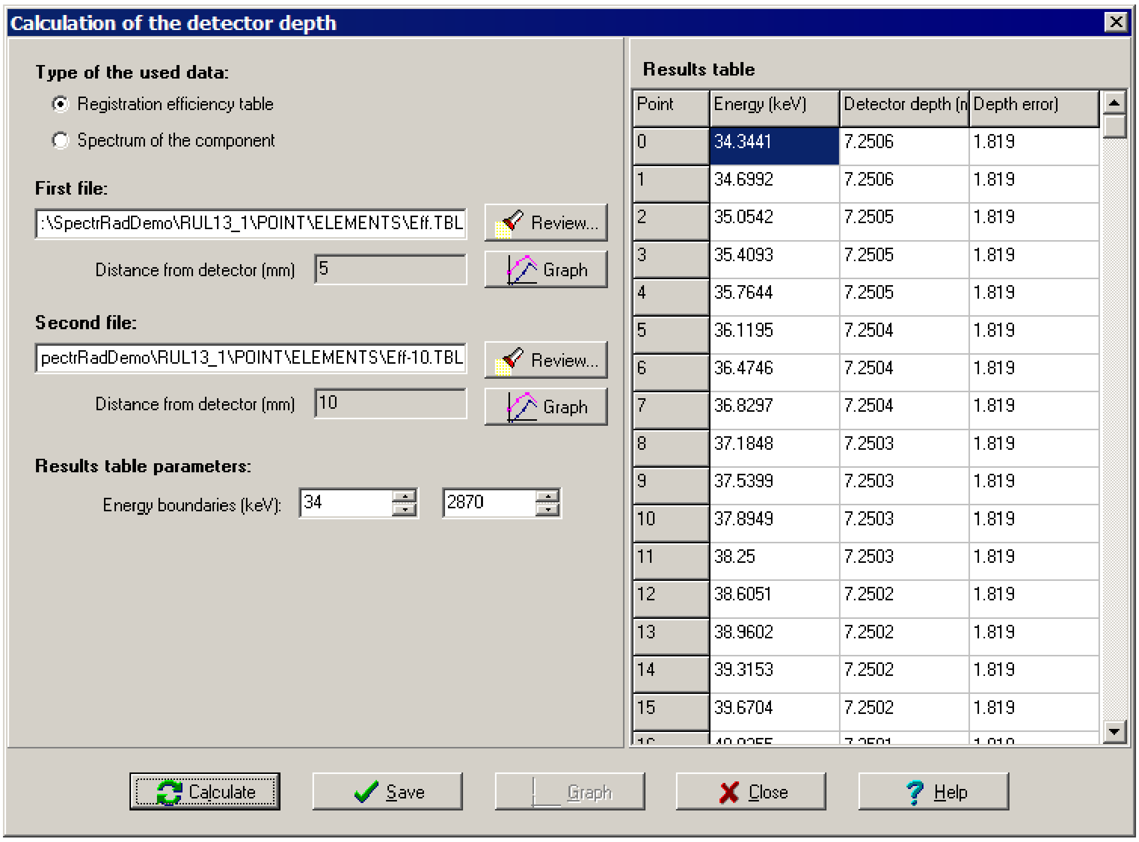
Results table parameters:
Energy boundaries (keV): 0.0001 4000

Results table

Point	Energy (keV)	Detector depth (n	Depth error)

The operator must select the type of data to use: **Registration efficiency table** in peaks of total absorption or **Spectrum of the component**. The spectra of the components can be used if there are no calibrations of the recording efficiency (scintillation spectrometry). Select the **first** and **second calibration file** with different values of the **distance from the detector**, set the parameters of **the result table** and click on the "**Calculate**" button.

The form will have the following form, for example:



Calculation of the detector depth

Type of the used data:

● Registration efficiency table

○ Spectrum of the component

First file: :\SpectrRadDemo\RUL13_1\POINT\ELEMENTS\Eff.TBL

Distance from detector (mm): 5

Second file: pectrRadDemo\RUL13_1\POINT\ELEMENTS\Eff-10.TBL

Distance from detector (mm): 10

Results table parameters:

Energy boundaries (keV): 34 2870

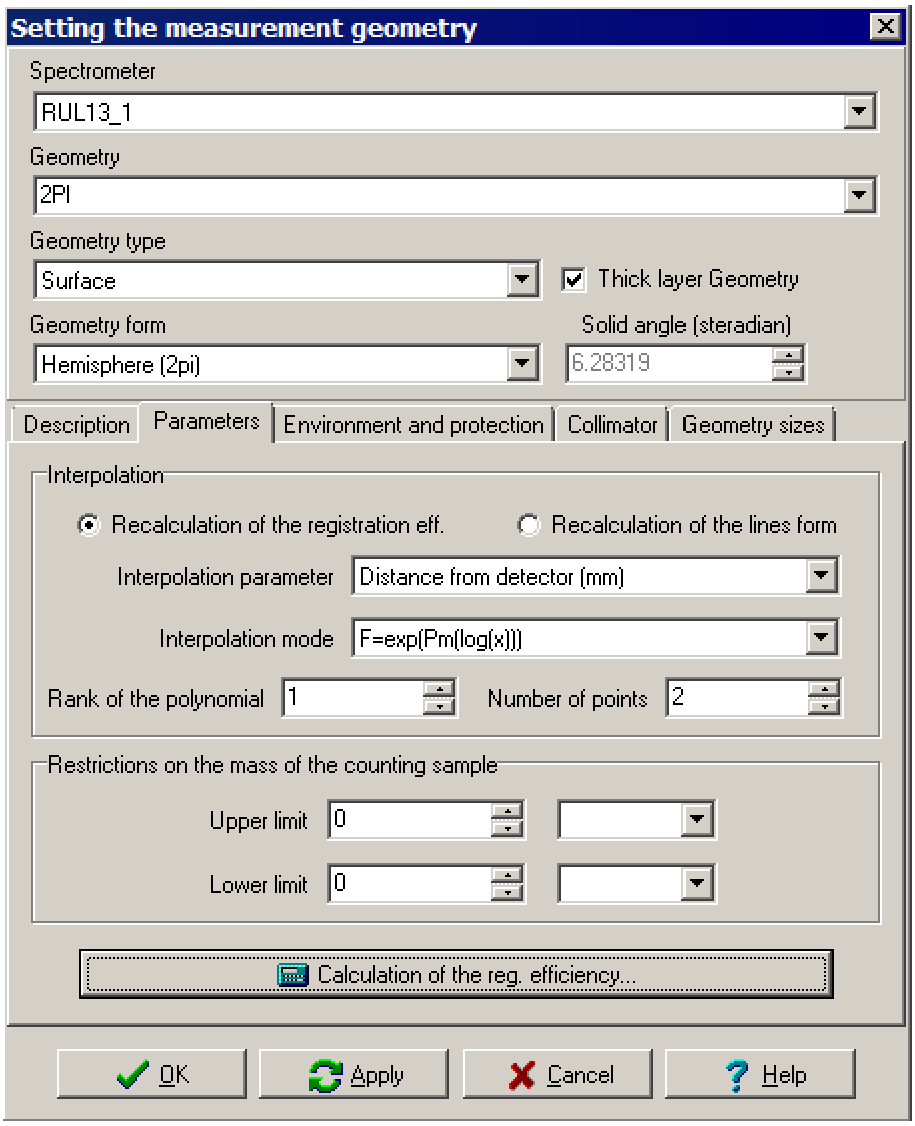
Results table

Point	Energy (keV)	Detector depth (n	Depth error)
0	34.3441	7.2506	1.819
1	34.6992	7.2506	1.819
2	35.0542	7.2505	1.819
3	35.4093	7.2505	1.819
4	35.7644	7.2505	1.819
5	36.1195	7.2504	1.819
6	36.4746	7.2504	1.819
7	36.8297	7.2504	1.819
8	37.1848	7.2503	1.819
9	37.5399	7.2503	1.819
10	37.8949	7.2503	1.819
11	38.25	7.2503	1.819
12	38.6051	7.2502	1.819
13	38.9602	7.2502	1.819
14	39.3153	7.2502	1.819
15	39.6704	7.2502	1.819

The operator must save the calculated table. The table is saved under the name "**DetectorDepth.tbl**" in the spectrometer folder. The operator can visualize the table and the spectrum files or registration efficiency tables used for calculation. At the same time, since the initial spectra or efficiency tables are reduced to zero radiation absorption during the calculation, the view of source files before and after the calculation will differ by the values of the absorption of radiation quanta.

Recalculation of the registration efficiency for a given geometry

After calibrating the registration efficiency for the point geometry and calculating the "detector depth", a procedure for calculating the effectiveness of detector registration for other geometry types becomes available. The shape of the geometry installation in this case has the following form:



Setting the measurement geometry

Spectrometer: RUL13_1

Geometry: 2PI

Geometry type: Surface

☑ Thick layer Geometry

Geometry form: Hemisphere (2pi)

Solid angle (steradian): 6.28319

Interpolation

● Recalculation of the registration eff. ○ Recalculation of the lines form

Interpolation parameter: Distance from detector (mm)

Interpolation mode: F=exp(Pm(log(x)))

Rank of the polynomial: 1

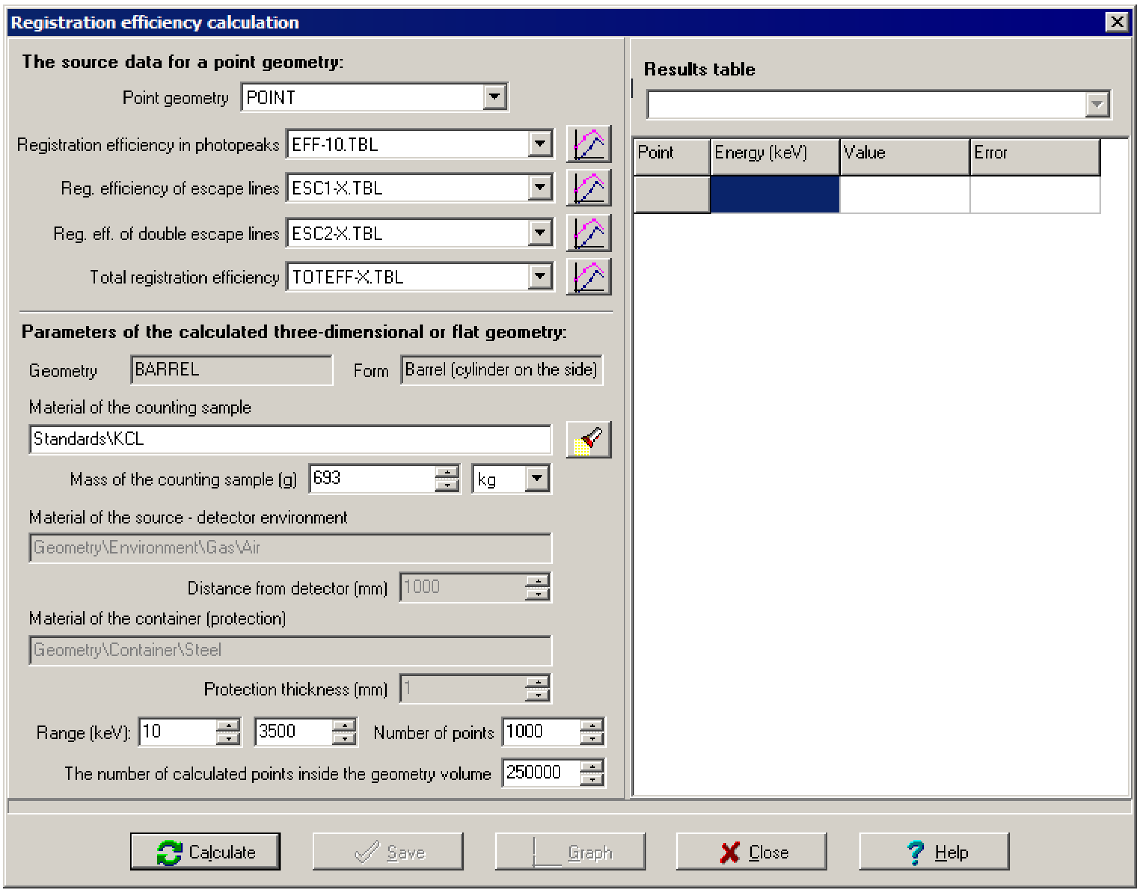
Number of points: 2

Restrictions on the mass of the counting sample

Upper limit: 0

Lower limit: 0

Clicking on the button "**Calculation of the reg. efficiency...**" brings up the form of the calculation procedure:



The source data for a point geometry:

Point geometry: POINT
Registration efficiency in photopeaks: EFF-10.TBL
Reg. efficiency of escape lines: ESC1-X.TBL
Reg. eff. of double escape lines: ESC2-X.TBL
Total registration efficiency: TOTEFF-X.TBL

Parameters of the calculated three-dimensional or flat geometry:

Geometry: BARREL
Form: Barrel (cylinder on the side)
Material of the counting sample: Standards\KCL
Mass of the counting sample (g): 693 kg
Material of the source - detector environment: Geometry\Environment\Gas\Air
Distance from detector (mm): 1000
Material of the container (protection): Geometry\Container\Steel
Protection thickness (mm): 1
Range (keV): 10 3500
Number of points: 1000
The number of calculated points inside the geometry volume: 250000

Point	Energy (keV)	Value	Error

The operator must select one of the existing **point geometries**, **registration efficiency** files for the point geometry, set the type of material for the calculated data (**Material of the counting sample**), **mass of the counting sample**, energy **range**, **number of points** of the calculated tables and the **number of calculated points inside the geometry volume**.

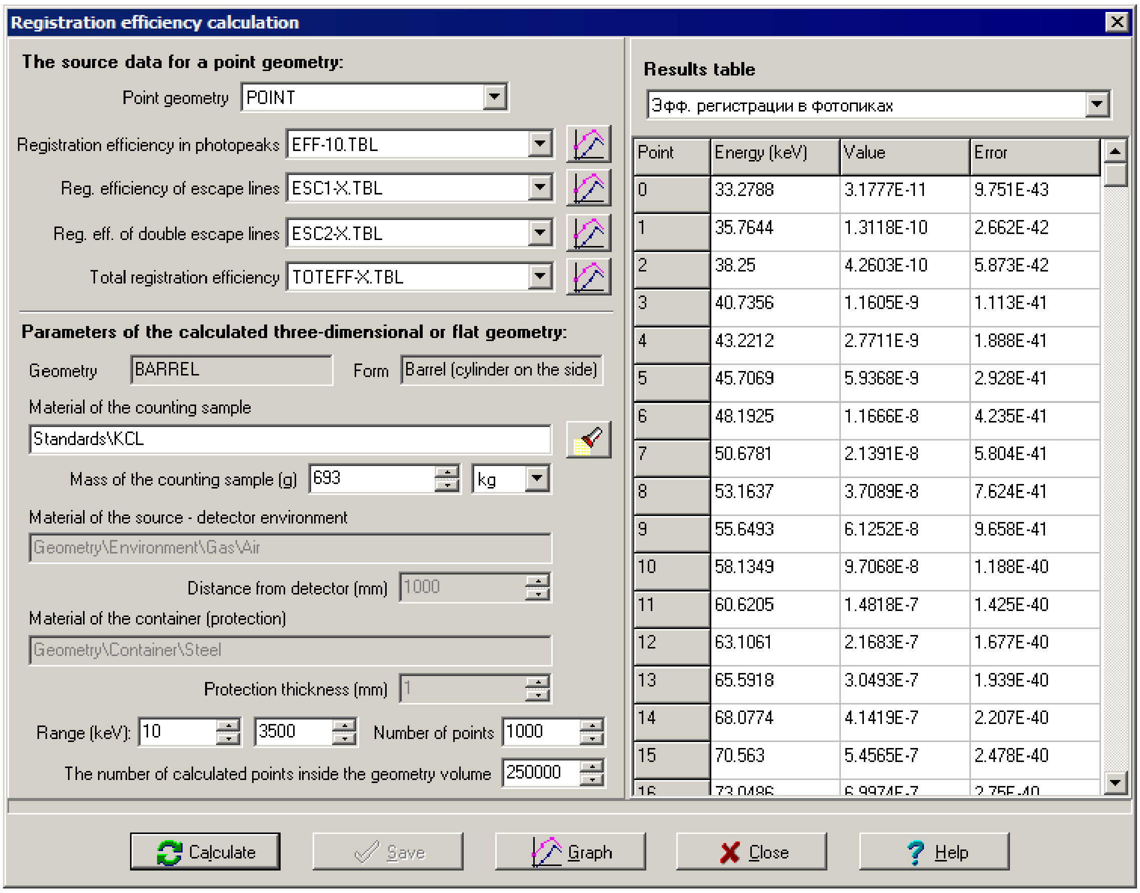
The calculation of the registration efficiency for volumetric or planar geometry is performed by averaging the point registration efficiency for a selected number of points within the volume of the calculated geometry, taking into account the distance to the effective center of the detector and the absorption in the substance of the counting sample, the container (protection) and the environment in which the counting sample and the detector are located.

The number of points of the calculated table (the density of the calculated table) and the number of calculated points inside the geometry volume determine the duration of the calculation. The more points are used, the more accurate, but the longer the calculation. Therefore, the number of points is chosen from a compromise between accuracy and speed.

The 📈 button allows you to visualize the selected data file, the button 🔦 find the required file with data on the counting sample material.

The calculation procedure is started by clicking on the "**Calculate**" button. The calculation procedure can be interrupted by pressing the "**Esc**" key on the computer keyboard.

Upon completion of the calculation procedure, the form will have the following view, for example:



The source data for a point geometry:

Point geometry: POINT

Registration efficiency in photopeaks: EFF-10.TBL

Reg. efficiency of escape lines: ESC1-X.TBL

Reg. eff. of double escape lines: ESC2-X.TBL

Total registration efficiency: TOTEFF-X.TBL

Parameters of the calculated three-dimensional or flat geometry:

Geometry: BARREL

Form: Barrel (cylinder on the side)

Material of the counting sample: Standards\KCL

Mass of the counting sample (g): 693 kg

Material of the source - detector environment: Geometry\Environment\Gas\Air

Distance from detector (mm): 1000

Material of the container (protection): Geometry\Container\Steel

Protection thickness (mm): 1

Range (keV): 10 3500

Number of points: 1000

The number of calculated points inside the geometry volume: 250000

Results table

Эфф. регистрации в фотопиках

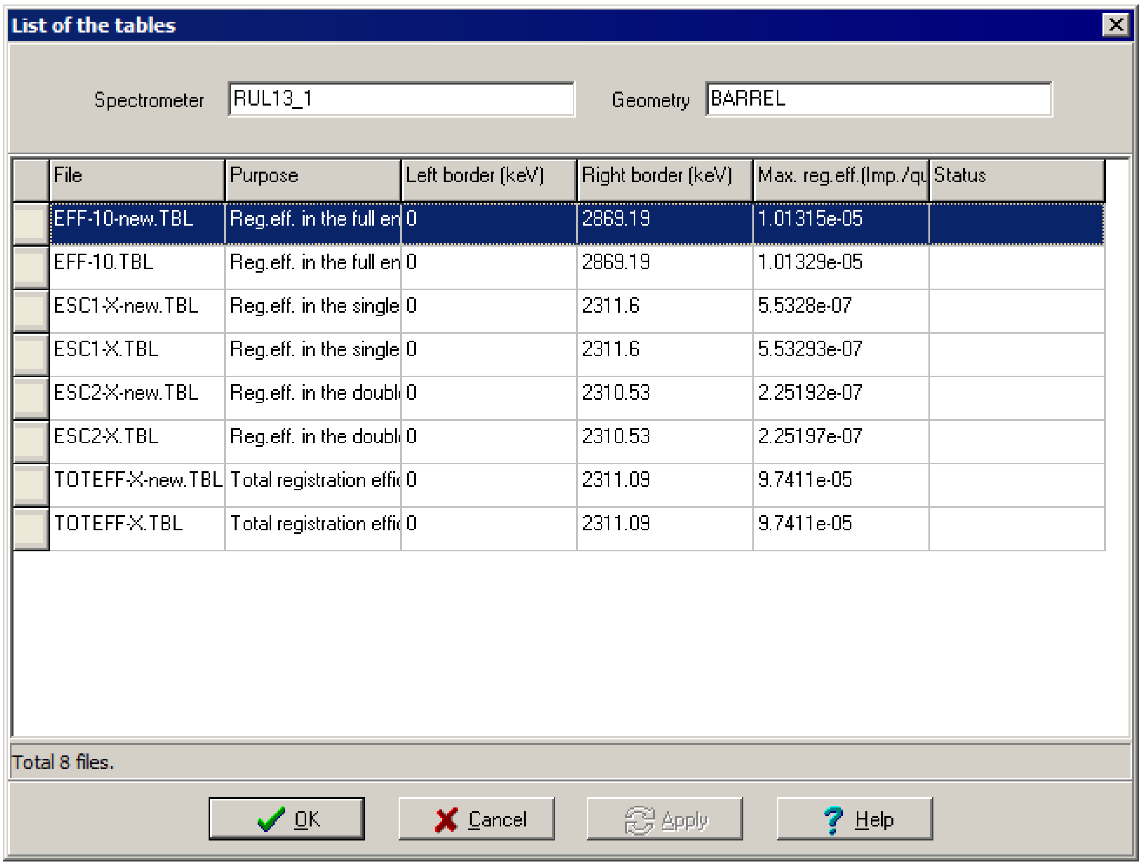
Point	Energy (keV)	Value	Error
0	33.2788	3.1777E-11	9.751E-43
1	35.7644	1.3118E-10	2.662E-42
2	38.25	4.2603E-10	5.873E-42
3	40.7356	1.1605E-9	1.113E-41
4	43.2212	2.7711E-9	1.888E-41
5	45.7069	5.9368E-9	2.928E-41
6	48.1925	1.1666E-8	4.235E-41
7	50.6781	2.1391E-8	5.804E-41
8	53.1637	3.7089E-8	7.624E-41
9	55.6493	6.1252E-8	9.658E-41
10	58.1349	9.7068E-8	1.188E-40
11	60.6205	1.4818E-7	1.425E-40
12	63.1061	2.1683E-7	1.677E-40
13	65.5918	3.0493E-7	1.939E-40
14	68.0774	4.1419E-7	2.207E-40
15	70.563	5.4565E-7	2.478E-40
16	73.0486	6.9974E-7	2.75E-40

If a table of the efficiency of registration of gamma quanta in photo peaks was also present in the source data set, the procedure, in addition to the efficiency of registration in photo peaks (peaks of total absorption of gamma quantum energy), also calculates a table of correction coefficients of registration efficiency for effects associated with registration of gamma quanta coinciding in time.

The operator must save the calculated tables. The registration efficiency tables are saved in the "**Elements**" folder of the corresponding geometry of the spectrometer. The table of registration efficiency correction coefficients is saved in the spectrometer geometry folder called "**CoincFactor.tbl**". The operator can visualize the calculated tables and the registration efficiency tables used for calculation.

To connect the calculated registration efficiency tables to the spectrum processing procedure, you can call up a list of files saved in the "**Elements**" folder of the corresponding geometry of the spectrometer. The list is formed by calling the main menu item "**Calibration / List of efficiency tables...**".

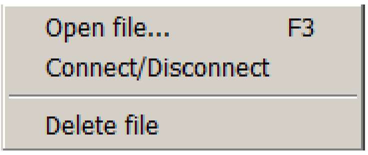
The list may look like this, for example:



Spectrometer RUL13_1 Geometry BARREL

File	Purpose	Left border (keV)	Right border (keV)	Max. reg.eff.(Imp./qu	Status
EFF-10-new.TBL	Reg.eff. in the full en	0	2869.19	1.01315e-05	
EFF-10.TBL	Reg.eff. in the full en	0	2869.19	1.01329e-05	
ESC1-X-new.TBL	Reg.eff. in the single	0	2311.6	5.5328e-07	
ESC1-X.TBL	Reg.eff. in the single	0	2311.6	5.53293e-07	
ESC2-X-new.TBL	Reg.eff. in the doubl	0	2310.53	2.25192e-07	
ESC2-X.TBL	Reg.eff. in the doubl	0	2310.53	2.25197e-07	
TOTEFF-X-new.TBL	Total registration effi	0	2311.09	9.7411e-05	
TOTEFF-X.TBL	Total registration effi	0	2311.09	9.7411e-05	

Total 8 files.

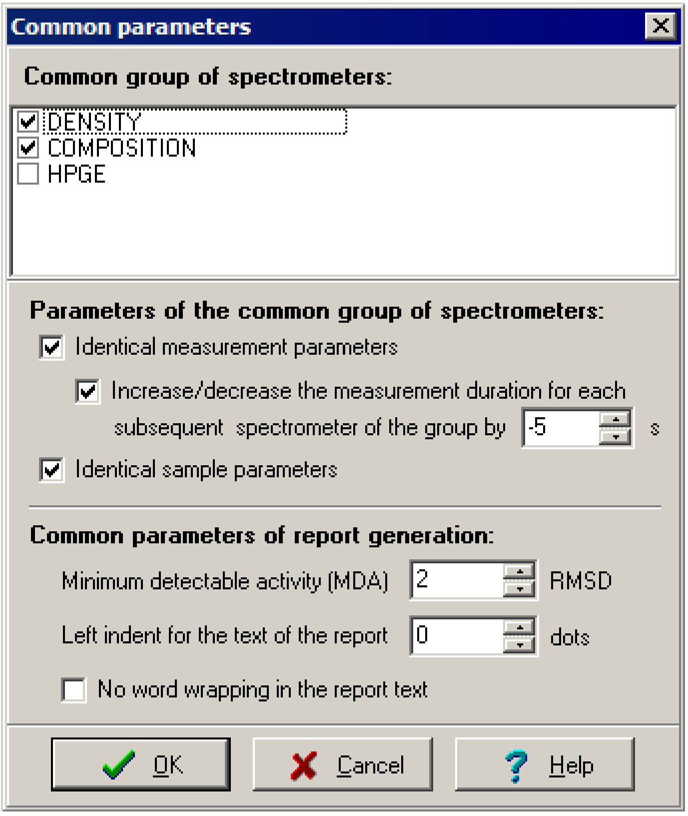


Using the pop-up menu (menu item "**Connect / Disconnect**"), the operator can connect the required tables or elementary spectra.

Setting up the measurement procedure

Setting up common parameters

The procedure is used to form a common group of spectrometers and set the parameters used in the formation of all reports. The procedure is called by the menu item "**Device / Configuration / Common parameters...**". At the same time, the procedure form appears on the screen:



Common parameters

Common group of spectrometers:

☑ DENSITY
☑ COMPOSITION
☐ HPGE

Parameters of the common group of spectrometers:

☑ Identical measurement parameters
☑ Increase/decrease the measurement duration for each subsequent spectrometer of the group by -5 s
☑ Identical sample parameters

Common parameters of report generation:

Minimum detectable activity (MDA) 2 RMSD
Left indent for the text of the report 0 dots
☐ No word wrapping in the report text

Common group of spectrometers is a group in which all operations related to the launch of measurements are synchronized – performed simultaneously. The measurement stop by the operator will also be synchronous. The measurements will be completed simultaneously if the "**Identical measurement parameters**" checkbox is selected. In this case, all measurement parameters in the group will be identical. If the "**Increase/decrease the measurement duration for each subordinate spectrometer of the group by n s**" checkbox is selected (**n** is the set value, a negative value of **n** reduces the duration of measurements), the measurement parameters in the spectrometers of the group will differ in the duration of the acquisition. This allows you to organize the streamline processing of spectra, which is important when implementing sequential processing of spectra in a group of spectrometers. For example, in Bayesian estimation, when the measurement results in the previous spectrometer is used as a priori data for spectrum processing in the current spectrometer.

If the "**Identical sample parameters**" checkbox is selected, the sample parameters will be entered only for one spectrometer from the group. The data collected will be used for other spectrometers of the group.

To create a common group of spectrometers, the operator must tick the appropriate spectrometers. Creating and editing a group is only available in **Full access** mode.

Common parameters of report generation:

- **Minimum detectable activity (MDA) -** minimum detectable activity in terms of **R**oot **M**ean **S**quare **D**eviation.
- **Left indent for the text of the report -** indentation from the left border of the form to the text of the report. The value is set in points. This parameter is used if the report is not included in the report template (in this case, its position is determined by the position of the label **{Report}** or **{Table}**).
- **No word wrapping in the report text -** setting or disabling automatic word wrapping in a paragraph

Setting up the cyclic measurement mode

Calibration of the spectrometer efficiency of recording radiation from nuclides (or quanta of various energies) will require measurements of reference sources. Moreover, in order to minimize the contribution of the error (uncertainty) of elementary spectra (efficiency functions) to the error in estimating sample activities, the spectra of the standards should be measured with very good statistics, which will require long-term measurements of the standards. Long-term measurements are also required for the study of certain types of samples with very strict safety standards.

Measurements of samples containing short–lived nuclides require, in order to effectively assess the time-varying activities of nuclides, the implementation of a measurement scheme at specified time intervals - an amplitude-time analysis scheme.

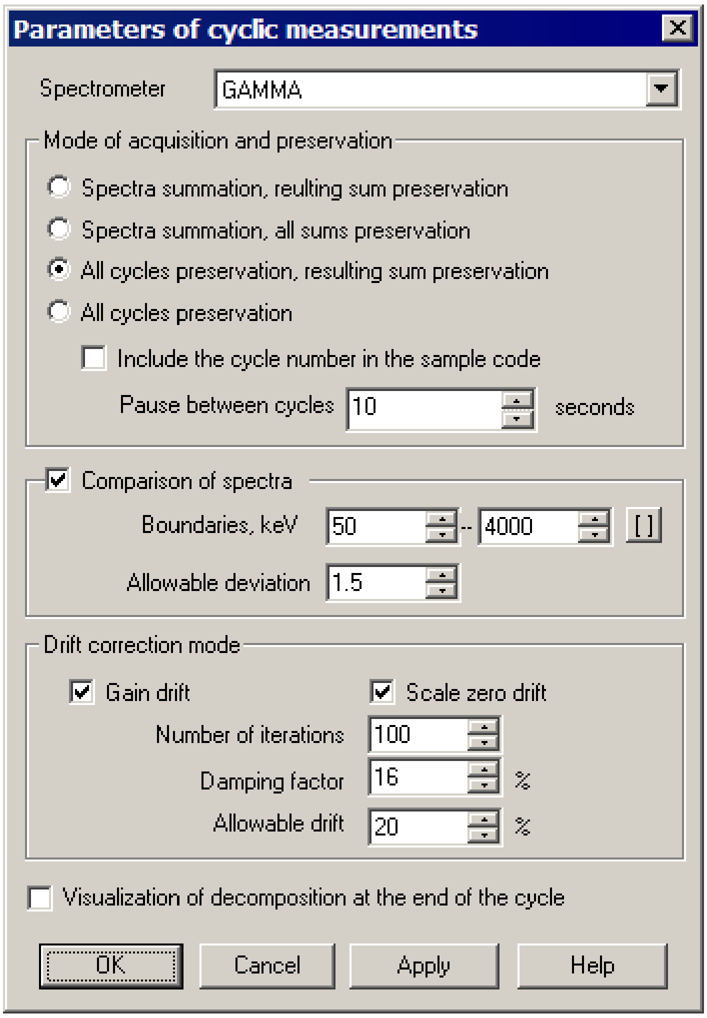
The organization of the control (monitoring) mode of technological processes requires continuous measurements or measurements at specified time intervals.

For these purposes, the SPECTRRAD package provides a cyclic measurement procedure. The essence of cyclic measurements is that the measurements of the sample are carried out a predetermined number of cycles of certain duration and the measurement results in individual cycles are either summarized and stored, or stored without summation. In this case, the program can compare the spectrum measured in the last cycle with the one accumulated earlier (or measured in the penultimate cycle) and thus control the stability of the spectrometer load (which is related to the stability of the spectrometer tract), and correct the energy drift of the spectrometer. The procedure for comparing spectra and, accordingly, correcting drift assumes the immutability (or insignificant changes) of the nuclide composition and the ratio of nuclide activity in the sample (radioactive equilibrium in the chains of nuclides present in the sample). If this condition is not met (short-lived nuclides are present in the sample), the operations of spectrum comparison and drift correction can be disabled.

Cyclic measurements allow you to save the accumulated spectrum in case of an accident of the spectrometer (power was lost, the computer was hopelessly frozen, etc.), since all the cycles accumulated by the time of the accident are already stored in the measurement archive and only the last cycle will be lost. After the accident has been eliminated (in principle, at any time, if there was no accident), the operator can continue measuring the sample in cyclic mode. To do this, you need to run the measurements of their archive, selecting the record of the desired sample as a working record and continue accumulating in the same spectrum file in the archive.

It is possible to process the spectrum after each cycle (when setting the processing template in the sample parameters), which can be useful for express analysis of the nuclide composition, analysis of changes in the nuclide composition or process monitoring mode. In the event that drift correction according to the procedure for comparing the accumulated spectrum and the spectrum of the last cycle is impossible due to the variability of the spectrum, correction of the drift of the spectrometer during cyclic measurements can be carried out after each cycle based on the results of processing the total spectrum.

Before performing cyclic measurements, it is necessary to set the necessary parameters of the cyclic measurement mode. To do this, by selecting the menu item "**Device / Configuration / Cyclic measurement...**", you must fill in the fields of the "**Parameters of cyclic measurements**" form for the selected spectrometer:



Parameters of cyclic measurements

Spectrometer: GAMMA

Mode of acquisition and preservation

- ○ Spectra summation, reulting sum preservation
- ○ Spectra summation, all sums preservation
- ● All cycles preservation, resulting sum preservation
- ○ All cycles preservation
- ☐ Include the cycle number in the sample code

Pause between cycles: 10 seconds

☑ Comparison of spectra

Boundaries, keV: 50 -- 4000 [ ]

Allowable deviation: 1.5

Drift correction mode

☑ Gain drift ☑ Scale zero drift

Number of iterations: 100

Damping factor: 16 %

Allowable drift: 20 %

☐ Visualization of decomposition at the end of the cycle

The form has three groups of parameters. In the "**Mode of acquisition and preservation**" group, the operator can choose one of four cyclic measurement modes:

- **Spectra summation, resulting sum preservation** is the main mode in which the program accumulates into one final spectrum, usually with correction of the energy drift of the spectrometer after each cycle.
- **Spectra summation, all sums preservation -** a mode in which all intermediate spectra of sums are saved.
- **All cycles preservation, resulting sum preservation -** saving all spectra accumulated in each measurement cycle, saving the sum of all cycles in a separate spectrum file.
- **All cycles preservation -** preservation of all spectra accumulated in each measurement cycle.

For modes with saving files for each cycle, when the "**Include the cycle number in the sample code**" checkbox is checked, the sample code (name) for the spectrum file of each cycle will be supplemented with the cycle number.

The "**Pause between cycles**" field allows you to set the time interval between measurement cycles, which may be necessary when implementing an amplitude-time analysis scheme, synchronizing measurements with the operation of an automatic sample changer or a measurement scheme related to the control of any processes.

The "**Comparison of spectra**" group - when the checkbox is selected, the spectrum comparison mode is enabled, which allows you to correct the energy drift of the spectrometer and evaluate the stability of the spectrometer tract. The group contains two parameters:

- **Boundaries** in units of the energy scale define the energy range in which the measured in the last cycle and the accumulated spectrum are compared. The "button" [ ] is used to substitute marker positions as processing boundaries. It is recommended to use the entire energy range with the exception of the regions of the beginning and end of the spectrum, which, due to the drift of the spectrometer, may leave the region of the spectrum set. Since the processing boundaries are set in units of the energy scale, the operator will have to return to setting the parameters of cyclic measurements after the initial calibration of the spectrometer.
- **Permissible deviation** - the maximum permissible level of the ratio of the real spectrum discrepancy to the theoretical one (normalized rooted mean square deviation $G = \sqrt{\sum((X_i - X_m)^2 / G_i^2)/(n-m)}$). The recommended value is from 1.5 to 2.0. If the discrepancy exceeds the specified threshold, the program will consider the process of comparing spectra to have failed and suspend cyclic measurements. In this case, the operator will be asked to decide whether to continue or stop measuring. If the operator decides to stop measuring, the last failed cycle will not be added to the accumulated spectrum, but will be saved in a separate file. If you decide to continue measuring, the spectra will be added up and the measurements will continue.

In the "**Drift correction mode**" group, the operator must determine the parameters for correcting the energy drift of the spectrometer during measurement.

- First of all, select the "drifting" parameters of the spectrometric tract: **Gain drift** and (or) **Scale zero drift**. When the appropriate checkboxes are selected, the program will adjust the drift of the gain coefficient of the tract, and (or) the drift of the zero. Usually both parameters drift and it is recommended to check both boxes.
- **Number of iterations** – limits the process of refining drift parameters to a given number of iterations. Setting a small number of iterations makes sense for computers with low performance.
- **Damping factor** - a constant (set as a percentage) increases the stability of the solving process. It makes sense if the process has an oscillatory character, which can happen if the system is poorly conditioned (a slight change in the shape of the spectrum with large changes in the drift parameters or an almost identical change in the shape of the spectra with changes in various parameters).
- **Allowed drift** - if the drift exceeds the specified threshold, the program will consider the drift correction process to have failed and interrupt cyclic measurements.

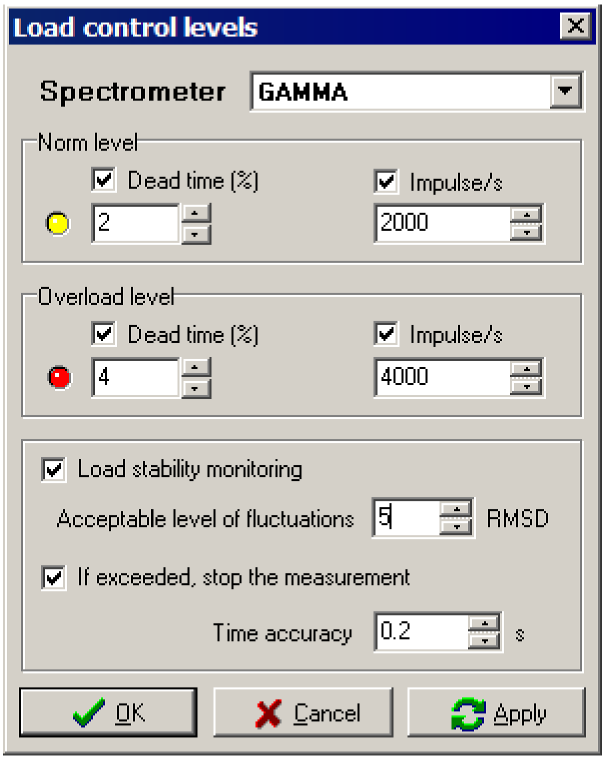
Checking the box "**Visualization of decomposition at the end of the cycle**" enables the visualization mode for comparing spectra and correcting drift at the end of the cycle.

Since the drift correction mode is based on comparing the shape of the spectrum measured in the last cycle with the shape of the accumulated spectrum, it is assumed that the nuclide composition of the sample remains unchanged during measurement. If the sample spectrum changes during measurement (short-lived nuclides are present in the sample), drift correction should be disabled.

Loading monitoring

Spectrometer loading is a term related to the intensity of the pulse flux (radiation quanta) recorded by the spectrometer and the time characteristics of the spectrometer. Processing of each pulse registered by the detector requires a certain time, during which the spectrometer cannot register other pulses. This time is the "**dead time**" of the spectrometer. Accordingly, the time when the spectrometer is open for recording pulses is "**live time**", less than the **real** (astronomical) **time** by the amount of "dead".

The item "**Device / Configuration / Loading monitoring...**" of the main menu (item "**Loading monitoring...**" of the popup menu of the "**Spectrometers state**" window) displays a window for setting the control levels of loading spectrometers:



Spectrometer: GAMMA

Norm level
☑ Dead time (%): 2
☑ Impulse/s: 2000

Overload level
☑ Dead time (%): 4
☑ Impulse/s: 4000

☑ Load stability monitoring
Acceptable level of fluctuations: 5 RMSD
☑ If exceeded, stop the measurement
Time accuracy: 0.2 s

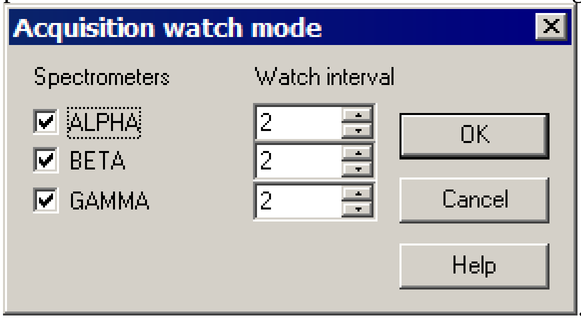
The operator must set two control levels of the spectrometer load: "**Norm level**" and "**Overload level**" and can set the **Load stability monitoring** mode by setting the appropriate "checkboxes". If both "checkboxes" are set: for monitoring by "**Dead time (%)**" and by absolute loading (**Impulse/s**), the program will issue an appropriate warning if any of the thresholds are exceeded.

In the **load stability monitoring** mode, the spectrometer after a certain time (load measurement time) compares the load levels in pulses/sec for the past and elapsed period and, if they differ by an amount greater than that specified in the "**Acceptable level of fluctuations**" field (in units of Rooted Mean Square Deviation), the monitoring program issues a warning message and, if the "**If exceeded, stop the measurements**" checkbox is selected, suspends the measurements until the operator decides to continue or abort the measurements. In the "**Time accuracy**" field, the error of the time interval in seconds is set.

Watching the spectrum acquisition

The program allows you to monitor the spectrum acquisition in all the included spectrometers (you can connect up to twelve spectrometers and take measurements simultaneously in all spectrometers).

The time parameters of the acquisition monitoring mode are set by calling the item "**Device / Configuration / Watch mode...**" in the main menu. If, for example, three spectrometers "ALPHA", "BETA" and "GAMMA" are connected in the program, the window for setting the parameters of the set monitoring mode may look like this:



Acquisition watch mode

Spectrometers	Watch interval
☑ ALPHA	2
☑ BETA	2
☑ GAMMA	2

.

The operator has the opportunity to turn on or off the acquisition monitoring mode by clicking the left mouse button and putting or removing the "tick" in the square window in front of the name of the spectrometer.

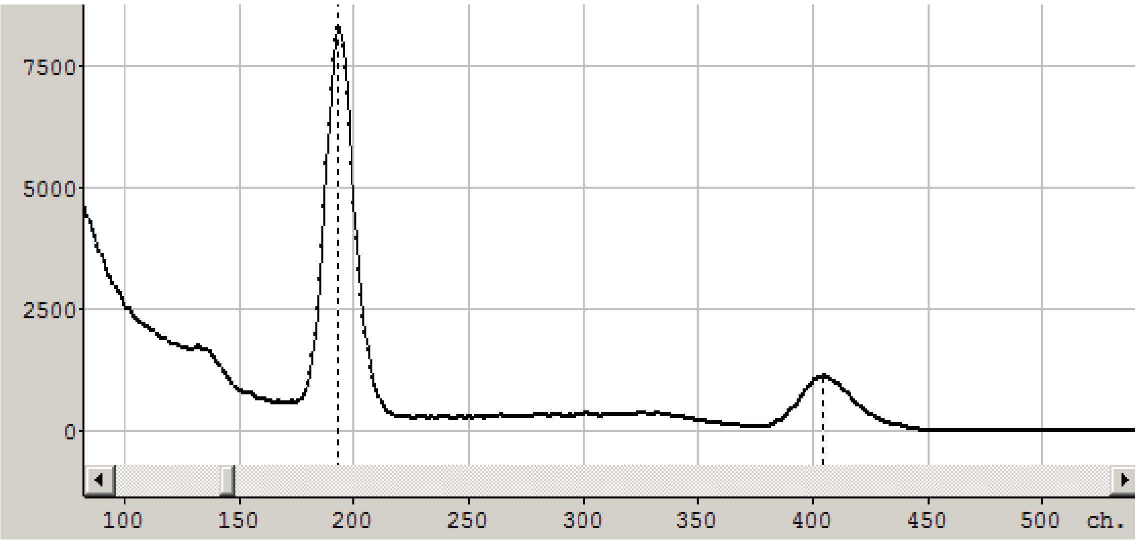
The observation period (the time after which the spectrum from the spectrometer will be read into the program window) is set in the window to the right of the name of the spectrometer.

Calibration of the spectrometer

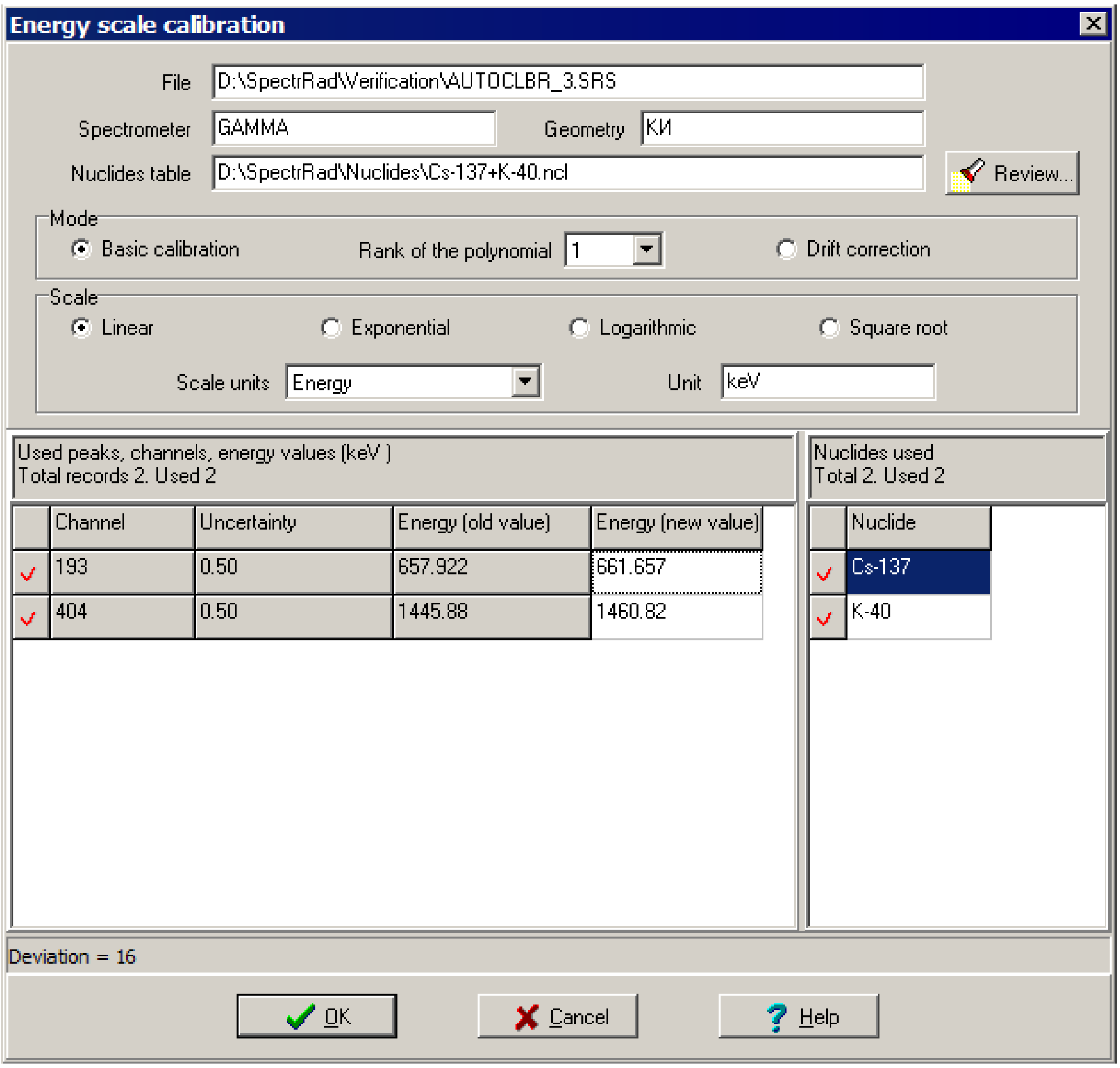
Energy calibration

The energy calibration of the spectrometer (or selected spectrum) is used to determine the correspondence between the channels of the spectrometer (spectrum) and the energy of the recorded radiation. In the "SPECTRRAD" package, it is assumed that the spectrum can be a distribution of the number of impulses not only by energy, but also by some other parameter - for example, time (time analysis), date, etc. Therefore, the abscissa scale can be not only an energy scale, but also a scale of other specified parameters.

After selecting the energy range and setting the parameters of the spectrometric tract, it is necessary to perform an initial energy calibration of the spectrometer. To do this, after measuring the calibration source, it is required to mark with a movable marker the channels of the spectrum corresponding to known energies: peaks or medians of peaks of known energies, boundary energies for beta spectra (for example, as in the figure).



Then, by selecting the menu item "**Calibration / Scale X (Energy) / By entered data...**", call the energy calibration procedure. The window (form) of the procedure will look like this:



Energy scale calibration

File D:\SpectrRad\Verification\AUTOCLBR_3.SRS

Spectrometer GAMMA

Geometry KИ

Nuclides table D:\SpectrRad\Nuclides\Cs-137+K-40.ncl

Mode

● Basic calibration

Rank of the polynomial 1

○ Drift correction

Scale

● Linear ○ Exponential ○ Logarithmic ○ Square root

Scale units Energy

Unit keV

Used peaks, channels, energy values (keV)
Total records 2. Used 2

	Channel	Uncertainty	Energy (old value)	Energy (new value)
✓	193	0.50	657.922	661.657
✓	404	0.50	1445.88	1460.82

Nuclides used
Total 2. Used 2

	Nuclide
✓	Cs-137
✓	K-40

Deviation = 16

The two upper fields of the energy calibration procedure form: "**File**" and "**Spectrometer**" are informational and contain the name of the spectrum file for which calibration is performed and the name of the spectrometer to which this spectrum belongs.

The "**Nuclides table**" field indicates the nuclide table used. The Review... button allows you to select the desired table. Using the nuclide table during calibration makes the calibration procedure more convenient: the operator can substitute the required energy value directly from the table, can select the peaks required for calibration using the information contained in the nuclide table. The nuclide table used for calibration must be prepared beforehand. It should contain information about calibration lines - the most powerful gamma or alpha lines, which the operator, when creating or editing the table, assigned calibration lines and indicated for them the energy range in which the calibration procedure will look for the most powerful peak in the spectrum to link the line energy to the peak position. By default, the table specified when setting the measurement geometry is used as the nuclide table.

There are two **modes** of energy calibration:

- **Basic calibration -** generates the basic calibration of the spectrometer. The basic calibration is a valid calibration for all elementary spectrometer spectra (including the autocalibration file) and is performed during the initial calibration of the spectrometer after setting the parameters of the spectrometer ADC. For initial calibration, you need to set the "**Rank of the polynomial**" (it can take values from 1 to 3), which, together with the number of points used for calibration, determines the real rank of the calibration polynomial. If the number of points is equal to or less than the specified rank, the rank of the calibration polynomial will be one less than the number of calibration points.

- **Drift correction** is used during operation to correct an excessively large energy drift of the spectrometer, in the event that the autocalibration procedure fails to cope with such a drift. After manual drift correction, it is recommended to perform an autocalibration of the spectrometer to clarify the drift parameters.

Below the "**Mode**" parameter group is the "**Scale**" parameter group, which determines the nature of the conversion of quantum energy into the magnitude of an electric pulse by the spectrometer:

Scale	**The reverse conversion function**[16]
Linear	$E = Pn(z)$
Exponential	$E = \exp(Pn(z))$
Logarithmic	$E = \log(Pn(z))$
Square root	$E = \sqrt{Pn(z)}$

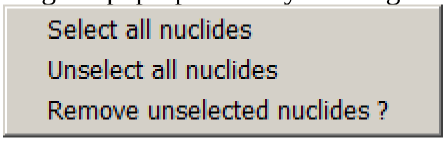
Here: **E**- energy (abscissa); ***z*** is the position of the pulse on the channel scale; **Pn(z)** is a polynomial.

By default, the linear scale is used $E = Pn(z)$.

At the bottom of the "**Scale**" group, the drop-down list is "**Scale units**" and the "**Unit**" field. The "**Scale units**" list has three lines: "**Energy**", "**Date/Time**" and "**Custom**", available only in the initial calibration mode. The "**Unit**" field, when selecting the "**Custom**" value, is used to enter the name of the unit of measurement of the scale. When selecting the values "**Energy**" or "**Date / Time**", the "**Unit**" field is informative.

There are two tables in the central part of the calibration procedure form: a table of peaks (channels) used and their corresponding energies and a table of nuclides used in calibration. Only marked table entries participate in the calibration procedure. The marked records are highlighted with a red check mark in the first column of the tables.

The operator can specify the **nuclides** (in the right table of the form) present in the calibration source. The selection of nuclides is made by double-clicking the left mouse button or by calling the pop-up menu by clicking the right mouse button:



The operator must select the "**Basic calibration**" mode and enter the energy values of the labeled spectrum channels in kiloelectronvolts[17] in the "**Energy (new value)**" column. The energy values can be substituted from the nuclide table used for calibration. Double-clicking on the cell of the column "**Energy (new value)**" or right-clicking on the menu (menu item "**Select**

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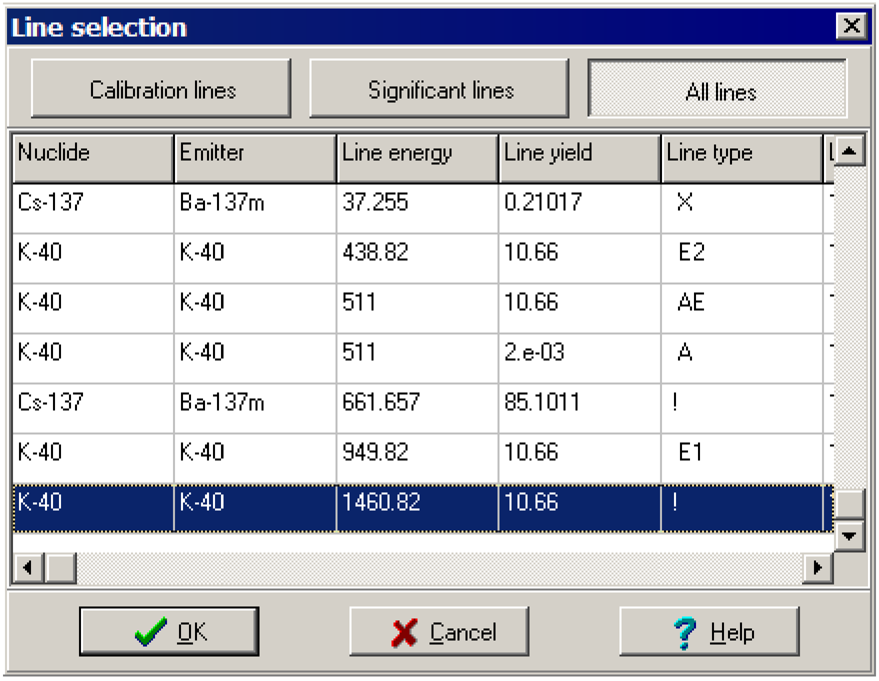
[16] The energy calibration uses a **reverse conversion function** that relates the energy of the quanta to the position of the pulses on the channel scale. In the name of the scale of a particular spectrometer, a direct transformation can also be indicated, and in this case, the exponential scale will be called logarithmic, and the logarithmic scale will be called exponential.

[17] The energy measurement units for the spectrometer scale should be the same as the energy measurement units in the nuclide tables used. Since the nuclide tables are included in the delivery package, in which the energy of the lines is set in kiloelectronvolts, it is recommended to calibrate the spectrometer scale also in kiloelectronvolts.

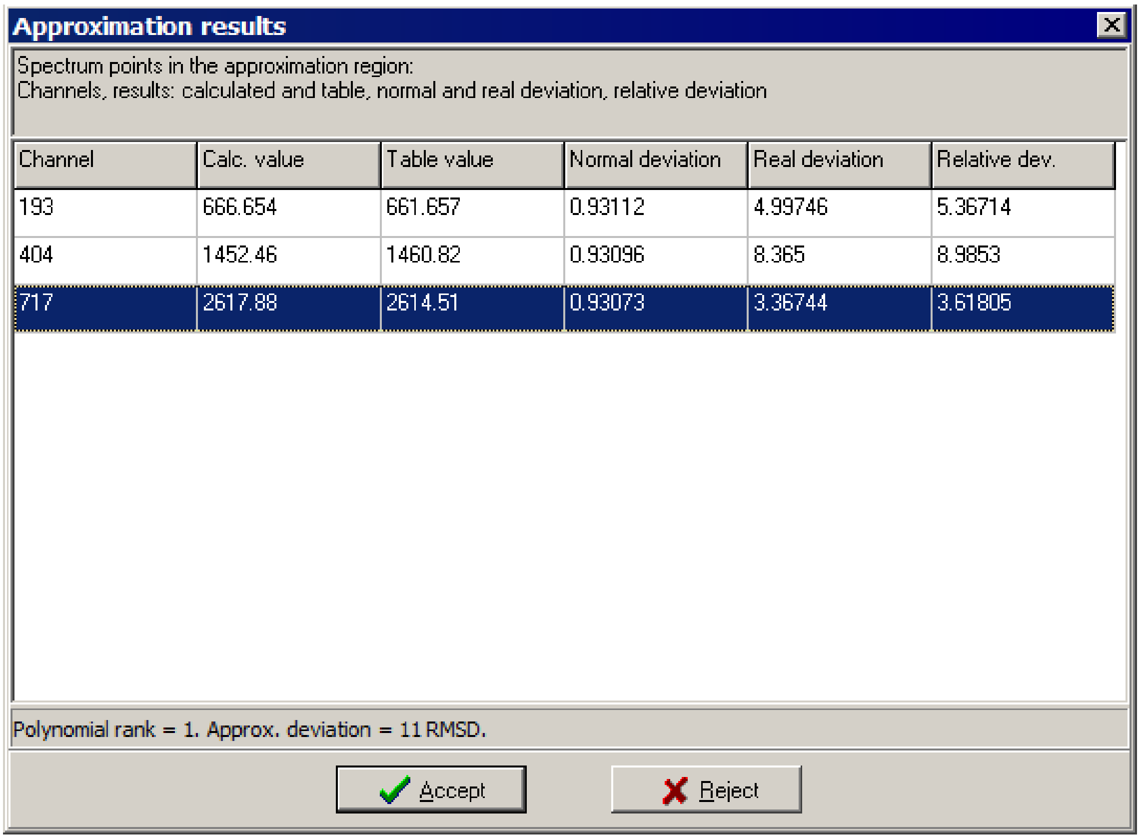
line...") allows you to substitute the required energy value. At the same time, a table is displayed on the screen



Nuclide	Emitter	Line energy	Line yield	Line type
Cs-137	Ba-137m	37.255	0.21017	X
K-40	K-40	438.82	10.66	E2
K-40	K-40	511	10.66	AE
K-40	K-40	511	2.e-03	A
Cs-137	Ba-137m	661.657	85.1011	!
K-40	K-40	949.82	10.66	E1
K-40	K-40	1460.82	10.66	!

The table displays the lines of the nuclides marked with the operator (the marked entries are highlighted with a red check mark in the first column of the list) of the nuclide table used. For the convenience of selecting a line, the operator can switch to the display mode of only calibration lines by pressing the "**Calibration lines**" key or significant lines by pressing the "**Significant lines**" button. Calibration lines are marked in the "**Line type**" column with an exclamation mark. Significant lines are marked in the "**Line type**" column with a "percentage - %" sign or an exclamation mark (since significant lines include calibration lines).

Clicking on the "**OK**" button of the main form of the calibration procedure starts the program for calculating the calibration polynomial. If the number of points used for calibration exceeds the rank of the calibration polynomial by more than one, that is, the number of points is excessive for calculating the coefficients of the polynomial, the calibration procedure calculates them using the least squares method and calculates the approximation discrepancy. At the same time, the form is displayed on the screen: with a table of approximation results:



Spectrum points in the approximation region:
Channels, results: calculated and table, normal and real deviation, relative deviation

Channel	Calc. value	Table value	Normal deviation	Real deviation	Relative dev.
193	666.654	661.657	0.93112	4.99746	5.36714
404	1452.46	1460.82	0.93096	8.365	8.9853
717	2617.88	2614.51	0.93073	3.36744	3.61805

Polynomial rank = 1. Approx. deviation = 11 RMSD.

The "**Normal deviation**" column contains the permissible energy deviation calculated from the error of setting the position of the calibration points. The position error determined by the marker is assumed to be equal to 0.5 channels. "**Real deviation**" is the deviation of the tabular energy value from the calculated one using the approximating polynomial. "**Relative dev.**" **-** the actual deviation divided by the normal one. The rank of the calibration polynomial and the average normalized approximation discrepancy are indicated at the bottom of the table.

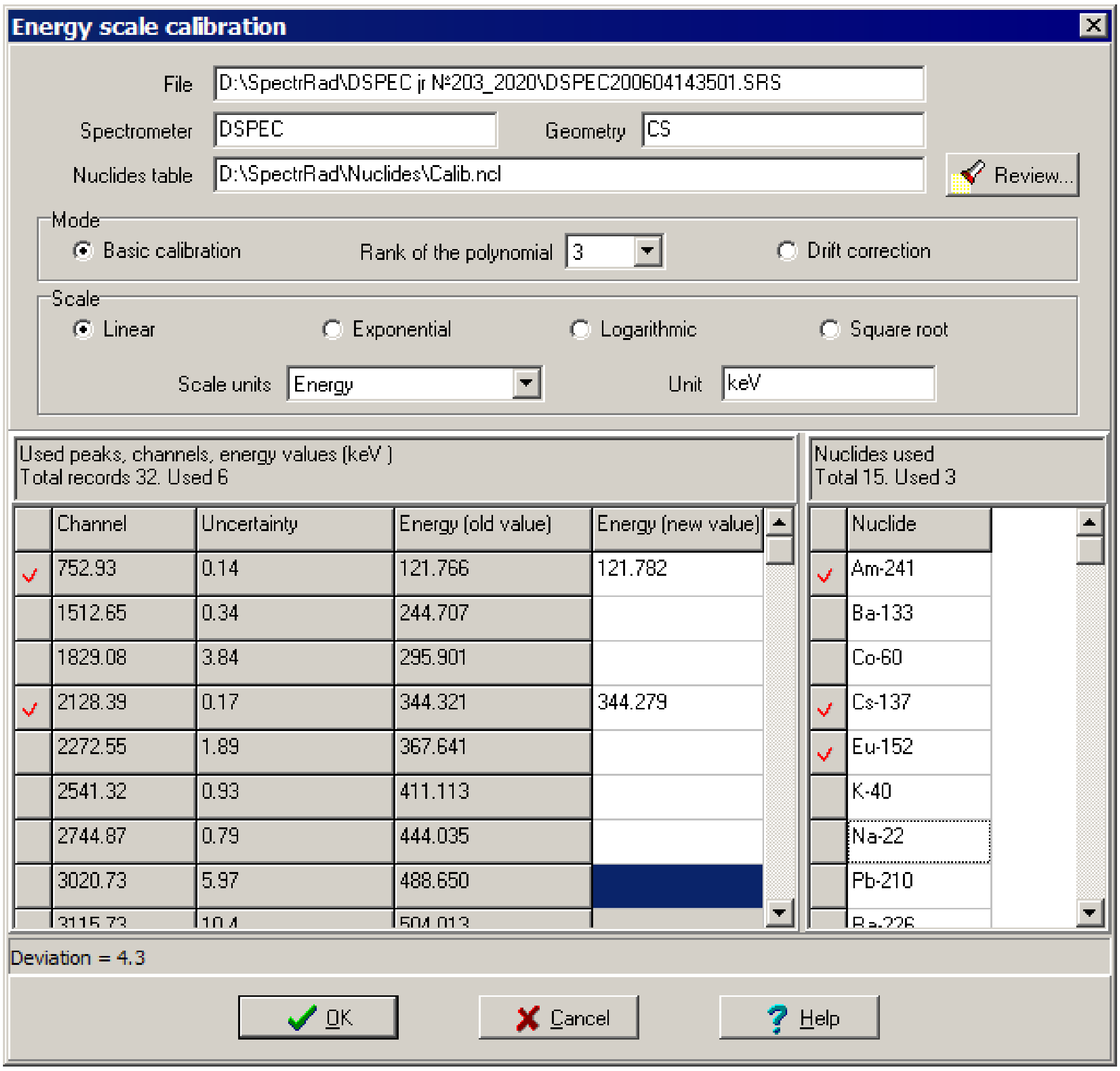
The operator can accept or reject the calibration results. If the results are rejected, the program returns to the form of the calibration procedure, and the operator has the opportunity to correct the calibration data or change the rank of the polynomial.

When you press the "**Accept**" key, the program will prompt you to save the calibration accepted for the used spectrum as a spectrometer calibration that must be performed.

If desired, the calibration curve graph can be viewed by selecting the menu item "**Calibration / Scale X (Energy) / Visualization**".

For poorly resolved or continuous spectra (scintillation gamma spectrometry, beta spectrometry), the energy calibration of the spectrometer can be considered complete. For permitted linear spectra (HPGe gamma spectrometry), the energy calibration of the spectrometer will have to be returned more than once: more accurate calibration by peak positions and even more accurate – by the positions of calculated line models require additional calibrations and program settings.

Therefore, after calibrating the peak widths, setting up the peak search procedure and spectrum processing using the "**Peaks search**" procedure for resolved spectra, we must return to the energy calibration procedure of the spectrometer. And if, for example, we used Eu-152 to calibrate a gamma spectrometer with a cooled semiconductor detector, the form for energy calibration may look like this:



Energy scale calibration

File: D:\SpectrRad\DSPEC jr №203_2020\DSPEC200604143501.SRS

Spectrometer: DSPEC Geometry: CS

Nuclides table: D:\SpectrRad\Nuclides\Calib.ncl

Mode: ● Basic calibration Rank of the polynomial: 3 ○ Drift correction

Scale: ● Linear ○ Exponential ○ Logarithmic ○ Square root

Scale units: Energy Unit: keV

Used peaks, channels, energy values (keV)
Total records 32. Used 6

	Channel	Uncertainty	Energy (old value)	Energy (new value)
✓	752.93	0.14	121.766	121.782
	1512.65	0.34	244.707	
	1829.08	3.84	295.901	
✓	2128.39	0.17	344.321	344.279
	2272.55	1.89	367.641	
	2541.32	0.93	411.113	
	2744.87	0.79	444.035	
	3020.73	5.97	488.650	
	3115.73	10.4	504.013	

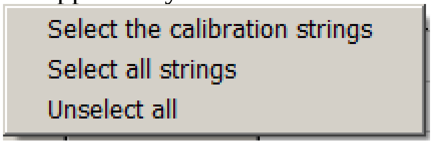
Nuclides used
Total 15. Used 3

	Nuclide
✓	Am-241
	Ba-133
	Co-60
✓	Cs-137
✓	Eu-152
	K-40
	Na-22
	Pb-210
	Ra-226

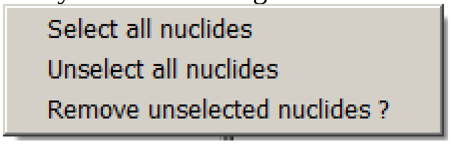
Deviation = 4.3

To select the peaks used for calibration, the operator can pre–mark them in the spectrum, but can enable or exclude them directly in the form: double-clicking on the row with the desired record in the area of the first four columns switches the recording state: enabled recording is excluded, and not enabled recording is enabled.

In addition, the operator has the opportunity to select calibration peaks using the pop-up menu activated by right-clicking: . Calibration string is a string with a minimum error in the position of the peak (or calibration point) and the energy value corresponding to the current calibration "**Energy (old value)**", falling within the range specified for the calibration line at the nuclide table.



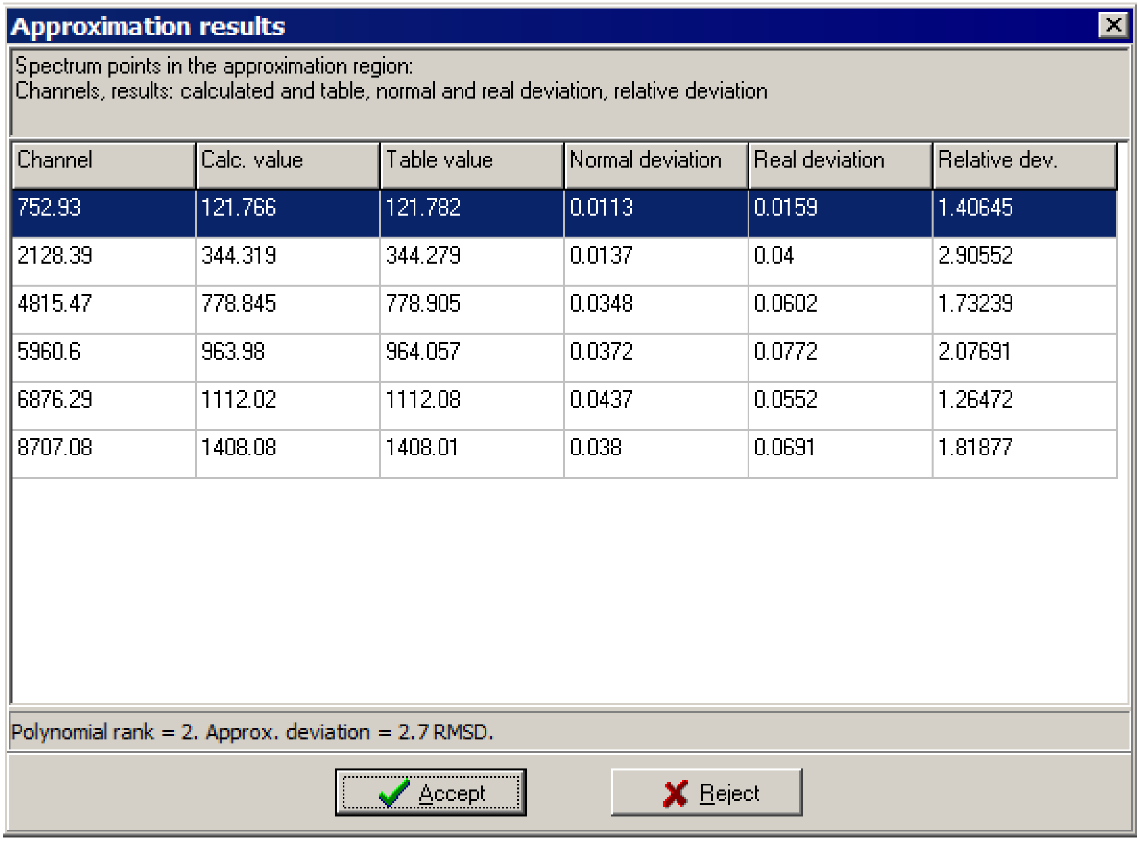
Previously, the operator can, using the Review... key, to select the required nuclide table (by default, the nuclide table specified during geometry installation is used) and specify the nuclides (in the right table of the form) present in the calibration source. The selection of nuclides is made by double-clicking the left mouse button or by calling the pop-up menu by right-clicking:



Then select the "**Basic calibration**" mode and set the rank of the polynomial. It is recommended to try calibration with a minimum rank – linear calibration, and only in case of unsatisfactory results increase the rank of the calibration polynomial

Next, you need to enter the energy values of the marked peaks in kiloelectronvolts in the "**Energy (new value)**" column. The energy values can be substituted from the nuclide table used for calibration.

Pressing the "**OK**" button starts the procedure for calculating the calibration polynomial and a table of approximation results is displayed on the screen:



Spectrum points in the approximation region:
Channels, results: calculated and table, normal and real deviation, relative deviation

Channel	Calc. value	Table value	Normal deviation	Real deviation	Relative dev.
752.93	121.766	121.782	0.0113	0.0159	1.40645
2128.39	344.319	344.279	0.0137	0.04	2.90552
4815.47	778.845	778.905	0.0348	0.0602	1.73239
5960.6	963.98	964.057	0.0372	0.0772	2.07691
6876.29	1112.02	1112.08	0.0437	0.0552	1.26472
8707.08	1408.08	1408.01	0.038	0.0691	1.81877

Polynomial rank = 2. Approx. deviation = 2.7 RMSD.

The operator can either not accept the results and return to the energy calibration form and correct the data, or accept and save it as a spectrometer calibration.

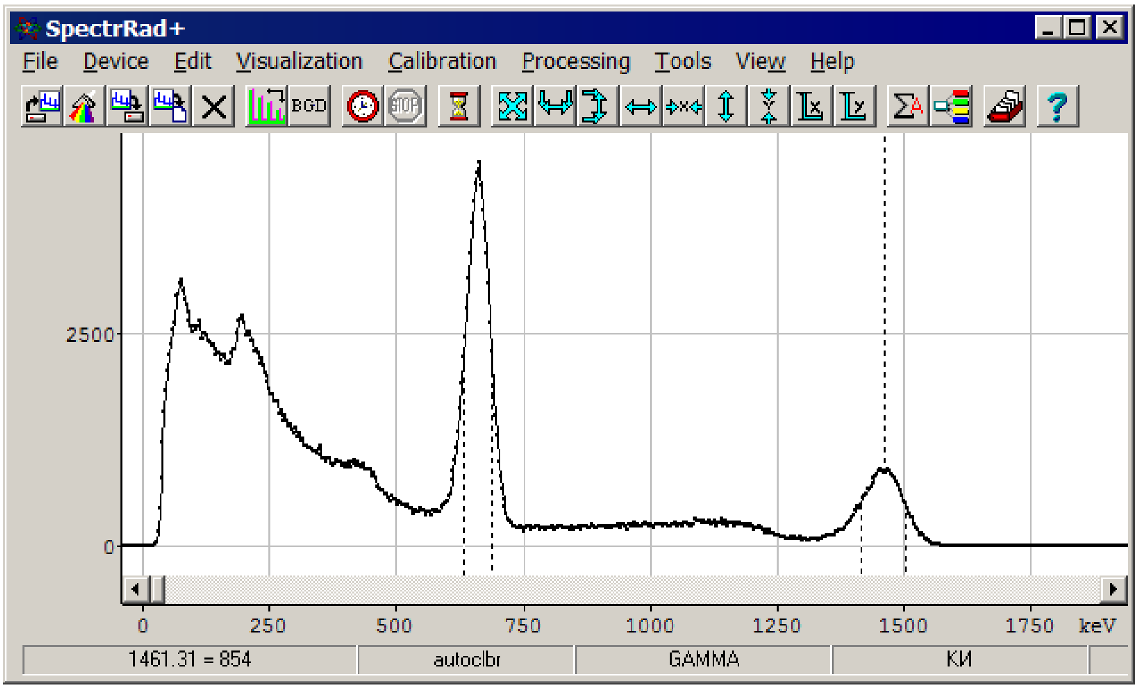
Further calibration of the spectrometer will require measurements of the background spectra and reference sources. All measurements require prior energy calibration of the spectrometer. For these purposes, the procedure of automatic energy calibration of the spectrometer is used - autocalibration. Automatic calibration of the spectrometer simplifies and speeds up the calibration procedure.

To set up the autocalibration procedure, first of all, it is necessary, having measured with good statistics (according to the cyclic measurement mode, if the required measurement time significantly exceeds the working measurement time) the reference source, which will later be used for autocalibration, process the spectrum according to the "**Calibration / Autocalibration / Setup...**" mode.

During installation, the spectrum of the calibration source is saved as a reference for subsequent calibrations. The recommended nuclide for autocalibration of scintillation gamma tracts is Th-232, beta tracts are dot Sr-90, gamma spectrometers with a cooled HPGe detector are Eu-152.

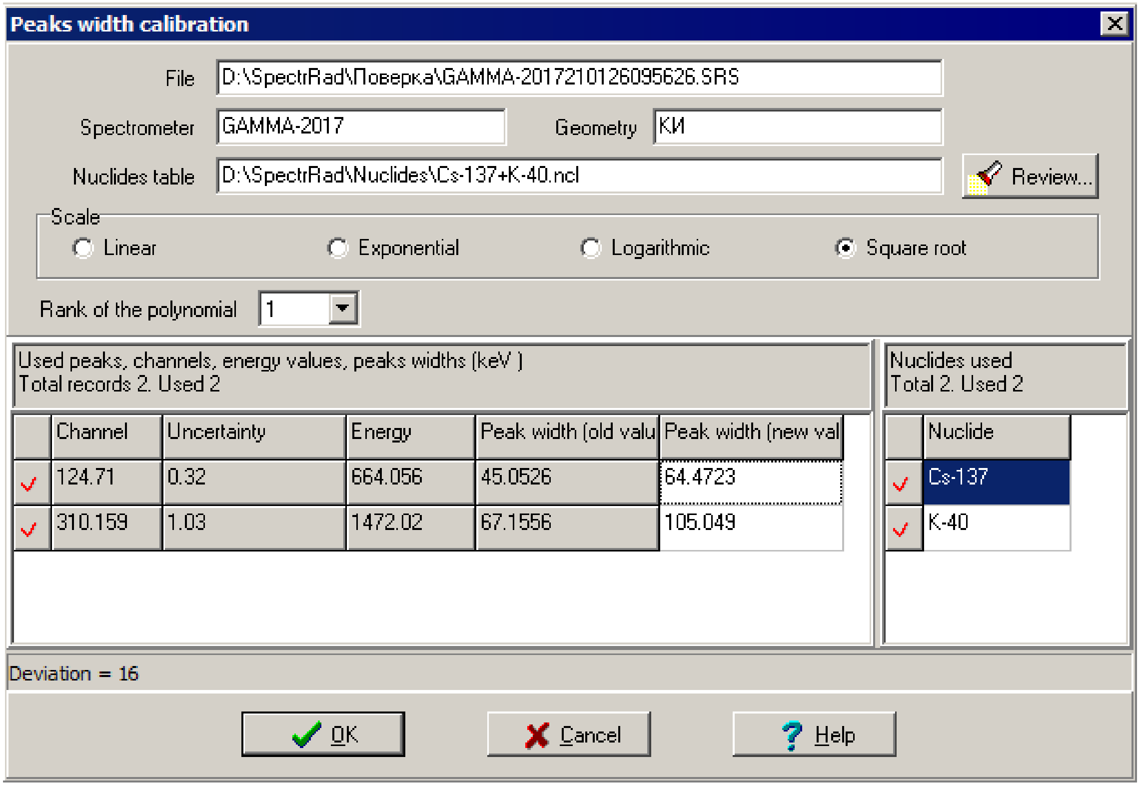
Peaks width calibration

After spectrometer energy calibration, for a gamma or alpha spectrometer it is necessary to calibrate the dependence of the width of peaks formed by gamma (alpha) radiation lines on the energy of the lines. To do this, after measuring the calibration source, it is required to mark with a movable marker the channels of the spectrum corresponding to half the height of the peaks to the left and right of the vertices of the single peaks (for example, as in the figure).



1461.31 = 854 | autoclbr | GAMMA | КИ

Then select the menu item "**Calibration / Peaks width / By entered data...**" and in the form that opens,



File: D:\SpectrRad\Поверка\GAMMA-20172101260956626.SRS

Spectrometer: GAMMA-2017

Geometry: КИ

Nuclides table: D:\SpectrRad\Nuclides\Cs-137+K-40.ncl

Scale: ○ Linear ○ Exponential ○ Logarithmic ● Square root

Rank of the polynomial: 1

Used peaks, channels, energy values, peaks widths (keV)
Total records 2. Used 2

	Channel	Uncertainty	Energy	Peak width (old valu	Peak width (new val
✓	124.71	0.32	664.056	45.0526	64.4723
✓	310.159	1.03	1472.02	67.1556	105.049

Nuclides used
Total 2. Used 2

	Nuclide
✓	Cs-137
✓	K-40

Deviation = 16

select the type of dependence of the peak width on energy in the "**Scale**" parameter group (by default, the square root is suggested - $FWHM = \sqrt{\mathrm{Pn(E)}}$) and, if necessary, adjust the values of the peak width at half the height in energy units ("keV"); click the "**OK**" button. To the program's question: "**Save as spectrometer calibration?**", answer "**Yes**".

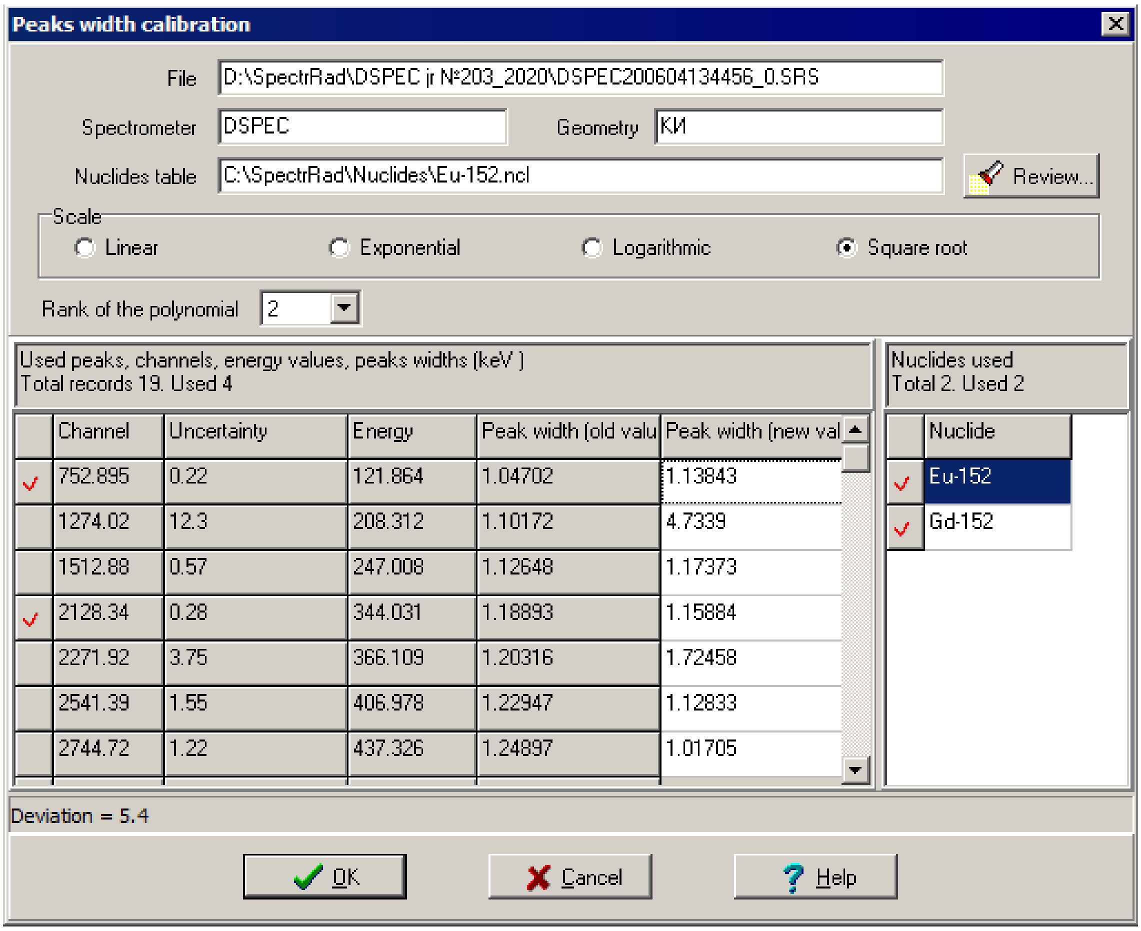
If desired, the calibration curve graph can be viewed by selecting the menu item "**Calibration / Peaks width / Visualization**". If the energy scale of the abscissa scale is set, the width of the peaks is also displayed in energy units, if the scale "X" is displayed in channels, the width of the peaks will also be represented in channels.

When processing linear spectra without peak search (scintillation spectrometry), peak width calibration is used to automatically generate spectra of nuclides missing from the list of nuclides for which elementary spectra are calculated from reference spectra (see "Creating a decomposition templates").

When processing linear spectra with peak search, peak width calibration is used at almost all processing stages. The search for peaks in the spectrum is impossible without pre-calibration of the peak width, at the same time, the most accurate calibration of the peak width is possible only after performing the peak search procedure in the calibration spectrum. Therefore, for linear spectra, after the initial calibration of the peak width and setting the peak search parameters, it is necessary to repeat the calibration procedure by processing the calibration spectrum using the "**Processing / Peaks search / Search**" mode. When calibrating the peak width of the spectrum processed in this way, data is taken from the processing results file.

The operator can mark the peaks that will be used during calibration with markers, and one marker in the peak area is enough, rather than two as in the initial calibration, since in this case the operator simply points to the peak with a marker, and does not set the peak width with markers. You don't have even to specify peaks with markers, because there is such a possibility in the form for calibrating the width of peaks.

The form, when calibrating, for example using Eu-152, in this case may look like this:



File: D:\SpectrRad\DSPEC jr №203_2020\DSPEC200604134456_0.SRS

Spectrometer: DSPEC

Geometry: КИ

Nuclides table: C:\SpectrRad\Nuclides\Eu-152.ncl

Scale: ○ Linear ○ Exponential ○ Logarithmic ● Square root

Rank of the polynomial: 2

Used peaks, channels, energy values, peaks widths (keV)
Total records 19. Used 4

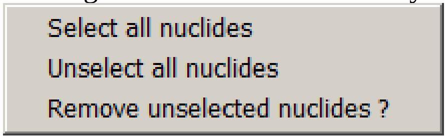
	Channel	Uncertainty	Energy	Peak width (old valu	Peak width (new val
✓	752.895	0.22	121.864	1.04702	1.13843
	1274.02	12.3	208.312	1.10172	4.7339
	1512.88	0.57	247.008	1.12648	1.17373
✓	2128.34	0.28	344.031	1.18893	1.15884
	2271.92	3.75	366.109	1.20316	1.72458
	2541.39	1.55	406.978	1.22947	1.12833
	2744.72	1.22	437.326	1.24897	1.01705

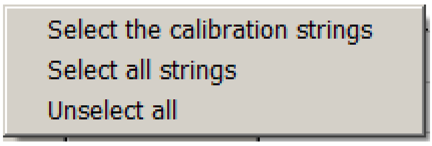
Nuclides used
Total 2. Used 2

	Nuclide
✓	Eu-152
✓	Gd-152

Deviation = 5.4

The **nuclides table** used in calibration is required to select calibration peaks. Previously, the operator using the Review... key can select the desired nuclide table (by default, the nuclide table specified during geometry installation is used) and specify the nuclides (in the right side table) present in the calibration source. The selection of nuclides is made by double-clicking the left mouse button or by calling the pop-up menu by clicking the right mouse button: . Then select the calibration peaks using the pop-up menu activated by right-clicking .



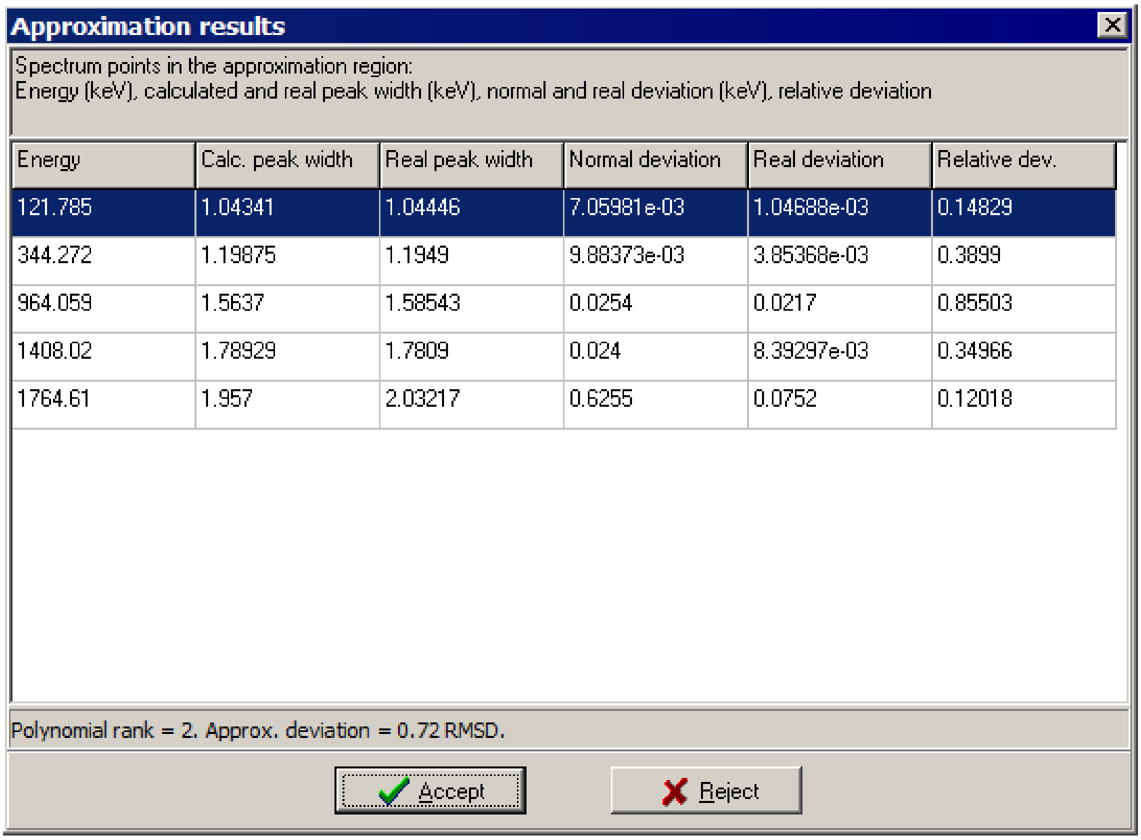


Calibration line is a line with a minimum error of the peak width and an energy value that falls within the range specified for the calibration line of the nuclide table.

The **rank of the polynomial** (can take values from 1 to 3), together with the number of points used for calibration, determines the real rank of the calibration polynomial. If the number of points is equal to or less than the specified rank, the rank of the calibration polynomial will be one less than the number of calibration points. It is recommended to use the minimum rank for calibration and only in case of unsatisfactory calibration results try to increase the rank of the polynomial.

The peak widths for the allowed linear spectra are taken from the processing results file, if it exists. If such a file does not exist, the peak width is calculated as the energy difference of the labeled channels, and the peak position is calculated as the average of the energies of the left and right labeled channels. The operator can, if necessary, adjust the values of the peak widths.

Pressing the "**OK**" button starts the procedure for calculating the calibration polynomial and a table of approximation results is displayed on the screen:



Spectrum points in the approximation region:
Energy (keV), calculated and real peak width (keV), normal and real deviation (keV), relative deviation

Energy	Calc. peak width	Real peak width	Normal deviation	Real deviation	Relative dev.
121.785	1.04341	1.04446	7.05981e-03	1.04688e-03	0.14829
344.272	1.19875	1.1949	9.88373e-03	3.85368e-03	0.3899
964.059	1.5637	1.58543	0.0254	0.0217	0.85503
1408.02	1.78929	1.7809	0.024	8.39297e-03	0.34966
1764.61	1.957	2.03217	0.6255	0.0752	0.12018

Polynomial rank = 2. Approx. deviation = 0.72 RMSD.

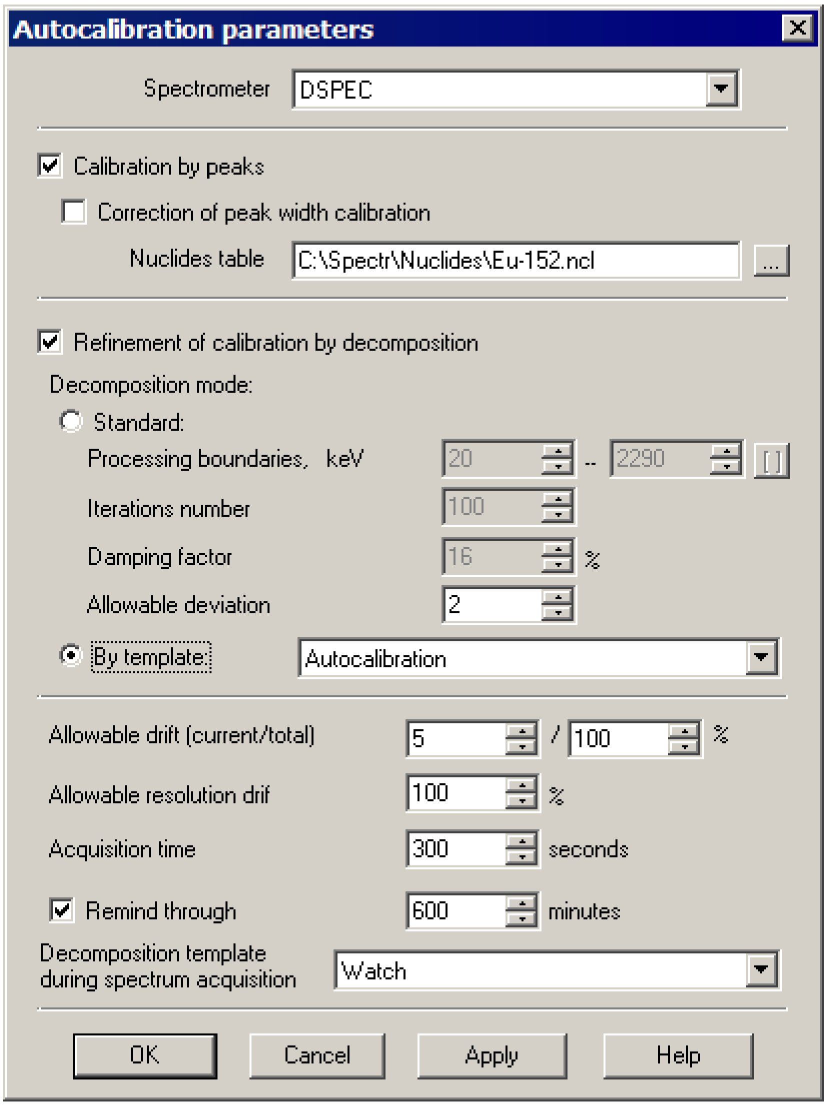
The operator can either reject the results and return to the peak width calibration form and correct the data, or accept and save it as a spectrometer calibration.

Calibration by peak widths calculated by the peak processing procedure is much more accurate than manual calibration by the operator, but it also contains a significant drawback – the peak used for calibration can be formed by several close lines (be a hidden multiplet) and, accordingly, be wider than the peak formed by a single line. Therefore, the final stage of peak width calibration is performed in the peak model calculation procedure. The procedure for calculating peak models calculates the response to exactly one radiation line, subtracting all possible interferences, and calibration based on peak models is free from this disadvantage.

Setting auto calibration parameters

The "**autocalibration"** procedure is used for automatic energy calibration of the spectrometer according to the reference source and verification of the spectrometer. Depending on the setting, it either compares the spectrum measured from the reference source with the same spectrum measured when installing the spectrometer, or performs spectrum processing, determining the activity of nuclides of the reference source, and based on the results of processing, corrects the energy calibration of the spectrometer and evaluates its operability, allowing or prohibiting operational measurements.

Before starting the auto-calibration procedure for the first time, the operator must set the auto-calibration parameters. The menu item "**Calibration / Autocalibration / Configure...**" calls the procedure for setting the parameters of the automatic energy calibration of the spectrometer. The operator needs to fill in the fields of the "**Autocalibration parameters**" table. For spectrometers with a linear type of spectra, the parameter table may look like:



Autocalibration parameters

Spectrometer DSPEC

☑ Calibration by peaks

☐ Correction of peak width calibration

Nuclides table C:\Spectr\Nuclides\Eu-152.ncl

☑ Refinement of calibration by decomposition

Decomposition mode:

○ Standard:

Processing boundaries, keV 20 -- 2290

Iterations number 100

Damping factor 16 %

Allowable deviation 2

● By template: Autocalibration

Allowable drift (current/total) 5 / 100 %

Allowable resolution drif 100 %

Acquisition time 300 seconds

☑ Remind through 600 minutes

Decomposition template during spectrum acquisition Watch

When autocalibrating spectrometers recording spectra having a linear character (alpha and gamma radiation), the operator can choose two modes of autocalibration: "**Calibration by peaks**" and (or) "**Refinement of calibration by decomposition**".

The "calibration by peaks" procedure searches for peaks in the spectrum of the reference source (the parameters of the peak search procedure must first be set and the peak width calibrated) and assigns the medians of the selected peaks of the energy spectrum of the calibration lines from the specified line table (**Nuclides table**). The table should contain lines marked as **calibration lines** that correspond to the peaks of the spectrum used in calibrating the spectrometer. The calibration procedure for each line in the table searches for the most powerful peak of the spectrum within the specified boundaries (E_{lin}-DE < E< E_{lin}+DE) and assigns it the specified energy E_{lin}.

When calibrating by peaks, the operator can also set the peak width calibration correction mode by selecting the appropriate checkbox – "**Correction of peak width calibration**".

The procedure for clarifying the energy calibration by decomposition determines the parameters of the energy drift of the spectrometer by decomposing the spectrum into spectra with a known energy calibration and estimating the displacement of the energy calibration parameters relative to the corresponding parameters of the component spectra. In this case, the operator must select the **decomposition mode** and set a number of parameters:

- **Standard** is a simplified auto-calibration mode that does not take into account background changes and decay of the calibration source. The measured spectrum in the standard mode is compared with the spectrum of the calibration source. When installing the spectrometer (measurement geometries have not yet been set, the background has not been measured), only the "**Standard**" mode is available. In this case, you need to set the following parameters:
- **Processing boundaries -** the boundaries of the spectrum area that will be used for auto-calibration. The "button" [] is used to substitute marker positions as processing boundaries. It is recommended to use the entire energy range with the exception of the regions of the beginning and end of the spectrum, which, due to the drift of the spectrometer, may leave the region of the spectrum acquisition.
- **Iterations number** - the number of repetitions of the procedure for clarifying the drift parameters. Limiting the number of iterations makes sense only for computers with low performance.
- **Damping factor** is a constant (set as a percentage) that increases the stability of the auto-calibration procedure. It makes sense if the system of equations solving process has an oscillatory character, which can happen if the system is poorly conditioned (a slight change in the shape of the spectrum with large changes in the drift parameters or an almost identical change in the shape of the spectra with changes in various parameters).
- **By template** - auto-calibration mode, in which the spectrum of the calibration source is processed according to a decomposition template created by the user (see section "Creating a decomposition templates"). This takes into account the background change and decay of the reference source during operation. In this case, the processing parameters are set in the parameters of the decomposition template. At the end of the spectrometer setup (geometry settings, reference samples measurements), it is recommended to create a template for auto-calibration and set the appropriate auto-calibration mode.

The last group of parameters is common to both types of calibration (calibration by peaks and standard calibration mode by spectrum decomposition):

- **Allowable deviation -** the maximum permissible level of the ratio of the real divergence of the spectra to the theoretical one (normalized by standard deviation $G = \sqrt{\sum((X_i - X_m)^2 / G_i^2)/(n-m)}$). The recommended value is from 1.5 to 3.0.
- **Allowable drift (current/total)** - the maximum allowable level of the total energy drift of the gain factor and zero of the spectrometer scale as a percentage. **Current drift** – the drift of the spectrometer over the time since the previous calibration (auto-calibration). The recommended value is twice the resolution of the spectrometer (from 15% to 30% for scintillation detectors). **Total drift** - the drift of the spectrometer since the initial calibration of the spectrometer. If the total drift of the spectrometer exceeds the set level, measurements in the restricted access mode will be prohibited.

- **Acquisition time n seconds** is the working time of measuring the reference source during autocalibration. The measurement time should ensure an average of at least 50 pulses per channel in the operating range of the spectrum.
- **Remind through n minutes -** a checkbox and a field for entering the duration of the interval, after which the program will require the spectrometer to be autocalibrated (provided that the checkbox is selected).
- **Decomposition template during spectrum acquisition** – the operator has the option to select a decomposition template from the drop-down list that will be used when processing the spectrum during the spectrum acquisition process.

For spectrometers with a continuous type of recorded spectra (beta radiation), only one type of calibration is available – **Refinement of calibration by decomposition**

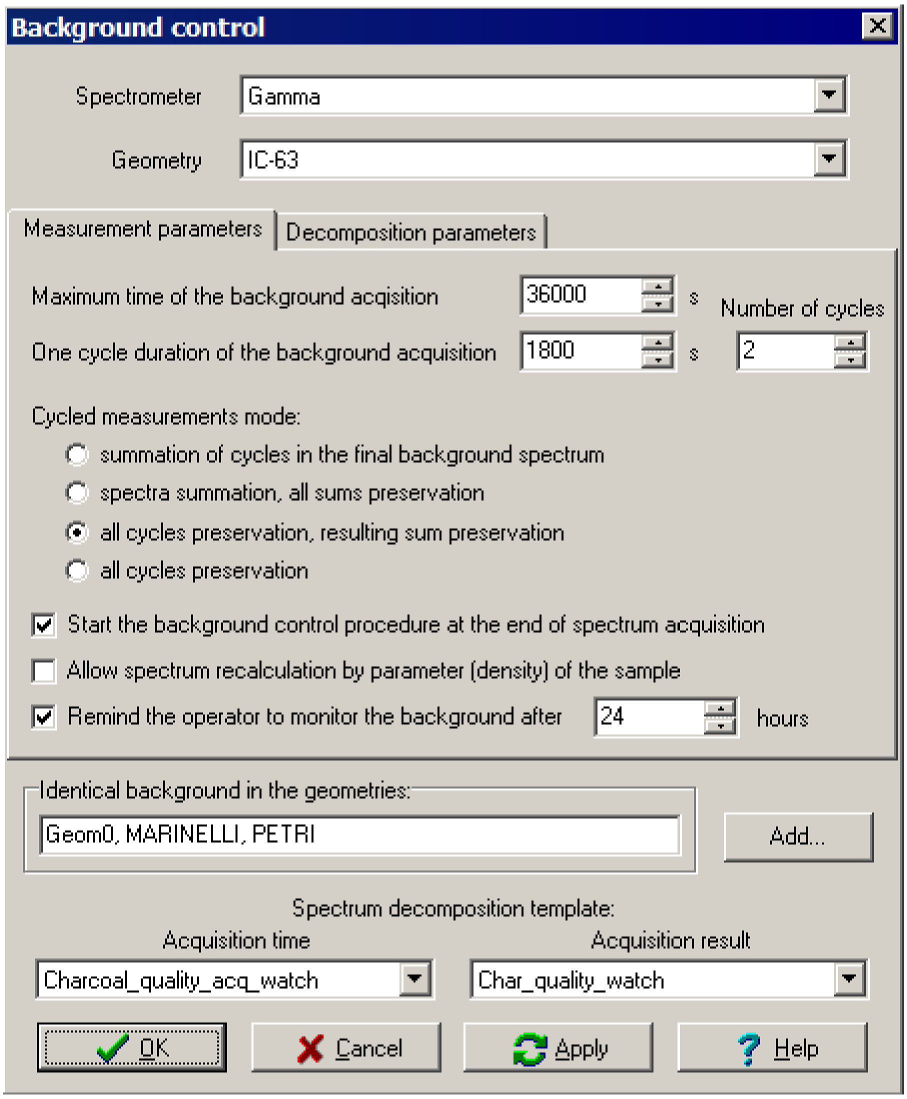
If both types of calibration are marked, calibration by peaks is performed first and then the energy calibration parameters are refined by decomposition.

The procedure for clarifying calibration by decomposition, in addition to the task of clarifying energy calibration, verifies the spectrometer, determining a number of parameters of the spectrometer (line shape stability, registration efficiency), which are extremely important for quality control of spectrometry and evaluation of the spectrometer's operability.

Setting the parameters of the background radiation control

Background spectrum is the spectrum of radiation recorded by the detector from all sources except the sample: cosmic radiation, radiation from the earth, building materials, detector structural materials, etc., etc. The measured spectrum is the sum of the radiation spectra from the sample and the background spectrum. The background spectrum is subtracted by the processing program from the measured spectrum. Therefore, it is necessary to measure and install the background spectrum in the program.

Previously, by selecting the menu item "**Calibration / Background / Configure...**", it is necessary to set the parameters of the procedure for background radiation measurement and control for the selected measurement geometry. The table of background radiation control parameters can look like this:



Background control

Spectrometer: Gamma

Geometry: IC-63

Maximum time of the background acqisition: 36000 s

One cycle duration of the background acquisition: 1800 s

Number of cycles: 2

Cycled measurements mode:

○ summation of cycles in the final background spectrum
○ spectra summation, all sums preservation
● all cycles preservation, resulting sum preservation
○ all cycles preservation

☑ Start the background control procedure at the end of spectrum acquisition

☐ Allow spectrum recalculation by parameter (density) of the sample

☑ Remind the operator to monitor the background after 24 hours

Identical background in the geometries: Geom0, MARINELLI, PETRI

Spectrum decomposition template:

Acquisition time: Charcoal_quality_acq_watch

Acquisition result: Char_quality_watch

At the bottom there is a line with a list of geometries, the background of which, within the required accuracy, can be considered the same: "**Identical background in the geometries:**". In general, due to the shielding of the detector by the sample substance, the presence of radionuclides in the measuring vessels, the background depends on the geometry. But these differences can be negligible in comparison with statistical fluctuations of the background, and specifying the identity of the background allows (when controlling the background) not to measure the background for each geometry, but, having measured only for one geometry of the list, to perform a background control operation (mixing or replacing the background) for all geometries from the list. Clicking on the button adds the selected geometry to the list.

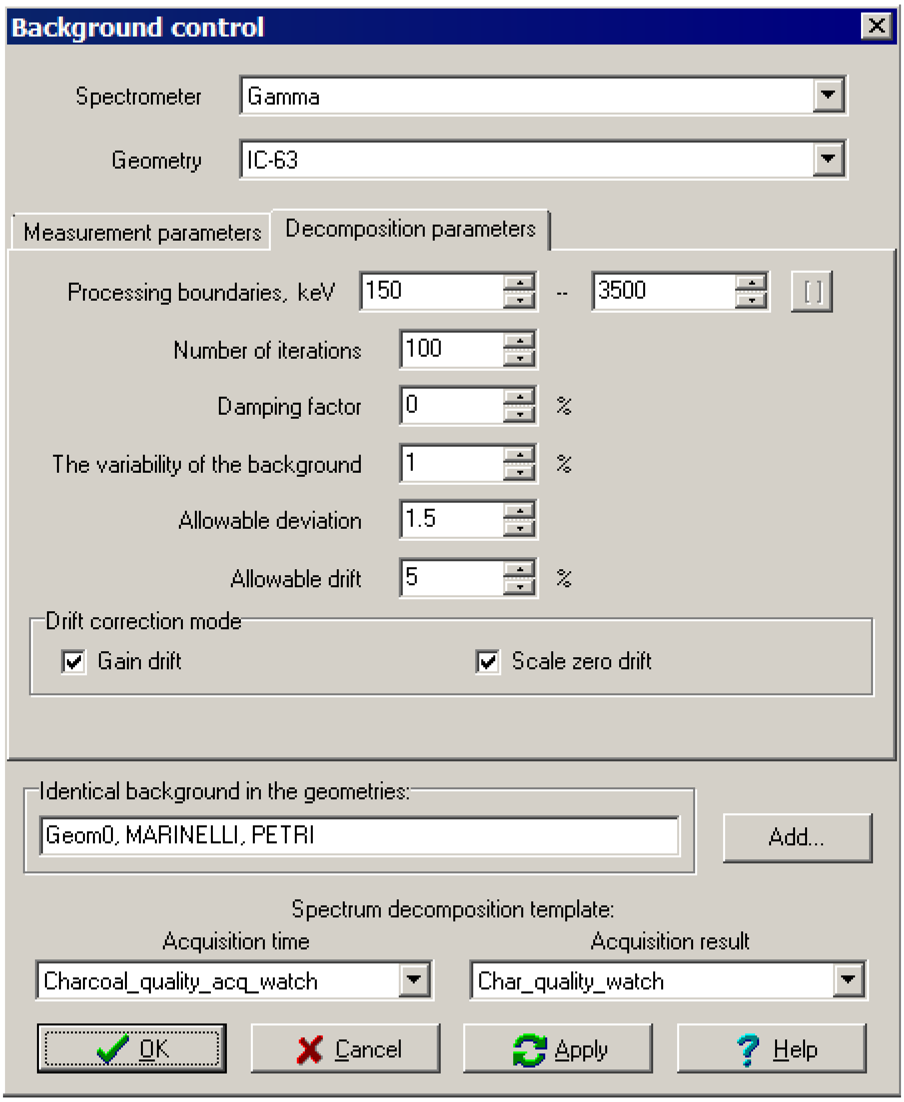
Two drop-down lists "**Spectrum decomposition template:**" allow you to set the procedure for processing the spectrum during the **acquisition time** and after completion of measurements of the background spectrum (**Acquisition result**). The processing template during spectrum acquisition is used to monitor the acquisition process. Upon completion of the background spectrum measurements, the "**background control**" procedure is started. The "**background control**" procedure compares the measured background spectrum with the working background spectrum (formed earlier), if it exists, and based on the results of the comparison suggests that the operator either mix the measured spectrum with the existing one, or replace the working background spectrum with the newly measured one. Spectrum processing according to the measurement result processing template, if the template is specified, is started before the "**background control**" procedure is performed and is used to evaluate additional parameters that are not taken into account in the standard "**background control**" procedure (for example, the amount of residual radon in activated carbon when measuring radon fluxes).

The central part of the form contains two pages: "**Measurement parameters**" and "**Decomposition parameters**".

On the first page, the operator must set the parameters for measuring the background spectrum:

- **Maximum time of the background acquisition** is the time before which the previously measured background spectrum can be summed with the newly measured one, and when exceeded, it can be mixed in proportion determined by the ratio of the measurement time to the maximum background accumulation time.
- **One cycle duration of the background acquisition** and **Number of cycles** determine the working time of the background sample measurement during background control. The recommended measurement time should ensure an average of at least 5 pulses per channel in the operating range of the spectrum (for alpha radiometry, you can limit yourself to the requirement of at least 16 pulses in the operating range). If the number of cycles is greater than one, background measurements will be carried out in cyclic mode. In this case, the operator must select the **Cycled measurement mode:**
    - **Summation of the cycles in the final background spectrum** – the measurement results in individual cycles will be combined in the final background spectrum.
    - **Spectra summation, all sums preservation** – all sums of spectra obtained at the end of each cycle will be saved in separate files of measurement archive.
    - **All cycles preservation, resulting sum preservation** – background spectra measured in separate cycles will be saved in separate files of measurement archive. Additionally, the spectrum of the sum of cycles will be preserved.
    - **All cycles preservation** – background spectra measured in separate cycles will be saved in separate measurement archive files.
- **Start the background control procedure at the end of the spectrum acquisition** – the background control procedure will not be started upon completion of measurements if the checkbox is not selected. In this case, the operator will have to start the background control procedure itself from the measurement archive at the end of the measurements.
- **Allow spectrum recalculation by parameter (density) of the sample -** a checkbox allowing (when set) the mode of enabling the newly measured spectrum as a separate file for calculating the background spectrum by interpolation or averaging over several spectra having different geometric parameters (densities) of background samples.
- **Remind the operator to monitor the background after n hours -** a checkbox and a field for entering the duration of the interval after which the program will require measurements of the background spectrum (provided that the checkbox is selected).

On the "**Decomposition parameters**" page, the operator must set the parameters of the procedure for comparing the working and measured spectra - the "**background control**" procedure:



Background control

Spectrometer: Gamma

Geometry: IC-63

Processing boundaries, keV: 150 -- 3500

Number of iterations: 100

Damping factor: 0 %

The variability of the background: 1 %

Allowable deviation: 1.5

Allowable drift: 5 %

Drift correction mode

☑ Gain drift ☑ Scale zero drift

Identical background in the geometries: Geom0, MARINELLI, PETRI

Spectrum decomposition template:

Acquisition time: Charcoal_quality_acq_watch

Acquisition result: Char_quality_watch

- **Processing boundaries** - the left and right energy boundaries of the background spectrum processing. The "button" **[ ]** is used to substitute marker positions as processing boundaries.
- **Number of iterations** - the maximum allowed number of iterations to refine the estimates. Limiting iterations makes sense for computers with low performance.
- **Damping factor** is a constant (set as a percentage) that increases the stability of the drift correction procedure. It makes sense if the system of equations solving process has an oscillatory character, which can happen if the system is poorly conditioned (a slight change in the shape of the spectrum with large changes in the drift parameters or an almost identical change in the shape of the spectra with changes in various drift parameters).
- **The variability of the background** is a value characterizing the instability of the background in the detector. It is assumed that background changes are caused by statistical fluctuations (Poisson statistics) plus **additional background variability** (set as a percentage) due, for example, to instability of radon concentration in the detector area or fluctuations in the cosmic component of the background.

- **Allowable deviation** (maximum allowable discrepancy value) and **Allowable drift** (maximum allowable energy drift value) are comparison parameters, if exceeded, the procedure for comparing two spectra (new and old background) will be considered failed (new and old background differ significantly from each other).
- **Drift correction mode: Gain drift** and **Scale zero drift** are checkboxes that allow (when installed) or prohibit (when removed) correction of the corresponding parameters of the energy drift of the spectrometer (gain drift and zero drift of the scale) during the background control procedure.

Then it is required to perform an autocalibration of the spectrometer (measure and process the calibration source according to the procedure "**Calibration / Autocalibration / Start...**" - button). Next, measure the background sample in the selected geometry for at least the measurement time of the working samples (BGD button, menu item "**Calibration / Background / Start...**").

At the end of the measurements, or upon launching the background control procedure from the measurement archive by the operator (in the case of cyclic measurements with each cycle saved), the program compares the previously accumulated background spectrum with the newly measured with the parameters set by the operator and, depending on the results of the comparison, offers the operator either to replace the background spectrum with a new one, either mix it with the old one, or install it as a separate file. If the previously set spectrum does not exist, the program suggests setting the measured spectrum as the background spectrum. The systematic excess of permissible parameters (drift and discrepancy) and, accordingly, the prohibition of background mixing indicate either incorrect parameter settings or unsatisfactory operation of the spectrometer (unstable background or electronic noise of the tract, large drift). Some types of measurements require the installation of a new background spectrum for a certain group of measurements (radon measurements on activated carbon or activation analysis, etc.).

Calibration of registration efficiency

The spectra obtained by measuring samples on a spectrometer with a **linear type of spectra** set in the parameters of the spectrometer are processed with preliminary subtraction from the sample spectrum of a continuous spectrum on which the resonant sections of the spectrum are peaks. The decomposition of the spectrum into components (decomposition) is carried out for the spectrum of peaks. For gamma-ray spectra, in the processing of which, as a rule, this method is used, photons of certain energy form a number of peaks in the spectrum. For example, photons with an energy exceeding 1022 keV can form more than four peaks in the spectrum: a peak of total absorption (photopic) with an energy corresponding to the photon energy, a peak of single escape with an energy 511 keV less, a peak of double escape with an energy 1022 keV less than the energy of the peak of total absorption, an annihilation peak with an energy equal to 511keV and peaks of addition of cascade transitions.

In the "SPECTRRAD" software package, four quantum registration efficiency functions can be calculated: the efficiency of registering quanta of a certain energy in peaks of total absorption **Eff(e)=S(e)/Q(e)**, the total registration efficiency **EffTot(e) = STot(e)/Q(e)**, the registration efficiency in peaks of single escape **EffEsc1(e-511)=Sesc1(e-511)/Q(e)** and peaks of double escape **EffEsc2(e-1022)=Sesc2(e-1022)/Q(e)**. Here: **e** is the energy of the line, **S(e)**, **STot(e)**, **Sesc1(e-511)**, **Sesc2(e-1022) -** respectively: the peak area of total absorption, the total area of the line registration spectrum, the peak areas of single and double escape, corresponding to the number of radiation quanta **Q(e)** of this energy.

The full registration efficiency function is required for the correct calculation of the effects associated with the registration of cascade transitions. The efficiency of registration in escape peaks is required because the effect of pair formation, which leads to the appearance of escape peaks, occurs not only in the sample material, but also in the structural materials of the detector. And a correct calculation of this effect, without calibrating the efficiency of recording in escape peaks, would require knowledge of both the materials and the design of the detector, which in practice is not always known.

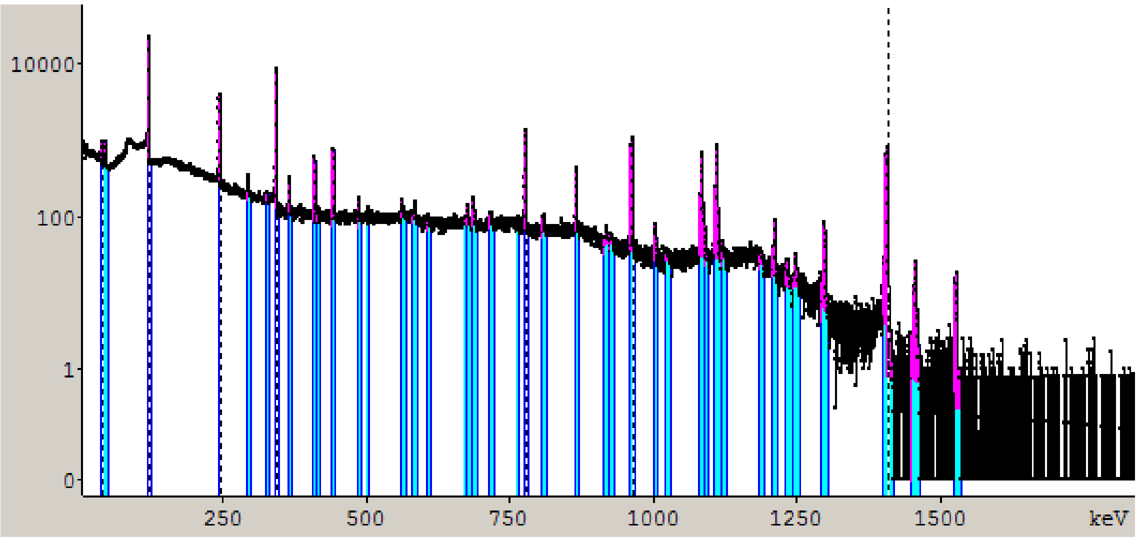
The program for calculating registration efficiency functions takes into account the effects associated with the registration of cascade transitions. Information about cascade transitions should be present in the nuclide worksheet.

There are two most common methods for calculating the registration efficiency function: calculation based on standards with the geometry of the corresponding measurement geometry and calculation based on the geometry of a point source. The second method is available if the registration efficiency functions for the point source are calculated using the first method and the "detector depth" function is calculated. A significant disadvantage of calculating registration efficiency functions based on standards with the geometry of the corresponding measurement geometry is that a set of standards is required for each of the geometries. The following text refers to the calculation of registration efficiency functions based on standards with the geometry of the corresponding measurement geometry. Calculation of registration efficiency functions for a given geometry using the registration efficiency functions for point geometry is given in the chapter "**Installing the measurement geometry /Recalculation of the registration efficiency for a given geometry**".

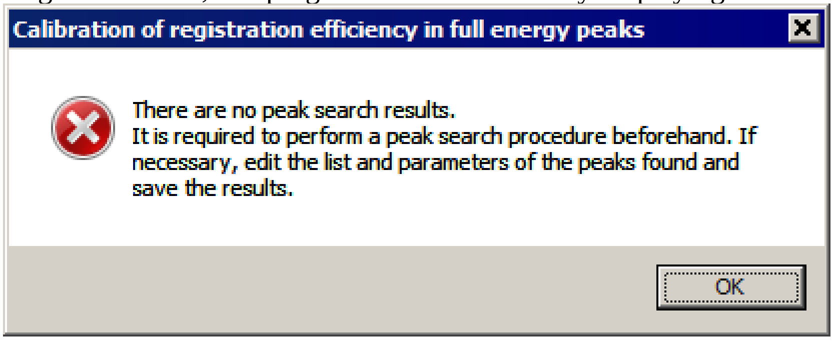
The recording efficiency depends both on the geometric parameters of the counting sample or the geometry of the measurements and on the absorption of radiation in the sample substance. The absorption of radiation in the sample substance depends on the density of the counting sample (for measurement geometries in the "thin" and intermediate layers) and on the charge of the nucleus of the sample elements (Z). One of the geometric parameters of the geometry or the density of the substance of the counting sample can be used as **interpolation parameters** determined when setting the measurement geometry. The effects associated with the absorption of radiation in the sample substance, depending on the density of the sample, are calculated using radiation absorption formulas, if the sample density is not defined as an **interpolation parameter**. For a correct assessment of the registration efficiency corresponding to the interpolation parameter of the measured spectrum of the working sample, calibration of the registration efficiency must be performed several times using standards with different values of the **interpolation parameter**.

Initially, the registration efficiency is calibrated at full absorption peaks. It is previously required to perform an autocalibration of the spectrometer and set the parameters of the peak search procedure. Then measure a reference sample of the activity of a nuclide or a mixture of nuclides (standard) having a sufficient number of peaks in the operating energy range, in a given geometry, for a sufficient time to set at least 1000 pulses in the peaks to be used for calibration, according to the cyclic measurement mode with a cycle duration equal to the average measurement time of the working sample. For the range from 30 to 1500 keV, a mixture of Am-241 with Eu-152 is usually used.

As an example of building a registration efficiency table, we use the Eu-152 spectrum. We will first mark the peaks that will be used for calibration with markers. The spectrum, in this case, may look like:



We will process the measured spectrum according to the "**Calibration / Quanta registration efficiency / in full energy peaks...**" mode. To calculate the table of the efficiency of registration of gamma quanta in peaks, it is necessary to pre-perform the procedure for searching for peaks in the spectrum (menu item "**Processing/ Peak Search/ Search**"). If we forgot to do this, the program will remind us by displaying a warning message on the screen


Calibration of registration efficiency in full energy peaks

There are no peak search results.
It is required to perform a peak search procedure beforehand. If necessary, edit the list and parameters of the peaks found and save the results.

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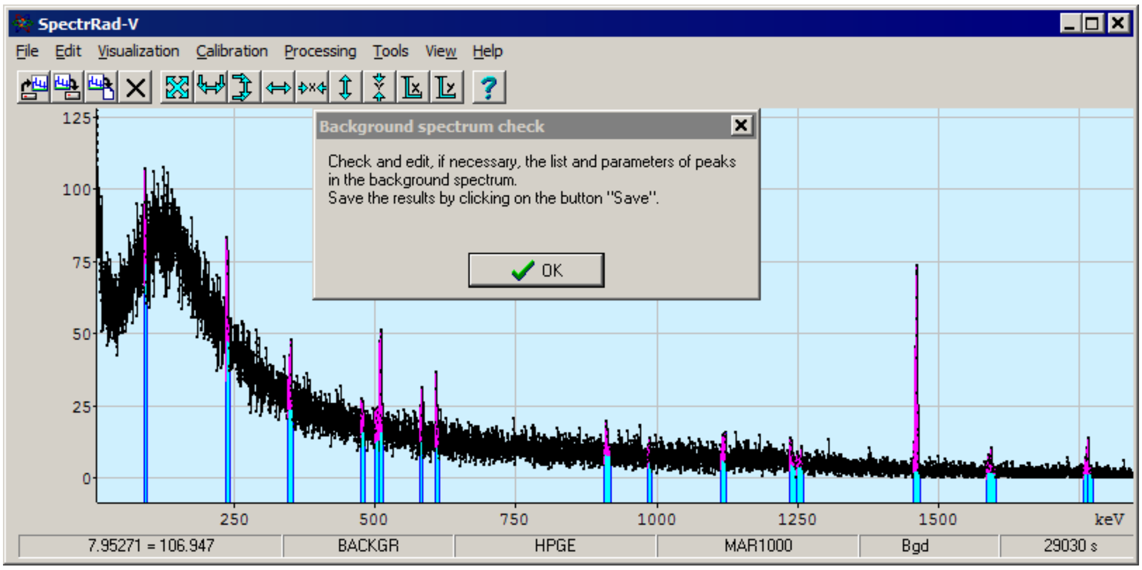
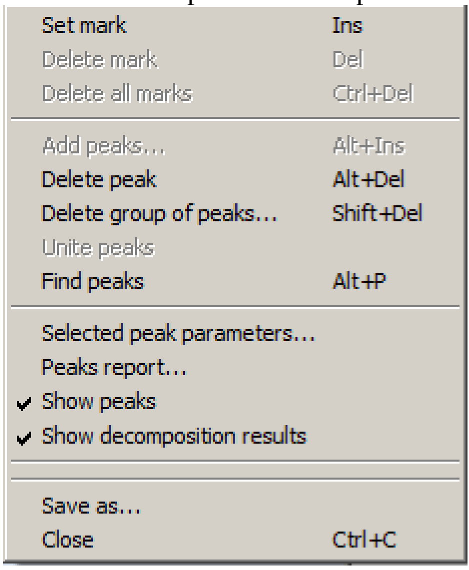
If the procedure for searching for peaks in the spectrum has been performed, calling the procedure for calibrating the registration efficiency in photo peaks will open two additional windows: the "**Background spectrum check**" dialog box and the **SpectrRad-V** program window with the background spectrum used in calculating the registration efficiency table.

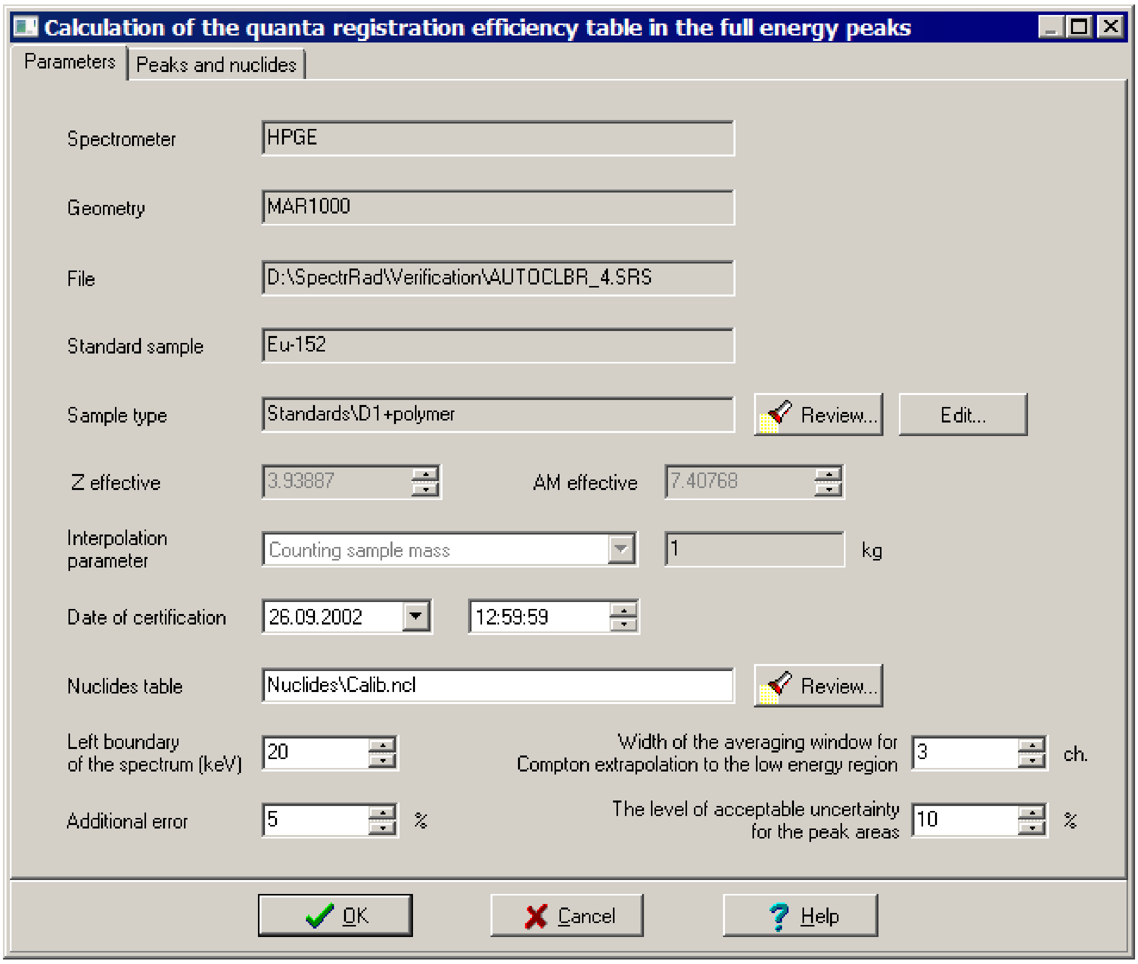


Check and edit, if necessary, the list and parameters of peaks in the background spectrum.
Save the results by clicking on the button "Save".

If necessary, the operator can edit the list and parameters of peaks found in the background spectrum using the pop-up menu: 

. The dialog box can be closed only after the **SpectRad-V** window is closed. If the list or parameters of peaks have been changed, they must first be saved by clicking on the "**Save**" button in the **SpectRad-V** program window.

After that, the form of the program for calculating the registration efficiency table is displayed on the screen. The form has two pages. The first page of "**Parameters**" may look like this:



Spectrometer: HPGE

Geometry: MAR1000

File: D:\SpectrRad\Verification\AUTOCLBR_4.SRS

Standard sample: Eu-152

Sample type: Standards\D1+polymer

Z effective: 3.93887

AM effective: 7.40768

Interpolation parameter: Counting sample mass 1 kg

Date of certification: 26.09.2002 12:59:59

Nuclides table: Nuclides\Calib.ncl

Left boundary of the spectrum (keV): 20

Width of the averaging window for Compton extrapolation to the low energy region: 3 ch.

Additional error: 5 %

The level of acceptable uncertainty for the peak areas: 10 %

The operator must select from the suggested list or specify:

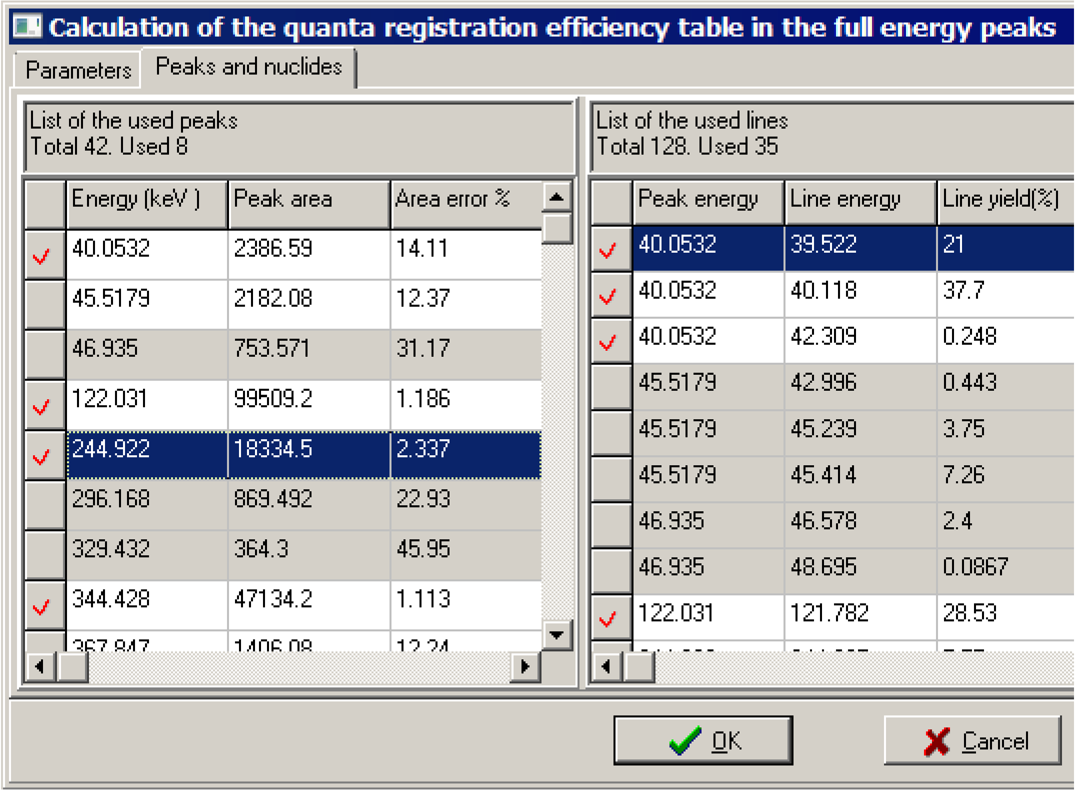
- **Interpolation parameter** – a parameter according to the value of which the registration efficiency function for a specific specimen will be calculated when calculating the registration efficiency from several registration efficiency tables with different values of the interpolation parameter. The interpolation parameter can be the mass or density of the sample, a geometric parameter specified during the installation of the geometry (the distance of the sample from the detector, the height of the filling, etc.).
- **Date of certification -** the date of certification of the measured standard (a reference sample of activity).
- Select the **Nuclides table** containing information about the nuclides of the reference sample. Since when recalculating the nuclide activities of the standard entered on the date of certification to the values of the average nuclide activity during the measurement of the standard necessary for calculating the registration efficiency, the program takes into account the processes of decay and accumulation of nuclides, the nuclide table must contain a correct scheme of nuclide decay.
- Set the **left boundary of the spectrum** and the **width of the averaging window for Compton extrapolation to the low energy region**. These parameters are necessary for the correct calculation of the value of the total efficiency of registration of gamma quanta in the spectrum. Since any spectrometer has a so-called "low-level signal discriminator" that cuts off noise, the spectrum is set not from zero energy, but from some left boundary energy. In addition, most nuclides have soft X-ray lines in their composition, which are almost impossible to account for correctly. Therefore, to calculate the full efficiency of recording gamma quanta, including Compton scattering quanta with very low energy, extrapolation of the Compton scattering spectrum to the left of the established boundary is used by the average value for the section of the Compton scattering spectrum from the left boundary to the left boundary plus the width

of the averaging window. The left boundary should be selected in such a way as to cut off the X-ray lines of the nuclide used in calibration.

- Set an **additional error** - the error of weighing, geometry violations, etc.
- Set **the level of acceptable uncertainty for peaks areas** – peaks of the spectrum with a relative error in determining the area exceeding the specified level will be excluded from the list of peaks used.

The **Sample type** field is associated with information about the chemical composition of the reference substance. This information is necessary to correctly account for the absorption of radiation in the sample substance. The lack of information about the chemical composition of the standard means that we neglect the effects associated with the photo absorption of gamma quanta in the sample substance. Photo absorption is the most significant effect at low energies (up to 100 keV) and large Z. You can set the chemical composition of the standard by clicking on the Edit... button, or select the type of standard with the correct chemical composition by clicking on the Review... button.

Switching to the second page of "**Peaks and nuclides**", enter information about the peaks used, the lines and the activities of the nuclides forming them. The "**Peaks and nuclides**" page has three columns: "**List of the used peaks**", "**List of the used lines**", and "**List of the used nuclides**". In the example, the Eu-152 standard is used for calibration. In this case, the "**List of the used peaks**" column may look like:


Calculation of the quanta registration efficiency table in the full energy peaks

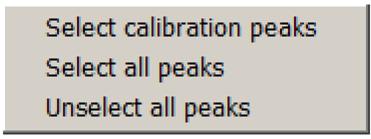
List of the used peaks
Total 42. Used 8

	Energy (keV)	Peak area	Area error %
✓	40.0532	2386.59	14.11
	45.5179	2182.08	12.37
	46.935	753.571	31.17
✓	122.031	99509.2	1.186
✓	244.922	18334.5	2.337
	296.168	869.492	22.93
	329.432	364.3	45.95
✓	344.428	47134.2	1.113
	367.847	1406.08	12.24

List of the used lines
Total 128. Used 35

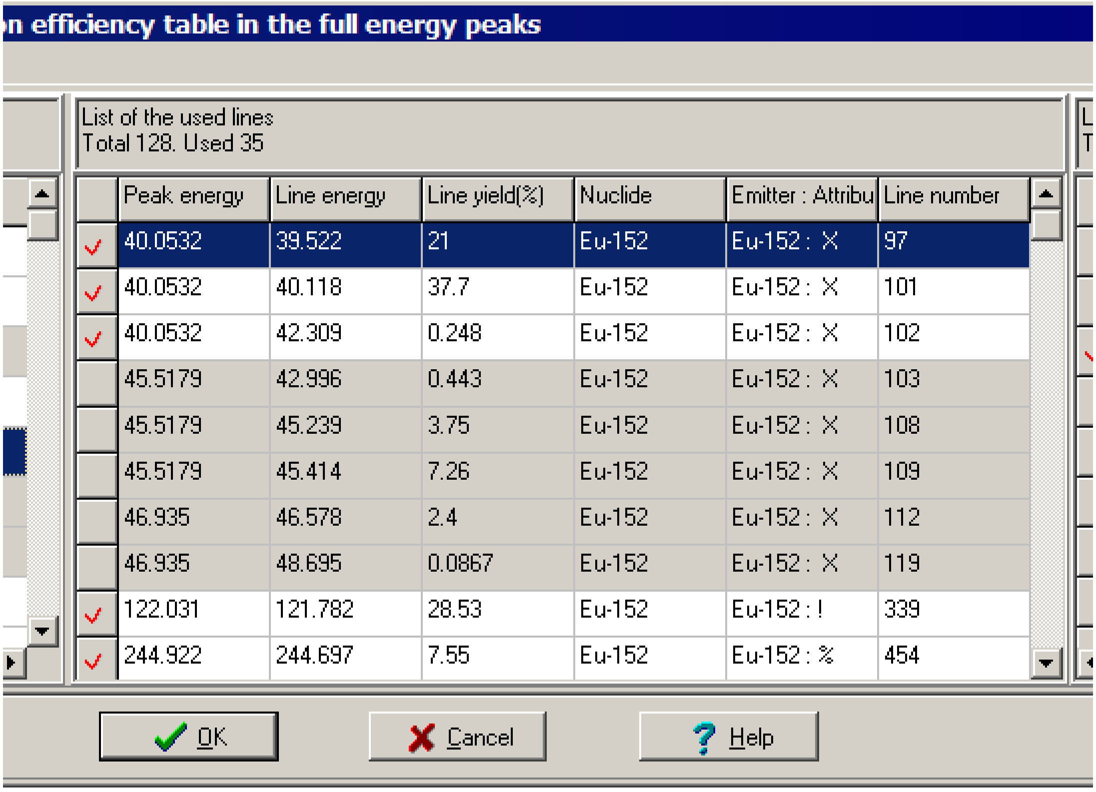
	Peak energy	Line energy	Line yield(%)
✓	40.0532	39.522	21
✓	40.0532	40.118	37.7
✓	40.0532	42.309	0.248
	45.5179	42.996	0.443
	45.5179	45.239	3.75
	45.5179	45.414	7.26
	46.935	46.578	2.4
	46.935	48.695	0.0867
✓	122.031	121.782	28.53

Peaks that cannot be used are marked in gray (peaks of undisclosed multiplets, escape peaks, cascading addition, weak peaks, etc.). Red check marks in the left column indicate the peaks used. The crossed out check mark ☒ indicates that the peak was marked by the operator, but the program cannot or does not recommend using it for some reason. The operator can deselect or add the desired peak by double-clicking on the line with information about the peak. You can use the "**Insert**" key on the computer keyboard, pressing which changes the state of the current line.



The right mouse button displays a small menu, with which the operator can select or deselect either the calibration or all peaks. Calibration peaks are considered to be the most powerful peaks whose energy is in the range specified for the calibration lines of the nuclide table.

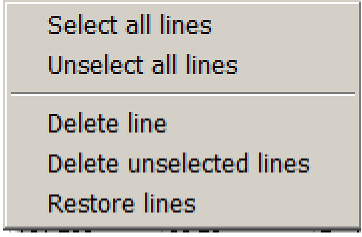
The second column has the form:



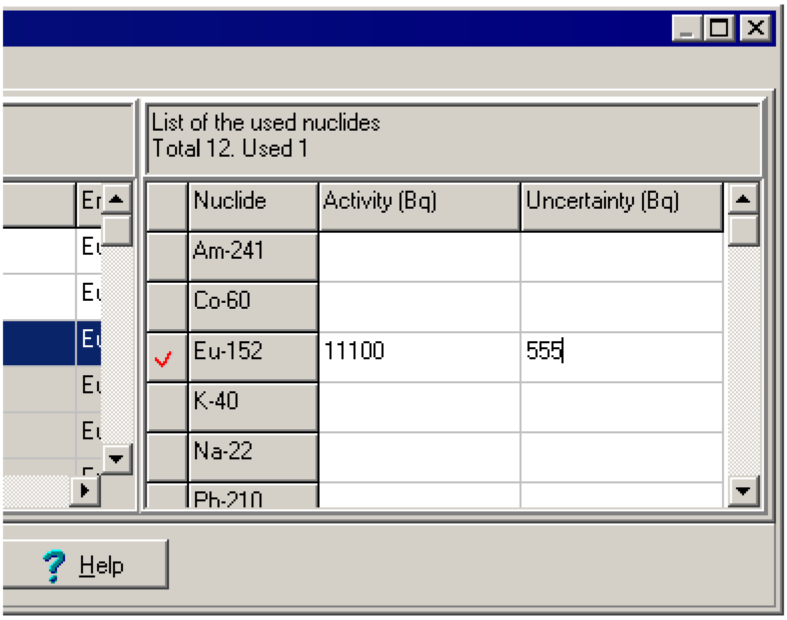
List of the used lines
Total 128. Used 35

	Peak energy	Line energy	Line yield(%)	Nuclide	Emitter : Attribu	Line number
✓	40.0532	39.522	21	Eu-152	Eu-152 : X	97
✓	40.0532	40.118	37.7	Eu-152	Eu-152 : X	101
✓	40.0532	42.309	0.248	Eu-152	Eu-152 : X	102
	45.5179	42.996	0.443	Eu-152	Eu-152 : X	103
	45.5179	45.239	3.75	Eu-152	Eu-152 : X	108
	45.5179	45.414	7.26	Eu-152	Eu-152 : X	109
	46.935	46.578	2.4	Eu-152	Eu-152 : X	112
	46.935	48.695	0.0867	Eu-152	Eu-152 : X	119
✓	122.031	121.782	28.53	Eu-152	Eu-152 : !	339
✓	244.922	244.697	7.55	Eu-152	Eu-152 : %	454

The operator can also double-click on the line information line to edit the list of lines forming the selected peaks. The right mouse button displays a small menu, with which the operator can select, deselect or delete lines.



The third column contains a list of nuclides forming the selected lines.


List of the used nuclides
Total 12. Used 1

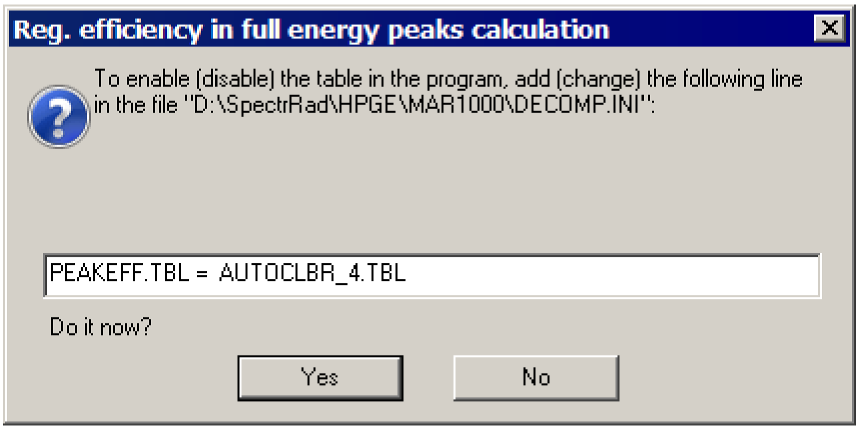
	Nuclide	Activity (Bq)	Uncertainty (Bq)
	Am-241		
	Co-60		
✓	Eu-152	11100	555
	K-40		
	Na-22		
	Pb-210		

Nuclides missing at the standard used for calibration can be removed by right-clicking on the nuclide table. The popup menu that is called contains three items: "**Select all nuclides**", "**Unselect all nuclides**" and "**Delete unselected nuclides**". Nuclides are selected by double-clicking on the name of the nuclide.

The operator must enter the value of the activities and errors of the nuclides present in the reference sample at the date of certification. For the geometries of measurements in the "thin" and intermediate layers enter the total activity of nuclides in the standard in Becquerel, for the geometry of measurements in the "thick" layer - the specific activity of nuclides in the standard in Bq/kg. If a standard certificate has been pre-formed for the nuclide table used, the program will substitute data on the activities and errors of nuclides from the existing standard certificate.

Pressing the "**OK**" key starts the procedure for calculating the registration efficiency tables (when calculating the registration efficiency in photo peaks, the table of the total efficiency of quantum registration in the detector is also calculated), after which the program suggests saving the generated tables in the "**Elements**" folder and adding the necessary lines in the "**Decomp.ini**" file to connect the calculated tables with the specified interpolation parameter with the processing program.

When saving the table, the program generates a window with information about the proposed modification of the corresponding line in the "**Decomp.ini**" file. For example:


Reg. efficiency in full energy peaks calculation

To enable (disable) the table in the program, add (change) the following line in the file "D:\SpectrRad\HPGE\MAR1000\DECOMP.INI":

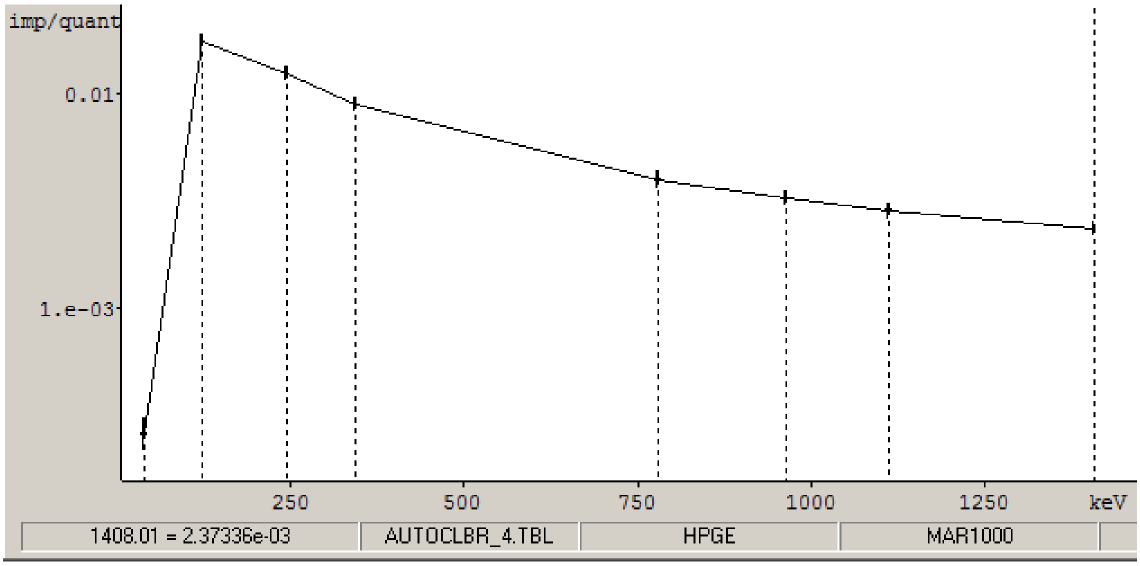
PEAKEFF.TBL = AUTOCLBR_4.TBL

Do it now?

The operator can agree with the proposed modification of the "**Decomp.ini**" file or edit the line himself.

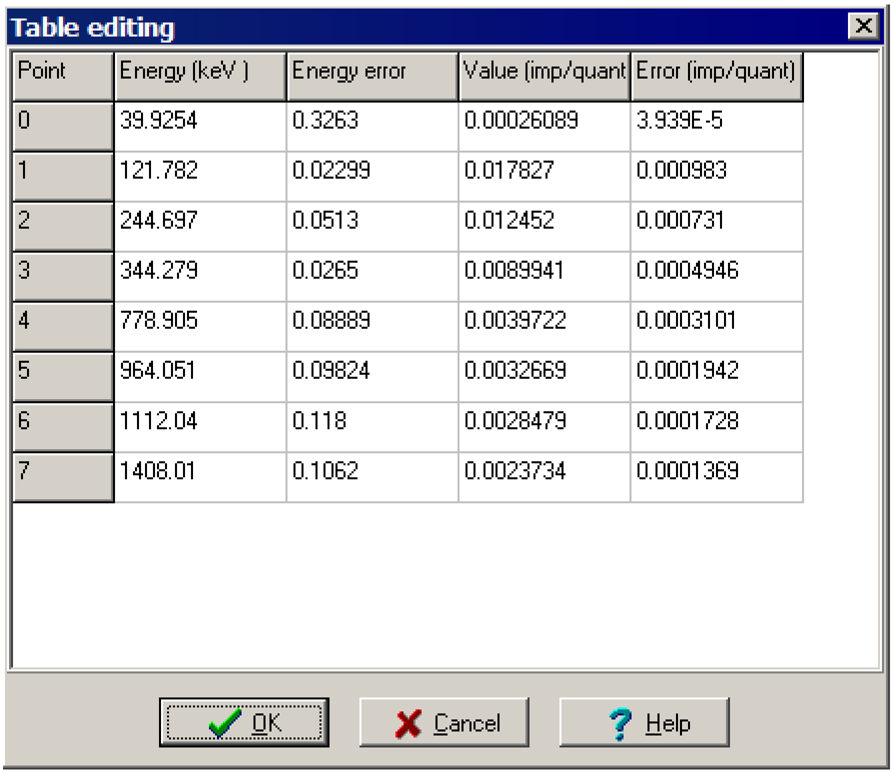
In addition to the quantum registration efficiency table in photo peaks, the procedure calculates the full registration efficiency for the average line energy of all nuclides of the standard sample and also suggests saving the calculated table and connecting it to the program by modifying the "**Decomp.ini**" file. Full registration efficiency is required to correctly account for the effects associated with simultaneous registration of several gamma quanta during cascade transitions. The most accurate full registration efficiency is calculated when calibrating according to reference source containing only one powerful line including 90 percent or more of the gamma quanta output. Therefore, if such standard sample is available, it is better to use them to calibrate the full efficiency of registration, and ignore the full efficiency calculated according to Eu-152 and not connect it to the program.

The view of the generated table in the piecewise linear visualization mode (namely, piecewise linear interpolation is used to calculate intermediate values of functions specified in a tabular manner) is not very pretty (the figure shows the mode of piecewise linear interpolation on a logarithmic scale):



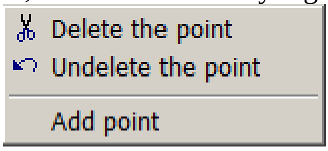
The table can be edited manually using the procedure for editing tables and spectra (Menu item "**Edit / Edit data...**"). Only the selected section of the table or spectrum is edited (the area between the two points of the table closest to the movable marker), and since in our case all points of the table are selected, if you do not deselect, only the last point of the table can be edited. Therefore, before editing, delete the marks (Menu item "**Edit / Delete mark**" or "**Edit / Delete all marks**").

The window of the editing procedure looks like this:

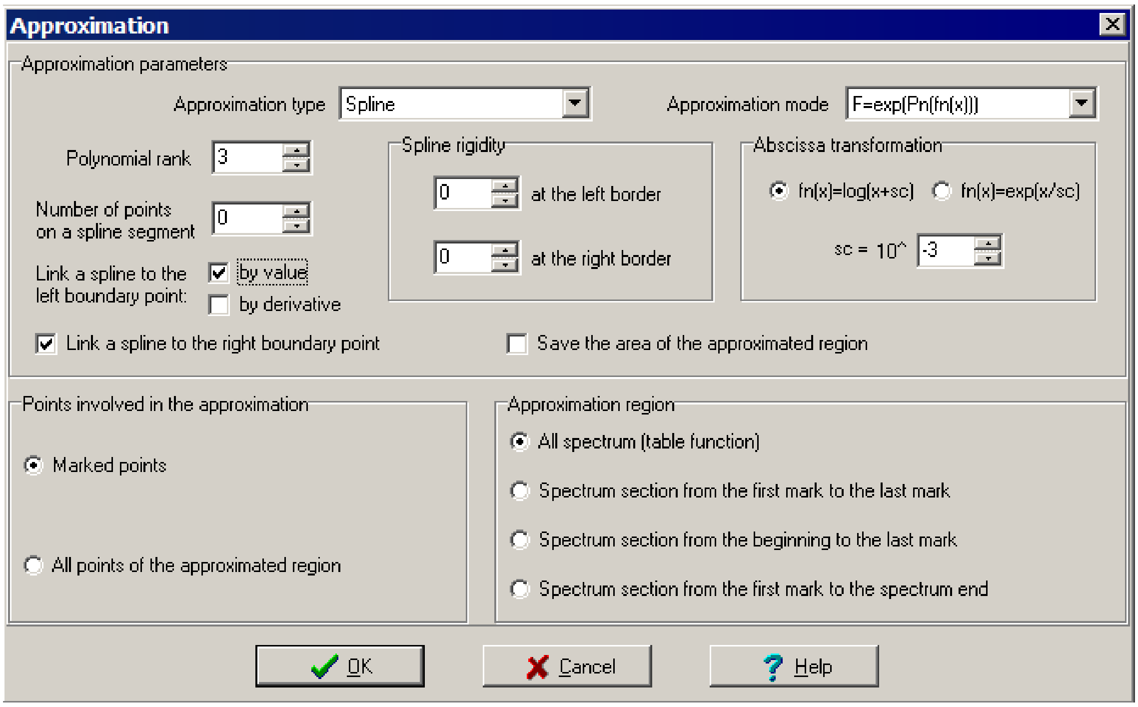


Point	Energy (keV)	Energy error	Value (imp/quant	Error (imp/quant)
0	39.9254	0.3263	0.00026089	3.939E-5
1	121.782	0.02299	0.017827	0.000983
2	244.697	0.0513	0.012452	0.000731
3	344.279	0.0265	0.0089941	0.0004946
4	778.905	0.08889	0.0039722	0.0003101
5	964.051	0.09824	0.0032669	0.0001942
6	1112.04	0.118	0.0028479	0.0001728
7	1408.01	0.1062	0.0023734	0.0001369

The operator can change the data of any point in the table, insert additional points into the table, or delete entries using the pop-up menu, which is called by right-clicking on the left column (point number) of any row in the table .



After editing, if necessary, it is required to approximate the table with a polynomial or spline. Approximation is required, on the one hand, to give the table a more decent appearance, and on the other hand, a smooth curve more adequately reflects a smooth continuous function of registration efficiency. Previously, the operator must mark with a marker the points of the table that will participate in the approximation. The approximation procedure is called by the menu item "**Edit / Approximate...**". At the same time, the procedure window appears on the screen:



Approximation parameters

Approximation type: Spline

Approximation mode: F=exp(Pn(fn(x)))

Polynomial rank: 3

Number of points on a spline segment: 0

Link a spline to the left boundary point: ☑ by value ☐ by derivative

☑ Link a spline to the right boundary point

Spline rigidity: 0 at the left border; 0 at the right border

Abscissa transformation: ● fn(x)=log(x+sc) ○ fn(x)=exp(x/sc)

sc = 10^ -3

☐ Save the area of the approximated region

Points involved in the approximation
- ● Marked points
- ○ All points of the approximated region

Approximation region
- ● All spectrum (table function)
- ○ Spectrum section from the first mark to the last mark
- ○ Spectrum section from the beginning to the last mark
- ○ Spectrum section from the first mark to the spectrum end

The form contains three groups of parameters: "Approximation parameters", "Points involved in the approximation" and "Approximation region".

In the "Approximation parameters" group, the operator must choose one of two possible types of approximation: "Spline" or "Polynome" (a spline is a function stitched from segments of polynomials, a spline is more flexible than a polynomial function, which is both an advantage and a disadvantage at the same time). Choose one of nine possible types of approximation (**Approximation mode**):

F=Pm(x)
F=Pm(fn(x))
F=exp(Pm(x))
F=exp(Pm(fn(x)))
F=1/Pm(x)
F=1/Pm(fn(x))
F=1/exp(Pm(x))
F=1/exp(Pm(fn(x)))
F=F0*(1-exp(-k*x))

And select the type of energy scale transformation function (**Abscissa transformation**) - **fn(x)**.

It is believed that the double logarithmic scale of the polynomial approximation **F=exp(Pm(fn(x))) fn(x) = log(x+sc)** is best suited for approximating registration efficiency functions in the range of 30-3000 keV. The constant **sc** (scale coefficient) set by the operator determines the range of variation of the abscissa for the polynomial - the larger the value of **sc**, the narrower the range of variation of the abscissa and, accordingly, the more rigid the polynomial (spline) and vice versa.

If it is possible to approximate the table with an asymmetric Gaussian with acceptable accuracy (**exp(Pn(log(x+sc)**, the **rank of the polynomial** is 2), then this is wonderful. If it fails, you can increase the rank of the polynomial. But increasing the rank is dangerous because at the boundaries of the range the polynomial may not bend in the right direction. If it is not possible to approximate the table with a polynomial, you must select **spline**. If the number of approximation points is sufficient to form a cubic spline, it is recommended to set the spline rank (**Polynomial rank**) to **3**.

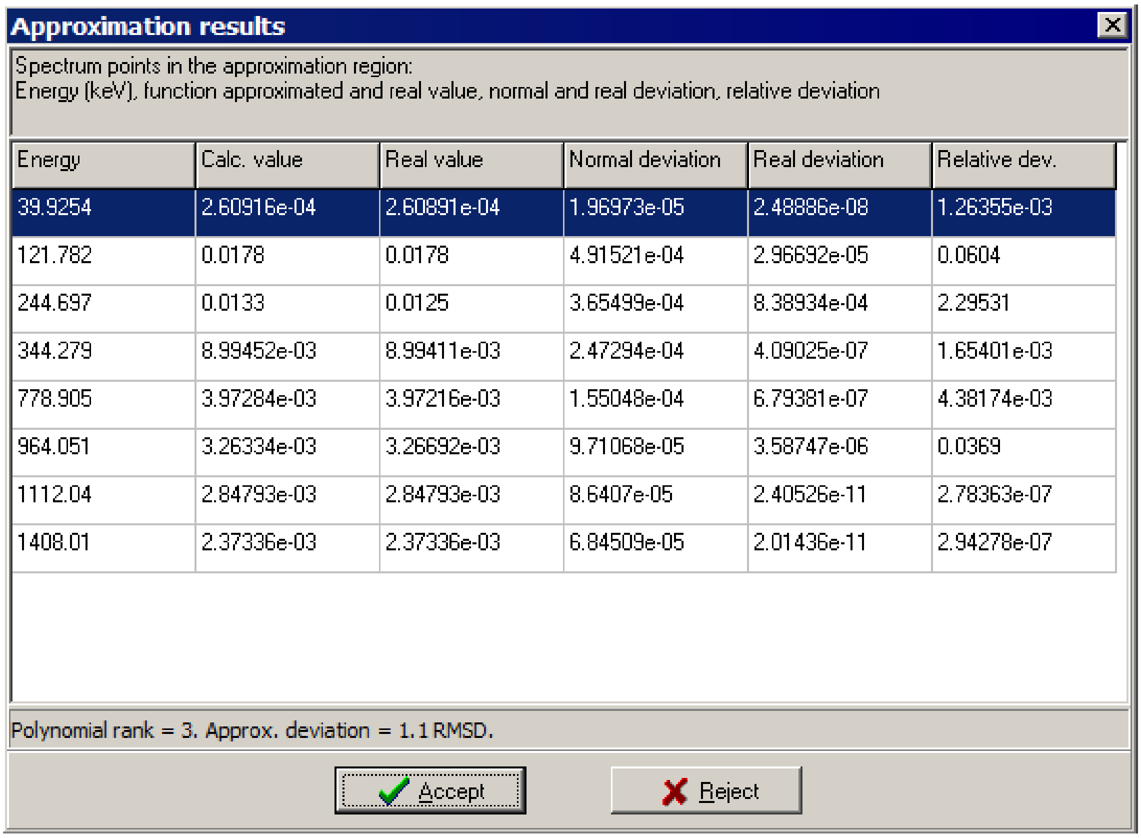
Number of points on a spline segment - the number of points of the original table used to calculate the parameters of the spline segment. The "**Spline rigidity**" parameter determines the stiffness of the spline. The stiffness of a polynomial or spline is determined by the constant set by the operator, used in the weight function of suppressing the curvature of the spline or polynomial. Two values of the stiffness constant are set for the spline: **at the left border** of the approximation area and **at the right border** of the approximation area. The value of the stiffness constant for a specific segment of the spline is calculated by linear interpolation from the specified values.

The spline can be linked to the left (**Link a spline to the left boundary point**) and (or) to the right boundary point (**Link a spline to the right boundary point**) of the approximated section. The spline can be bound to the left boundary point both **by value** and **by** the first **derivative**. To the right - only by value. Binding the spline to the left boundary point in both value and derivative allows the operator to independently create cross linked polynomials with different stiffness – a flexible polynomial for the low–energy region and a rigid one for high energies. If the derivative binding of the spline is set, and there are no points to the left of the left boundary point of the approximated section (the derivative on the left cannot be calculated), the derivative is considered equal to zero.

Selecting the "**Save the area of the approximated region**" checkbox allows you to save the area of the approximated curve, which is necessary when approximating line models and elementary spectra. In this case, you should not check the box.

In the "**Approximation region**" group, the operator must select which section of the table will be approximated. Since we marked the necessary points of the table with a marker, you need to select "**All spectrum (table function)**" and in the "**Point involved in the approximation**" group, select the "**Marked points**" mode. If the points in the table are not marked, and all are necessary for approximation, select the "**All points of the approximated region**" mode.

Pressing the "**OK**" key generates an approximation table and a form containing the results of the approximation:



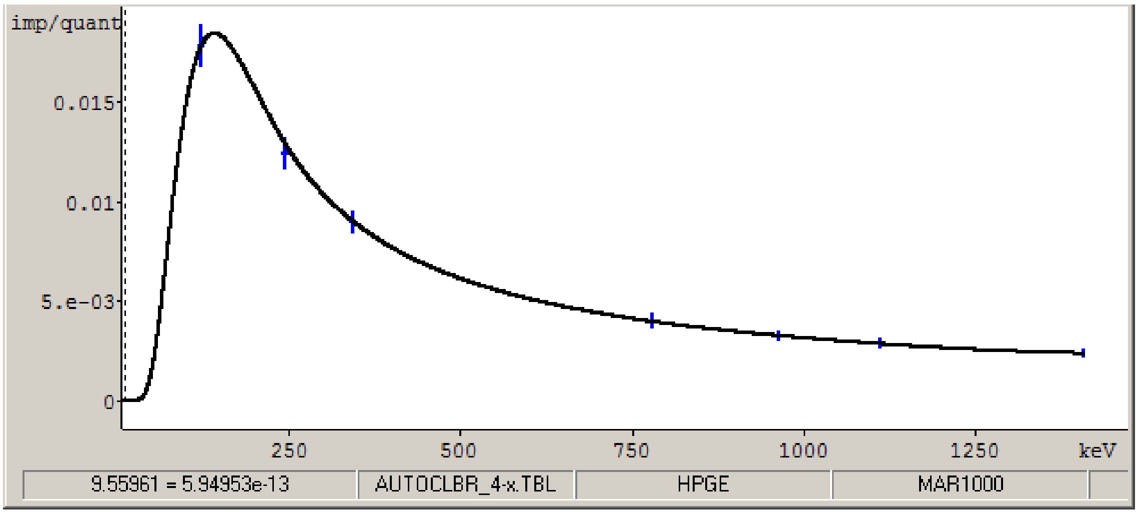
Spectrum points in the approximation region:
Energy (keV), function approximated and real value, normal and real deviation, relative deviation

Energy	Calc. value	Real value	Normal deviation	Real deviation	Relative dev.
39.9254	2.60916e-04	2.60891e-04	1.96973e-05	2.48886e-08	1.26355e-03
121.782	0.0178	0.0178	4.91521e-04	2.96692e-05	0.0604
244.697	0.0133	0.0125	3.65499e-04	8.38934e-04	2.29531
344.279	8.99452e-03	8.99411e-03	2.47294e-04	4.09025e-07	1.65401e-03
778.905	3.97284e-03	3.97216e-03	1.55048e-04	6.79381e-07	4.38174e-03
964.051	3.26334e-03	3.26692e-03	9.71068e-05	3.58747e-06	0.0369
1112.04	2.84793e-03	2.84793e-03	8.6407e-05	2.40526e-11	2.78363e-07
1408.01	2.37336e-03	2.37336e-03	6.84509e-05	2.01436e-11	2.94278e-07

Polynomial rank = 3. Approx. deviation = 1.1 RMSD.

The operator may or may not accept the results, and in the latter case, return to the original form of the approximation procedure, edit the data and try again.

When deciding to accept the results of the approximation, the program suggests saving the approximating table in a file. It should be saved under the same name as the original table, since this is the name of the file included in the "**Decomp.ini**" configuration file, but we cannot always be sure of the successful outcome of the approximation (the approximation was successful or not, it is visually checked), therefore it is recommended to create a backup copy of the original table. As a result, the approximated table takes the form:



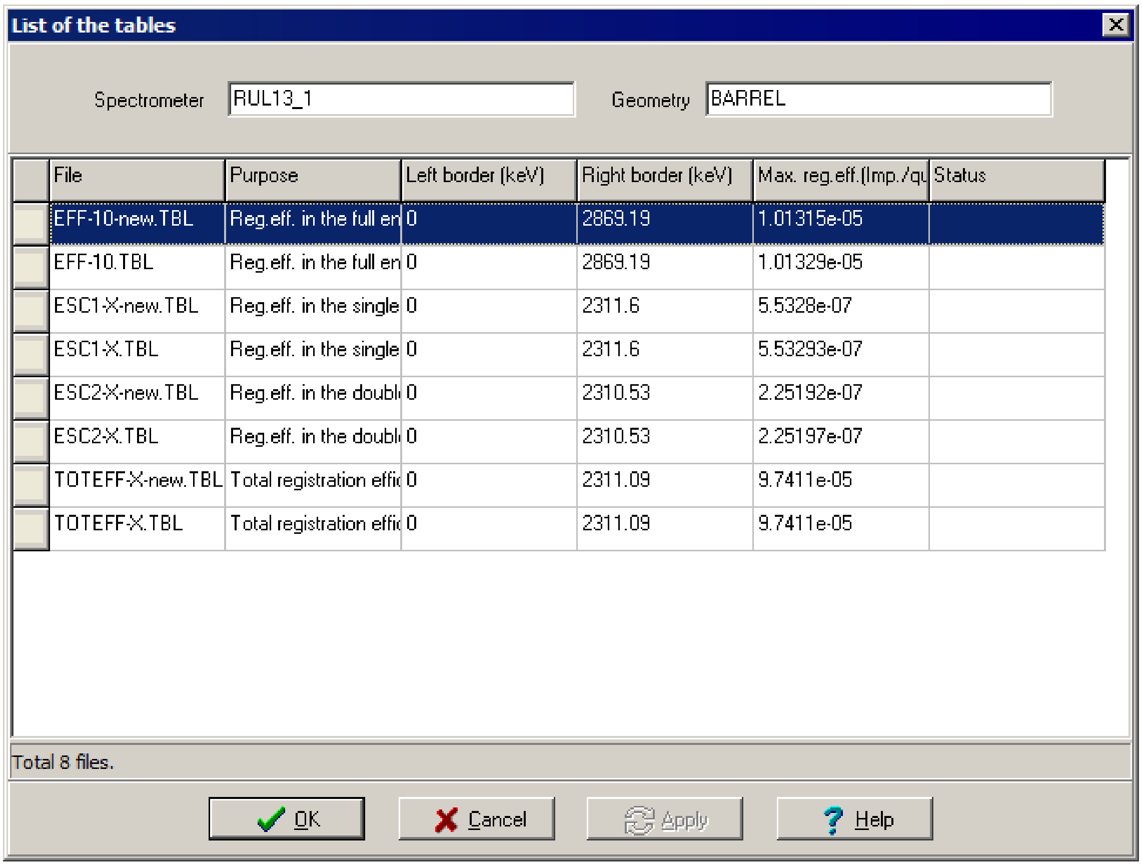
To correctly compare the two tables (the original and the approximated one), it is necessary to use the "**Normal**" scale of the ordinate axis. For clarity of comparison, the "**Dots**" visualization mode is selected (Menu item "**Visualization /Dots**"). From comparing the tables, it can be seen that the approximation is quite successful - the approximated function runs inside all rectangles with the exception of one point (at this scale of the X-axis, the rectangles look like vertical lines), which reflect the positions and errors of the points in the original table.

In the event that nuclides with cascading transitions were used in the calibration of efficiency, after installing the approximated table in the program, it is recommended to repeat the calibration of the registration efficiency. During recalibration, the existing table of registration efficiency in photo peaks, tables of full registration efficiency is taken into account and the effects associated with cascade transitions are taken into account more correctly.

The calibration of the quantum registration efficiency in escape peaks should be carried out after calibration of the quantum registration efficiency in full absorption peaks. The gamma line table used should contain information about the escape lines. The standard samples used for calibration must contain nuclides having lines with energies exceeding 1022 keV.

The calibration procedure does not differ from the calibration procedure for recording efficiency in total absorption peaks, except that the operator must use peaks containing escape lines for calibration.

The list of calculated quantum registration efficiency tables can be viewed by clicking on the menu item "**Calibration / List of efficiency tables...**". The view form can look like:

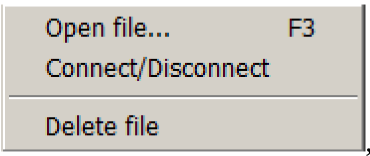


Spectrometer: RUL13_1

Geometry: BARREL

File	Purpose	Left border (keV)	Right border (keV)	Max. reg.eff.(Imp./qu	Status
EFF-10-new.TBL	Reg.eff. in the full en	0	2869.19	1.01315e-05	
EFF-10.TBL	Reg.eff. in the full en	0	2869.19	1.01329e-05	
ESC1-X-new.TBL	Reg.eff. in the single	0	2311.6	5.5328e-07	
ESC1-X.TBL	Reg.eff. in the single	0	2311.6	5.53293e-07	
ESC2-X-new.TBL	Reg.eff. in the doubl	0	2310.53	2.25192e-07	
ESC2-X.TBL	Reg.eff. in the doubl	0	2310.53	2.25197e-07	
TOTEFF-X-new.TBL	Total registration effic	0	2311.09	9.7411e-05	
TOTEFF-X.TBL	Total registration effic	0	2311.09	9.7411e-05	

Total 8 files.



Using the small pop-up menu, the operator has the opportunity to view the file, connect it to processing procedures or disable, delete the file. You can delete a file only after it is disabled.

Features of calibration of registration efficiency for detectors with high registration efficiency

In detectors with high registration efficiency (more than 30%), gamma quantum registration processes for nuclides with a cascade decay scheme play a significant role (and most nuclides have a cascade decay scheme). To correctly account for the nuances in the registration process of cascading gamma quanta, calibration of the full efficiency of gamma quanta registration in the spectrometer is required.

In the SPECTRRAD package, the total registration efficiency is calculated when calibrating the efficiency in photo peaks and is taken into account when calculating the registration efficiency in photo peaks. But if, when calibrating spectrometers with detectors with low registration efficiency (10%-20%), the approximation of estimating the full registration efficiency from a single nuclide with a lot of lines used in calibration of registration efficiency in photo peaks, for example Eu-152, is acceptable, since the redistribution of recorded pulses due to cascade transitions is insignificant, for detectors with high efficiency registration requires a special approach. For such detectors, and for any detectors, if the measurement accuracy is very important for us, it is first necessary to correctly calibrate the full efficiency of gamma quanta registration in the spectrometer.

In the "SPECTRRAD" package, as already mentioned, it is calculated when calibrating the efficiency in photo peaks. In this case, the average output of gamma quanta for the average energy is calculated. This approach is quite acceptable either at close line energies or at high line energies.

The accuracy of estimating the total recording efficiency for a particular energy will be the higher the greater the output of gamma quanta belongs to one line. Ideally, it is the only line in the radiation spectrum of the nuclide. The ideal option is practically not found. Recommended set of nuclides for calibration of the full registration efficiency are: Am-241, Cd-109, Co-57, Ce-139, Sn-113, Cs-137, Mn-54, Zn-65, Co-60, K-40.

It is required to measure and calibrate the registration efficiency in photo peaks using standards made on the basis of these nuclides (not mixtures of nuclides, but single nuclides). In the procedure for calculating the registration efficiency, it is important to correctly set the left boundary energy of the spectrum. It should cut off soft X-ray radiation (despite the fact that X-ray peaks can be used to calibrate the recording efficiency in photo peaks). As a result, we will get a set of points of full efficiency of registration of gamma quanta for various energies.

The resulting data set will include files of full registration efficiency and quantum registration efficiency in photo peaks. After calibrating the spectrometer according to the proposed set of nuclides, it is possible to calibrate the spectrometer according to standard samples made from a mixture of nuclides or based on nuclides with several powerful lines, for example, the same Eu-152 and combine the data obtained.

The standard procedure for including calculated data in the general data set for the registration efficiency function allows you to include no more than six files of efficiency tables – a sufficient option for calibration of efficiency in photo peaks. The proposed set of nuclides is more than six. In the event that the number of files to be merged containing information about the effectiveness of registration exceeds six, it is recommended to merge the tables manually (menu item "**Edit/Addition ...**") and to approximate the final tables. The most suitable type of approximation for the energy range from 0 to 2000 keV in this case is **F=F0*(1–exp(-k*x))**. This type of approximation is available only in the "**Polynome**" mode.

It is recommended to combine the files of the registration efficiency tables in photo peaks in any case for the purpose of approximating the final table.

Calculation of registration efficiency for volumetric or planar geometries based on the registration efficiency of a point source

In gamma spectrometry, the registration efficiency for volumetric or planar geometry can be calculated by integrating the registration efficiency for points within the geometry. The parameters that will determine the final registration efficiency are: the distance from the calculated point to the effective center of the detector, the distance that the gamma quantum flies in the material of the counting sample, in the material of the container and medium between the detector and the counting sample, the chemical composition and density of the material of the counting sample, container and medium.

It is assumed that the radiation in vacuum from the selected point is attenuated in proportion to the square of the distance from the point to the effective center of the detector. To calculate this distance, in advance, when calibrating the registration efficiency for a point source, the "**detector depth**" is calculated - the distance from the detector boundary to the effective center of the detector. This distance is a function of the energy of gamma quanta and depends on the relative position of the point and the detector. It would be more correct to calculate the depth of the detector for different directions along the axes of the detector. In practice, it is extremely difficult to do this – the detector protection and the collimator interfere. Therefore, the SPECTRRAD software package uses the depth calibration of the detector only along one main axis.

To calculate the depth of the detector, the recording efficiency is calibrated for two positions of the point source with different distances of the source from the detector along the main axis of the detector. The procedure for calculating the depth of the detector is described in detail in the chapter "**Installing the measurement geometry / Calculating the detector depth**".

A detailed description of the procedure for calculating the registration efficiency for volumetric and planar geometries based on the registration efficiency of a point source is given in the chapter "**Installing the measurement geometry / Recalculation of the registration**

efficiency for a given geometry". The procedure allows you to recalculate four tables of registration efficiency for the specified parameters of volumetric or planar geometry (in photo peaks, in peaks of single and double escape, and total efficiency). In addition, a correction factor is calculated for the efficiency of recording total gamma quanta during cascade transitions, which allows for more accurate consideration of the effects associated with cascade transitions.

Calculation of elementary spectra from reference spectra

If the components of the spectrum decomposition procedure (decomposition) are the spectra of the spectrometer response per unit of nuclide activity - elementary spectra, estimates of the contributions of the components to the spectrum will be the activity of nuclides. Therefore, the calibration of the spectrometer includes a procedure for calculating elementary spectra from the spectra of standards (reference samples of activity). The calculation of elementary spectra from reference spectra is a much more accurate procedure than the generation of elementary spectra from nuclide tables and spectrometer calibrations. And if, when processing well-resolved linear spectra, the procedure for generating peak spectra from the nuclide table and the registration efficiency function works well, for continuous spectra, generation sins with large errors, due to the need to generate a complete response to line radiation, including a continuous spectrum (the spectrum of Compton scattering of gamma quanta and bremsstrahlung of beta particles). In any case (and for well-resolved linear spectra), the use of elementary spectra calculated from the spectra of standards increases the accuracy of decomposition.

For measurement geometries in the "thick" layer, the specific activity - Becquerel/kg is used as the unit of activity (the response of the spectrometer depends on the specific activity of the sample and does not depend on the total activity, since only particles of the upper layer of the counting sample are recorded). For the geometries of the "thin" and intermediate layers, the Becquerel (Bq) is used as the unit of activity.

For geometries of the "thick" layer, the response of the spectrometer per unit of specific activity of the nuclide does not depend on the density or mass of the counting sample, but depends on the geometric parameters of the counting sample or the geometry of measurements (if geometry with a variable geometric parameter is used) and the loading of the spectrometer. The response of the spectrometer to 1 nuclide decay (for the geometries of the "thin" and intermediate layers) depends both on the density of the counting sample and on the geometric parameters of the counting sample or the geometry of measurements and on the loading of the spectrometer - on the **interpolation parameters** set in the geometry parameters. Therefore, for the correct calculation of elementary spectra corresponding to the interpolation parameter of the measurements, the calculation of the elementary spectra must be carried out several times using standard samples with different values of the **interpolation parameter**.

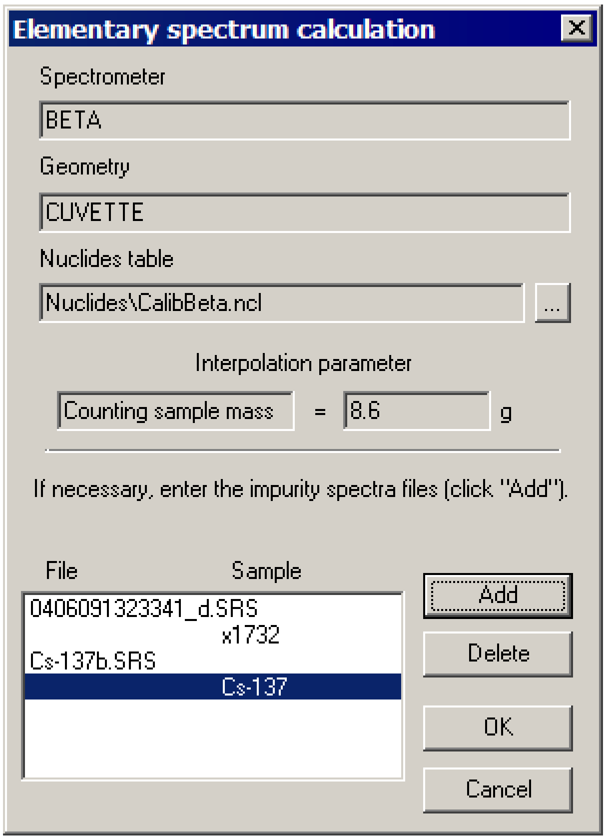
Since the calculation of the elementary spectrum also calculates the average radiation energy of the standard used when taking into account radiation absorption in determining the "total" alpha and beta activity, for the correct calculation of the average radiation energy, non-detectable low energy lines of the standard sample nuclides must be removed from the nuclides table used when calibrating the spectrometer.

It is previously required to perform an auto-calibration of the spectrometer.

Then measure a reference sample of the activity of the required nuclide in a given geometry for a time sufficient to set at least 200 pulses per channel in the operating range of the spectrum according to the cyclic measurement mode with a cycle duration equal to the average measurement time of the working sample.

In the case of complex standards containing mixtures of nuclides, repeat this procedure for all standards containing interconnected mixtures of nuclides.

Then process the spectra of the standards according to the "**Calibration / Elementary spectrum / Calculate by acquired spectra...**" mode. At the same time, the following table is displayed on the screen:



Elementary spectrum calculation

Spectrometer
BETA

Geometry
CUVETTE

Nuclides table
Nuclides\CalibBeta.ncl

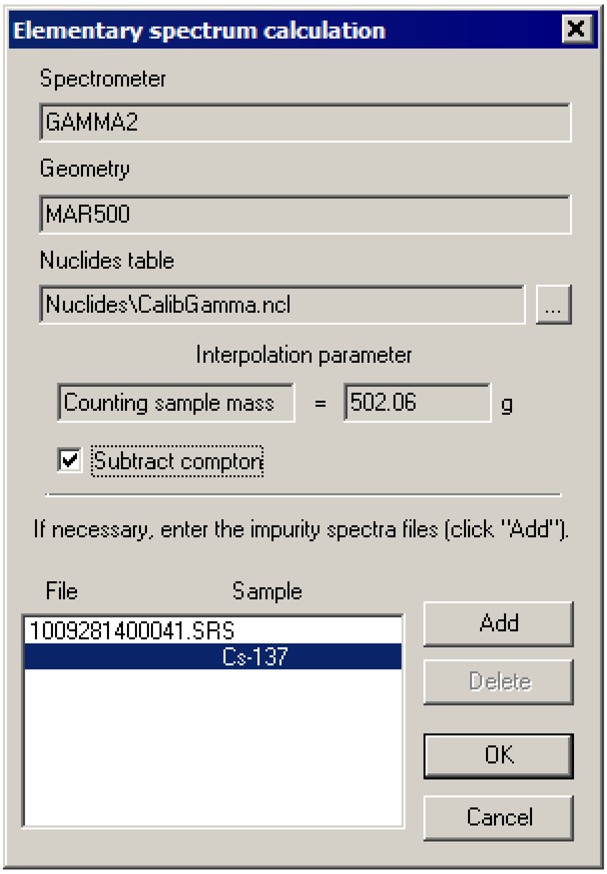
Interpolation parameter
Counting sample mass = 8.6 g

If necessary, enter the impurity spectra files (click "Add").

File	Sample
0406091323341_d.SRS	x1732
Cs-137b.SRS	Cs-137

The ... button allows you to select the required nuclide table. Since, when recalculating the nuclide activities of the standard entered on the date of certification to the values of the average nuclide activity necessary for calculating elementary spectra during the measurement of the standard, the program takes into account the processes of decay and accumulation of nuclides, the nuclide table must contain a correct scheme of nuclide decay.

For gamma–ray spectrometry, the procedure for calculating elementary spectra allows us to calculate either the full responses of the spectrometer, including both the spectrum of continuous scattering (Compton gamma quanta and bremsstrahlung X-ray of beta particles), and peak spectra - the responses of the spectrometer with the subtracted spectrum of continuous scattering. In this case, the first form of the calculation procedure may look like:


Elementary spectrum calculation

Spectrometer: GAMMA2

Geometry: MAR500

Nuclides table: Nuclides\CalibGamma.ncl

Interpolation parameter: Counting sample mass = 502.06 g

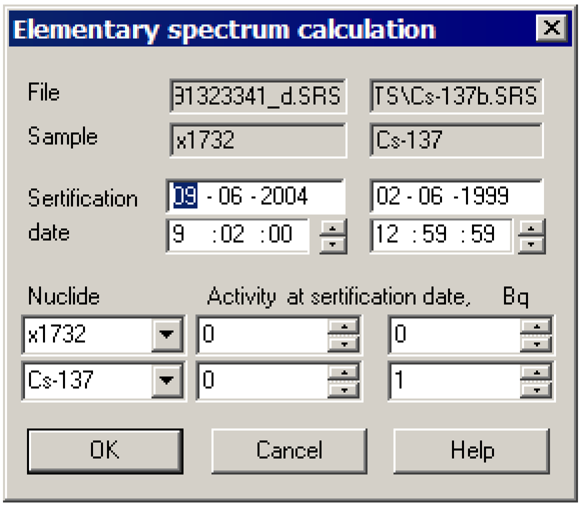
☑ Subtract compton

If necessary, enter the impurity spectra files (click "Add").

File	Sample
1009281400041.SRS	Cs-137

When the "**Subtract compton**" check mark is set, the calculation of elementary (normalized per unit of activity) spectra of peaks will be performed. In this case, a search for peaks in the spectrum of the standard must be carried out beforehand. Since the background spectrum must be subtracted from the measured spectrum, in the case of peak spectra calculation, peak search must also be performed for the background spectrum used. Therefore, the calculation procedure will display the background spectrum used in the **SpectrRad-V** program window and prompt the operator to edit it if necessary (the procedure for editing the background spectrum is described in detail in the chapter "Calibration of registration efficiency").

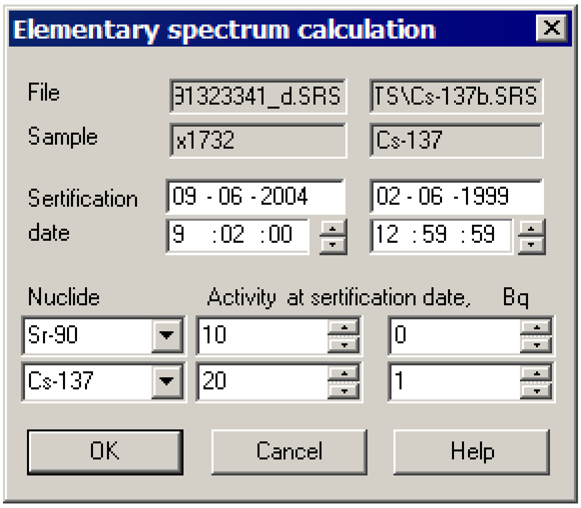
In the case of standards containing mixtures of nuclides, the operator must add files containing spectra of impurities (up to 4 files) to the list. In this case, the operator can specify either previously calculated elementary spectra of impurity nuclides, or files of spectra of standards containing impurity nuclides. If the reference consists of nuclides forming a decay chain, additional files may be spectra of the same reference measured at different times. The period between measurements is determined by the half-life of the nuclides in the reference. Upon completion of the file input, a table is displayed for entering the values of the activity of nuclides in the standards. Its appearance depends on the number of reference files, for two files it may look like this:


Elementary spectrum calculation

File	31323341_d.SRS	TS\Cs-137b.SRS
Sample	x1732	Cs-137
Sertification date	09 - 06 - 2004 9 :02 :00	02 - 06 -1999 12 :59 :59

Nuclide	Activity at sertification date, Bq	
x1732	0	0
Cs-137	0	1

The operator must enter the names of the nuclides contained in the set of standards and the values of the activity of the nuclides (in the example **Sr-90** and **Cs-137**) on the date of certification for the standard sample **x1732** and the standard **Cs-137**. For example, the **x1732** reference sample contains 10 Bq **Sr-90** and 20 Bq **Cs-137**, and the **Cs-137b.src** file contains the elementary spectrum of **Cs-137**. In this case, the table with the entered data should look like this:


Elementary spectrum calculation

File	31323341_d.SRS	TS\Cs-137b.SRS
Sample	x1732	Cs-137
Sertification date	09 - 06 - 2004 9 :02 :00	02 - 06 -1999 12 :59 :59

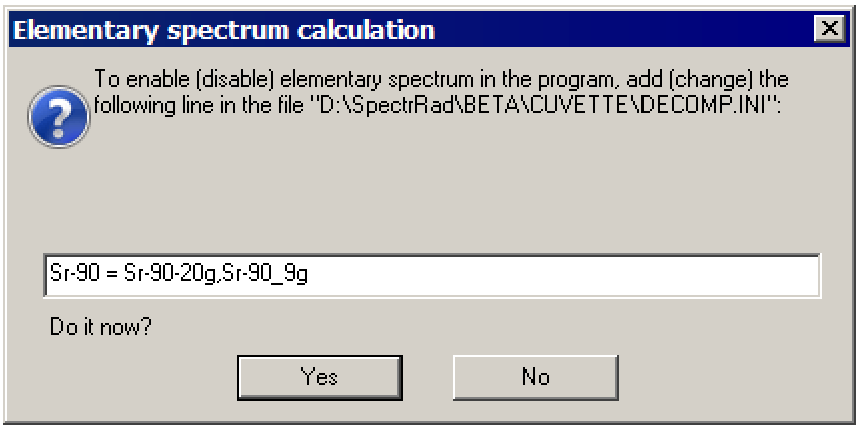
Nuclide	Activity at sertification date, Bq	
Sr-90	10	0
Cs-137	20	1

After entering the activity values, the program will request the input of the values of errors of the certified activity of nuclides in a table of a similar type.

For the geometries of the "thick" layer, the program will request the values of the nuclides specific activity of the standards sample in Bq/kg.

Upon completion of entering all data, the program calculates the elementary spectrum of the nuclide saves it in the "**Elements**" folder of this spectrometer and this geometry and suggests changing the "**Decomp.ini**" file accordingly, including information about the new elementary spectrum.

When saving the spectrum, the program generates a window with information about the proposed modification of the corresponding line in the "**Decomp.ini**" file. For example:



Elementary spectrum calculation

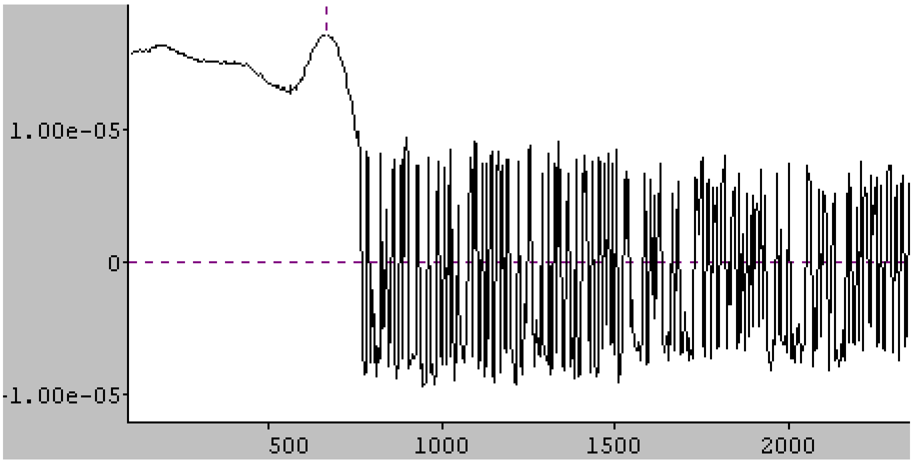
To enable (disable) elementary spectrum in the program, add (change) the following line in the file "D:\SpectrRad\BETA\CUVETTE\DECOMP.INI":

Sr-90 = Sr-90-20g,Sr-90_9g

Do it now?

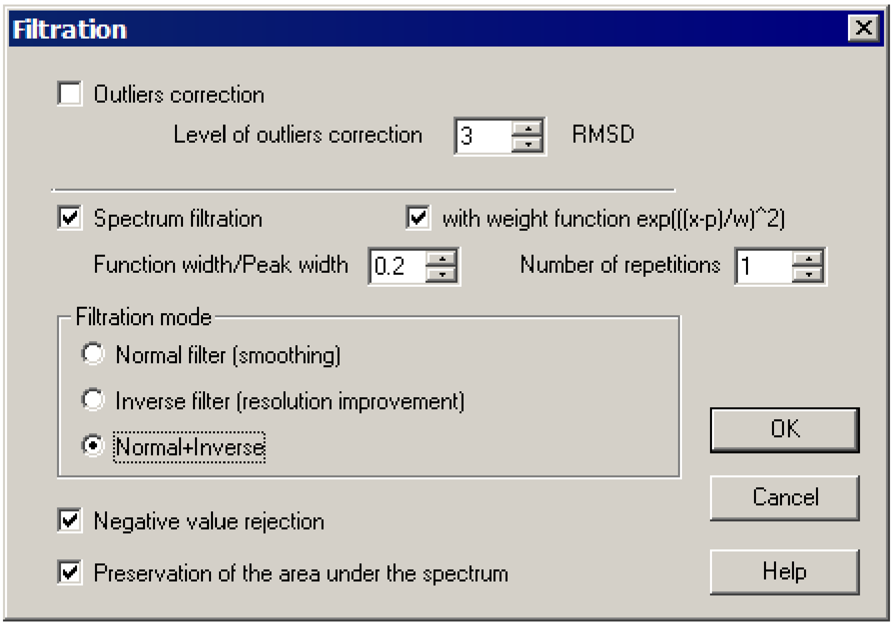
The operator can agree with the proposed modification of the "**Decomp.ini**" file or edit the line himself.

The resulting elementary spectrum contains statistical fluctuations and may look like this, for example (in the example, the Cs-137 spectrum on a logarithmic scale):



Since derivatives of elementary spectra are calculated during the processing of working sample spectra, it is recommended to filter it using the "**Edit / Filtrate...**" command or approximate it with a spline (menu item "**Edit / Approximate...**"). When approximating with a spline, it is necessary to set the mode of preserving the area of the approximated area in the approximation parameters. Then "clean" the spectral regions that do not contain statistically significant positive values with the "**Edit / Erase ...**" procedure, which allows you to more accurately set the significant region of the spectrometer's response function to the radiation of a given nuclide and, accordingly, more accurately calculate the errors in the estimates of the activities of this nuclide.

The window (form) of the filtering procedure looks like:



Filtration

☐ Outliers correction

Level of outliers correction 3 RMSD

☑ Spectrum filtration ☑ with weight function exp(((x-p)/w)^2)

Function width/Peak width 0.2 Number of repetitions 1

Filtration mode

○ Normal filter (smoothing)

○ Inverse filter (resolution improvement)

● Normal+Inverse

☑ Negative value rejection

☑ Preservation of the area under the spectrum

Spectrum filtering is performed for the selected section of the spectrum and allows you to:

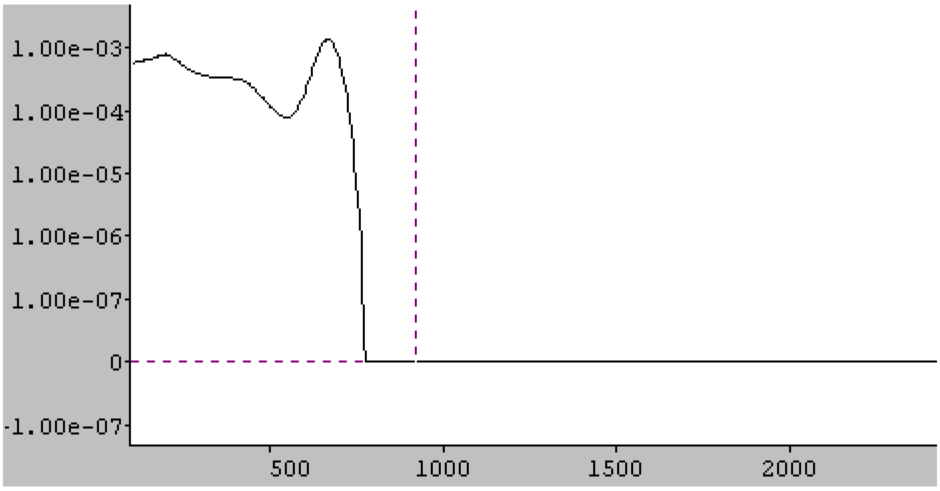
- **Correct the outliers** (the "**Outliers correction**" checkbox is selected). An outlier will be considered a value in the spectrum channel that deviates from the average value in three adjacent channels (left, right and under study) by an amount greater than the **Levels of outliers correction** set by the operator in terms of standard deviations (**RMSD**) under the assumption of Poisson spectrum statistics. The “average" in this procedure is calculated as the average value in the sense of least modules, not least squares. The outlier value will be replaced by the average value. The area of the spectrum is not preserved during outlier’s correction.
- **Spectrum filtration** - filtering the spectrum by averaging over a given **number of points** or **with a** given **weight function** $\exp(((x-p)/w)^2)$ suppresses high-frequency spectrum noise (smooth the spectrum), but slightly degrades the resolution. If the spectrum is linear and calibrated by peak width, when smoothing **with a weight function**, the operator sets the ratio of the width of the function to the width of the peaks of the spectrum (**Function width/Peak width** $w/fwhm$, w is the width of the weight function, $fwhm$ - the width of the peak at half the height). The operation is performed for a specified **number of repetitions**.
- If the “**Inverse filter (resolution improvement)**” checkbox is selected, the reverse smoothing operation is performed (the filtering operator is pre-inverted). If smoothing reduces noise and slightly degrades resolution, then the inverse operation, accordingly, increases noise and slightly improves resolution.
- Zeroing negative values (the “**Negative value rejection**” checkbox). The operation of zeroing negative values changes the area of the spectrum. To restore the original area of the spectrum, the operator must check the box “**Preservation of the area under the spectrum**".

The application of forward and reverse filtering to the spectrum does not lead to the restoration of the original spectrum due to poor condition number of the inverse matrix, the presence of edge effects. As a result, the application of a composite filter (**Normal+Inverse**) to the spectrum, with proper selection of the width of the weight function, allows noise suppression without compromising the resolution of the spectrum.

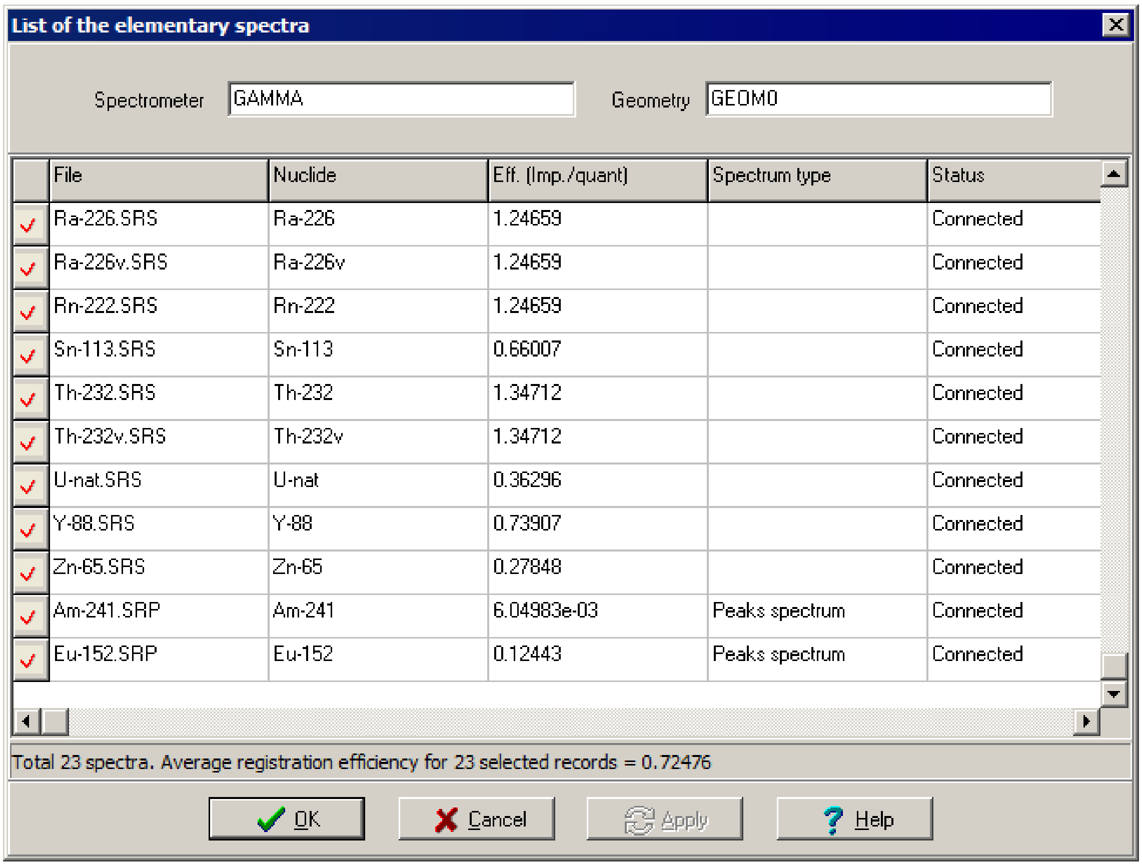
Smoothing and reverse filtering operations preserve the area of the spectrum.

The order of operations: correction of outliers, smoothing and cutting of negative values.

Recommended parameter values are given in the example form of the filtering procedure. After filtration and cleaning procedures, the spectrum takes the form:



The list of calculated elementary spectra can be viewed by clicking on the menu item "**Calibration / List of elementary spectra...**". The viewing form may look like:

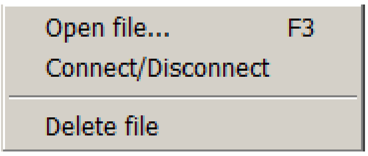


Spectrometer: GAMMA

Geometry: GEOM0

	File	Nuclide	Eff. (Imp./quant)	Spectrum type	Status
✓	Ra-226.SRS	Ra-226	1.24659		Connected
✓	Ra-226v.SRS	Ra-226v	1.24659		Connected
✓	Rn-222.SRS	Rn-222	1.24659		Connected
✓	Sn-113.SRS	Sn-113	0.66007		Connected
✓	Th-232.SRS	Th-232	1.34712		Connected
✓	Th-232v.SRS	Th-232v	1.34712		Connected
✓	U-nat.SRS	U-nat	0.36296		Connected
✓	Y-88.SRS	Y-88	0.73907		Connected
✓	Zn-65.SRS	Zn-65	0.27848		Connected
✓	Am-241.SRP	Am-241	6.04983e-03	Peaks spectrum	Connected
✓	Eu-152.SRP	Eu-152	0.12443	Peaks spectrum	Connected

Total 23 spectra. Average registration efficiency for 23 selected records = 0.72476



Using a small pop-up menu the operator has the opportunity to view the file, connect it to the processing procedures or disable, delete the file. You can delete a file only after it is disabled.

Calculation the models of the peaks

The model of the line (line model) is the response of a spectrometer to radiation of a certain energy. When processing the allowed linear spectra, a part of the line model is used – the model of the peak (peak model). Peak models are used both in the search for peaks and in the generation of peak spectra for nuclides suspected of forming the spectrum.

The approach common in the past to use a superposition of elementary functions as a peak model (usually a Gaussian stitched at the edges with exponents) is bad because the real shape of the peak is more complicated than any superposition of elementary functions, and using a large number of parameters to provide the necessary flexibility of an artificially constructed peak model worsens the conditionality of the system.

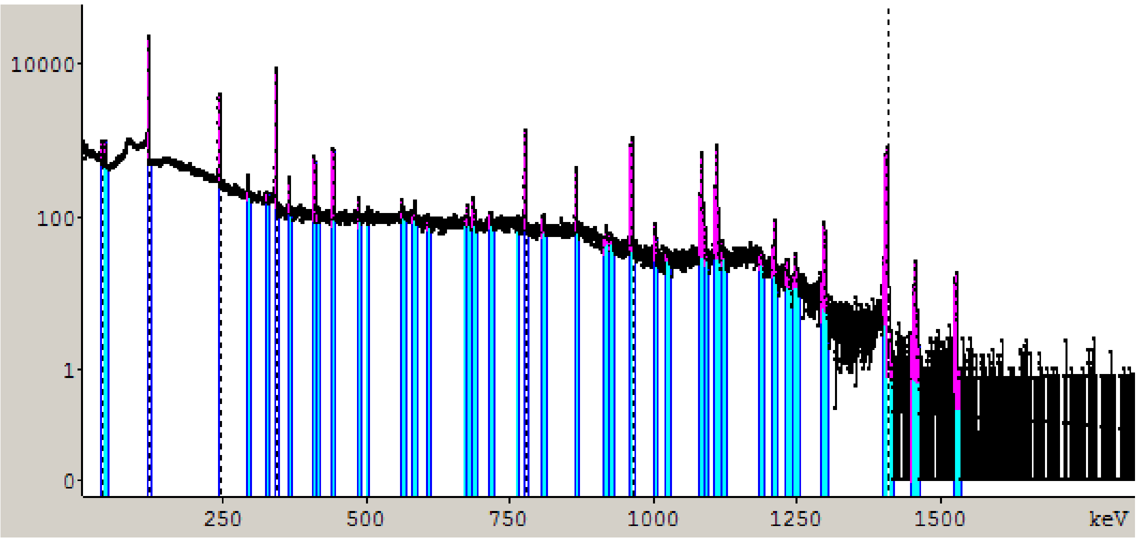
The software package "SpectrRad" uses either a Gaussian or a really measured response of the spectrometer to radiation of certain energy as a peak model. The use of the measured response of the spectrometer to radiation of certain energy removes all problems of discrepancy between the shape of the real peak and the model used. For resolved gamma (X-ray) spectra, the peak model is calculated from the peak spectra (the Compton scattering spectrum is pre-subtracted). At the same time, it is assumed (and confirmed by experience) that within the limits used to calculate the model, peak or multiplet, all shape changes are accurately described by an affine type deformation $\varphi(z) = \varphi(\frac{x-p}{w})$. Accounting for more complex shape changes depending on the energy and type of line is ensured by the fact that not one model is used, but a set of peak models for different energies and types of lines (gamma, X-ray or annihilation) and the peak model for a specific energy and type of line is calculated by interpolation from neighboring peak models for this type of line.

The shape of the peak spectrum, in general, depends on the density of the counting sample and on the geometric parameters of the counting sample or the geometry of measurements (if geometry with a variable geometric parameter is used) and on the load of the spectrometer - depending on the **interpolation parameter** set in the geometry parameters, therefore, in order to correctly calculate the peak spectra corresponding to the interpolation parameter of the measured spectrum of the working sample, it is recommended to calculate the peak spectra several times using standards with different values of the **interpolation parameter**.

Note that the accuracy of the description of the peak shape is higher the more spectrum channels are used in the formation of the peak model. Therefore, the number of channels of the spectrometer and the energy range used must provide at least 5 points of the spectrum per half-width of the peak. For example: we have a spectrometer with a number of channels of 8192 and a resolution of 1.2 keV at the beginning of the range used. In this case, we will have to limit ourselves to the upper energy equal to 8192*1,2/5 = 1966 keV.

It is previously required to perform an auto calibration of the spectrometer and set the parameters of the peak search procedure, if they have not yet been set. Then measure a reference sample of the activity of a nuclide or a mixture of nuclides (standard) having a sufficient number of peaks in the operating energy range, in a given geometry, for a sufficient time to set peaks that will be used to calculate the spectra of lines, at least 1000 pulses, according to the cyclic measurement mode with a cycle duration equal to the average measurement time of the working sample. For the range from 30 to 1500 keV, a mixture of Am-241 with Eu-152 is usually used. Since the annihilation peaks are somewhat wider than usual, it is recommended to form a model of the annihilation peak using, for example, a standard based on Na-22.

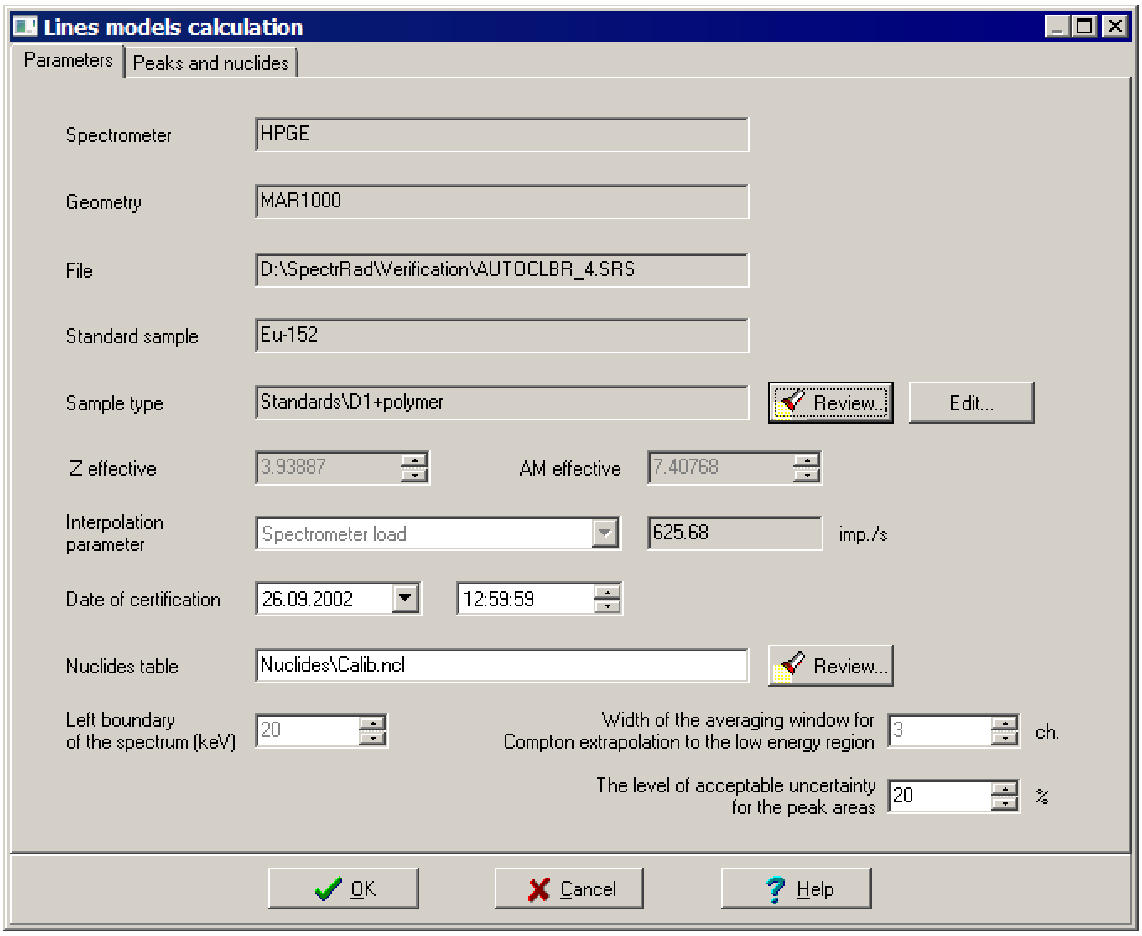
As an example of calculating line spectra, we use the Eu-152 spectrum. We will first mark the peaks that will be used for peaks models with markers. The spectrum, in this case, may look like:



The calculation procedure is called by the menu item "**Calibration / Calculate peaks spectra...**". Previously, a search for peaks in the spectrum must be performed. Since the background spectrum must be subtracted from the measured spectrum, for the case of calculating peak models, peak search must also be performed for the background spectrum used. Therefore, the calculation procedure will display the background spectrum used in the **SpectrRad-V** program window and prompt the operator to edit it if necessary (the procedure for editing the background spectrum is described in detail in the chapter "Calibration of registration efficiency").

The program window depends on the nature of the spectrum. For linear spectra, the window has the same appearance as for calibration of registration efficiency and has two pages.

The first page of "**Parameters**" may look like this:

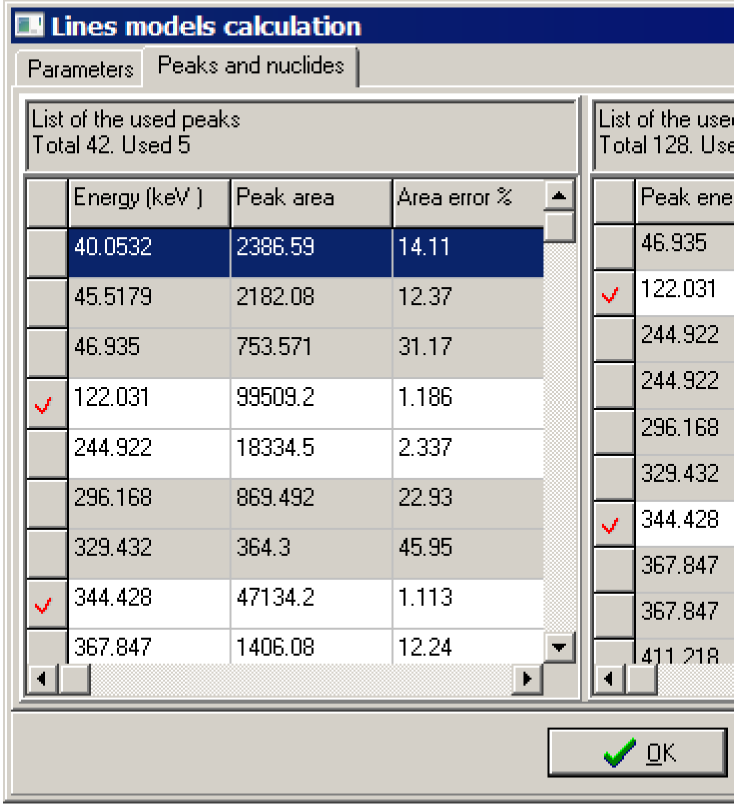


Spectrometer: HPGE
Geometry: MAR1000
File: D:\SpectrRad\Verification\AUTOCLBR_4.SRS
Standard sample: Eu-152
Sample type: Standards\D1+polymer
Z effective: 3.93887
AM effective: 7.40768
Interpolation parameter: Spectrometer load; 625.68 imp./s
Date of certification: 26.09.2002; 12:59:59
Nuclides table: Nuclides\Calib.ncl
Left boundary of the spectrum (keV): 20
Width of the averaging window for Compton extrapolation to the low energy region: 3 ch.
The level of acceptable uncertainty for the peak areas: 20 %

The operator must select from the suggested list or specify:

- **Interpolation parameter** – the parameter on which the shape of the line depends. The interpolation parameter can be the mass or density of the sample, a geometric parameter specified during the installation of the geometry (the distance of the sample from the detector, the height of the filling, etc.), the loading of the spectrometer.
- **Date of certification -** the date of certification of the measured standard (a reference sample of activity).
- Select the **Nuclides table** containing information about the nuclides of the reference sample. Since when recalculating the nuclide activities of the standard entered on the date of certification to the values of the average nuclide activity during the measurement of the standard necessary for calculating the registration efficiency, the program takes into account the processes of decay and accumulation of nuclides, the nuclide table must contain a correct scheme of nuclide decay.
- Set **the level of acceptable uncertainty for peaks areas** – peaks of the spectrum with a relative error in determining the area exceeding the specified level will be excluded from the list of peaks used.

Switching to the second page of "**Peaks and nuclides**", enter information about the peaks used, the lines and the activities of the nuclides forming them. The "**Peaks and nuclides**" page has three columns: "**List of the used peaks**", "**List of the used lines**", and "**List of the used nuclides**". In the example, the Eu-152 standard is used for calibration. In this case, the "**List of the used peaks**" column may look like:



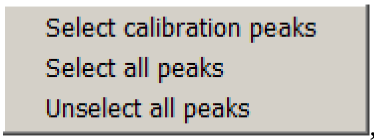
List of the used peaks
Total 42. Used 5

	Energy (keV)	Peak area	Area error %
	40.0532	2386.59	14.11
	45.5179	2182.08	12.37
	46.935	753.571	31.17
✓	122.031	99509.2	1.186
	244.922	18334.5	2.337
	296.168	869.492	22.93
	329.432	364.3	45.95
✓	344.428	47134.2	1.113
	367.847	1406.08	12.24

List of the use
Total 128. Use

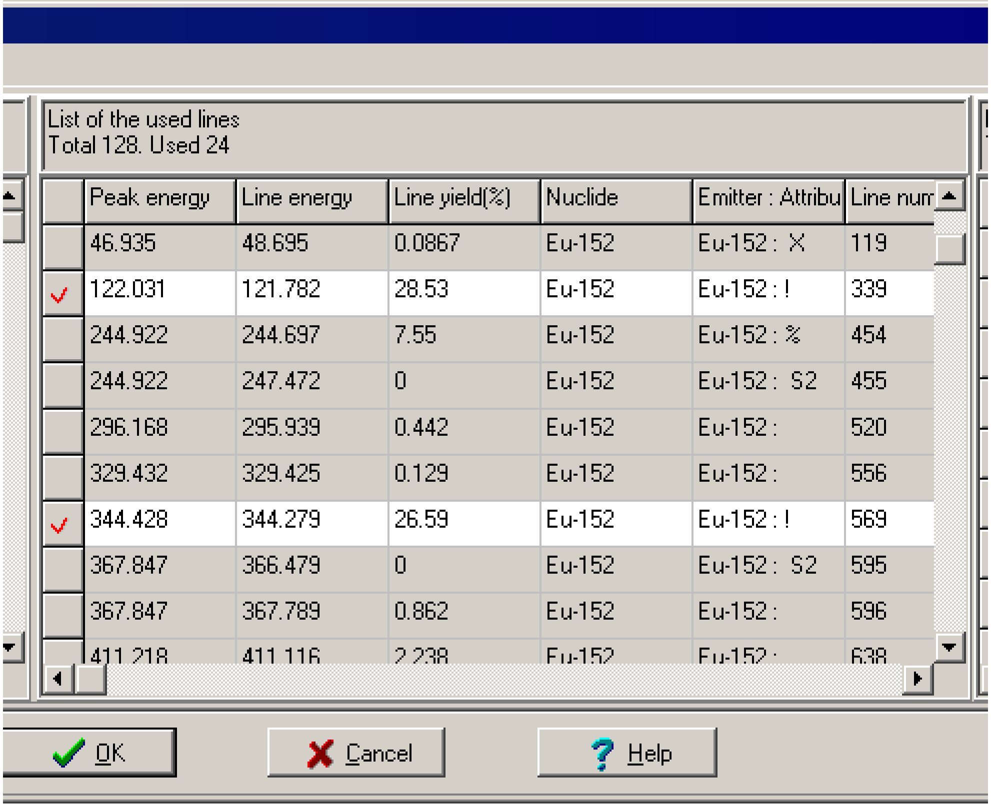
	Peak ene
	46.935
✓	122.031
	244.922
	244.922
	296.168
	329.432
✓	344.428
	367.847
	367.847
	411.218

Peaks that cannot be used are marked in gray (peaks of undisclosed multiplets, escape peaks, cascading addition, weak peaks, etc.). Red check marks in the left column indicate the peaks used. The crossed out check mark indicates that the peak was marked by the operator, but the program cannot or does not recommend using it for some reason. The operator can deselect or add the desired peak by double-clicking on the line with information about the peak. You can use the "**Insert**" key on the computer keyboard, pressing which changes the state of the current line.



The right mouse button displays a small menu, with which the operator can select or deselect either the calibration or all peaks. Calibration peaks are considered to be the most powerful peaks whose energy is in the range specified for the calibration lines of the nuclide table.

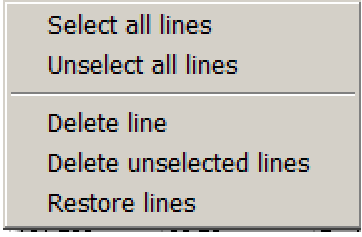
The second column has the form:



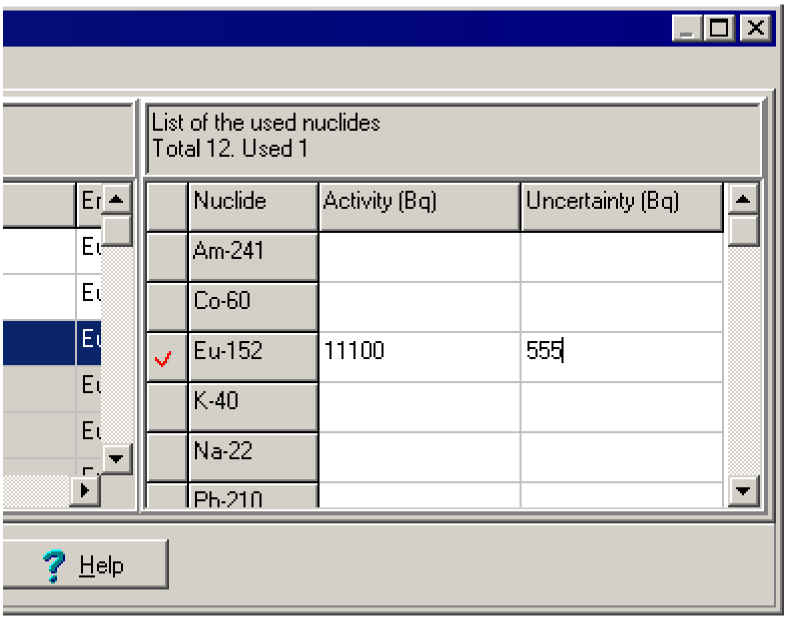
List of the used lines
Total 128. Used 24

	Peak energy	Line energy	Line yield(%)	Nuclide	Emitter : Attribu	Line num
	46.935	48.695	0.0867	Eu-152	Eu-152 : X	119
✓	122.031	121.782	28.53	Eu-152	Eu-152 : !	339
	244.922	244.697	7.55	Eu-152	Eu-152 : %	454
	244.922	247.472	0	Eu-152	Eu-152 : S2	455
	296.168	295.939	0.442	Eu-152	Eu-152 :	520
	329.432	329.425	0.129	Eu-152	Eu-152 :	556
✓	344.428	344.279	26.59	Eu-152	Eu-152 : !	569
	367.847	366.479	0	Eu-152	Eu-152 : S2	595
	367.847	367.789	0.862	Eu-152	Eu-152 :	596
	411.218	411.116	2.238	Eu-152	Eu-152 :	638

The operator can also double-click on the line information line to edit the list of lines forming the selected peaks. The right mouse button displays a small menu, with which the operator can select, deselect or delete lines.



The third column contains a list of nuclides forming the selected lines.



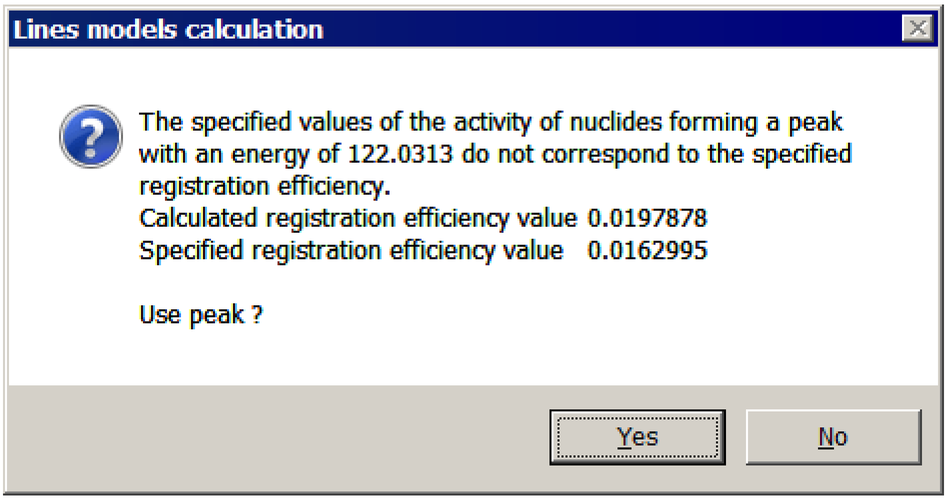
List of the used nuclides
Total 12. Used 1

	Nuclide	Activity (Bq)	Uncertainty (Bq)
	Am-241		
	Co-60		
✓	Eu-152	11100	555
	K-40		
	Na-22		
	Pb-210		

Nuclides missing at the standard used for calibration can be removed by right-clicking on the nuclide table. The popup menu that is called contains three items: "**Select all nuclides**", "**Unselect all nuclides**" and "**Delete unselected nuclides**". Nuclides are selected by double-clicking on the name of the nuclide.

The operator must enter the value of the activities and errors of the nuclides present in the reference sample at the date of certification. For the geometries of measurements in the "thin" and intermediate layers enter the total activity of nuclides in the standard in Becquerel, for the geometry of measurements in the "thick" layer - the specific activity of nuclides in Bq/kg. If a standard certificate has been pre-formed for the nuclide table used, the program will substitute data on the activities and errors of nuclides from the existing standard certificate.

Pressing the "**OK**" key starts the procedure for calculating line spectra. At the same time, the program checks the compliance of the registration efficiency values calculated from the generated spectrum of lines with the existing calibration of registration efficiency and, if they do not match, issues a warning message. For example:



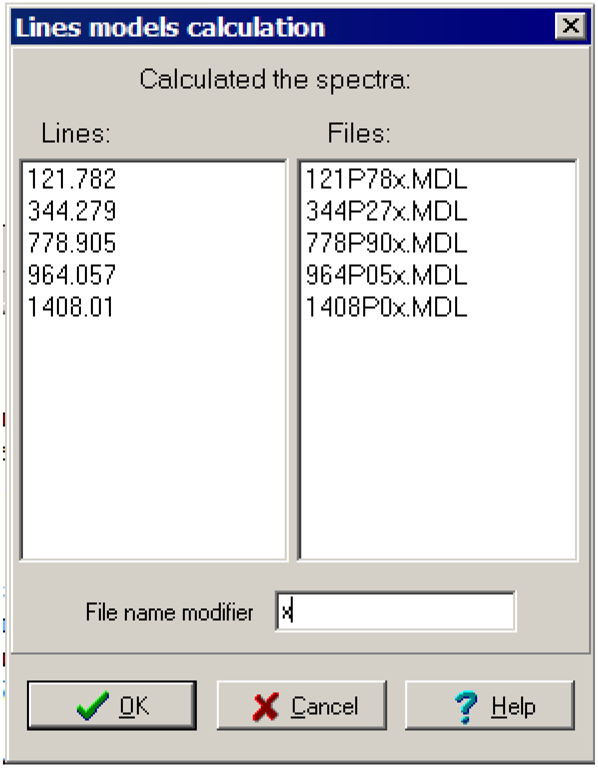
The specified values of the activity of nuclides forming a peak with an energy of 122.0313 do not correspond to the specified registration efficiency.
Calculated registration efficiency value 0.0197878
Specified registration efficiency value 0.0162995

Use peak ?

.

Such a discrepancy may be caused by the fact that not all the lines forming it are taken into account in the peak used. And if the energies of such unaccounted lines differ from the energies of the accounted lines as a line model, we will get a response to several lines – an erroneous broader line model. Therefore, only if we are sure that such a discrepancy is not caused by an erroneous determination of the peak-forming lines, peak boundaries and the approximation of Compton scattering, the peak can be used as a model of the line spectrum.

Upon completion of the calculation, the program suggests saving the generated line spectra in the "**Elements**" folder and adding the necessary lines in the "**Decomp.ini**" file to connect the calculated spectra corresponding to the **interpolation parameter** set in the calibration spectrum (**density** or "**size**" of the sample) to the processing program. The window of the saving procedure may look like:



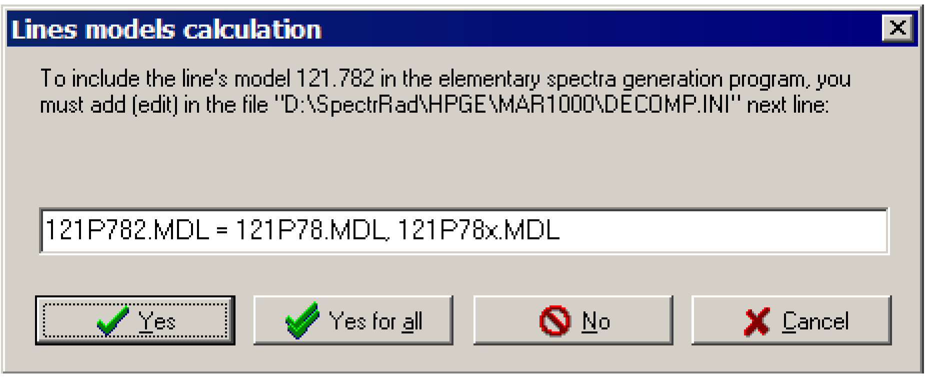
Calculated the spectra:

Lines:	Files:
121.782	121P78x.MDL
344.279	344P27x.MDL
778.905	778P90x.MDL
964.057	964P05x.MDL
1408.01	1408P0x.MDL

File name modifier: x

File names for saving spectra are formed from line energies and, when forming the same set of line spectra for different interpolation parameters, in order for the newly created files not to overwrite existing line models, but to be included separately to recalculate the shape of the lines depending on the interpolation parameter, a field is provided in the form for the operator to enter a **files name modifier**.

When saving the spectra, the program generates a window with information about the proposed modification of the corresponding line in the "**Decomp.ini**" file. For example:



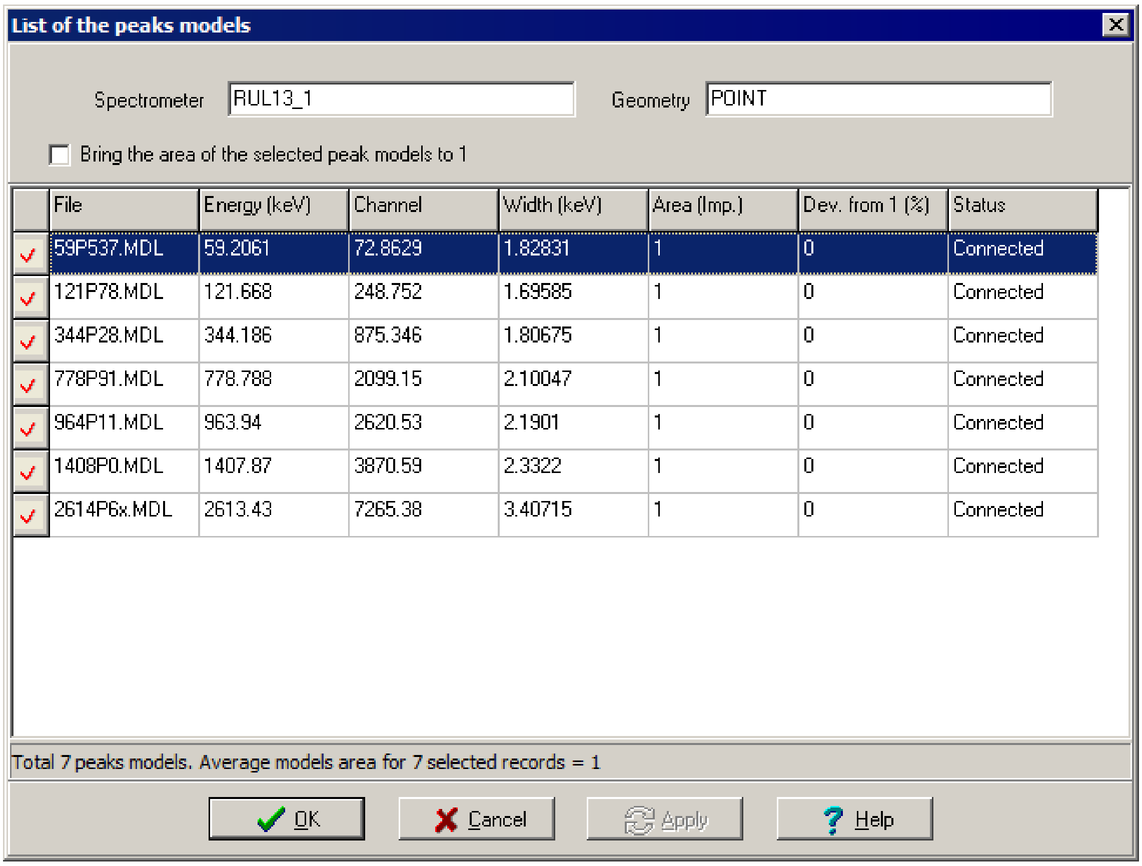
To include the line's model 121.782 in the elementary spectra generation program, you must add (edit) in the file "D:\SpectrRad\HPGE\MAR1000\DECOMP.INI" next line:

121P782.MDL = 121P78.MDL, 121P78x.MDL

The operator can agree with the proposed modification of the "**Decomp.ini**" file or edit the line himself.

The calculated peak of the total absorption of radiation of quanta of defined energy – the line model for the resolved spectra most accurately relates the position of the line on the channel scale to the line energy and the peak width corresponds to the width of one line. Therefore, after saving the formed lines, the program prompts the operator to refine the energy calibration of the spectrometer and the calibration of the peak width. When specifying calibration based on line models, all generated models are used, not only those generated by this procedure. Therefore, if the operator assumes to calculate the spectra of the lines according to other standards, the refinement of the energy calibration can be postponed until the final calculation of the line models. Such calibration can be performed at any time after the calculation of the lines is completed, using the main menu items: "**Calibration / Scale X (Energy) / By peak models...**" and "**Calibration / Peaks width / By peak models…**».

The list of calculated peak models can be viewed by clicking on the menu item "**Calibration / List of peaks spectra...**". The view form can look like:



List of the peaks models

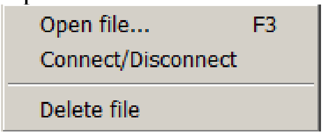
Spectrometer RUL13_1   Geometry POINT

☐ Bring the area of the selected peak models to 1

	File	Energy (keV)	Channel	Width (keV)	Area (Imp.)	Dev. from 1 (%)	Status
✓	59P537.MDL	59.2061	72.8629	1.82831	1	0	Connected
✓	121P78.MDL	121.668	248.752	1.69585	1	0	Connected
✓	344P28.MDL	344.186	875.346	1.80675	1	0	Connected
✓	778P91.MDL	778.788	2099.15	2.10047	1	0	Connected
✓	964P11.MDL	963.94	2620.53	2.1901	1	0	Connected
✓	1408P0.MDL	1407.87	3870.59	2.3322	1	0	Connected
✓	2614P6x.MDL	2613.43	7265.38	3.40715	1	0	Connected

Total 7 peaks models. Average models area for 7 selected records = 1

The area of the peaks should be equal to one. If, for some reason, it differs from one, clicking on the "**Apply**" button with the check mark "**Bring the area of the selected peak models to 1**" brings the area of the peak models to one.



Using a small pop-up menu the operator has the opportunity to view the file, connect it to the processing procedures or disable, delete the file. You can delete a file only after it is disabled.

Calculation the models of the lines

The spectrum of the line (or line model) for poorly resolved linear spectra is the full response of the spectrometer to one quantum of radiation of a certain energy, that is, the line model is a function of the efficiency of recording radiation of a given energy in the channels of the spectrometer. For such spectra, the spectrum is processed without searching for peaks and the continuous scattering spectrum for the line (the "Compton" spectrum for gamma lines) is included in the spectrometer response.

The calculation of line spectra for processing linear spectra without searching for peaks is necessary if we do not have the opportunity to calculate the elementary spectrum of a nuclide directly from the spectra of standards. In this case, the package provides the user with the opportunity to generate the necessary spectra from the library of nuclides and the available elementary spectra. At the same time, it should be borne in mind that this procedure, in addition to all those errors that were included in the calculated elementary spectra of nuclides, complements the generated spectra with errors related to the uncertainty of the nuclide libraries, features of the formation of spectrograms on this spectrometer (escape peaks, cascade transitions, etc.), errors of interpolation - extrapolation of data.

The essence of the method is to calculate the response to radiation of a certain energy by interpolation (extrapolation) from the nearest known response spectra to reference energies e_1 and e_2.

$$f(e,i) = ((e_2 - e)\cdot f(e_1,k_1,i) + (e_1 - e)\cdot f(e_2,k_2,i))/(e_2 - e_1), \ldots k_1 = e/e_1,\ k_2 = e/e_2 \quad (1)$$

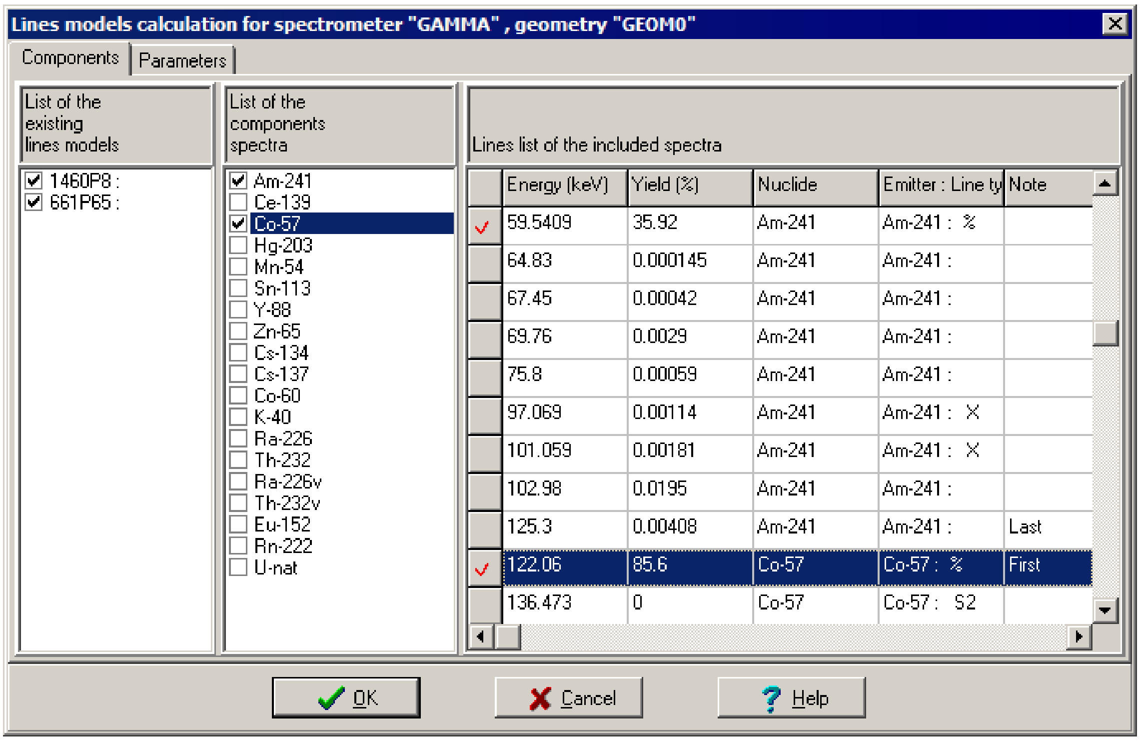
The spectrum of a nuclide $F = \sum A_j \cdot f_j$ is the sum of the responses with the corresponding quantum yield of all lines of a given nuclide.

The more reference lines we have in the operating range of the spectrometer, the more accurate the interpolation will be. Unfortunately, for example, there are practically no single-line nuclides for gamma spectrometry. Therefore, the gamma line responses are also calculated from the reference spectra using the same assumption (1). For example: we have as a reference a nuclide with two gamma lines e_1 and e_2. It is necessary to calculate the spectrometer's response to radiation e_1. Due to Compton scattering, the line spectra overlap each other and, as a result, we have **n** equations and **2n** unknowns. But, expressing by formula (1) the response e_2 from through e_1, we will get just **n** unknowns. The real procedure combines into a common system of equations up to 10 spectra of standards and, if necessary, already calculated responses to lines of known energies. To calculate the line spectra, it is necessary to select nuclides having one strong line and a small number of weak ones.

The spectrum of the line depends both on the density of the counting sample and on the geometric parameters of the counting sample or the geometry of measurements (if geometry with a variable geometric parameter is used) and on the loading of the spectrometer - on the **interpolation parameter** set in the geometry parameters, therefore, for the correct calculation of the line models corresponding to the interpolation parameter of the measured spectrum of the working sample, line models calculation must be performed several times with different values of the **interpolation parameter**

The procedure for calculating line models uses already formed elementary spectra of nuclides (they must be formed beforehand) and previously calculated line models. Elementary spectra and existing line models are pre-calculated according to the **interpolation parameter** selected at the geometry installation, and the calculated set of spectra is used to calculate the spectra of lines with the specified interpolation parameter. The accuracy of the calculation depends on the nature of the elementary spectra - the fewer peaks; the greater the relative output of the calculated line, the greater the accuracy of the calculation. Recommended set of elementary spectra for scintillation gamma spectrometry is: Am-241, Ce-139, Co-57, Cs-137, K-40.

The generation procedure is called by the menu item "**Calibration / Calculate lines spectra...**". The window of the line spectra calculation program has two pages. The first page of "**Components**" may look like this:



List of the existing lines models

☑ 1460P8 :
☑ 661P65 :

List of the components spectra

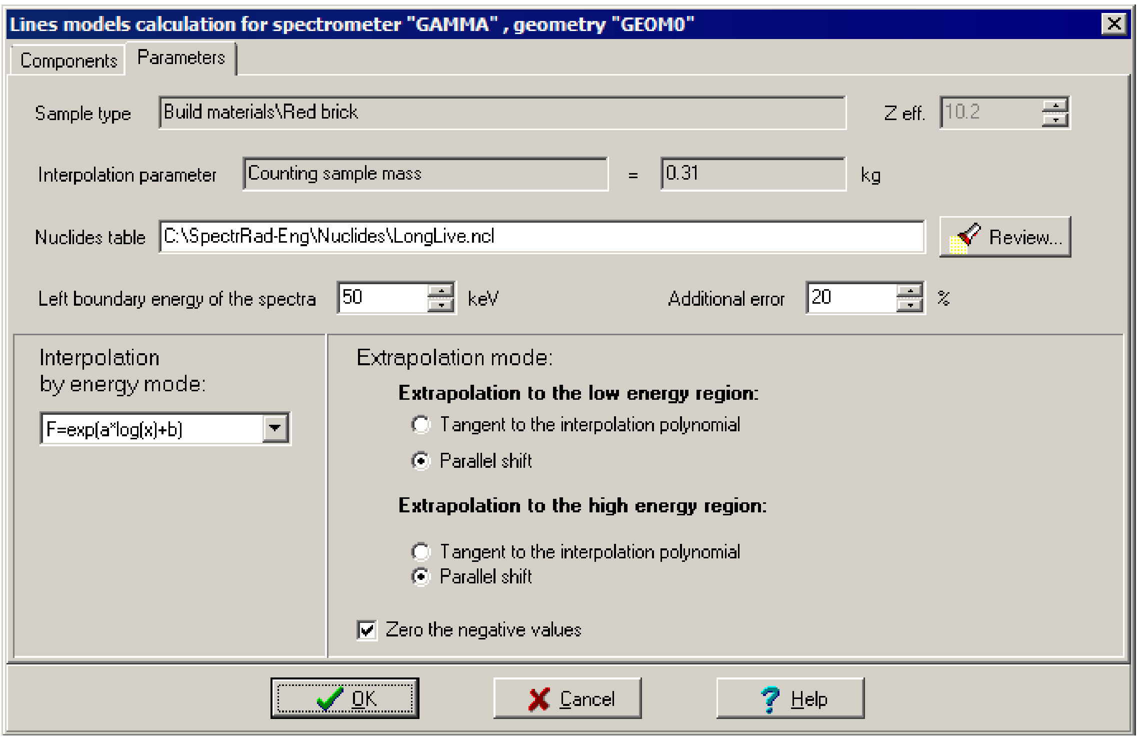
☑ Am-241
☐ Ce-139
☑ Co-57
☐ Hg-203
☐ Mn-54
☐ Sn-113
☐ Y-88
☐ Zn-65
☐ Cs-134
☐ Cs-137
☐ Co-60
☐ K-40
☐ Ra-226
☐ Th-232
☐ Ra-226v
☐ Th-232v
☐ Eu-152
☐ Rn-222
☐ U-nat

Lines list of the included spectra

	Energy (keV)	Yield (%)	Nuclide	Emitter : Line ty	Note
✓	59.5409	35.92	Am-241	Am-241 : %	
	64.83	0.000145	Am-241	Am-241 :	
	67.45	0.00042	Am-241	Am-241 :	
	69.76	0.0029	Am-241	Am-241 :	
	75.8	0.00059	Am-241	Am-241 :	
	97.069	0.00114	Am-241	Am-241 : X	
	101.059	0.00181	Am-241	Am-241 : X	
	102.98	0.0195	Am-241	Am-241 :	
	125.3	0.00408	Am-241	Am-241 :	Last
✓	122.06	85.6	Co-57	Co-57 : %	First
	136.473	0	Co-57	Co-57 : S2	

The operator in the column "**List of the existing lines models**", if the list is not empty, must mark the lines that will be used to calculate the additionally generated line spectra, and in the column "**List of the components spectra**" - nuclides elementary spectra containing the calculated lines.

In the "**Lines list of the included spectra**" section, the operator must mark the necessary lines. Lines are included (or excluded from generation) by double-clicking on a list row in the area of any column except the first one highlighted in gray. You can also change the state of the selected line by pressing the "**Insert**" key on the computer keyboard. The included lines are marked with a red "tick" in the leftmost column. The operator must select the most powerful nuclide lines. In the event that there are no previously formed line models and there are no nuclides with only one line in the list of elementary spectra, the operator must select either the first or the last lines in the spectrum of each nuclide (see "Mathematics", "Calculation spectra of the lines").



Lines models calculation for spectrometer "GAMMA" , geometry "GEOM0"

Sample type: Build materials\Red brick
Z eff. 10.2
Interpolation parameter: Counting sample mass = 0.31 kg
Nuclides table: C:\SpectrRad-Eng\Nuclides\LongLive.ncl
Left boundary energy of the spectra: 50 keV
Additional error: 20 %

Interpolation by energy mode: F=exp(a*log(x)+b)

Extrapolation mode:

Extrapolation to the low energy region:
○ Tangent to the interpolation polynomial
● Parallel shift

Extrapolation to the high energy region:
○ Tangent to the interpolation polynomial
● Parallel shift

☑ Zero the negative values

On the second page of "**Parameters**", the operator must select one of the four possible modes for interpolating line models by energy:

F=a*x+b

F=exp(a*x+b)

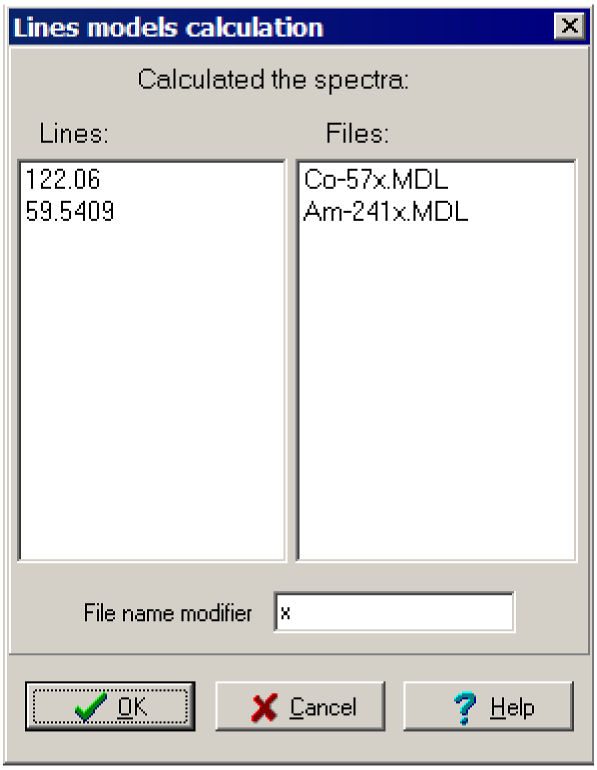
F=a*log(x)+b

F=exp(a*log(x)+b) Here: **F** is the value of the function, **x** is the energy, **a** and **b** are the parameters of linear interpolation (piecewise linear interpolation is used).

And set the extrapolation mode to the low and high energy regions (**Extrapolation mode**): either **tangent to the interpolation polynomial**, or **parallel shift**. In parallel transfer, only one nearest line model is used, compressed or stretched according to a given energy. Since the interpolated functions are always positive and defined for positive abscissa values, it is recommended to use linear interpolation on a double logarithmic scale (**F=exp(a*log(x)+b)**), parallel transfer for extrapolation to the low and high energy regions.

Pressing the "**OK**" key starts the procedure for calculating line spectra. Upon completion of the calculation, the program suggests saving the generated line spectra in the "**Elements**" folder and adding the necessary lines in the "**Decomp.ini**" file to connect the calculated spectra corresponding to the specified interpolation parameter (sample density or spectrometer loading) to the processing program.

The window of the save procedure may look like:



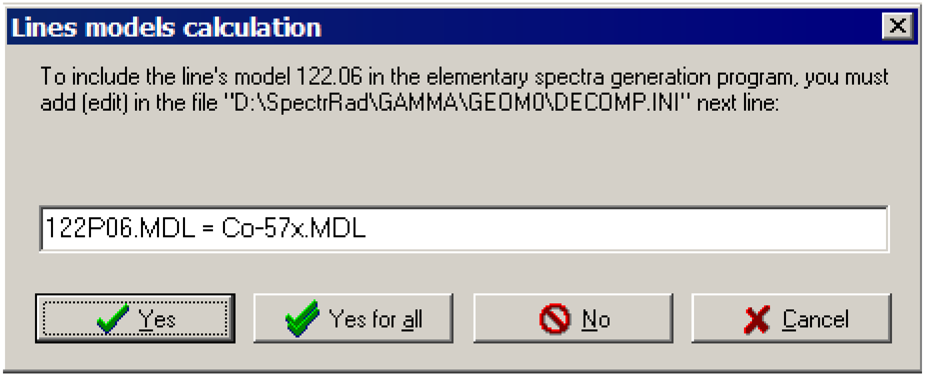
122.06
59.5409

Co-57x.MDL
Am-241x.MDL

File name modifier x

The file names for saving line spectra are formed from the file names of the elementary spectra used and, when forming the same set of line spectra for different interpolation parameters, in order for the newly created files not to overwrite existing line models, but to be included separately for recalculating lines depending on the interpolation parameter, an input field in the form "**File name modifier**" is provided for operator.

When saving the spectra, the program generates a window with information about the proposed modification of the corresponding line in the "**Decomp.ini**" file. For example:

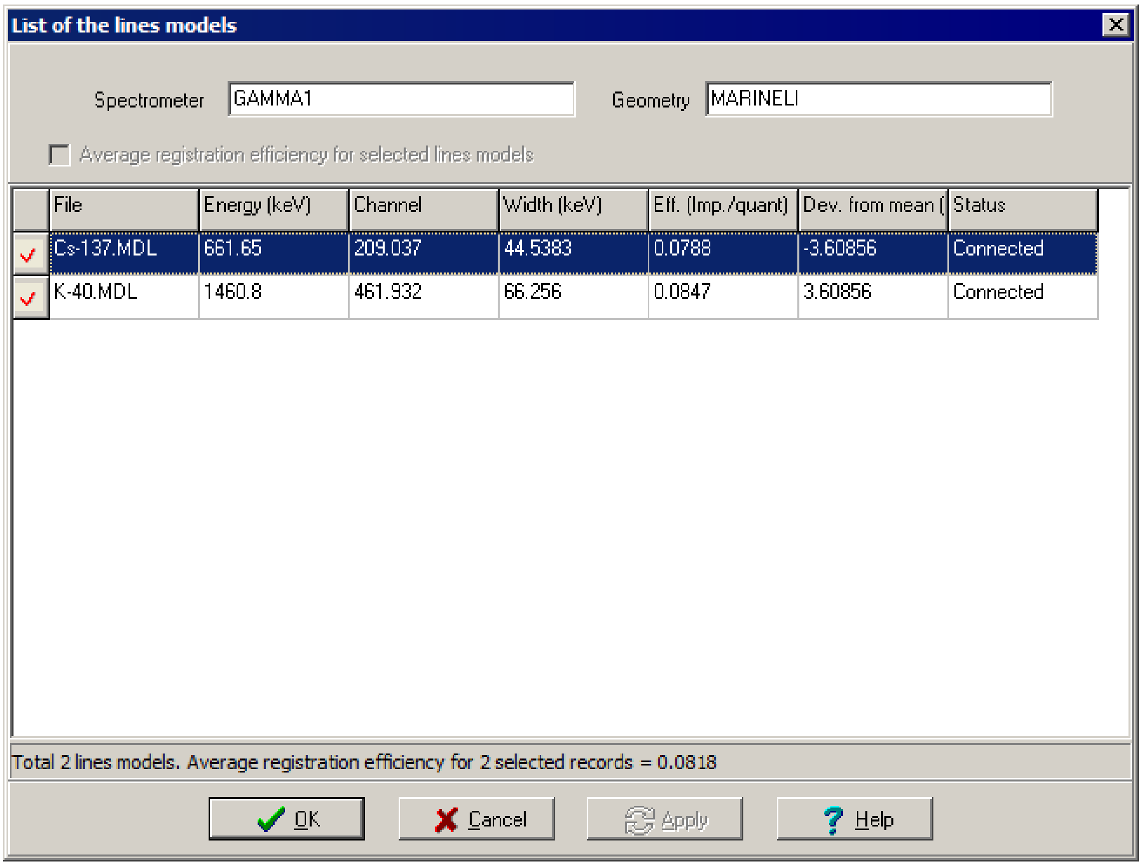


To include the line's model 122.06 in the elementary spectra generation program, you must add (edit) in the file "D:\SpectrRad\GAMMA\GEOM0\DECOMP.INI" next line:

122P06.MDL = Co-57x.MDL

The operator can agree with the proposed modification of the "**Decomp.ini**" file or edit the line himself.

Upon completion of the calculation procedure, the program displays a list of all generated line models:



Spectrometer GAMMA1

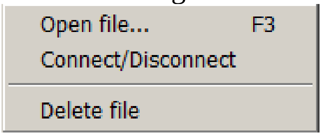
Geometry MARINELI

☐ Average registration efficiency for selected lines models

	File	Energy (keV)	Channel	Width (keV)	Eff. (Imp./quant)	Dev. from mean (	Status
✓	Cs-137.MDL	661.65	209.037	44.5383	0.0788	-3.60856	Connected
✓	K-40.MDL	1460.8	461.932	66.256	0.0847	3.60856	Connected

Total 2 lines models. Average registration efficiency for 2 selected records = 0.0818

The operator can edit the value of the registration efficiency for the line, average the registration efficiency for the selected lines (it is believed that in alpha spectrometry, the registration efficiency weakly depends on the energy of the lines). The record is selected by double-clicking on the leftmost cell of the selected row. Using the small pop-up menu , the operator can open the file of the selected model or delete the file. You can only delete the line model file that is not connected to the spectrum processing procedures.



Calculation the models of the lines for alpha spectra

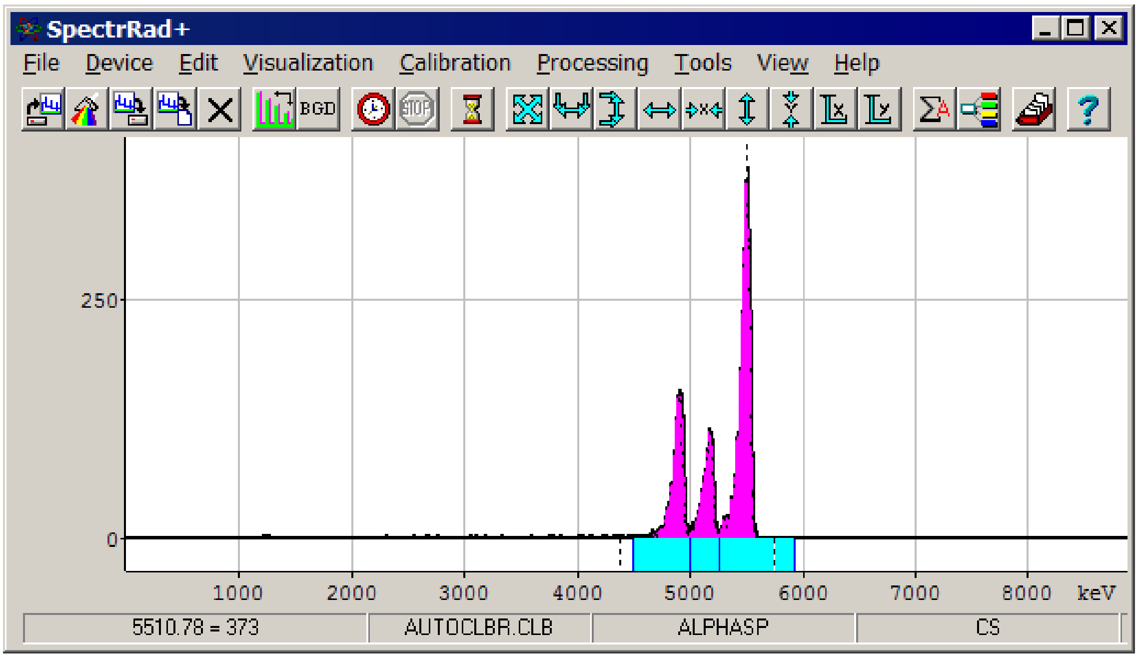
Alpha spectra usually have a resolution better than scintillation gamma spectra with NaI(Tl) detectors, but worse than the resolution of gamma spectra with cooled detectors made of especially pure germanium. Therefore, two variants of calculating line models are implemented for them: calculation based on elementary spectra for poorly resolved linear spectra (and for spectra without a linear structure) and calculation based on the measured spectrum of the reference similar to the calculation of lines for resolved spectra. The choice of the calculation option is determined by the type of spectrum selected by the operator in the main window of the program: if the already calculated elementary spectrum is selected, the calculation will be based on the elementary spectrum, if the measured spectrum of the reference sample is selected, the calculation will be based on the spectrum of the reference sample.

The deformation of the line model depending on the energy of the line is assumed to be an affine type deformation $\varphi(z) = \varphi(\frac{x-p}{w})$. Accounting for more complex shape changes depending on the energy of the line can be provided with a set of line models for different energies.

As a line model, the response of the spectrometer to one quantum of alpha radiation is calculated, that is, the line model will also contain the registration efficiency. Since the recording efficiency and the shape of the spectrum of the line depend both on the amount of material deposited on the substrate and on the geometric parameters of the counting sample or the geometry of measurements and on the loading of the spectrometer - on the **interpolation parameter** set in the geometry parameters, therefore, for the correct calculation of the line models corresponding to the interpolation parameter of the measured spectrum of the working sample, line models calculation must be performed several times with different values of the **interpolation parameter**.

It is previously required to perform an autocalibration of the spectrometer, measure the background and set the parameters of the peak search procedure, if they have not yet been set. Then measure a reference sample of the activity of a nuclide or a mixture of nuclides (standard). As an example of calculating line spectra, we use the spectrum of plutonium: Pu-238, Pu-240 and Pu-242.

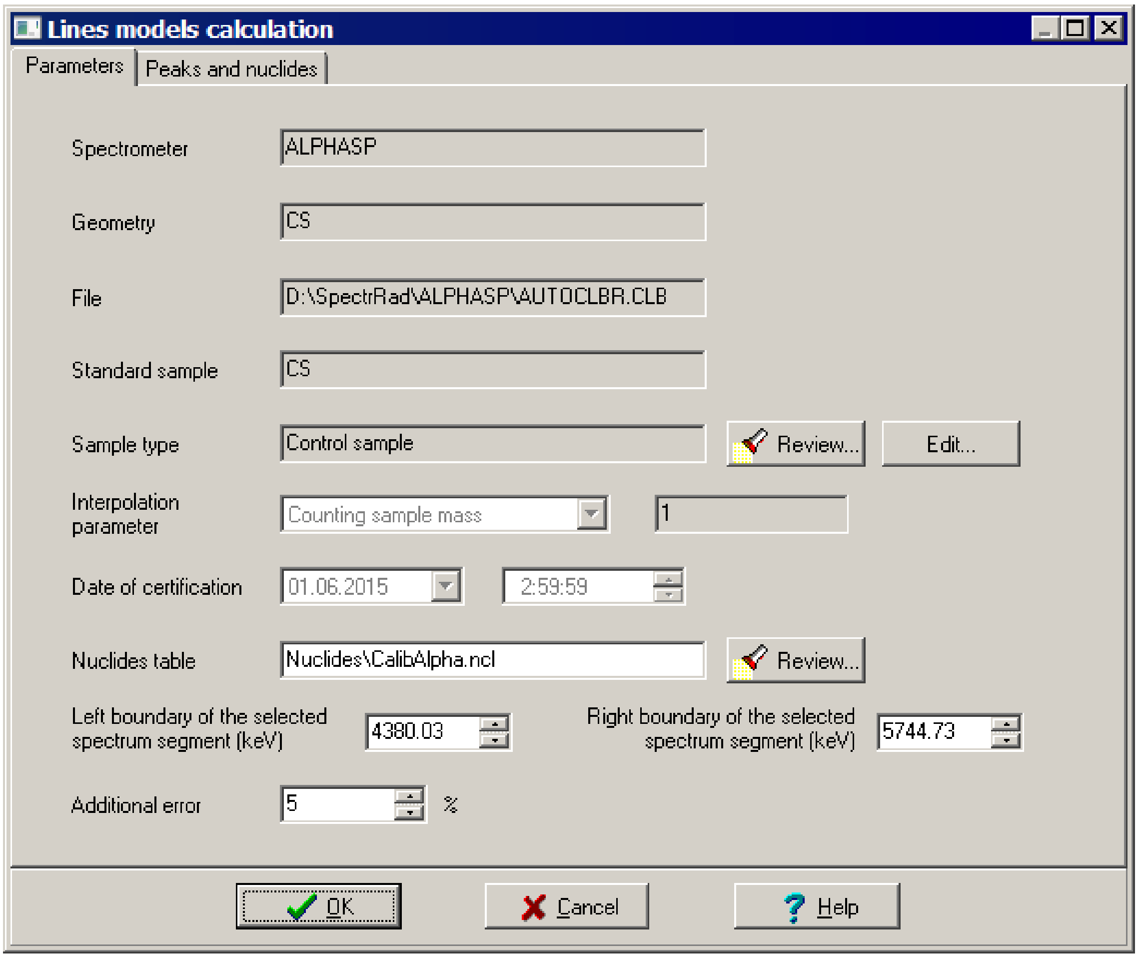
The operator must mark the multiplet used to calculate the line model with markers and set the marker to the most powerful peak in the multiplet. The most powerful alpha line forming this peak will be recommended by the processing procedure for calculating the line model. It is desirable that this peak be extreme in the multiplet, since the matrix formed by the calculation procedure in this case will have a triangular character and will be more conditioned, which will eventually affect the accuracy of the calculation. The spectrum, in this case, may look like:



5510.78 = 373 | AUTOCLBR.CLB | ALPHASP | CS

The calculation procedure is called by the menu item "**Calibration / Calculate lines spectra...**". The calculation procedure window has two pages.

The first page of "**Parameters**" may look like this:



Spectrometer ALPHASP

Geometry CS

File D:\SpectrRad\ALPHASP\AUTOCLBR.CLB

Standard sample CS

Sample type Control sample

Interpolation parameter Counting sample mass 1

Date of certification 01.06.2015 2:59:59

Nuclides table Nuclides\CalibAlpha.ncl

Left boundary of the selected spectrum segment (keV) 4380.03

Right boundary of the selected spectrum segment (keV) 5744.73

Additional error 5 %

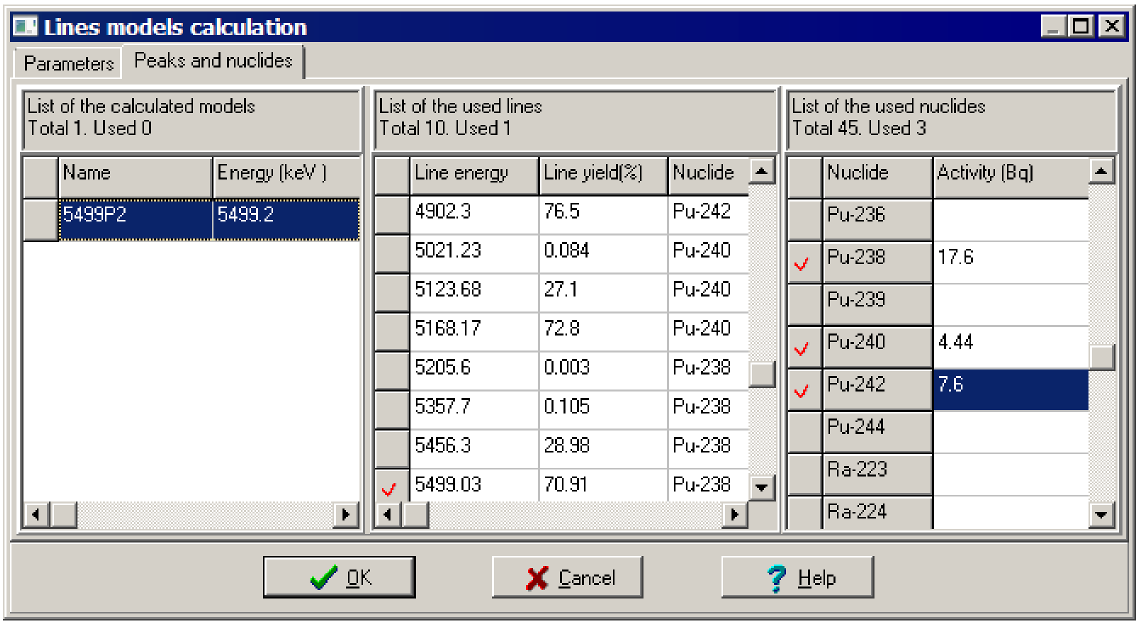
The operator must select from the suggested list or specify:

- **Date of certification -** the date of certification of the measured standard (a reference sample of activity).
- Select the **Nuclides table** containing information about the nuclides of the reference.
- Specify the boundaries of the selected section of the spectrum
- Set the value of additional uncertainty (**Additional error**) for the calculated line model.

Switching to the second page of "**Peaks and nuclides**", enter information about previously used and calculated line models, lines and activities of nuclides forming the selected part of the spectrum.

The Peaks and nuclides page has three columns: "**List of the calculated models**", "**List of the used lines**", and "**List of the used nuclides**". The example uses the standard (a reference sample of activity) Pu-238, Pu-240 and Pu-242.

In the first column, the operator can mark the line models that have already been calculated and will be used to calculate the new line model. At the same time, if any of the lines forming the multiplet is located closer to the calculated line model; its contribution will be subtracted from the spectrum. This will increase the conditionality of the equation system and the accuracy of the line calculation. In the example, the line model is recalculated for energy equal to 5499.2 keV, so it is useless to use the already calculated model – in this case it will not be taken into account.



List of the calculated models
Total 1. Used 0

	Name	Energy (keV)
	5499P2	5499.2

List of the used lines
Total 10. Used 1

	Line energy	Line yield(%)	Nuclide
	4902.3	76.5	Pu-242
	5021.23	0.084	Pu-240
	5123.68	27.1	Pu-240
	5168.17	72.8	Pu-240
	5205.6	0.003	Pu-238
	5357.7	0.105	Pu-238
	5456.3	28.98	Pu-238
✓	5499.03	70.91	Pu-238

List of the used nuclides
Total 45. Used 3

	Nuclide	Activity (Bq)
	Pu-236	
✓	Pu-238	17.6
	Pu-239	
✓	Pu-240	4.44
✓	Pu-242	7.6
	Pu-244	
	Ra-223	
	Ra-224	

The second column contains a list of lines of selected nuclides forming a given section of the spectrum.

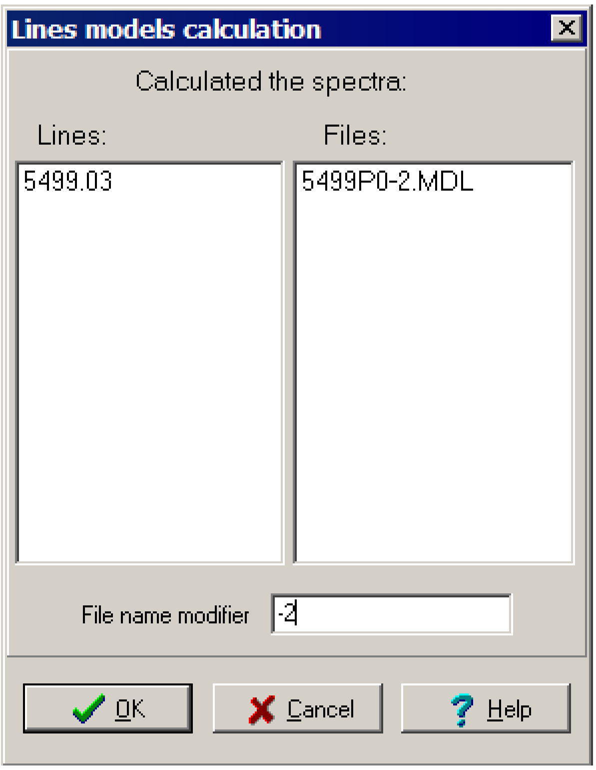
The operator can double-click on the line with information about the line to select the line for which the model will be calculated. It is recommended to choose the extreme line with the most powerful output (taking into account the activity of the nuclide). Using the pop-up menu, the operator can delete unimportant, but interfering lines (menu item "**Delete line**"), or restore the list of lines ("**Restore lines**").

The third column contains a list of nuclides forming the selected lines.

Nuclides that are not needed for calibration can be deleted by right-clicking on the nuclide table. The popup menu that is called contains three items: "**Select all nuclides**", "**Unselect all nuclides**" and "**Delete unselected nuclides**". Nuclides are selected by double-clicking on the name of the nuclide.

The operator must enter the value of the nuclide activities present in the reference at the date of certification. For the geometries of measurements in the "thin" and intermediate layers enter the total activity of nuclides in the standard in Becquerel, for the geometry of measurements in the "thick" layer - the specific activity of nuclides in Bq/kg.

Pressing the "**OK**" key starts the procedure for calculating line spectra. Upon completion of the calculation, the program suggests saving the generated line spectra in the "**Elements**" folder and adding the necessary lines in the "**Decomp.ini**" file to connect the calculated spectra corresponding to the **interpolation parameter** set in the calibration spectrum (density or "size" of the sample) to the processing program. The window of the saving procedure may look like:



Calculated the spectra:

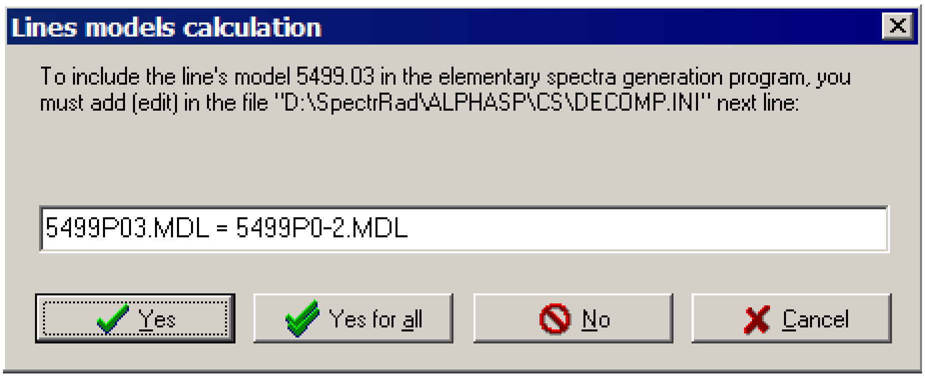
Lines: 5499.03

Files: 5499P0-2.MDL

File name modifier: -2

File names for saving spectra are formed from line energies and, when forming the same set of line spectra for different interpolation parameters, in order for the newly created files not to overwrite existing line models, but to be included separately to recalculate the shape of the lines depending on the interpolation parameter, a field is provided in the form for the operator to enter a **files name modifier**.

When saving the spectra, the program generates a window with information about the proposed modification of the corresponding line in the "**Decomp.ini**" file. For example:

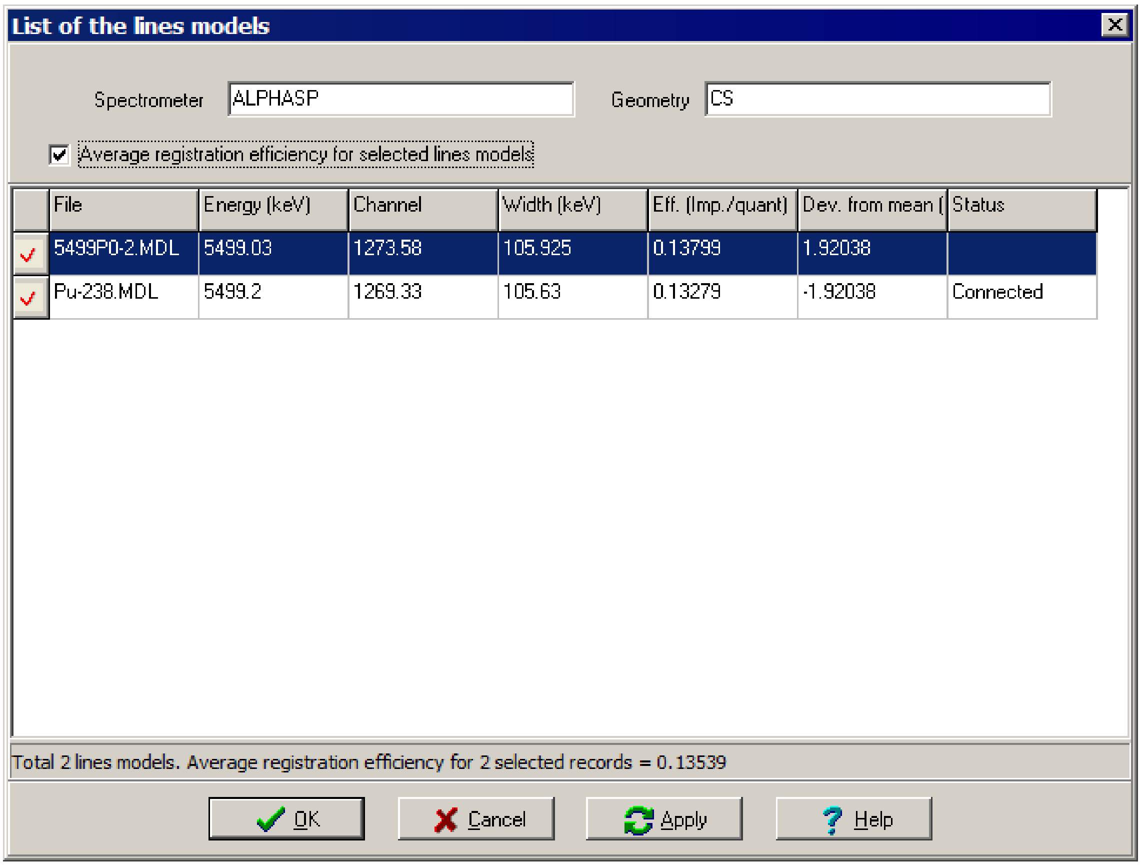


To include the line's model 5499.03 in the elementary spectra generation program, you must add (edit) in the file "D:\SpectrRad\ALPHASP\CS\DECOMP.INI" next line:

5499P03.MDL = 5499P0-2.MDL

The operator can agree with the proposed modification of the "**Decomp.ini**" file or edit the line himself.

Upon completion of the calculation procedure, the program displays a list of all generated line models:



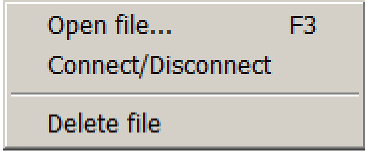
Spectrometer: ALPHASP
Geometry: CS

☑ Average registration efficiency for selected lines models

	File	Energy (keV)	Channel	Width (keV)	Eff. (Imp./quant)	Dev. from mean (	Status
✓	5499P0-2.MDL	5499.03	1273.58	105.925	0.13799	1.92038	
✓	Pu-238.MDL	5499.2	1269.33	105.63	0.13279	-1.92038	Connected

Total 2 lines models. Average registration efficiency for 2 selected records = 0.13539

The operator can edit the value of the registration efficiency for the line, average the registration efficiency for the selected lines (it is believed that in alpha spectrometry, the registration efficiency weakly depends on the energy of the lines). The record is selected by double-clicking on the leftmost cell of the selected row. Using a small pop-up menu, the operator can open the file of the selected model, connect or disconnect from processing procedures, or delete the file. You can only delete the line model file that is not connected to the spectrum processing procedures.



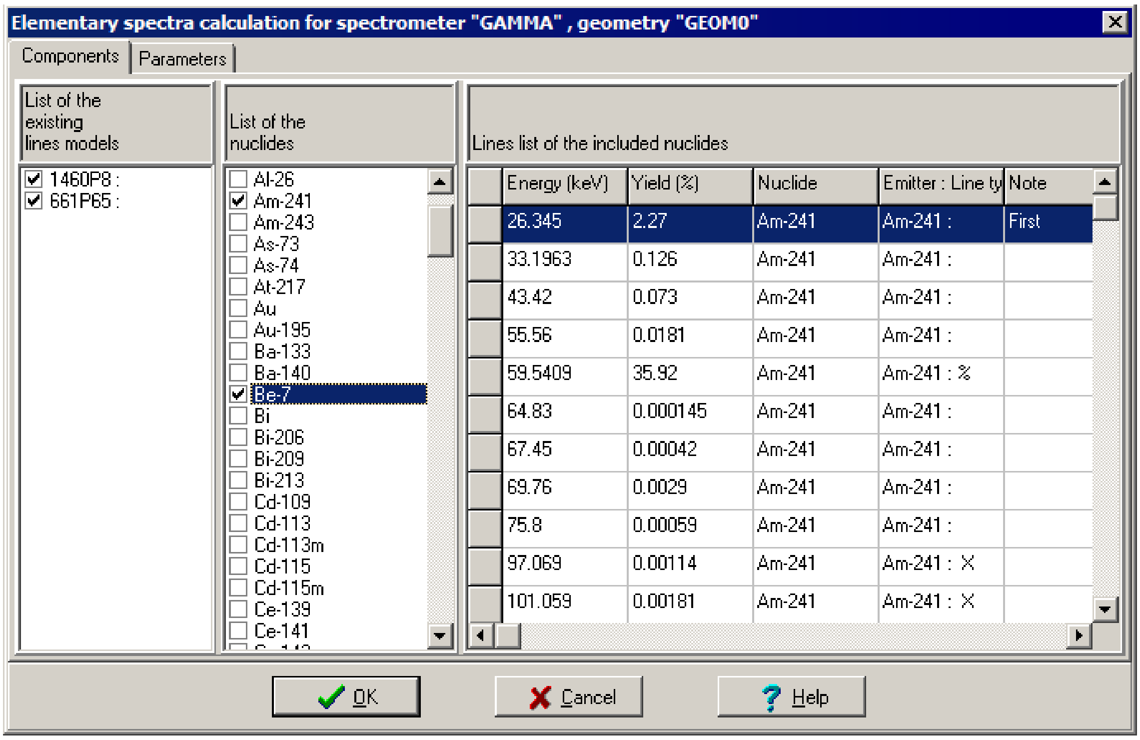
The calculated line model most accurately relates the position of the line on the channel scale to the energy of the line and the width of the peak corresponds to the width of one line. Therefore, after saving the formed lines, the operator is recommended to clarify the energy calibration of the spectrometer and the calibration of the peak width. When specifying calibration based on line models, all generated models are used, not only those generated by last procedure. Therefore, if the operator assumes to calculate line spectra using other standards, the refinement of energy calibration and peak width calibration can be postponed until the final calculation of line models. This calibration can be performed using the main menu items: «**Calibration / Scale X (Energy) / By peak models…**» и «**Calibration / Peaks width / By peak models…**».

Calculation of elementary spectra by the table of lines

The spectrum processing procedures calculate the necessary elementary spectra automatically. In the event that the necessary elementary spectra calculated from the standards exist, the program primarily uses them, but if they are not available, the necessary elementary spectra of nuclides are calculated from the tables of lines and calibrations of the spectrometer - "**generated**". The procedure for preliminary calculation of elementary spectra according to the line table reduces the processing time of the spectra and can be recommended for spectrometers using computers with limited performance and for calculating frequently used nuclide spectra. In addition, when calling the procedure for calculating elementary spectra by the lines table, the operator sets the necessary calculation parameters, which are stored in the configuration file and will be used in the future when calling the procedure for automatically generating the necessary elementary spectra. Therefore, it is possible not to generate any elementary spectra, but it is recommended to call the procedure for calculating elementary spectra according to the line table to set the parameters for generating spectra.

The generation of spectra is possible only after all calibrations have been performed, line spectra have been calculated and the necessary nuclide tables have been created. The processing of spectra with different interpolation parameters requires several elementary spectra to calculate the spectrum corresponding to the interpolation parameter (density or size of the counting sample or loading of the spectrometer). Therefore, it is recommended to calculate the elementary spectra by the table of lines as many times as we have sets of models of lines, with the same values of the interpolation parameter as the sets of models of lines. For example, we have two sets of standards: with a density of 1 g/cubic cm and 2 g/cubic cm. In this case, we can calculate two sets of elementary spectra, two registration efficiency functions, two sets of line models and, accordingly, we can calculate two sets of additional elementary spectra from two sets of line models.

The generation procedure is called by the menu item "**Calibration / Elementary spectrum / Generate by nuclides table / By lines models...**" to calculate full spectra or "**Calibration / Elementary spectrum / Generate by nuclides table / By peaks models...**" to calculate peak spectra. The generation procedure window has two pages. The first page of "**Components**" can look like:



List of the existing lines models

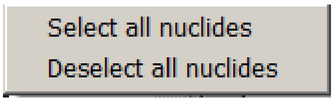
- ☑ 1460P8 :
- ☑ 661P65 :

List of the nuclides

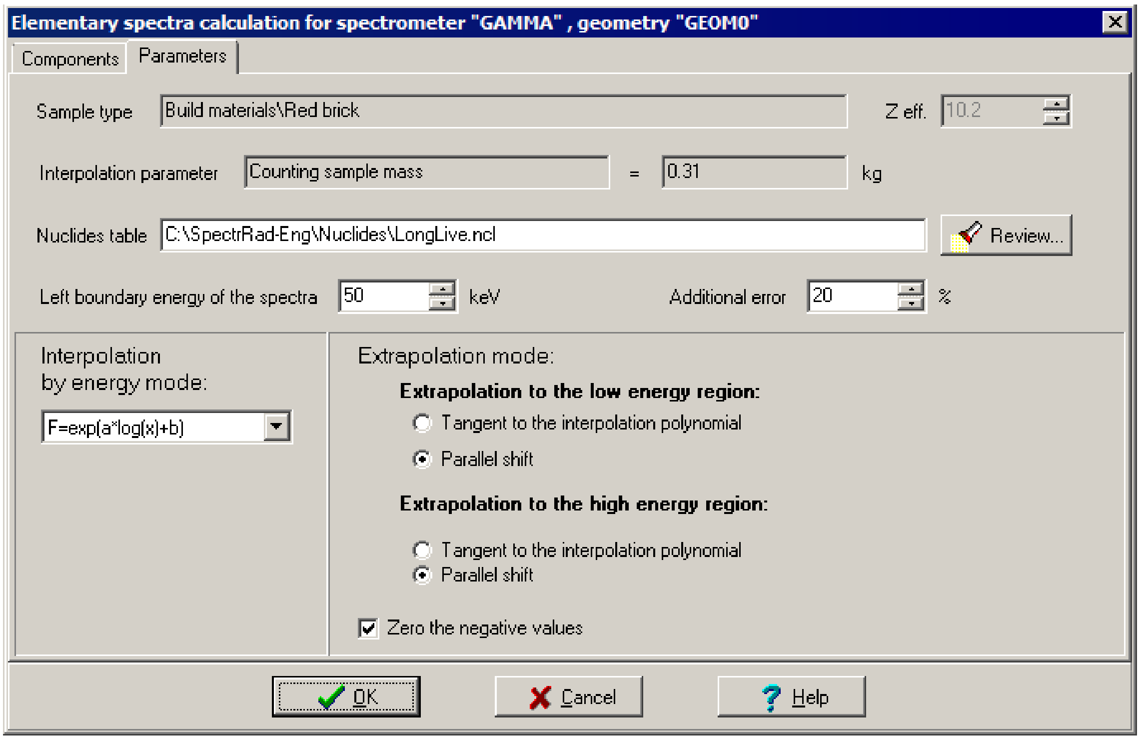
- ☐ Al-26
- ☑ Am-241
- ☐ Am-243
- ☐ As-73
- ☐ As-74
- ☐ At-217
- ☐ Au
- ☐ Au-195
- ☐ Ba-133
- ☐ Ba-140
- ☑ Be-7
- ☐ Bi
- ☐ Bi-206
- ☐ Bi-209
- ☐ Bi-213
- ☐ Cd-109
- ☐ Cd-113
- ☐ Cd-113m
- ☐ Cd-115
- ☐ Cd-115m
- ☐ Ce-139
- ☐ Ce-141

Lines list of the included nuclides

Energy (keV)	Yield (%)	Nuclide	Emitter : Line ty	Note
26.345	2.27	Am-241	Am-241 :	First
33.1963	0.126	Am-241	Am-241 :	
43.42	0.073	Am-241	Am-241 :	
55.56	0.0181	Am-241	Am-241 :	
59.5409	35.92	Am-241	Am-241 : %	
64.83	0.000145	Am-241	Am-241 :	
67.45	0.00042	Am-241	Am-241 :	
69.76	0.0029	Am-241	Am-241 :	
75.8	0.00059	Am-241	Am-241 :	
97.069	0.00114	Am-241	Am-241 : X	
101.059	0.00181	Am-241	Am-241 : X	

The operator in the column "**List of the existing lines models**", if the list is not empty, should mark the lines that will be used to generate elementary spectra of nuclides (it is recommended to use all lines), and in the column "**List of the nuclides**" - the nuclides for which elementary spectra will be calculated. You can select all the nuclides (or deselect the entire list) using the pop-up menu , which is called by clicking on the right mouse button.

The section "**Lines list of the included nuclides**" is informative. It displays a list of spectral lines of the generated nuclides. In the event that the nuclide spectrum has lines with energies that lie far from the energy range of the line models, generation for spectra that do not have a pronounced linear character (scintillation spectrometry) will be very approximate. If no nuclides are selected, there is no section.



Elementary spectra calculation for spectrometer "GAMMA" , geometry "GEOM0"

Sample type: Build materials\Red brick
Z eff.: 10.2
Interpolation parameter: Counting sample mass = 0.31 kg
Nuclides table: C:\SpectrRad-Eng\Nuclides\LongLive.ncl
Left boundary energy of the spectra: 50 keV
Additional error: 20 %
Interpolation by energy mode: F=exp(a*log(x)+b)

Extrapolation mode:

Extrapolation to the low energy region:
○ Tangent to the interpolation polynomial
● Parallel shift

Extrapolation to the high energy region:
○ Tangent to the interpolation polynomial
● Parallel shift

☑ Zero the negative values

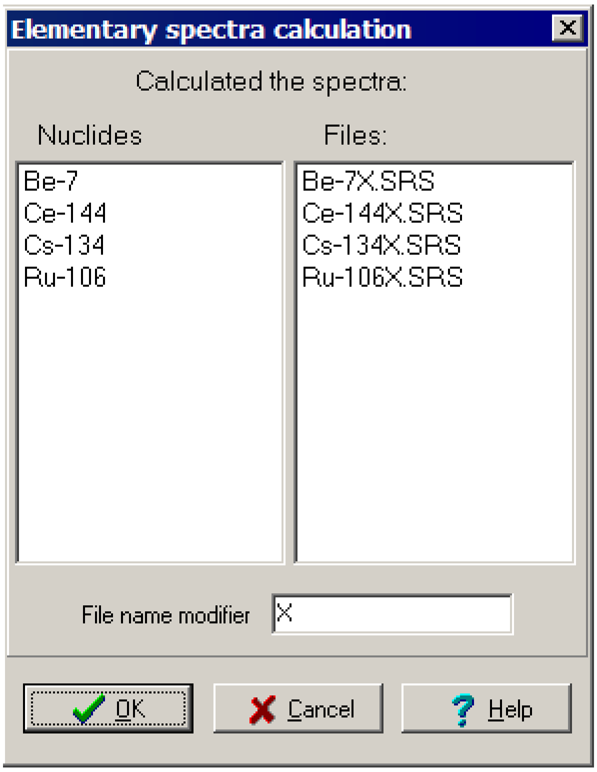
When calculating peak spectra, the chemical composition of the counting sample specified in the "**Sample type**" column is also taken into account, if it is specified (**Z eff.** > **0**). In the future, when using the calculated elementary spectra in the decomposition procedure, only the **interpolation parameter** will be taken into account. For the correct calculation of the elementary spectra corresponding to the interpolation parameter of the counting sample, it is recommended to calculate at least two sets of elementary spectra with different values of the interpolation parameter.

On the second page of "**Parameters**", the operator must select one of the four possible modes for interpolating line models:

F=a*x+b
F=exp(a*x+b)
F=a*log(x)+b
F=exp(a*log(x)+b) Here: **F** is the value of the function, **x** is the energy, **a** and **b** are the parameters of linear interpolation (piecewise linear interpolation is used).

Set the extrapolation mode to the low and high energy regions (**Extrapolation mode**): either **tangent to the interpolation polynomial**, or **parallel shift**. In parallel transfer, only one nearest line model is used, compressed or stretched according to a given energy. Since the interpolated functions are always positive and defined for positive abscissa values, it is recommended to use linear interpolation on a double logarithmic scale (**F=exp(a*log(x)+b)**), parallel transfer for extrapolation to the low and high energy region

Pressing the "**OK**" key starts the procedure for calculating the nuclide spectra. Upon completion of the calculation, the program suggests saving the generated spectra in the "**Elements**" folder and adding the necessary lines in the "**Decomp.ini**" file to connect the calculated spectra corresponding to the specified interpolation parameter (density or "size" of the sample) to the processing program. The window of the save procedure may look like:

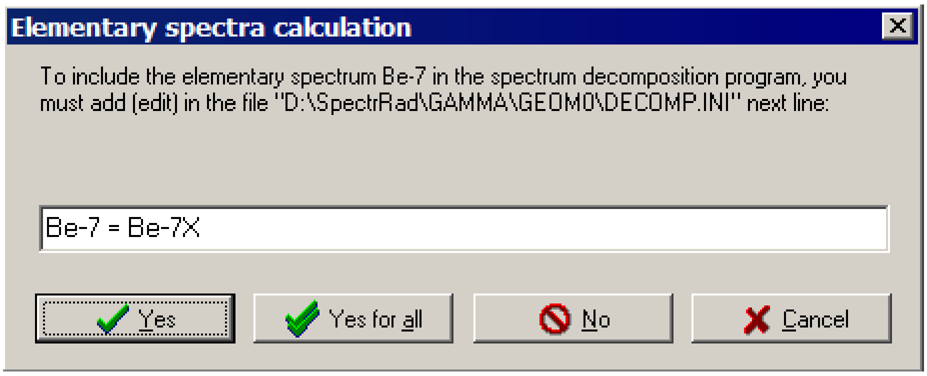


Nuclides	Files:
Be-7	Be-7X.SRS
Ce-144	Ce-144X.SRS
Cs-134	Cs-134X.SRS
Ru-106	Ru-106X.SRS

File name modifier: X

File names for saving nuclide spectra are formed from the names of nuclides and, when forming the same set of nuclide spectra for different interpolation parameters, in order for the newly created files not to overwrite existing spectra, but to be included separately for recalculating spectra depending on the interpolation parameter, an input field in the form "**File name modifier**" is provided for operator.

When saving the spectra, the program generates a window with information about the proposed modification of the corresponding line in the "**Decomp.ini**" file. For example:



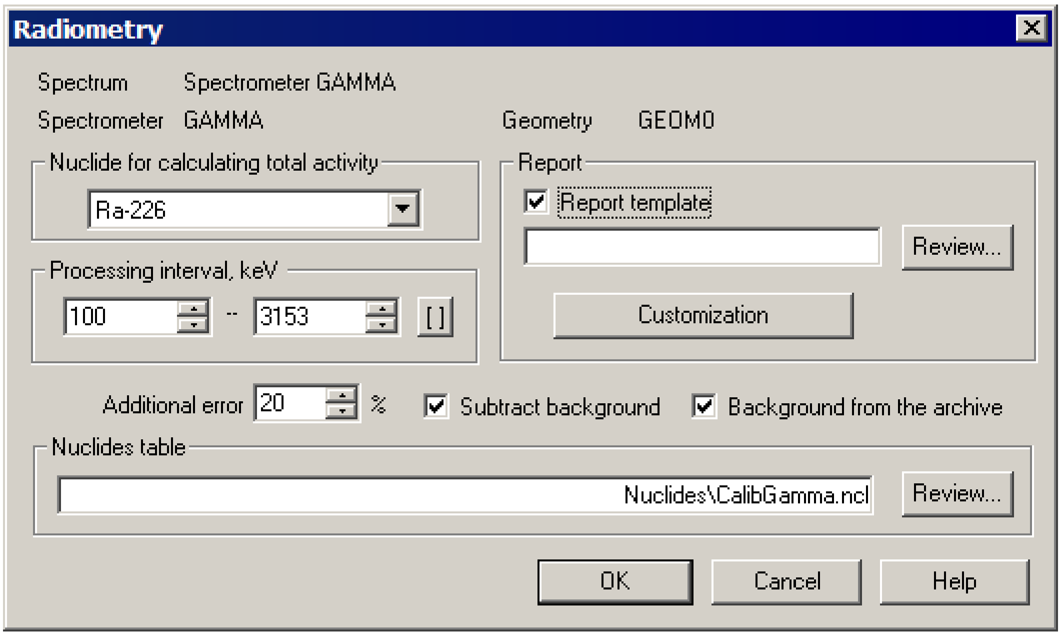
To include the elementary spectrum Be-7 in the spectrum decomposition program, you must add (edit) in the file "D:\SpectrRad\GAMMA\GEOM0\DECOMP.INI" next line:

```
Be-7 = Be-7X
```

The operator can agree with the proposed modification of the "**Decomp.ini**" file or edit the line himself.

Setting up the "Radiometry" procedure

The menu item "**Processing / Radiometry / Configure...**" allows the operator to set the necessary parameters for the procedure of calculating the "total activity" of the sample. At the same time, the following window is displayed on the screen:



Spectrum Spectrometer GAMMA
Spectrometer GAMMA
Geometry GEOM0
Nuclide for calculating total activity: Ra-226
Processing interval, keV: 100 -- 3153 [ ]
Report: ☑ Report template
Additional error 20 %
☑ Subtract background
☑ Background from the archive
Nuclides table: Nuclides\CalibGamma.ncl

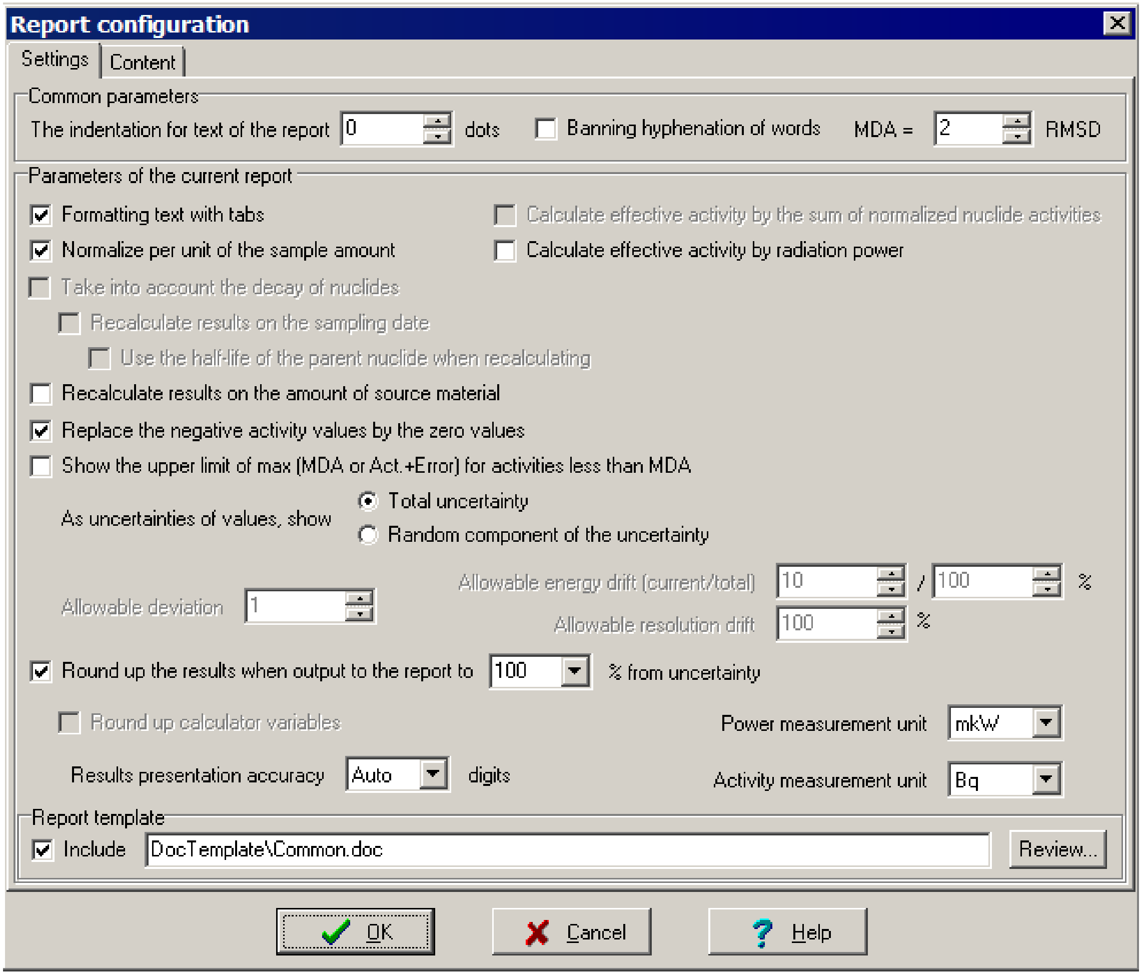
The operator needs to select a **nuclide to calculate the total activity** in a given energy **processing interval**. The [ ] button is used to substitute marker positions as processing boundaries.

Select the **nuclides table** containing data on the selected nuclide. The Review... button allows you to find the nuclide table file on your computer.

The operator must specify an additional to statistical error (**Additional error**) as a percentage of activity. Set the background subtraction mode (the "**Subtract background**" checkbox), specify which background to use: the saved **background from the archive** or the **current background**.

Report template - the operator, if desired, can specify the report template file, or find it using the Review... button.

The "**Customization**" button allows you to generate the contents of the report. In this case, the following table is displayed on the screen:



Report configuration

Settings | Content

Common parameters

The indentation for text of the report: 0 dots
☐ Banning hyphenation of words
MDA = 2 RMSD

Parameters of the current report

☑ Formatting text with tabs
☐ Calculate effective activity by the sum of normalized nuclide activities
☑ Normalize per unit of the sample amount
☐ Calculate effective activity by radiation power
☐ Take into account the decay of nuclides
  ☐ Recalculate results on the sampling date
    ☐ Use the half-life of the parent nuclide when recalculating
☐ Recalculate results on the amount of source material
☑ Replace the negative activity values by the zero values
☐ Show the upper limit of max (MDA or Act.+Error) for activities less than MDA

As uncertainties of values, show
● Total uncertainty
○ Random component of the uncertainty

Allowable deviation: 1
Allowable energy drift (current/total): 10 / 100 %
Allowable resolution drift: 100 %

☑ Round up the results when output to the report to 100 % from uncertainty
☐ Round up calculator variables
Power measurement unit: mkW
Results presentation accuracy: Auto digits
Activity measurement unit: Bq

Report template

☑ Include DocTemplate\Common.doc

The form has two pages: "**Settings**" and "**Content**". There are two groups on the "**Settings**" page:

Common parameters - parameters used in generating radiometry and decomposition reports:

- **The indentation for text of the report** - indentation from the left border of the form to the text of the report. The value is set in points. This parameter is used if the report is not included in the report template (in this case, its position is determined by the position of the {**Report**} or {**Table**} label).
- **Banning hyphenation of words** - setting or disabling the automatic word wrapping mode in a paragraph.
- **MDA =** - setting the value of the minimum detectable activity in terms of standard deviations.

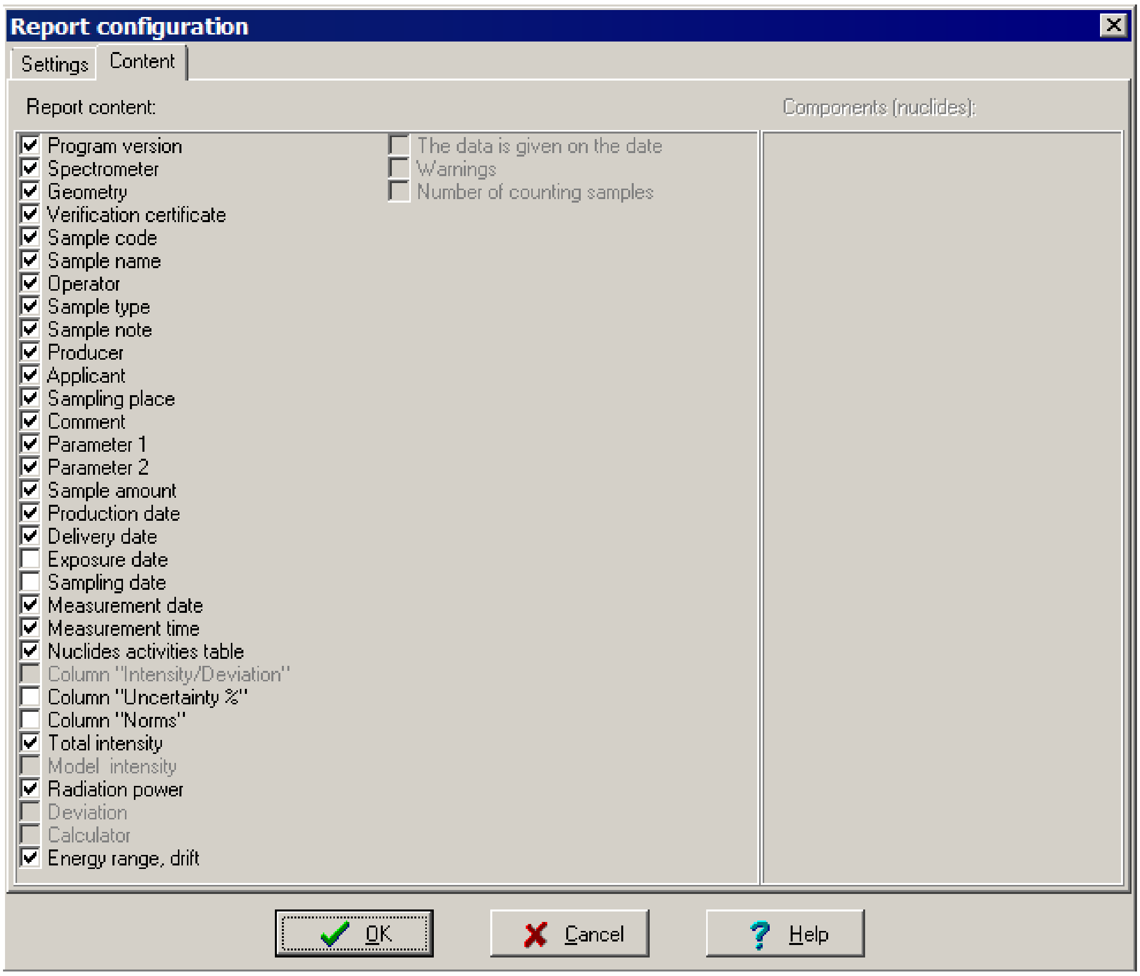
Parameters of the current report - parameters used in generating radiometry reports for a given spectrometer and a given measurement geometry:

- **Formatting text with tabs** – when the checkbox is selected, the procedure for generating a report before each new paragraph of text containing descriptions of the sample, spectrometer, and measurement conditions will include a tab character to align the text with the first tab position (the position of the "red" line).
- **Normalize per unit of the sample amount** - output values of the specific or total activity of the sample. For the usual type of geometry (thin or intermediate layer), normalization by sample amount means dividing the estimated activity of the counting sample by the mass of the counting sample – that is, calculating the specific activity of the counting

sample. For the geometry of the "thick" layer, normalization by sample amount means multiplying the estimated specific activity of the counting sample by the mass of the counting sample, that is, determining the total activity of the counting sample. If the "**Normalize per unit of the sample amount**" and "**Recalculate results on the amount of source material**" check boxes are checked simultaneously, the estimated specific activity of the sample source material is displayed in the report in any case.

- **Recalculate results on the amount of source material** – output of the nuclide activities of the initial sample material (at the marked point) or the nuclide activities in the substance of the counting sample.
- **Replace the negative activity values by zero values** – when the checkbox is set, negative activity values in the report will be replaced with zero values.
- **Show the upper limit of max (MDA or Act.+Error) for activities less than MDA**. When the checkbox is set, the upper limit of values for values with activity estimates less than the minimum detectable in accordance with ISO and IEC recommendations will be given in the report. For such values, the report shows either **MDA** or **Activity+Error** with a "<" sign or the word "less", depending on which value is greater. The MDA value in units of mean-square deviations is set in the archive settings.
- **Calculate effective activity by radiation power**. When you check the box, the report will show the total effective activity of the sample for the selected nuclide. The activity of nuclides equivalent in energy output to the activity of the selected nuclide is accepted as effective (for gamma radiation, Ra-226 is used as a comparison nuclide).
- **As uncertainties of values, show "Total uncertainty"** or "**Random component of the uncertainty**" **-** the operator is given a choice of one of two options for presenting the error in the report. If you select a random error component, the activity table in the report will be displayed in blue font.
- **Round up the results when output to the report to nn % from uncertainty** – setting the mode and form of rounding the measurement results in the report. When 100% rounding is set, the values of activities and errors in the report will be given in accordance with the requirements of MI 2453-2000.
- **Results presentation accuracy** – select the number of digits to represent the results in the report. The value "**Auto**" corresponds to the automatic determination of the required accuracy of the presentation of the results. In this case, insignificant zeros are not output.
- **Power measurement unit** – select the unit of measurement of the radiation power from the sample calculated by the procedure (**keV/s, MeV/s, mcW** or **W**) in which the power will be shown in the report. The radiation power is calculated within the selected energy range.
- **Activity measurement unit** – select the unit of measurement (Becquerel or Curie) in which the activity of nuclides in the report will be shown.
- **Report template -** the operator, if desired, can specify the report template file. The file must contain the template text saved in RTF format or as a Word document (DOC, DOCX). An example of a report template is provided in the appendix. Review... button **-** overview of existing report templates

On the "**Content**" page, the operator can set the rows and columns of the radiometry output form, which will be shown in the report:



Report content:

☑ Program version
☑ Spectrometer
☑ Geometry
☑ Verification certificate
☑ Sample code
☑ Sample name
☑ Operator
☑ Sample type
☑ Sample note
☑ Producer
☑ Applicant
☑ Sampling place
☑ Comment
☑ Parameter 1
☑ Parameter 2
☑ Sample amount
☑ Production date
☑ Delivery date
☐ Exposure date
☐ Sampling date
☑ Measurement date
☑ Measurement time
☑ Nuclides activities table
☐ Column "Intensity/Deviation"
☐ Column "Uncertainty %"
☐ Column "Norms"
☑ Total intensity
☐ Model intensity
☑ Radiation power
☐ Deviation
☐ Calculator
☑ Energy range, drift

☐ The data is given on the date
☐ Warnings
☐ Number of counting samples

Search for peaks. Setting parameters

The spectra with a linear type of spectra set in the parameters of the spectrometer are processed with preliminary subtraction from the acquired spectrum of a continuous spectrum[18] on which the resonant sections of the spectrum are peaks. The decomposition of the spectrum into components is carried out for the spectrum of peaks[19].

Before processing the linear spectra, it is necessary to set the necessary peak search parameters for the selected spectrometer and measurement geometry. To do this, by selecting the menu item "**Processing / Peaks search / Configure...**", you must fill in the fields of the "**Peaks search parameters**" table:

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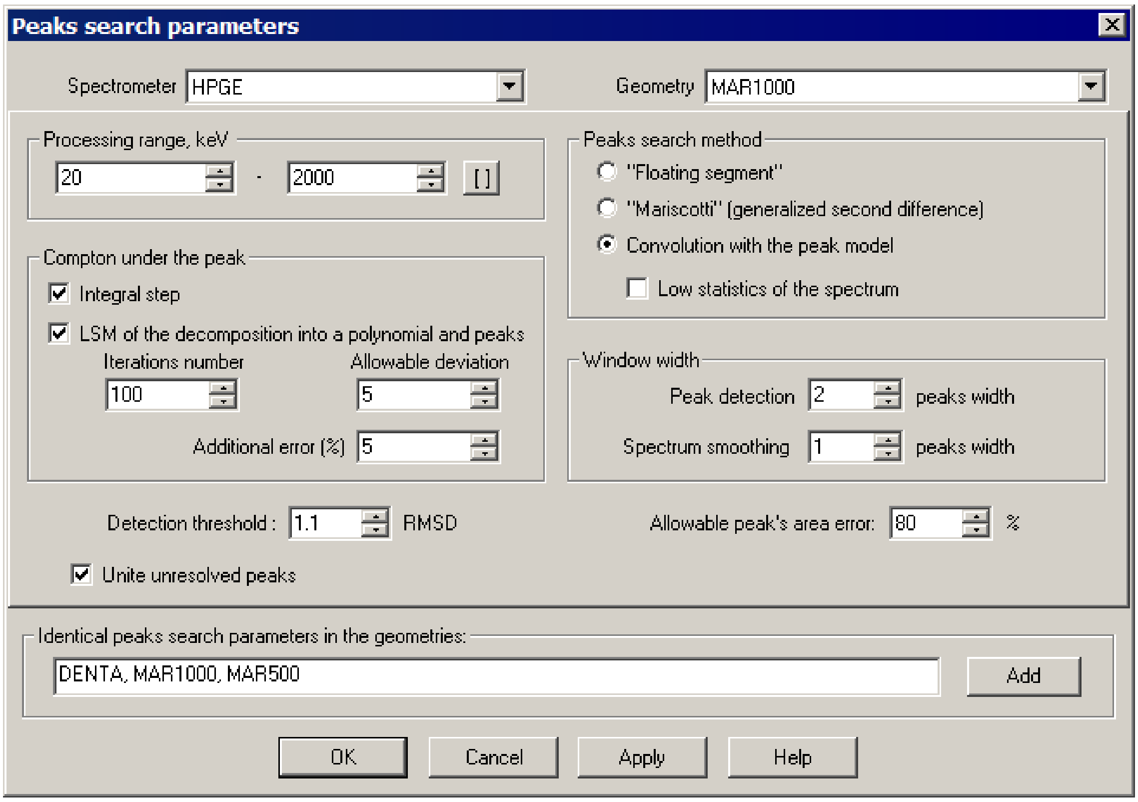
[18] For gamma spectra, the **continuous spectrum** is the spectrum of Compton scattering of gamma quanta and bremsstrahlung of beta particles. In the peak region, the continuous spectrum is approximated by a spline, a Philippotte integral step, a polynomial, or the sum of an integral step and a polynomial.

[19] The procedure of preliminary subtraction of the continuous scattering spectrum significantly increases the conditionality of the decomposition matrix and significantly facilitates the task of generating spectra, but is applicable only if it is possible to isolate peaks or groups of peaks in the sample spectrum.


Peaks search parameters

Spectrometer: HPGE
Geometry: MAR1000

Processing range, keV: 20 - 2000

Peaks search method:
○ "Floating segment"
○ "Mariscotti" (generalized second difference)
● Convolution with the peak model
☐ Low statistics of the spectrum

Compton under the peak:
☑ Integral step
☑ LSM of the decomposition into a polynomial and peaks
Iterations number: 100
Allowable deviation: 5
Additional error (%): 5

Window width:
Peak detection: 2 peaks width
Spectrum smoothing: 1 peaks width

Detection threshold : 1.1 RMSD
Allowable peak's area error: 80 %

☑ Unite unresolved peaks

Identical peaks search parameters in the geometries: DENTA, MAR1000, MAR500

Processing range - the maximum permissible limits of spectrum processing when searching for peaks. When processing according to the selected template, the common area of the processing interval specified in the peak search parameters and in the decomposition template is used. The "button" [ ] is used to substitute marker positions as processing boundaries.

Peaks search method - the operator has the option to choose one of three peak search methods:

- **"Floating segment"** is the essence of the method in calculating the ratio of the area of the spectrum over a straight line segment moving along the spectrum to the error of its determination.
- **"Mariscotti" (generalized second difference)** – search for peaks by the second derivative. The numerical implementation of the method was proposed by Mariscotti in the 60s of the last century.
- **Convolution with the peak model -** convolution of a section of the spectrum within a given window with a peak model. It is believed that the third method is more sensitive and reliable, since in addition to the integral area estimation, the peak shape is also analyzed. This is true, but only for single peaks, since spectrum convolution is performed with a peak model for a single line. In the case of a multiplet, shape analysis can only confuse the situation. In principle, it is possible to construct a multiplet of arbitrarily complex shape, on which any peak search method will break off its teeth (such a multiplet is the spectrum of any soil sample measured on a scintillation gamma spectrometer). For very complex multiplets, we can recommend a method for processing spectra without searching for peaks and for resolved linear spectra.

Compton under the peak - the operator can choose one of four methods for constructing a continuous scattering spectrum under the peak:

- The check mark "**Integral step**" is set – the Compton spectrum under the peak region is approximated by the integrated Philipott step.
- The check mark "**LSM of the decomposition into a polynomial and peaks**" is set – approximation by a polynomial. When approximated by a polynomial, the portion of the spectrum containing peaks is decomposed by the least squares method into the sum of

the peak spectra and the polynomial of the continuous scattering spectrum. In this case, the operator must specify the number of iterations (**Iterations number**) and the amount of **allowable deviation**. If the decomposition discrepancy exceeds the permissible one, the Compton spectrum under the peak is approximated by an integral step or a linear function.

- If both check boxes are set, the background under the peaks is approximated by the sum of the integral step and the polynomial.
- If none of the ticks are set, the background under the peaks is approximated by a linear function.

Additional error (%) is an additional to statistical error of the Compton scattering area under the peaks (and, accordingly, the peak area) associated with the uncertainty of constructing the continuous scattering spectrum. It is difficult to estimate this value in advance, since it strongly depends on the resolution of the spectrometer and on the complexity of the spectrum. The actual value is determined during operation of the spectrometer.

Window width - the operator must specify the width of two windows (in units of peak width at half height) used when searching for peaks:

- **Peak detection -** with the convolution method, the window width determines the range of convolution of the spectrum with the peak model, for the generalized second difference method – the width of the "Mariscotti" function, and for the "floating segment" method - the length of the segment. The recommended value is ~2.5 for the "floating segment" and convolution methods with the peak model and ~2.2 for the "Mariscotti" method.
- **Spectrum smoothing -** the width of the window determines the number of points by which the count values in the spectrum channels are averaged for the spectrum smoothing procedure. The recommended value is ~1.0 for the "floating segment" methods, convolution with the peak model and for the "Mariscotti" method.

Detection threshold n.n RMSD is the value level of the peak detection function[20] normalized for the error of its calculation (mean square deviation), above which the search procedure will register the presence of a peak in the spectrum. For small values of the detection threshold, the search procedure may include false peaks in the list of peaks found, and for large ones, skip weak peaks. Recommended value: from 1 to 3.

Allowable peak's area error – the value of the error in determining the peak area as a percentage, if exceeded, the peaks will not be included in the list of peaks found.

Unite unresolved peaks is a checkbox that allows you to set the mode for combining unresolved peaks. Unresolved peaks in this case are considered to be peaks forming a multiplet without a gap between the peaks. Such peaks are formed by the processing procedure in the mode of spectrum decomposition on peak models and Compton scattering polynomials. The error in determining the areas of such unresolved peaks is significantly higher than the error in determining the area of the total peak. Therefore, for procedures where the accuracy of peak area estimation is important (for example, calibration of registration efficiency), it is recommended to check the box.

Peak search parameters can be set separately for each of the measurement geometries in spectrometers with a linear character of the spectra. The "**Identical peaks search parameters in the geometries**" parameter group, which includes a row with a list of geometries and the "**Add**" button, allows you to set identical peak search parameters for several geometries. Clicking on the "**Add**" button adds the current geometry to the list of geometries with identical peak search parameters.

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[20] **Detection function –** depending on the setting, either the peak area above a segment of a straight line moving along the spectrum and with a length equal to the width of the peak, or the convolution of the spectrum within the peak width with the peak model, or the second difference (Mariscotti function).

Creating decomposition templates

General concepts

Decomposition is the decomposition of the measured spectrum into the emission spectra of individual nuclides or equilibrium chains of nuclides (spectra of components). At the same time, the program evaluates the contribution of each component to the spectrum, and if the decomposition components are normalized per unit of nuclide activity (the parent nuclide for the nuclide chain); the nuclide activity will be the contribution estimate.

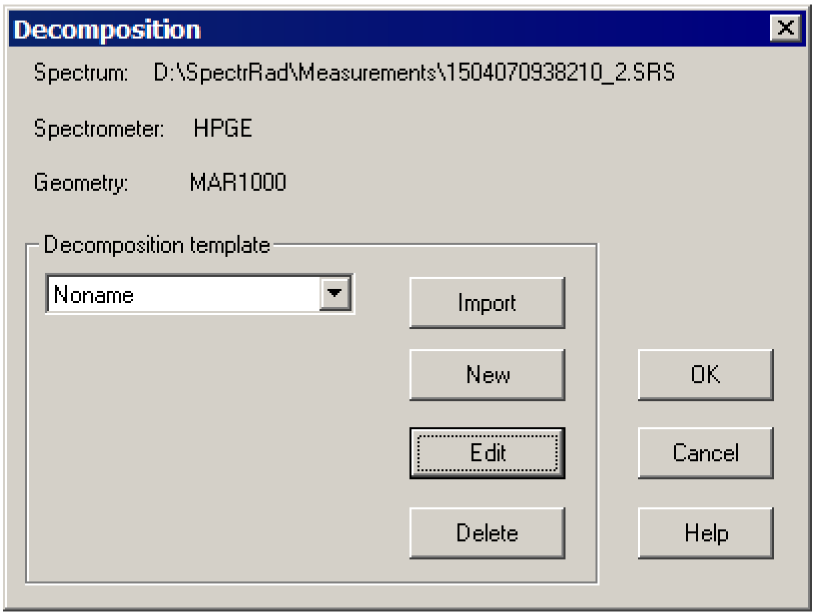
The **decomposition template** is a list of decomposition components, a set of processing parameters, report forms and a program for additional processing of the results of activity estimates stored in the **Decomp.par** file.

Pre-creation of the necessary processing templates for the selected spectrometer and the selected measurement geometry allows the operator not to waste time setting processing parameters each time the decomposition procedure is called, but simply to select one of the existing templates.

When processing the spectrum according to the decomposition mode (decomposition of the spectrum into components), the operator can either choose one of the existing processing templates, or independently create the necessary **decomposition templates**.

Calling the procedure for creating a decomposition template

When clicking on the button (selecting the menu item "**Processing / Decomposition...**"), the following window is displayed:



Spectrum: D:\SpectrRad\Measurements\1504070938210_2.SRS

Spectrometer: HPGE

Geometry: MAR1000

Decomposition template: Noname

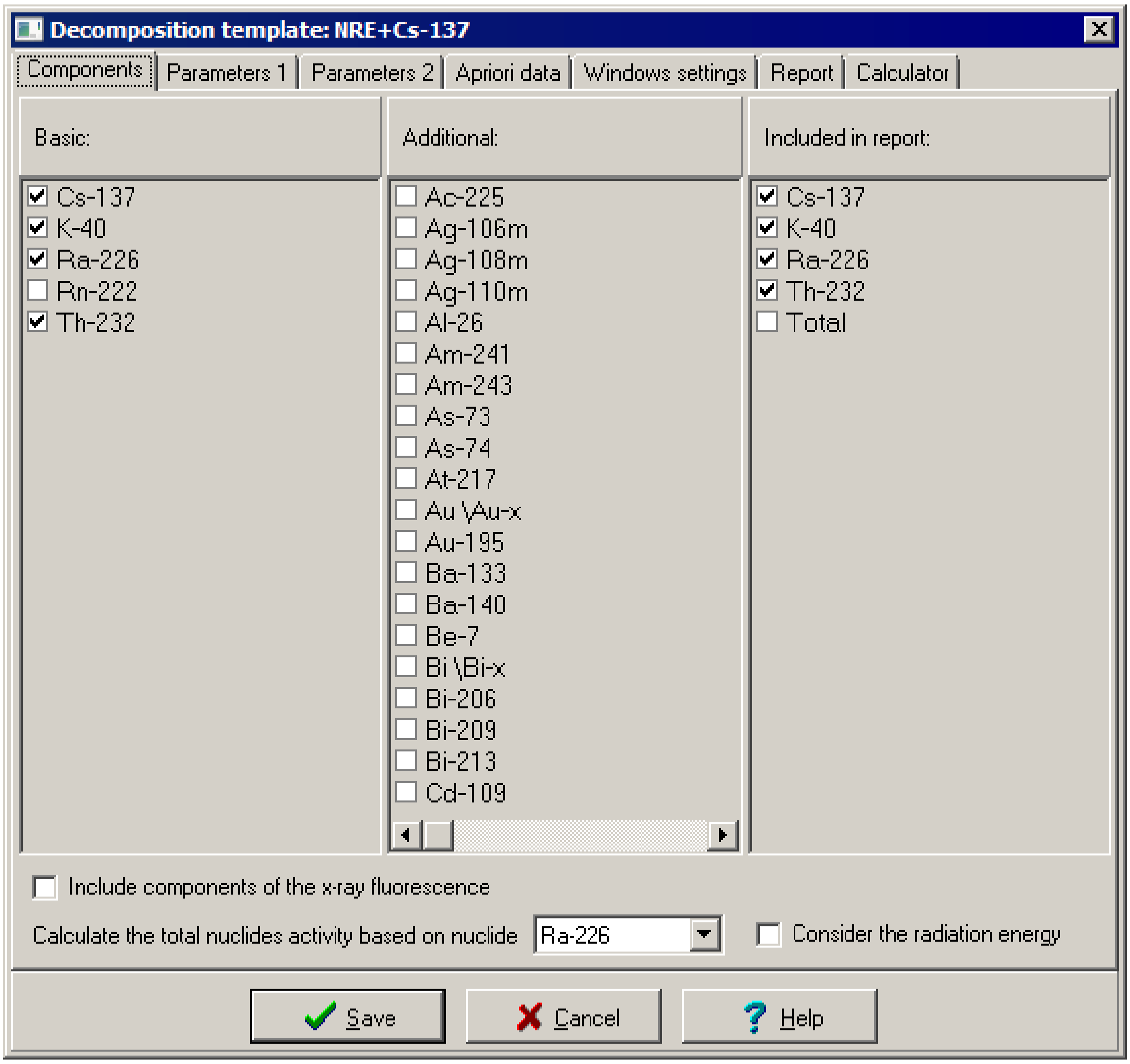
When installing the spectrometer, the list of decomposition templates contains only one "**Noname**" element containing the default processing parameters. The operator can either edit an existing template by clicking on the "**Edit**" key, or create a new one by clicking on the "**New**" key. You can delete an unnecessary template by clicking on the "**Delete**" key.

The "**Import**" key allows you to import processing templates from the **Decomp.par** file selected by the operator into this set of templates.

Clicking on the "**New**" or "**Edit**" key displays a form for creating or editing decomposition templates. The form contains 7 pages: "**Components**", "**Parameters 1**", "**Parameters 2**", "**Apriori data**", "**Windows settings**", "**Report**" and "**Calculator**".

Selection of decomposition components

On the first page of the form, the operator must select the components that will participate in the decomposition procedure.



Basic:

- ☑ Cs-137
- ☑ K-40
- ☑ Ra-226
- ☐ Rn-222
- ☑ Th-232

Additional:

- ☐ Ac-225
- ☐ Ag-106m
- ☐ Ag-108m
- ☐ Ag-110m
- ☐ Al-26
- ☐ Am-241
- ☐ Am-243
- ☐ As-73
- ☐ As-74
- ☐ At-217
- ☐ Au \Au-x
- ☐ Au-195
- ☐ Ba-133
- ☐ Ba-140
- ☐ Be-7
- ☐ Bi \Bi-x
- ☐ Bi-206
- ☐ Bi-209
- ☐ Bi-213
- ☐ Cd-109

Included in report:

- ☑ Cs-137
- ☑ K-40
- ☑ Ra-226
- ☑ Th-232
- ☐ Total

☐ Include components of the x-ray fluorescence

Calculate the total nuclides activity based on nuclide: Ra-226

☐ Consider the radiation energy

The page contains three lists of elementary spectra of nuclides (chains of nuclides) and a number of additional parameters:

- **Basic** - elementary nuclide spectra pre-calculated for selected spectrometer and geometry (in the example, the list for the scintillation gamma spectrometer). Elementary spectra can be calculated from reference spectra or generated from spectrometer calibrations and nuclide tables. As a rule, this list contains elementary spectra calculated from the spectra of standards. For well-resolved gamma spectra, when using the processing method with pre-subtraction of the continuous scattering spectrum (Compton scattering of gamma quanta and bremsstrahlung X-ray of beta particles), it is not necessary to pre-calculate elementary spectra, therefore this list may be empty. The list can include up to 500 components.
- **Additional** - a list of all nuclides included in the nuclide table used in this processing template. The elementary spectra of the nuclides marked by the operator in this list will be calculated by the generation program using the nuclides table. The list can include an unlimited number of components. In the processing method with approximation of the continuous scattering spectrum by a spline (see "**Decomposition parameters**"), the main list will include the full spectrometer responses (including the continuous scattering spectrum) to nuclide radiation, and when selecting a nuclide from the list of

additional ones, the peak spectrum (without the continuous scattering spectrum) will be calculated for it. Thus, the operator has the opportunity to choose the response of the spectrometer to nuclide radiation and both types of elementary spectra can participate in the decomposition procedure.

- **Included in report** - a list of nuclides from the first two lists that will be included in the decomposition report.
- **Include components of the x-ray fluorescence** – when the “tick” is set, the list of nuclides will be supplemented with X-ray fluorescence components of the counting sample material. The calculation of the X-ray fluorescence components is possible if the chemical composition of the substance of the counting sample is specified and the nuclide table used contains a list of X-ray fluorescence lines. Such calculation is necessary if the sample material contains heavy elements and the activity of the sample is sufficient for significant X-ray fluorescence.
- **Calculate the total nuclides activity based on nuclide "*name*" -** calculation of the "total activity" of the sample in accordance with the coefficient calculated by the efficiency of radiation registration in the established energy range. The operator must specify the nuclide name, the elementary spectrum and quantum yield of which will be used to calculate the "total activity" and "effective total activity". It is recommended to use a "virtual" nuclide as such a nuclide. The "virtual" nuclide does not participate in the procedures for the automatic determination of the nuclide composition and is intended primarily for comparison purposes.
- Selecting the "**Consider the radiation energy**" checkbox sets the mode for estimating the average radiation energy of the counting sample by the median of the spectrum when calculating the total activity of the sample and the corresponding recalculation of the registration efficiency. For alpha radiation, the calculation is performed only if the radiation energy is not specified in the spectrum parameters.

The operator must tick the elementary spectra that will be used in the decomposition (up to 100 spectra from two lists can be included) and mark the necessary nuclides in the list "**Included in report"**.

When setting the automatic spectrum composition analysis mode, the processing procedure can supplement the list of nuclides to be determined. In this case, the components included by the operator, unlike the components included in the composition analysis procedure, the processing program does not have the right to remove the decomposition component from the list and, if the component is not present in the spectrum, the value of the minimum detectable activity (MDA) will be calculated for it.

Calculation of total activity

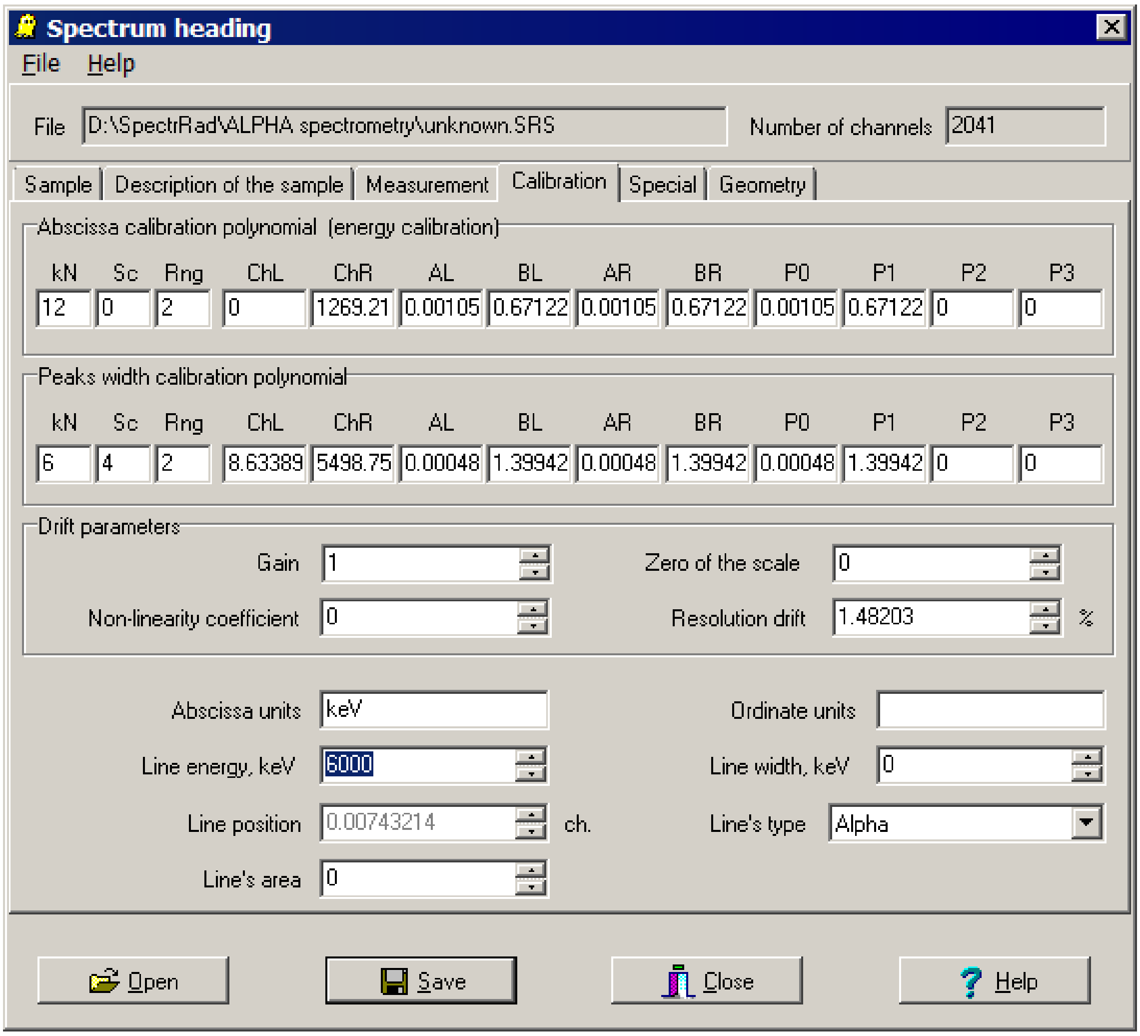
In accordance with current legislation (SanPiN 2.1.4.559-96 and SP 2.6.1 758-99 "Radiation Safety Standards (NRB-99)"), fresh natural waters for domestic drinking purposes in Russia, among other indicators, should be monitored for "total alpha activity" – 0.2 Bq/l and "total beta activity" – 1 Bq/l. "Total activity" refers to the number of radiation particles formed in a sample as a result of radioactive decay per unit of time: for total alpha activity – the number of alpha particles, for total beta – the number of beta particles. The Becquerel unit of measurement for "total activity" does not mean decay per second, but a particle per second. Accordingly, the concepts of specific total activity are defined. By analogy, we can define the concept of "total gamma activity" - the number of gamma quanta per unit of time.

The concept of "total activity" is very conditional, because if alpha radiation can be recorded by existing alpha radiometers for the entire possible energy range, then soft beta radiation by beta radiometers is simply not recorded. We can talk about a reliable determination of the total beta activity of the sample only on the assumption that both the sample and the standard used for calibration have identical beta emitters. It should also be taken into account that the water sample preparation required to achieve the desired "accuracy" sends both radioactive gases dissolved in water and radioactive isotopes of hydrogen present in water to ventilation.

The "**Calculate the total nuclides activity based on nuclide *name***" checkbox allows you to calculate the "total activity" of the sample in accordance with the coefficient calculated by the efficiency of radiation registration in the specified energy range. For the resolved linear spectra, radiation registration efficiency in the peaks is used to calculate the "total activity". The specified nuclide ***name*** for such spectra is used to calculate the "effective total activity" as a standard unit of "effective total activity". For poorly resolved spectra and for spectra that do not have a linear structure, the elementary spectrum and the quantum yield of a given nuclide will be used to calculate the "total activity". Since the elementary spectra are normalized per decay, and not per a quantum of radiation, for correct recalculation it is required to set a table of nuclides corresponding to the selected elementary spectrum in the decomposition parameters. For example, if we specified Sr-90 as the nuclide for calculating the total activity, and the elementary spectrum of Sr-90 contains the total response of Sr-90 and Y-90, in the table of nuclides used, Sr-90 should be represented as an equilibrium chain Sr90+Y90. Non–detectable low energy lines should be removed from the line table for the selected nuclide - for example, electrons with energy of 2.66 keV for K-40. To calculate the "total beta activity", it is recommended to use K-40 as a reference.

Both alpha and beta radiation are significantly attenuated by the substance of the counting sample. The absorption of radiation in the space of the measured sample is determined by the physical properties of sample substance (density, average effective atomic number and average effective atomic mass) and radiation energy (see "Norms and materials"). When calibrating the spectrometer, the parameters of the reference (physical constants and average radiation energy) are stored in the reference spectrum file. For a sample substance physical constants are taken from the files of norms and materials associated with the **sample type**. These data should be formed either in advance or at the stage of entering sample parameters.

For alpha spectra, the operator can also set, if known, the average alpha radiation energy of the sample in the parameter "**Line energy, keV**" spectrum parameters (menu item "**Tools / Spectrum parameters ...**".



File: D:\SpectrRad\ALPHA spectrometry\unknown.SRS
Number of channels: 2041

Abscissa calibration polynomial (energy calibration)

kN	Sc	Rng	ChL	ChR	AL	BL	AR	BR	P0	P1	P2	P3
12	0	2	0	1269.21	0.00105	0.67122	0.00105	0.67122	0.00105	0.67122	0	0

Peaks width calibration polynomial

kN	Sc	Rng	ChL	ChR	AL	BL	AR	BR	P0	P1	P2	P3
6	4	2	8.63389	5498.75	0.00048	1.39942	0.00048	1.39942	0.00048	1.39942	0	0

Drift parameters

Gain: 1
Zero of the scale: 0
Non-linearity coefficient: 0
Resolution drift: 1.48203 %

Abscissa units: keV
Ordinate units:
Line energy, keV: 6000
Line width, keV: 0
Line position: 0.00743214 ch.
Line's type: Alpha
Line's area: 0

If the alpha radiation energy is set in this way for the parameters of the spectrometer, it will be valid for all samples measured after that on the spectrometer until a new setting of a different value.

The average radiation energy of the reference is calculated and stored in the "**Line energy, keV**" parameter when calibrating the spectrometer (calculating the elementary spectrum). In order to correctly calculate the average radiation energy, non-detectable low energy lines must be removed from the line table used in calibration of the spectrometer for nuclides of the standard sample.

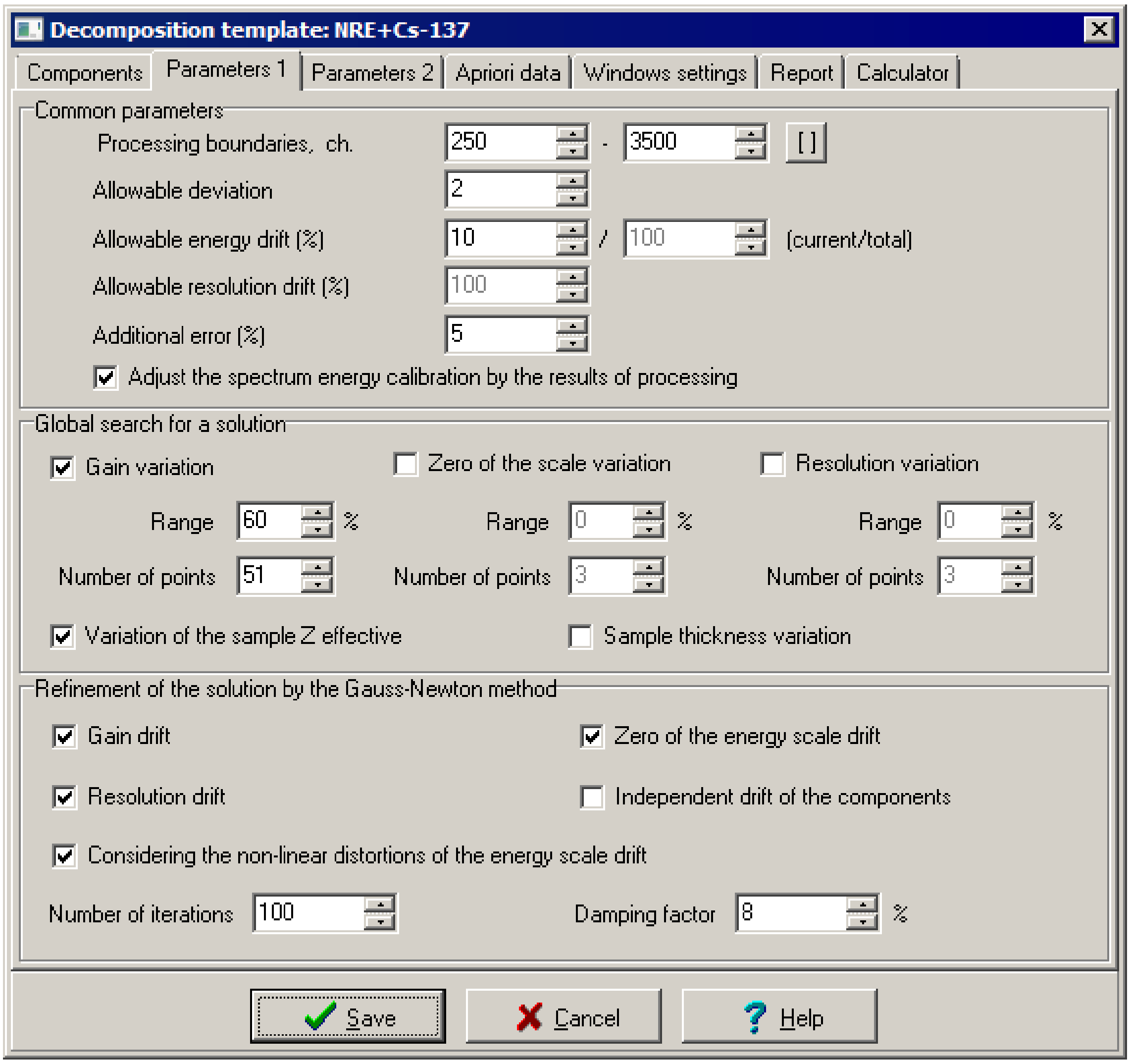
The radiation energy of the sample can be calculated from the medians of the spectra of the sample and the reference, if the "**Consider the radiation energy**" checkbox is selected in the parameters of the decomposition template. For alpha radiation, the calculation is performed only if the radiation energy is not specified in the parameters of the sample spectrum.

The calculation of radiation absorption in the substance of the counting sample is performed if the physical constants of the substance and the counting sample and the reference are set (the average effective atomic number and the average effective atomic mass of the substance). If the physical constants of the substance of the counting sample are not specified, they are assumed to be the same as those of the standard. If the radiation energy is not set or the "**Consider the radiation energy**" checkbox is not checked, no recalculation of the radiation energy is performed and the average radiation energy of the counting sample is assumed to be equal to the average radiation energy of the reference.

The integral of the elementary spectrum is calculated according to the energy range specified in the processing template; the energy range of the integral for the sample spectrum is multiplied by the stretching-compression coefficient calculated from the quartiles of the spectra of the sample and the reference. To reduce additional errors, while calculating the total activity, associated with the recalculation of the energy range for the sample, the operator must select a nuclide having radiation energy close to the estimated energy of the recorded radiation.

Decomposition parameters

The parameters of the processing procedure occupy four pages: "**Parameters 1**", "**Parameters 2**", "**Apriori data**" and "**Windows settings**". The "**Parameters 1**" page may look like:



Common parameters

Processing boundaries, ch. 250 - 3500 [ ]

Allowable deviation 2

Allowable energy drift (%) 10 / 100 (current/total)

Allowable resolution drift (%) 100

Additional error (%) 5

☑ Adjust the spectrum energy calibration by the results of processing

Global search for a solution

☑ Gain variation ☐ Zero of the scale variation ☐ Resolution variation

Range 60 % Range 0 % Range 0 %

Number of points 51 Number of points 3 Number of points 3

☑ Variation of the sample Z effective ☐ Sample thickness variation

Refinement of the solution by the Gauss-Newton method

☑ Gain drift ☑ Zero of the energy scale drift

☑ Resolution drift ☐ Independent drift of the components

☑ Considering the non-linear distortions of the energy scale drift

Number of iterations 100 Damping factor 8 %

In the first group, the operator must set "**Common parameters**" - the general decomposition parameters:

- **Processing boundaries** are the left and right energy boundaries of the spectrum decomposition region. The "button" [ ] is used to substitute marker positions as processing boundaries.
- **Allowable deviation** - the maximum allowable deviation[21] value at which decomposition is considered successful.
- **Allowable energy drift (%) (current/total)** - the maximum value (in percent) of the energy drift (the total change in the gain factor and zero of the spectrometer scale). If

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[21] **Deviation** of the calculated model from the object normed on the estimated value of the standard deviation. $G=\sqrt{\sum((X_i-X_m)^2/G_i^2)/(n-m)}$.

exceeded, the decomposition will be considered unsuccessful, and the program will not refine the calibration of the spectrum based on the results of spectrum processing. **Current drift** – the drift over the time since the last calibration of the spectrum (spectrometer). **Total drift -** the drift over the time since the initial calibration of the spectrometer. The value of the total drift is for reference (not editable). It is set in the auto-calibration parameters.

- **Allowable resolution drift (%) -** the maximum value (in percent) of the change in the resolution of the spectrometer. If exceeded, the program will not refine the calibration of the spectrometer based on the results of spectrum processing. The value of the allowed resolution drift is for reference (not editable). It is set in the auto-calibration parameters.
- **Additional error (%) -** an error set by the operator, additional to the measurement error calculated by the program, associated with errors in determining sample parameters: weight, sample volume, geometry violations, etc.
- **Adjust the spectrum energy calibration by the result of processing -** a checkbox that allows you to change the parameters of the energy calibration of the spectrum (spectrometer) based on the results of processing.

The second group allows you to include the **Global search for a solution** mode in the decomposition procedure and set global search parameters[22]:

- **Gain variation** – the program will decompose the spectrum into components for a given **number of points** evenly distributed in a given range of variation (**Range**) of the spectrometer gain. The range of variation is understood in a multiplicative sense, that is, for example, a 100 percent range means a variation from 0.5 to 2 times the gain value. The number of points is always rounded to an odd value so that the initial value falls in the middle of the range of variation.
- **Zero of the scale variation** is a similar procedure for varying the zero of the energy scale of a spectrometer. The range of variation is understood in an additive sense as a percentage of the processing range.
- **Resolution variation** is a similar procedure for varying the resolution of a spectrometer. The range of variation is understood in an additive sense as a percentage of the current resolution.
- **Variation of the sample Z effective, Sample thickness variation** is a procedure allowed only for gamma spectrum processing patterns. When varying the Z effective and the thickness of the sample, accounting for photo absorption and Compton scattering of gamma quanta is calculated for different values of the Z effective and/or effective thickness of the counting sample, and values are selected that ensure a minimum deviation in the decomposition of the spectrum. The thickness of the counting sample varies from 50% to 200% of the geometry of the average thickness of the counting sample specified during installation. A necessary condition for varying the Z-value and thickness of the sample is the presence of lines with different energies in the spectra of the components.

The third group is used to set the modes and parameters of the solution refinement procedure by the Gauss-Newton method (**Refinement of the solution by the Gauss-Newton method**). The operator can set different processing modes by ticking the enabled processing procedures:

- **Gain drift** is a procedure for estimating and correcting the drift of the spectrometer gain factor.

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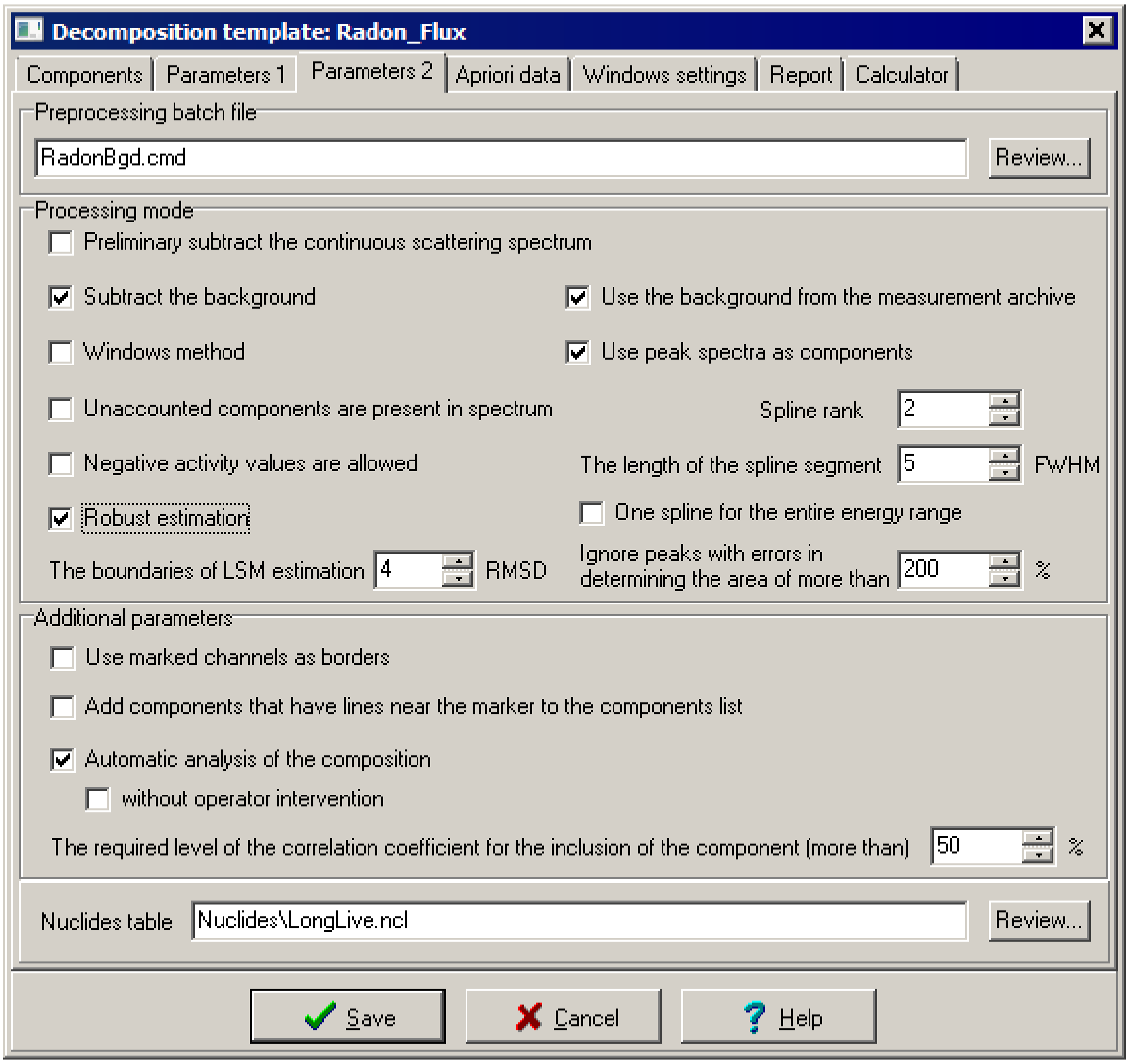
[22] The **global search for a solution** and the **refinement of the solution by the Gauss-Newton method** are necessary to correct the parameters of the spectrometric tract (first of all, the energy drift). A global search finds the parameters of the initial approximation for the Gauss-Newton solution refinement procedure.

- **Zero of the energy scale drift -** estimation and correction of the zero drift of the energy scale of the spectrometer.
- **Resolution drift -** estimation and correction of the resolution drift of the spectrometer.
- **Considering the non-linear distortions of the energy scale drift**. With a significant load on the spectrometric tract, the energy drift becomes nonlinear. The nonlinearity of the energy scale of the spectrometer is also taken into account in the basic energy calibration of the spectrometer, but with a significant change in the load, the nature of nonlinear distortions also changes. Selecting this check box enables the procedure for evaluating such distortion.
- **Independent drift of the components** is a processing mode in which the independent drift of the components is evaluated. Of course, the parameters of the spectrometer tract change (drift), but if we are not sure that all the elementary spectra (including the background), the components of the decomposition, are in a single energy scale, the values of the drift parameters for them may be different and in this case it is reasonable to use this processing mode. Such uncertainty may arise if the measurement methodology of the standard samples is not followed. In this processing mode, the stability of the decomposition procedure is significantly reduced and, therefore, its use is justified either for spectra with good line resolution or with a small number of decomposition components. A side effect of this processing mode is that in this case, the spectra of the components are formed in the "**Comp**" folder, reduced to a single energy scale (the scale of the sample spectrum). The operator can use them as refined elementary spectra by moving them to the "**Elements**" folder.
- **Number of iterations -** the maximum allowed number of iterations to refine the decomposition estimates in the energy drift correction procedure by the Gauss-Newton method. The program terminates the procedure in the absence of significant changes in the estimates of the parameters being determined, or when the specified number of iterations is exceeded. Limiting iterations makes sense for computers with low performance.
- **Damping factor** is a constant (set as a percentage) that increases the stability of the decomposition procedure. The value of the damping coefficient should be greater, the less the conditionality of the system of equations to be solved (a large number of decomposition components, a similar shape of the components, a slight change in the shape of the spectra with large changes in drift parameters, or an almost identical change in the shape of the spectra with changes in various drift parameters). When the "**Independent drift of the components**" checkbox is selected, it is recommended to set the damping coefficient to at least 10%.

The "**Parameters 2**" page may look like:


Decomposition template: Radon_Flux

Preprocessing batch file: RadonBgd.cmd

Processing mode

☐ Preliminary subtract the continuous scattering spectrum

☑ Subtract the background

☑ Use the background from the measurement archive

☐ Windows method

☑ Use peak spectra as components

☐ Unaccounted components are present in spectrum

Spline rank: 2

☐ Negative activity values are allowed

The length of the spline segment: 5 FWHM

☑ Robust estimation

☐ One spline for the entire energy range

The boundaries of LSM estimation: 4 RMSD

Ignore peaks with errors in determining the area of more than: 200 %

Additional parameters

☐ Use marked channels as borders

☐ Add components that have lines near the marker to the components list

☑ Automatic analysis of the composition

☐ without operator intervention

The required level of the correlation coefficient for the inclusion of the component (more than): 50 %

Nuclides table: Nuclides\LongLive.ncl

If the **Preprocessing batch file** is specified, the processing program will call the external procedure specified in the command file after calculating the spectra of the decomposition components, but before the start of the spectrum decomposition procedure into components and wait for the end of the external procedure.

The command file can control the operation of external equipment, for example, run an automatic sample changer or run a program that preprocesses spectra.

The standard version of the "SPECTRRAD" software package includes two command files **RadonBgd.cmd** and **CtrlBgd.cmd**, which are used to calculate the background spectrum when measuring radon on coal adsorbers and monitoring residual radon in activated carbon (see "Radon measurement, background spectrum preprocessing").

In the second group, the operator can set various **processing modes** by setting the appropriate "checkboxes":

- **Preliminary subtract the continuous scattering spectrum** – for gamma spectra, when the check mark is set, the continuous scattering spectrum (the spectrum of Compton scattering of gamma quanta and the spectrum of bremsstrahlung X-ray emission of beta particles) is preliminarily subtracted from the measured spectrum. The peak spectrum is decomposed into the peak spectra of the components. For resolved linear spectra, this is the default mode.
- **Subtract the background** – when the check mark is set, the list of decomposition components will be supplemented with a background spectrum. In this case, the background spectrum is considered as a component of decomposition with a known

intensity, but with unknown energy drift parameters (if the energy drift parameter estimation mode is set).

- **Use the background from the measurement archive** – when the check mark is set, when processing spectra stored in the archive, the background saved for this spectrum in the archive is also used. The background for this sample is archived during the first processing of the sample spectrum. Since the background for some types of measurements (for example, when measuring radon on coal adsorbers) can vary greatly, using the current background when re-processing samples measured earlier may lead to incorrect results. If unchecked, the current background (accumulated recently) will be used.
- **Windows method** - spectrum decomposition is not channel-by-channel, but with preliminary integration of spectra in specified energy windows. In the spectrum processing mode with peak search, windows are formed automatically in accordance with the nuclides defined in the spectrum and the nuclide table used. To process continuous or poorly resolved spectra, windows must be set on the "**Windows settings**" page. The method works well when processing resolved linear spectra. For scintillation gamma spectrometry this method can be recommended when decomposition procedure use as components spectra generated according to the nuclides table (generation flaws are hidden in the integral windows). In principle, the method is not recommended for scintillation spectrometry, since it does not provide advantages, and losses in the effectiveness of estimates are obvious - pre-integration violates the condition of the Gauss-Markov theorem on effective estimates.
- **Use peak spectra as components** are a mode for gamma spectra when it is difficult or impossible to correctly separate the peak spectrum from the continuous scattering spectrum in the processed spectrum. When the check mark is set, the program calculates peak spectra as decomposition components for nuclides marked in the "**Additional:**" list on the "**Components**" page (elementary spectra without a continuous scattering spectrum). And decomposes the measured spectrum into elementary nuclide spectra marked in the "**Basic:**" list, which may include both the continuous scattering spectrum and peak spectra for nuclides marked in the second list, the background spectrum and a spline approximating the continuous scattering spectrum. Peak spectra are much easier to calculate taking into account the absorption of gamma quanta in the counting sample material, medium, protection and container. Peak spectra can be calculated if the recording efficiency of the spectrometer has been calibrated. The method can also be used for well-resolved gamma spectra.
- **Spline rank** is a parameter related to the degree of polynomials in the spline and the procedure for subsequent processing of the spline. When the rank is set to zero, one, or two, a piecewise linear approximation is performed. Since the function is not smooth in this case, after being constructed with a rank greater than zero, it is smoothed by the number of points corresponding to the half-width of the peak (the rank equal to one) or approximated by a cubic spline (with a rank equal to two). When setting a rank equal to three, a parabolic spline is constructed, and with a rank equal to four– a cubic spline is constructed. The higher the degree of the polynomial, the more flexible the spline is and the less conditioned the system of equations is.
- **One spline for the entire energy range** – when the checkbox is selected, the entire spectrum processing range will be one energy window and will be approximated by one continuous spline, otherwise a number of splines approximating areas not separated by unused energy windows. In this case, the assessment of activities and the calculation of residuals are performed using the entire energy interval without taking into account energy windows, which are visualized only for informational purposes.
- **The length of the spline segment** is an additional parameter for the modes of the decomposition using spline. The value is set in the half–widths of the peaks (more precisely, in the values of the full width of the peaks at half the height **- FWHM**). The shorter the spline segment, the more flexible and less stable the spline is. When the

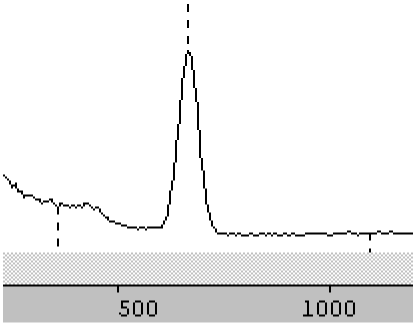
length of the spline segment is set to exceed the length of the processed part of the spectrum, the spline degenerates into a polynomial.

- **Ignore peaks with errors in determining the area of more than nnn%** – the parameter that is used when decomposing the spectrum into peak spectra (the "**Preliminary subtract the continuous scattering spectrum**" or "**Use peak spectra as components**" checkbox is selected). In this case, the processing procedure will ignore the lines that form peaks with relative errors in determining the area above a given level. The level is set as a percentage. As a result, the spectrum is more correctly marked up into "**significant**" and "**insignificant**" windows, since the large number of lines used makes such marking difficult. Such line filtering is performed after the initial assessment of the nuclide activities, since the contribution of the line to the spectrum can be estimated only by knowing the activity of the nuclide.
- **Unaccounted components are present in spectrum -** a mode in which the program, at a deviation level exceeding a specified threshold, tries to minimize the distance between the sample spectrum and the model by supplementing the model with a spline and suppressing negative residuals (it is assumed that there cannot be negative activities), if the "**Negative activity values are allowed**" checkbox is not selected. The most optimal processing mode is for a pre-known situation about the presence of nuclides in the spectrum that are not included in the list of components.
- **Negative activity values are allowed -** in normal mode (the flag is not set), the program suppresses negative activity values, but in order to verify the correctness of estimates of activity values by the program for samples with a known nuclide composition, or when using a non-orthogonal set of components (components contain, in some ratios, each other), it is required to allow the use of negative activity values - check the box.
- **Robust estimation** – setting a check mark enables the mode of noise-resistant Huber type estimation. **The boundaries of LSM estimation *n* RSMD -** the boundaries of the LSM estimation in terms of standard deviations determine the range of the LSM estimation. Beyond the boundaries of the range, the evaluation is performed using the method of least modules. If the check mark is unchecked, the least squares method (LSM estimation) is used to evaluate the parameters.

Different combinations of the included procedures and processing modes form different processing methods. For example:

- **Linear estimation** (none of the procedures are included) is a linear assessment of the contributions of the decomposition components to the sample spectrum. The most stable decomposition procedure. It is used when the matrix of elementary spectra is poorly conditioned (a large number of poorly resolved scintillation gamma spectra, decomposition of beta spectra without a priori data).
- **Drift correction** (the boxes for correction of the gain factor and/or zero of the scale, resolution of the spectrometer and/or nonlinear distortions of energy drift are set) - in addition to estimating the intensities of the components, the program determines the parameters of the energy drift of the spectrometric tract. Correction of energy drift works perfectly with the decomposition of gamma and alpha spectra. For beta spectra, it is recommended to use drift correction when including a priori data in the processing process.
- **Drift correction+Unaccounted components -** (drift correction procedures and evaluation of unaccounted components are included) is a mode in which the program, if the linear decomposition fails, tries to correct the situation by attempting to **correct the energy drift**, and in case of failure, by enabling the "**Unaccounted components are present in spectrum**" method.

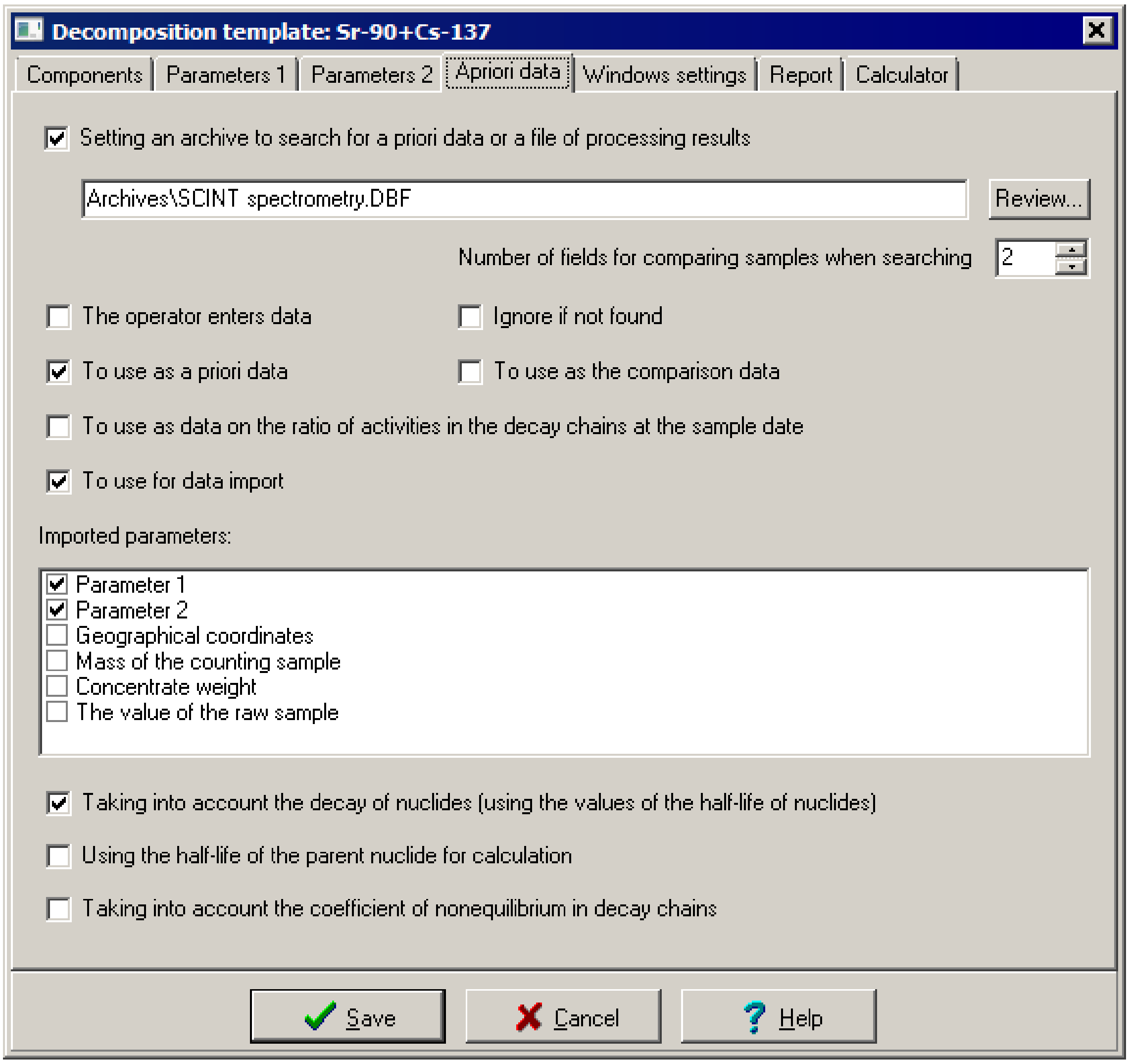
Additional parameters:

- The "**Use marked channels as borders**" checkbox allows you to change the spectrum processing area without changing the template. When the check box is selected, the operator must mark the spectrum processing area before starting the decomposition procedure (for example, as in the picture ), the "**Processing boundaries**" parameters in this case serve as the extreme values of the possible range of the processing area.
- The "**Add components that have lines near the marker to the components list**" checkbox allows you to include nuclides that have lines in the marker area in the component list. When the checkbox is selected, the program searches the table of lines and supplements the list of components with nuclides that have significant lines (lines marked with the attributes "Significant line") in the energy range **Em-FWHM(Em) < E < Em+FWHM(Em)** (here: **Em** is the energy of the marker, **FWHM(Em)** is the peak width for **Em** energy). Previously, the operator must set a marker on the analyzed peak. The mode is allowed if the peak width has been calibrated.
- It is recommended to set the "**Automatic analysis of the composition**" checkbox only for linear spectra (when installing the spectrometer, the linear type of spectra is specified). When the check box is selected, the program supplements the list of components specified by the operator with an additional list of nuclides from the specified **library of nuclides** having lines falling into the peak regions of the spectrum.
- When the "**Automatic analysis of the composition**" mode is set, the operator can select the additional "**without operator intervention**" checkbox. In this case, the program will not offer the operator to correct the list of suspected nuclides, but will immediately proceed to the procedure of spectrum decomposition into spectra of suspected components.
- **Required level of correlation coefficient to include a component (more than) nnn %** - when the automatic composition analysis mode is set and the list of components is supplemented with nuclides with "significant" lines, determines the level of the correlation coefficient (**Test1**) used for nuclide rejection. Nuclides with a **Test1** value less than the specified level will be excluded from the list of "suspected" nuclides.

Nuclides table - the nuclide table used in this processing mode. The nuclide library defines a set of additional nuclides on the "**Components**" page. The Review... key is an overview of existing nuclide tables.

The mode of using **a priori data** allows you to take into account the results of processing spectra of samples from the same material measured on different spectrometers or at different times (taking into account the results of processing gamma spectra when processing beta spectra, the results of processing the "hard" region of the spectrum when processing "soft", etc.).

The "**Apriory data**" page may look like:



☑ Setting an archive to search for a priori data or a file of processing results

Archives\SCINT spectrometry.DBF

Number of fields for comparing samples when searching: 2

☐ The operator enters data

☐ Ignore if not found

☑ To use as a priori data

☐ To use as the comparison data

☐ To use as data on the ratio of activities in the decay chains at the sample date

☑ To use for data import

Imported parameters:

- ☑ Parameter 1
- ☑ Parameter 2
- ☐ Geographical coordinates
- ☐ Mass of the counting sample
- ☐ Concentrate weight
- ☐ The value of the raw sample

☑ Taking into account the decay of nuclides (using the values of the half-life of nuclides)

☐ Using the half-life of the parent nuclide for calculation

☐ Taking into account the coefficient of nonequilibrium in decay chains

When checking the boxes "**To use as a priori data**", "**To use as the comparison data**", "**To use as data on ratio of activities in the decay chain at the sample date**" and (or) "**To use for data import**", the program will either request from the operator or find data in the measurement archive that will be used in spectrum processing.

If the "**To use as a priori data**" checkbox is selected, the data will be used to calculate the activities of the nuclides being determined in accordance with the Bayesian estimation method.

The **comparison data** is used in the formation of verification protocols and the creation of Shewhart control charts.

Data on ratio of activities in the decay chain at the sample date are used if the decomposition components contain nuclides that are part of the decay chain. Accounting for the ratios of nuclide activities in decay chains differs depending on whether a group of spectra is being processed together or a single spectrum is being processed. When processing a group of spectra, the data on this ratio is recalculated as of the date of measurement of each spectrum of the group, the list of decomposition components does not change. When processing one spectrum for each chain of nuclides, only one elementary spectrum of the parent nuclide is calculated, including the radiation of all daughter nuclides in accordance with the ratio of activities established in the chain at the date of sample measurement. The daughter nuclides of the chains are excluded from the list of components (their radiation is included in the parent nuclide), which significantly increases the evaluation efficiency.

When the "**To use for data import**" checkbox is selected, the selected data from the a priori results file from the **imported parameters** list will be transferred to the processing procedure before processing begins (before calculating the decomposition components), since such a parameter as the mass of the counting sample affects radiation absorption and must be taken into account when calculating the decomposition components. And in such devices, for example, as core analyzers in geology, the core density is determined on a separate channel of the spectrometer and it must be taken into account before processing the spectrum of the sample measured on the main channel of the analyzer.

A priori data, comparison data and imported data are available through predefined variables of the programmable calculator.

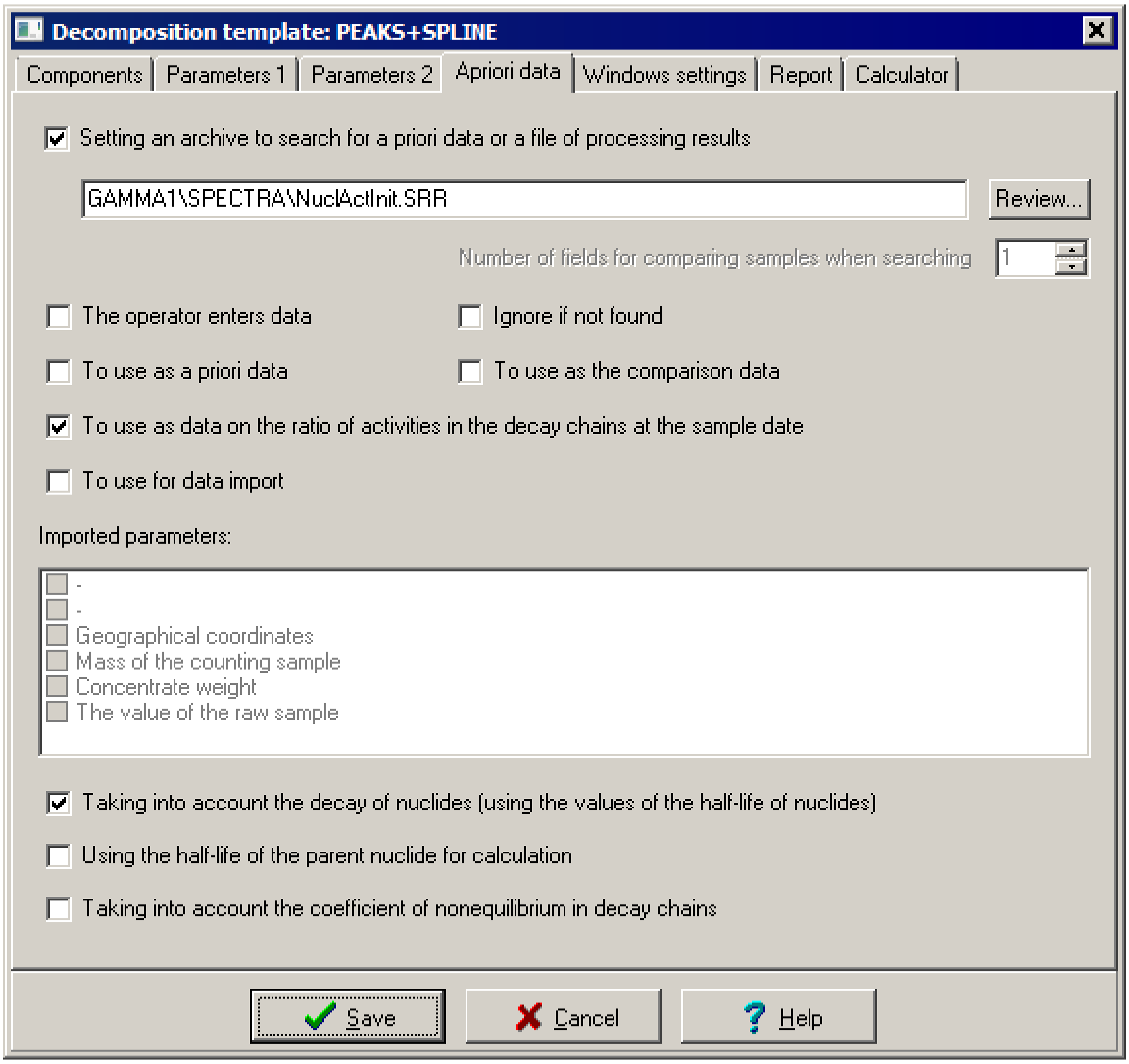
The operator can select a priori results (comparison data, data on ratio of activities in the decay chain at the sample date) from the measurement archive or enter them manually during spectrum processing (when the "**The operator enters data**" checkbox is selected).

The program can search for the necessary data in the measurement archive itself. To do this, select the checkbox "**Setting an archive to search for a priory data or a file of processing result**", specify the full path to the desired archive of measurements to search for records and set the **number of fields for comparing samples when searching** in the archive. When searching for data in the archive, the program searches from the end of the specified archive and uses the first found processing results as a priori data, which have data matching the processed spectrum by sample type and by a specified number of fields out of seven fields of the sample description: "Sample code", "Sample name", "Sample note", "Producer", "Applicant", "Sampling place" and "Comment" (the initial names of the archive columns are indicated). The comparison by the "Sample type" field is performed in any case.

Data on the rate of decay of nuclides make it possible to recalculate the activities of nuclides at a given date, increase the efficiency of activity estimates when setting the initial activity ratios at the sample date and when processing a group of spectra together. The accounting mode is set by setting a "check mark" in the item "**Taking into account the decay of nuclides (using the values of the half-life of nuclides)**)". In the event that only single nuclides and equilibrium chains of nuclides are used in the decomposition components, it is recommended to check the box "**Using the half-life of the parent nuclide for calculation** ". This reduces the amount of calculations and, accordingly, increases the processing speed.

By checking the box "**Taking into account the coefficient of nonequilibrium in decay chains**", it is possible to take into account the imbalance in the decay chain that is not taken into account when calculating equilibrium chains (emanation, leaching of nuclides, etc.), if the activity of a nuclide is determined by the radiation of another nuclide of the equilibrium chain. In this case, the activity of the nuclide is calculated taking into account the coefficient of nonequilibrium. The coefficient of nonequilibrium is related to the type of sample and is given as "**Kneq.(Norm 5)**" when forming standards and constants for the selected type of sample and a specific nuclide (menu item " **Tools/Norms and materials...**").

If you have to regularly use the same comparison data or a priori data, for example, when checking a spectrometer, you can save the a priori data under some name (menu item "**File / Save as...**"), and in the processing template, check the box "**Setting an archive to search for a priori data or a processing result file**" and specify the full path to the saved file with a priori data (the file type of a priori data coincides with the file type of processing results – "**.SRR**"). In this case, the form may look like:



☑ Setting an archive to search for a priori data or a file of processing results

GAMMA1\SPECTRA\NuclActInit.SRR

Number of fields for comparing samples when searching 1

☐ The operator enters data

☐ Ignore if not found

☐ To use as a priori data

☐ To use as the comparison data

☑ To use as data on the ratio of activities in the decay chains at the sample date

☐ To use for data import

Imported parameters:

☐ -
☐ -
☐ Geographical coordinates
☐ Mass of the counting sample
☐ Concentrate weight
☐ The value of the raw sample

☑ Taking into account the decay of nuclides (using the values of the half-life of nuclides)

☐ Using the half-life of the parent nuclide for calculation

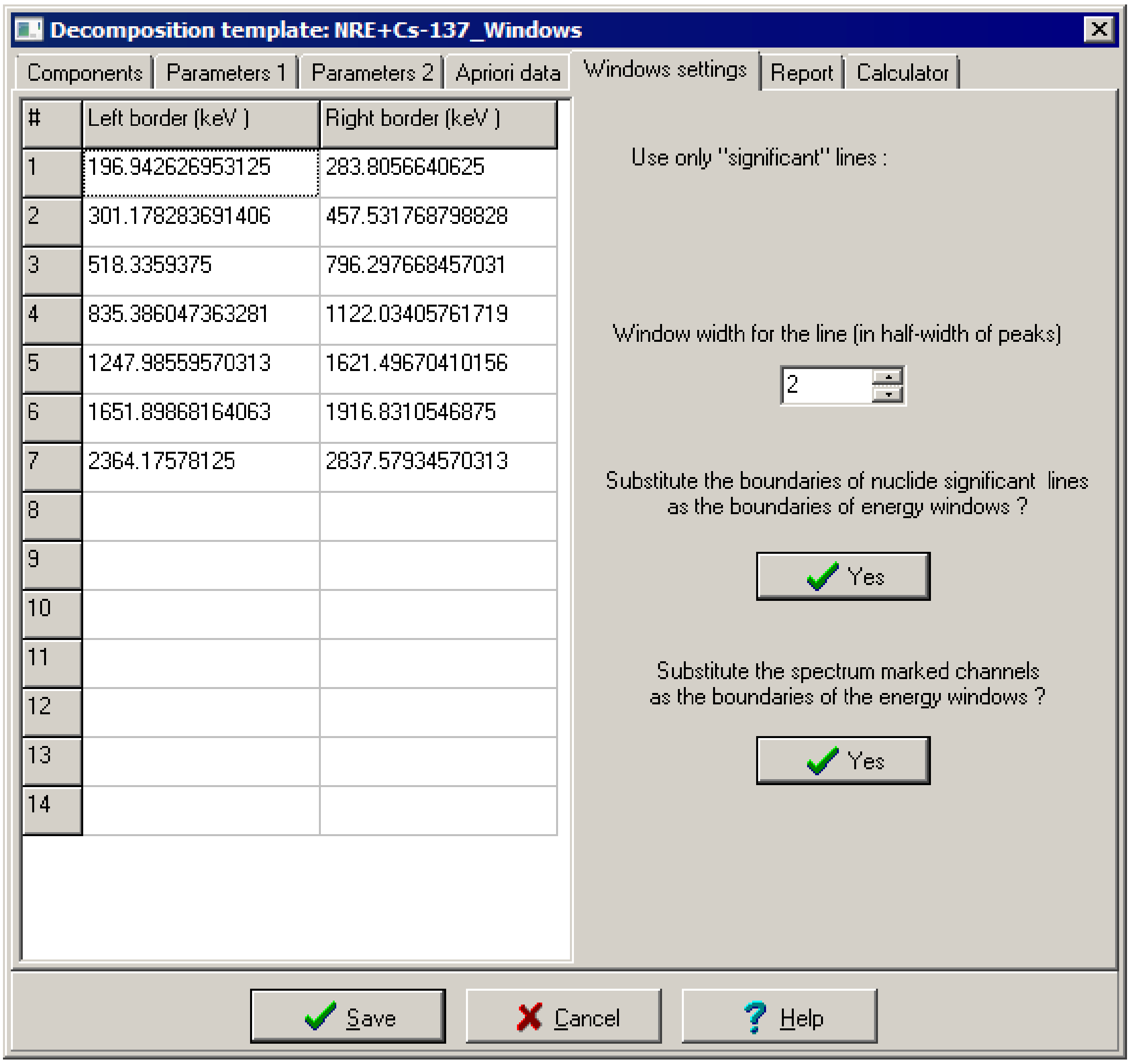
☐ Taking into account the coefficient of nonequilibrium in decay chains

The "**Review...**" key allows you to find the necessary archive file or the results of spectrum processing.

In the event that a priori data are not found in the search mode, or the archive file for searching for a priori data is not specified, the program will prompt the operator to find them itself or enter them manually if the "**Ignore if not found**" checkbox is not selected.

It should be borne in mind that the program recalculates the activity values by the value of the initial sample material. This allows you to use the measurement results of native samples when processing counting samples from a concentrated substance, but it can serve as a source of errors if the operator forgot to indicate that one of the samples is concentrated or the nuclide composition of the sample has changed as a result of concentration.

When processing continuous or poorly resolved spectra, the "**Widows settings**" page is used in the window processing mode (**Windows method**) to set energy windows.



#	Left border (keV)	Right border (keV)
1	196.942626953125	283.8056640625
2	301.178283691406	457.531768798828
3	518.3359375	796.297668457031
4	835.386047363281	1122.03405761719
5	1247.98559570313	1621.49670410156
6	1651.89868164063	1916.8310546875
7	2364.17578125	2837.57934570313
8		
9		
10		
11		
12		
13		
14		

Use only "significant" lines :

Window width for the line (in half-width of peaks) 2

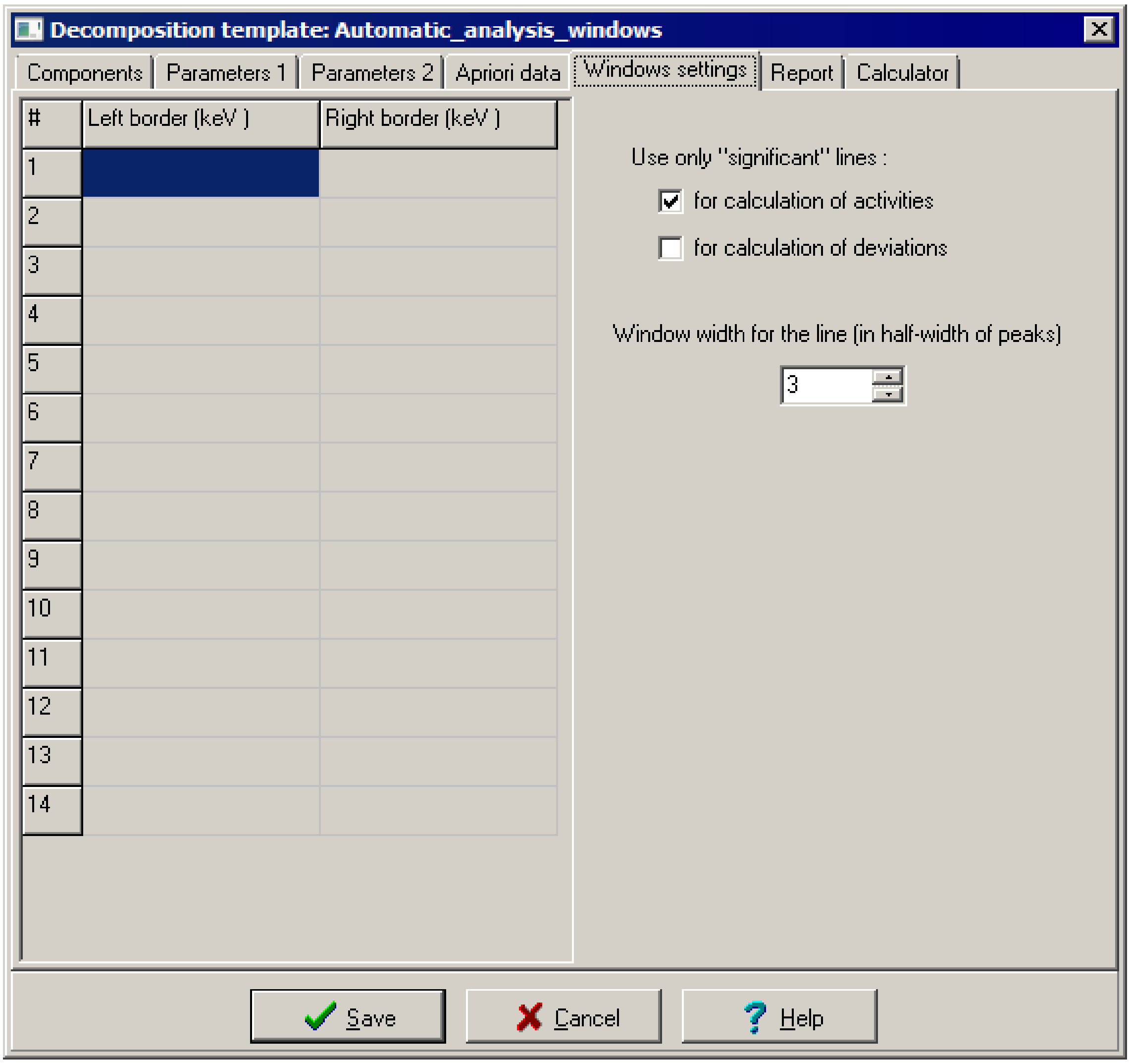
Substitute the boundaries of nuclide significant lines as the boundaries of energy windows ?

Substitute the spectrum marked channels as the boundaries of the energy windows ?

The operator has the opportunity to set the energy boundaries of the windows or substitute as such boundaries the energy boundaries of the significant nuclide lines of the decomposition components used (for gamma and alpha spectra), or the marked channels of the spectrum, by clicking on the appropriate key ✓ Yes. When defining window boundaries by nuclide lines, the operator must set the **window width for the line** in the values of the width of peaks at half height (**in half width of peaks**). A total of 14 windows can be defined. The window borders should increase sequentially. The right border of the window may coincide with the left border of the next window. Keep in mind that the number of windows cannot be less than the number of components being defined. The most characteristic regions in the component spectra are used as windows.

Right-clicking on the window number causes a pop-up menu: Delete window Insert window which allows you to either delete the selected energy window, or insert a new one in place of the current window by moving the windows down in the table.

When decomposing linear spectra into peak spectra, windows are formed automatically in accordance with the assumed nuclide composition of the spectrum, and the page is used to set the parameters of the window formation mode, if the operator has not set the mode of one energy window (**One spline for the entire energy range**).



#	Left border (keV)	Right border (keV)
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
11		
12		
13		
14		

Use only "significant" lines :

☑ for calculation of activities

☐ for calculation of deviations

Window width for the line (in half-width of peaks)

3

The operator must set the width of the windows in the values of the peak widths - the parameter "**Window width for the line (in half width of peaks)**" (the term "**half width**" is used - the width of the peak at half height) and specify all nuclide lines or only those marked as "**significan**t" will be used to form windows and, accordingly, for calculation of nuclide activities and partial residuals when setting the appropriate checkboxes.

Radon measurement, background spectrum preprocessing

When measuring the volumetric concentration of radon-222 in the air or radon fluxes using techniques based on radon adsorption on activated carbon, activated carbon is measured from several adsorbers (coal containers). Radon measurement can be performed for different amounts of activated carbon adsorbers (different amounts of activated carbon). This requires recalculation by the amount of coal and the radon elementary spectrum and background spectrum. Background spectrum recalculation is required because coal (fresh or after regeneration) contains residual radon-222 before the start of measurements and may contain some amount of cesium-137 and potassium-40. The elementary spectrum of Rn-222 remains unchanged, but the background changes both due to the deterioration of coal characteristics and due to its variability for a number of reasons.

The background spectrum should, under the standard procedure for calculating the background spectrum, be measured separately for each number of adsorbers used, which would lead to a significant increase in analysis time.

As part of the "SPECTRRAD" package there is a program **RadBgd.exe**, which allows calculating the background spectrum for a specific number of adsorbers. The calculation is performed as follows:

- the "pure" background spectrum is subtracted from the background spectrum measured for a given (maximum) number of adsorbers;
- the remainder is normalized to a given (maximum) number of adsorbers;
- multiplied by the number of adsorbers in the sample spectrum;
- complemented by a "pure" background spectrum (background spectrum without carbon adsorbers).

The program must contain five parameters when called:
RadBgd "Back0" "BackAdsElem" "BackAdsComp" nAdsSample nAsdsBgd.

Here:

Back0 is the address of the background file without coal. The file path may not contain the path to the spectrometer folder. For example: "**CS\ELEMENTS\backgr.srs**"
BackAdsElem is the path to the charcoal background file. For example: "**IC-63\ELEMENTS\backgr.srs**"
BackAdsComp is the path to the file of the calculated background spectrum in the "**Comp**" folder (the "Comp" folder contains files used in spectrum processing). For example: "**IC-63-63\COMP\backgr.srs**"
nAdsSample is the number of adsorbers in the measured sample.
nAdsBgd is the number of adsorbers for the background with coal.

The background spectrum calculation program can be called from the processing procedure either by including the program call string with the necessary parameters in the **Preprocessing batch file** in the parameters of the decomposition template, or by including a command file (a text file with the extension "**cmd**") containing the **RadBgd.exe** program call with the required parameters.

When the "SPECTRRAD" package is running, the "working" folder (the folder in which data and program files are searched if the full path is not specified in the file address) is the head folder of the "SPECTRRAD" software package, but for the preprocessing batch file, the "working" folder is assigned to the folder of the corresponding spectrometer. Therefore, it is recommended to place the preprocessing command files in the spectrometer folders.

When calling the **RadBgd.exe** program from the decomposition procedure, a number of call string parameters can be omitted:

- **BackAdsComp** – if the address of the background spectrum calculation result is omitted, the calculated background spectrum will be recorded in the "**Comp**" folder, designed to save all the spectra used in processing.
- **nAdsSample** – if there is no parameter for the number of adsorbers (amount of coal) in the sample spectrum, it will be taken from the parameter "**Parameter 1**" of the sample spectrum.
- **nAsdsBgd** – if there is no number of adsorbers (amount of coal) in the background spectrum of adsorbers with coal, it will be taken from the parameter "**Parameter 1**" of the background spectrum of adsorbers with coal**.**

In the standard delivery version, the "SPECTRRAD" software package contains two command files:

- **RadonBgd.cmd**, which contains the string **RadBgd "CS\ELEMENTS\backgr.srs" "IC-63\COMP\backgr.srs"**.
  The **RadonBgd.cmd** command file is used to calculate the background spectrum when processing activated carbon spectra after exposure (to calculate the volumetric activity of radon in the air or radon fluxes). The entry stands for as follows: the pure background (without coal) **backgr.srs** is taken from the **ELEMENTS** folder of the **CS** geometry, the background with coal **backgr.srs** is taken from the **COMP** folder of the **IC-63** geometry, the number of adsorbers is not set, so it is taken from the **Parameter 1** of the sample spectra and the background with coal. Before the procedure starts, the background spectrum in the **IC-63\COMP** folder is either a copy of the background spectrum in the

IC-63\ELEMENTS folder (the file of the current background spectrum with coal), or a copy of the background spectrum with coal from the measurement archive, if the "**Use the background from the measurement archive**" mode is set in the decomposition parameters.

- **CtrlBgd.cmd** – contains the string **RadBgd "CS\ELEMENTS\backgr.srs" "IC-63\COMP\backgr.srs" "IC-63\COMP\backgr.srs" 0**.
  The **CtrlBgd.cmd** command file is used to calculate the background spectrum for the coal quality control procedure. Since the value "**0**" is set as the amount of activated carbon in the spectrum, the "pure" background spectrum will be calculated.

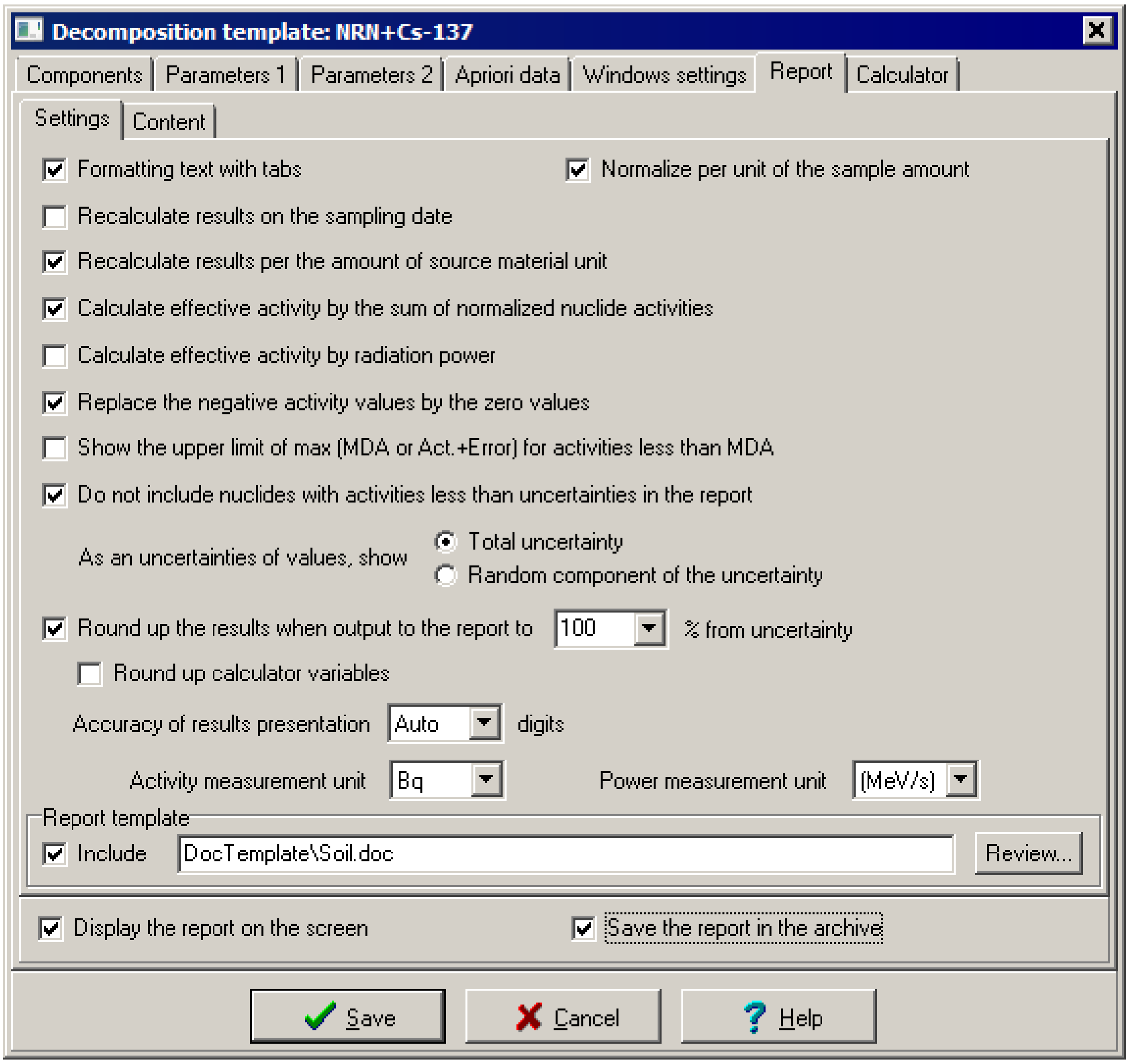
To use the supplied command files, the operator needs to edit them in accordance with the actual addresses of the background spectra without coal and with coal (it is necessary to replace the names of geometries (**CS**, **IC-63**) with real ones in the call strings).

Customizing a decomposition report

In the "SpectrRad" package, the operator has the ability to create any form of measurement results reports. The principle of forming a report is that data on the results of processing, sample, measuring instrument, regulatory documentation, etc. can be included in a pre-generated document (report template). The selection of the desired report template can be made by the calculator program, depending on the group to which the sample type belongs (for example, for the "Products" group one form of the template, and for the "Soils" group another) and on the result of spectrum processing (compliance or non-compliance with any standards).

Of course, for a lazy user, a report can be generated without a report template, but, nevertheless, in this case, it remains possible to specify its content and form.

The "**Report**" page contains two bookmarks: "**Settings**" and "**Content**".



☑ Formatting text with tabs
☑ Normalize per unit of the sample amount
☐ Recalculate results on the sampling date
☑ Recalculate results per the amount of source material unit
☑ Calculate effective activity by the sum of normalized nuclide activities
☐ Calculate effective activity by radiation power
☑ Replace the negative activity values by the zero values
☐ Show the upper limit of max (MDA or Act.+Error) for activities less than MDA
☑ Do not include nuclides with activities less than uncertainties in the report

As an uncertainties of values, show
● Total uncertainty
○ Random component of the uncertainty

☑ Round up the results when output to the report to 100 % from uncertainty
☐ Round up calculator variables

Accuracy of results presentation Auto digits

Activity measurement unit Bq
Power measurement unit (MeV/s)

Report template
☑ Include DocTemplate\Soil.doc Review...

☑ Display the report on the screen
☑ Save the report in the archive

On the first tab there are a number of parameters that define the form of the report:

- **Formatting text with tabs** – when the checkbox is selected, the procedure for generating a report before each new paragraph of text containing descriptions of the sample, spectrometer, and measurement conditions will include a tab character to align the text with the first tab position (the position of the "red" line).
- The "**Normalize per unit of the sample amount**" checkbox determines the type of representation of nuclide activity in the report. The type of representation depends on the type of geometry. For measurement geometries in the "thin" and intermediate layers, the total activity if unchecked, the specific activity if checked. For measurement geometries in the "thick" layer, the inverse relationship is: the checkbox is not selected - specific activity, the checkbox is selected - the total activity of nuclides in the counting sample.

- **Recalculate results on the sampling date** – if the "tick" is set, the nuclide activity will be recalculated on the date of sampling, otherwise – on the date of the beginning of measurements.
- The "**Recalculate results per amount of source material unit**" checkbox allows you to report nuclide activities in raw material calculated from nuclide activities in concentrated (or diluted) counting samples.
- **Calculate effective activity by the sum of normalized nuclide activities**. When you check the box, the report will show the total effective gamma activity of the sample. The activity of nuclides equivalent to the activity of Ra-226 is considered to be effective. The calculation program takes data on the equivalence coefficients for nuclides from the working library of nuclides and, if the gamma coefficient of the Ra-226 equivalent for a nuclide is different from zero, the contribution of the nuclide to the total effective activity of the sample will be taken into account. It should be borne in mind that such a calculation of effective activity for a standard set of coefficients (three coefficients: 1 for Ra–226, 1.3 for Th-232 and 0.09 for K–40) will be correct only if only K-40, Ra–226 and Th-232 are present in the sample in a state of radioactive equilibrium with daughter nuclides.
- **Calculate effective activity by radiation power** – when the "tick" is set, the program calculates the total effective activity by the power of alpha, beta or gamma radiation in comparison with the power of the selected type of radiation of 1 Bq of the specified comparison nuclide.
- **Replace the negative activity values by zero values** – in the event that negative activity values are allowed during spectrum processing, when the "check mark" is set, the negative activity values in the report will be replaced with zero. It should be understood that banning negative values in spectrum processing is not at all equivalent to replacing negative activity values with zero ones - banning negative values in spectrum processing protects against blunders with incomplete or incorrect spectrum model, but does not allow for full-fledged statistical processing of measurement results.
- The "**Show the upper limit of max(MDA or Act+Error) for activities less than MDA**" checkbox sets the form of output of results in the report for values with activity estimates less than the minimum detectable in accordance with ISO and IEC recommendations. For such values, the report shows either **MDA** or **Activity+Error** with a "<" sign or the word "**less**", depending on which value is greater. The **MDA** value in units of mean-square deviations is set when setting up the archive (see "Archive of measurement results". "Configuring the archive").
- If the "**Do not include nuclides with activities less than uncertainties in the report**" checkbox is selected, the report will contain entries only for nuclides with a relative error of determining activity of less than 100%.
- As an uncertainty of values, show "**Total uncertainty**" or "**Random component of the uncertainty**" **-** the operator is given a choice of one of two options for presenting the error in the report. If you select a random error component, the activity table in the report will be displayed in blue font.
- **Round up the results when output to the report to *nn* % from uncertainty** – setting the mode and form of rounding estimates of nuclide activities in the report. When 100% rounding is set, the values of activities and errors in the report will be given in accordance with the requirements of MI 2453-2000. If the list of nuclides to be determined is formed by automatic composition determination procedures, turning on/off the rounding results mode and rounding accuracy also affect the list of nuclides that will be shown in the report. When the rounding mode is turned off, the entire list of nuclides is shown, when turned on, only those nuclides added by the automatic composition determination procedures, the relative error in determining the activity of which is less than a certain level associated with the rounding accuracy.
- **Round up calculator variables** – when the checkbox is selected, the variables of the programmable calculator will also be rounded when output to the report. Since the

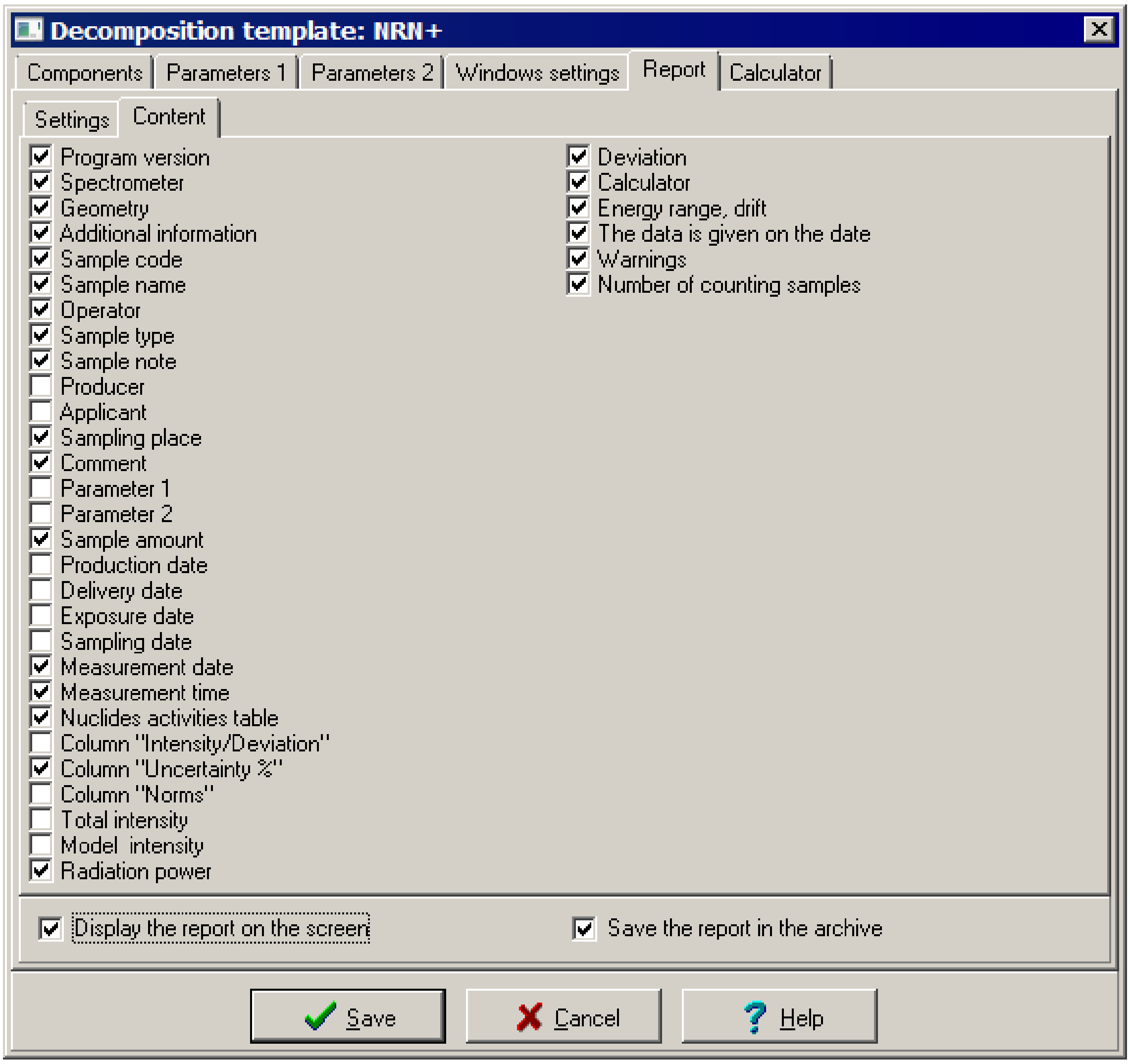
rounding procedure in this case has no information about the error of the rounded value, the value of the value will be rounded with a relative accuracy of 10% of the specified rounding accuracy. For example, if 100% rounding is set and the value of the value is 353.265, and then this value will be rounded to 10% accuracy in the report and presented as 350. For correct rounding of the values calculated in the calculator, it is necessary to use the rounding functions existing in the calculator.

- **Accuracy of results presentations** – select the number of digits to represent the results in the report. The value "**Auto**" corresponds to the automatic determination of the required accuracy of the presentation of the results. In this case, insignificant zeros are not output.
- **Activity measurement unit** – select the unit of measurement of activity (Becquerel or Curie) or content (grams) in which the activity (content) of nuclides in the sample will be shown in the report.
- **Power measurement unit** – select the unit of measurement of the radiation power from the sample calculated by the procedure (keV/s, MeV/s, mcW or W) in which the power will be shown in the report. The radiation power is calculated within the selected energy range.

Report template - the operator, if desired, can specify the report template file. The file must contain the template text saved in RTF format or as a Word document (DOC). The report template in the form of a Word document has much more formatting options. The disadvantage of such a template is that the report is created in the Word program and the "SpectrRad" program cannot track all the actions of the operator in another program. An RTF template can contain formatted text including drawings, but, of course, not all Microsoft Word features are supported ("Framing", inserting a frame, columns, etc., etc. are not supported).

The Review... button is an overview of existing report templates.

The "**Content**" table allows you to set the rows and columns of the output form for the results of spectrum processing, which will be shown in the report.



☑ Program version
☑ Spectrometer
☑ Geometry
☑ Additional information
☑ Sample code
☑ Sample name
☑ Operator
☑ Sample type
☑ Sample note
☐ Producer
☐ Applicant
☑ Sampling place
☑ Comment
☐ Parameter 1
☐ Parameter 2
☑ Sample amount
☐ Production date
☐ Delivery date
☐ Exposure date
☐ Sampling date
☑ Measurement date
☑ Measurement time
☑ Nuclides activities table
☐ Column "Intensity/Deviation"
☑ Column "Uncertainty %"
☐ Column "Norms"
☐ Total intensity
☐ Model intensity
☑ Radiation power
☑ Deviation
☑ Calculator
☑ Energy range, drift
☑ The data is given on the date
☑ Warnings
☑ Number of counting samples

☑ Display the report on the screen
☑ Save the report in the archive

When the "**Display the report on the screen**" checkbox is selected in the normal spectrum processing mode, the report window is displayed on the display screen. In the spectrum processing mode, while monitoring the spectrum acquisition the report is displayed in the upper-right corner of the main window of the SPECTRRAD program, regardless of whether the checkbox is selected.

The checkbox in the "**Save the report in the archive**" column allows you to save the report in the archive at the end of the spectrum processing procedure. For cyclic measurements, the spectrum, along with the processing results, if spectrum processing is ordered, is archived at the end of each cycle, regardless of whether the checkbox is selected.

Report template labels

The formation of a report in the form of an MSWord document in the "SPECTRRAD" package is based on the fact that in a pre-prepared MSWord document (the **report template**) part of the text is replaced with a specific text. Such a replaceable text is:

- Certain words enclosed in curly brackets are labels of the report template, for example **{Act[Cs–137]}**. The report template labels are used to insert sample parameters, measurement conditions, and spectrum processing results into the template text.
- An arithmetic expression consisting of numbers and labels replaced by numerical values associated with symbols of arithmetic operations and functions in accordance with the

syntax and spelling of the built-in programmable calculator, enclosed in operator brackets “~<” and “>~”, for example **~<2*({Act[Cs-137]}+{Err[Cs-137]})+100>~**

A report template can consist of two parts: general and repeatable (the repeatable part of the template may be missing). The repeatable part of the report template is enclosed in double angle brackets, for example **<<{Nucl} {Act} {Err}>>**. Both the common and repeatable parts of the report template can contain arbitrary text, including labels.

The report is generated as follows:

- All labels of the report template are replaced with data from the processing results. If the report template contains a repeatable part, the labels of the repeatable part are replaced with data for the first nuclide from the processing results table.
- The repeatable part, if present, is copied, and the labels of the repeatable part are replaced with data for the second nuclide of the table.
- The process is repeated until the end of the entries in the result table.
- Arithmetic expressions are replaced by calculated values.
- Labels containing spelling errors are removed from the text.

Using report templates that include a repeatable part is useful if the number of nuclides that will be determined in the sample is unknown in advance. This situation will happen when using processing templates that include procedures for automatic determination of the nuclide composition.

A number of labels only make sense if they are included in a repeatable part of the report template:

Label	***Description***
{SN}	The sequential number of the record in the table.
{Nucl}	The name of the nuclide for the current record.
{Act} **{Activ}**	Nuclide activity
{SAct}	The activity of the nuclide. The difference from the {Act} label is that the {Act} label can be replaced either by the activity of the nuclide or by the value of the Act.+Err. depending on the report setting, and the {SAct} label is always replaced by the nuclide activity.
{StErr}	The statistical uncertainty of estimating the activity of a given nuclide in units of activity.
{TotErr}	The total error in estimating the activity of a given nuclide in units of activity. The total error includes statistical uncertainty, the error of the measuring instrument and the measurement method.
{Err} **{AbsErr}**	The error (uncertainty) of estimating the activity of a nuclide in units of activity. The error is either complete, statistical, or absent, depending on the settings of the report form.
{SErr}	The error in estimating the activity of a given nuclide in units of activity. The error is either complete or statistical, depending on the setting of the report form, the difference from the {Err} label is the same as for the {Sact} label.

{Act&Err}	The activity and error of estimating the activity of a nuclide in the form: Act±Err (for example 125±15).
{RelErr}	The relative error in estimating the nuclide activity as a percentage.
{Mass}	The mass of the nuclide in the counting sample. For the geometry of the "thin" layer, the mass is given in kilograms, for the geometry of the "thick" layer in relative fractions of the mass of the counting sample.
{MassErr}	The error in estimating the mass of a given nuclide in units of mass.
{Norm1}-{Norm5}	Five norms for the nuclide of the current record.

Labels of the general part of the report template:

Label	***Description***
{Image}	Image of the main window of the spectrum decomposition program.
{File}	The name of the report file.
{Date}	Report creation date.
{Program}	Program version.
{DecTemplate}	The name of the processing template used.
{NuclidesTable}	The table of nuclides used in the processing.
{Analyser}	Name and description of the spectrometer. The text is copied from the description of the spectrometer entered during installation.
{AnalNick}	The short name of the spectrometer.
{Geometry}	Name and description of the measurement geometry. The text is copied from the geometry description entered when installing the geometry.
{GeomNick}	The short name of the measurement geometry.
{Info}	Information about the verification of the spectrometer. The text is copied from the column "Verification certificate" of the description of the spectrometer entered during its installation.
{AddNote}	Additional information about the spectrometer. The text is copied from the "Additional information" column of the description of the spectrometer entered during its installation.
{SampleCode}	The sample code.

{Sample}	The name of the sample.
{Operator}	Operator - the data of the operator (laboratory assistant) who carried out the measurements.
{SampleType}	The type of sample and information about the standards associated with this type of sample. Information about the standard is copied from the "Comment" column of the corresponding standard.
{SampleNote}	Description of the sample.
{Producer}	Manufacturer.
{ProductionDate}	Date of production.
{Declarant}	The applicant is an organization or an individual who has submitted an application for a sample study.
{DeliveryDate}	Delivery date.
{SampleArea}	Sampling place.
{Comment}	Note.
{Size}	Parameter 1.
{SParam}	Parameter 2.
{RawValue}	The amount of starting material used in the concentration of the sample.
{ConcMass}	The mass of the concentrate obtained by concentrating the starting material.
{ChemYield}	The yield of the released substance (%) during chemical concentration.
{SampleMass}	The mass of the counting sample.
{Weight}	The mass of the counting sample or the amount of the starting material used in the concentration of the sample, depending on how the specific activity values are presented in the processing results.
{ExposeDate}	The date of the beginning of sampling (exposure).
{SampleDate}	The end date of sampling (exposure).
{MeasDate}	The measurement start date.
{MeasEndDate}	The end date of the measurement.
{ActualDate}	The date on which the values of nuclide activities and radiation intensities are given. The date of the activity value can coincide

	either with the date of the beginning of measurements or with the date of sampling.
{MeasTime}	The duration of the measurement in seconds.
{Report}	The results of the Processing. The {Report} label is replaced by the full text of the report, which includes both a table of nuclide activities, and information about the sample, measuring instruments, etc.
{Table}	Table of nuclide activities. The activity table includes, in addition to the activities themselves, the results of the calculator program and additional information: the intensity of the model, background, deviation, energy range, number of samples, warnings about exceeding the specified control parameters.
{Calculator}	The results of the calculator program execution.
{Calc1}, {ErCalc1}... **{Calc8}, {ErCalc8}**	The values of the stored variables of the calculator program.
{Calc&Err1},… **{Calc&Err8}**	The values of the stored variables of the calculator program in the form: Calc±ErCalc (for example 125±15).
{AUnit}	The unit of the activity of nuclides.
{Nucl[i]} **{Nucl[Name]}**	The name (synonym) of the **i**-th nuclide or, alternatively, the synonym of the nuclide **Name**. **i** is the sequence number of the nuclide entry in the activity table. The numbering starts from one. For example, **{Nucl[1]}** for the list of nuclides starting with Cs-137 will be replaced by the synonym of the nuclide **Cs-137**, and **{Nucl[SumAct-G]}** with the text "**Total gamma**".
{Act[i]} **{Act[Name]}** **{Activ[i]}** **{Activ[Name]}**	The activity of the **i**–th nuclide (for example **{Act[1]}**) or in an alternative form **-** the activity of the nuclide **Name** (for example **{Act[Cs-137]}**). The names of conditional nuclides are reserved for the total activity: **SumAct-A**, **SumAct-B** and **SumAct-G** – total in alpha, beta and gamma.
{SAct[i]} **{SAct[Name]}**	The activity of the nuclide. The difference from the {Activ[]} label is that in the report, the {Activ[]} label can be replaced either by the nuclide activity or by the Act+Err value, depending on the report setting, and the {Sact[]} label is always replaced by the nuclide activity.
{StErr[i]} **{StErr[Name]}**	The statistical uncertainty of estimating the activity of a given nuclide in units of activity.
{TotErr[i]} **{TotErr[Name]}**	The total error in estimating the activity of a given nuclide in units of activity. The total error includes statistical uncertainty, the error of the measuring instrument and the measurement method.
{Err[i]}	The error (uncertainty) of estimating the activity of a nuclide in

{Err[Name]} **{AbsErr[i]}** **{AbsErr[Name]}**	units of activity. The error is either complete, statistical, or absent, depending on the settings of the report form.
{SErr[i]} **{SErr[Name]}**	The error in estimating the activity of a given nuclide in units of activity. The difference from the {Err[]} label is the same as for the {Sact[]} label.
{Act&Err[i]} **{Act&Err[Name]}**	The activity and error of estimating the activity of a nuclide in the form: Act±Err (for example 125±15).
{RelErr[i]} **{RelErr[Name]}**	The relative error in estimating the nuclide activity as a percentage.
{Mass[i]} **{Mass[Name]}**	The mass of the **i**–th nuclide in the counting sample or in an alternative form - the mass of the nuclide **Name** (for example **{Mass[Cs-137]}**). For the geometry of the "thin" layer, the mass is given in kilograms, for the geometry of the "thick" layer in relative fractions of the mass of the counting sample.
{MassErr[i]} **{MassErr[Name]}**	The error in estimating the mass of a given nuclide in units of mass.
{Norm1[i]}-{Norm5[i]} **{Norm1[Name]}-** **-{Norm5[Name]}**	Five norms for a given nuclide.
{AEff}	The total effective activity of nuclides in the sample is calculated in accordance with the values of the gamma equivalent of nuclide radiation according to Ra-226 set in the table of nuclides used in processing. Either the AEff value itself or the upper threshold (AEff+AeffErr) can be used as AEff, depending on the setting of the report parameters.
{SAEff}	The total effective activity of nuclides in the sample. The AEff value is always used directly as SAEff.
{AEffErr} **{AEffAbsErr}**	The error in estimating AEff in units of activity.
{SAEffErr}	The error in estimating AEff in units of activity. The AEff error value is always used directly as the SAEffErr.
{AEff&Err}	The activity and error of estimating the total effective activity of nuclides in the form: Act±Err (for example 125±15).
{AEffRelErr}	The relative error of the AEff estimate as a percentage.
{InputRate}	The total intensity of the radiation registered by the spectrometer in the imp./c.
{SumIntens}	The total intensity of the recorded radiation from the counting sample and the background in a given energy range in imp./c.

{BgdIntens}	The intensity of background radiation in a given energy range.
{ModelIntens}	The intensity of radiation from the nuclides of the formed model in a given energy range.
{ComptonIntens}	The intensity of the Compton scattering spectrum in a given energy range.
{RadPower}	The radiation power from the sample.
{Residuals}	Decomposition discrepancy.
{GlbResiduals}	The general discrepancy.
{EnergyPar}	The energy range used in the processing and energy drift parameters .
{Drift}	Energy drift parameters.
{Zeff}	The estimated effective Z value of the counting sample.
{NumberOfSamples}	The number of counting samples, the measurement results of which were used to generate the report.
{Warnings}	The text of messages generated by the processing procedure when the specified permissible levels of deviation, energy drift and deterioration of the resolution of the spectrometer are exceeded.
{Note}	The text of information messages generated by the processing procedure.

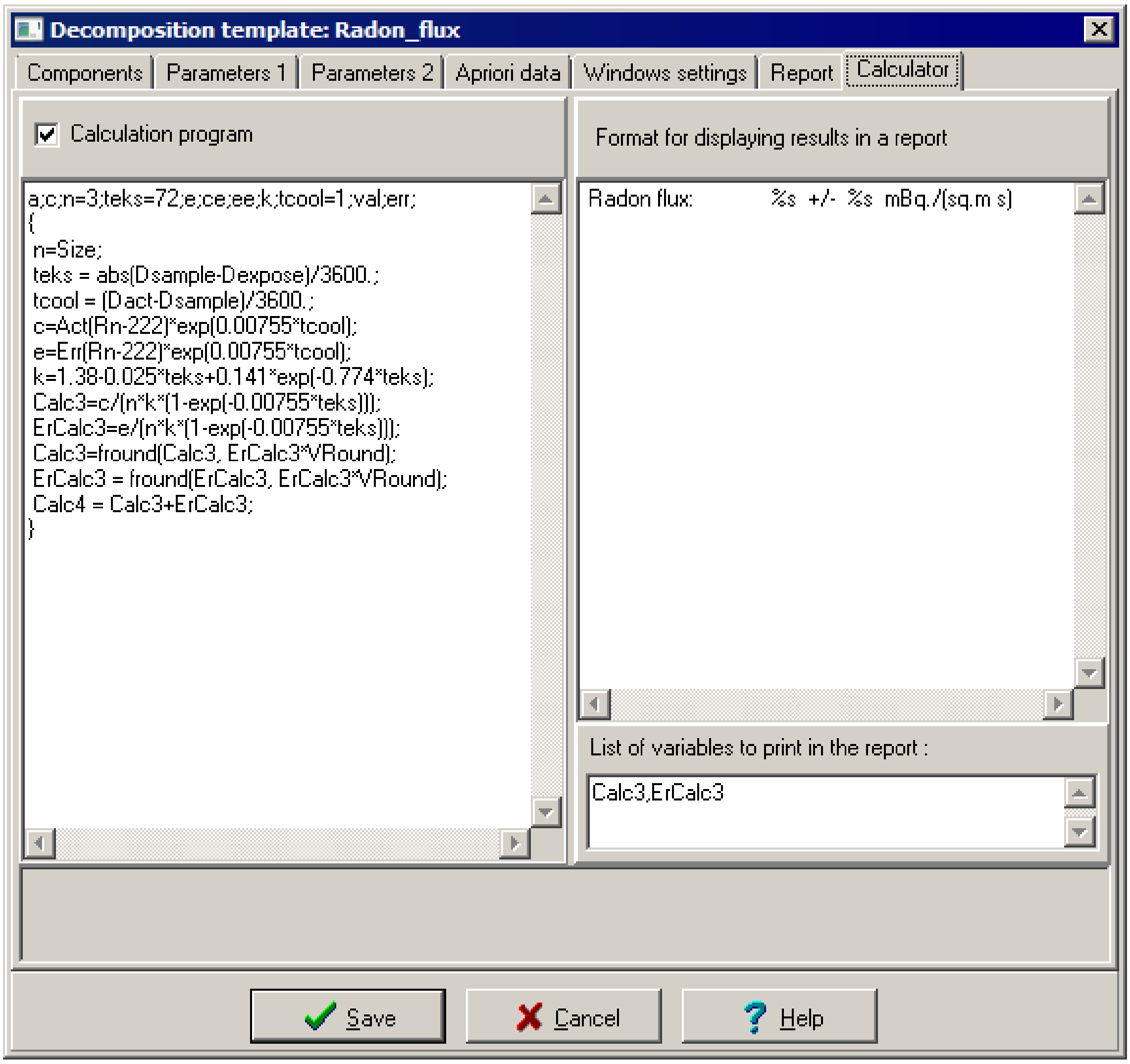
The text associated with the corresponding label replaces the label text when generating the report, inheriting the style and font of the label text. Since the names of fields ("Spectrometer", "Geometry", "Sample code", etc.) in the "SpectrRad" software package can change, for labels, from the **{Analyser}** label to the **{MeasTime}** label, there are additional labels of the form **{lbxxxx}**, which are replaced by the current name of the corresponding field. For example: the label **{lbAnalyser}** will be replaced with the text "Spectrometer" or "Analyzer", and the label **{lbSize}** with the text "Sample size", "Well depth" or "Number of adsorbers", depending on the settings of the measurement archive. The case in the label name does not matter – the **{Analyser}** label and the **{analyser}** label are identical labels.

The report on the results of spectrum processing, replacing the **{Report}** label, can also contain all the fields related to sample parameters and measurement conditions, therefore, in order to avoid duplication of information, the report template and the setting of the "**Content**" table of the "**Report**" page must be consistent with each other.

The calculator program

The operator has the ability to calculate additional parameters from the estimated values of nuclides activities and additional variables, control the selection of a report template, manage external processes and the duration of the measurement procedure using the capabilities of the built-in calculator.

The "**Calculator**" page looks like:



☑ Calculation program

```
a;c;n=3;teks=72;e;ce;ee;k;tcool=1;val;err;
{
 n=Size;
 teks = abs(Dsample-Dexpose)/3600.;
 tcool = (Dact-Dsample)/3600.;
 c=Act(Rn-222)*exp(0.00755*tcool);
 e=Err(Rn-222)*exp(0.00755*tcool);
 k=1.38-0.025*teks+0.141*exp(-0.774*teks);
 Calc3=c/(n*k*(1-exp(-0.00755*teks)));
 ErCalc3=e/(n*k*(1-exp(-0.00755*teks)));
 Calc3=fround(Calc3, ErCalc3*VRound);
 ErCalc3 = fround(ErCalc3, ErCalc3*VRound);
 Calc4 = Calc3+ErCalc3;
}
```

Format for displaying results in a report

```
Radon flux:          %s  +/-  %s  mBq./(sq.m s)
```

List of variables to print in the report :

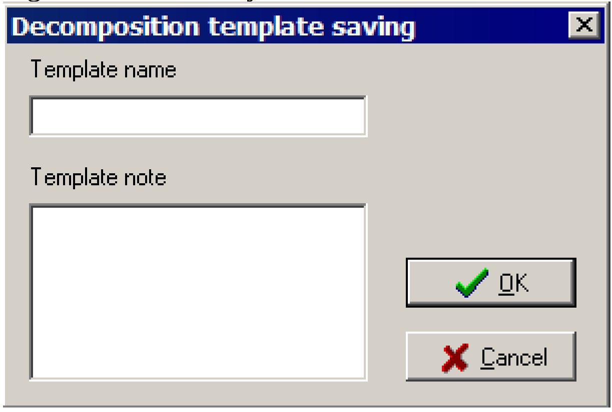
```
Calc3,ErCalc3
```

To record a program, the operator must select the "**Calculation program**" checkbox.

The text of the calculator program is written in the left window of the form (the example shows a program for generating a report depending on the value of the effective activity of the sample). The right window is "**Format for displaying results in a report**" to record the text output format and calculated parameters specified in the **list of variables to print in the report**. The lower panel is used to display error messages when compiling the program.

Saving the decomposition template

The processing parameters set by the operator can be saved as a decomposition template by clicking on the "**Save**" key. At the same time, a window is displayed on the screen



.

The operator must enter the **template name** (spaces in the template name are not allowed) and an arbitrary comment (**Template note**).

Calculator

Purpose

The built-in programmable calculator provides the user with a number of additional features:

- The ability to create programs to calculate the necessary additional parameters based on the results of sample processing. For example, the calculation of the parameter of compliance of the amount of radionuclides in a sample with SanPiN standards, the volumetric activity of radon in the air by the activity of radon decay products in carbon filters, the activity of nuclides in the test material based on the results of sample analysis after radiochemical separation, etc., etc.
- The processing of spectra during cyclic measurements or during the observation of a set provides the user with the ability to control the measurement process - stop measurements when necessary conditions are met, save or not save the measurement results in the archive.
- Calling an external procedure from the calculator program allows you to control external processes that may depend on the results of the analysis of the measured spectra (for example, turning on the siren, etc.)

The ability to independently create and edit such programs, including forming the necessary forms for displaying results, allows you to automate most of the necessary additional calculations, organize the printing of results in a user-friendly form.

The inclusion of calculation results from the calculator program in the database allows them to be used in more powerful database maintenance programs (Excel, Foxpro, etc.).

Terms

Variable	A number in floating-point format, accessible from the calculator program via a name unique in the context of the program. All variables used must be listed (declared) at the beginning of the program.
Expression	A sequence of mathematical operations written according to certain rules (see the syntax of the calculator program).
Assigning expression	An expression of type **A = Expression** where **A** is the name of the variable.

The structure of the calculator program

The calculator program consists of two parts: the **initialization section** and the **calculation section**.

The **initialization section** is located at the beginning of the program text and is intended for declaring and initializing variables. All variables must be declared here, except the predefined ones that are used in the calculation section. To declare a variable, enter a name and, additionally, an initializing expression. Any arithmetic operations and functions can be used in the initializing expression, but variable names, including predefined ones, cannot be used.

Examples:

A;B;C=10;Pi=3.141596;E=exp(1);

4 variables **A, B, C, Pi** are declared; **C, Pi** and **E** are initialized with constant expressions, the values of variables **A** and **B** are undefined.

A=pow(2,10)*5;
B=sin(3.14/2);

Variables **A**, **B** are declared and initialized;

Initializing of the type

A = 10;
B = A/100;

it is not allowed, since **A** is a variable and its value may not be defined at the time of initialization.

The initialization section may be missing. The symbol "{" indicates the end of initialization and the beginning of the calculation section. The **calculation section** continues from the first "{" to the last "}". The **calculation section** consists of a sequence of assignment expressions, conditional **if and else** statements, **while** cycle operators, I/O operators, procedures, and functions.

Predefined variables

When creating the program, the following variables are automatically declared:

nNucl	The number of nuclides in the table of spectrum processing results (including conditional nuclides of total activity).
iNucl(I)	The name of the nuclide with the serial number **I** in the results table. The numbering of nuclides begins with one. An alternative way to access the values of the result table is convenient when viewing measurement results in the **while** loop statement.
iElement(I)	The name of the element containing the nuclide with the specified abundance value for the nuclide with the sequence number **I** in the results table. The numbering of nuclides begins with one.
Act(Nucl)	The activity of the nuclide **Nucl** at the date of the activity values (predefined variable **Dact**) in Becquerel for the geometry of the "thin layer" and in Bq/kg for the geometries of the "thick layer". **Nucl** is the name of the nuclide (for example, **Act(Cs-137)** is the activity of cesium-137).
AprAct(Nucl)	The activity of the nuclide **Nucl** in a priori data (comparison data) at the date of **Dact** in Becquerels for "thin layer" geometries and in Bq/kg for "thick layer" geometries.
iAct(I)	The activity of the nuclide with the sequence number **I** in the results table on the date of **Dact**. The numbering of nuclides begins with one. An alternative way to access the values of the result table is convenient when viewing measurement results in the while loop statement.
iAct0(I)	The activity of the nuclide with sequence number **I** in the results table at the date of the spectrum acquisition start.
iAprAct(I)	The activity of the nuclide in the a priori data (comparison data) with the sequence number **I** in the results table on the date of the activity values.
Err(Nucl)	The error in estimating the activity of the **Nucl** nuclide in the same units on the same date **Dact**. As an error, the program returns the value of either a random component of uncertainty, or a complete uncertainty, depending on the report settings. The checkbox that determines the type of error can also be changed directly in the calculator program (**SetRandomError(flag)** function).
AprErr(Nucl)	The error (uncertainty) in estimating the activity of the **Nucl** nuclide in a priori data (comparison data) at the date of **Dact**. As an error, the program returns the value of the random component of the uncertainty. If the error is less than or equal to zero, there is no a priori data.

iErr(I)	The error in estimating the activity of the nuclide with sequence number **I** in the results table at the date of **Dact**.
iErr0(I)	The error in estimating the activity of the **I**-th nuclide in the results table at the date of the spectrum acquisition start
iAprErr(I)	The random component of the error in estimating the activity of the **I**-th nuclide of a priori data (comparison data) in the results table. If the error is less than or equal to zero, there is no a priori data.
IsVisible(I)	The flag of the presence of the **I**-th nuclide in the report: 1 - nuclide is presented in the report, 0 - nuclide is missing.
EffAct	The specific effective activity at the date of the activity values in Becquerels per unit of the specimen value (for example, in Bq/kg, if the specimen value unit is kg).
ErrEffAct	The error in estimating the specific effective activity in the same units.
SumAct(N)	The specific total activity of the sample at the start date of measurements in Becquerels per unit of the sample value (for example, in Bq/kg, if the sample value unit is kg). **N** = 1 is the total alpha activity. **N** = 2 is the total beta activity. **N** = 3 is the total gamma activity. **N** = 0 **-** the type of total activity (alpha, beta or gamma) is determined by the type of radiation of the sample spectrum.
ErrSumAct(N)	The error in estimating the specific total activity in the same units.
NuclMass (Nucl)	The mass of the nuclide **Nucl** at the date of activity values (predefined variable **Dact**) in kilograms for the geometry of the "thin layer" and in relative mass fraction for the geometries of the "thick layer".
iNuclMass (I)	The mass of the nuclide with the ordinal number **I** in the nuclide table (numbering of nuclides begins with one) on the date of the activity values.
ErrNuclMass (Nucl)	The error in estimating the mass of the **Nucl** nuclide in the same units on the same date **Dact**.
iErrNuclMass (I)	The error in estimating the mass of a nuclide with ordinal number **I** in the table of nuclides in the same units on the same date **Dact**.
NormGroup	The number of the group of standards associated with the specified type of sample.
Norm1(Nucl) - **- Norm5(Nucl)**	Five standards (SanPiN, NPB, etc.) for a given type of sample for nuclide **Nucl**.
Norm(I, J)	The **j**-th standard out of five standards for the **i-**th nuclide in the results table.
NormSumAct(N,I)	The **I**-th standard of five standards for specific total activity **N** (**N** is the type of total activity). The numbering of the parameters starts from one.
NormEffAct(I)	The **I**-th standard of four standards for specific effective gamma activity. The numbering of standards begins with one.
HalfLife(Nucl)	The half-life in seconds of the nuclide **Nucl**.

iHalfLife(I)	The half-life in seconds of a nuclide with the ordinal number **I** in the nuclide table (numbering of nuclides begins with one).
ActSection(Nucl)	The activation cross section in the barns of a stable nuclide **Nucl**.
AtomMass(Nucl)	The atomic weight of the nuclide **Nucl**.
Abundance(Nucl)	The abundance of the nuclide **Nucl** in the corresponding element (for natural radioactive nuclides).
iAbundance(I)	The abundance of a nuclide with the ordinal number **I** in the nuclide table (numbering of nuclides begins with one) in the corresponding element (for naturally radioactive nuclides) as a percentage.
GEquRa(Nucl)	The gamma equivalent of radium for the nuclide **Nucl**.
iGEquRa(I)	The gamma equivalent of radium for a nuclide with the ordinal number **I** in the nuclide table (the numbering of nuclides begins with one).
SampleMass	The mass of the counting sample in kilograms.
ConcMass	The mass of the resulting concentrate (or the entire sample) in kilograms.
RawValue	The value (mass, volume or area) of the source material, corresponding to the mass of the counting sample.
SampleValue	Either the **SampleMass** value or the **RawValue** value is passed to **SampleValue**, depending on the setting of the "*Recalculate results by concentration factor*" parameter in the processing template or the position of the corresponding button () in the report form.
Size	Parameter 1 of the sample.
SParam	Parameter 2 of the sample.
Tmeas	Live measurement time in milliseconds.
TmeasReal	Real measurement time in milliseconds.
Dexpose	Start date of sampling (exposure). The date format used in the calculator is the number of days from December 30, 1899 (TDateTime format).
Dsample	End date of sampling (exposure).
Dmeas	Measurement start date.
DAprMeas	The date of measurement of the a priori data. If the date is zero, there is no a priori data.
Dact	The date of the activity values. The date of the activity values coincides with either the measurement start date (**Dmeas**) or the sampling date (**Dsample**), depending on the setting of the processing parameters.
UseMHL	The value of the activity conversion mode flag for a specified date defined in the report settings: if the **UseMHL** is different from zero, the half–life of the parent nuclide (if it is present in the spectrum) is used in the calculation, otherwise the half-life of the nuclide for which the calculation is performed is used.
VRound	The rounding level of the results is set in the report parameters. The value is set in relative units: 0 – rounding is not set, 1 – 100 percent

	rounding).
InputRate	The average load of the spectrometer during the spectrum acquisition, in pulses per second.
RateWarnLevel	The "warning threshold" set for the spectrometric tract in pulses per second. When the spectrometer is loaded above this threshold, the yellow indicator lights up and the "Warning" sound circuit turns on.
RateAlarmLevel	The "alarm threshold" set for the spectrometric tract in pulses per second. When the spectrometer is loaded above this threshold, the red indicator lights up and the "Alarm" sound circuit turns on.
DTWarnLevel	The "warning threshold" set for the spectrometric tract as a percentage of the "dead time" of the spectrometer. The threshold warning circuit is activated when any of the levels is exceeded: "dead time" or the intensity of the recorded pulses.
DTAlarmLevel	The "alarm threshold" set for the spectrometric tract as a percentage of the "dead time" of the spectrometer.
TotalInt	The intensity of the pulses (imp./s) recorded in the energy window used for spectrum processing. For the resolved linear spectra, the intensity of the pulses recorded in peaks.
GlobalResiduals	The total discrepancy (deviation of the spectrum from the model) calculated over the entire processing range used. The discrepancy is given in standard deviations.
NormalResiduals	Decomposition discrepancy.
ResAlarmLevel	The maximum allowable level of discrepancy.
Drift	The energy drift of the spectrometer as a percentage, estimated from the decomposition results.
DriftAlarmLevel	The maximum allowable drift level.
ADrift	The parameter "A" of the linear drift (A*X+B) of the energy calibration is the gain drift.
BDrift	The linear drift parameter "B" is the zero drift of the scale.
Calc1-Calc8, **ErCalc1-ErCalc8**	Calculated variables that will be stored in the archive of measurement results. Variables **ErCalc1-ErCalc8** are recommended to be used for error values of **Calc 1-Calc 8** values.

The syntax of the program

The calculator program may consist of the following elements:

Element	**Description**
{	The beginning of the calculation section, the **if** block, the **else** block, the **while** block.
}	The end of the calculation section, the **if** block, the **else** block, the **while** block.
=	Assignment.
;	The end of the expression.
***** **/** + **-**	Multiplication, division, addition, subtraction.

( )	Parentheses specify the order of calculations, the expression in parentheses is calculated first.
> < >= <= == != & |	Logical operations "greater than", "less than", "greater than or equal to", "less than or equal to", "equal to", "not equal to", logical "AND", logical "OR". Logical operations should be used together with the conditional **if/else** operator and the **while** loop operator. The result of logical operations is 1 if the condition is met (true), or 0 if the condition is not met (false). You should avoid using '==' to compare variables due to the limited accuracy of calculations. It is acceptable to compare a variable with a constant.
The name of the variable	The sequence of letters and numbers must start with a letter.
Number	It is allowed to enter numbers in the range -1.e38, +1.e38 in floating point or exponential form.
Predefined variables, operators, functions and procedures	The calculator defines a number of mathematical functions, predefined variables, a conditional **if/else** operator, a **while** loop operator, operators for input/output of variable values, and a number of procedure operators for controlling the measurement process and external processes.
Separator	The space and newline characters are considered delimiters of the expression elements. Delimiters are ignored during calculations and can occur anywhere in the expression
//	Two slashes in a row indicate the beginning of the comment. The comment text is ignored during calculations and can be arbitrary, the comment continues to the end of the line.

The sequence of operations

1.	Expression in parentheses ( ), function.	Top priority.
2.	*, /	multiplication, division.
3.	+, -	addition, subtraction.
4.	>=, >, <, <=, ==, !=	comparison operations.
5.	&, |	logical operations "AND", "OR"

Within the brackets, the sequence of operations in the expression is the same as indicated.

Conditional operator

It is intended for branching the calculator program depending on the current value of some expression called "**condition**":

The conditional operator has four forms of writing:

1.

if(condition) <expression>;
<expression> calculated if the **condition** is true**;**

2.

if(condition)
{
<expression_1>;

```
...
<expression_p>;
}
```

<expression_1> - <expression_p> are calculated if the **condition** is true**;**

3.

```
if(condition) <expression 1>;
else <expression 2>;
```

<expression 1> is calculated if **condition** is true**,**
<expression 2> is calculated if **condition** is false**;**

4.

```
if(condition)
{
<expression_1>;
...
<expression_p>;
}
else
{
<else_expression_1>;
...
<else_expression_n>;
}
```

<expression_1> - <expression_n> are calculated if the **condition** is true**,**
<else_expression_1> - <else_expression_n> are calculated if the **condition** is false**.**

Cycle operator

It is designed to repeat a part of the calculator program a set number of times depending on the current value of some expression called "condition":

```
while(condition)
{
<expression_1>;
...
<expression_p>;
}
```

<expression -1> - <expression n> is calculated if the **condition** is true and the calculations will be repeated until the **condition** becomes false.

Functions

Function	**Description**
lg(X)	Decimal logarithm **X**, **X**>0;
ln(X)	The natural logarithm **X**, **X**>0;
pow(X, Y)	**X** to the power of **Y**;
exp(X)	Exponent **X**;
sqrt(X)	The square root of **X**, **X**>=0;
abs(X)	Absolute value **X**;
sin(X)	The sine **X**, **X** is given in radians, 180° = 3.141596 radians;
cos(X)	The cosine of **X**, **X** is given in radians;

tg(X)	The tangent of **X**, **X** is given in radians;
asin(X)	The Arcsinus **X**;
acos(X)	Arccosine **X**;
atg(X)	Arctangent **X**;
mod(X, Y)	The remainder of dividing **X** by **Y**;
round(X)	The largest integer not exceeding **X**.
fround(Val, Err)	The value of **Val** rounded to the accuracy of **Err**.
NuclNameCmp("Name",Var)	Comparing the value of the **Var** variable with the text string "**Name**". In the calculator, all variables are 8 bytes long. This function interprets a variable as a string of characters up to 8 bytes long. The comparison is case-insensitive and is used to compare the names of nuclides. The function returns a non-zero value if the strings are identical.
SetRandomError(Flag)	Setting a flag that determines the calculation of uncertainties (errors). If the value of the **Flag** variable is different from zero, the error will include only a random component, otherwise it will include complete uncertainty. The function returns the flag value that was set in the program before it was redefined.
SetNuclDecayFlag(Flag)	Setting the flag defining the value of the activities transmitted to the calculator program. If the value of the **Flag** variable is different from zero, the activity values will correspond to the specified date of the **Dact**, otherwise – the average over the measurement time. The function returns the flag value that was set in the program before it was redefined.
SetEffSumActMode(Flag)	Setting a flag that determines the calculation of total activity. If the value of the **Flag** variable is different from zero, the total effective activity is calculated, otherwise the usual total activity is calculated. The function returns the flag value that was set in the program before it was redefined.
SetMassActUnit(Flag)	Setting a flag that determines the output in the report of nuclide activity in units of activity or nuclide content in grams. If the value of the **Flag** variable is different from zero, the values are output in grams, otherwise in units of activity measurement (Bq or Ci). The function returns the flag value that was set in the program before it was redefined.
RecalcAct(Date)	Recalculation of activity values and errors for a given date. The function returns a value other than zero if the recalculation is successful. If the **Date** value is zero, the recalculation is performed on the sampling date or the measurement date, depending on the report setting.

Procedures

Procedures differ from functions in that they do not perform calculations, but perform certain actions related to the results of calculations and, in addition, are performed only when starting the calculator from the spectrum processing program (the entire calculator program, with the exception of procedures, is executed every time the report is opened, and not only when processing the spectrum).

Procedure	Description
Print("format", X1, …Xn)	Printing the values **X1,...Xn** in accordance with the format string "**format**". The list of variables may be missing. Any text entered in the "**format**" line will be included in the report. In this case, special combinations of two characters **%c** , **%s** or **%d** indicate the place in the text where the next variable from the list of variables to print **X1, ...Xn** will be printed. The **%c** combination is replaced by the text value of the expression (the name of the nuclide). The **%s** combination is replaced by the numeric value of the expression. The **%d** combination interprets the value as a date. When forming the report, the **%u** symbols are replaced by the abbreviated designation of the unit of measurement of sample activity ("Bq", "Ci", "Bq/kg", "Ci/g", "Bq/cub m", "Bq/l", "Ci/sq m", etc.)
SetMass(Val, Unit)	Setting the mass of the counting sample to **Val**. **Unit:** 1 – kg, 2 – g, 3 – mg.
SetSize(Val)	Setting the Size parameter (Parameter 1) to **Val**.
SetSParam(Val)	Setting the parameter SParam (Parameter 2) to **Val**.
SetAutoSaveFlag()	Setting the flag for automatic saving of spectrum processing results in the archive. The procedure allows the user to decide whether to save the measurement results in the archive or not after analyzing the measured spectrum without the operator's participation. To do this, the flag for saving measurement results in the archive should be unchecked when starting measurements and the flag for automatically saving processing results in the decomposition template should be unchecked. The calculator program should be included in the processing template performed at the end of the measurements, where the issue of the need to save the measurement results and spectrum processing will be resolved – performing the procedure will save the spectrum and processing results in the archive without displaying the results on the computer display.
ClearAutoSaveFlag()	Zeroing the flag for automatic saving of spectrum processing results in the archive. The procedure serves the same purpose as the previous one. It removes the flag for automatic saving of results in the decomposition template, if it is set and allows the operator to decide whether to save the data.
StopMeas()	Calling the measurement completion procedure, if measurements are enabled, for the tract on which the processed spectrum was measured.
PlaySound(«SoundFile»)	Starts playback of a sound file of the **Wave** type (files with

	the **.wav** extension). The file name "**SoundFile**" may not contain the full path to the file. In this case, the program searches for it in the folder corresponding to the processed spectrum of the spectrometer, and if it does not find it, in the head folder of the "SPECTRRAD" package. The file will be played either before the operator intervenes or before the spectrum processing report is closed. The **PlaySound** procedure allows you to create the required sound scheme for accompanying events based on the results of spectrum processing.
MessageBox («Message»)	Displaying the **Message** on the screen. **MessageBox** allows you to inform the operator about any activity values in the measured sample that require the operator's attention. When the **MessageBox** procedure window is closed, the audio file stops playing if it was started earlier by the **PlaySound** procedure.
Procedure("Command")	Calling an external program. **Command** – a command line that includes the full path to the program being called and the necessary arguments. An external program can control the equipment, for example, turning on the siren, etc.
IgnoreCalc()	The procedure sets a flag canceling the results of the calculator program: the calculator variables will not be saved in the measurement archive and will not be displayed in the report on the results of spectrum processing.

Input, output

An expression of the form **X=input("PROMPT")** allows the operator to enter the necessary values of variables in the calculation process using the calculator program. Here: **X** is the name of an arbitrary variable, and **prompt** is a hint that will be displayed as the title of the window generated by the **input** operator.

The i**nputdate("PROMPT")** operator is used to enter dates. When you enter the date value, it is converted to the number of days since 12.30.1899 12:00:00. Therefore, for example, the expression **Duration=(Dsamle-inputdate("Start date of the exposition"))*24** will be the number of hours from the start of exposure to sampling.

The **Report("FILE")** operator allows you to set a report template that will include a report on measurement results and calculation results according to the calculator program. The **FILE** variable is the name of the report template file. If the file name does not specify the file path or extension, then the file path and extension are taken from the file specified in the decomposition template. For example, if the report template "**C:\SpectrRad\DocTemplate\Soil.doc**" was set in the decomposition template, then the **Report("Build materials")** statement will replace the report template with "**C:\SpectrRad\DocTemplate\Build materials.doc**». If the extension is not explicitly specified anywhere, "**.RTF**" is used by default for the file name extension.

You can use the **Print** statement to print the values of variables and text that you want to include in the report (see "**Procedures**"). The **Print** statement can also be used in a loop statement. The **Print** statement is available for the 8th version of the package and above.

For compatibility with older versions of the package, the old printing mode is also retained. The variables to be included in the report at the end of the calculator should be listed in the column "**List of variables to print in the report**". Up to 16 variables can be enabled. When listing variables, they must be separated from each other by commas or spaces. The output format is set in the field "**Format for displaying results in a report**". Any text entered in this field will be included in the report. Special combinations of two characters **%c, %s** or **%d** indicate the place in the text where the next variable from the list of variables to be printed will be printed. The **%c** combination is replaced by the text value of the expression (the name of the nuclide). The **%s** combination is replaced by the numeric value of the expression. The **%d** combination interprets the value as a date. In order to include the **%** symbol in the text, you must print it twice **%%**. When forming the report, the **%u** symbols are replaced by the abbreviated designation of the unit of sample activity ("Bq", "Ci", "Bq/kg", "Ci/g", "Bq/cub m", "Bq/l", "Ci/sq km", etc.).

Error messages

Undefined variable	The variable name is not specified in the initialization section and is not the name of a predefined variable.
The variable is already defined	Redeclaring a variable or declaring a predefined variable.
Assignment operation for a predefined variable	An attempt to change the value of a predefined variable in the calculator program.
Incorrect syntax **Error in expression**	The calculator cannot interpret the expression.
There must be a left bracket **There must be a right bracket**	By the context of the expression, a parenthesis is expected.
Division by zero	In the process of calculations, an erroneous situation of division by zero arose.
The value of the expression is out of range	The argument of the function is outside the scope of the function definition (the logarithm of a negative or zero number, the square root of a negative number).
Incorrect number	Acceptable range of numbers: -1.e38, +1.e38.
There must be `{`	A parenthesis is expected to start the calculation section.
Superfluous `{`	The number of opening brackets '{' must be equal to the number of closing brackets '}'.
Too many variables	The program declares too many variables, in the current version the limit is 512.
Incorrect ending, **Must be `}`**	Expected '}'.
Variable name is too long	The allowed length of the name is 32 characters.
Must be a variable name	According to the context of the program, the name of the variable is expected.
Must be `;`(semicolon)	The expression must end with a semicolon.
Must be `=`(assignment)	At the beginning of an expression, the variable name is usually followed by '='.
Must be constant	An attempt to initialize a variable with an expression containing references to variables.

Must be `,`(comma)	The arguments of the function must be separated by a comma.
The program is too long	The volume of the program text exceeds the allowed one.

Program example

Calculation program

```
// Initialization section
    p;a;e;a1;e1;i;
// Calculation section
    a = 0;
    e = 0;
    i = 1;
    while (i <= nNucl)
    {
      if (IsVisible(i))
      {
         p = Norm(i,1);
         if (p > 0)
         {
            a1 = iAct(i)/p;
            if (a1 < 0)
              a1 = 0;
            a = a + a1;
            e1 = iErr(i)/p;
            e = e+e1*e1;
         }
      }
      i = i+1;
    }
    e=sqrt(e)/SampleValue;
    a = a/SampleValue;
    e1 = VRound*e;
    ErCalc1 = fround(e, e1);
    Calc1 = fround(a, e1);
    Calc2=Calc1+ErCalc1;
    Calc3=Calc1-ErCalc1;
   }
```

Format for displaying result in a report

```
--------------------------------------------------
Conformity parameter:    %s(Act.) + %s(Error) = %s
--------------------------------------------------
```

List of variables to print in the report

```
Calc1, ErCalc1, Calc2
```

Norms and materials

Registration of the results of sample measurements in the form of a completed document requires access to radiation safety standards, sanitary and hygienic standards, intra-industry standards, etc., etc. All these standards are related to the **type of test sample (Sample type)**.

Correct accounting of absorption in the substance of a counting sample requires knowledge and specification of the elemental composition of the sample and the associated cross sections of the reactions of radiation interaction with the substance. Since different types of samples associated with radiation standards have different chemical compositions, in the software package "SPECTRRAD" these data are set in one procedure and stored in one structure.

The menu item "**Tools / Norms and materials**" calls the program for forming and editing the structure (tree) of standards (SanPiN, NRB, etc.) and the chemical composition and density of the specimen substance, specimen container (shield) or media between sample and detector.

Structure

In the "SPECTRRAD" package, data on norms and constants are stored in the files **Norms.nrm** and **Norms.txt** (in **Norms.txt -** a comment on the sample type and the **Norms.nrm** table of standards). The path to the file is determined by the sample type as follows **-** the sample type is part of the full path to the file **Norm.nrm**, starting (but not including) the "**Sample types**" folder. Accordingly, the sample type must have the form of a file path and all file path restrictions are imposed on the text of the sample type.

The "**Sample types**" folder should be located in the main folder of the package and, if it does not exist, it is created when the program is first launched.

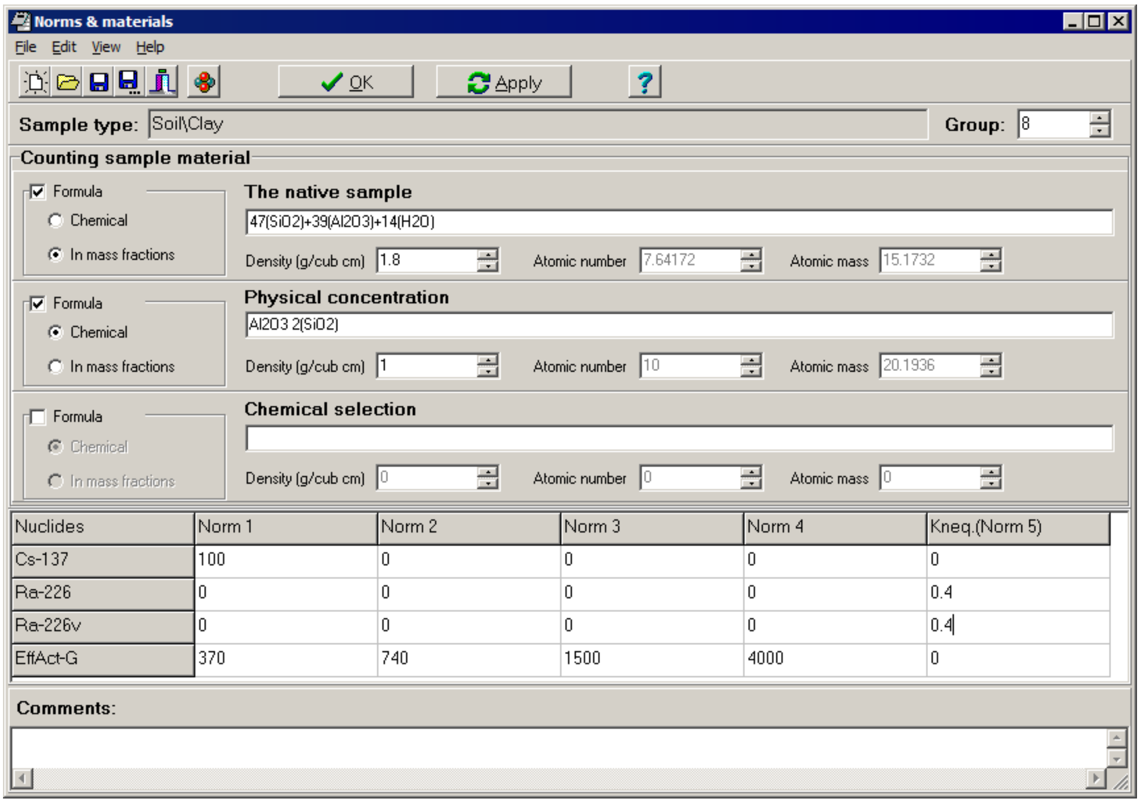
For example:

C:\SpectrRad \ Sample types\6.Products\1.Meat products\1.Meat\1.Bones\Norms.nrm
is a file of standards and chemical composition for samples of type
6.Products\1.Meat products\1.Meat\1.Bones (the head folder of the package-**C:\SpectrRad**).

Access to these standards is provided through predefined variables **Norm1(Nucl) -- Norm5(Nucl)** (**Nucl** is the name of the nuclide) in the calculator program.

Main window

The window of the program for the formation of standards and constants, depending on the type of sample of the working spectrum, may look like this, for example:



Sample type: Soil\Clay **Group:** 8

Counting sample material

The native sample
☑ Formula ○ Chemical ● In mass fractions
47(SiO2)+39(Al2O3)+14(H2O)
Density (g/cub cm) 1.8 Atomic number 7.64172 Atomic mass 15.1732

Physical concentration
☑ Formula ● Chemical ○ In mass fractions
Al2O3 2(SiO2)
Density (g/cub cm) 1 Atomic number 10 Atomic mass 20.1936

Chemical selection
☐ Formula ● Chemical ○ In mass fractions
Density (g/cub cm) 0 Atomic number 0 Atomic mass 0

Nuclides	Norm 1	Norm 2	Norm 3	Norm 4	Kneq.(Norm 5)
Cs-137	100	0	0	0	0
Ra-226	0	0	0	0	0.4
Ra-226v	0	0	0	0	0.4
EffAct-G	370	740	1500	4000	0

At the top of the form there are menus and toolbar buttons. Below is the "**Sample type**" panel, the "**Counting sample material**" panel, the norms panel and the comments to the norms. The dimensions of the form can be changed by the operator (with the left mouse button pressed, you can drag the boundaries of the form, changing its size). The height of the norms panel is also adjusted by moving the border between the norms and comments panels. In addition, you can visualize either only the materials panel, or only the norms panel, or both panels using the "**View / Materials panel**" and "**View / Norms panel**" menu items.

A number of similar sample types are grouped into a **group**, for example, group 1 "**Food raw materials and food products**". The group number is available to the user in a programmable calculator and allows, for example, changing the form of the report depending on its value. A comment on the standards can be included in the report of the results of spectrum processing, if the decomposition parameters are adjusted accordingly.

The operator has the opportunity to enter or change the values of the group number, five values of standards for the selected sample type, set formulas for the elemental composition of the sample substance for three types of counting samples, enter an arbitrary comment and save the entered data by pressing the "**OK**" key or using the "**File / Save**" menu item.

Menu

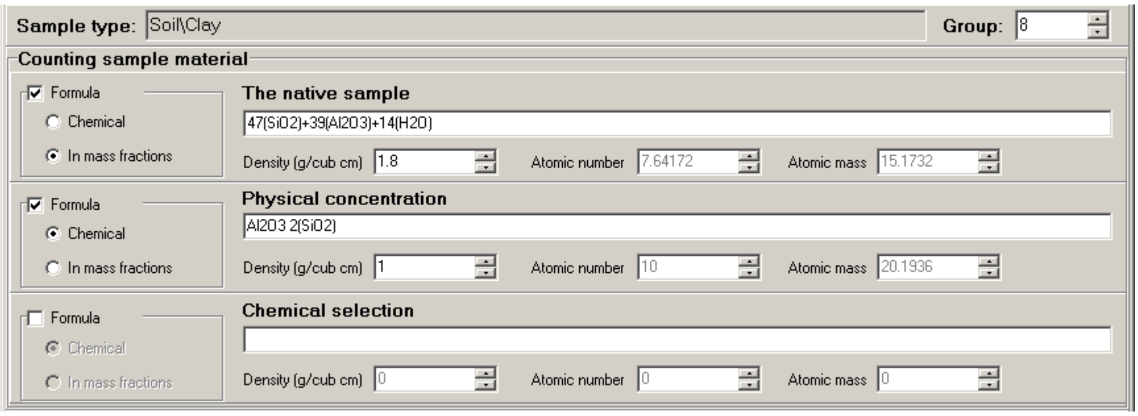
The menu and button panel provide the operator with the opportunity to create files of standards for a new type of sample or open and edit existing ones.

Menu item	*Action*
File:	
Create	Create a new "sample type".
Open…	Open one of the existing "sample type".
Save	Save the "sample type".
Save as…	Save the data as a new "sample type".
Delete	Delete the "sample type".
Exit	Close the "Norms and Materials" window.
Edit:	
Cross-sections	
Calculate…	Calculate the cross-section tables of the reactions of radiation interaction with matter according to the given formulas.
Edit…	Edit tables of cross sections of reactions of radiation interaction with matter.
Add / Delete nuclides…	Change the list of nuclides for the table of norms.
Edit group…	Change the value of the group number for the entire selected group of norms.
Import	
Norms…	Import data on norms from the selected sample type.
Materials…	Import data on the chemical composition of the substance of the selected sample type.
View:	
Materials panel	Visualization of the chemical composition of the substance panel.
Norms panel	Visualization of the norms panel.
Help **F1**	Description of the program.

Entering formulas for the chemical composition of the sample

Correct accounting of the absorption of alpha, beta and gamma radiation in the sample substance requires knowledge of the chemical composition of the substance of the counting sample and its density.

The "**Counting sample material**" panel,



Sample type: Soil\Clay **Group:** 8

Counting sample material

☑ Formula ○ Chemical ● In mass fractions

The native sample

47(SiO2)+39(Al2O3)+14(H2O)

Density (g/cub cm) 1.8 Atomic number 7.64172 Atomic mass 15.1732

☑ Formula ● Chemical ○ In mass fractions

Physical concentration

Al2O3 2(SiO2)

Density (g/cub cm) 1 Atomic number 10 Atomic mass 20.1936

☐ Formula ● Chemical ○ In mass fractions

Chemical selection

Density (g/cub cm) 0 Atomic number 0 Atomic mass 0

allows the operator to enter this data by entering the formula of the chemical composition of the sample substance for three types of counting samples: "**The native sample**", "**Physical concentration**" and "**Chemical selection**". For the medium and protection material, only the first formula is used – the native sample.

The formula of the chemical composition of the substance can be entered in two versions:

Chemical - in the form of the number of atoms and molecules.

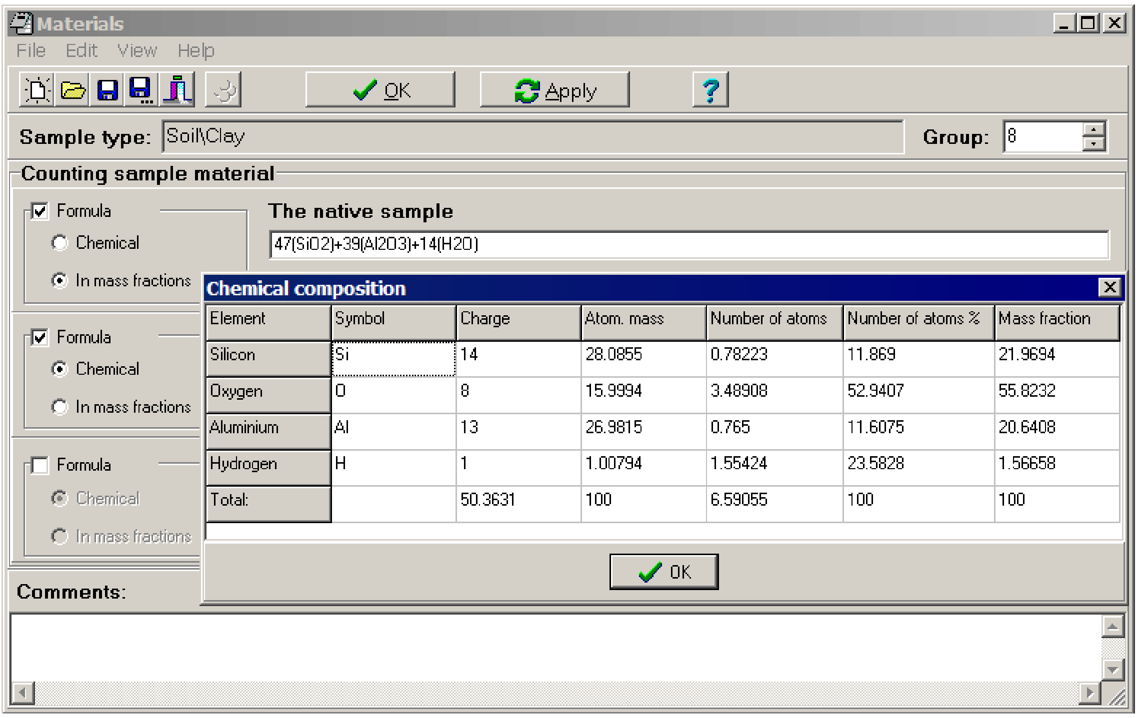
In mass fractions – the composition of a molecule (a molecule can be one chemical element) in the form of a chemical formula, and the number of molecules in mass fractions. The molecules must be enclosed in parentheses and the mass fraction of the molecules is indicated as a number before the formula of the molecule. For example: **2(H) 1(O)**, will be interpreted as two mass fractions of hydrogen and one of oxygen, which, of course, is not water, and **1(H2O) -** as one mass fraction of water.

The formula of the chemical composition of the molecule is entered in accordance with the accepted rules for writing chemical formulas, except that the procedure does not allow you to enter numbers in the form of a subscript. The formula of water will look like **H2O**. This restriction somewhat reduces the ambiguity of entries, so it is recommended not to hesitate in using parentheses when writing formulas.

Acceptable symbols when writing formulas are the accepted designations of chemical elements, numbers, parentheses, spaces and the plus sign (+). For example: **2(K3(Fe(CN)6))+5(H2O)** or **2(K3(Fe(CN)6)) 5(H2O)**. Depending on the choice of the type of formula (chemical or in mass fractions), the record will be interpreted either as two molecules of potassium ferrocyanide **K3(Fe(CN)6)** and five water molecules **(H2O)** – chemical formula, or as two-seventh by weight of potassium ferrocyanide molecules **K3(Fe(CN)6)** and five-sevenths by weight of water molecules **(H2O)**. The number of molecules in a chemical formula can only be an integer, the mass fraction can also be a fractional number.

When entering the formula, the program calculates the number of chemical elements and the effective atomic number and the effective atomic mass of the substance in accordance with the specified formula.

Double-clicking on the formula of the substance displays a table of the chemical composition of the sample:



Sample type: Soil\Clay

Group: 8

The native sample

47(SiO2)+39(Al2O3)+14(H2O)

Chemical composition

Element	Symbol	Charge	Atom. mass	Number of atoms	Number of atoms %	Mass fraction
Silicon	Si	14	28.0855	0.78223	11.869	21.9694
Oxygen	O	8	15.9994	3.48908	52.9407	55.8232
Aluminium	Al	13	26.9815	0.765	11.6075	20.6408
Hydrogen	H	1	1.00794	1.55424	23.5828	1.56658
Total:		50.3631	100	6.59055	100	100

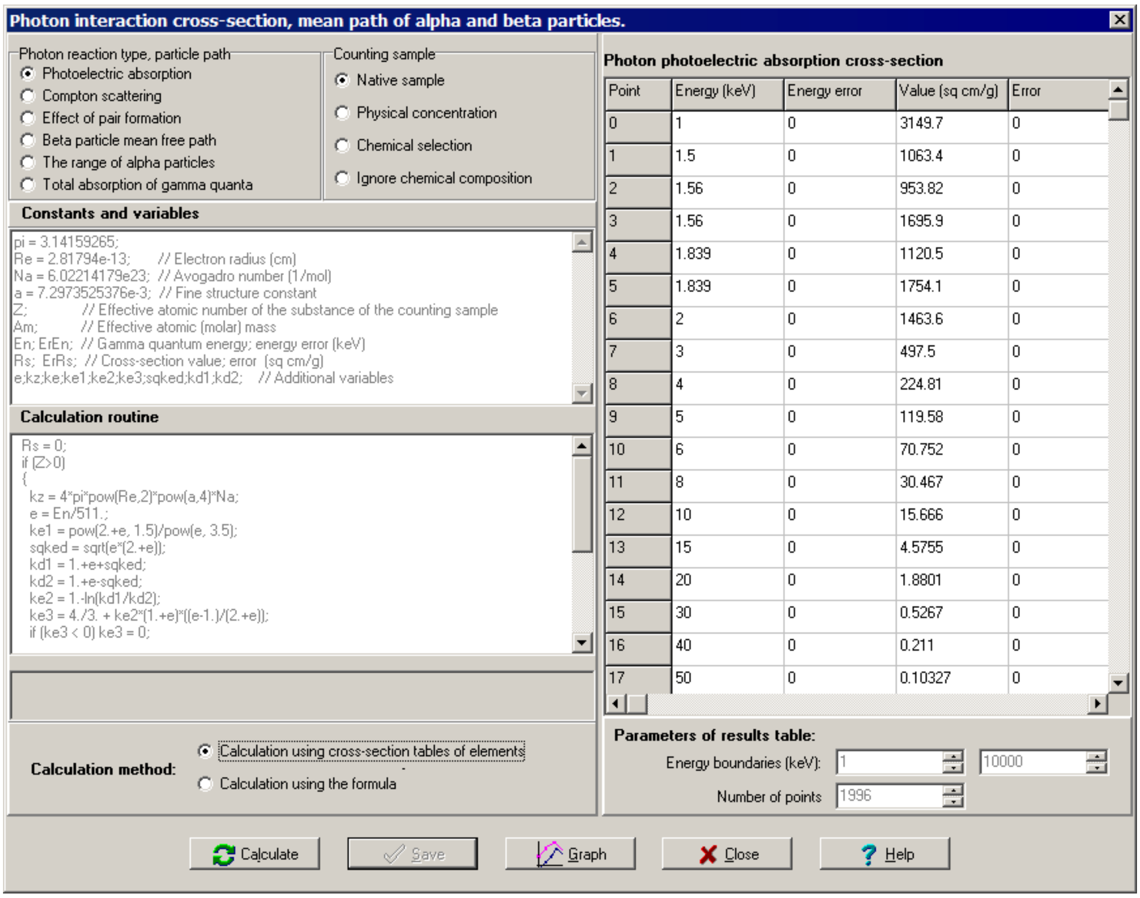
The lines with the name of the element in the "**Charge**" column show the charge of the atoms of the element, in the "**Atom. mass**" column - the atomic mass of the atoms of the element. The "**Number of atoms**", depending on the type of formula, contains either the number of atoms of an element in a substance molecule (**Chemical formula**) or the number of atoms in a conventional weight unit (**Formula in mass fractions**). The columns "**Number of atoms %**" and "**Mass fraction**" contain the percentage values of the corresponding values.

The line "**Total:**" contains the total values:

- in the "**Charge**" column $\sum Z_i \cdot n_i$, where Z_i is the charge of the element atom, n_i is the number of atoms of the element;
- in the column "**Atom. mass**" $\sum Am_i \cdot n_i$, where Am_i is the atomic mass of an element;
- in the column "**Number of atoms**" $\sum n_i$, "**Number of atoms%**" is always equal to 100%.
- The total "**Mass fraction**" is also always equal to 100%.

Calculation of the reaction cross section

The menu items "**Edit / Cross-sections / Calculate...**" and "**Edit / Cross-sections / Edit...**" allow the operator to create or change formulas for calculating cross sections of reactions of gamma radiation interaction with matter (mass coefficients of gamma radiation attenuation in matter in sq.cm/g), the mean free path of beta and alpha particles in matter (g/sq.sm) or tables of such cross sections and mean free path values for the selected sample type. Calling the procedure using the menu item "**Edit / Cross-sections / Edit...**" does not allow you to change the cross-section calculation program and calculate the reaction cross-section, calling the procedure using the menu item "**Edit / Cross-sections / Calculate...**" allows all operations. At the same time, the form of the procedure for calculating and editing the cross section of reactions of interaction of gamma radiation with matter, the path of alpha and beta particles is displayed on the screen:



Photon interaction cross-section, mean path of alpha and beta particles.

Photon reaction type, particle path
● Photoelectric absorption
○ Compton scattering
○ Effect of pair formation
○ Beta particle mean free path
○ The range of alpha particles
○ Total absorption of gamma quanta

Counting sample
● Native sample
○ Physical concentration
○ Chemical selection
○ Ignore chemical composition

Constants and variables

```
pi = 3.14159265;
Re = 2.81794e-13;       // Electron radius (cm)
Na = 6.02214179e23;  // Avogadro number (1/mol)
a = 7.2973525376e-3;  // Fine structure constant
Z;              // Effective atomic number of the substance of the counting sample
Am;            // Effective atomic (molar) mass
En; ErEn;  // Gamma quantum energy; energy error (keV)
Rs;  ErRs;  // Cross-section value; error  (sq cm/g)
e;kz;ke;ke1;ke2;ke3;sqked;kd1;kd2;    // Additional variables
```

Calculation routine

```
Rs = 0;
if (Z>0)
{
  kz = 4*pi*pow(Re,2)*pow(a,4)*Na;
  e = En/511.;
  ke1 = pow(2.+e, 1.5)/pow(e, 3.5);
  sqked = sqrt(e*(2.+e));
  kd1 = 1.+e+sqked;
  kd2 = 1.+e-sqked;
  ke2 = 1.-ln(kd1/kd2);
  ke3 = 4./3. + ke2*(1.+e)*((e-1.)/(2.+e));
  if (ke3 < 0) ke3 = 0;
```

Calculation method:
● Calculation using cross-section tables of elements
○ Calculation using the formula

Photon photoelectric absorption cross-section

Point	Energy (keV)	Energy error	Value (sq cm/g)	Error
0	1	0	3149.7	0
1	1.5	0	1063.4	0
2	1.56	0	953.82	0
3	1.56	0	1695.9	0
4	1.839	0	1120.5	0
5	1.839	0	1754.1	0
6	2	0	1463.6	0
7	3	0	497.5	0
8	4	0	224.81	0
9	5	0	119.58	0
10	6	0	70.752	0
11	8	0	30.467	0
12	10	0	15.666	0
13	15	0	4.5755	0
14	20	0	1.8801	0
15	30	0	0.5267	0
16	40	0	0.211	0
17	50	0	0.10327	0

Parameters of results table:

Energy boundaries (keV): 1 10000
Number of points 1996

The operator has the ability to calculate cross-section tables for three types of reactions of interaction of gamma radiation with matter and the mean free path of alpha and beta particles:

- **Photoelectric absorption** – absorption of a gamma quantum as a result of a photoelectric effect in the substance.
- **Compton scattering** – scattering of gamma quanta on electrons of atoms.
- **Effect of pair formation** – formation of electron+positron pairs by gamma quanta in the substance.
- **Beta particle mean free path** – the extrapolated mean free path of beta particles in the substance;
- **The range of alpha particles** – the mean free path of alpha particles in the substance.
- **Total absorption of gamma quanta** – the sum of the cross sections of the photoelectric effect, Compton scattering and the effect of pair formation.

Since various methods of preparing counting samples change its chemical composition, cross-section tables are calculated one way or another for three types of preparation of a counting sample: **native sample**, **physical concentration** and **chemical selection**. Since the Compton scattering and the beta particle mean free path are weakly dependent on the chemical composition of the counting sample, it is possible to create cross-section tables for them without taking into account the chemical composition (**Ignore chemical composition**).

The basic procedure provides two calculation methods: **calculation using cross-sections tables of elements** and **calculation using formula**. The calculation according to the tables of sections for the elements is performed according to the tables published on the website https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html.

If, for some reason, the operator does not trust the data from this site, he can either manually enter any cross-section tables, or calculate them using a given formula.

The calculation according to the formula takes place according to the **calculation procedure (Calculation routine)** specified by the operator. When the form is first called, the calculation procedures will contain formulas used by the "SPECTRRAD" program by default. The operator can create his own calculation procedure and save it by pressing the  key. At this, three files corresponding to the selected radiation-substance interaction reaction are saved in the "**Sample types**" folder: **Name.h, Name.c** and **Name.obj**. The **name** is determined by the type of reaction:

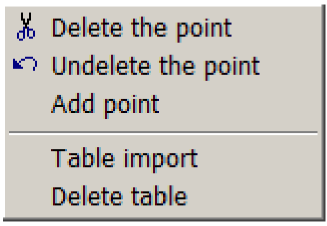
Type of reaction	**Files names**
Photo effect	RsPhoto
Compton scattering	RsCompton
Effect of pairs formation	RsPair
Beta particle mean free path	RsBeta
Alpha particle mean free path	RsAlpha

The **Name.h** file contains a list of variables used in the calculation loaded in the "**Constants and variables**" field, the file **Name.c** is the text of the calculation procedure in the language of the built–in programmable calculator and **Name.obj** is the compiled module of the cross-section calculation procedure, which will be used by the program when calculating the absorption of radiation in the substance of the counting sample, media substance or shield material.

On subsequent calls to the reaction cross-section calculation form, the text from the corresponding files **Name.h** and **Name.c** will be loaded into the fields of the form "**Constants and variables**" and "**Calculation routine**".

The  button starts the calculation procedure using the generated formulas of the cross-section table of selected reactions for a given type of procedure for preparing counting samples: **native sample, physical concentration** and **chemical selection**, or without taking into account the chemical composition (**Ignore chemical composition**). The calculation is performed for the selected type of sample with a specified chemical composition of the counting sample in the specified **energy boundaries** with a specified **number of points** in the table.

Such a table is stored in a folder of the appropriate sample type. The table can be edited, imported from the section tables downloaded from the site https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html or just enter it manually, if we know the data of such sections for the selected material (**sample type**). To edit or create a table, use a small menu called by right-clicking on the leftmost cell of the selected table row:



. Switching to the data editing mode in a table cell is performed by clicking the left mouse button on the selected cell.

To save the calculated or edited table, press the ✓ Save key. The Graph button allows you to view the table as a graph. You can open the saved table by clicking on the Open button (in the mode of calling the table editing procedure "**Edit / Cross-sections / Edit...**").

The reaction cross-section table for a given sample material can most correctly display the real values of such cross-sections (the formula, even very complex, cannot display the resonant sections present in the real functions of the dependence of the cross-sections on the radiation energy). Therefore, in the "SPECTRRAD" package, the procedure for calculating the attenuation of radiation in the substance, first of all, searches in the folder of a given type of sample for a cross-section table for the required reaction. If it does not find it, it uses the calculation formula created by the operator (the **Name.obj** file in the "**Sample types**" folder). And if the formula is not specified by the operator, it uses built-in formulas to calculate cross sections and mean free path values. For Compton scattering and beta particle mean free path, if the program has not found a cross-section table in the folder of a given sample type, it tries to find a cross-section table common to all materials (excluding chemical composition) in the "**Sample types**" folder. And only if there is no general table of sections (mean free path), the calculation is performed using formulas.

Norms

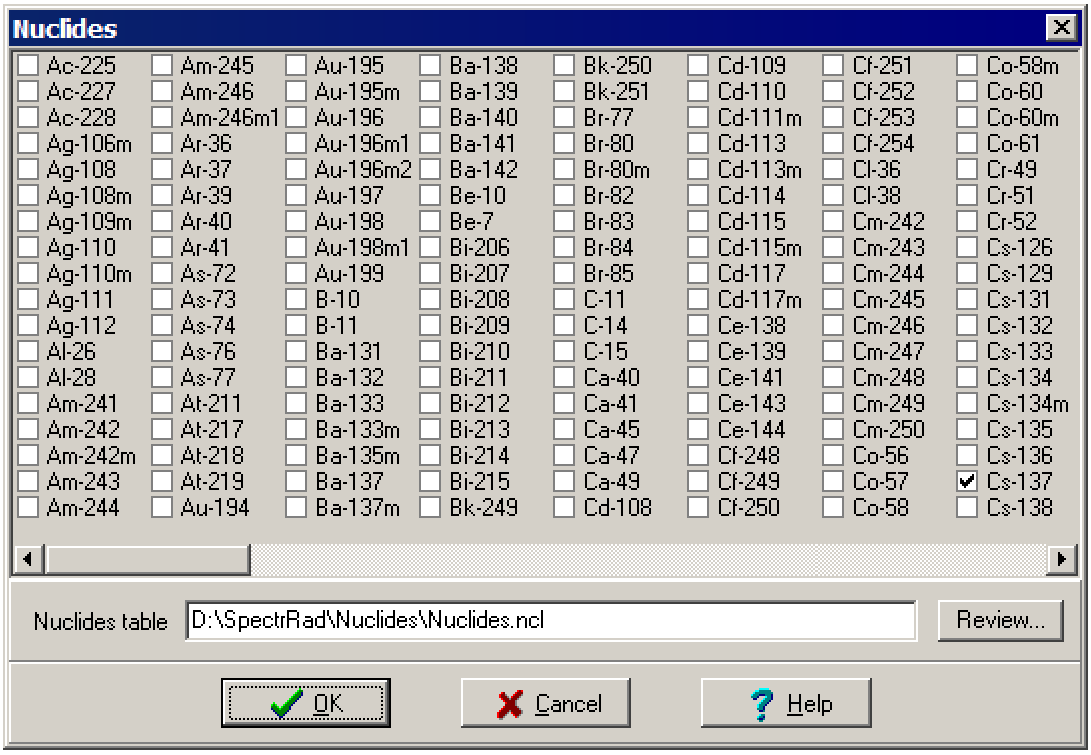
Four constants (**Norm 1 – Norm 4**) for the selected set of nuclides set the boundary values for determining the class of the sample material according to the level of radiation safety. The values of all four levels are available only through a programmable calculator. The value of the first level (**Norm 1**) is used by the report generation procedures as an acceptable level for all types of samples (SanPiN standards, standards of the Technical Regulations of the customs agreement, etc.).

Norm 5 is used by the report generation procedure as the coefficient of nonequilibrium **Kneq**. In the event that the activity of a nuclide A_{N1} in the equilibrium chain is determined through the activity of another nuclide A_{N2}, the nonequilibrium coefficient *N2* relative to *N1* is defined as $K_{neq} = \frac{A_{N1} - A_{N2}}{A_{N1}}$. In this case, the activity of nuclide *N1* is calculated using the formula $A_{N1} = A_{N2} / (1 - K_{ntq})$ (1).

The nonequilibrium coefficient is determined by processes that are not taken into account by the procedures for calculating the response of the spectrometer to radiation from the equilibrium chain of nuclides: the emanation of gaseous decay products from the sample, different solubility of nuclides in solvents, etc. A well–known example is the determination of the activity of Ra-226 by the express method (without 20 days exposure in an airtight vessel) from the radiation of daughter Rn-222. In this case, the nonequilibrium coefficient will be mainly determined by the emanation coefficient Rn-222 from the counting sample. The calculation according to formula (1) is performed only if the "**Take into account the coefficient of nonequilibrium**" checkbox is selected in the report generation parameters.

Editing the list of nuclides

The menu item "**Edit / Add/Delete nuclides...**", the button allows the operator to change the list of nuclides for the selected sample type. At the same time, a window with a table of the working library of nuclides is displayed on the screen:



☐ Ac-225
☐ Ac-227
☐ Ac-228
☐ Ag-106m
☐ Ag-108
☐ Ag-108m
☐ Ag-109m
☐ Ag-110
☐ Ag-110m
☐ Ag-111
☐ Ag-112
☐ Al-26
☐ Al-28
☐ Am-241
☐ Am-242
☐ Am-242m
☐ Am-243
☐ Am-244
☐ Am-245
☐ Am-246
☐ Am-246m1
☐ Ar-36
☐ Ar-37
☐ Ar-39
☐ Ar-40
☐ Ar-41
☐ As-72
☐ As-73
☐ As-74
☐ As-76
☐ As-77
☐ At-211
☐ At-217
☐ At-218
☐ At-219
☐ Au-194
☐ Au-195
☐ Au-195m
☐ Au-196
☐ Au-196m1
☐ Au-196m2
☐ Au-197
☐ Au-198
☐ Au-198m1
☐ Au-199
☐ B-10
☐ B-11
☐ Ba-131
☐ Ba-132
☐ Ba-133
☐ Ba-133m
☐ Ba-135m
☐ Ba-137
☐ Ba-137m
☐ Ba-138
☐ Ba-139
☐ Ba-140
☐ Ba-141
☐ Ba-142
☐ Be-10
☐ Be-7
☐ Bi-206
☐ Bi-207
☐ Bi-208
☐ Bi-209
☐ Bi-210
☐ Bi-211
☐ Bi-212
☐ Bi-213
☐ Bi-214
☐ Bi-215
☐ Bk-249
☐ Bk-250
☐ Bk-251
☐ Br-77
☐ Br-80
☐ Br-80m
☐ Br-82
☐ Br-83
☐ Br-84
☐ Br-85
☐ C-11
☐ C-14
☐ C-15
☐ Ca-40
☐ Ca-41
☐ Ca-45
☐ Ca-47
☐ Ca-49
☐ Cd-108
☐ Cd-109
☐ Cd-110
☐ Cd-111m
☐ Cd-113
☐ Cd-113m
☐ Cd-114
☐ Cd-115
☐ Cd-115m
☐ Cd-117
☐ Cd-117m
☐ Ce-138
☐ Ce-139
☐ Ce-141
☐ Ce-143
☐ Ce-144
☐ Cf-248
☐ Cf-249
☐ Cf-250
☐ Cf-251
☐ Cf-252
☐ Cf-253
☐ Cf-254
☐ Cl-36
☐ Cl-38
☐ Cm-242
☐ Cm-243
☐ Cm-244
☐ Cm-245
☐ Cm-246
☐ Cm-247
☐ Cm-248
☐ Cm-249
☐ Cm-250
☐ Co-56
☐ Co-57
☐ Co-58
☐ Co-58m
☐ Co-60
☐ Co-60m
☐ Co-61
☐ Cr-49
☐ Cr-51
☐ Cr-52
☐ Cs-126
☐ Cs-129
☐ Cs-131
☐ Cs-132
☐ Cs-133
☐ Cs-134
☐ Cs-134m
☐ Cs-135
☐ Cs-136
☑ Cs-137
☐ Cs-138

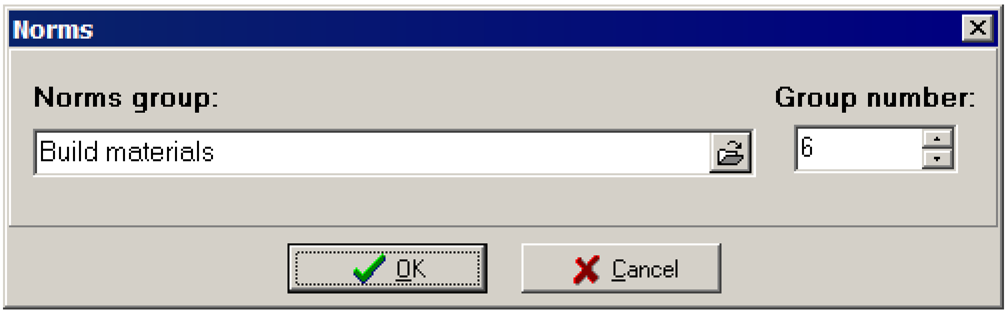
Nuclides table: D:\SpectrRad\Nuclides\Nuclides.ncl

To set the norms of total and effective activity, the list of nuclides of the working library is supplemented with four conditional "nuclides": **SumAct-A, SumAct-B, SumAct-G** and **EffEct-G**, corresponding to three types of total activity (alpha, beta and gamma) and effective (reduced by ionization effect to Ra-226 radiation) the gamma of activity.

The operator must mark the necessary nuclides with "ticks" to include them in the list

Editing a group of standards

The menu item "**Edit / Edit group...**" allows the operator to change the group number for the selected group of sample types. At the same time, the following window is displayed on the screen:



Norms group: Build materials

Group number: 6

The operator has the opportunity to select a group of standards and set its number. When you press the "**OK**" key, the group number for all standards included in the selected group will be changed to the specified one.

The value of a group of standards is used in a programmable calculator. In the processing templates provided in the installation package, the group number is used to select the report template. The following values of the group numbers are used:

0 - the group is not defined, the report in the form of an MS Word document is not generated.
1 - food raw materials and food products.
2 - not used.
3 - baby food products.
4 - forestry products.
5 - ceramic products.
6 - building materials.
7 - materials with a high content of NRE.
8 - soil.
9 - water.
10 - snow.

Tables of nuclides

In spectrometric complexes designed to measure the radionuclide composition of samples, nuclide tables are necessary both for calibration of spectrometers and for processing the spectra of working samples. Accounting for the decay of nuclides during the time from sampling or certification of the nuclides activity to the moment of measurement, the decay of nuclides during measurement, the decay of reference sources during operation, the generation of spectra from line tables all requires data on nuclides, which are stored in nuclide tables.

Several such tables are required, since different types of samples, sampling methods, and sample preparation methods form equilibrium radioactive chains of nuclides in samples in different ways. For example: it is reasonable to determine the activity of Th-232 in soil samples on a gamma spectrometer for all daughter nuclides of the decay chain, since Th-232 is usually in a state of radioactive equilibrium in soils, in water, with a high probability, the equilibrium is disturbed, and somewhere in a laboratory for the production of radioisotopes this thorium can to be completely without children.

In the software package "**SPECTRRAD**", the menu item "**Tools / Nuclides table...**" calls the program "**SpectrRadNucl**" (executable file "**SpectrRadNucl.exe**") - a program for viewing, creating and editing nuclide tables.

Data available on the Internet can be used to create nuclide tables - http://www.nndc.bnl.gov/ensdf /.

Tables structure

In the "**SPECTRRAD**" package, information about nuclides (atomic weight, half-life, gamma equivalent of radium, abundance, energy, and quantum yield of lines) is stored in five files linked by a common name. The file with the extension "**ncl**" contains information about atomic weights, half-lives, abundance, gamma equivalent of radium, and the decay pattern of nuclides. The file with the "**gml**" extension contains information about the X-ray and gamma lines of the nuclide, the file with the "**btl**" extension contains information about the beta lines of the nuclide, the file with the "**aln**" extension contains information about the alpha lines of the nuclide, and the text file with the "**txt**" extension contains a description of the table.

Each entry in the isotope table (file with the extension "**ncl**") has the following structure:

Field name	Length (bytes)	Description
Nuclide	**8**	The short name of the nuclide.
Synonym	**40**	The name of the nuclide.
Atomic mass	**4**	The atomic weight of the nuclide.
Half-life	**8**	The value and abbreviated name of the unit for the half-life of the nuclide.
Element	**2**	The name of the element for naturally radioactive nuclides, which includes a nuclide.
Abundance	**4**	The amount of naturally radioactive nuclide in the element as a percentage.
Gamma-Eq. Ra-226	**4**	The gamma equivalent of Ra-226 is the gamma coefficient of the nuclide yield relative to the yield of Ra-226. If the coefficient is different from zero, the contribution of the nuclide will be taken into account by the procedure for calculating the total effective activity of the sample.
Attributes	**4**	Four symbols defining some characteristics of the

		nuclide. The attribute values are given in the following table.
First child	**12**	The name of the 1st child nuclide and the branching coefficient as a percentage.
Second child	**12**	The name of the 2nd child nuclide and the branching coefficient.
Third child	**12**	The name of its 3-child nuclide and the corresponding branching coefficient.

Attribute	Meaning	Description
Attribute 1	**Space**	The nuclide is included in the list of active ones.
	@	The nuclide is excluded. The nuclide is present in the list of isotopes, but is not taken into account by spectrum processing programs and equilibrium chain formation procedures. The operator has the option to include a nuclide by changing its attribute.
Attribute 2	**0-9**	The rank of a nuclide is a number from zero to nine. The larger the number, the higher the rank of the nuclide. The processing program uses the rank of the nuclide if it is necessary to remove the nuclide from the list of equations determined in case of degeneracy of the solved system of equations (nuclides have matching lines). A nuclide with a lower rank is removed. If the nuclides are of equal rank, the program will give the operator a choice.
Attribute 3	**Space**	A single nuclide.
	P	The nuclide forms an equilibrium decay chain.
	C	The nuclide is included in the equilibrium chain (all nuclide lines are included in the list of lines forming the nuclide chain).
	p	The nuclide forms a copy of a part of the equilibrium decay chain included in another equilibrium chain. Since individual nuclides and parts of equilibrium chains can be used in the formation of other equilibrium chains, the program generates copies of such nuclides or parts of chains, if necessary.
	n	A nuclide is a copy of a nuclide included in the equilibrium chain.
	V	A "virtual" nuclide. A virtual nuclide can be either a single nuclide or a formed chain of nuclides. The virtual nuclide has no kinship relations and does not participate in the procedures for the automatic determination of the nuclide composition of the spectrum.
Attribute 4		The number of nuclides included in the equilibrium chain.

The line table entries (files with the extension "**aln**", "**btl**" and "**gml**") have the following structure:

NN	Type of radiation	Field name	Length (bytes)	Description
1	**All kinds**	**Nuclide**	**8**	The name of a single nuclide or nuclide

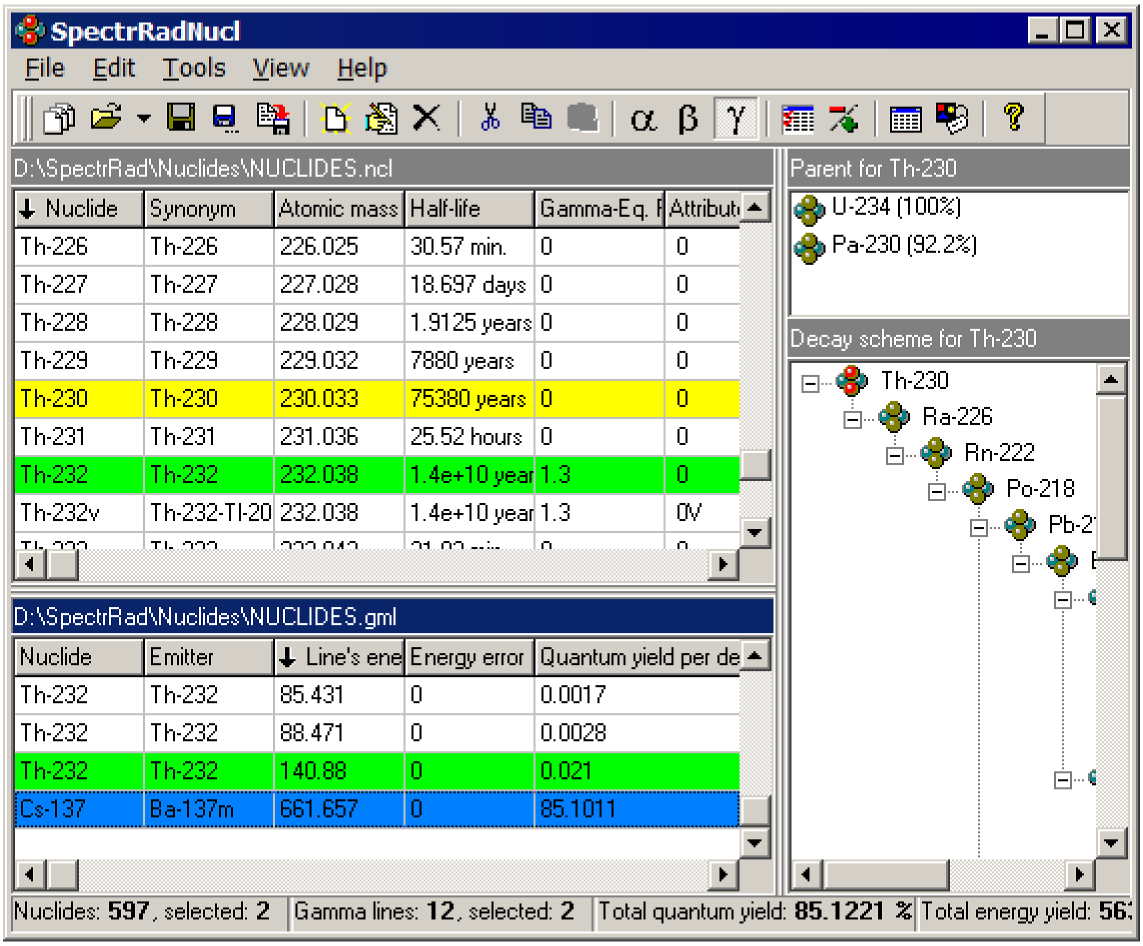
				forming an equilibrium chain.
2	**All kinds**	**Emitter**	**8**	The name of the nuclide emitter for this line. In the case of a chain, the name of the emitter nuclide may differ from the name of the nuclide.
3	**Alpha**	**Line’s energy**	**4**	The energy of the alpha line.
	Beta	**Beta’s maximum energy**		The boundary energy of the beta line.
	Gamma	**Line’s energy**		The energy of the gamma line.
4	**All kinds**	**Energy error**	**4**	The error of the energy value in the same units as the energy. The energy error for calibration lines is used by calibration procedures as the energy range in which the peak corresponding to this line will be searched.
5	**All kinds**	**Quantum yield per decay**	**4**	The quantum yield of the line as a percentage. For gamma escape lines, the output of the mother line is indicated. For the gamma line of cascade addition, the output of the first line in the cascade.
6	**All kinds**	**Yield error**	**4**	Uncertainty of the quantum output
7	**Alpha**		**4**	Not used.
	Beta	**Beta’s mean energy**		The average energy of the beta line.
	Gamma	**Internal conversion coefficient**		The internal conversion coefficient is equal to the ratio of the number of internal conversion electrons to the number of gamma quanta during the transition of the nucleus from one excited state to another.
8	**Alpha**		**4**	Not used.
	Beta			Not used.
	Gamma	**List of the cascade transitions**		A pointer to the list of cascading transitions.
9	**All kinds**	**Attributes**	**4**	Four symbols defining some characteristics of the line. The attribute values are given in the following table.

Attribute	Meaning	Description
Attribute 1	**Space** **0-9**	The line is included in the list of active ones. For gamma lines, the number from 0 to 9 is the number from the list of nuclear reactions that formed the gamma line.
	@	The line is excluded. The line is present in the list of lines, but is not taken into account by spectrum processing programs and

		equilibrium chain formation procedures. The operator has the option to enable the line by changing its attribute.
Attribute 2	**Space**	The simple line.
	%	A "significant" line. When creating a processing template, the operator has the opportunity to use only "significant" lines to evaluate nuclide activities. Only the "significant" lines are used to create a list of nuclides forming an unknown peak in scintillation gamma spectrometry.
	!	The "calibration" line. The "calibration" line is also "significant". Calibration lines are used for automatic energy calibration of spectrometers.
	?	A line with an unknown or unreliable quantum output. It is not used for evaluating activities.
Attribute 3-4	**Spaces**	The simple gamma or alpha line.
	0-9	The gamma line. The letters from "**A**" to "**Z**" - the transition level are used instead of a space in order to mark as different gamma lines with the same energies, but related to different decay schemes, Such energy-matching lines may have different cascade transitions and therefore they cannot be combined.
	X	The X-ray line.
	A	The annihilation line.
	E1	Single escape line.
	E2	Double escape line.
	S2	The addition line for two cascading transitions.
	S3	The addition line for three cascading transitions.
	B+	Beta positron.
	B-	Beta electron.
	e	Electron.

"SpectrRadNucl" program. Main window

The program window depends on the program settings and may, for example, look like:



D:\SpectrRad\Nuclides\NUCLIDES.ncl

Nuclide	Synonym	Atomic mass	Half-life	Gamma-Eq. f	Attribut
Th-226	Th-226	226.025	30.57 min.	0	0
Th-227	Th-227	227.028	18.697 days	0	0
Th-228	Th-228	228.029	1.9125 years	0	0
Th-229	Th-229	229.032	7880 years	0	0
Th-230	Th-230	230.033	75380 years	0	0
Th-231	Th-231	231.036	25.52 hours	0	0
Th-232	Th-232	232.038	1.4e+10 year	1.3	0
Th-232v	Th-232-Tl-20	232.038	1.4e+10 year	1.3	0V

D:\SpectrRad\Nuclides\NUCLIDES.gml

Nuclide	Emitter	Line's ene	Energy error	Quantum yield per de
Th-232	Th-232	85.431	0	0.0017
Th-232	Th-232	88.471	0	0.0028
Th-232	Th-232	140.88	0	0.021
Cs-137	Ba-137m	661.657	0	85.1011

Nuclides: **597**, selected: **2** | Gamma lines: **12**, selected: **2** | Total quantum yield: **85.1221 %** | Total energy yield: 56

In the upper part of the window there are menus and toolbar buttons, providing more convenient access to the main menu items.

In the upper left part of the window there is an isotope table of the open nuclide table (**D:\SpectrRad\Nuclides\Nuclides.ncl**), in the lower left - a table of nuclide lines, in the right part of the window: at the top - a list of parent for the selected nuclide, at the bottom - a decay scheme of the selected nuclide. At the bottom is a line of information about the number of nuclides and lines in the table and the number of selected records.

In the table of isotopes and lines, one of the entries (rows of the table) is working (or active). Such an entry is marked in yellow (if the current entry is one of a group of selected entries, its color changes to blue). The list of parent nuclides and the decay scheme in the right part of the window refer to the nuclide of the working entry of the nuclide table. The cursor keys up and down on the computer keyboard move the work record accordingly. Pressing the "**Home**" and "**End**" keys makes the first or last record of the table active, respectively. Clicking on an entry makes it active.

The operator can select a group of records (one record is a special case of a group), marking them with the mouse when the "**Ctrl**" key is pressed, you can mark the group by clicking on the last record in the group when the "**Shift**" key is pressed - the group from the current record to the last one will be marked. Moving the cursor up or down the table while pressing the "**Shift**" key or pressing the "**Insert**" key, operator can change the selection of records. The selected records are marked in green and participate in group operations of editing records, copying or clipping to the clipboard.

The alpha, beta or gamma lines of either all or selected nuclides of the isotope table are displayed in the line table, depending on the position of the switch (menu item "**View / All lines**"). The type of radiation is determined by the switch α β γ (menu items: "**View / Alpha lines / Beta lines / Gamma lines**"). If the output mode of the selected nuclide lines is set, but there are no selected nuclides, the nuclide lines of the working record are output, if there are selected nuclides, the nuclide lines of the working record are not included in the list of lines.

The width of the columns (fields) of the table can be adjusted by the operator. To do this, place the mouse pointer on the border between the fields, while the mouse pointer will take the form and, holding down the left mouse button, drag the border to the desired position.

The table entries can be sorted by the values of any column in the table - just click on the button with the column name. The sorting direction is indicated by an arrow to the left of the column name.

The right mouse button opens a menu, the contents of which change depending on the position of the mouse pointer and the moment of the call. Some of the menu items duplicate the functions of the main menu.

Double-clicking on any entry in the nuclide or line table triggers the editing procedure for either the selected nuclides or lines, or the line or nuclide of this entry, if there are no selected entries.

Clicking on the nuclide icon in the list of parent nuclides or the decay scheme makes the entry of this nuclide active in the isotope table. In this case, the principle is violated that the list of maternal and the decay scheme refer to the active entry of the isotope table - in this case, neither the list of maternal nor the decay scheme are changed. This is done specifically so that the operator can view information about the nuclides of the decay scheme or the list of parent ones. The decay scheme and the list of parent ones will be generated for the active record only if it is selected by the operator directly in the isotope table window.

When forming the decay scheme, two types of pictograms are used: the icon is used to indicate a single nuclide, and the icon is used to indicate the equilibrium chain of nuclides[23]. The nucleons of unstable nuclei are drawn in two different colors, while the nucleons of stable nuclei are drawn in one color. The icon of the selected nuclide stands out in brighter colors - . To the right of the nuclide icon, its name is displayed (the name of the nuclide forming the chain for chains) and in parentheses the branching coefficient as a percentage, if it is not equal to 100%. On the left is an icon indicating whether the decay scheme of this nuclide is open or collapsed. The ⊞ sign in front of the nuclide icon indicates that the scheme is not disclosed. To open it, click on the ⊞ icon. Double-clicking on the nuclide icon either reveals the decay scheme if it is collapsed, or collapses if the scheme is opened.

The information bar at the bottom of the program window contains information about the number of nuclides and lines in the table, the number of selected and excluded entries:  Nuclides: **599**, selected: **2**, excluded: **2** Gamma lines: **12**, selected: **2**, excluded: **1** and the total quantum and energy output of the selected lines. The energy output of a line is the product of the energy of the line and its intensity.

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[23] An **equilibrium chain** is a chain of nuclides in a state of radioactive equilibrium (the activity of the daughter is in dynamic equilibrium with the activity of the parent nuclide). In the equilibrium chain, the radiation of daughter nuclides is included in the list of maternal lines in accordance with the quantum yield of the daughter lines, the branching coefficient in the decay chain and the ratio of half-lives assuming a radioactive equilibrium between the parent nuclide and daughter nuclides.

Menu

Menu item	*Action*
File:	
New	Create a new nuclide table.
Open… **Ctrl+O**	Open an existing nuclide table. Clicking on the right side of the ▾ button displays a list of previously opened nuclide tables.
Save **Ctrl+S**	Save changes to the nuclide table.
Save as…	Save the table under a new name.
Exit	Close the program.
Edit:	
Save selected… **Shift+Ctrl+S**	Save the selected nuclides in a new nuclide table.
New nuclide… **New line…** **Ctrl+N**	Create a new entry in the isotope or line table.
Edit… **Ctrl+E**	Editing records. If there are no selected entries, the working (active) one is edited. If there are selected ones, the selected ones are edited. If several records are selected, only the fields of the table are available for editing, which may be the same for a group of records.
Rename nuclide… **Ctrl+R**	Rename the nuclide. The synonym of the nuclide does not change.
Save nuclide as virtual…	Create a "virtual" nuclide based on the selected nuclide or the formed chain of nuclides. A virtual nuclide, unlike a conventional one, has no kinship relationships and does not participate in the procedures for automatic analysis of the nuclide composition of spectra.
Delete… **Shift+Del**	Delete selected entries.
Cut **Ctrl+X**	Move the selected part of the records to the clipboard.
Copy **Ctrl+C**	Copy the selected part of the records to the clipboard.

---

[24] The save, clipboard, and delete operations for the isotope table also include operations with alpha, beta, and gamma lines of the corresponding nuclides.

Paste 📋 **Ctrl+V**	Paste entries from the clipboard. You cannot insert nuclide records into the line table and line records into the isotopes table. Gamma lines cannot be inserted into the alpha or beta lines table. Lines of a certain type can only be inserted into a table of lines of the same type. Therefore, before inserting, it is necessary to switch to the required table of isotopes or lines.
Find:	
First child	Find the 1st child for the selected nuclide. You can switch to the child by clicking on the child nuclide in the decay scheme, but for excluded nuclides, the search works, but there is no decay scheme.
Second child	Find the 2nd child for the selected nuclide.
Third child	Find the 3rd child for the selected nuclide.
Orphan lines	Find the lines related to the nuclides missing from the isotopes table. Such lines can be formed during incorrect line insertion operations and are ballast, since they will not participate in spectrum processing operations.
Select:	
Select all ***Ctrl+A***	Select all entries.
Decay chain	Select the decay chain of the selected nuclide.
Invert selection ***Ctrl+I***	Invert the selection of records.
Unselect all ***Del***	Deselect all records.
Tools:	
Nuclides activity…	Calculate the activity of the nuclides of the selected branch of the decay scheme on a given date.
Nuclides equilibrium chain:	
Construct…	Form an equilibrium chain from the nuclide decay scheme.
Deconstruct…	Disband the equilibrium chain of the nuclide into a decay scheme.
Deconstruct all chains…	Disband all the equilibrium chains of nuclides formed in the table.
Nuclides mixture…	Create a conditional nuclide, which is a mixture of two or three nuclides selected by the operator in a given ratio.

Escape lines:	
Include in the table...	Include single and double escape lines in the gamma line table for all gamma lines with energy exceeding the specified threshold.
Delete from the table	Remove single and double escape lines from the table.
Addition lines of cascading transitions:	
Include in the table...	Include the lines corresponding to the peaks of summation of two and three cascade transitions in the gamma line table.
Delete from the table	Remove the addition lines of cascading transitions from the table.
Certificate of the standard source…	Creating or editing a "certificate of reference" is a procedure that allows you to supplement the nuclide table with data on the activities and errors of the nuclide activities of the table. The "Certificate of reference" makes the spectrometer calibration procedure more convenient.
Text table…	Generate a text table for selected nuclides or lines to print or transfer to WORD or EXCEL.
Customising…	Setting up the view of nuclide tables and lines table.
License…	View the current license.

View:

Alpha lines α	Switch to the alpha line table. The program form allows you to show only one of the three line tables of the nuclide table. The pressed state of the key means that alpha lines of nuclides are displayed in the line table.
Beta lines β	Switch to the beta line table.
Gamma lines γ	Switch to the gamma line table.
All lines **Ctrl+M**	The line table displays either the lines of the selected nuclides of the isotope table, or the lines of all nuclides. The pressed state of the key corresponds to the output of all lines.
Decay tree	Show the scheme of nuclide decay.
Show excluded records	Enabling or disabling the output mode for entries marked as "excluded". When the "excluded" mode is enabled, entries are displayed with the icon ❌ or ❎ in the Attributes column. The ❌ icon means that the nuclide is excluded by the operator. The ❎ icon means that the nuclide is included in the decay chain

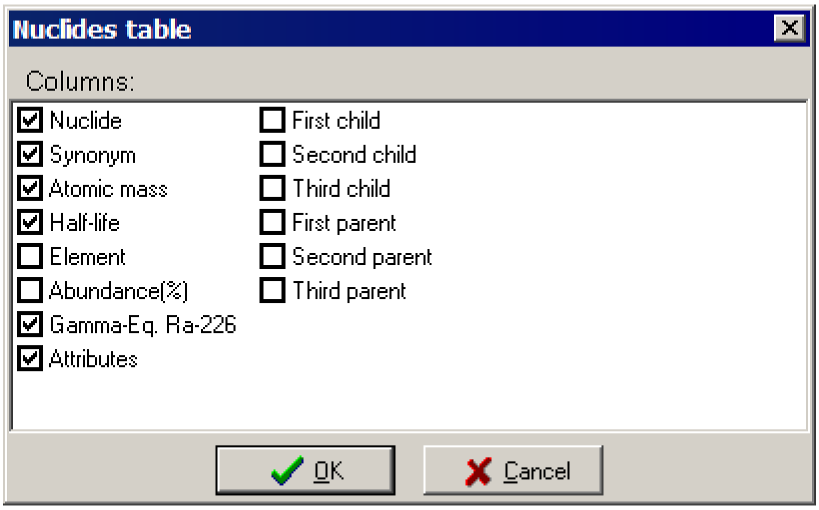
Help:

Content ?	**F1**	Description of the program.
About nuclides table…		Description of the nuclide table.
About program…		Brief information about the program.

Configuring the program

The number of columns to be visualized and their names in the lists of isotopes and lines are set by the operator in the program setup procedure. The procedure is called by clicking on the menu item "**Tools / Customizing...**" or on the button "**Customize table**" - . Depending on which table is active (the active table is highlighted in the header color), either the procedure for configuring the nuclide table or the line tables is called.

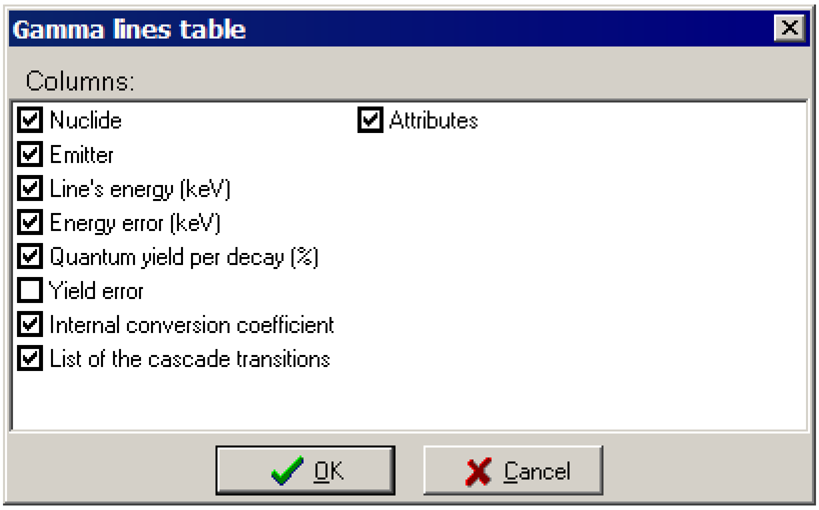
The window of the procedure for setting up the nuclide table may look like:



☑ Nuclide
☑ Synonym
☑ Atomic mass
☑ Half-life
☐ Element
☐ Abundance(%)
☑ Gamma-Eq. Ra-226
☑ Attributes
☐ First child
☐ Second child
☐ Third child
☐ First parent
☐ Second parent
☐ Third parent

Left-clicking on the square to the left of the column name enable or disable the column display mode in the table. Double-clicking on the column name allows editing the name. The operator can name the column as he likes, but its purpose will remain the same. The initial column names are restored when you enter an “empty” name.

The view of the window for setting up line tables depends on the type of radiation (alpha, beta or gamma). For gamma lines, the window can look like:



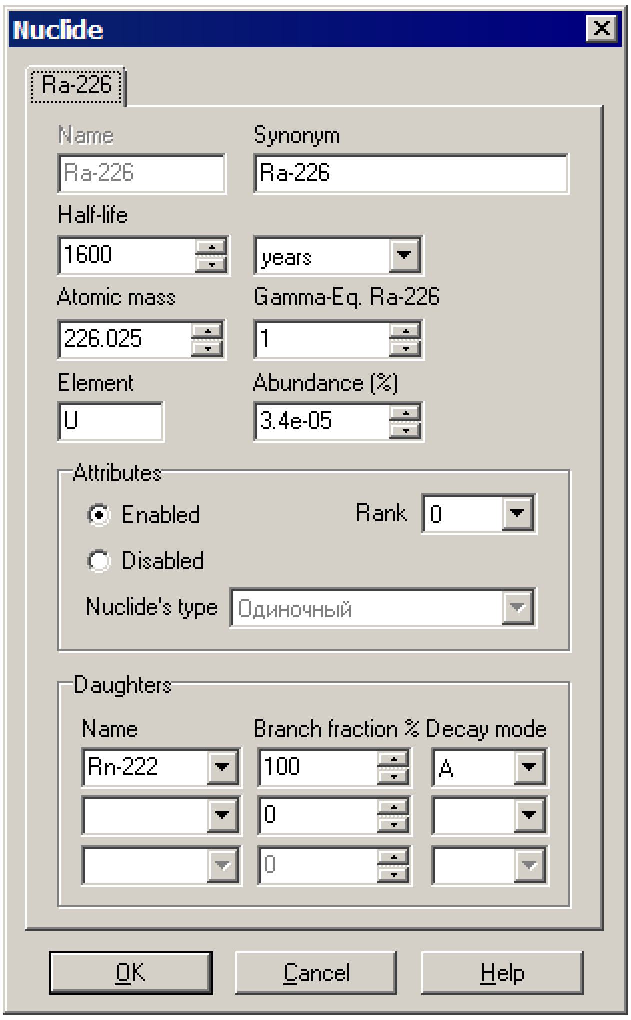
☑ Nuclide
☑ Emitter
☑ Line's energy (keV)
☑ Energy error (keV)
☑ Quantum yield per decay (%)
☐ Yield error
☑ Internal conversion coefficient
☑ List of the cascade transitions
☑ Attributes

The setup procedure is identical for all tables.

Editing records

The menu item "**Edit / Edit...**" or mouse click on the button "**Edit selected nuclides (Lines)**" opens the program for editing table entries. If there are selected records in the table, the selected ones are edited. If several records are selected, only the fields of the table are available for editing, which may be the same for a group of records. If there are no selected records, the working (active) record of the table is edited. Depending on which table is active (the active table is highlighted in the header color), either the procedure for editing the nuclide table or the line tables is called.

The window of the editing procedure for a single entry of the isotope table may look like:



Name: Ra-226
Synonym: Ra-226
Half-life: 1600 years
Atomic mass: 226.025
Gamma-Eq. Ra-226: 1
Element: U
Abundance (%): 3.4e-05
● Enabled
○ Disabled
Rank: 0
Nuclide's type: Одиночный

Name	Branch fraction %	Decay mode
Rn-222	100	A
	0	
	0	

The structure and purpose of the nuclide parameters are described in the chapter "Table structure". Type of nuclide: single, forms decay chain or is included in the decay chain, is formed by the equilibrium chain formation procedure and it is not recommended to change it manually.

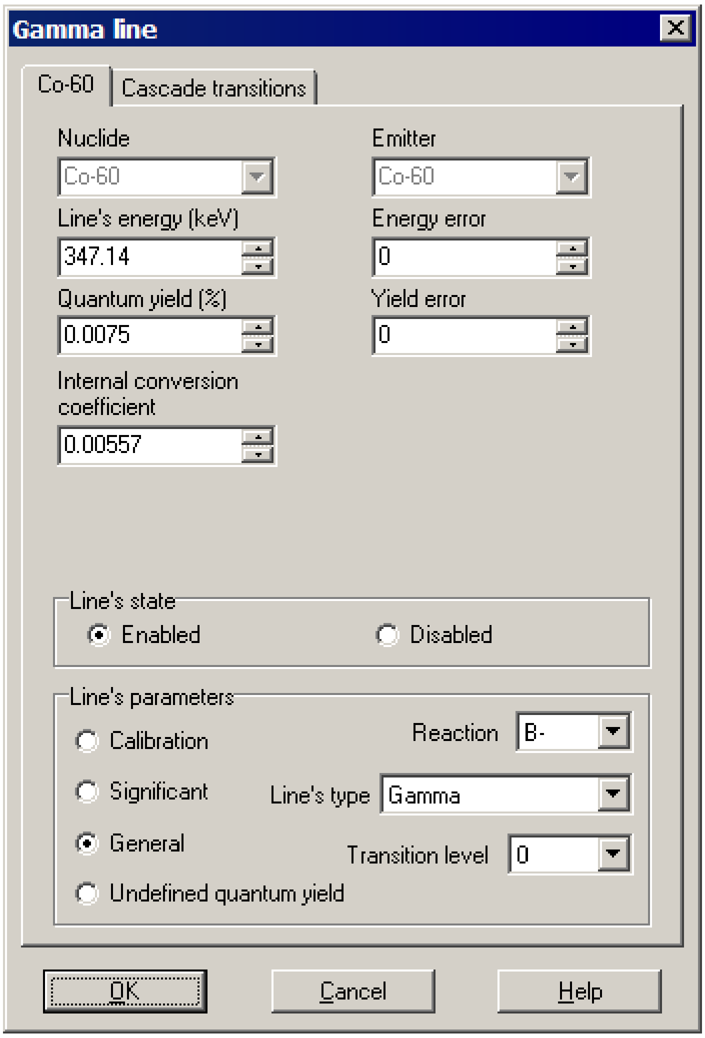
The type of decay (**Decay mode**) has the following values:

Designation	**Decay mode**
	not defined
A	alpha decay
B-	beta decay
B+	positron beta decay
EC	electron capture

EC+B+	electron capture + positron beta decay
IT	isomeric transition
SF	spontaneous fission
p	proton decay
n	neutron decay

The child nuclide must be present in the table; the type of decay and the name of the child nuclide are not controlled by the editing procedure.

The view of the window for editing line table entries depends on the type of radiation (alpha, beta or gamma). For gamma lines, the window can look like:



Nuclide: Co-60

Emitter: Co-60

Line's energy (keV): 347.14

Energy error: 0

Quantum yield (%): 0.0075

Yield error: 0

Internal conversion coefficient: 0.00557

Line's state: ● Enabled ○ Disabled

Line's parameters:
- ○ Calibration
- ○ Significant
- ● General
- ○ Undefined quantum yield

Reaction: B-

Line's type: Gamma

Transition level: 0

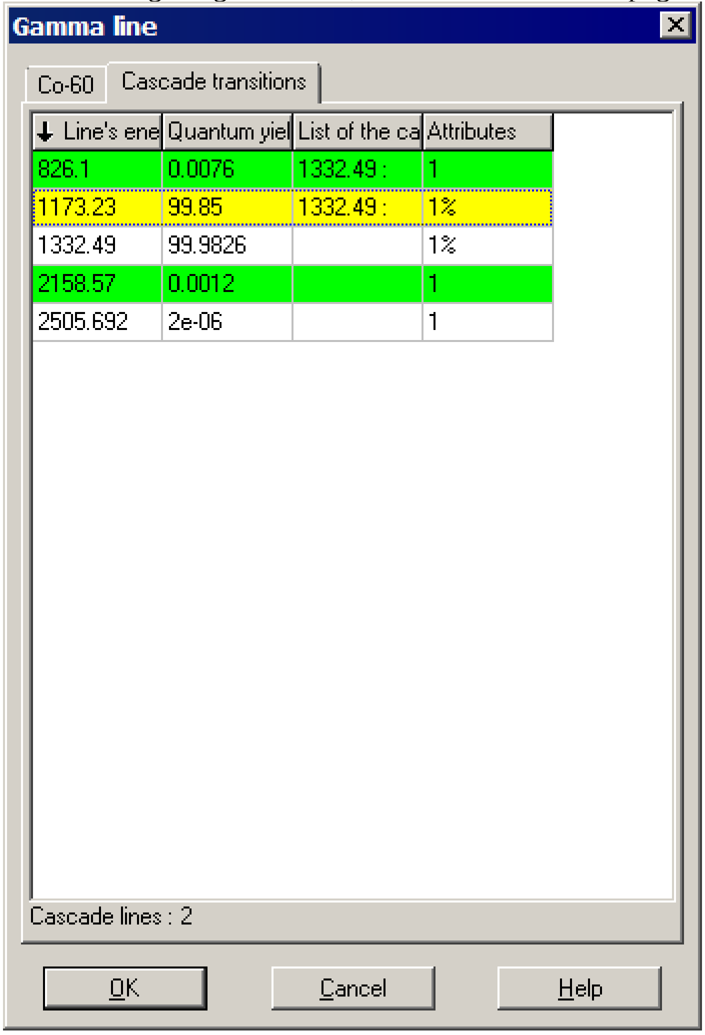
The structure and purpose of the line parameters are described in the chapter "Table Structure". The "**Reaction**" drop-down list includes symbols for nuclear reactions in which this gamma line is formed:

Reaction number	**Designation**	**Nuclear reaction**
		not defined
0	A	alpha decay

1	B-	beta decay
2	B+	positron beta decay
3	EC	electron capture
4	EC+B+	electron capture + positron beta decay
5	IT	isomeric transition
6	SF	spontaneous fission
7	p	proton decay
8	n	neutron decay

When editing in a group (multiple records are selected), only the fields of the table are available, which may be the same for a group of records. It is forbidden to change the line parameters created by the procedures for forming escape lines or adding cascading lines.

When editing the gamma line, the form has a second page "**Cascade transitions**":

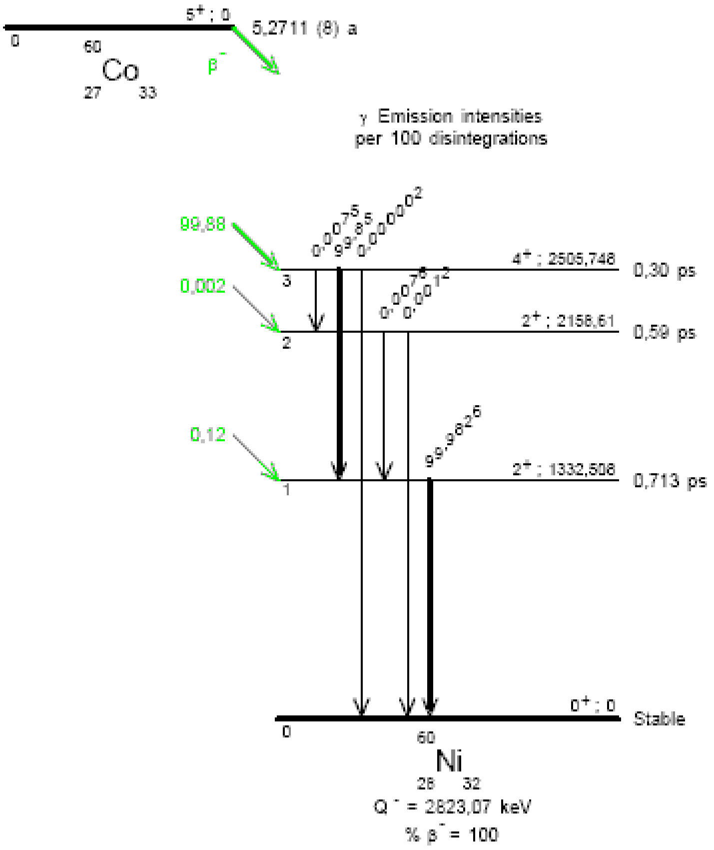


↓ Line's ene	Quantum yiel	List of the ca	Attributes
826.1	0.0076	1332.49 :	1
1173.23	99.85	1332.49 :	1%
1332.49	99.9826		1%
2158.57	0.0012		1
2505.692	2e-06		1

Cascade lines : 2

The table contains a list of all nuclide lines except the one being edited. The lines that form a direct cascade with the editable line are highlighted in green or blue. The operator can include the line in the cascade list or exclude it from it by double-clicking on the line or using the pop-up menu.

It must be remembered that it is required to mark as cascading only the lines that form a direct cascade with the editable one. For example, in the decay scheme of Co-60:



for the line formed by the transition from the 3rd level to the 2nd (Q=0.0075), it is required to specify as cascade lines formed by the transition of the nuclide from the 2nd level to the first (Q=0.0076) and from the second to the zero (Q=0.0012).

The procedure for forming a new record in the isotope or line table uses the form of the record editing procedure. The only difference is that in the form for creating a record about a new nuclide, the "**Name**" or "**Nuclide**" field is also available for modification, for entering the name of a new nuclide.

Construction of equilibrium chains

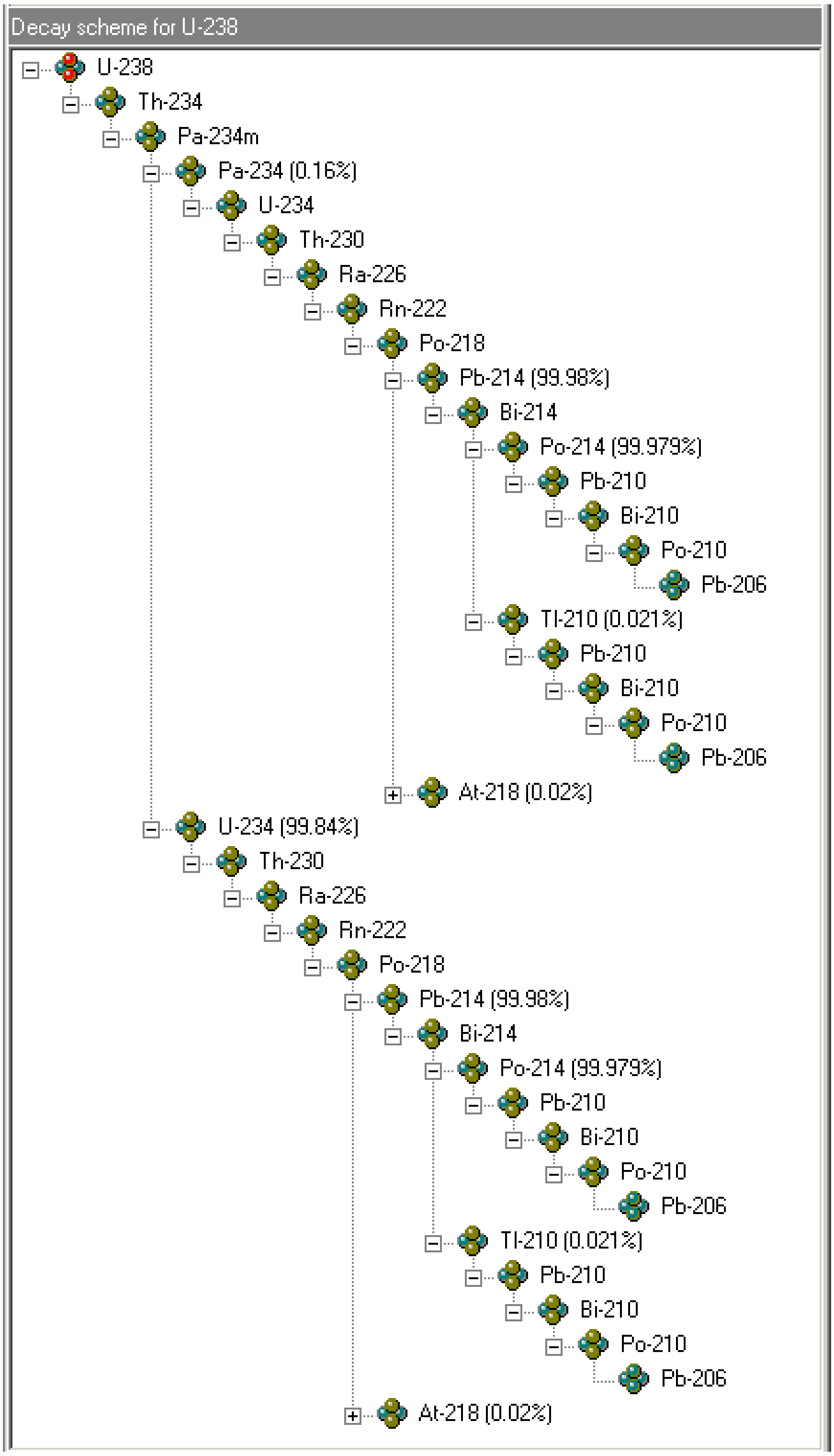
The theory of estimation rightly asserts that we will get effective estimates of measurement results (estimates with minimal uncertainty) when we minimize the number of unknowns to be determined and use all available reliable information to the maximum. Therefore, neglecting information about the relationships established at the time of measurement between the activities of nuclides in the decay chains of parent nuclides means sacrificing the effectiveness of estimates.

An equilibrium chain is a chain of nuclides in a state of radioactive equilibrium (the activity of the daughter is in dynamic equilibrium with the activity of the parent nuclide). In the equilibrium chain, the radiation of daughter nuclides is included in the list of maternal lines in accordance with the quantum yield of daughter lines and the values of the activities of daughter nuclides, assuming a radioactive equilibrium between the parent nuclide and daughter nuclides. A nuclide forming an equilibrium chain may not have its own alpha, beta or gamma radiation lines suitable for evaluating its activity, and radiation from daughter nuclides is used to determine activity. For example, in gamma spectrometry, the activity of Cs-137 is determined by the gamma radiation of the daughter Ba-137m, with which Cs-137 is almost always in a state of radioactive equilibrium.

Different types of samples, sampling methods, and sample preparation methods form equilibrium radioactive chains of nuclides in samples in different ways. For example: it is reasonable to determine the activity of Th-232 in soil samples on a gamma spectrometer for all daughter nuclides of the decay chain, since Th-232 is usually in a state of radioactive equilibrium in soils, in water, with a high probability, the equilibrium is disturbed, and somewhere in a laboratory for the production of radioisotopes this thorium can to be completely without daughter nuclides.

Therefore, the ability to create nuclide work tables with different equilibrium chains is mandatory for the program of creating and editing nuclide tables. In the program "**SpectrRadNucl**", the menu item "**Tools / Nuclides equilibrium chain / Construct...**" calls the procedure for forming an equilibrium chain from a nuclide decay scheme. The procedure for forming an equilibrium chain is performed either for **all nuclides of the disclosed tree** of the decay scheme, or only for the selected branch, depending on the selected nuclide of the scheme. If the parent nuclide of the decay tree is selected, the quantum yield is calculated for all nuclides in all branches of the disclosed decay scheme tree and the quantum yield of identical nuclides in different decay branches is summed up. If one of the nuclides in any branch of the decay scheme is selected, an equilibrium chain is formed for the nuclides of the selected part (from the selected to the parent) of this branch of the decay scheme. Stable nuclides are not included in the equilibrium chains. Therefore, if the decay branch ends with a stable nuclide, you need to choose the nuclide preceding the stable one.

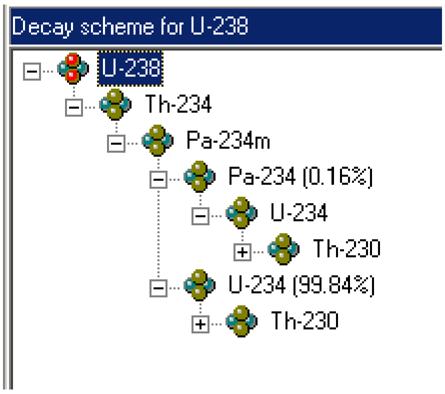
Let's consider the process of forming equilibrium chains using the example of creating such chains from the U-238 decay scheme.



Decay scheme for U-238

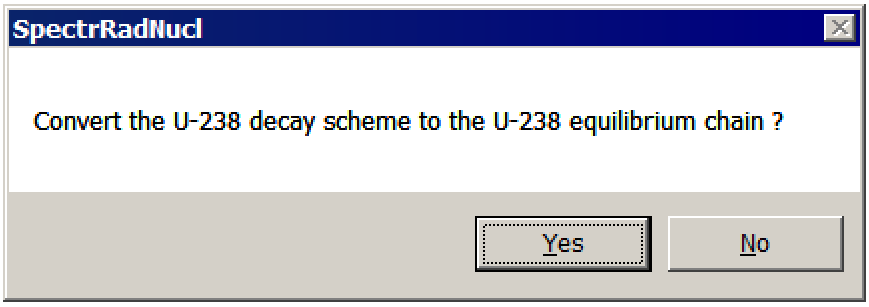
- U-238
  - Th-234
    - Pa-234m
      - Pa-234 (0.16%)
        - U-234
          - Th-230
            - Ra-226
              - Rn-222
                - Po-218
                  - Pb-214 (99.98%)
                    - Bi-214
                      - Po-214 (99.979%)
                        - Pb-210
                          - Bi-210
                            - Po-210
                              - Pb-206
                      - Tl-210 (0.021%)
                        - Pb-210
                          - Bi-210
                            - Po-210
                              - Pb-206
                  - At-218 (0.02%)
      - U-234 (99.84%)
        - Th-230
          - Ra-226
            - Rn-222
              - Po-218
                - Pb-214 (99.98%)
                  - Bi-214
                    - Po-214 (99.979%)
                      - Pb-210
                        - Bi-210
                          - Po-210
                            - Pb-206
                    - Tl-210 (0.021%)
                      - Pb-210
                        - Bi-210
                          - Po-210
                            - Pb-206
                - At-218 (0.02%)

The radioactive balance between U-238 and Ra-226 is often disturbed. Therefore, we will include U-238, Th-234, Pa-234m, Pa-234, U-234 and Th-230 in the first chain. To do this, collapse the decay scheme below Th-230 by left-clicking on the icon to the left of the Th-230 icon. As a result, the scheme will look like:



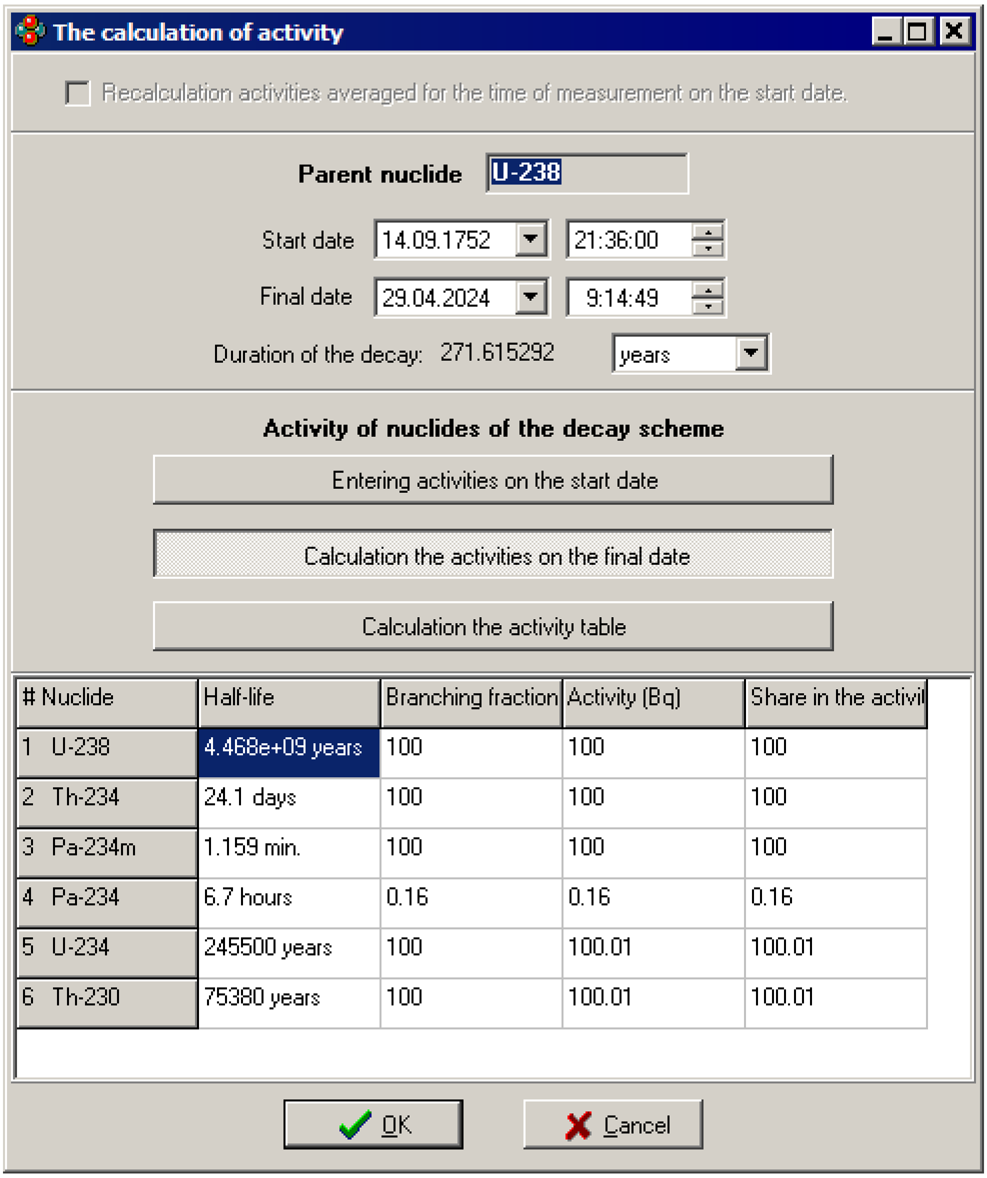
The chain formation procedure does not include nuclides in the chains that are not displayed in the decay scheme. Therefore, the fact that we have collapsed the decay scheme for Th-230 will lead to the fact that only Th-234, Pa-234m, Pa-234, U-234 and Th-230 will be included in the equilibrium chain of U-238.

Let's start the procedure for forming an equilibrium chain from the main menu or by calling the pop-up menu by right-clicking on the U-238 icon. At this the program will ask you to confirm the seriousness of our intentions



Convert the U-238 decay scheme to the U-238 equilibrium chain ?

The answer "Yes" starts the chain formation procedure and displays a window for calculating the nuclide activity of the selected part of the decay scheme on the current date with an initial date corresponding to the requirement of the required decay duration for the formation of the equilibrium state of the chain



☐ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide: U-238

Start date: 14.09.1752 21:36:00

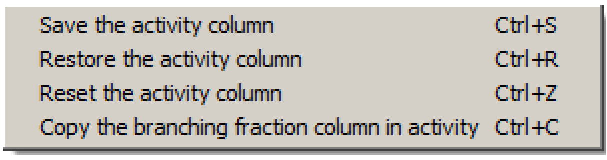
Final date: 29.04.2024 9:14:49

Duration of the decay: 271.615292 years

# Nuclide	Half-life	Branching fraction	Activity (Bq)	Share in the activi
1 U-238	4.468e+09 years	100	100	100
2 Th-234	24.1 days	100	100	100
3 Pa-234m	1.159 min.	100	100	100
4 Pa-234	6.7 hours	0.16	0.16	0.16
5 U-234	245500 years	100	100.01	100.01
6 Th-230	75380 years	100	100.01	100.01

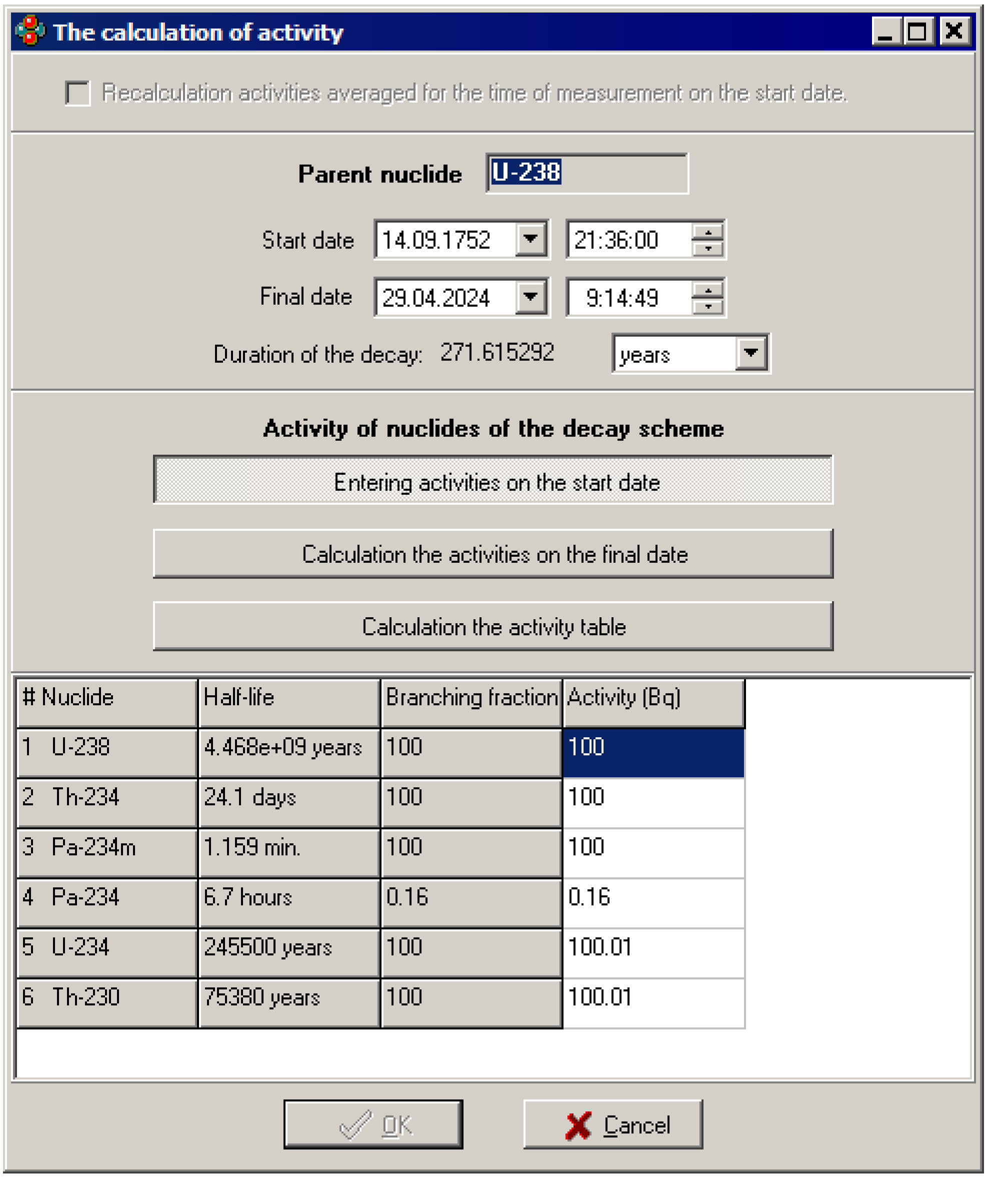
In accordance with the values of the last column of the table "**Share in the activity of the parent (%)**", the quantum yields for the nuclide lines included in the equilibrium chain are calculated. It can be noted that the activity of U-234 and Th-230 in our example is slightly higher than 100% (fraction in decay) - this always happens after some time required for the formation of equilibrium in the chain due to some predominance of the accumulation of daughter nuclides in the chain over the decay process. There is no such thing as absolute equilibrium. If the half-life of the parent nuclide in the chain is more than ten times longer than the half-life of the longest-lived of the daughter nuclides, it is considered that the requirement necessary for the formation of radioactive equilibrium in the chain is fulfilled. Otherwise, the program will inform you that the radioactive equilibrium in the chain will never occur and will prompt the operator to set the required decay duration and, accordingly, the state of the ratio of nuclide activities in the chain.

The form has a small menu associated with the nuclide table, and is available when entering the initial activities of the nuclide chain



, that helps to manipulate the column of the initial activity of the nuclide chain, which is necessary for calculating nonequilibrium chains. The menu item "**Restore the activity column**" restores the values of the initial activities saved by calling the menu item "**Save the activity column**".

If we do not agree with the calculation, or we need to form a non-equilibrium chain, we can set other dates for the beginning and end of the decay and the initial activities at the beginning of the decay by pressing the "**Entering activities on the start date**" key. The form will take the form:



☐ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide U-238

Start date 14.09.1752 21:36:00

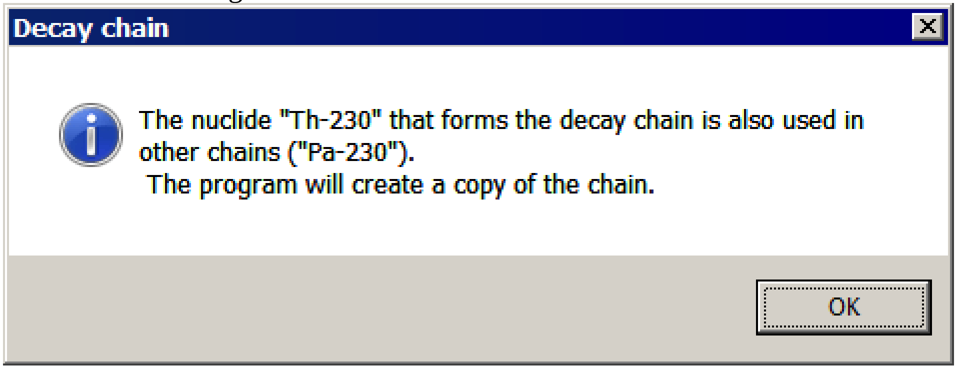
Final date 29.04.2024 9:14:49

Duration of the decay: 271.615292 years

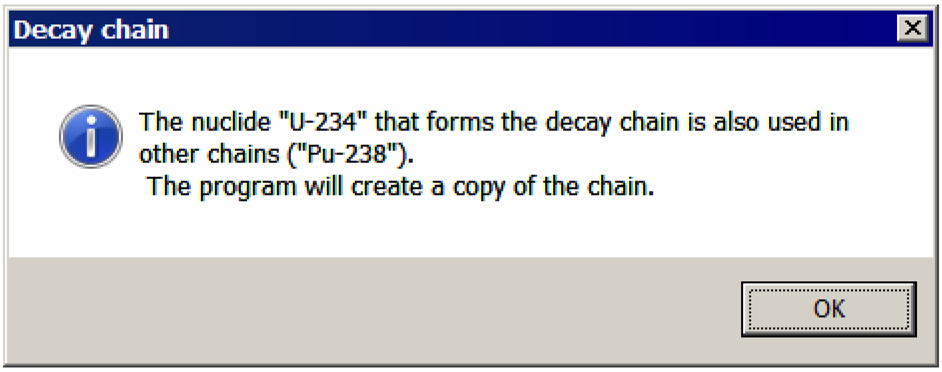
# Nuclide	Half-life	Branching fraction	Activity (Bq)
1 U-238	4.468e+09 years	100	100
2 Th-234	24.1 days	100	100
3 Pa-234m	1.159 min.	100	100
4 Pa-234	6.7 hours	0.16	0.16
5 U-234	245500 years	100	100.01
6 Th-230	75380 years	100	100.01

After entering the initial values of the activities and the dates of the beginning and end of the decay, press the "**Calculating the activities on the final date**" key. The program will recalculate the activity values for the specified end date and allow the formation of a chain. If necessary, you can preview the decay charts by pressing the "**Calculating the activity table**" key and select the desired end date.

Pressing the "**OK**" key starts the chain formation process. In the process of chain formation, the program finds out that some nuclides or chains of nuclides are included in the decay schemes of other nuclides and, in this case, form copies of them. In our case, we will receive such messages:



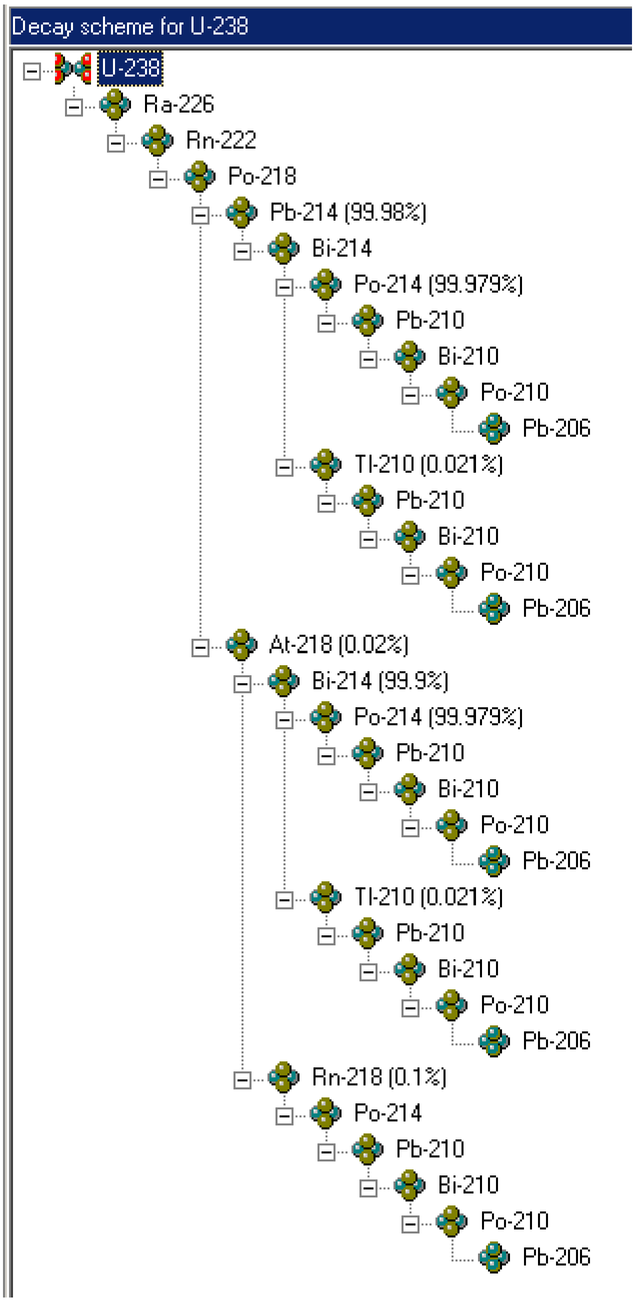
The nuclide "Th-230" that forms the decay chain is also used in other chains ("Pa-230").
The program will create a copy of the chain.



The nuclide "U-234" that forms the decay chain is also used in other chains ("Pu-238").
The program will create a copy of the chain.

The nuclides included in the chain copies may be required to form other equilibrium chains. When creating a "copy of the chain", in fact, not a copy of the nuclides of the chain is created, but the attributes of the nuclides change in such a way that the nuclide acquires the status of a "copy of the nuclide", instead of the status "included in the equilibrium chain". This should be taken into account if you want to delete or edit the nuclide yourself.

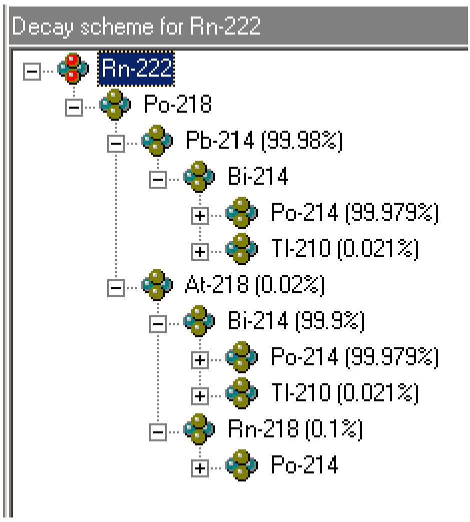
Upon completion of the process, we obtain the following decay scheme for U-238:



Decay scheme for U-238

- U-238
  - Ra-226
    - Rn-222
      - Po-218
        - Pb-214 (99.98%)
          - Bi-214
            - Po-214 (99.979%)
              - Pb-210
                - Bi-210
                  - Po-210
                    - Pb-206
            - Tl-210 (0.021%)
              - Pb-210
                - Bi-210
                  - Po-210
                    - Pb-206
        - At-218 (0.02%)
          - Bi-214 (99.9%)
            - Po-214 (99.979%)
              - Pb-210
                - Bi-210
                  - Po-210
                    - Pb-206
            - Tl-210 (0.021%)
              - Pb-210
                - Bi-210
                  - Po-210
                    - Pb-206
          - Rn-218 (0.1%)
            - Po-214
              - Pb-210
                - Bi-210
                  - Po-210
                    - Pb-206

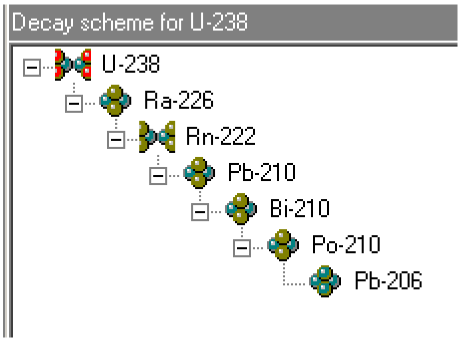
All lines Th-234, Pa-234m, Pa-234, U-234 and Th-230 are switched on according to the quantum yield and the share in the activity of the parent U-238. The Rn-222 - Po-214 chain can also be combined into an equilibrium one. To do this, we will switch to Rn-222 in the isotope table and collapse the decay scheme below Po-214 and Tl-210. We get the following decay scheme:



Decay scheme for Rn-222

- Rn-222
  - Po-218
    - Pb-214 (99.98%)
      - Bi-214
        - Po-214 (99.979%)
        - Tl-210 (0.021%)
    - At-218 (0.02%)
      - Bi-214 (99.9%)
        - Po-214 (99.979%)
        - Tl-210 (0.021%)
      - Rn-218 (0.1%)
        - Po-214

. By calling the equilibrium chain construction procedure for Rn-222, we will eventually obtain the U-238 decay scheme



Decay scheme for U-238

- U-238
  - Ra-226
    - Rn-222
      - Pb-210
        - Bi-210
          - Po-210
            - Pb-206

, comprising two equilibrium chains U-238-Th-230 and Rn-222 -Po-214.

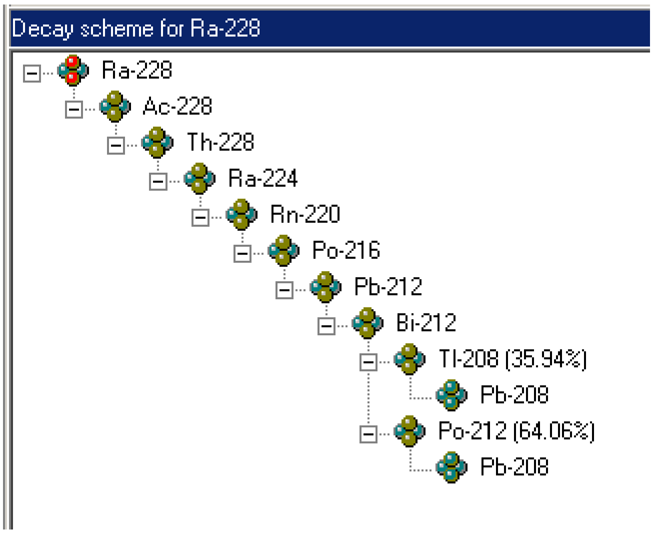
The formed equilibrium chain is easily converted back into a set of individual nuclides by calling the menu item "**Tools / Nuclides equilibrium chain / Deconstruct...**".

Construction of nonequilibrium chains

Often we need to calculate the decomposition component based on the decay chain, the radioactive equilibrium in which has not been established or, in principle, cannot be established. For example: after radiochemical separation of a nuclide, or calcinations of a sample to remove radioactive gases, etc. In this case, the state of the chain is calculated for a given duration of decay from the initial state.

Let's consider the process of forming a nonequilibrium chain using the example of the decay chain of Ra-228 after chemical separation of radium from a sample. This procedure is used in hygiene and epidemiology centers to control the radium content in water. The SanPiN standards for radium are very strict (0.49 Bq/l for Ra-226 and 0.2 Bq/ l for Ra-228), therefore, in order to obtain the required accuracy, radium has to be separated from a large volume of water and the resulting material analyzed for the content of Ra-226 and Ra-228. And for this, it is necessary to calculate the elementary spectra (spectrometer responses to 1 nuclide decay) for the decay chains Ra-226 and Ra-228 on a given date.

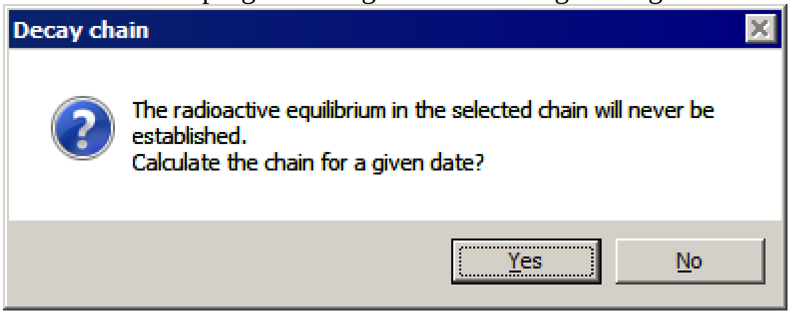
This is what the Ra-228 decay tree looks like:



Decay scheme for Ra-228

- Ra-228
  - Ac-228
    - Th-228
      - Ra-224
        - Rn-220
          - Po-216
            - Pb-212
              - Bi-212
                - Tl-208 (35.94%)
                  - Pb-208
                - Po-212 (64.06%)
                  - Pb-208

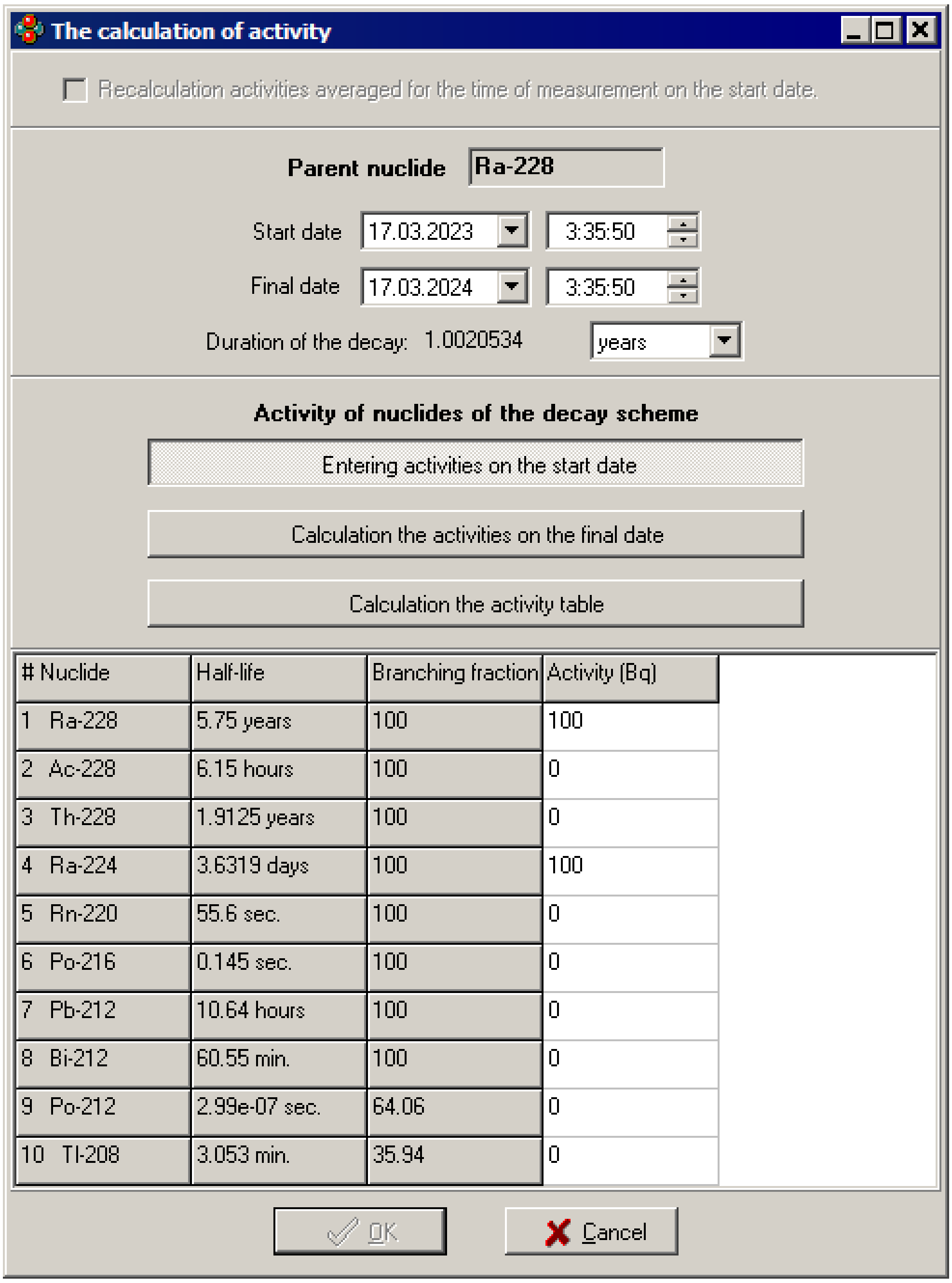
Let's start the chain formation procedure from the main menu (menu item "**Tools / Nuclides equilibrium chain / Construct...**") or by calling the pop-up menu by right-clicking on the icon Ra-228. The program will give us a warning message:



Decay chain

The radioactive equilibrium in the selected chain will never be established.
Calculate the chain for a given date?

. Click on the "**Yes**" button and enter the initial values of Ra-228 and Ra-224 after the chemical separation of radium in the form that opens. We do not need absolute values; we need a ratio of nuclide activities in the Ra-228 decay chain in water:



The calculation of activity

☐ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide Ra-228

Start date 17.03.2023 3:35:50

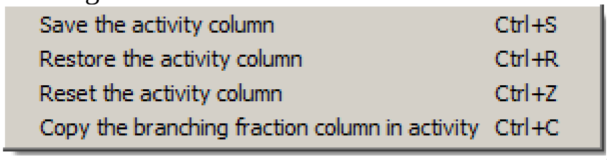
Final date 17.03.2024 3:35:50

Duration of the decay: 1.0020534 years

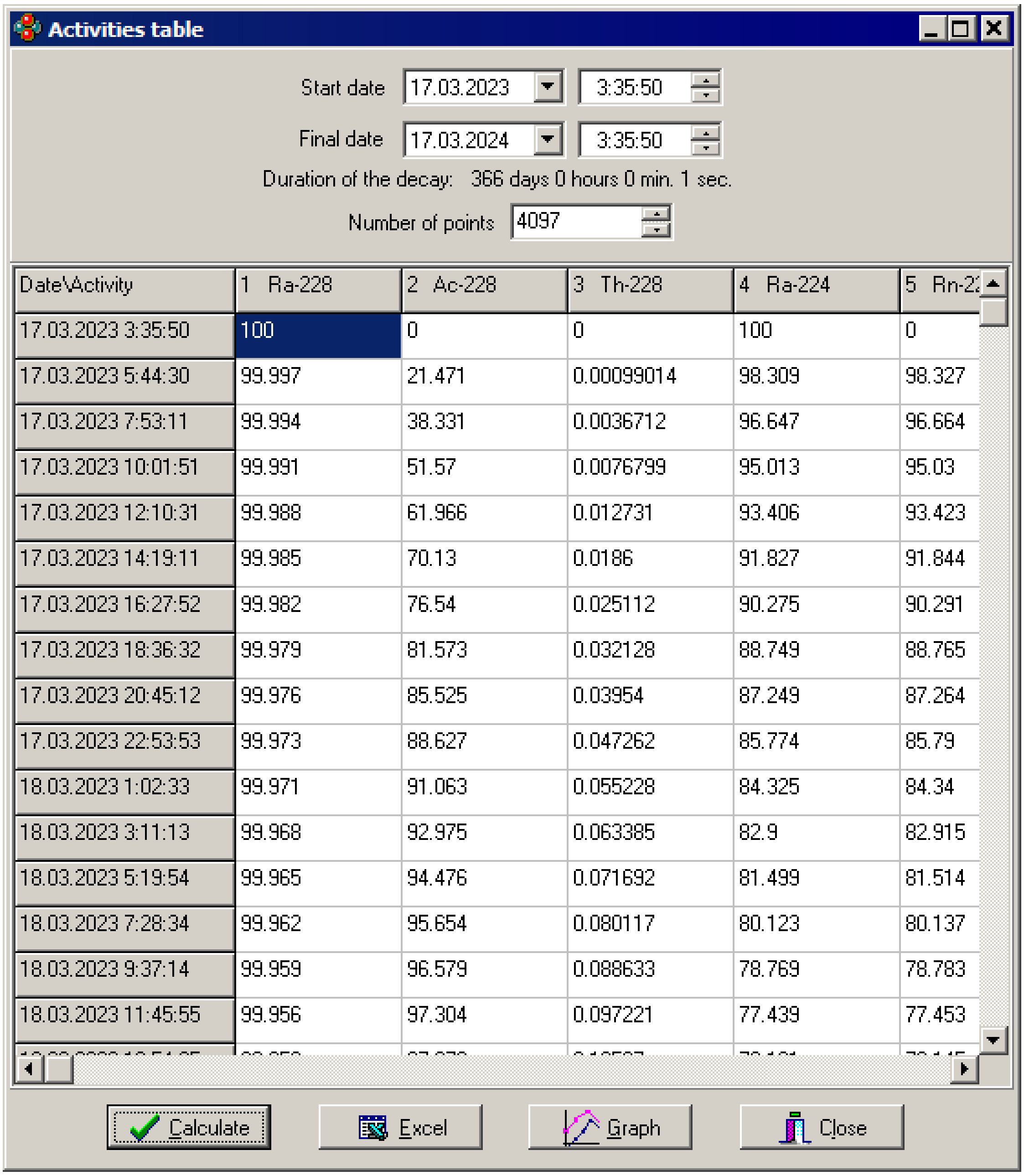
Activity of nuclides of the decay scheme

# Nuclide	Half-life	Branching fraction	Activity (Bq)
1 Ra-228	5.75 years	100	100
2 Ac-228	6.15 hours	100	0
3 Th-228	1.9125 years	100	0
4 Ra-224	3.6319 days	100	100
5 Rn-220	55.6 sec.	100	0
6 Po-216	0.145 sec.	100	0
7 Pb-212	10.64 hours	100	0
8 Bi-212	60.55 min.	100	0
9 Po-212	2.99e-07 sec.	64.06	0
10 Tl-208	3.053 min.	35.94	0

The form has a small menu associated with the nuclide table, and is available when entering the initial activities of the nuclide chain, which helps to manipulate the column of the initial activity of the nuclide chain, which is necessary for calculating nonequilibrium chains. The menu item "**Restore the activity column**" restores the values of the initial activities saved by calling the menu item "**Save the activity column**". In this case, the menu item "**Reset the activity column**" is useful to us - reset the activity column to zero values.



We need to determine the date of measurement of the sample so that Rn-222 from Ra-226 has time to accumulate and all short-lived Ra-228 in the decay tree have a minimum rate of change in activity (a state of quasi-equilibrium has occurred). To do this, calculate the activity table by clicking on the corresponding key:



Activities table

Start date 17.03.2023 3:35:50

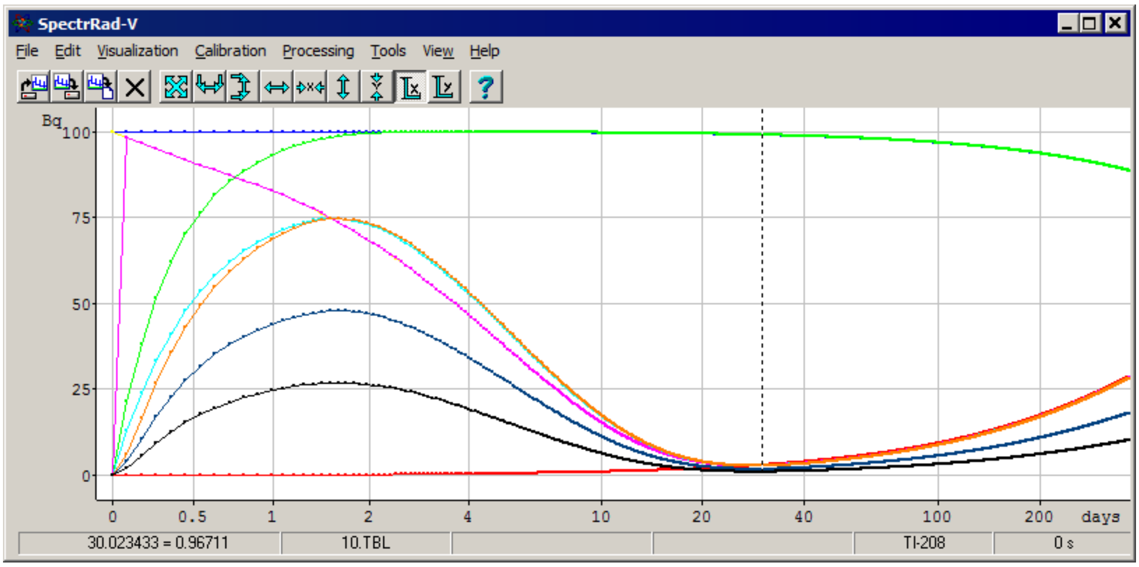
Final date 17.03.2024 3:35:50

Duration of the decay: 366 days 0 hours 0 min. 1 sec.

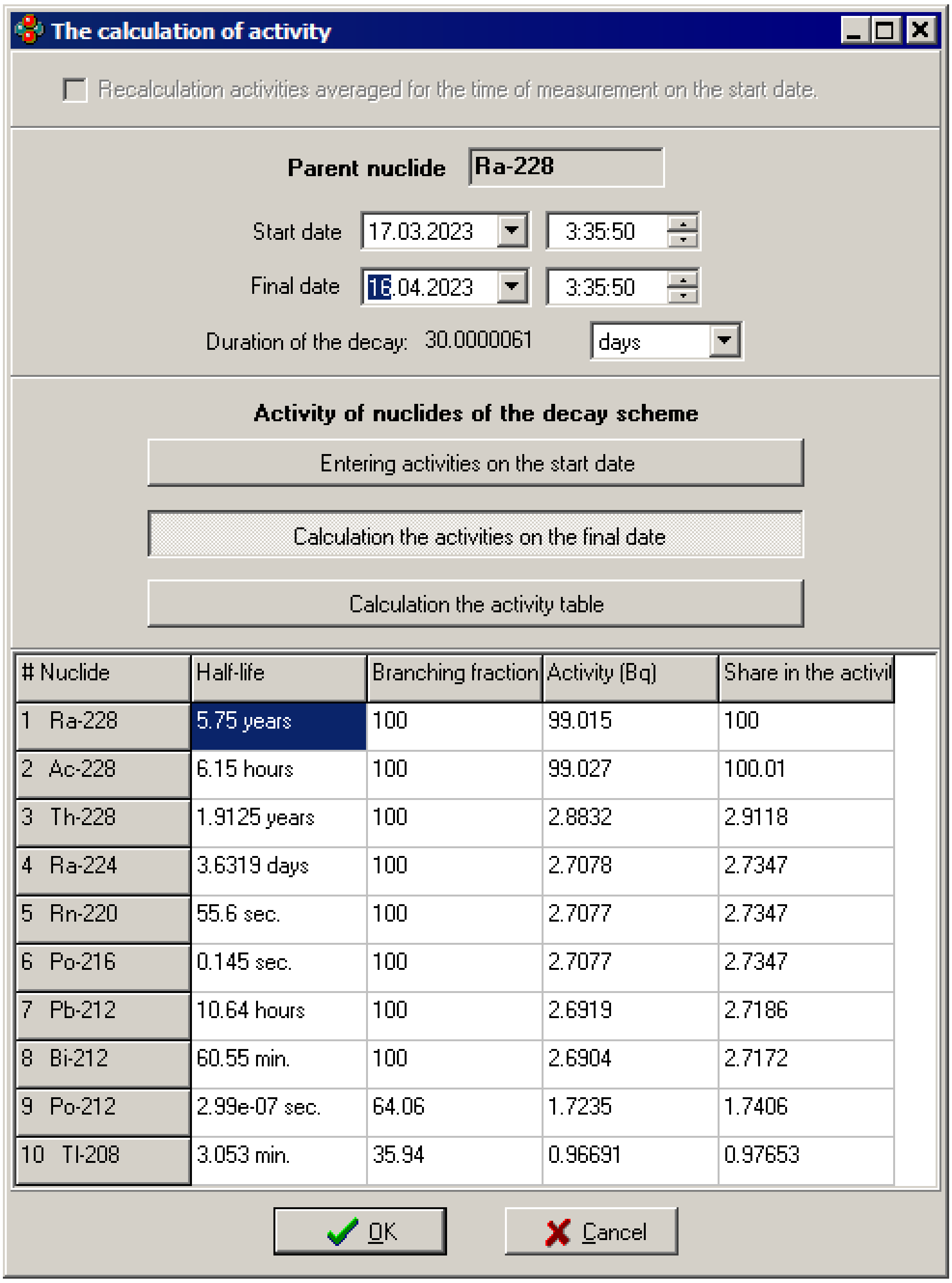
Number of points 4097

Date\Activity	1 Ra-228	2 Ac-228	3 Th-228	4 Ra-224	5 Rn-2
17.03.2023 3:35:50	100	0	0	100	0
17.03.2023 5:44:30	99.997	21.471	0.00099014	98.309	98.327
17.03.2023 7:53:11	99.994	38.331	0.0036712	96.647	96.664
17.03.2023 10:01:51	99.991	51.57	0.0076799	95.013	95.03
17.03.2023 12:10:31	99.988	61.966	0.012731	93.406	93.423
17.03.2023 14:19:11	99.985	70.13	0.0186	91.827	91.844
17.03.2023 16:27:52	99.982	76.54	0.025112	90.275	90.291
17.03.2023 18:36:32	99.979	81.573	0.032128	88.749	88.765
17.03.2023 20:45:12	99.976	85.525	0.03954	87.249	87.264
17.03.2023 22:53:53	99.973	88.627	0.047262	85.774	85.79
18.03.2023 1:02:33	99.971	91.063	0.055228	84.325	84.34
18.03.2023 3:11:13	99.968	92.975	0.063385	82.9	82.915
18.03.2023 5:19:54	99.965	94.476	0.071692	81.499	81.514
18.03.2023 7:28:34	99.962	95.654	0.080117	80.123	80.137
18.03.2023 9:37:14	99.959	96.579	0.088633	78.769	78.783
18.03.2023 11:45:55	99.956	97.304	0.097221	77.439	77.453

Let's look at the decay graphs of Ra-228 and its subsidiaries by clicking on the "**Graph**" key:



The quasi–equilibrium state occurs 25 days after the release of radium - the minimum rate of change in the activities of the nuclides of the decay chain occurs after this time. Therefore, returning to the plate with the input of initial activities, we will enter a decay duration equal to 30 days (it does not matter what duration is in the range from 25 to 35 days) and calculate the activity of nuclides for a given decay duration.



☐ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide: Ra-228

Start date: 17.03.2023 3:35:50

Final date: 16.04.2023 3:35:50

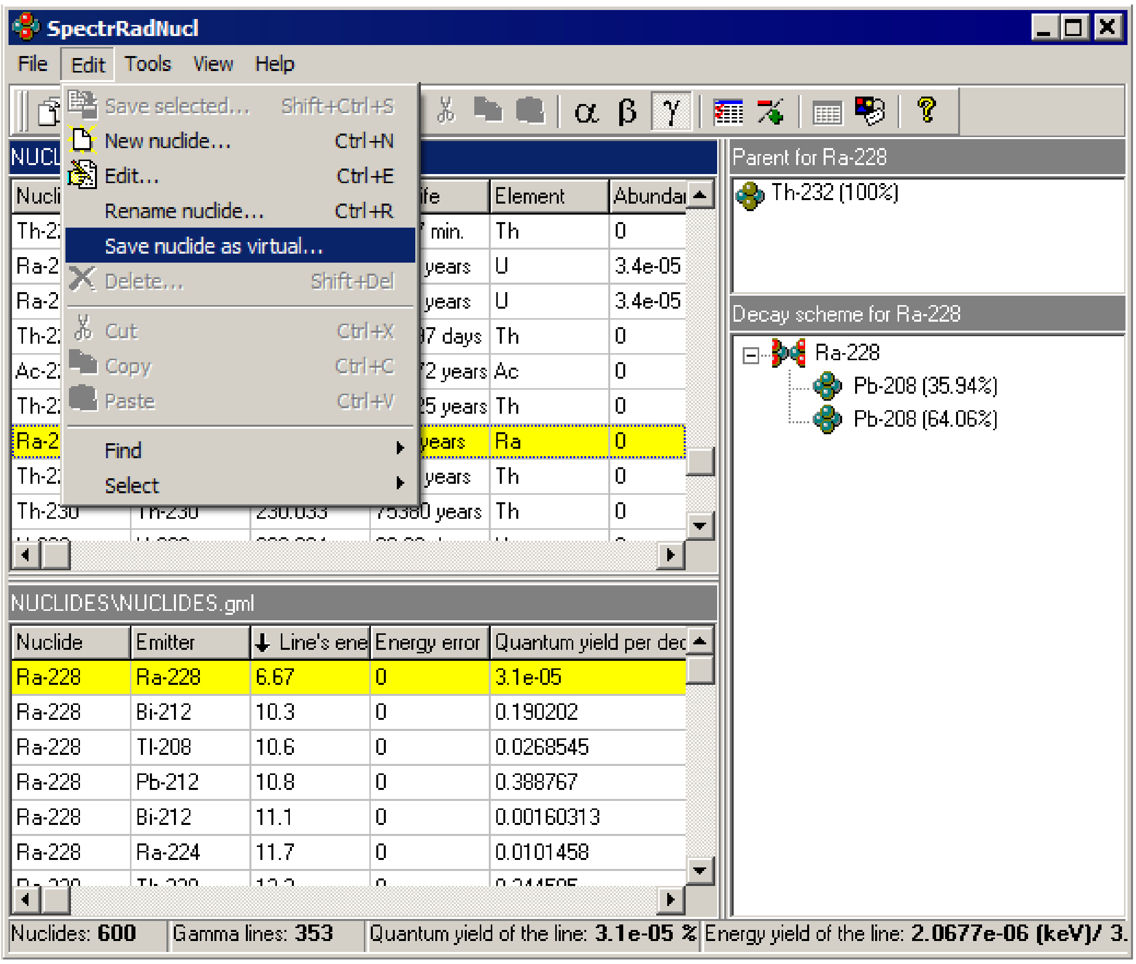
Duration of the decay: 30.0000061 days

#	Nuclide	Half-life	Branching fraction	Activity (Bq)	Share in the activi
1	Ra-228	5.75 years	100	99.015	100
2	Ac-228	6.15 hours	100	99.027	100.01
3	Th-228	1.9125 years	100	2.8832	2.9118
4	Ra-224	3.6319 days	100	2.7078	2.7347
5	Rn-220	55.6 sec.	100	2.7077	2.7347
6	Po-216	0.145 sec.	100	2.7077	2.7347
7	Pb-212	10.64 hours	100	2.6919	2.7186
8	Bi-212	60.55 min.	100	2.6904	2.7172
9	Po-212	2.99e-07 sec.	64.06	1.7235	1.7406
10	Tl-208	3.053 min.	35.94	0.96691	0.97653

As a result, we obtain a nonequilibrium chain of Ra-228, in which the outputs of the daughter nuclide lines 30 days after the start of the decay of the parent are included in the list of maternal lines.

It is recommended to save the nuclide as a virtual one (virtual nuclides are excluded from the automatic search for nuclides in the sample spectrum).

]



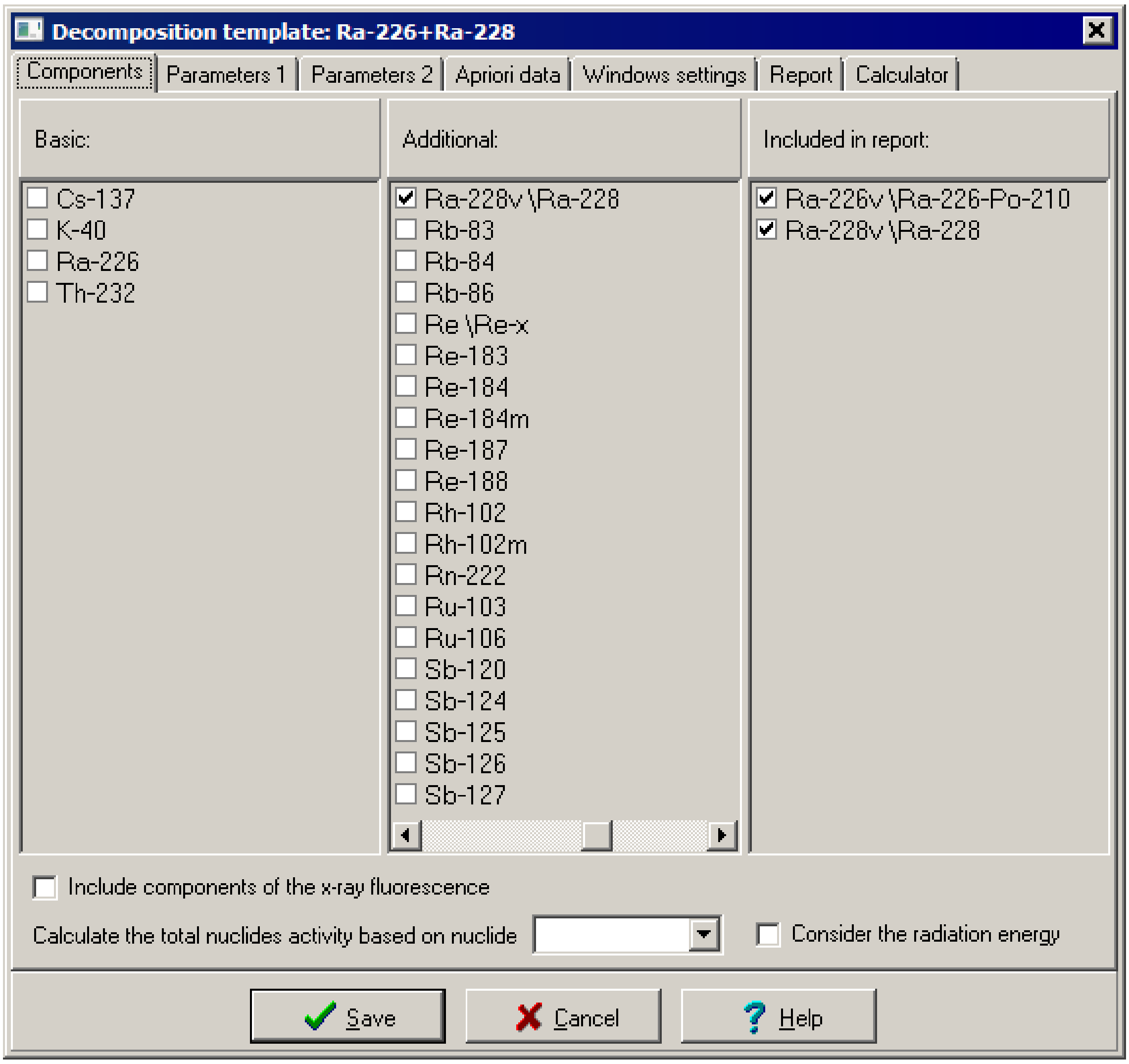
Nucli			ife	Element	Abunda
Th-2			min.	Th	0
Ra-2			years	U	3.4e-05
Ra-2			years	U	3.4e-05
Th-2			7 days	Th	0
Ac-2			2 years	Ac	0
Th-2			5 years	Th	0
Ra-2			years	Ra	0
Th-2			years	Th	0
Th-230	Th-230	230.033	75380 years	Th	0

Nuclide	Emitter	↓ Line's ene	Energy error	Quantum yield per dec
Ra-228	Ra-228	6.67	0	3.1e-05
Ra-228	Bi-212	10.3	0	0.190202
Ra-228	Tl-208	10.6	0	0.0268545
Ra-228	Pb-212	10.8	0	0.388767
Ra-228	Bi-212	11.1	0	0.00160313
Ra-228	Ra-224	11.7	0	0.0101458

Nuclides: **600** | Gamma lines: **353** | Quantum yield of the line: **3.1e-05 %** | Energy yield of the line: **2.0677e-06 (keV)/ 3.**

As a result, we can include the generated virtual nuclide as a component of the decomposition of the sample spectrum, having previously copied it into the nuclide worksheet, and not forgetting to include the escape lines of annihilation gamma quanta and the summation lines of cascade transitions.

And we can specify it as a decomposition component when creating a template for processing spectra on Ra-226 and Ra-228:



Decomposition template: Ra-226+Ra-228

Basic:

☐ Cs-137
☐ K-40
☐ Ra-226
☐ Th-232

Additional:

☑ Ra-228v \Ra-228
☐ Rb-83
☐ Rb-84
☐ Rb-86
☐ Re \Re-x
☐ Re-183
☐ Re-184
☐ Re-184m
☐ Re-187
☐ Re-188
☐ Rh-102
☐ Rh-102m
☐ Rn-222
☐ Ru-103
☐ Ru-106
☐ Sb-120
☐ Sb-124
☐ Sb-125
☐ Sb-126
☐ Sb-127

Included in report:

☑ Ra-226v \Ra-226-Po-210
☑ Ra-228v \Ra-228

☐ Include components of the x-ray fluorescence

Calculate the total nuclides activity based on nuclide

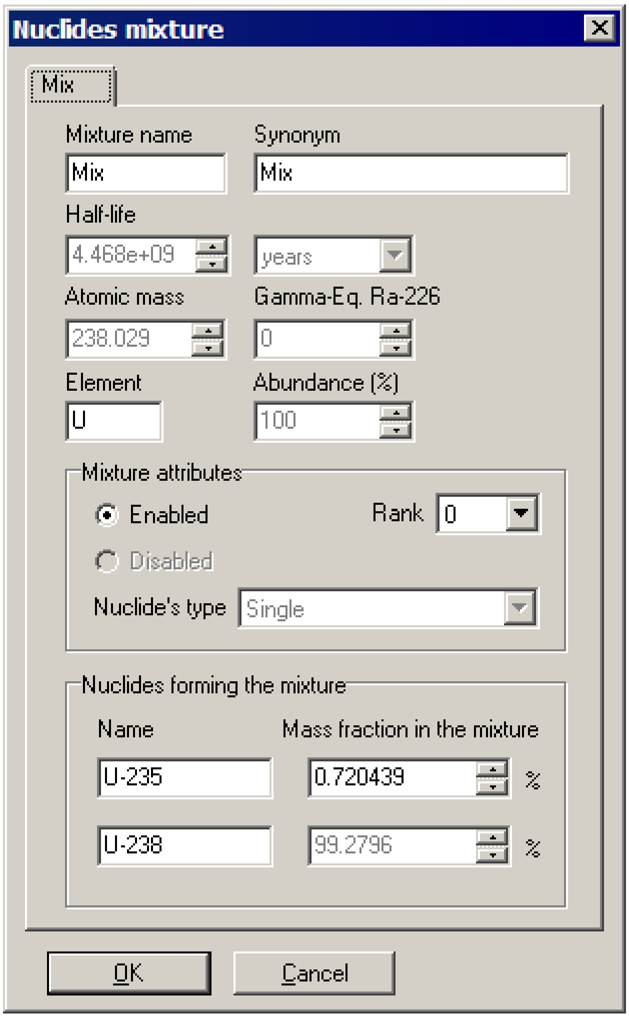
☐ Consider the radiation energy

At the same time, we should not forget that, calculated from the generated data of the nonequilibrium chain of Ra-228, the elementary spectrum corresponds to reality only on the 30th day of chemically selected Ra-228. Since the rate of change in the activities of all nuclides in the chain at this time is minimal, differences in activities during ± 5 days will not be significant.

Creating a mixture of nuclides

The menu item "**Tools / Nuclides mixture...**" calls the program for the formation of a conditional nuclide, which is a mixture of two or three nuclides selected by the operator.

The window of the procedure for creating a mixture of nuclides is almost identical to the window of the procedure for editing data for nuclides:



Mixture name: Mix
Synonym: Mix
Half-life: 4.468e+09 years
Atomic mass: 238.029
Gamma-Eq. Ra-226: 0
Element: U
Abundance (%): 100

Mixture attributes
● Enabled
○ Disabled
Rank: 0
Nuclide's type: Single

Nuclides forming the mixture

Name	Mass fraction in the mixture
U-235	0.720439 %
U-238	99.2796 %

The difference of the window is that some of the items are prohibited for editing and in place of the lower group, instead of specifying the children, nuclides marked by the operator are given to form a mixture. The operator must specify the name of the nuclide for the mixture to be formed and specify the proportion of nuclides (atomic mass as a percentage) in the mixture. Since the sum of the fractions must be equal to 100%, for two nuclides it is allowed to change the proportion of the first nuclide (the proportion of the second is automatically calculated), for three – to change the proportion of the first and second nuclides. By default, if the percentage of nuclide abundance is specified, it is substituted as a fraction in the mixture. As a result of the procedure, a conditionally equilibrium chain of nuclides is formed, in which a mixture nuclide is created having the maximum decay time, with daughter nuclides included in the chain forming the mixture.

Since the chain being formed is not in equilibrium, the fraction in decay for daughter nuclides is recalculated in accordance with the ratio of half-lives. The proportion calculated in this way naturally changes over time, and therefore, when forming mixtures of relatively short-lived nuclides, this must be taken into account.

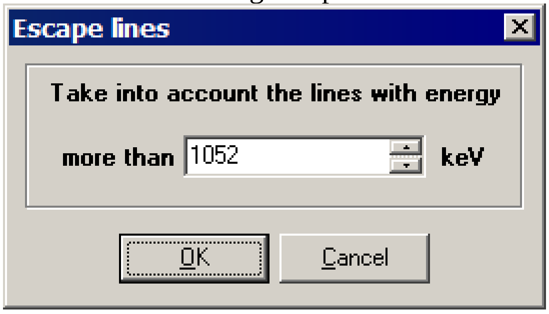
Unlike the equilibrium chain, where the activity of the chain is considered to be the activity of the parent nuclide, the activity of the mixture is considered to be the total activity of the nuclides included in the mixture.

The formation of mixtures increases the conditionality of the system being solved and, accordingly, increases the effectiveness of estimates. For example, the proportion of U-238 and U-235 in natural (non-enriched) uranium is constant with rare exceptions. Therefore, for example, when solving the problem of determining uranium in soils, it is reasonable not to separate the uranium, but to determine directly a mixture of uranium.

Accounting for escape lines and cascade summing lines

The effects associated with the formation of an annihilation peak and escape peaks for gamma lines with an energy exceeding the energy of electron-positron pair formation and the appearance of summation peaks for cascade transition lines must be taken into account in gamma spectrum processing procedures. In the "**SPECTRRAD**" software package, to reduce the processing time of spectra, information about the energies of escape lines and cascade transition summation lines is formed in advance, and the effects associated with the redistribution of gamma quanta are finally calculated in the spectrum processing procedure.

The menu item "**Tools / Escape lines / Include in the table...**" calls the program that complements the table of gamma lines of nuclides with lines of single and double escape. At the same time, the program suggests introducing boundary energy for the lines that will be taken into account when forming escape lines.



The menu item "**Tools / Addition lines of cascading transitions / Include in the table**" is used to include lines with energies corresponding to the summation energies of two and three cascade transition lines in the table. Information about cascading transitions should be indicated in the gamma line entries.

The procedure for forming the addition of cascade lines calculates the conditional quantum outputs of the second and third stages (the probabilities of gamma quanta in the second and third stages, provided that the gamma quantum is released in the first cascade transition) for all possible cascade transitions.

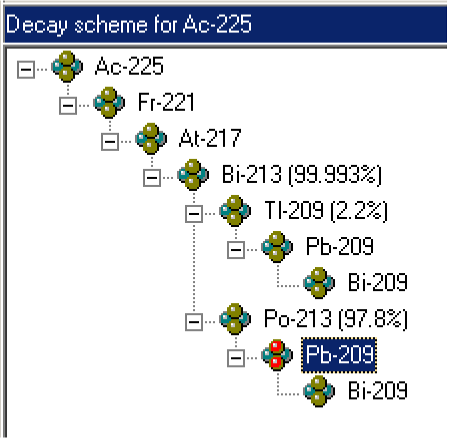
The formed lines are included in the table with the corresponding attributes: "annihilation", "escape line" or "cascade addition".

Menu item "**.../ Delete from the table**" removes previously formed escape or summing of cascades lines from the line table.

The inclusion of escape and cascade addition lines in the table must be carried out after the formation of equilibrium chains and mixtures of nuclides, since only in this case the quantum outputs of the included lines will be correctly calculated. If we have re-formed the table: we have created new equilibrium chains or disbanded the old ones, it is necessary to remove the old escape and cascade addition lines from the table and include them again.

Calculation of the activity of nuclides of the decay scheme

The menu item "**Tools / Nuclide activity...**" calls the procedure for calculating the activity of nuclides of the decay scheme on a given date. The calculation is performed either for all nuclides of the scheme, or only for the selected branch, depending on the selected nuclide of the scheme. If the parent nuclide of the decay tree is selected, the activities for all nuclides in all branches of the decay are calculated and the activities of identical nuclides in different branches of the decay are summarized in the final table. If one of the nuclides in any branch of the decay scheme is selected, the nuclide activity of the selected part (from the parent to the selected one) of the selected branch of the decay scheme is calculated. For example, in the decay scheme of Ac-225, we choose Pb-209 as the last nuclide:

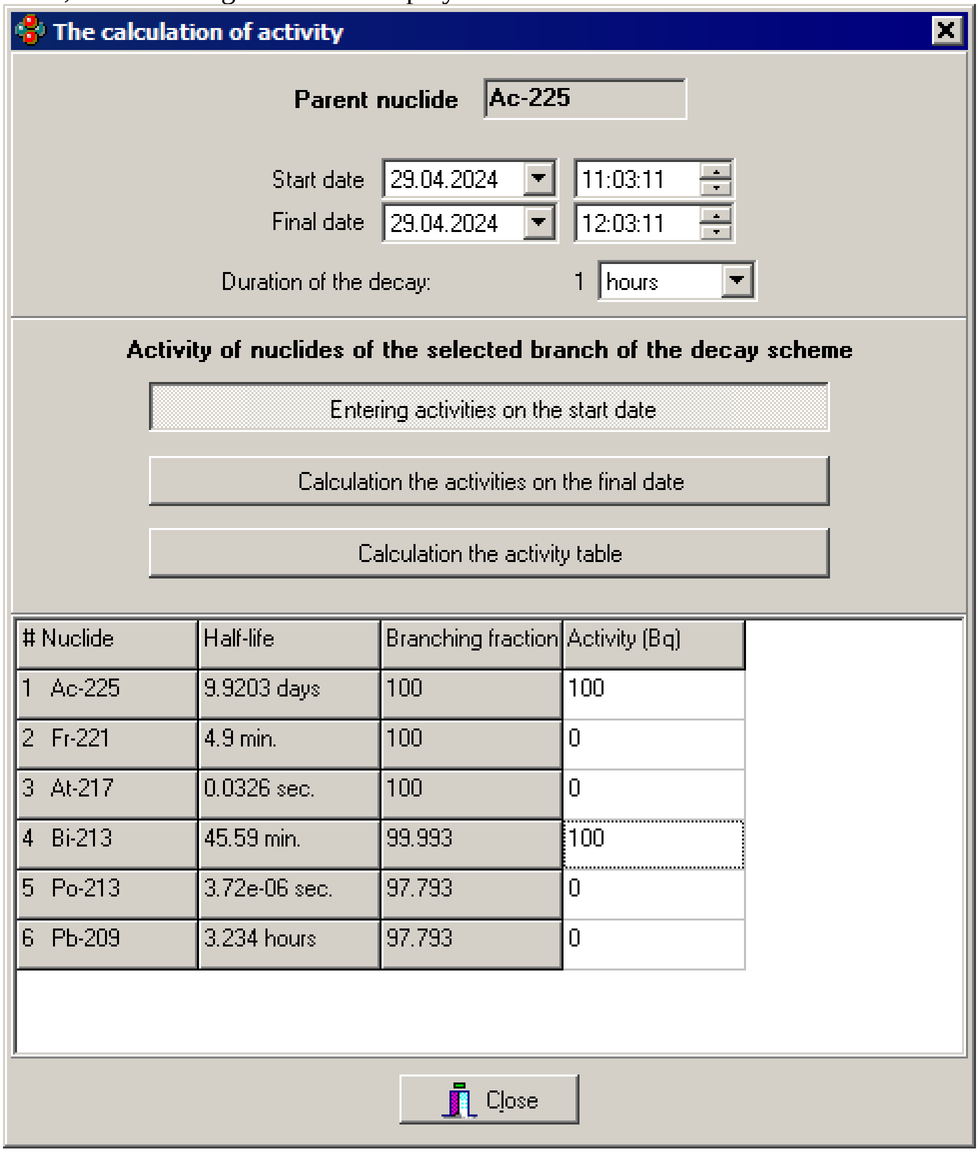


Decay scheme for Ac-225

- Ac-225
  - Fr-221
    - At-217
      - Bi-213 (99.993%)
        - Tl-209 (2.2%)
          - Pb-209
            - Bi-209
        - Po-213 (97.8%)
          - Pb-209
            - Bi-209

In this case, the activity calculation will be performed for the chain Ac-225 >Fr-221 >At-217 >Bi-213 >Po-213 >Pb-209.

At this, the following window is displayed on the screen:



The calculation of activity

Parent nuclide Ac-225

Start date 29.04.2024 11:03:11

Final date 29.04.2024 12:03:11

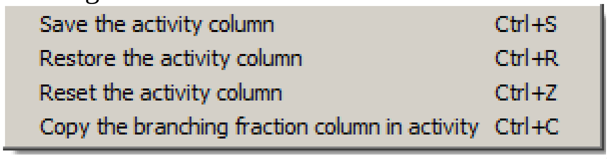
Duration of the decay: 1 hours

Activity of nuclides of the selected branch of the decay scheme

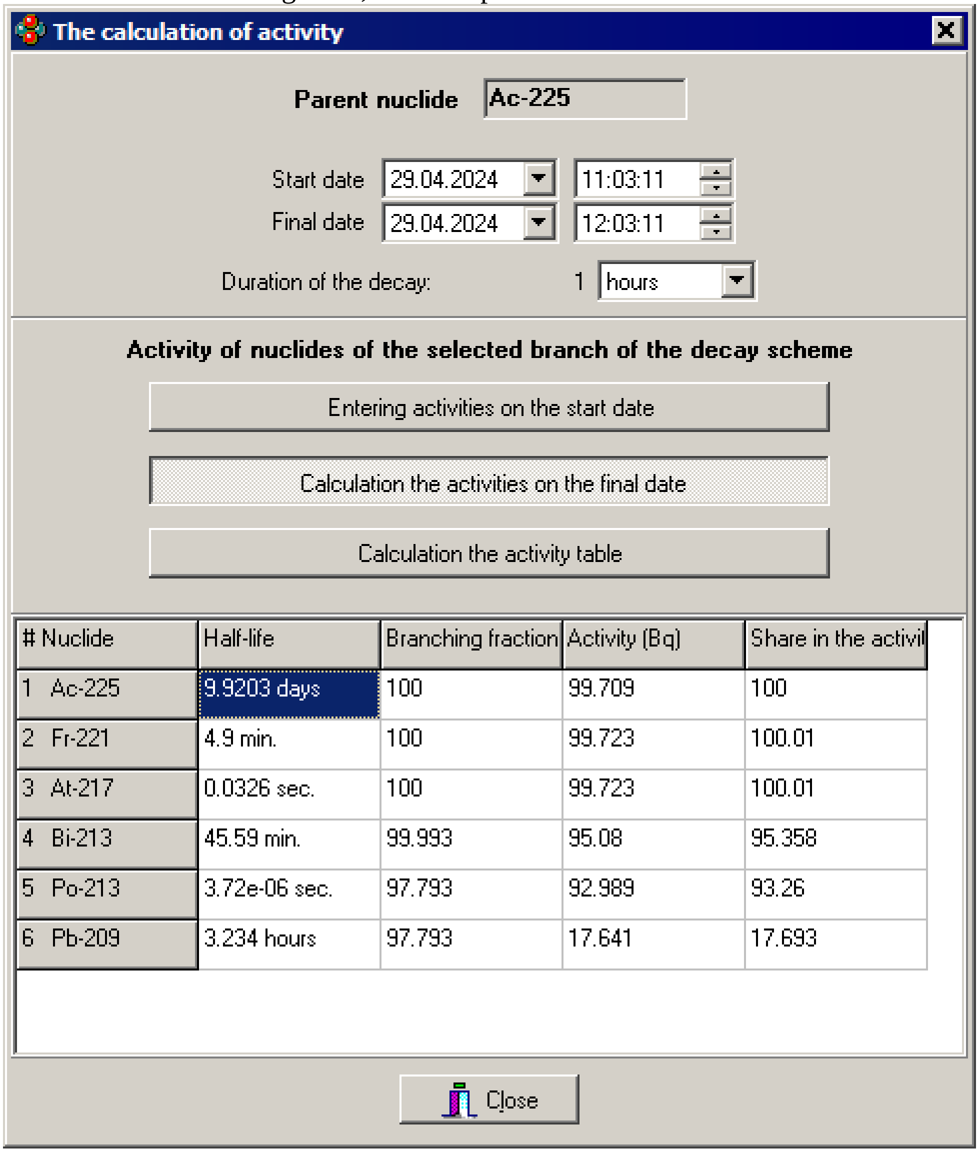
# Nuclide	Half-life	Branching fraction	Activity (Bq)
1 Ac-225	9.9203 days	100	100
2 Fr-221	4.9 min.	100	0
3 At-217	0.0326 sec.	100	0
4 Bi-213	45.59 min.	99.993	100
5 Po-213	3.72e-06 sec.	97.793	0
6 Pb-209	3.234 hours	97.793	0

The operator must specify the initial and final decay date and the activity of the nuclides of the decay scheme (or the nuclides of the selected branch) on the initial date.

The form has a small menu associated with the nuclide table, and is available when entering the initial activities of the nuclide chain , which helps to manipulate the column of the initial activity of the nuclide chain. The menu item "**Restore the activity column**" restores the values of the initial activities saved by calling the menu item "**Save the activity column**".



The activity on the end date is calculated by clicking on the button . The form of the activity calculation procedure takes the following form, for example:



Parent nuclide: Ac-225

Start date: 29.04.2024 11:03:11

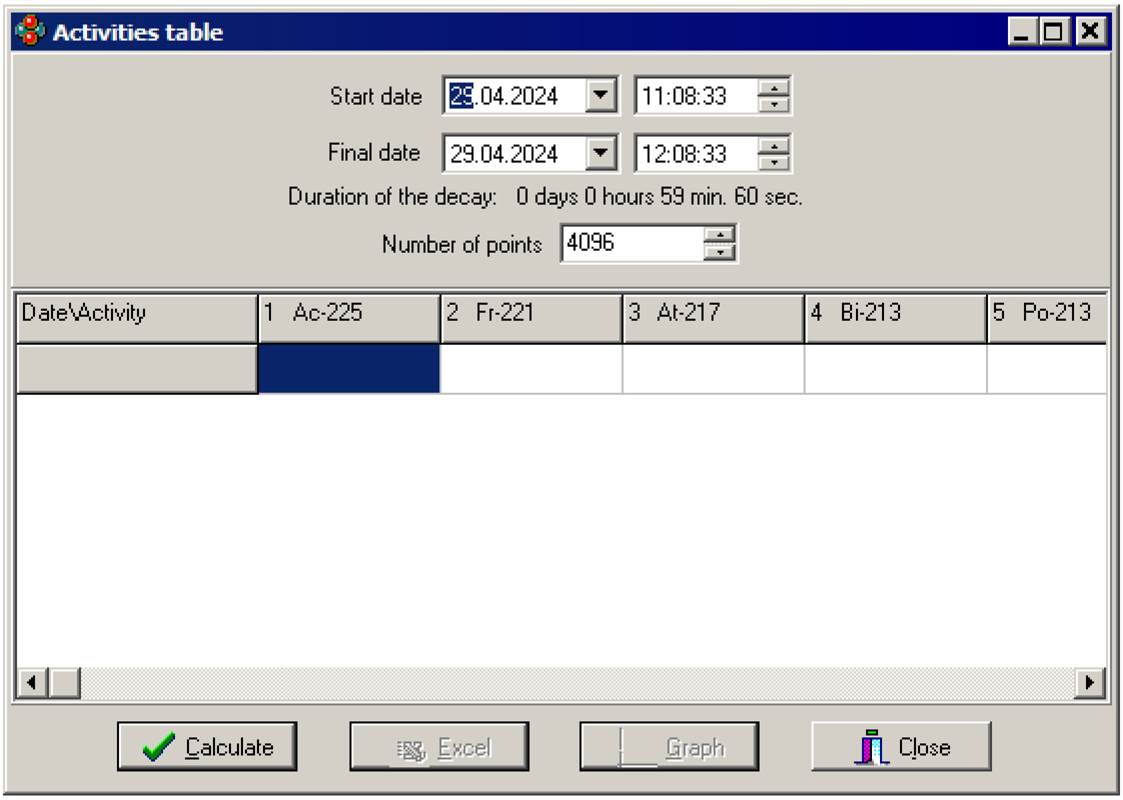
Final date: 29.04.2024 12:03:11

Duration of the decay: 1 hours

# Nuclide	Half-life	Branching fraction	Activity (Bq)	Share in the activi
1 Ac-225	9.9203 days	100	99.709	100
2 Fr-221	4.9 min.	100	99.723	100.01
3 At-217	0.0326 sec.	100	99.723	100.01
4 Bi-213	45.59 min.	99.993	95.08	95.358
5 Po-213	3.72e-06 sec.	97.793	92.989	93.26
6 Pb-209	3.234 hours	97.793	17.641	17.693

The column "**Activity (Bq)**" contains the activity of a specific nuclide in the chain of nuclides on the final date. The column "**Share in the activity of the parent (%)**" shows the relative activity of the nuclide (relative to the activity of the parent) at a given time (**Final date**).

The Calculation the activity table button allows you to calculate the activity table for a given time interval with a given number of points. The following form appears on the screen when you click on the button:



Activities table

Start date 29.04.2024 11:08:33

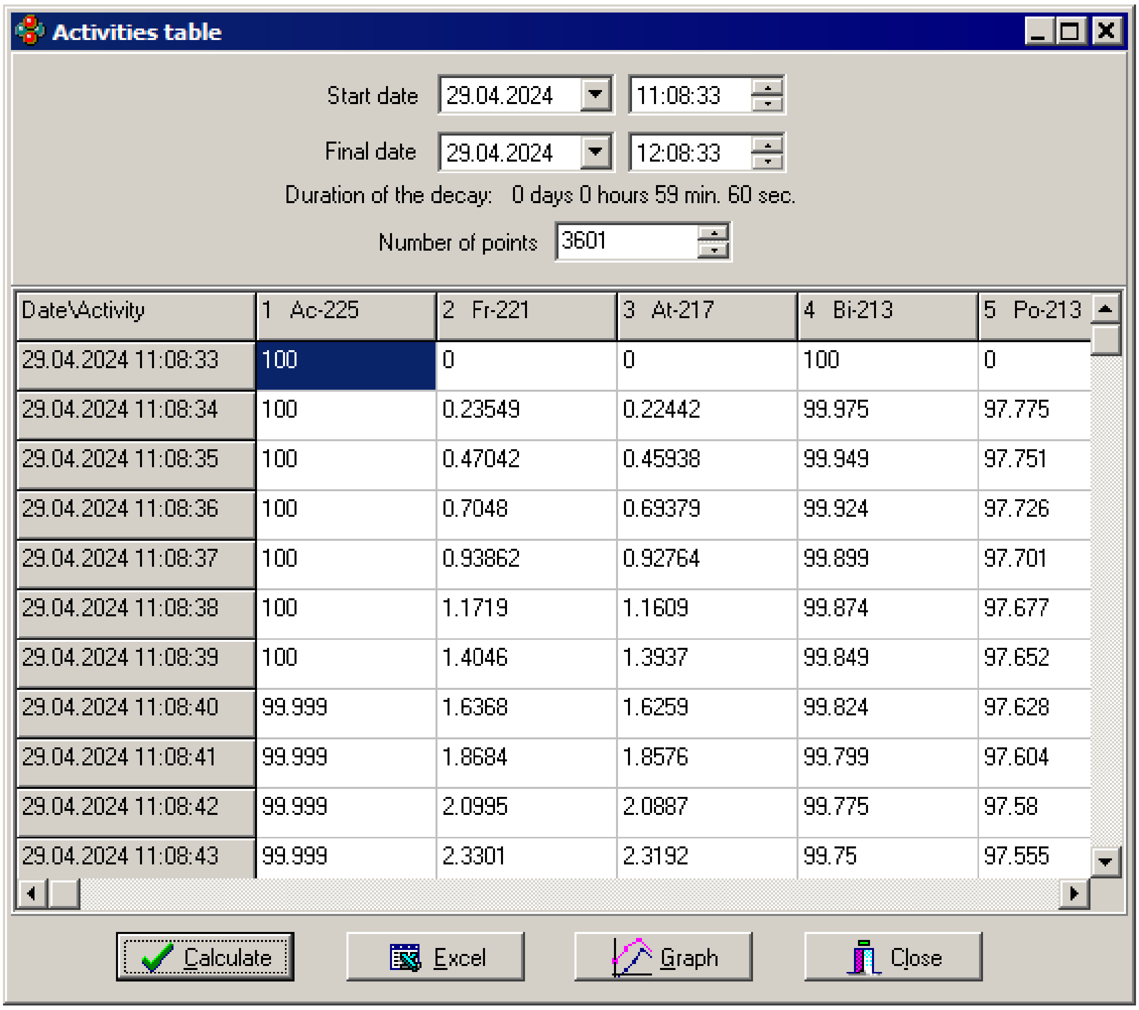
Final date 29.04.2024 12:08:33

Duration of the decay: 0 days 0 hours 59 min. 60 sec.

Number of points 4096

Date\Activity	1 Ac-225	2 Fr-221	3 At-217	4 Bi-213	5 Po-213

The operator can change the date range (negative decay time values are also allowed) and set the required number of points in the table. Clicking on the ✓ Calculate button starts the calculation procedure and upon completion the form will take the following form:



Start date 29.04.2024 11:08:33

Final date 29.04.2024 12:08:33

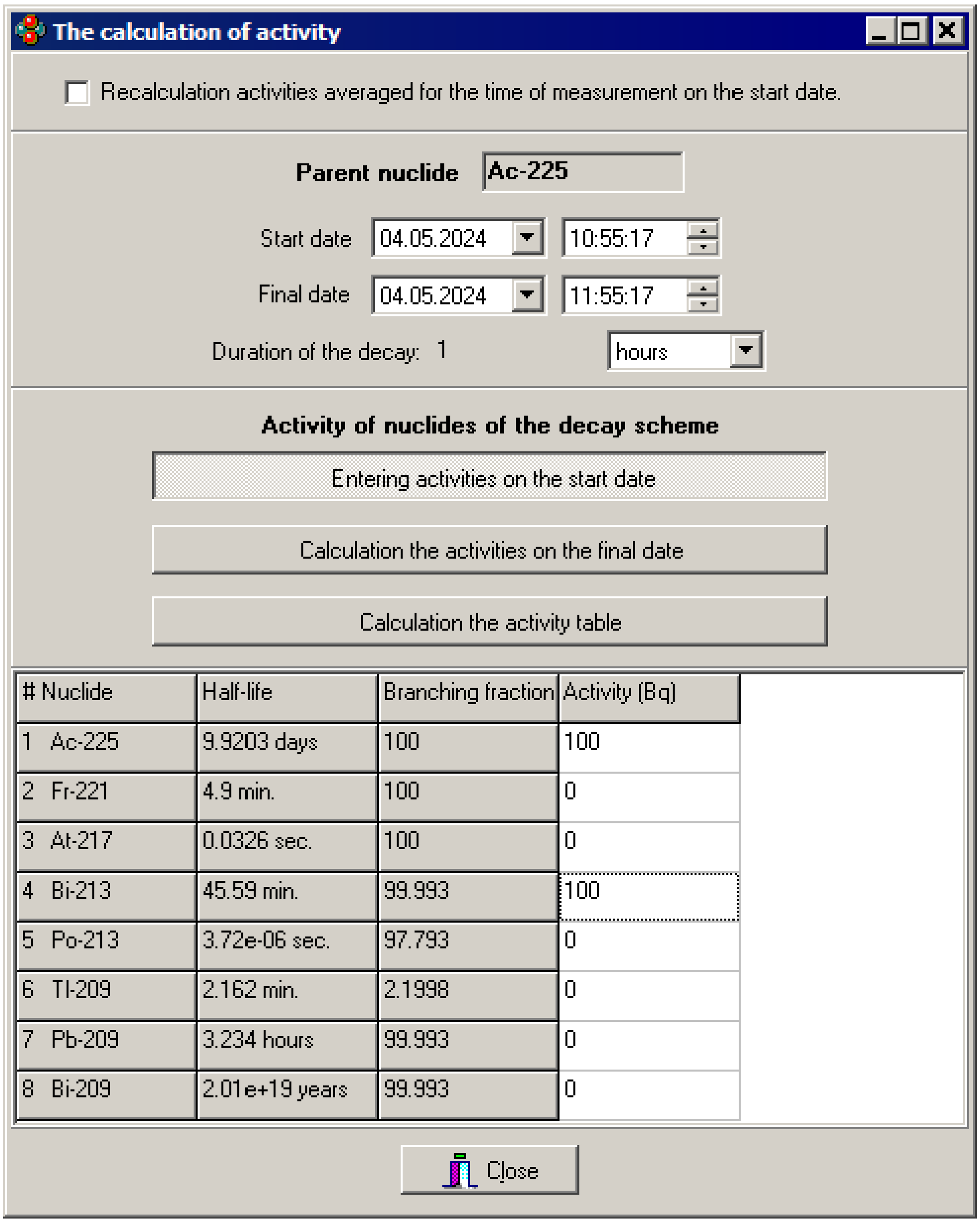
Duration of the decay: 0 days 0 hours 59 min. 60 sec.

Number of points 3601

Date\Activity	1 Ac-225	2 Fr-221	3 At-217	4 Bi-213	5 Po-213
29.04.2024 11:08:33	100	0	0	100	0
29.04.2024 11:08:34	100	0.23549	0.22442	99.975	97.775
29.04.2024 11:08:35	100	0.47042	0.45938	99.949	97.751
29.04.2024 11:08:36	100	0.7048	0.69379	99.924	97.726
29.04.2024 11:08:37	100	0.93862	0.92764	99.899	97.701
29.04.2024 11:08:38	100	1.1719	1.1609	99.874	97.677
29.04.2024 11:08:39	100	1.4046	1.3937	99.849	97.652
29.04.2024 11:08:40	99.999	1.6368	1.6259	99.824	97.628
29.04.2024 11:08:41	99.999	1.8684	1.8576	99.799	97.604
29.04.2024 11:08:42	99.999	2.0995	2.0887	99.775	97.58
29.04.2024 11:08:43	99.999	2.3301	2.3192	99.75	97.555

Clicking on the Excel button exports the contents of the table to Excel, and the Graph button allows you to view the decay functions as graphs. The operator can change the start and end dates of the decay and recalculate the results by clicking on the Calculate key.

The form for calculating the activities of all nuclides of the decay scheme is as follows:



☐ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide Ac-225

Start date 04.05.2024 10:55:17

Final date 04.05.2024 11:55:17

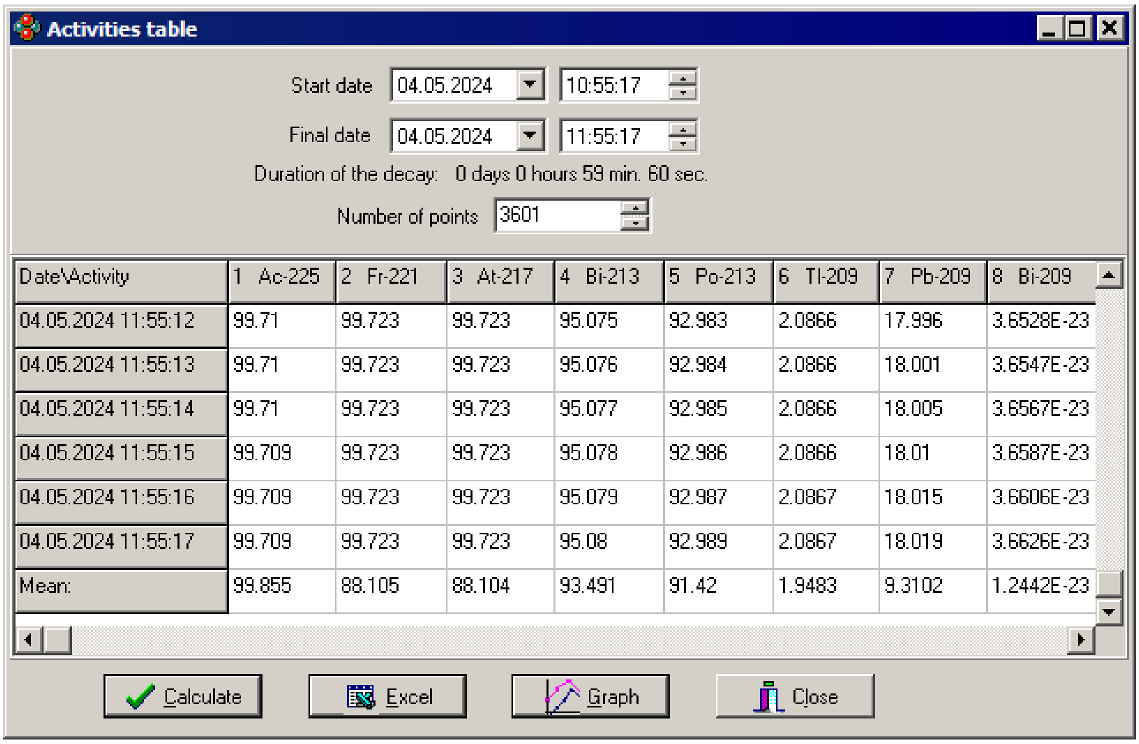
Duration of the decay: 1 hours

Activity of nuclides of the decay scheme

# Nuclide	Half-life	Branching fraction	Activity (Bq)
1 Ac-225	9.9203 days	100	100
2 Fr-221	4.9 min.	100	0
3 At-217	0.0326 sec.	100	0
4 Bi-213	45.59 min.	99.993	100
5 Po-213	3.72e-06 sec.	97.793	0
6 Tl-209	2.162 min.	2.1998	0
7 Pb-209	3.234 hours	99.993	0
8 Bi-209	2.01e+19 years	99.993	0

The form differs in the heading of the nuclide activity table – instead of the heading "**Activity of nuclides of the selected branch of the decay scheme**", the heading "**Activity of nuclides of the decay scheme**" is displayed and, accordingly, the nuclide table will contain all the nuclides of the decay scheme, and not just the selected branch. In addition, the procedure allows you to calculate the activity of the nuclides of the decay scheme at the beginning of measurements based on the average values of the activities during the measurement. To do this, set the "tick" in the item "**Recalculation activities averaged for the time of measurement on the start date**", enter the spectra calculated by the program, averaged over the time of activity measurement and click on the "**Calculation the activities on the measurement start**" button. Such a calculation, taking into account the processes of accumulation and decay of nuclides in the chain during measurement, is generally impossible directly in the spectrum processing procedure, since processing, for example, the gamma radiation spectrum does not allow us to evaluate the activity of nuclides in a chain without gamma lines, and for correct calculation knowledge of the activities of all nuclides of the decay scheme is required.

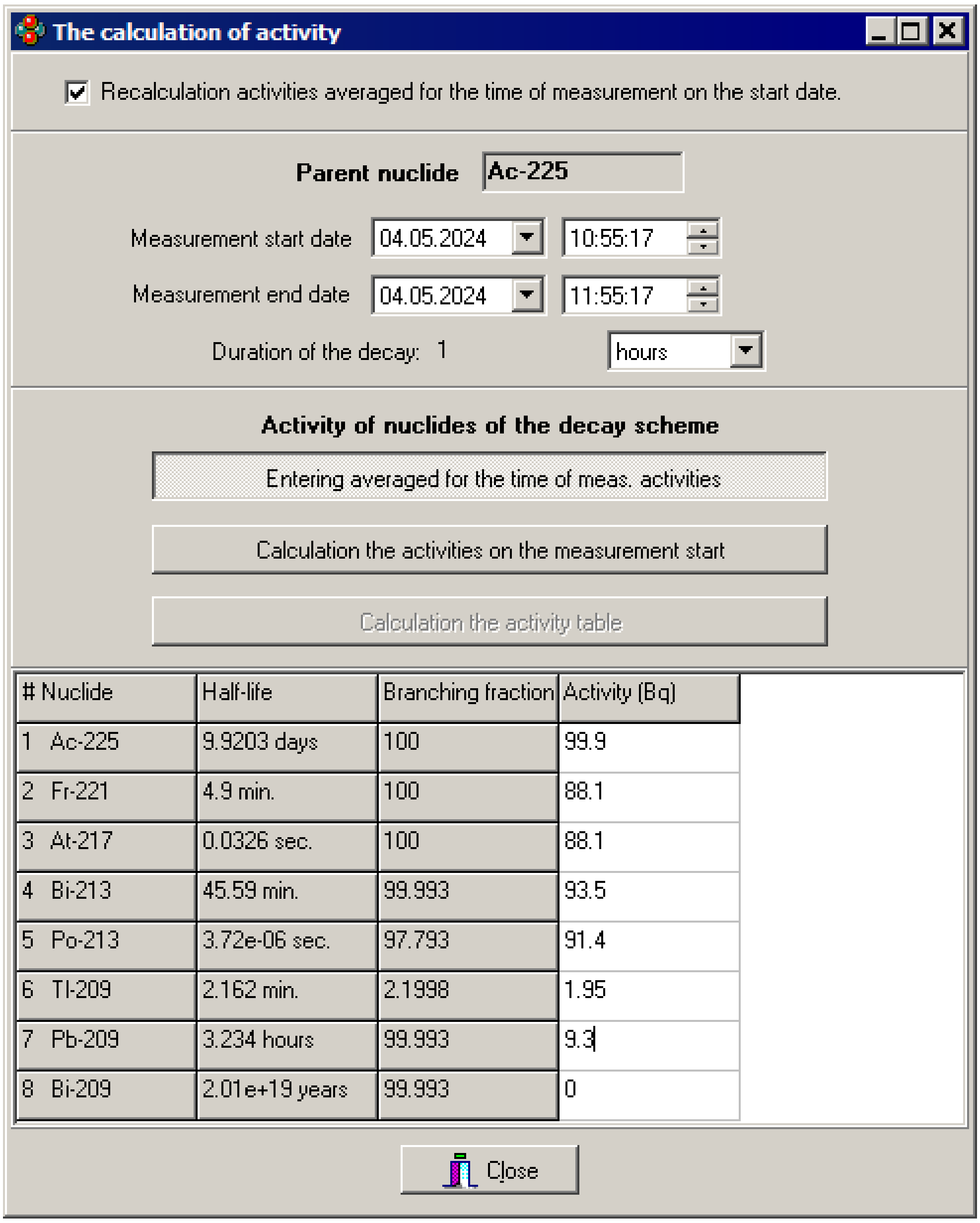
The activity table calculation procedure also calculates the average values of activities during the decay. Under our initial conditions (100 Bq Ac-225 and Bi-213), the average per hour decay (decay during sample measurement) will have the following values:



Start date 04.05.2024 10:55:17
Final date 04.05.2024 11:55:17
Duration of the decay: 0 days 0 hours 59 min. 60 sec.
Number of points 3601

Date\Activity	1 Ac-225	2 Fr-221	3 At-217	4 Bi-213	5 Po-213	6 Tl-209	7 Pb-209	8 Bi-209
04.05.2024 11:55:12	99.71	99.723	99.723	95.075	92.983	2.0866	17.996	3.6528E-23
04.05.2024 11:55:13	99.71	99.723	99.723	95.076	92.984	2.0866	18.001	3.6547E-23
04.05.2024 11:55:14	99.71	99.723	99.723	95.077	92.985	2.0866	18.005	3.6567E-23
04.05.2024 11:55:15	99.709	99.723	99.723	95.078	92.986	2.0866	18.01	3.6587E-23
04.05.2024 11:55:16	99.709	99.723	99.723	95.079	92.987	2.0867	18.015	3.6606E-23
04.05.2024 11:55:17	99.709	99.723	99.723	95.08	92.989	2.0867	18.019	3.6626E-23
Mean:	99.855	88.105	88.104	93.491	91.42	1.9483	9.3102	1.2442E-23

Let's enter this value into the calculation table by checking the box "Recalculation activities averaged for the time of measurement on the start date":



☑ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide Ac-225

Measurement start date 04.05.2024 10:55:17

Measurement end date 04.05.2024 11:55:17

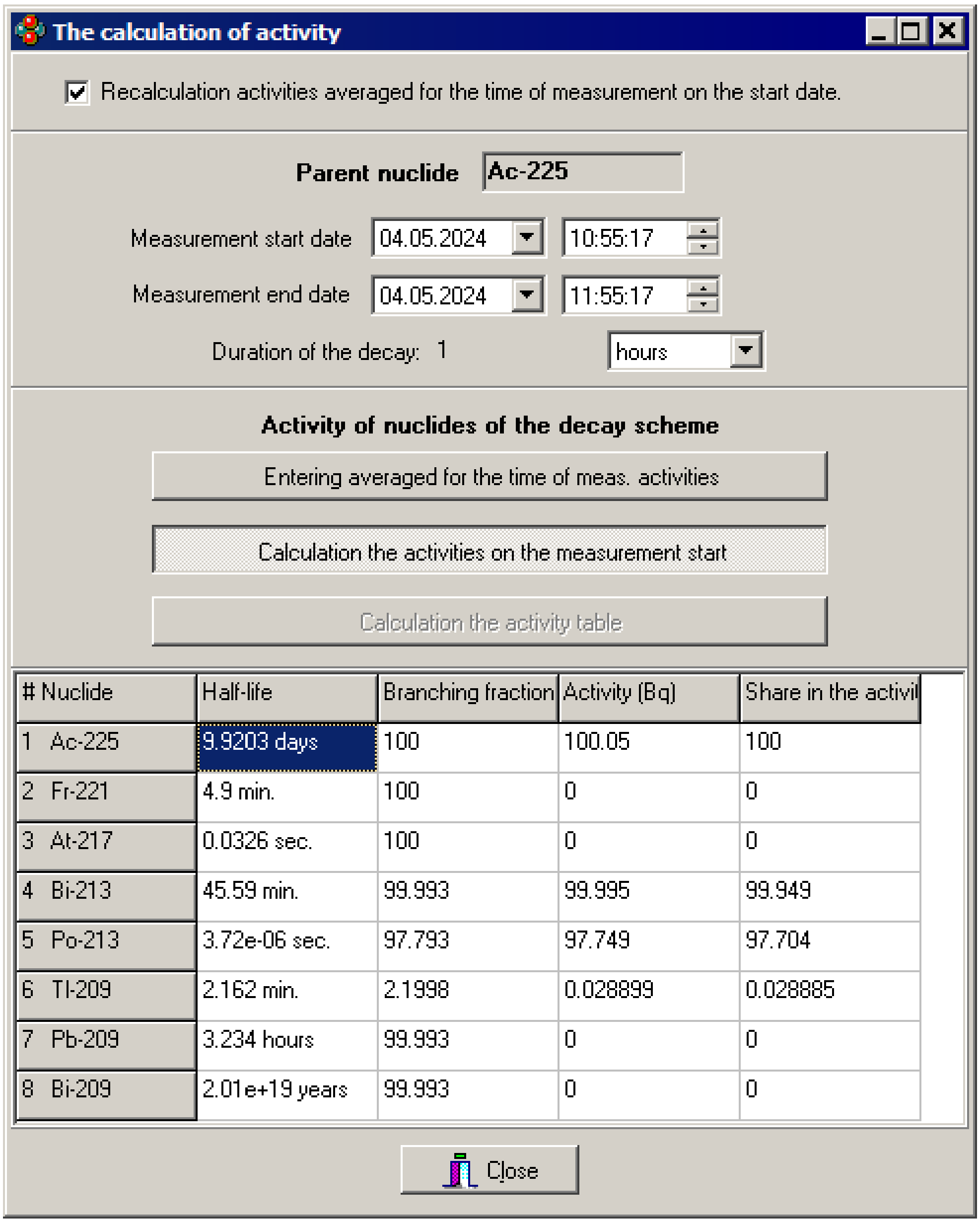
Duration of the decay: 1 hours

Activity of nuclides of the decay scheme

#	Nuclide	Half-life	Branching fraction	Activity (Bq)
1	Ac-225	9.9203 days	100	99.9
2	Fr-221	4.9 min.	100	88.1
3	At-217	0.0326 sec.	100	88.1
4	Bi-213	45.59 min.	99.993	93.5
5	Po-213	3.72e-06 sec.	97.793	91.4
6	Tl-209	2.162 min.	2.1998	1.95
7	Pb-209	3.234 hours	99.993	9.3
8	Bi-209	2.01e+19 years	99.993	0

And calculate the activity at the beginning of the measurements by clicking on the Calculation the activities on the measurement start key.

We will get the result:



☑ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide: Ac-225

Measurement start date: 04.05.2024 10:55:17

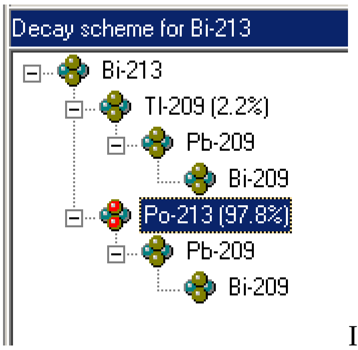
Measurement end date: 04.05.2024 11:55:17

Duration of the decay: 1 hours

# Nuclide	Half-life	Branching fraction	Activity (Bq)	Share in the activi
1 Ac-225	9.9203 days	100	100.05	100
2 Fr-221	4.9 min.	100	0	0
3 At-217	0.0326 sec.	100	0	0
4 Bi-213	45.59 min.	99.993	99.995	99.949
5 Po-213	3.72e-06 sec.	97.793	97.749	97.704
6 Tl-209	2.162 min.	2.1998	0.028899	0.028885
7 Pb-209	3.234 hours	99.993	0	0
8 Bi-209	2.01e+19 years	99.993	0	0

The conditionality of the matrix of the system of integral equations that must be solved during the calculation may be low and the calculation results may have significant uncertainties. In the given example, the average activities are calculated from the activity value at the initial date of Ac-225 and the activity of Bi-213 equal to 100 Bq with zero activities of other subsidiaries. The reverse calculation gave the initial value of the activity of Po-213 equal to 97.7 Bq, which, of course, differs significantly from the initial zero, but the half-life of Po-213 is only 3.72 microseconds, therefore, the introduced errors of the average values during the measurement are quite sufficient to obtain such initial values. The initial conditions were set incorrectly for demonstration purposes (in reality, Po-213 is always in equilibrium with Bi-213). But in practice, it must be borne in mind that the uncertainty of the measurement results will affect the solution of the inverse problem.

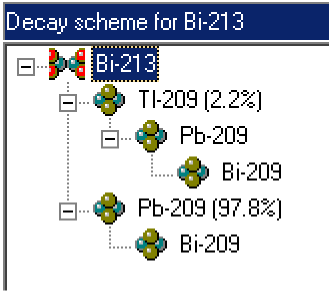
Let's correct the initial data so that the task is correct – first of all, we will form the equilibrium chain B-213-Po-213.



Decay scheme for Bi-213

- Bi-213
  - Tl-209 (2.2%)
    - Pb-209
      - Bi-209
  - Po-213 (97.8%)
    - Pb-209
      - Bi-209

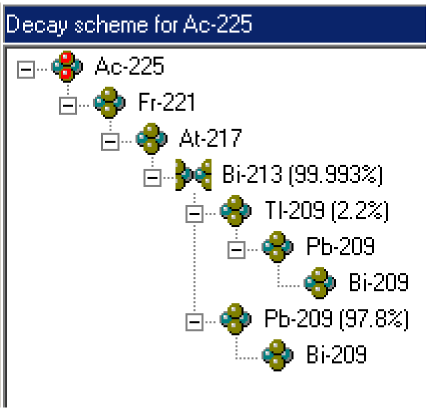
In this case, it is necessary to form an equilibrium chain from one branch of the Bi-213 decay. Therefore, we will select Po-213 and start the procedure for forming an equilibrium chain. We obtain the following Bi-213 decay scheme



Decay scheme for Bi-213

- Bi-213
  - Tl-209 (2.2%)
    - Pb-209
      - Bi-209
  - Pb-209 (97.8%)
    - Bi-209

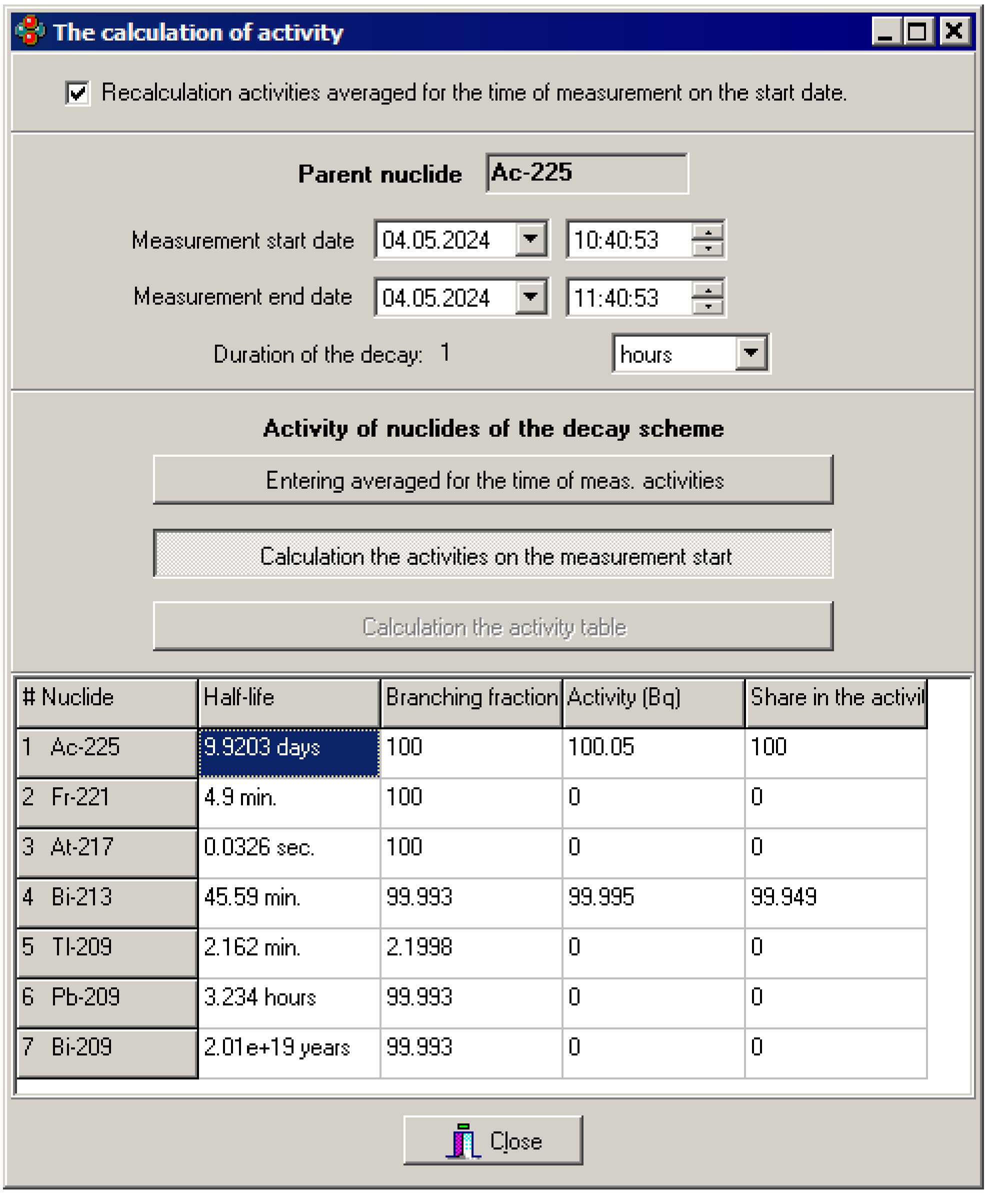
And the corresponding Ac-225 decay scheme



Decay scheme for Ac-225

- Ac-225
  - Fr-221
    - At-217
      - Bi-213 (99.993%)
        - Tl-209 (2.2%)
          - Pb-209
            - Bi-209
        - Pb-209 (97.8%)
          - Bi-209

Repeating the calculation of the activities at the beginning of the measurements according to the average activities during the measurement, we get a completely correct result of the activities at the beginning of the measurement:



☑ Recalculation activities averaged for the time of measurement on the start date.

Parent nuclide Ac-225

Measurement start date 04.05.2024 10:40:53

Measurement end date 04.05.2024 11:40:53

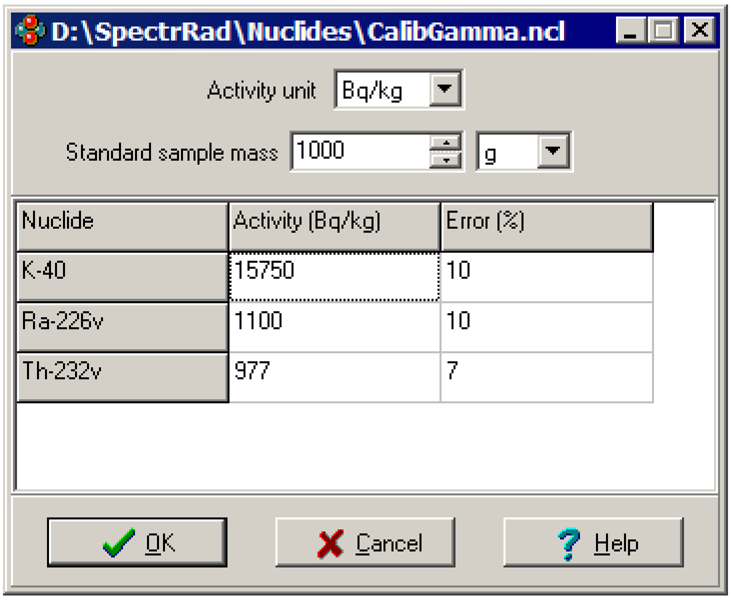
Duration of the decay: 1 hours

Activity of nuclides of the decay scheme

#	Nuclide	Half-life	Branching fraction	Activity (Bq)	Share in the activi
1	Ac-225	9.9203 days	100	100.05	100
2	Fr-221	4.9 min.	100	0	0
3	At-217	0.0326 sec.	100	0	0
4	Bi-213	45.59 min.	99.993	99.995	99.949
5	Tl-209	2.162 min.	2.1998	0	0
6	Pb-209	3.234 hours	99.993	0	0
7	Bi-209	2.01e+19 years	99.993	0	0

Certificate of the standard source

The menu item "**Tools / Certificate of the standard source...**" allows the operator to supplement information about nuclides with information about the activities and activity errors of selected nuclides in the table. At the same time, a form for entering activities will appear on the screen:



Activity unit: Bq/kg

Standard sample mass: 1000 g

Nuclide	Activity (Bq/kg)	Error (%)
K-40	15750	10
Ra-226v	1100	10
Th-232v	977	7

The operator can select the **units of activity (Activity unit)** of nuclides in the standard: "**Bq**" or "**Bq/kg**", set the **Standard sample mass**, if necessary, and enter data on the activities and errors of the activities of the selected nuclides. The absence of data in the "**Activity**" column or a zero activity value means that there is no information about the activity of this nuclide and, if necessary, the calibration procedure will request the missing information from the operator. The number of rows in the table for entering activities depends on whether the nuclide table entries have been pre-selected or not. When pre–selecting table rows, only selected records are copied to the table for entering activities, if there are no selected ones, all records of the nuclide table are copied. Setting the mass of the standard allows you to calculate the activity of a counting sample prepared from the standard if the not the entire standard sample is used as a counting sample.

Using the nuclide tables with the generated certificate as a working table, when installing geometry in the SPECTRRAD software package, greatly simplifies calibration procedures, since the operator does not have to enter data on the activities of nuclides present in the standard when calculating elementary spectra or calibrating the registration efficiency. In any case, the operator must specify the date of certification of the standard (the date on which the activity values are given) in the "Sampling date" column when starting the measurement of the standard.

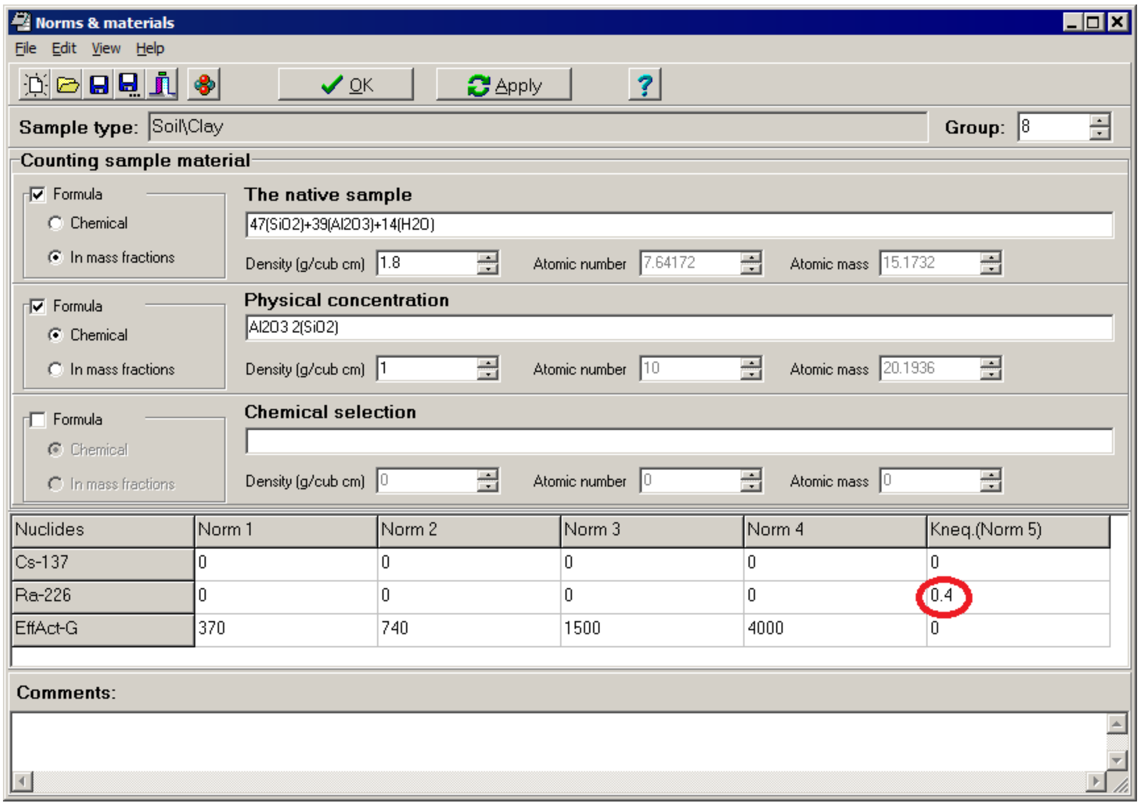
Appendix

Evaluation the activity of Ra-226 by gamma-ray spectrometric methods

Ra-226 has only one significant gamma line (186.211 keV, 3.64%), which almost coincides with the most powerful gamma line U-235 (185.715 keV, 57%) and a number of weak lines of daughter U-238: Pa-234 (186.15 keV, 1.85%), (Th-230 (186.53 keV, 0.0088%), Pa-234m (184.7 keV, 0.00168 %).

There is practically no possibility of decomposing the **scintillation spectrum** into U-235, U-238 (or U-nat) and Ra-226. Therefore, the evaluation the activity of Ra-226 is used by radiation of daughter Rn-222 (Pb-214, Bi-214). But Rn-222 has a fairly long half-life (3.82 days) and may well fly out of the sample material and from the measuring vessel. The standard procedure for determining Ra-226 by Rn-222 requires a 20-day exposure of the counting sample in an airtight measuring vessel. As practice has shown, standard plastic Marinelli vessels do not have the required tightness. Metal vessels with an airtight lid are required. The method of rapid assessment of the content of Ra-226 suggests using the average coefficient of emanation of Rn-222 equal to 0.75±0.25 and, accordingly, the uncertainty of the coefficient of emanation (≈30%) is added to the measurement error.

In recent years, many studies of radon emanation coefficients for various materials have been published, for example, "The influence of clay rock properties on radon emanation" by P.S. Miklyaev, T.B. Petrova, and others, "Features of radon emanation from soils in areas mined by coal mines (using the example of the Leninsk–Kuznetsky district)" by T.V. Leshchukov, A.V. Larionov and others, etc. It is more correct to use a different radon emission coefficient for different materials rather than an average one. The "SPECTRRAD" package provides such an opportunity - in the structure of the standards of the "SPECTRRAD" package, **Norm 5** is used by the report generation procedure as the **Kneq** disequilibrium coefficient.



Sample type: Soil\Clay

Group: 8

Counting sample material

The native sample

☑ Formula
○ Chemical
● In mass fractions

47(SiO2)+39(Al2O3)+14(H2O)

Density (g/cub cm) 1.8 Atomic number 7.64172 Atomic mass 15.1732

Physical concentration

☑ Formula
● Chemical
○ In mass fractions

Al2O3 2(SiO2)

Density (g/cub cm) 1 Atomic number 10 Atomic mass 20.1936

Chemical selection

☐ Formula
● Chemical
○ In mass fractions

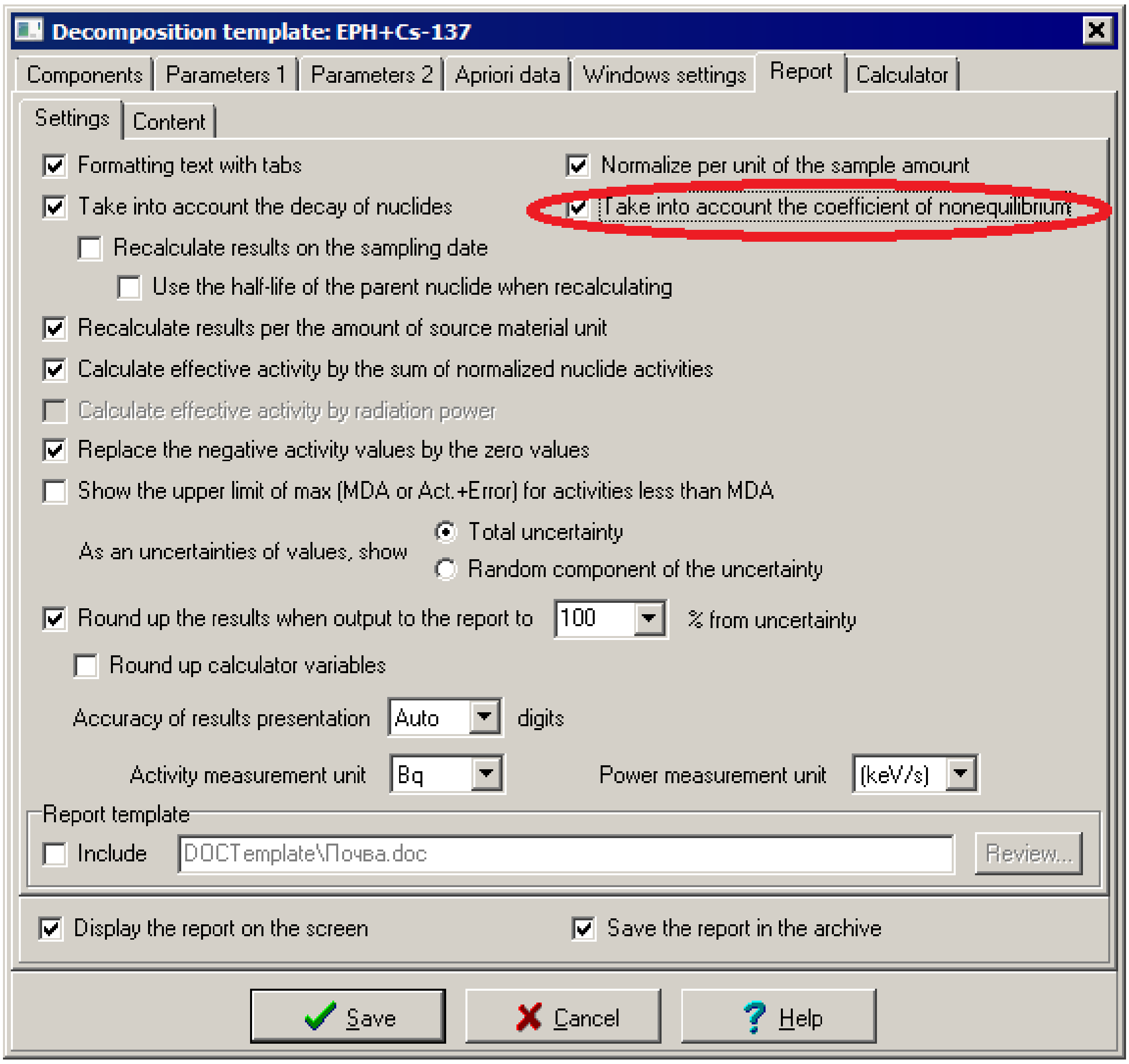
Density (g/cub cm) 0 Atomic number 0 Atomic mass 0

Nuclides	Norm 1	Norm 2	Norm 3	Norm 4	Kneq.(Norm 5)
Cs-137	0	0	0	0	0
Ra-226	0	0	0	0	0.4
EffAct-G	370	740	1500	4000	0

Comments:

In the event that the activity of a nuclide A_{N1} in the equilibrium chain is determined through the activity of another nuclide A_{N2}, the nonequilibrium coefficient *N2* relative to *N1* is defined as $K_{neq} = \frac{A_{N1} - A_{N2}}{A_{N1}}$. In this case, the activity of nuclide *N1* is calculated using the formula $A_{N1} = A_{N2} /(1 - K_{ntq})$ (1).

The nonequilibrium coefficient is determined by processes that are not taken into account by the procedures for calculating the response of the spectrometer to radiation from the equilibrium chain of nuclides: the emanation of gaseous decay products from the sample, different solubility of nuclides in solvents, etc. A well–known example is the definition of the activity of Ra-226 by the express method (without 20 days exposure in an airtight vessel) from the radiation of daughter Rn-222. In this case, the nonequilibrium coefficient will be mainly determined by the emanation coefficient Rn-222 from the counting sample. The calculation according to formula (1) is performed only if the "**Take into account the coefficient of nonequilibrium**" checkbox is selected in the report generation parameters.



☑ Formatting text with tabs

☑ Normalize per unit of the sample amount

☑ Take into account the decay of nuclides

☑ Take into account the coefficient of nonequilibrium

☐ Recalculate results on the sampling date

☐ Use the half-life of the parent nuclide when recalculating

☑ Recalculate results per the amount of source material unit

☑ Calculate effective activity by the sum of normalized nuclide activities

☐ Calculate effective activity by radiation power

☑ Replace the negative activity values by the zero values

☐ Show the upper limit of max (MDA or Act.+Error) for activities less than MDA

As an uncertainties of values, show ● Total uncertainty ○ Random component of the uncertainty

☑ Round up the results when output to the report to 100 % from uncertainty

☐ Round up calculator variables

Accuracy of results presentation Auto digits

Activity measurement unit Bq

Power measurement unit (keV/s)

Report template

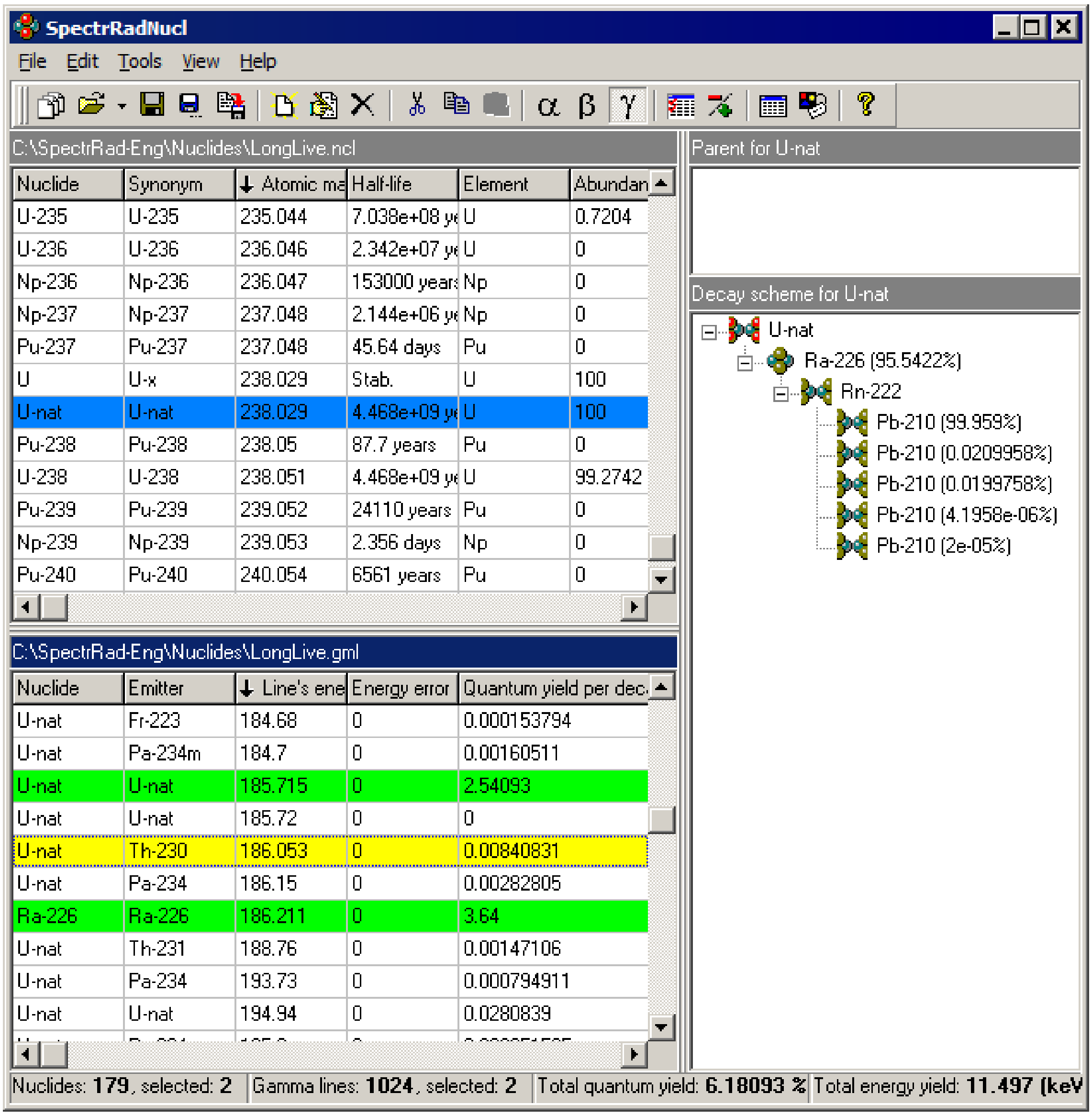
☐ Include DOCTemplate\Почва.doc Review...

☑ Display the report on the screen

☑ Save the report in the archive

For gamma-ray spectra **measured on spectrometers with cooled detectors made of HPGe**, it is possible to use own Ra-226 line.

U-238 and U-235 in uranium are in a certain ratio, and therefore, if the uranium is not enriched, it is wiser not to separate the uranium in the library, but to use a natural mixture of uranium – U-nat:



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Nuclide	Synonym	Atomic ma	Half-life	Element	Abundan
U-235	U-235	235.044	7.038e+08 ye	U	0.7204
U-236	U-236	236.046	2.342e+07 ye	U	0
Np-236	Np-236	236.047	153000 years	Np	0
Np-237	Np-237	237.048	2.144e+06 ye	Np	0
Pu-237	Pu-237	237.048	45.64 days	Pu	0
U	U-x	238.029	Stab.	U	100
U-nat	U-nat	238.029	4.468e+09 ye	U	100
Pu-238	Pu-238	238.05	87.7 years	Pu	0
U-238	U-238	238.051	4.468e+09 ye	U	99.2742
Pu-239	Pu-239	239.052	24110 years	Pu	0
Np-239	Np-239	239.053	2.356 days	Np	0
Pu-240	Pu-240	240.054	6561 years	Pu	0

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Nuclide	Emitter	Line's ene	Energy error	Quantum yield per dec.
U-nat	Fr-223	184.68	0	0.000153794
U-nat	Pa-234m	184.7	0	0.00160511
U-nat	U-nat	185.715	0	2.54093
U-nat	U-nat	185.72	0	0
U-nat	Th-230	186.053	0	0.00840831
U-nat	Pa-234	186.15	0	0.00282805
Ra-226	Ra-226	186.211	0	3.64
U-nat	Th-231	188.76	0	0.00147106
U-nat	Pa-234	193.73	0	0.000794911
U-nat	U-nat	194.94	0	0.0280839

Parent for U-nat

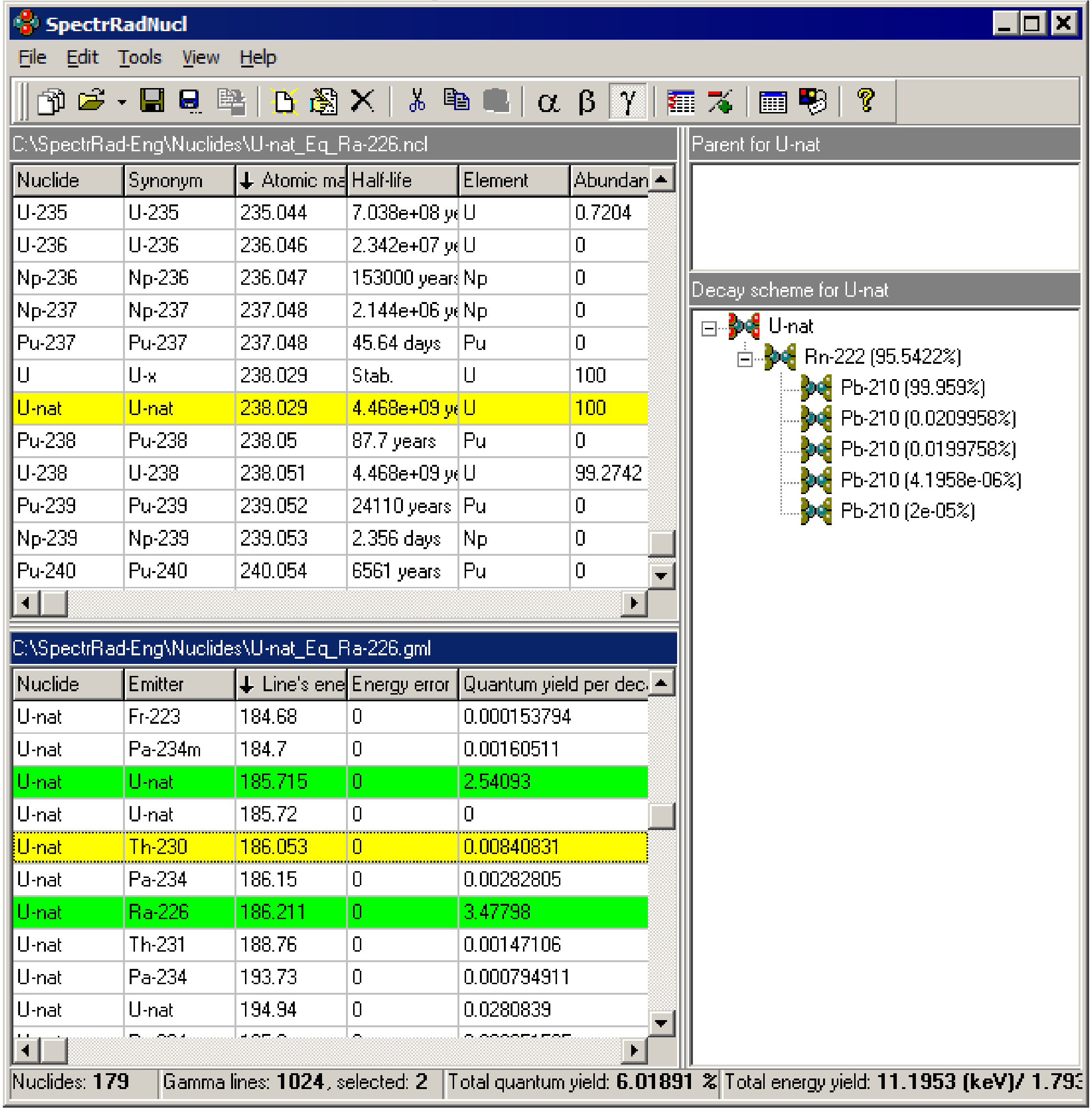
Decay scheme for U-nat

- U-nat
  - Ra-226 (95.5422%)
    - Rn-222
      - Pb-210 (99.959%)
      - Pb-210 (0.0209958%)
      - Pb-210 (0.0199758%)
      - Pb-210 (4.1958e-06%)
      - Pb-210 (2e-05%)

Nuclides: **179**, selected: **2** | Gamma lines: **1024**, selected: **2** | Total quantum yield: **6.18093 %** | Total energy yield: **11.497 (keV**

Since the chemical properties of Ra-226 differ from those of uranium (it can be leached out in the soil), radium is isolated as a separate nuclide in the decay chain.

If we are sure that Ra-226 is in equilibrium with U-that, we can include Ra-226 in U-nat:



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Nuclide	Synonym	Atomic ma	Half-life	Element	Abundan
U-235	U-235	235.044	7.038e+08 ye	U	0.7204
U-236	U-236	236.046	2.342e+07 ye	U	0
Np-236	Np-236	236.047	153000 years	Np	0
Np-237	Np-237	237.048	2.144e+06 ye	Np	0
Pu-237	Pu-237	237.048	45.64 days	Pu	0
U	U-x	238.029	Stab.	U	100
U-nat	U-nat	238.029	4.468e+09 ye	U	100
Pu-238	Pu-238	238.05	87.7 years	Pu	0
U-238	U-238	238.051	4.468e+09 ye	U	99.2742
Pu-239	Pu-239	239.052	24110 years	Pu	0
Np-239	Np-239	239.053	2.356 days	Np	0
Pu-240	Pu-240	240.054	6561 years	Pu	0

Parent for U-nat

Decay scheme for U-nat

- U-nat
  - Rn-222 (95.5422%)
    - Pb-210 (99.959%)
    - Pb-210 (0.0209958%)
    - Pb-210 (0.0199758%)
    - Pb-210 (4.1958e-06%)
    - Pb-210 (2e-05%)

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Nuclide	Emitter	Line's ene	Energy error	Quantum yield per dec
U-nat	Fr-223	184.68	0	0.000153794
U-nat	Pa-234m	184.7	0	0.00160511
U-nat	U-nat	185.715	0	2.54093
U-nat	U-nat	185.72	0	0
U-nat	Th-230	186.053	0	0.00840831
U-nat	Pa-234	186.15	0	0.00282805
U-nat	Ra-226	186.211	0	3.47798
U-nat	Th-231	188.76	0	0.00147106
U-nat	Pa-234	193.73	0	0.000794911
U-nat	U-nat	194.94	0	0.0280839

Nuclides: **179** | Gamma lines: **1024**, selected: **2** | Total quantum yield: **6.01891 %** | Total energy yield: **11.1953 (keV)/ 1.79**

This increases the conditionality of the task and, consequently, the accuracy of the definition of Ra-226.

An example of a program for calculating parameters of compliance

A calculator program that calculates the parameters of compliance of Cs-137 and Sr-90 quantities with SanPiN safety standards may look like this:

Calculation program

```
// Initialization section
p1; // CL for Sr-90
p2; // CL for Cs-137
p;a;e;a1;a2;e1;e2;
// Calculation section
{p1=Norm1(Sr-90);   // Read the standard.
 if(p1==0)           // If the standard is not defined,
{
  p1=100;            // define the default value,
  p1=input("Reference level for Sr-90 (Bq/kg)");// ask the
operator
 }
 p2= Norm2(Cs-137);
 if(p2==0)
 {
   p2=100;
   p2=input("Reference level for Cs-137 (Bq/kg)");//  }
 a1=Act(Sr-90)/p1;
 a2=Act(Cs-137)/p2;
 e1=Err(Sr-90)/p1;
 e1=e1*e1;
 e2=Err(Cs-137)/p2;
 e2=e2*e2;
 Calc1=round(100*(a1+a2)/SampleValue)/100;
 ErCalc1=round(100*sqrt(e1+e2)/SampleValue)/100;
 Calc2=Calc1+ErCalc1;
 if(Calc2 > 1)          // If it does not meet the requirements,
   Report("Does not meet the requirements"); // use the
appropriate report template
}
```

Format for displaying result in a report

```
__________________________________________________
  Parameters of compliance (B)
RL for Sr-90 - %s Bq/kg, RL for Cs-137 - %s Bq/kg
B   =  %s(Act.)  +  %s(Error)  =  %s
```

List of variables to print in the report

```
p1,p2,Calc1, ErCalc1, Calc2
```

The program saves the calculation results in columns Calc 1 - Calc 2 of the measurement results archive. It is recommended to rename the archive column data accordingly:

Calc 1 is the compliance parameter.

ErCalc1 is the error of the compliance parameter.

Calc 2 is the total compliance parameter.

An example of a program for calculating the volume activity of radon

A calculator program that calculates the volumetric and volumetric equivalent activity of radon based on the results of measuring the activity of radon (Rn-222) in carbon filters using the passive method according to the method proposed by Pavlov I.V. (STC "Niton") may look like this:

Calculation program

```
// Initialization section
a;c;n=3;dexpos;teks;tcool=1;m1=20;m2=21;m;e;ce;ee;
// Calculation section
{
 n=input("Number of adsorbers");
 dexpos = Dsample;                // default value
 dexpos = inputdate("Start date of the exposure");
 m1=input("Mass of adsorbers before exposure (g)");
 m2=input("Mass of adsorbers after exposure (g)");
 teks = (Dsample-dexpos)/3600.;
 tcool = (Dact-Dsample)/3600.;
 m=(m2-m1)/n;
 c=1000*Act(Rn-222)*exp(0.00755*tcool);
 e=1000.*Err(Rn-222)*exp(0.00755*tcool);
 m1=1.58+0.307*ln(teks)-0.923*sqrt(m);
 m2=2.04*sqrt(m)*exp(-0.0438*teks);
 Calc3=round(c/(n*exp(m1-m2))+0.5);
 ErCalc3=round(e/(n*exp(m1-m2))+0.5);
 Calc8=0.4*Calc3;
 ErCalc8=0.4*ErCalc3;}
```

Format for displaying result in a report

```
------------------------------------------------------------
 Volumetric radon activity = %s  +/-  %s (Bq./cubic meters)
 Equiv.equil. vol. radon activity = %s  +/-  %s (Bq./cubic meters)
------------------------------------------------------------
```

List of variables to print in the report

```
Calc3,ErCalc3,Calc8,ErCalc8
```

The program saves the calculation results in Calc3 - ErCalc8 columns of the measurement results archive. It is recommended to rename the archive column data accordingly:

Calc 3 is the volume activity of radon.

ErCalc3 is the error of volume activity.

Calc8 is the equivalent equilibrium volume activity of radon.

ErCalc8 is the error of the equivalent equilibrium volume activity.

Example of a report template

MINISTRY OF HEALTH OF THE RUSSIAN FEDERATION

Moscow Center for State Sanitary and Epidemiological Surveillance

129626, Moscow, Grafsky lane, 4/9 phone (095)-287-78-34

Department of Radiation Hygiene

PRODUCT TEST REPORT N {Sample} dated {Date}

{Program}

{lbAnalyser}:	{Analyser}
{lbGeometry}:	{Geometry}
{lbInfo}:	{Info}
{lbAddNote}:	{AddNote}
{lbSampleType}:	{SampleType}
{lbSampleNote}:	{SampleNote}
{lbSampleArea}:	{SampleArea}
{lbComment}:	{Comment}
{lbSize}:	{Size}
{lbMeasTime}:	{MeasTime}

Нуклид	**Активность ({AUnit})**	**Погрешность ({AUnit})**	**(%)**
<<{Nucl}	{Activ}	{AbsErr}	{RelErr}

>>{Calculator}

{Warnings}
{ActualDate}
{NumberOfSamples}

Operator:

Conclusion of the sanitary doctor:

The studied food samples in terms of the content of radionuclides of caesium-137 and strontium-90 comply with the current SanPiN 2.3.2.560-96.

Head of the Department

Example of a statistical report template

MINISTRY OF HEALTH OF THE RUSSIAN FEDERATION

Moscow Center for State Sanitary and Epidemiological Surveillance

129626, Moscow, Grafsky lane, 4/9 phone (095)-287-78-34

Department of Radiation Hygiene

PRODUCT TEST REPORT N {Sample} dated {Date}

Spectrometer: {Analyzer}
Applicant: {Declarant}
Sampling location: {Sample Area}
Date of measurement: {MeasDate}

TEST RESULTS

Sample	**Eff. activity {AUnit}**	**Radionuclides activity, {AUnit}**			
		Cs137	**K40**	**Ra226**	**Th232**
<<{Sample}	{Aeff&Err}	{Act&Err[Cs-137]}	{Act&Err[K-40]}	{Act&Err[Ra-226]}	{Act&Err[Th-232]}

>>

Number of records	{N[Aeff]}	{N[Cs-137]}	{N[K-40]}	{N[Ra-226]}	{N[Th-232]}
Minimum value	{XMin[Aeff]} ±{GMin[Aeff]}	{XMin[Cs-137]} ±{GMin[Cs-137]}	{XMin[K-40]} ±{GMin[K-40]}	{XMin[Ra-226]} ±{GMin[Ra-226]}	{XMin[Th-232]} ±{GMin[Th-232]}
Maximum value	{XMax[Aeff]} ±{GMax [Aeff]}	{XMax[Cs-137]} ±{GMax [Cs-137]}	{XMax [K-40]} ±{GMax [K-40]}	{XMax [Ra-226]} ±{GMax [Ra-226]}	{XMax [Th-232]} ±{GMax [Th-232]}
Mean	{X0[Aeff]} ±{G0[Aeff]}	{X0[Cs-137]} ±{G0[Cs-137]}	{X0[K-40]} ±{G0[K-40]}	{X0[Ra-226]} ±{G0[Ra-226]}	{X0[Th-232]} ±{G0[Th-232]}
RMSD	{Sx[Aeff]}	{Sx[Cs-137]}	{Sx[K-40]}	{Sx[Ra-226]}	{Sx[Th-232]}
Stat. error	{USx[Aeff]}	{USx[Cs-137]}	{USx[K-40]}	{USx[Ra-226]}	{USx[Th-232]}
Tot. error	{UTx[Aeff]}	{UTx[Cs-137]}	{UTx[K-40]}	{UTx[Ra-226]}	{UTx[Th-232]}

Operator:

Example of a control chart template

REFERENCE SOURCE ACTIVITY MEASUREMENTS GRAPH

{Programm}

{lbSampleCode}:**{SampleCode}**
{lbSample}:**{Sample}**
{lbSampleNote}: **{SampleNote}**
{lbSampleType}: **{SampleType}**
{lbComment}: **{Comment}**
{lbSampleDate}: **{SampleDate}**

Measuring tool	
Spectrometer	Verification certificate
{Analyser}	{Info}

{Image}

Additional error:	{AddError} %
Minimum:	{Ymin}±{YminErr} {Yunit}
Maximum:	{Ymax}±{YmaxErr} {Yunit}
Mean:	{Ymid}±{YErrmid} {Yunit}
Bias:	{Bias} {Yunit} ({BiasPercent} %)
RMSD:	{StDvn} {Yunit}
Stat. error:	{ExStDvn} {Yunit}
Total error:	{ExTotDvn}{Yunit}

Control levels:

Nominal level:	{Level1} {Yunit}
Upper level:	{Level2} {Yunit}
Lower level:	{Level3} {Yunit}

{EnergyPar}

{Warnings}

The activities shown on the graph have been recalculated as of the date of certification of the reference source.

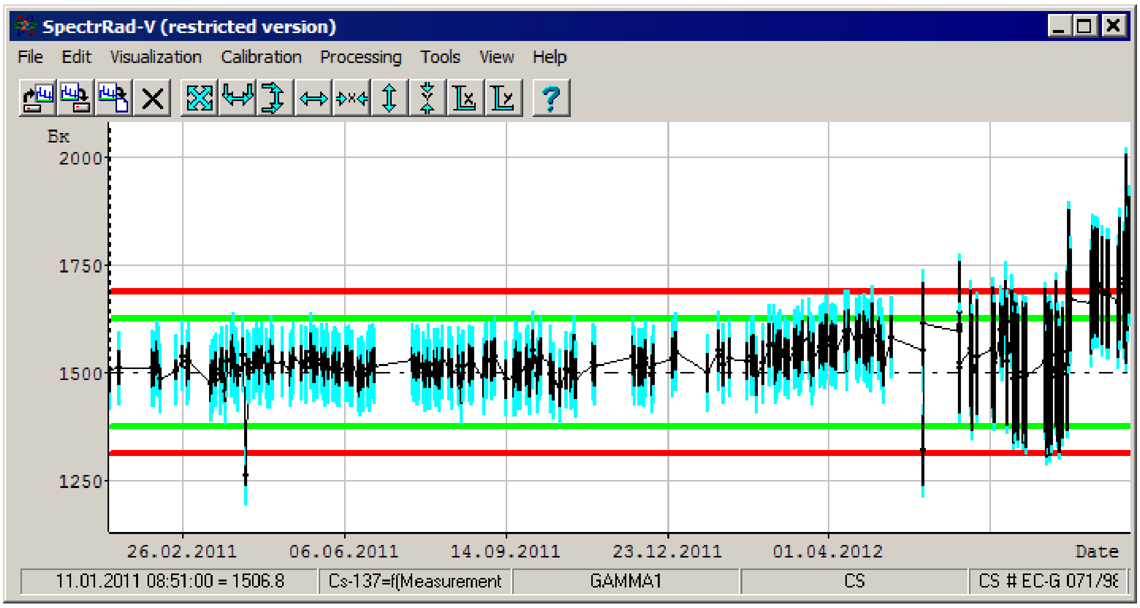
Responsible for the report	Operator	{Operator}	____________
	post	name	signature

Control chart specimen

REFERENCE SOURCE ACTIVITY MEASUREMENTS GRAPH

Sample code:**CS # EC-G 071/98**
Sample name:**Act. Cs-137 = 1500 Bq.,Act. K-40 = 16500 Bq.**
Sample note: **Reference source Cs-137+K-40 # EC-G 071/98 Act. Cs-137 = 1500 Bq.,Act. K-40 = 16500 Bq.**
Sample type: **Reference source**
Comment: **Act(Cs-137)=f(Meas. date)**
Sample date: **11.01.2011 8:51:00**

Measuring tool	
Spectrometer	Verification certificate
0781-AR-B-G	3004845



11.01.2011 08:51:00 = 1506.8
Cs-137=f(Measurement
GAMMA1
CS
CS # EC-G 071/9

Minimum:	1261 ± 70 (20) Bq
Maximum:	1800 ± 160 (130) Bq
Mean:	1537 ± 100 (70) Bq
Bias:	37 Bq (2,45 %)
RMSD:	58.9
Stat. error:	118

Control levels:

Nominal:	1500 Bq
The upper limit of the warning level:	1625 Bq
The lower limit of the warning level:	1375 Bq
The upper limit of the action level:	1688 Bq
The lower limit of the action level :	1313 Bq

Time range: 11.01.2011 - 04.10.2012 (5.46043e+07 c)

Responsible for the report Operator Vasileva N.A. ____________
name signature

Mathematics

Energy calibration

The energy calibration of the spectrometer (or the selected spectrum) determines the relationship between the channels of the spectrometer (spectrum) and the energy of the detected radiation. Energy calibration is divided into two types: **Basic** and **Drift correction**.

Four variants of the communication function are used for the initial calibration $E = \varphi(Pn(z))$:

Scale	**Function**
Linear	$\mathrm{E} = \mathrm{Pn(z)}$
Exponential	$\mathrm{E} = \exp(\mathrm{Pn(z)})$
Logarithmic	$\mathrm{E} = \log(\mathrm{Pn(z)})$
Square root	$\mathrm{E} = \sqrt{\mathrm{Pn(z)}}$

By default, a linear scale is used $\mathrm{E} = \mathrm{Pn(z)}$.

$\mathrm{Pn(z)}$ - a polynomial of rank no higher than 3, which is replaced by a tangent at the extreme calibration points.

$\mathrm{z} < \mathrm{z}_0$	$\mathrm{Pn} = \mathrm{P'n(z_o)} \cdot \mathrm{z} + \mathrm{Pn(z_o)} - \mathrm{P'n(z_o)} \cdot \mathrm{z_o}$
$\mathrm{z} < \mathrm{z}_0 < z_n$	$\mathrm{Pn} = \mathrm{Pn(z)}$
$\mathrm{z} > \mathrm{z_n}$	$\mathrm{Pn} = \mathrm{P'n(z_n)} \cdot \mathrm{z} + \mathrm{Pn(z_n)} - \mathrm{P'n(z_n)} \cdot \mathrm{z_n}$

Here: *E*- energy; $\mathrm{z} = \mathrm{x} - (\mathrm{x}_0 + \mathrm{x_n})/2$; x_0, ($\mathrm{z}_0 = (\mathrm{x}_0 - \mathrm{x_n})/2$) - the first calibration point, x_n, ($\mathrm{z_n} = (\mathrm{x_n} - \mathrm{x}_0)/2$) - the last calibration point; $\mathrm{Pn(z)}$ - the polynomial; $\mathrm{P'n(z)}$ - derivative of a polynomial: $\mathrm{P'n(z_0)}$ - derivative at a point z_0, $\mathrm{P'n(z_n)}$ - derivative at a point z_n.

The coefficients of the polynomial are determined by the least squares method

$$k_{Pn} = (A^T \cdot W^T \cdot W \cdot A)^{-1} \cdot A^T \cdot W^T \cdot W \cdot e$$

Here:

$$A_{ij} = \sum_{k=1}^{n} P^i(z_k) \cdot P^j(z_k);$$

n is the number of calibration points;

$P^j(z_k)$ - an orthogonal Chebyshev polynomial of rank *j* at a point z_k

$W = K_z^{-1/2}$ - the matrix of weights;

$K_z = D_z \cdot I$ (I – identity matrix, D_z – vector of variances);

K_z - covariance matrix of the positions of labeled peaks or channels. The energies of the labeled peaks or channels are considered known, and all calibration uncertainty is related to the uncertainty of the peak positions used to calibrate the linear spectra or channels selected by the operator. If the channels selected by the operator are used for calibration, the position uncertainty is assumed to be half the channel.

e - a vector of energies used to calibrate peaks or channels.

If the error in determining the coefficient at the highest degree of the polynomial exceeds its value, the rank of the polynomial is lowered and a new energy calibration polynomial is calculated.

The drift of the energy calibration during the operation of the spectrometer is assumed to be nonlinear: $\mathrm{x} = \mathrm{a} \cdot \mathrm{ch} + \mathrm{b} + \mathrm{c} \cdot \mathrm{ch}^2$ (ch - spectrometer channel, a-1 - gain drift, b - scale zero drift, c – nonlinear distortion coefficient). During the initial calibration $\mathrm{x} = \mathrm{ch}$.

Peaks width calibration

The width of the peaks at half the height is used as the width of the peaks. Peak width calibration determines the relationship between peak width and peak energy.

Four communication function options are used to calibrate the peak widths. $FWHM = \varphi(Pn(z))$:

Scale	**Function**
Linear	$\mathrm{E} = \mathrm{Pn(z)}$
Exponential	$\mathrm{E} = \exp(\mathrm{Pn(z)})$
Logarithmic	$\mathrm{E} = \log(\mathrm{Pn(z)})$
Square root	$\mathrm{E} = \sqrt{\mathrm{Pn(z)}}$

By default, a square root scale is used $FWHM = \sqrt{\mathrm{Pn(z)}}$.

$\mathrm{Pn(z)}$ - a polynomial of rank no higher than 3, which is replaced by a tangent at the extreme calibration points.

$\mathrm{z} < \mathrm{z}_0$ $\quad \mathrm{Pn} = \mathrm{P'n}(\mathrm{z_o}) \cdot \mathrm{z} + \mathrm{Pn}(\mathrm{z_o}) - \mathrm{P'n}(\mathrm{z_o}) \cdot \mathrm{z_o}$

$\mathrm{z} < \mathrm{z}_0 < z_n$ $\quad \mathrm{Pn} = \mathrm{Pn(z)}$

$\mathrm{z} > \mathrm{z_n}$ $\quad \mathrm{Pn} = \mathrm{P'n}(\mathrm{z_n}) \cdot \mathrm{z} + \mathrm{Pn}(\mathrm{z_n}) - \mathrm{P'n}(\mathrm{z_n}) \cdot \mathrm{z_n}$

Here: FWHM - width of the peaks; x - energy; $\mathrm{z} = \mathrm{x} - (\mathrm{x_0} + \mathrm{x_n})/2$; x_0, ($\mathrm{z_0} = (\mathrm{x_0} - \mathrm{x_n})/2$) - the first calibration point, x_n, ($\mathrm{z_n} = (\mathrm{x_n} - \mathrm{x_0})/2$) - the last calibration point; $\mathrm{Pn(z)}$ - the polynomial; $\mathrm{P'n(z)}$ - derivative of a polynomial: $\mathrm{P'n}(\mathrm{z_0})$ - derivative at a point z_0, $\mathrm{P'n}(\mathrm{z_n})$ - derivative at a point z_n.

The calculation of the coefficients of the polynomial is the same as in the energy calibration procedure (see "Energy calibration").

Calibration of registration efficiency

Four quantum detection efficiency functions can be calculated in the SPECTRAD software package:

- the efficiency of recording quanta of a certain energy at the peaks of total energy absorption *Eff(e) = S(e)/Q(e),*
- in single escape peaks, *EffEsc1(e-511) = Sesc1(e-511)/Q(e),*
- at the peaks of the double escape, *EffEsc2(e-1022) = Sesc2(e-1022)/Q(e).*
- full efficiency of recording quanta of a certain energy in the spectrum *Eff(e) = S/Q(e).*

Here: *e* is the line energy in keV, *S(e), Sesc1(e-511), Sesc2(e-1022)*, *S* are, respectively, the area of the total absorption peak, the areas of the single and double escape peaks, the area of the spectrum including compton and all peaks corresponding to the number of radiation quanta *Q(e)* the given energy.

In the "SPECTRRAD" package, the registration efficiency function is set in tabular form. With a low density of points in the table, it is recommended to approximate the table with a spline (a spline is understood to be a polynomial stitched up to the values of the function or the first derivatives, depending on the rank of the spline). The spline has an approximating character - it does not pass through all the points of the table, but approximates it by forming a segment of the spline using the weighted least squares method from orthogonal Chebyshev polynomials for a given number of points.

It is believed that the double logarithmic scale of the polynomial approximation *F=exp(Pm(log(x)))* is best suited for approximating the efficiency functions of quantum registration at peaks of total absorption in the range of 30-3000 keV, and the logarithmic scale of the polynomial approximation *F=Pm(log(x)* is best suited for approximating the efficiency functions of quantum registration at peaks of single and double escape.

Calculation of elementary spectra from reference spectra

We assume that the alpha, gamma, or beta spectrum accumulated by the spectrometer is a linear sum of elementary spectra. $\mathrm{s} = \mathrm{F} \cdot \mathrm{x} + \mathrm{b}$

Here:

F - matrix of elementary nuclide spectra,
x - vector of nuclide activities,
b - background spectrum.

A necessary condition for calculating elementary spectra is the requirement of non-degeneracy of the activity matrix of the calculated elementary spectra in the working set of standards. The most desirable option is the orthogonality of the activity matrix.

The formula for calculating: $\mathrm{F} = \mathrm{R}\{(\mathrm{S} - \mathrm{B}) \cdot \mathrm{C}^{-1}\}$

Here:

R - the operator of projecting the obtained values to constraints. In this case, zeroing values less than the specified statistical level (<**G**) is used to set the range of values of the elementary spectrum.

C^{-1} - the matrix is the inverse of the matrix of averages during the measurement of nuclide activities in the standards:

$$C_{nm} = A_{nm} \left\{ \sum_{k=0}^{l} \lambda_l \int_{Tm}^{Te} \left(\frac{X_k}{\lambda_k} \cdot \prod_{i=0}^{k-1} \beta_i \cdot \lambda_i \cdot \left(\sum_{i=0}^{k} \frac{\exp(-\lambda_i \cdot (t - T_p))}{\prod_{\substack{j=0 \\ j \neq i}}^{k} (\lambda_j - \lambda_i)} \right) \right) \cdot dt \right\} / (T_E - T_M)$$

A_{nm} - the activity of the *n*-th nuclide in the *m*-th standard at the certification date; the *n*-th nuclide in the activity matrix is the *l*-th nuclide in the chain of decay of the nuclides contained in the *m*-th standard;

λ_j - the decay constant of the *j*-th nuclide in the decay chain;

β_i - the proportion of the selected transition (branch) in this node of the decay tree.

T_P - date of certification of the standard;

T_M - the date of the beginning of measurements of the standard;

T_E - the date of the end of measurements.

S - a matrix of spectra of measured standards normalized for live measurement time.

B – a matrix of background spectra normalized for live measurement time.

The calculation of the errors of elementary spectra is based on the condition that the statistical fluctuations of the spectrum are negligible in comparison with the error of the certification of the standards (the spectra of the standards must be measured with good statistics), and, accordingly, the relative error of the values in the channels of the spectra of the standards is equal to the relative error of the certification of the standards.

Accordingly

$$D_{Aij} = \sum_k D((S - B)_{ik}) \cdot (X_{kj}^{-1})^2 .$$

D_{Aij} - the variance of the *i*-th channel of the *j*-th elementary spectrum.

$D((S - B)_{ik})$ - variance of the *k*-th element of the *i*-th row of the matrix $(S - B)$.

Calculation spectra of the lines

The spectrum recorded by the spectrometer is described by the expression

$$S(x) = \int F(x,e) \cdot s(e) \cdot de$$

Here:

$F(x,e)$ - a function describing the process of recording radiation quanta s(e) in the form of an instrument spectrum – kernel of the conversion.

In the case of a linear spectrum $s(e) = A_i \cdot \delta(e - e_i)$, δ is the Dirac delta function.

$S(x) = \sum A_i \cdot F(x,e_i)$, where $F(x,e_i)$ are the cross sections of the conversion kernel for a given energy e_i, or, in other words, is the response of the spectrometer to radiation of a given energy - the spectrum of the line.

If we can calculate a certain number of such cross-sections of the conversion kernel (line spectra), then we can interpolate these cross-sections to calculate the instrument spectra of nuclides.

Based on the assumption of $F(x,e)$ continuity, the following parameterization is proposed:

- **For high-resolution linear spectra**.
  The spectrum refers to the spectrum of peaks (for gamma spectra, the spectrum with a pre-subtracted continuous scattering spectrum). For alpha spectra, the response of the spectrometer to one alpha particle of a given energy is calculated. For semiconductor gamma-ray spectrometry, the recording efficiency is stored in the recording efficiency tables and the peak of a given energy and width with a one unit area is calculated as a model of the line – model of the peak. The response of the spectrometer will be the product of the recording efficiency for a quantum of a given energy and the calculated models of the peak.

  $$F(x,e) = Eff(e) \cdot F((x - En^{-1}(e) + En^{-1}(e_i))/(W(e)/W(e_i))$$

  Here:

  $Eff(e)$ - registration efficiency function, for alpha spectrometry $Eff(e)$ = 1.

  $En(e)$ - energy calibration of the spectrometer,

  $W(e)$ - calibration of peak widths,

  e_i - line energy.

  Energy calibration of the spectrometer, peak width calibration, and detection efficiency calibration are used.

- **For linear spectra with poor resolution (processing without subtracting the continuous scattering spectrum).**
  The spectrum includes a continuous scattering spectrum. The cross section of the conversion kernel is the total response of the spectrometer to one quantum of radiation of a given energy (the cross section also includes the recording efficiency). $F(x,e) = F(e \cdot (x - En^{-1}(e) + En^{-1}(e_i))/e_i)$

  Only the energy calibration of the spectrometer is used.

For linear, well-resolved spectra, the line model is calculated from the spectra of total absorption peaks. It is assumed (and confirmed by experience) that within the limits of the peak line or multiplet used to calculate the model, all shape changes are accurately described by affine type deformation. $\varphi(z) = \varphi(\frac{x-p}{w})$.

The spectrum of the line $\varphi(i)$ under this assumption is calculated by solving a system of integral equations $B(i)=\int_{i}^{i+1}\sum_{j=1}^{n}\varphi\left(\frac{i-p(e_j)}{w(e_j)}\right)\cdot di$.

Here: $B(i)=S(i)-S_{compt}(i)-Bgd(i)+Bgd_{compt}(i)$

$S(i)$ - the spectrum of the reference sample, $S_{compt}(i)$ - the continuous scattering spectrum of the reference spectrum,

$Bgd(i)$ - the background spectrum, reduced to the measurement time of the reference spectrum,

$Bgd_{compt}(i)$ - continuous scattering spectrum for the background,

$p(e_j)$ - - the position of the energy line e_j on the channel scale,

$w(e_j)$ - the width of the energy line e_j.

The procedure calculates the desired function for the entire region of the single peak or multiplet used, determines the line parameters (energy, width, area). For gamma spectra, it normalizes the selected peaks per area. And saves them as models of the lines.

For poorly resolved spectra (processing without peaks search), the line spectra are calculated from elementary spectra. In this case, it may be that the entire set of elementary spectra does not contain spectra from a single line (of the set of nuclides commonly used for calibration of gamma-ray scintillation spectrometers, only the elementary spectrum of K-40 consists of a single line of 1460.8 keV). Therefore, the calculation procedure uses the described line parameterization to calculate the lines. Suppose the elementary spectrum contains n lines and there is not a single calculated line. The operator must select the most powerful line as the calculated one (the line with the index 0), while the program expresses all other lines using the described parameterization by extrapolating the calculated line spectrum. If the elementary spectrum s contains *k* channels, we obtain a system of *k* equations with *k* unknowns.

$$F(e_i\cdot(x-En^{-1}(e_i)+En^{-1}(e_i))/e_0)=s$$

Since all additional lines are obtained by extrapolating the main one, the solution will be acceptable if the following conditions are met:

- additional lines are located near the main one,
- the contribution of the additional lines is insignificant compared to the contribution of the main line.

If several lines from several elementary spectra are calculated, the procedure first calculates the most conditioned lines and uses the obtained spectra to interpolate the lines calculated later. The calculation procedure for increasing the conditionality of the matrix imposes another limitation - the system of equations being formed must be triangular in nature, that is, the selected lines must be extreme in the spectrum of the nuclide (either the first or the last).

Calculation of elementary spectra by the table of lines

In the event that the necessary for decomposition elementary spectra calculated from the standards exist, the program primarily uses them, but if they are not available, the necessary elementary spectra of nuclides are calculated from the tables of lines and calibrations of the spectrometer - "**generated**".

The procedure uses the method of piecewise linear interpolation (extrapolation) of the line spectra forming the elementary spectrum from the two preformed line spectra closest to the energy of the calculated line (see "Calculation spectra of the lines") of certain energies *e1* and *e2* in the interpolation mode specified by the operator:

*f=a*x+b*
*f=exp(a*x+b)*
*f=a*log(x)+b*
*f=exp(a*log(x)+b)*

The response to radiation of a certain energy is calculated by interpolation (extrapolation):

$$f(e,i) = ((e_2 - e)\cdot f(e_1,k_1,i) + (e_1 - e)\cdot f(e_2,k_2,i))/(e_2 - e_1),\ldots k_1 = e/e_1,\, k_2 = e/e_2$$

Nuclide spectrum $F = \sum A_j \cdot f_j$ - the sum of the responses with the corresponding quantum yield A_j of all lines of a given nuclide.

To calculate the line spectra of a given energy *e*, the following parameterization of the calculated line spectra is used:

- **For high-resolution linear spectra**.

  A spectrum is defined as a peak spectrum (a spectrum with a pre-subtracted continuous scattering spectrum). A line spectrum is a peak of a unit area of a given energy and width.

  $$F(e,x) = Eff(e)\cdot F(e_i,(x - En^{-1}(e) + En^{-1}(e_i))/(W(e)/W(e_i))$$

  Here:

  $Eff(e)$ - registration efficiency function, for alpha spectrometry $Eff(e) = 1$.

  $En(e)$ - energy calibration of the spectrometer,

  $W(e)$ - calibration of peak widths,

  e_i - line energy.

  Energy calibration of the spectrometer, peak width calibration, and detection efficiency calibration are used.

- **For linear spectra with poor resolution (processing without subtracting the continuous scattering spectrum).**

  The spectrum includes a continuous scattering spectrum..

  $$F(e,x) = F(e_i,(x - En^{-1}(e) + En^{-1}(e_i))/e_i)$$

  Only the energy calibration of the spectrometer is used.

Absorption of radiation in a substance

When passing through matter, radiation particles interact with electrons and nuclei of atoms of matter. When they interact, they are either absorbed or lose some of their energy and change direction. For a stream of particles N_0 passing through a unit area on a Δx path, the particles $\Delta n = N_0 \cdot (\rho \cdot N_a / A) \cdot \sigma \cdot \Delta x$ will react.

Here, *p* is the density of the medium, *N_a* is the Avogadro number, *A* is the molar mass of the atoms of the substance, *σ* is the total effective (averaged for all atoms of a substance) interaction cross section.

The value $\sigma \cdot \rho \cdot N_a / A$ is called the total linear attenuation coefficient of the radiation. The total linear attenuation coefficient depends on the density of the substance. Therefore, calculations use the value $\mu = \sigma \cdot N_a / A$ (sq.cm/g) – the mass cross-section of the interaction (or the mass attenuation coefficient). For alpha and beta radiation, it is customary to use the inverse of the mass attenuation coefficient – the particle free path in the substance (g/sq.cm.). The free path measured in g/sq.cm also does not depend on the density of the substance. To calculate the free path in terms of length, it must be divided by the density of the substance.

The efficiency of particle detection in the detector depends on the density of the counting sample and the mass attenuation coefficient (or path) of the particles in the substance of the counting sample:

$eff_1 = eff_0 \cdot k(\mu_0, \rho_0, \mu_1, \rho_1)$ or $eff_1 = eff_0 \cdot k(R_0, \rho_0, R_1, \rho_1)$

$k(\mu_0, \mu_1) = \mu_0 \cdot \rho_0 \cdot (1 - \exp(-\rho_1 \cdot \mu_1) / (\mu_1 \cdot \rho_1 \cdot (1 - \exp(-\rho_0 \cdot \mu_0))$ - the detection efficiency coefficient related to the mass attenuation coefficient of radiation in the reference μ_0 in square cm / g and in the counting sample μ_1 for the detection efficiency expressed in *(imp. / s)/ Bq* or *in imp./ quantum* measurements in a "thin" layer for gamma and beta radiation.

$k(\mu_0, \mu_1) = \mu_0 \cdot (1 - \exp(-\rho_1 \cdot \mu_1) / (\mu_1 \cdot (1 - \exp(-\rho_0 \cdot \mu_0))$ - the detection efficiency coefficient related to the mass attenuation coefficient of radiation in the reference μ_0 in sq.cm/g and in the counting sample μ_1 for the detection efficiency expressed in (imp./s)/(Bq/kg) or in imp./(quantum/kg) – measurements in the "thick" layer for gamma and beta radiation.

$k(R_0, R_1) = \dfrac{R_1 \cdot fAtten(\rho_1, R_1)}{R_0 \cdot fAtten(\rho_0, R_0)}$ - the registration efficiency coefficient related to the radiation free path in the reference R_0 in g/sq.sm and in the counting sample R_1 (measurements in the "thick" layer) for alpha radiation.

$fAtten(\rho, R) = 1 - sqrt(1 - (\rho / R)^2) + (\rho / R) \cdot \arccos(\rho / R)$ - for. < 0.8.

$fAtten(\rho, R) = 1 - \exp(-\alpha \cdot \rho / R)$ - for. > 0.8.

ρ - surface density in g/sq.cm, respectively, of the standard and sample.

α is a coefficient for combining two functions.

Gamma radiation

When passing through matter, gamma rays are either absorbed as a result of the photoelectric effect, or they lose some of their energy and change direction as a result of Compton scattering and the effect of electron–positron pair generation (there are a number of other effects, but the three most significant are mentioned). At low gamma-ray energies, the photoelectric effect is the most significant. At quantum energies Ey ≥1022 keV, the effect of the generation of electron-positron pairs occurs.The cross section of the combined effects is equal to the sum of the cross sections of the individual reactions:

$$\sigma = \sigma_{ф} + \sigma_{к} + \sigma_{пар}$$

$\sigma_{\text{ф}}, \sigma_{\text{к}}, \sigma_{\text{пар}}$ - cross sections of the photoelectric effect, Compton scattering, and the pair formation effect.

In the "SPECTRRAD" package, there are several ways to determine reaction cross-sections as functions of radiation energy for specified types of materials of counting samples.:

- definition in the form of a table,
- calculation based on the mass or chemical formula of a substance, taking into account the absorption for a specific element according to the tables https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html:
- calculation according to the procedure defined by the operator.

If the calculation procedure is not specified by the operator, the calculation is based on the mass or chemical formula of the substance according to the formulas proposed by the teachers of the Department of General Nuclear Physics of the Faculty of Physics of Moscow State University:

$$\sigma_{\text{ф}} = 4\pi r_0^2 a^4 Z^5 * \frac{(2+\varepsilon)^{3/2}}{\varepsilon^{7/2}} * \left[\frac{4}{3} + (1+\varepsilon) * \frac{(\varepsilon-1)}{(2+\varepsilon)} * \left(1 - \ln\left(\frac{1+\varepsilon+\sqrt{\varepsilon*(2+\varepsilon)}}{1+\varepsilon-\sqrt{\varepsilon*(2+\varepsilon)}}\right)\right)\right]$$

где:

$\varepsilon = \dfrac{E_\gamma}{(m_e * c^2)}$ - the dimensionless parameter of gamma-ray energy,

$r_0 = \dfrac{e^2}{(m_e * c^2)} = 2.81794092 * 10^{-15} \text{м}$ - classical electron radius,

Z - the charge of the nucleus of an element of the substance.

$a = \dfrac{e^2}{(h * c)} = \dfrac{1}{137.03598}$ - the fine structure constant,

E_γ - the energy of gamma radiation.

$m_e * c^2$ – the rest energy of the electrona,

$$\sigma_{\text{к}} = 2\pi r_0^2 Z * \left\{\frac{(1+\varepsilon)}{\varepsilon^2} * \left[2 * \frac{(1+\varepsilon)}{(1+2*\varepsilon)} - \frac{\ln(1+2*\varepsilon)}{\varepsilon}\right] + \frac{\ln(1+2*\varepsilon)}{2*\varepsilon} - \frac{(1+3*\varepsilon)}{(1+2*\varepsilon)^2}\right\}$$

$$\sigma_{\text{пар}} = r_0^2 \text{a} Z^2 * \left(\frac{28}{9} * \ln(2*\varepsilon) - \frac{218}{27}\right), \text{ for } 1 << \varepsilon < \frac{1}{a * Z^{1/3}}$$

$$\sigma_{\text{пар}} = r_0^2 \text{a} Z^2 * \left(\frac{28}{9} * \ln(183 * Z^{-1/3}) - \frac{218}{27}\right), \text{ for } \varepsilon > \frac{1}{a * Z^{1/3}}$$

The total cross-section of the three effects is used to calculate the registration efficiency table in photopics. The pair formation cross section is used to calculate the table of efficiency of registration in leakage peaks.

In scintillation spectrometry (when processing without peaks), the total cross-section of the three reactions cannot be used, since gamma rays that have experienced Compton scattering may not register in the detector, or they may register in the Compton scattering spectrum. In the same way, gamma quanta that have formed electron-positron pairs can register in the spectrum, but naturally in a different energy range. It is very difficult to calculate where the gamma quantum will register in the spectrum (if it does) after Compton scattering. For scintillation spectra in the "SPECTRRAD" package, the component spectra are recalculated (interpolated or extrapolated) to a given electron density (Compton scattering is proportional to the electron density) using component spectra calculated from standards of different densities reduced to a given effective atomic charge and effective atomic mass. And recalculation for a given effective charge and effective atomic mass, that is, photoabsorption is taken into account using the formula for radiation absorption in a substance for the photoelectric effect ($\sigma_{ф}$).

Beta radiation

The free path of beta particles is inversely proportional to the electron density. The default formula is:

$$R = 0.19272464 \ * E_{\beta}^{1.4} * \frac{A}{Z} \text{ for } E_{\beta} < 0.8 \text{ МэВ},$$

$$R = 0.4818116 \ * \left(0.54 * E_{\beta} - 0.133\right) \cdot \frac{A}{Z} \text{ for } E_{\beta} \geq 0.8 \text{ МэВ}.$$

Since the beta radiation spectrum is continuous, the calculation by formulas can be used (with caution) only when calculating the total activity. The spectra of the decomposition components for the beta spectra in the SPECTRAD package are calculated by interpolating or extrapolating the spectra of components with different electron density values to the electron density of the counting sample..

Alpha radiation

The free path of alpha particles in matter is calculated using the empirical formula of William Henry Bragg: $R = 0.0001 \cdot \sqrt{A \cdot E_{\alpha}^{3}}$ g/sq.cm (energy E_{α} at Mev).

Interpolation of tables and component spectra

Tables of registration efficiency and spectra of decomposition components reduced to a given value of a geometric parameter (interpolation parameter) are calculated from tables and elementary spectra with different values of the interpolation parameter in accordance with the selected geometric parameter of the sample. As a rule, the density of the counting sample is used as a geometric parameter, and if the effective atomic number and effective atomic mass of the substance of the standards and the counting sample are specified, in accordance with the electron density of the counting sample. The calculation is carried out by the piecewise polynomial interpolation (extrapolation) procedure for each channel of the spectrum or point of the table according to **n** (**n**<**7**) tables or elementary spectra with different values of the geometric parameter according to the selected formula:

F(S)=F([EXP](Pm[LOG](X)))

with parameters *Parameter*, *Rang*, *Mode*, *Points* and *Volume* set in the file “**decomp.ini**".

Here:

F(S)	Function of the interpolated values: (S - values of the approximated points of the spectrum).
X	An interpolation parameter (sample density or one of the sample sizes or variable geometry sizes).
Pm	Polynomial of rank *Rang*. The default value is *Rang* =1. *Rang* must be in the range from 0 to 3.
Mode	Interpolation mode: mode=0 – F=Pm(x), mode=1 – F=Pm(log(x)), mode=2 – F=exp(Pm(x)) – by default for gamma spectrometers, mode=3 – F=exp(Pm(log(x))), mode=4 – F=1/Pm(x), if *Points* = 2 and *Rang* = 1, then F=1/(ax+b)^2, mode=5 – F=1/Pm(log(x)), mode=6 – F=1/exp(Pm(x)), mode=7 – F=1/exp(Pm(log(x))), mode=8 – F=F0·(1-exp(-k·x)) - the default value for "thick layer" geometries»,

mode=9 – F=F0·(1-exp(-k·x))/(k·x) - default value for alpha and beta spectrometers.

Points	The number of points involved in the formation of the polynomial.
Volume	The volume of a standard sample vessel for this geometry.

Peaks search

The peaks search procedure uses three peaks search methods at the operator's choice:

- **«Floating segment»**.

$$f(i) = \left(\int_{i-w(i)/2}^{i+w(i)/2} (Sp(x) - Sbgd(x)) \cdot dx\right) / \sqrt{1 + \int_{i-w(i)/2}^{i+w(i)/2} Sp(x) \cdot dx}$$

Here:
f(i) - detection function.
i – spectrum channel, *w(i)* –peak width (in channels).
Sp -spectrum, *Sbgd* - the values of the "background" under the peak, approximated by a straight line segment fixed on the spectrum at points *i-w(i)/2* и *i+w(i)/2*.

- **Convolution with the peak model**.

$$f(e) = (\int_{e-w(e)/2}^{e+w(e)/2} F(x,e) \cdot (Sp(x) - Sbgd(x)) \cdot dx) / \int_{e-w(e)/2}^{e+w(e)/2} \sqrt{Sp(x) \cdot F(x,e)^2}\,) \cdot dx$$

Here:
f(e) - detection function.
e - energy, *w(e)* - peak width (in units of energy).
F(x,e) – model of the peak.

- **«Mariscotti» (generalized second difference)**.

$$f(e) = (\int_{e-2w(e)}^{e+2w(e)} M(x,e) \cdot Sp(x) \cdot dx) / \int_{e-2w(e)}^{e+2w(e)} \sqrt{Sp(x) \cdot M(x,e)^2}\,) \cdot dx$$

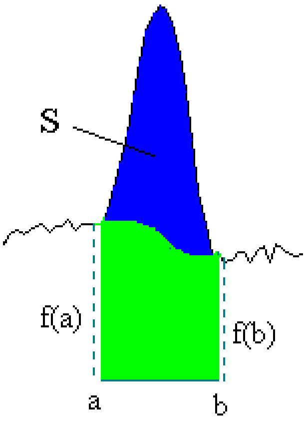
Here:
f(e) - detection function.
e - energy, *w(e)* - peak width (in units of energy).
M(x,e) – Mariscotti function.

A peak is considered to be present in the spectrum if the value of the detection function exceeds the threshold set by the settings.

Approximation of the continuous scattering spectrum

Two methods are used to approximate the continuous scattering spectrum under the peak:

- **Integral step**.



$$f_j(i) = f(a) - (s(i) - f_{j-i}(i)) \cdot (f(a) - f(b)) / S_{j-1}$$

Here:
f is the continuous scattering spectrum, ***i*** is the spectrum channel, and ***j*** is the iteration number.
s - spectrum; ***a, b*** - the beginning and end of the peak region.

$S = \sum_{a}^{b}(s(i) - b(i))$ - peak area.

- **Polynomial.** When approximated by a polynomial, the portion of the spectrum containing the peaks is decomposed by the least squares method into the sum of the peak spectra and the polynomial of the continuous scattering spectrum..

Accounting for cascading transitions

For linear gamma-ray spectra, the effects associated with cascading transitions (pulse leakage from total absorption peaks to cascade transition summation peaks) are taken into account both when processing spectra with peak search (efficiency calibration, spectrum generation, calculation of nuclide activities) and when processing spectra without peak search (spectrum generation, calculation of nuclide activities).

For two cascading transitions:

$N_1 = Ef_1 \cdot Q_1 - N_1^*$ - the probability of recording pulses recorded in the first peak, taking into account leakage.

$N_2 = Ef_2 \cdot Q_2 - N_2^*$ - the probability of recording pulses recorded in the second peak, taking into account leakage.

$N_{12} = Ef_1 \cdot K_1 \cdot Q_1 \cdot Ef_2 \cdot K_2 \cdot Q_{2/1}$ - the probability of recording pulses recorded at the peak of summation.

$N_1^* = Ef_1 \cdot K_1 \cdot Q_1 \cdot Ef_2^* \cdot K_2 \cdot Q_{2/1}$ - the probability of pulse leakage from the first peak.

$N_2^* = Ef_2 \cdot K_2 \cdot Q_2 \cdot Ef_1^* \cdot K_1 \cdot Q_{1/2}$ - the probability of pulse leakage from the second peak.

Q_1 - the probability of quantum output for the first cascade line.

Q_2 - the probability of quantum output for the second cascade line.

$Ef_1 = \iiint f(e_1) \cdot dv / Vol$ - the recording efficiency for the peak of total absorption averaged over the sample volume for the first cascade line.. Here: $f(e)$ - the efficiency of registering a quantum with energy *e* for a given point in the geometry, Vol - sample volume.

Ef_2 - the recording efficiency for the peak of total absorption averaged over the sample volume for the second cascade line.

Ef_1^* - the total registration efficiency averaged over the sample volume for the first cascade line (the probability of detecting a quantum in any region of the spectrum: the peak of total absorption, the Compton scattering spectrum, leakage peaks, and the annihilation peak).

Ef_2^* - the total recording efficiency for the second cascade line averaged over the sample volume.

$K(e) = \sqrt{(\iiint f(e) \cdot f(e) \cdot dv)/(\iiint f(e) \cdot dv \cdot \iiint f(e) \cdot dv)}$ - a geometric factor that takes into account the difference between the registration efficiency at a given point and the volume-averaged registration efficiency.

$Q_{2/1}$ - the conditional probability of a quantum output for the second cascade line under the condition of the output of the quanta for the first..

$Q_{1/2}$ - the conditional probability of a quantum output for the first cascade line under the condition of the output of the quanta for the second.

Equality is used in the calculation $Q_2 \cdot Q_{1/2} = Q_1 \cdot Q_{2/1}$. – the probability of simultaneous output of two gamma quanta

For three cascading transitions:

$N_1 = Ef_1 \cdot Q_1 \cdot (1 - Ef_2^* \cdot K_1 \cdot K_2 \cdot Q_{2/1}) \cdot (1 - Ef_3^* \cdot K_1 \cdot K_3 \cdot Q_{3/1})$ - the probability of detecting pulses recorded at the peak of total absorption, taking into account leakage (similarly for N_2 and N_3).

$N_{12} = Ef_1 \cdot K_1 \cdot Q_1 \cdot Ef_2 \cdot K_2 \cdot Q_{2/1} \cdot (1 - Ef_3^* \cdot K_3 \cdot Q_{3/1})$ - the probability of recording pulses recorded at the peak of the summation of two cascades (similarly for N_{13} and N_{23}).

$N_{123} = Ef_1 \cdot K_1 \cdot Q_1 \cdot Ef_2 \cdot K_2 \cdot Q_{2/1} \cdot Ef_3 \cdot K_3 \cdot Q_{3/1}$ - the probability of registering pulses recorded at the peak of the summation of three cascades.

$Q_{3/1}$ - the conditional probability of the output of the quanta of the third cascade line under the condition of the output of the quanta for the first.

Ef_3 - the recording efficiency for the peak of total absorption for the third cascade line.

Ef_3^* - total registration efficiency for the third cascade line.

Calculation of activities and estimation of uncertainties

The activity calculation method is based on the decomposition of the spectrum in the selected energy range into component spectra, assuming that the measured spectrum is the sum of the nuclide spectra of the counting sample and the background spectrum. The nuclide composition of the sample is assumed to be either known in advance or determined by the preliminary analysis procedures. It is assumed that the spectrum of the component does not change due to the presence of other nuclides in the sample, but depends on geometric factors (measurement geometry) of the chemical composition and density of the counting sample.

Metrics

A common approach in estimation is to find such parameters p_x of the model $M(p)$ (p is the vector of estimated model parameters) that would have minimal $D_{px} = \min(D_p)$ variances and satisfy the condition $\|M(p_x) - S\| < E$ ($\|..\|$ is the designation of the norm of the vector, S – the object, in our case, – the measured spectrum, E - the specified threshold of acceptability of the model). For the class of linear estimates (and for a somewhat broader class in the case of normality $M(p) - S$) these two conditions are combined into one . $\|K_x^{-1/2} \cdot (M(p_x) - S)\| = \min \|K_x^{-1/2} \cdot (M(p_x) - S)\|$.

Here K – vector ($M(p) - S$) covariance matrix.

Using Euclidean length as the norm and, accordingly, the least squares method as the procedure would provide us with minimal variances of estimates, but only under the assumption of a pre–known covariance matrix. The least squares method is a very unstable procedure with respect to violations of the initial assumptions, and therefore various kinds of noise-resistant (robust) estimation methods are currently being used. The Huber estimation is widespread, and it is also used in our program. The norm in the Huber metric looks like this:

||…|| = $(M(p) - S)^2$ in the case $0 > C_a < (M(p) - S) < C_b > 0$ - the least squares under the condition of a small deviation.

||…|| = $|M(p) - S|$ in the case $0 > C_a > (M(p) - S)$ or $(M(p) - S) > C_b > 0$ – the smallest modules for deviations exceeding the specified threshold.

In our methodology $C_a = -m \cdot G$, $C_b = n \cdot G$, where G is the estimated standard deviation, the values of *m* and *n* are set in the decomposition parameters (*m* and *n* can be set equal ∞, in this case the estimate will be an OLS estimate).

Object

We assume that the spectrum S has a diagonal covariance matrix $K_s = D_s \cdot I$ (I is the identity matrix, D_s is the variance vector), with $D_{Si} = F_i + \eta^2 F_i^2$ for $F_i > 0$ and $D_{Si} = 1$ for $F_i < 1$. $F_i = S_i$ for the first iteration and $F_i = M(p,i)$ for subsequent iterations.

Here:

S_i – The number of counts in the *i*-th channel of the spectrum S.

η – The coefficient of the linear component of statistics $(\eta \geq 0)$. That is, the spectrum has a composite: Poisson plus linear statistics. For the spectrum of the sample, it is determined by the differential nonlinearity of the spectrometer. For the background spectrum, it is the coefficient of background variability calculated by the procedure of statistical processing of background measurement results.

Model

We assume:

$$M(p,i) = \{\int (\Phi(x,w) \cdot f \cdot_0 (a_0 \cdot (i-x)^2 + b_0 \cdot (i-x) + c_0) +$$

$$k(Z,i) \cdot \sum A_j \cdot f_j(a_j \cdot (i-x)^2 + b_j \cdot (i-x) + c_j)) \cdot dx\} + S_{compt}(i) + Pn(i)$$

$$p = (Z, w, a_0, b_0, c_0, A_1, a_1, b_1, c_1, \ldots A_n, a_n, b_n, c_n, Pn_0, \ldots Pn_k).$$

Here:

$f_0 = B - B_{compt}$ – background spectrum with subtracted continuous scattering spectrum (B_{compt} is included in the model only in the mode of processing gamma spectra with peaks isolation).

$f_1, \ldots f_n$ – component spectra (radiation spectra of individual nuclides or chains of nuclides in a state of radioactive equilibrium normalized by the number of decays).

$A_1, \ldots A_n$ – the amplitudes of the corresponding components.

$a_0, \ldots a_n$, $b_0, \ldots b_n$ и $c_0, \ldots c_n$ – parameters of the energy drift of the spectrometer.

Multiplier $k(Z,i) = (1 - \exp(-\mu \cdot \rho \cdot Z^4 \cdot \Delta / f(E(i)))) / (\mu \cdot \rho \cdot Z^4 \cdot \Delta / f(E(i))$ is used only in the gamma spectrum processing mode.

Z is the deviation of the conditional *Z* effective sample from the *Z* effective standard used in calculating the registration efficiency. $E(i)$ - channel *i* energy. μ - linear absorption coefficient. ρ - the density of the counting sample. Δ - the thickness of the counter sample (set when setting the geometry).

$S_{compt}(i)$ – the continuous scattering spectrum for the sample spectrum (the continuous scattering spectrum is included in the model only in the mode of processing gamma-ray spectra with peaks isolation).

$Pn(i)$ - the spline. The spline is used when decomposing the gamma spectrum into peak spectra to approximate the continuous scattering spectrum if no preprocessing of the spectrum has been performed to search for peaks and calculate the continuous scattering spectrum. ($S_{compt}(i)$ =0).

i - the spectrum channel.

Convolution with the scattering function $\Phi(x,w)$ simulates the deterioration of the resolution of the spectrometer. With the exception of alpha spectrometry, the Gaussian $\exp(-(x/w)^2)$ is used as the scattering function. For alpha spectrometry, convolution is used with the spectrometer's response to the radiation quantum, the model of the peak $S((x-p)/w)$.

A nonlinear model is used, since in scintillation spectrometry (and not only in scintillation), the energy drift of the spectrometric tracts cannot be neglected (the usual operating drift in the range of 1-3% for scintillation spectra causes a distortion of estimates several times higher than the estimated statistical errors, even with 3-4 components in the model). In the general case, independent values of the drift parameters for all components are assumed, since the measurement of the standards took place at different times and at different loads of the spectrometer, respectively, at different values of the gain coefficients and zero of the spectrometer scale. In the event that, using the procedures of preliminary energy calibrations during measurements of standards, we have achieved, to some extent, a single energy scale for all decomposition components, the operator can indicate in the table of decomposition parameters that the spectra of the components are on a single scale, that is $a_0 = a_1 ... = a_n = 0$, $b_0 = b_1 ... = b_n$, $c_0 = c_1 ... = c_n$. The operator can exclude Z, w, $a_0, a_1,...a_n$ and (or) $b_0, b_1,...b_n$ and (or) $c_0, c_1,...c_n$ and Pn from the list of parameters by removing the corresponding check marks in the table of decomposition parameters.

The windowed processing method, which works well when decomposing high-resolution linear spectra of a recording detector (gamma-ray spectrometry with cooled HPGe detectors), uses a linear model.

$$M(p,i) = f_0(i) + \sum A_j \cdot f_j(i) + Comp(i); \quad p = (A_1,...A_n).$$

Here i – window number, $f_0, f_1,...f_n, Comp(i)$ – integral values in the *i*-th window, respectively, of the background, components, and continuous scattering spectrum.

When decomposing the spectra, nuclide activity values for the same sample material can be used, measured on other spectrometers or obtained by other methods. The model is supplemented with information about such a priori data: $X = X_0$; $K_x = G_0$.

X – activity values, K_x – the covariance matrix of the X.

Solution

We use the Gauss–Newton method. The initial value of the parameter vector p^0 is found using the global variation of the selected parameters in a given range with a given step. The speed of modern computers does not yet allow varying all parameters with sufficient grid density, so the operator can set the decomposition parameters to vary the four main parameters: Z effective, gain, zero scale and resolution of the spectrometer. We refine the approximation found using the Newtonian process.

$$p^{k+1} = p^k + R\left\{\lambda_k \cdot (M_{jl} + \beta_k \cdot D_{jl} + G_0^{-1})^{-1} \cdot F\right\}$$

Here:

p^k – the vector of parameters at the ***k*** -th iteration;

p^{k+1} – vector of parameters at the ***k+1*** -th iteration.

R – the operator of projecting the obtained parameter values to constraints.

λ_k – step on the ***k*** -th iteration $(0 < \lambda_k < 1)$.

$M_{jl} = (W \cdot \frac{dM}{dp})^T \cdot (W \cdot \frac{dM}{dp})$ **- t**he Gauss-Newton matrix;

$W = K^{-1/2}$ **-** the weight matrix. K **-** covariance matrix of the vector $M(p) - S$.

$\beta_k \cdot D_{jl}$ **-** the coefficient (set in the decomposition parameters) and the damping matrix of the ***k*** -th step.

G_0 **-** the covariance matrix of a priori data.

$$F = (W \cdot \frac{dM}{dP})^T \cdot (M(p) - S) + G_0^{-1} \cdot (A^k - X_0 \cdot b^k)\ \ for\, 0 > C_a < (M(p) - S) < C_b > 0.$$

$$F = (W \cdot \frac{dM}{dP})^T \cdot C_a + G_0^{-1} \cdot (A^k - X_0 \cdot b^k)\ \ for\, (M(p) - S) < C_a < 0.$$

$$F = (W \cdot \frac{dM}{dP})^T \cdot C_b + G_0^{-1} \cdot (A^k - X_0 \cdot b^k)\ \ for\, (M(p) - S) > C_b > 0.$$

X_0 - a priori data on component activities.

A^k - evaluation of the contribution of the components at the ***k***-th step,

b^k - estimation of the tract gain.

C_a, C_b - boundaries of OLS assessment.

The average activity of the ***k*** -th nuclide during the measurement:

$$\overline{X_k} = (\int_{El}^{Er} k(Z^n, e) \cdot A_k^n \cdot f_k(p^n) \cdot de / \int_{El}^{Er} f_k(p_0) \cdot de)\cdot;$$

Here:

El, Er - left and right energy boundaries of decomposition, *e* - energy;

$p^n = (w, a_j, b_j, c_j)$**.** - values of the energy drift parameters at the last iteration;

p_0 - initial values of energy drift parameters: $w = 0, a = 0, b = 1, c = 0$

A_k^n - assessment of the contribution of the ***k***-th component in the last step,

f_k - the spectrum of the ***k***-th component (the radiation spectrum of a nuclide or a chain of nuclides in a state of radioactive equilibrium, normalized by the number of decays);

Activity values at the start of measurements for single nuclides, equilibrium chain nuclides, and parent decay chain nuclides:

$X_k = \overline{X_k} \cdot (1 - \exp(-\lambda_k \cdot T_{meas})) / (\lambda_k \cdot T_{meas})$. Here:

λ_k - the decay constant of the nuclide (the decay constant of the parent nuclide, which ensures the radioactive equilibrium of the chain of nuclides, in the case of a chain of nuclides);

T_{meas} - measurement time.

For nuclides included in the decay chain, the solution is not described by an expression of elementary functions, but is a numerical solution of a system of integral equations.:

$$\overline{X_n} = \left\{ \lambda_n \cdot \sum_{k=0}^{n} \int_{0}^{Tmeas} \frac{X_k}{\lambda_k} \cdot \prod_{i=0}^{k-1} \beta_i \cdot \lambda_i \cdot \left(\sum_{i=0}^{k} \frac{\exp(-\lambda_i \cdot t)}{\prod_{\substack{j=0 \\ j \neq i}}^{k} (\lambda_j - \lambda_i)} \right) \cdot dt \right\} / T_{meas}$$

X_k - the desired solution;

λ_j - the decay constant of the ***j*** -th nuclide;

β_i - the proportion of the selected transition (branch) in this node of the decay tree.

Estimation of uncertainties

Our assumptions about the nature of the covariance matrix of the spectrum are formulated in the "**Object**" section.

The covariance matrix of the continuous scattering spectrum is also assumed to be diagonal $K_{comp} = D_{comp} \cdot I$ (I is the identity matrix, D_{comp} is the vector of variances), where $D_{COMPi} = \alpha^2 C_i^2$, C_i is the number of counts in the continuous scattering spectrum. α - the error in the calculation of the continuous scattering spectrum is set in the peak search parameters.

The values in the channels of the background spectrum are partially correlated (if the background has increased, then it has increased, plausibly, in all channels). $K_{i,j} = \beta^2 B_i \cdot B_j$ for $i \neq j$, $K_{i,i} = B_i + \beta^2 B_i^2$. This correlation preserves the property of composite Poisson statistics for variance $D(\sum B_i) = \sum B_i + \beta^2 (\sum B_i)^2$. The error introduced by the uncertainty of the continuous scattering spectrum for the background is neglected.

Here:

B_i – the number of counts in the ***i*** – th channel of the background spectrum.

β – background variability coefficient. The value of β is set in the settings of the spectrometer.

Finally:

$$K_p^n = \max(K_p^{n-1}, (p^n - p^{n-1}) \cdot (p^n - p^{n-1})^T + (M_{jl}^n + G_0^{-1})^{-1})$$

Here

K_p^n, K_p^{n-1} - estimates of the covariance matrix of the determined parameters at the last and penultimate steps of the solution procedure.

$p^n = (Z^n, w^n, A_1^n, \ldots A_N^n, a_1^n, \ldots a_N^n, b_1^n, \ldots c_N^n, c_1^n, \ldots c_N^n)$

and

$p^{n-1} = (Z^{n-1}, w^{n-1}, A_1^{n-1}, \ldots A_N^{n-1}, a_1^{n-1}, \ldots a_N^{n-1}, b_1^{n-1}, \ldots c_N^{n-1}, c_1^{n-1}, \ldots c_N^{n-1})$

parameter estimates at the last and penultimate steps of the solution procedure. That is, we use estimates of the errors of the linearized model supplemented by errors associated with the interruption of the iterative process (errors of the spectrometer drift).

$M_{ji}^n = (W \cdot \frac{dM}{dp})^T \cdot (W \cdot \frac{dM}{dp})$ - the Gauss-Newton matrix calculated at the last step of the solution procedure. Our solution procedure generates the covariance matrix of the parameters in the inverse matrix of the Gauss-Newton matrix.

$W = K_S^{-1/2}$ - the weight matrix. K_S - the covariance matrix of the vector $M(p) - S$. We consider it diagonal $K_S = D_S \cdot I$ (I – the identity matrix, D_S – the vector of variances) and $D_{Si} = S_i + \eta^2 \cdot S_i^2 + \alpha^2 \cdot C_i^2 + (B_i + \beta^2 \cdot B_i^2)/t^2$, here $t = t_B / t_S$ - the ratio of background and sample measurement time.

G_0 - the covariance matrix of a priori data.

Variances of estimates of averaged during measurement values of activity:

$\overline{Dxi} = \mathrm{Pr}es \cdot D_i / (b_i^n)^2$. Here:

$\mathrm{Pr}es$ - partial (calculated within the union of significant areas of determination of elementary spectra correlated with the ***i***-th component) residuals for a given nuclide. A significant area of definition is the area where the values of the elementary spectrum are nonzero.

$D_i = K_p^n(i,i)$ - the diagonal element of the covariance matrix of parameters for a parameter A_i^n in the spectrum processing mode without searching for peaks and subtracting the continuous scattering spectrum.

$D_i = \max(H_i, K_p^n(i,i))$ - the maximum value from the detection threshold of the ***i***-th nuclide and the diagonal element of the parameter covariance matrix for the parameter A_i^n in the spectrum processing mode with continuous scattering spectrum subtraction.

$H_i = \min(\{(h \cdot S_{compj} / ((k(Z,e_j) \cdot q_j^i \cdot Eff(e_j) \cdot T_{meas}))^2\}_{j=1..n})$ - the minimum threshold value of the values calculated for all ***n*** significant lines of the ***i***-th nuclide.

h - the value of the detection threshold set in the settings of the peak search procedure.

S_{compj} - the integral value of the continuous scattering spectrum in a region equal to three peak half-widths for the energy e_j of the ***j***-th line of the ***i***-th nuclide.

q_j^i - quantum yield of the ***j*** -th line of the ***i***-th nuclide.

$Eff(e_j)$ - registration efficiency for energy e_j.

b_i^n - the coefficient of linear energy drift ($z = b \cdot x + d$) of the ***i***-th component calculated as the coefficient of linear regression of the estimated nonlinear energy drift, n - the latest iteration;

T_{meas} - measurement time.

Variances of activity estimates at the start of measurements for single nuclides, equilibrium chain nuclides, and parent decay chain nuclides:

$$Dxi = \overline{Dxi} \cdot ((1 - \exp(-\lambda_i \cdot T_{meas})) / (\lambda_i \cdot T_{meas}))^2$$

λ_i - the decay constant of the nuclide (the decay constant of the parent nuclide, which ensures the radioactive equilibrium of the chain of nuclides, in the case of a chain of nuclides).

The Dxi variances for nuclides included in the decay chain are calculated by solving a system of integral equations describing the decay and accumulation of nuclides during measurement:

$$\overline{X_n} = \left\{ \lambda_n \cdot \sum_{k=0}^{n} \int_0^{Tmeas} \frac{X_k}{\lambda_k} \cdot \prod_{i=0}^{k-1} \beta_i \cdot \lambda_i \cdot \left(\sum_{i=0}^{k} \frac{\exp(-\lambda_i \cdot t)}{\prod_{\substack{j=0 \\ j \neq i}}^{k} (\lambda_j - \lambda_i)} \right) \cdot dt \right\} / T_{meas}$$

The solution is a linear transformation of $x = F \cdot \overline{x}$, respectively:

$Kx = F \cdot K\overline{x} \cdot F^T$, $Dxi = Kx_{ii}$

The final total uncertainty of the ***i*** - th activity:

$$G_{Xi} = \sqrt{(E_0 \cdot Xi)^2 + (E_i \cdot Xi)^2 + 4 \cdot Dxi}.$$

E_0 - *method error* is an additional relative error. E_0 - is associated with errors in determining the mass of the sample, geometry violations, etc., etc. In the "SPECTRRAD" package, E_0 is set as a decomposition parameter.

E_i - the relative error of the intensity values of the decomposition components calculated during the calibration of the spectrometer is related to the errors in the certification of standards, errors in the calculation of elementary spectra. E_i is the *error of the measuring instrument* for a particular nuclide.

The uncertainty estimate corresponds to a 95% confidence interval.

Calculation of the total activity of the sample

Total activity is the conditional activity of the sample equal to the intensity of the radioactive radiation from the sample. The total gamma activity is the number of gamma quanta emitted by the sample in 1 second, the total alpha and beta, respectively, is the number of alpha and beta particles per unit time. Since the spectrometer registers radiation in a limited energy range, we can talk about the total activity of the sample in a certain energy range.

When processing linear spectra with peak search and selection:

$$A_{sum} = \sum (S_i(e) - F(e)) / Eff(e, Am, Z)$$

Here:

$S_i(e)$ - the intensity of the ***i***-th peak with energy ***e***.

$F(e)$ - background intensity in the region of the ***i***-th peak with energy ***e***.

$Eff(e, Am, Z)$ - the efficiency of detecting radiation quanta with energy ***e*** in the peaks of total absorption for a countable sample with an effective atomic mass Am and an effective atomic number Z .

The sum is calculated for all peaks of the energy range of the spectrometer. Without analyzing the nuclide composition of the radiation, it is impossible to isolate the peaks of total absorption from the total set of peaks found in the sample spectrum, so the estimate of the total activity will be somewhat overestimated by including escape peaks in the calculation..

When processing spectra that do not have a linear structure or poorly resolved (processing without peak separation):

$$A_{sum} = k(R_0, R_1) \cdot (\int (S(e) - F(e)) \cdot de) / ((\int Elem(nucl, e) \cdot de) / \sum Q_i(nucl))$$

Here:

$k(R_0, R_1) = \dfrac{R_1 \cdot fAtten(\rho_1, R_1)}{R_0 \cdot fAtten(\rho_0, R_0)}$ - the detection efficiency coefficient related to the radiation free path in the standard R_0 in g/sqR_0 and in a counting sample R_1 when measured in a "thick" layer.

For gamma and beta radiation:

$fAtten(\rho, R) = 1 - \exp(-\rho / R)$

For alpha radiation:

$fAtten(\rho, R) = 1 - sqrt(1 - (\rho / R)^2) + (\rho / R) \cdot \arccos(\rho / R)$ - for. ρ / R < 0.8.

$fAtten(\rho, R) = 1 - \exp(-\alpha \cdot \rho / R)$ - for. ρ / R > 0.8.

ρ - surface density in g/sq.cm, respectively, of the standard and sample.

α - a coefficient for combining two functions.

$S(e)$ - the intensity of the sample spectrum (***e*** - energy).

$F(e)$ - background intensity.

$Elem(nucl, e)$ - he elementary spectrum of the nuclide ***nucl*** selected by the operator for calculating the total activity.

$Q_i(nucl)$ - the quantum yield of the ***i***-th nuclide line ***nucl***.

The path of the radiation quanta in the substance of the counting sample $R = f(E, Am, Z)$ is a function of the average initial radiation energy E and the values of the effective atomic mass Am and the effective number (charge) Z atoms of a substance of a counting sample.

The free path of radiation quanta in the “SPECTRAD” package is set by the user either in the form of tables or in the form of formulas in the procedure for entering and editing standards and constants for various types of samples (see "Norms and materials"). The following formulas are used by default:

For alpha radiation - $R = 10^{-4} \sqrt{Am \cdot E^3}$ g/sq.cm (William Bragg formula). Energy *E* in MeV.

For beta:

$R = 0{,}19272464 \cdot \mathrm{E}^{1.4} \cdot Am/Z$ for an initial electron energy of less than 0.8 MeV,

$R = 0.4818116 * (0.54 * E - 0.133) \cdot Am/Z$ for the initial electron energy of more than 0.8 MeV.

For gamma: the effect of pair formation is not taken into account, Compton scattering is taken into account by recalculating the elementary spectrum of the nuclide ***nucl*** on the electron density in the counting sample by interpolating from the spectra of standards with different electron densities, the effect of the photoelectric effect is calculated using the following formulas:

$$R = Am/(kz \cdot ke \cdot Z^5); \quad kz = 4\pi \cdot R_e^2 \cdot a^4 \cdot N_a,$$

Here: R_e - electron radius в см, a = 7.2973525376e-3 – the fine structure constant, N_a - Avogadro's number.

$$ke = \frac{(2+e)^{1,5}}{e^{3,5}} \cdot \left\{ \frac{4}{3} + (1+e) \cdot \frac{e-1}{2+e} \cdot \left[1 - \ln\left(\frac{1+e+\sqrt{e \cdot (2+e)}}{1+e-\sqrt{e \cdot (2+e)}} \right) \right] \right\}$$

$e = E/511$. energy E in keV.

The initial energy *E* for the nuclide ***nucl***, averaged over all lines falling within the specified energy range of quantum detection, is calculated during calibration of the spectrometer and stored in the parameters of the elementary spectrum. The average initial energy of the radiation quanta of the counting sample for beta particles is calculated by the processing procedure based on the positions of the medians of the elementary spectrum $Elem(nucl, e)$ and the spectrum of the sample $S(e) - F(e)$, for alpha particles it is either set by the operator in the parameters of the sample or the spectrometer, or calculated from the medians of the spectra, if not specified in the parameters of the sample.

The integral of the elementary spectrum is calculated according to the energy range specified in the processing template, the energy range of the integral for the sample spectrum is multiplied by the coefficient of tension-compression calculated from the quartiles of the spectra of the sample and the reference. To reduce the additional errors associated with recalculating the energy range for the sample, the operator must select a nuclide with a radiation energy close to the estimated energy of the detected radiation to calculate the total activity.

The sum of the quantum yield of the ***nucl*** nuclide is taken for all lines with line energy (for linear spectra) or boundary energy (for continuous spectra) exceeding the left energy limit of the selected range.

Since the elementary spectra are normalized for the decay of the nuclide, and not for the radiation quantum, for correct recalculation, it is necessary to specify a table of nuclides corresponding to the selected elementary spectrum in the decomposition parameters. For example, if we specified Sr-90 as the nuclide for calculating the total activity, and the elementary spectrum of Sr-90 contains the total response of Sr-90 and Y-90, in the table of nuclides used, Sr-90 should be represented as an equilibrium chain Sr90+Y90.

Calculation of the activity of the nuclide chain

The activity of nuclides in the selected branch of the parent nuclide decay chain is described by a system of differential equations:

$$\frac{dN_0}{dt} = -\lambda_0 \cdot N_0$$

$$\frac{dN_1}{dt} = \beta_0 \cdot \lambda_0 \cdot N_0 - \lambda_1 \cdot N_1$$

. . . .

$$\frac{dN_n}{dt} = \beta_{n-1} \cdot \lambda_{n-1} \cdot N_{n-1} - \lambda_n \cdot N_n$$

Here:

N - number of nuclide atoms,

λ - decay constant,

β - the proportion of the selected transition (branch) in this node of the decay tree.

The solution has the form:

$$N_n(t) = N_0 \cdot \prod_{i=0}^{n-1} \beta_i \cdot \lambda_i \cdot \left(\sum_{i=0}^{n} \frac{\exp(-\lambda_i \cdot t)}{\prod_{\substack{j=0 \\ j \neq i}}^{n} (\lambda_j - \lambda_i)}\right)$$

Activity $A(t) = \lambda \cdot N(t)$.

Content:

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