

# Kayzero for Windows

for reactor neutron activation analysis (NAA)

using

the  $k_0$  standardization method

Version 3.30

First Draft

User's Manual  
September 2017

Software developed by DSM Research, Geleen (NL)  
for NAA based on the  $k_0$  standardization method  
developed at the INW-RUG, Gent (B) and the AEKI, Budapest (H).

# Kayzero for Windows

## User's Manual

Kayzero for Windows, for calculating element concentrations  
in NAA analyses based on the  $k_0$  standardization method

Version 3.30  
**First Draft**

Distribution and support :

k0-ware  
R. van Sluijs  
Schaesbergerweg 25  
6415 AB Heerlen  
The Netherlands  
[www.kayzero.com](http://www.kayzero.com)

<b>1</b>	<b>Introduction .....</b>	<b>1</b>
<b>2</b>	<b>Installation and User Interface .....</b>	<b>2</b>
2.1	Installation.....	2
2.1.1	New user of Kayzero .....	2
2.1.2	Upgrade from older versions of Kayzero or Kayzero for Windows .....	2
2.2	Run The Program .....	3
2.3	User Interface .....	3
2.3.1	The 'MainMenu' .....	3
2.3.2	Program Output.....	3
2.3.3	(File)names .....	6
<b>3</b>	<b>Analysis Evaluation .....</b>	<b>7</b>
3.1	Menu Bar .....	7
3.2	Evaluating a Neutron Activation Analysis .....	10
3.3	Monitor Data .....	12
3.3.1	Monitor File .....	12
3.3.2	Entering Monitor Data.....	13
3.3.3	Peak summation.....	21
3.3.4	Calculating $F_c$ .....	23
3.3.5	Printing $F_c$ .....	24
3.4	Determination of the Element Concentrations .....	26
3.4.1	Order Input.....	27
3.4.2	Entering Measurement Data.....	28
3.4.3	Calculating the Element Concentrations .....	39
3.4.4	Printing the Element Concentrations.....	42
3.5	Select/reject analytical gamma lines.....	47
3.6	Order Report.....	57
3.6.1	Select Samples and Elements for Order Report.....	57
3.6.2	Print Order Report .....	58
<b>4</b>	<b>SolCoi .....</b>	<b>59</b>
4.1	General procedure .....	59
4.2	Effective Solid Angle and Coincidence Correction Factor Calculation .....	61
4.2.1	Data input and calculations.....	61
4.2.2	Data input for a detector/source-holder combination.....	62
4.2.3	Data input for a source geometry.....	67
4.2.4	Material composition input.....	69

4.2.5	Calculation of the effective solid angles for the reference position.....	71
4.2.6	Calculation of the effective solid angles and coincidence correction factors. ....	72
4.2.7	Printing the input and result data .....	73
4.2.8	Efficiency curve and Coincidence correction factors .....	74
4.2.9	Showing all available input and result files .....	77
4.3	Fine tuning.....	81
4.4	Reference efficiency and peak-to-total ratio curve fitting.....	84
4.4.1	Fit reference efficiency or PTT-curve .....	84
4.4.2	Saving fitted data in KAYZERO data file .....	88
4.4.3	Comparing stored reference efficiency fit or peak-to-total ratio fit data with measured data. ....	89
<b>5</b>	<b>History of detector and reactor calibrations .....</b>	<b>90</b>
5.1	Detector Calibration .....	90
5.2	Comparator Factors .....	94
5.3	Reactor Calibration Data .....	97
<b>6</b>	<b>Reference Guide .....</b>	<b>98</b>
6.1	Monitor Analysis Menu .....	98
6.1.1	Calculate f and alpha using the Zirconium-method .....	98
6.1.2	Calculate f and alpha using the 'Multi Monitor'-method ..	99
6.2	Kayzero Library.....	103
6.2.1	Printing the Full Library .....	103
6.2.2	Printing data for a specific Element.....	103
6.2.3	Gamma Line Listing.....	103
6.2.4	Excel output .....	103
6.3	Reports Menu .....	104
6.3.1	Print a list of Orders.....	104
6.3.2	Printing a list Measurements .....	105
6.3.3	Printing a list Measurements .....	105
6.3.4	Printing the peak table file .....	106
6.3.5	Printing Activities .....	108
6.4	Archive System .....	109
6.5	Special Options Menu .....	110
6.5.1	Energy Calibration (Series of Spectra).....	110
6.5.2	Spectrum Plot.....	112
6.5.3	Thermal neutron self-shielding.....	114
6.5.4	Calculation Parameters .....	114
6.5.5	Directories.....	115

<b>References.....</b>	<b>118</b>
<b>Appendix 1: Efficiency Calculation. ....</b>	<b>1</b>
<b>Appendix 2: Kayzero/SolCoi Files .....</b>	<b>2</b>
Description of Kayzero files .....	2
SolCoi Files in Efficiency Directory .....	5
File Formats for SOLANG and COINCALC.....	6
<b>Appendix 3: Algorithm and DataEvaluation .....</b>	<b>11</b>
K <sub>0</sub> Standardization.....	12
Efficiency.....	12
Spectrum Deconvolution .....	14
Comparator Factor .....	15
Evaluation .....	16
Isotope/Element Identification .....	16
Interference Correction .....	17
Weighted Mean Concentrations.....	18
<b>Appendix 4: Mass Absorption Coefficients.....</b>	<b>19</b>
<b>Appendix 5: Matrix Interpolation / Vials.....</b>	<b>20</b>
Density Interpolation.....	20
Matrix Interpolation.....	21
<b>Appendix 6: Parameters.....</b>	<b>22</b>
Calculation Parameters .....	22
Print Parameters .....	24
<b>Appendix 7: KAYZERO Library: Full listing .....</b>	<b>25</b>
<b>Appendix 8: KAYZERO Library: Gamma line listing ..</b>	<b>33</b>

# 1 Introduction

---

Kayzero for Windows is a program that helps the Neutron Activation Analyst in evaluating peak table data from measured gamma-ray spectra. In principle, Kayzero for Windows provides a list of concentrations and/or detection limits for all measurable elements in a sample, based on input consisting of sample data, irradiation data and measuring data.

Kayzero for Windows calculates concentrations using the  $k_0$ -standardization method according to De Corte and Simonits<sup>1,2</sup>. The method involves extensive calculations and the use of large data files. The Kayzero for Windows user is expected to be familiar with gamma spectroscopy, NAA and the  $k_0$  method. For practical guidelines regarding this method see the 'VADEMECUM FOR  $k_0$  USERS' by De Corte and Simonits<sup>3</sup>.

Chapter 2 explains the Installation and User Interface.

Chapter 3 explains the general use of the software after a detector was calibrated.

Chapter 4 explains detector calibration, which in general has to be performed only once. The detector calibration has to be done before doing anything else and consists of reference efficiency calibration, peak-to-total calibration and fine tuning.

Chapter 5, History of Detector and Reactor Calibrations, explains how detector and reactor calibration data can be monitored over a period of time.

Further information and details about all other options in the program can be found in Chapter 6, Reference Guide.

For extra help users can consult the Appendix, where detailed information is given on all algorithms and data file formats.

## 2 Installation and User Interface

---

### 2.1 Installation

Kayzero for Windows can be installed on a Personal Computer running under Windows (XP up too Windows10 64bit) with a free USB port. The installation is in fact nothing more than copying the unpacked program folder to the root-directory of a drive on your computer, inserting the USB copy-protection key and running the program KayWinVxx.Exe.

If you do not have a hardware copy-protection key (dongle) the program will be only a demonstration version with limited features.

The program can be downloaded from the website [www.kayzero.com](http://www.kayzero.com). Check the website regularly for updates of the Vade Mecum, this manual, demo data and the program itself. Please check the 'read.me'-file too.

#### 2.1.1 New user of Kayzero

The software is installed by copying the zipped KAYWINV3 folder downloaded from the [www.kayzero.com](http://www.kayzero.com) to the root-directory of a hard-disk or network drive.

Demo subdirectories should/will be created for the library, efficiency and example data.

#### 2.1.2 Upgrade from older versions of Kayzero or Kayzero for Windows

Do as mentioned under 2.1.1

Copy all non '.exe'-files from your current Kayzero for Windows folder to the new Kayzero for Windows folder.

**Note:** make sure that the selected library folder is the one in the latest program folder.

## 2.2 Run The Program

Run the Kayzero for Windows – software: ‘KayWinVxx.Exe’.

## 2.3 User Interface

Kayzero for Windows is a 100% windows program and works like any windows program. The program has NO built-in Help. This manual and the Vade-Mecum replace the Help.

### 2.3.1The ‘MainMenu’

The menu is almost identical organized as the DOS-menu of Kayzero, all options of the Solcoi-program are added in the SOLCOI –option (see Figure 2.2). The File-option, the Window-option, and the Help-option are new.

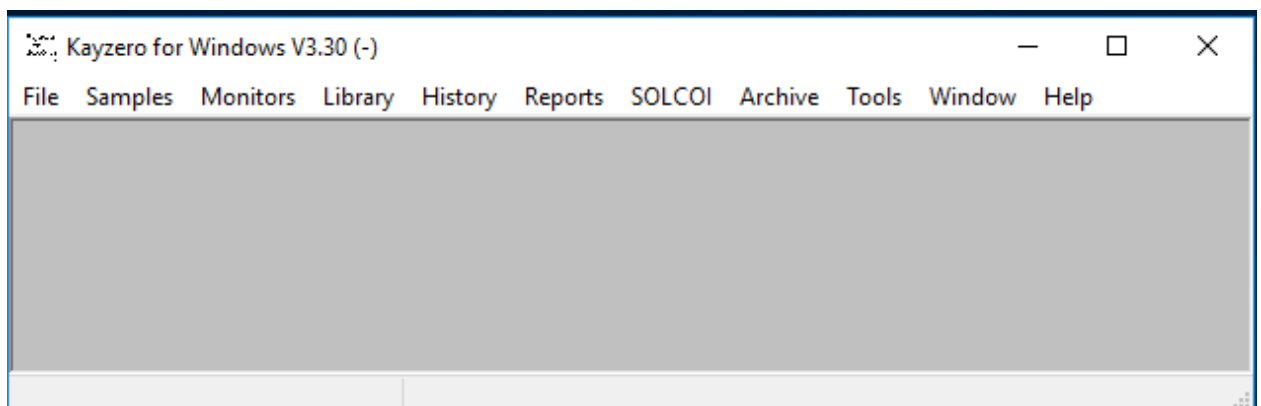


Figure 2.2: Main screen of Kayzero for Windows

### 2.3.2Program Output

All output of the program is first put on the main window of the program. There are several possibilities to print, save, edit or manipulate the presentation this output.

In figure 2.3 two typical types of output are shown. A graph and a text output.

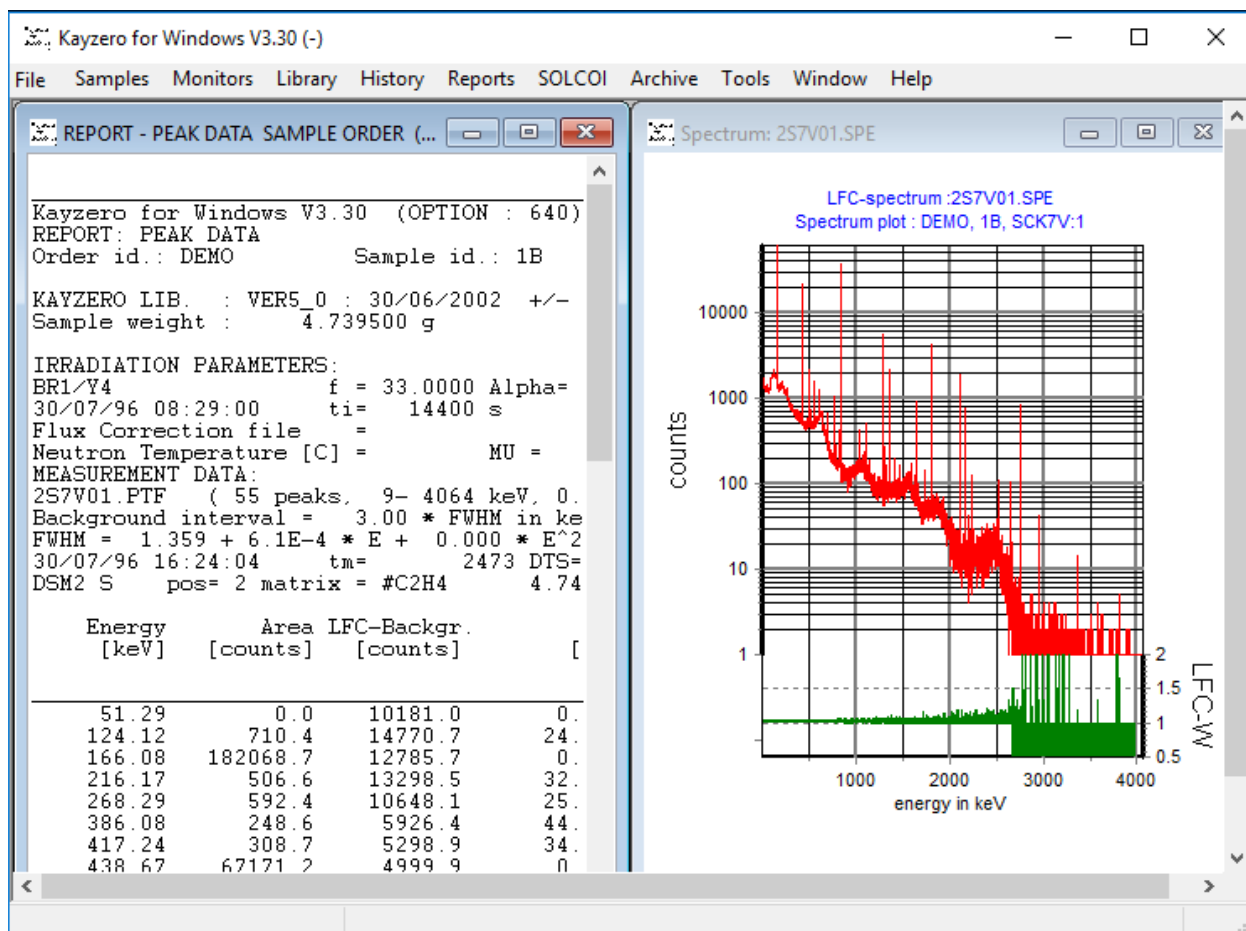


Figure 2.3: Kayzero for Windows: A spectrum plot and a print of the peak-table.

When pressing the right mouse button, a pop-up menu opens (see Figure 2.4). This pop-up menu is specific for each type of output.

The Edit option allows you to edit the graph, the other options are self-explanatory. In case of the text-output the data can be changed with 'Edit' but only after entering a password (:'ok').

The use and possibilities of the standard options as given in figure 2.5 need no extra explanation. The output windows can tiled horizontally, vertically (as shown in figure 2.3), cascaded or closed.

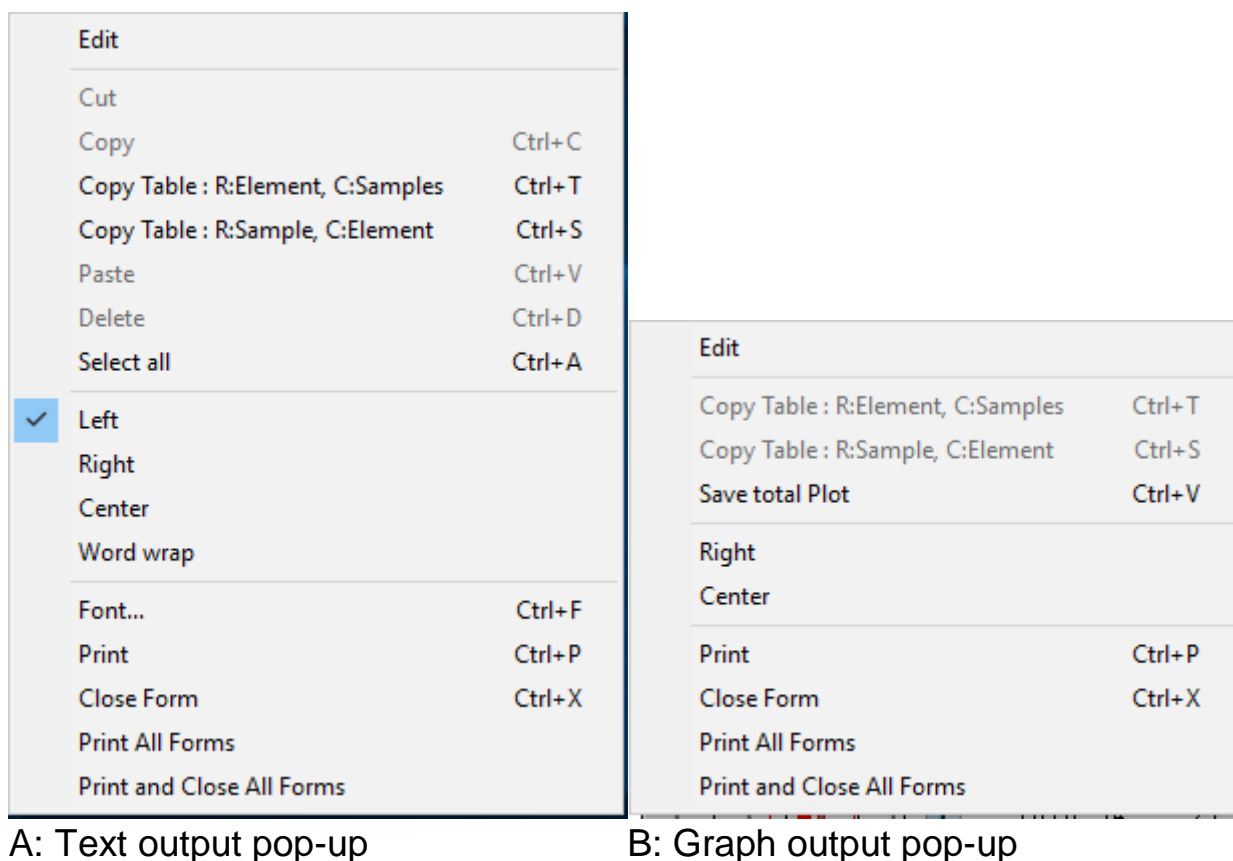
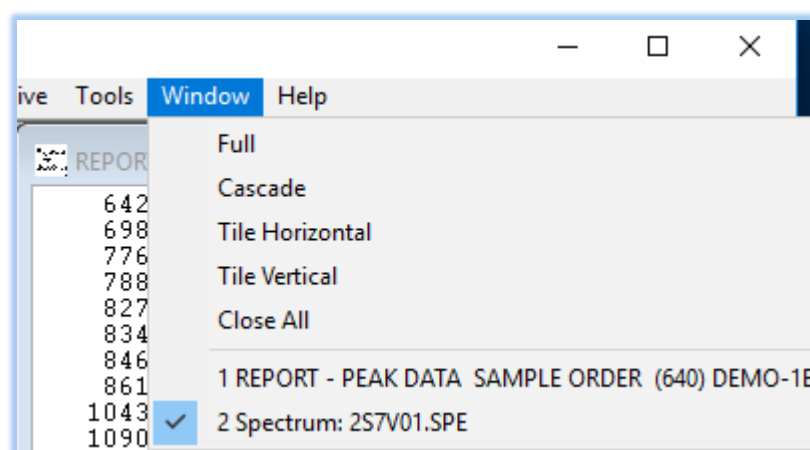


Figure 2.4: Kayzero for Windows: A spectrum plot and opened 'pop-up menu' (right-mouse button).



A: File- option                      B: Window-option

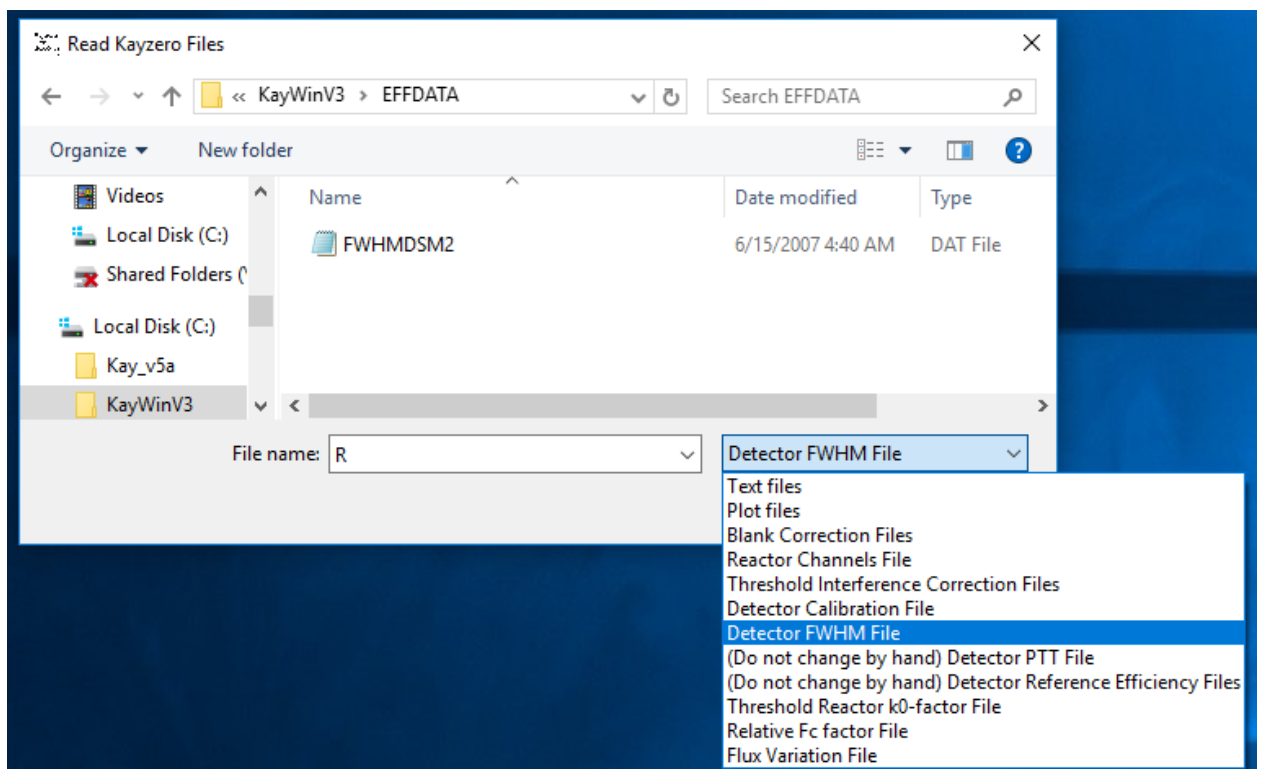
Figure 2.5: Kayzero for Windows: options for manipulating, rearranging output.

### 2.3.3(File)names

Although the program is a Windows program it is not possible to use long names. This is because of compatibility reasons:

- Orders, spectrum, samples, reactor, channel names max. 8 characters,
- Directory names should not exceed 60 characters,
- Sources max. 3 characters and
- Detectors max. 4 characters.

In general spaces have to be avoided.



## 3 Analysis Evaluation

This chapter describes the procedures to be followed when using Kayzero for Windows for the evaluation of an Neutron Activation Analysis (NAA).

### 3.1 Menu Bar

All options of Kayzero for Windows can be found through the menu bar (Figure 3.1). The programs version number is given in the program title but also on all printed output.

From the menu bar a choice can be made by using the mouse. The program can also be used without the use of a mouse.

You can use the arrow keys and <Enter> or by using the hotkeys: e.g. <Alt>+<S> . The hotkeys become visible after pressing <F10> or <Alt>, use them by pressing <Alt> and the underlined letter of the option, e.g. <Alt><R><P><S> for the option *PeakTable File Report*.

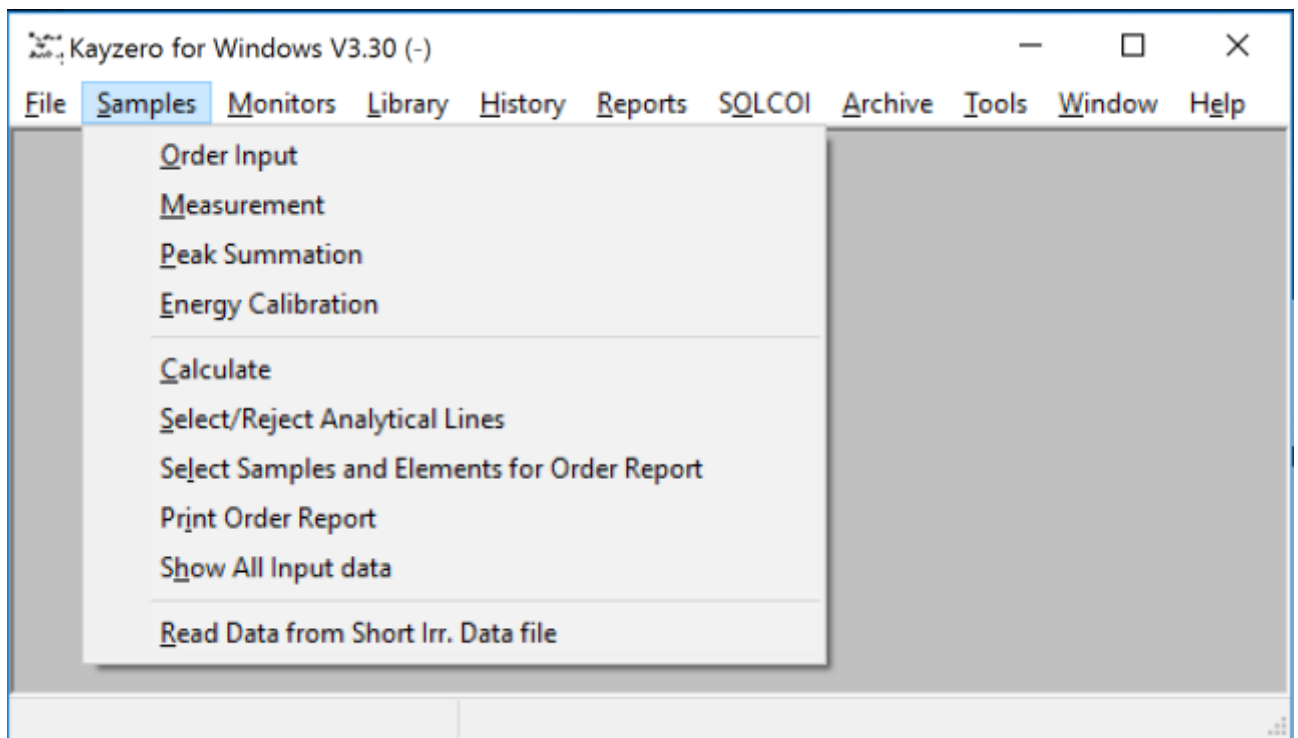


Figure 3.1 : Main screen of Kayzero for Windows after pressing <ALT><S>.

The menu bar contains the following menu options:

### File

The menu options can be used to open Kayzero specific or other text files. Once a file is opened new options will be available under *File*. The Right Mouse button can then also be used to open a popup menu.

### Samples

With this option you enter a dropdown menu. In this drop down menu you can enter the general data of the analysis job (*Order Input*), enter and edit the data of a measured spectrum (*Measurement*) and start the calculations (*Calculate*). It is also possible to combine peaks that were inserted to fit a spectrum peak but actually all refer to the same peak (*Peak Summation*), do a energy re-calibration (*Energy Calibration*), select the analytical lines that you want to use (*Select/Reject Analytical Lines*) and to print the result of the analysis for selected elements and samples (*Select Samples and Elements for Order Order Report*). Finally data from multiple measurements can be read from a database file (*Read Data from Short Irr. Data File*). Tables with all entered measurement data can be printed (*Show All Input Data*).

### Monitors

With the dropdown menu *Monitors* you can edit the general monitor information and enter and edit the monitor, irradiation and measurement data, calculate the comparator factor  $F_c$  and calculate alpha and f according to the 'Zirconium' method or the multi-monitor method (bare, sub-cadmium and Cd-ratio method).

### Library

The menu *Library* contains two different print options; a full library listing and a gamma line listing according to increasing energy.

### History

The detector and reactor calibration results can be printed and plotted as a function of time.

### Reports

The *Reports* submenu contains all the relevant printing options: printing an overview of jobs, an overview of sample data, peak table data files, results and an activity report. All output is directed to the main form of the program and can be printed or plotted from here.

### SolCoi

The solid-angle and coincidence correction calculation, the former SOLCOI program, is integrated in Kayzero for Windows. In this menu you will find also efficiency and peak-to-total-curve fitting and fine-tuning.

### Archive

Here you can change sample and monitor identification data, delete samples, monitors, jobs and files.

### Tools

This submenu contains the many utility functions like: performing a new energy calibration based on measured spectra; plotting the Compton background and the spectrum of a sample or monitor; changing the calculation parameter settings; changing data directories; and the material composition data.

### Window

Here you can select a report output window or organize the display.

Sample	: One physical portion of a material
Order	: Set of samples
Measurement	: Actually an irradiation of one sample resulting in one gamma spectrum
Measurement Id	: Combination of a sub-folder name where the spectrum is stored and a number
Monitor	: sample with a known, preferably certified, concentration of a comparator element used for determination of the comparator factor or flux
Monitor File	: a file containing several measurements of monitor, preferably all irradiated in the same channel

## 3.2 Evaluating a Neutron Activation Analysis

KAYZERO can be used for NAA data obtained using properly calibrated gamma-ray spectrometers and nuclear reactors (see VADE MECUM FOR K<sub>0</sub>-USERS).

In this manual the NAA data of an actual analyzed sample are used to explain the use of KAYZERO. The sample and a monitor were irradiated in channel Y4 of the BR1 reactor in Mol, Belgium. The sample and monitor were measured at DSM Research using detector 2, a properly calibrated High-Purity Germanium detector with a dual spectrum LFC system. The peak locations and peak areas were computed using Sampo-90.

The flux parameters,  $f$  and  $\alpha$ , for channel Y4 of the BR1 were predetermined and are assumed to be constant over time.

The calibration of a detector is not handled in this chapter since this is only done once. Detail like method to use, background and theory about detector calibration can be found in the Vademecum and the Laureate Thesis by Prof. F. De Corte. All needed tools can be found in the *SOLCOI* option. After the calibration of the detector all relevant data, the reference efficiency, the effective solid angles, peak-to-total-ratios and coincidence correction factor data were stored in the right format at the right locations (see Appendix 2). This is automatically done using the *SOLCOI* options. All starts with measuring efficiencies and peak-to-total ratios. K<sub>0</sub>-IAEA can produce this data as well.

The KAYZERO operating procedure (see Appendix 3) can be summarized as follows:

- make a new monitor file if needed in Kayzero <ALT><M><O>, here you can put for instance all monitors irradiated in one specific channel e.g. BR1Y4 or channel Y4 in the BR1, Belgian Reactor no. 1, this way you can follow the evaluation of  $F_c$  and  $f$  and  $\alpha$  in the *History*-option;
  - enter the measurement data of the monitor(s) <ALT><M><E> in the monitor file in KAYZERO;
  - check the spectra for split-up peaks (*Peak Summation*);
  - to determine  $F_c$ , calculate the flux parameters <ALT><M>,  $f$  and  $\alpha$  (using a gold/ zirconium monitor) or use predefined values of  $f$  and  $\alpha$  and e.g. a gold monitor for determination of  $F_c$  (only if the parameters  $f$  and  $\alpha$  can be considered to be constant);
  - print the flux parameters <ALT><M><I>;
- 
- make a new Order-file <ALT><S><O>, in this file you store all measurements related to a specific order or group of samples from a 'client'
  - enter the measurement data of the sample <ALT><S><M> and the determined flux parameters in KAYZERO;
  - calculate the element concentrations <ALT><S><C>;
  - check and correct (for blank concentrations, reaction interferences and outliers) the results <ALT><S><S>;
  - select the desired elements <ALT><S><L>;
  - print the element concentrations<ALT><S><I>

## 3.3 Monitor Data

Using the options given in the *Monitor* menu you can evaluate monitor-measurement data, see figure 3.2.

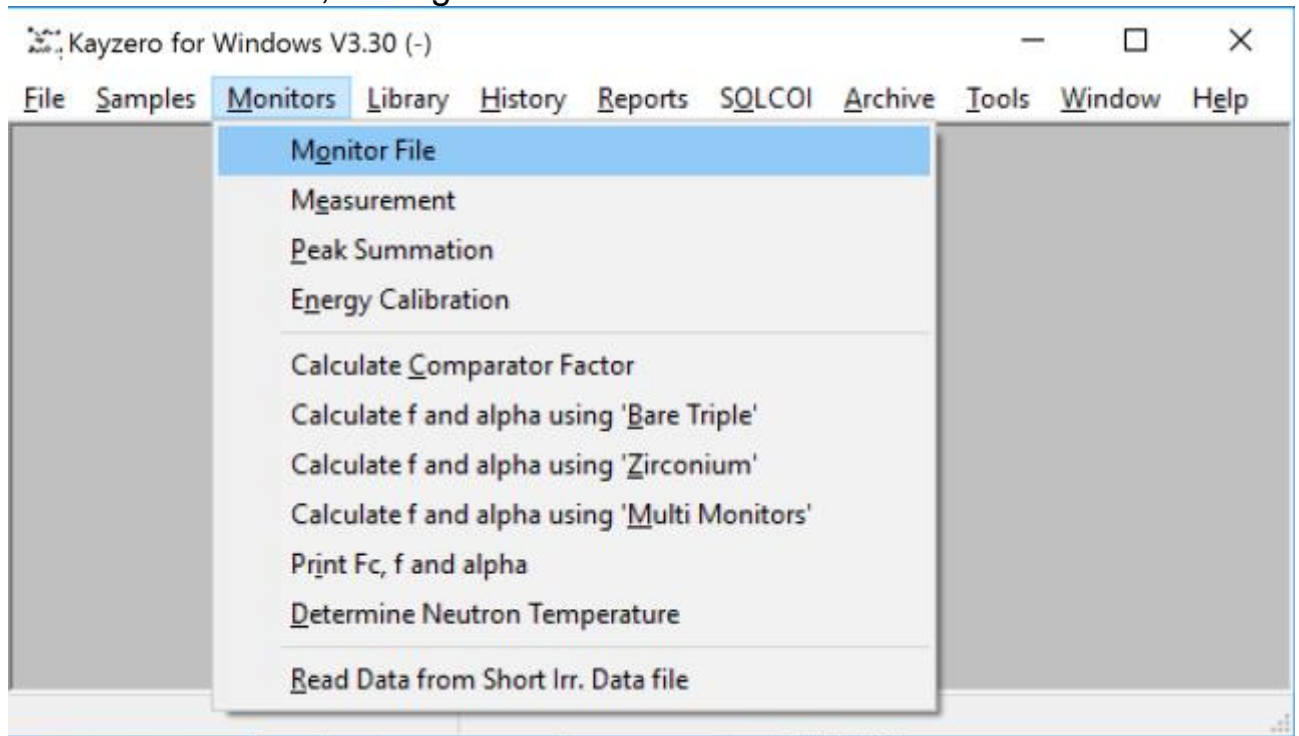


Figure 3.2: *Monitors* menu

The monitors-measurement data are stored in a monitor file. Per file some additional general information can be entered and stored (*Monitor File*). The comparator factor,  $F_c$ , can be calculated using only one monitor.

When three monitors are irradiated a full flux parameter set ( $F_c$ ,  $f$  and  $\alpha$ ) can be determined using 'Calculate  $f$  and  $\alpha$  using Multi Monitors' however three is the absolute minimum and results in high uncertainties for  $f$  and  $\alpha$ . Better is to use an Au/Zr monitor couple, using the special optimized Au/Zr technique. **Best** way to measure  $f$  and  $\alpha$  is to use the Cd-ratio method using several monitors (at least 4-5 monitors). See the VADE MECUM FOR  $k_0$ -USERS and Chapter 6.

### 3.3.1 Monitor File

A monitor file should contain the data of monitors irradiated in one particular channel. All data can then be compared and trends in  $F_c$ ,  $f$  or  $\alpha$  can be monitored. The name of the file can be best related to the channel used. In our example the file name is 'BR1Y4' for channel Y4 in Belgian Reactor No. 1 (BR1).

When choosing the first option *Monitor File* you can enter some general information about the set of monitors that was used (Figure 3.3). Please note the underline letters in the menu bar if you press <Alt>. You can enter the *Monitor File* option by pressing <Alt><M><O>.

First you need to select the monitor filename. This can be a new name or an existing file.

A monitor file named 'BR1Y4.STN' and an index file 'BR1Y4.SDX' are created in the job and monitor files data directory, see *Tools/Options/Directories*. The data entered is stored in the 'MONITOR.DIR' file (see Appendix 2).

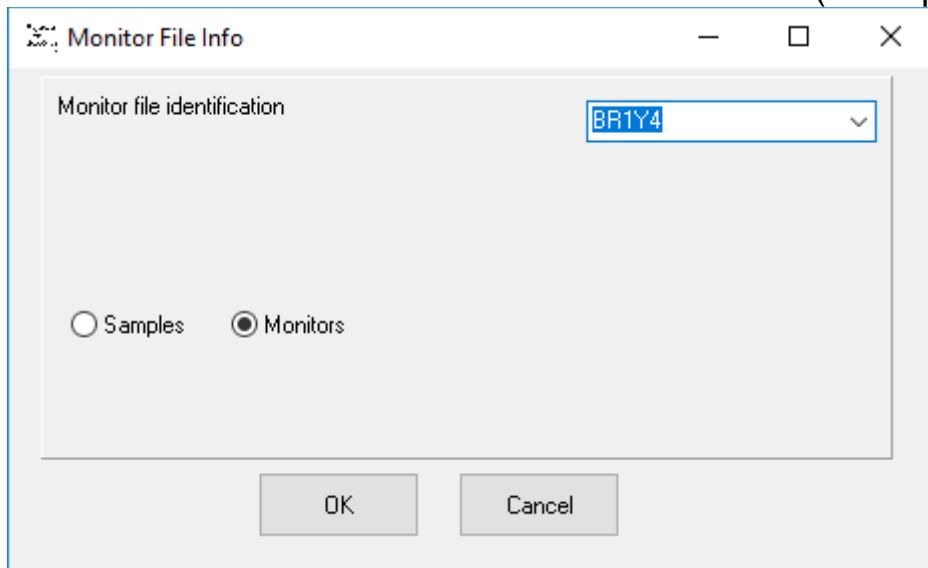


Figure 3.3A: Select Monitor filename.

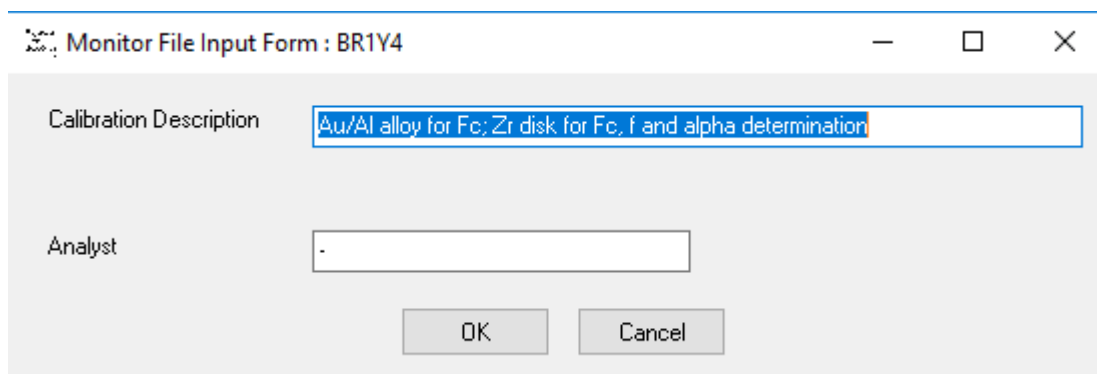


Figure 3.3B: Monitor file info.

### 3.3.2 Entering Monitor Data

You can enter data of measured monitors using *Measurement*. All data will be stored in the file 'BR1Y4.STN'. First, the monitor file identification (BR1Y4) must be specified. (See figure 3.4). Then KAYZERO demands a monitor identification (e.g. AU2). It is possible to enter letters and numerals.

The next input is the measurement identification. This may be a numeral (e.g.

1) but much better is to refer to the subdirectory where the spectrum data is stored. See the measurement data base directory specified in *Tools/Options/Directories*. In the latter case the measurement identification should contain the subdirectory and a measurement identification separated with a semicolon (e.g. SCK7V:1 where 'SCK7V' is the subdirectory and '1' the measurement number).

At DSM we store all spectra of samples irradiated in a specific channel during one irradiation day in a subdirectory. In this example the irradiation was code-named SCK7V and all measurement data was stored in the data directory '....\SCK7V\' (see the header of the input screen in figure 3.5). The measurement identification can thus be used to select all data of a particular irradiation (day). This monitor "AU2" was measured several times on different irradiation days and were different samples but all measured on detector 2.

You can pick your choice from a list of previously entered inputs.

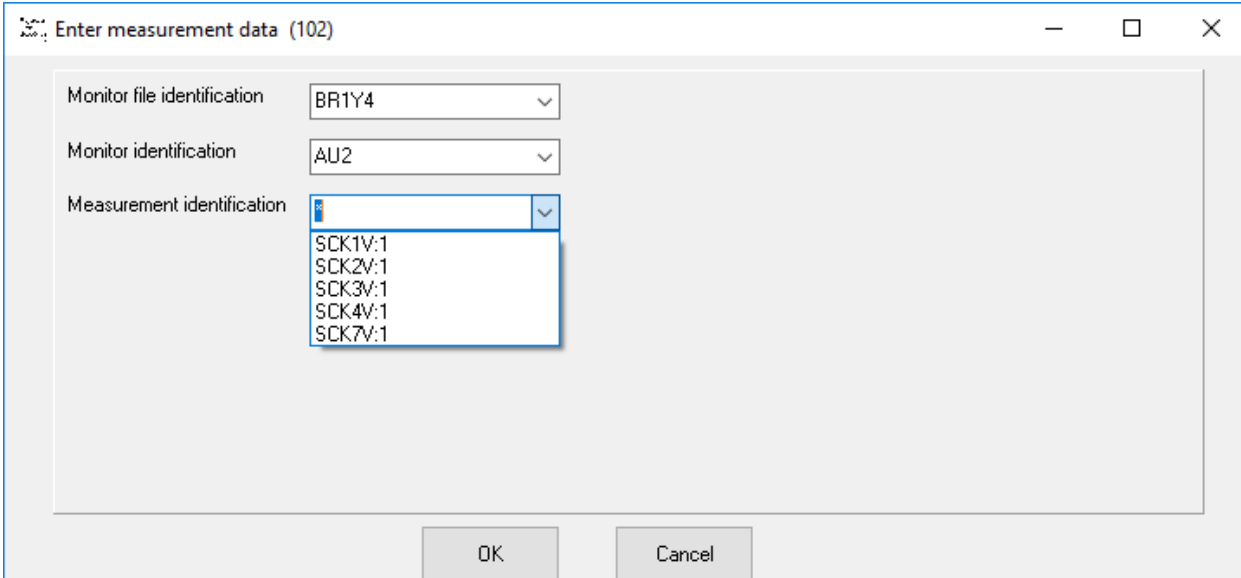
The image shows a software dialog box titled "Enter measurement data (102)". It has three dropdown menus. The first is labeled "Monitor file identification" and contains the text "BR1Y4". The second is labeled "Monitor identification" and contains the text "AU2". The third is labeled "Measurement identification" and is currently open, showing a list of options: "SCK1V:1", "SCK2V:1", "SCK3V:1", "SCK4V:1", and "SCK7V:1". At the bottom of the dialog box are two buttons: "OK" and "Cancel".

Figure 3.4 : Identification of the measurement data of a monitor

If the identification data have been entered correctly, you can proceed by pressing the 'OK'-button.

In the monitor measurement 'Edit Data' input screen (figure 3.5) the weight of the monitor element has to be entered in  $\mu\text{g}$  ( $72.48 \text{ mg} * 0.1 \% = 72.48 \mu\text{g}$ ). The self-absorption correction factors for thermal and epithermal neutrons may be entered (*Tools/Thermal Neutron Self Absorption*). It is also possible to enter a description and a label for the monitor selected.

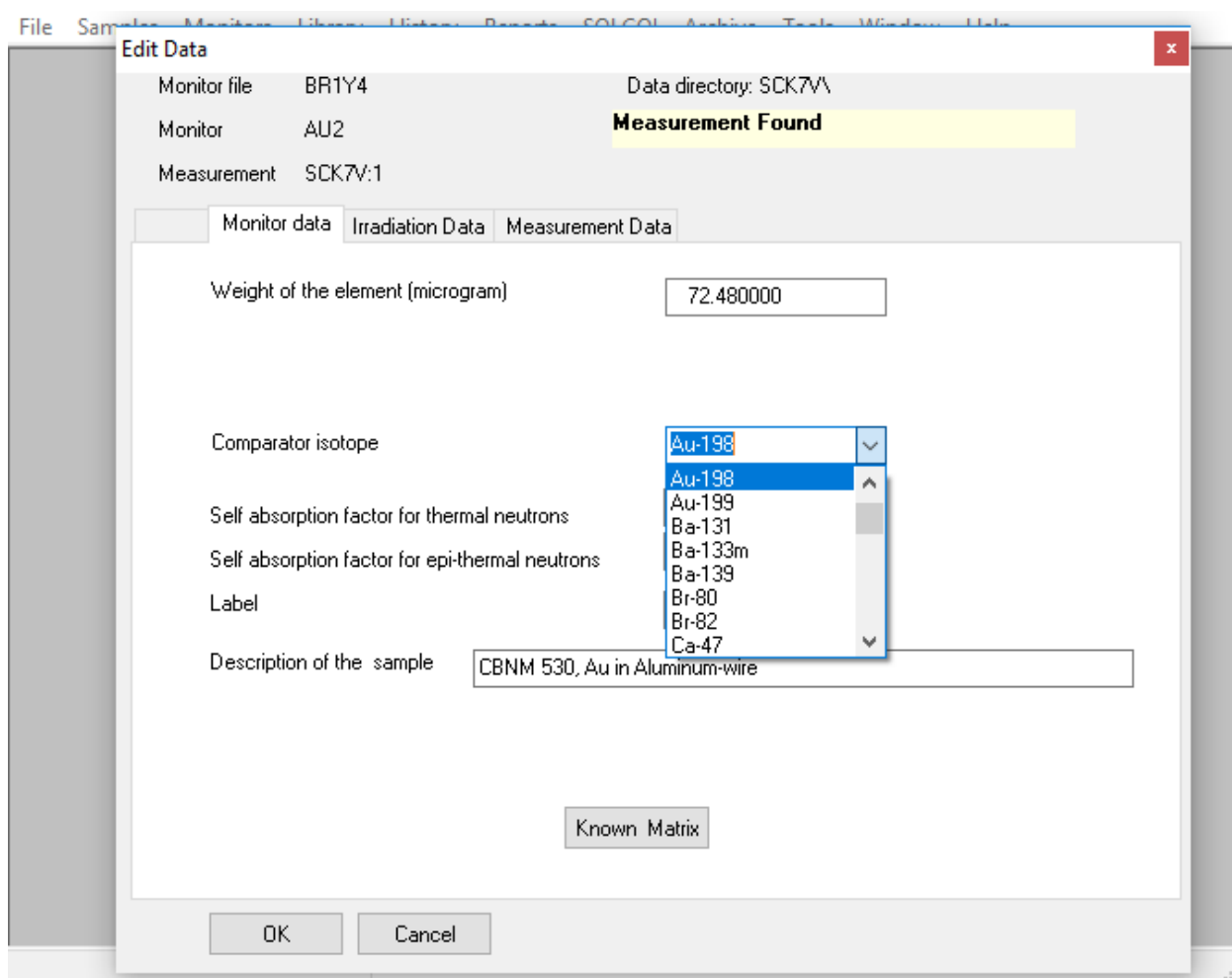


Figure 3.5: *Monitor Data*-tab with a list of possible comparator radioisotopes.

It is possible to choose the relevant comparator isotope from a list.

The self absorption factors for thermal and epi-thermal neutron can be entered in this screen as well. It is preferred to use elements that show little or no self absorption. For the calculation of these factors an input option is given with the *Known Matrix*-button. See figure 3.6.

In this screen known matrix elements can be entered. Sometimes elements are not measured but can affect the result through significant neutron and gamma absorption or interfering reactions. In these cases known matrix elements can be entered. In case of monitors the self absorption factors can be calculated.

Matrix Components

Matrix component or element	Concentration in %	Abs. Uncertainty in %	Use for Reaction Interference
#Au	0.1		<input type="checkbox"/>
			<input type="checkbox"/>
			<input type="checkbox"/>
			<input type="checkbox"/>
			<input type="checkbox"/>
			<input type="checkbox"/>
			<input checked="" type="checkbox"/>
			<input type="checkbox"/>
			<input type="checkbox"/>
			<input type="checkbox"/>

Sample Matrix Main Component

Aluminum 99.90000000 0.00000000 ☐

Use Neutron Self Absorption Data (1) for more than one measurement

- ☐ All Samples of this order
- ☐ All Measurements of this order in this Directory
- ☐ All Measurements of this Sample
- ☐ All Measurements of this Sample in this Directory
- ☒ Only this measurement
- ☐ Not Set

Gth Calculation Method (2)

- ☒ Original Kayzero Method
- ☐ Cornelia and Greg's Method

Use Matrix Compo. and Gth Method (2) for:

- ☐ All Samples in this order
- ☒ All Measurements of this sample

Neutron Self Absorption Data (1)

☒ Use Measurement Vial Dimensions

Radius [mm] 2.500

Height [mm] 1.000

Neutron Temperature [°C] 40.00

Sample Mass [g] 0.07248

Density [g/ml] 3.69

Gth 0.9966

G epi Au-198 = 0.9760

☒ Take over Gth ☒ Take over Gepi

OK Cancel

Figure 3.6: Input screen behind the *Known Matrix*-button.

The comparator element concentration, if entered as a known matrix component, is used to calculate the total mass of the sample.

The thermal self absorption correction factor can be calculated through the standard method as given by DeCorte or by the newer method by Chillian. The epi-thermal correction factor calculation method used is the one proposed by Chilian as well. The results can be taken over to the *Monitor Data* input tab.

In case the irradiation vial has different dimensions compared to the measurement vial this can be handled here. The yellow boxes are related. It is possible to select the option that this input is used for all samples in an order or for every measurement specific. The given matrix composition is used for the efficiency calculation if *Direct Calculation* is turned on and for the semi-automatic thermal neutron self absorption correction, see the final tab in the *Select Analytical Lines* option. The information for epi-thermal self absorption is also used in the option but now for every nuclide.

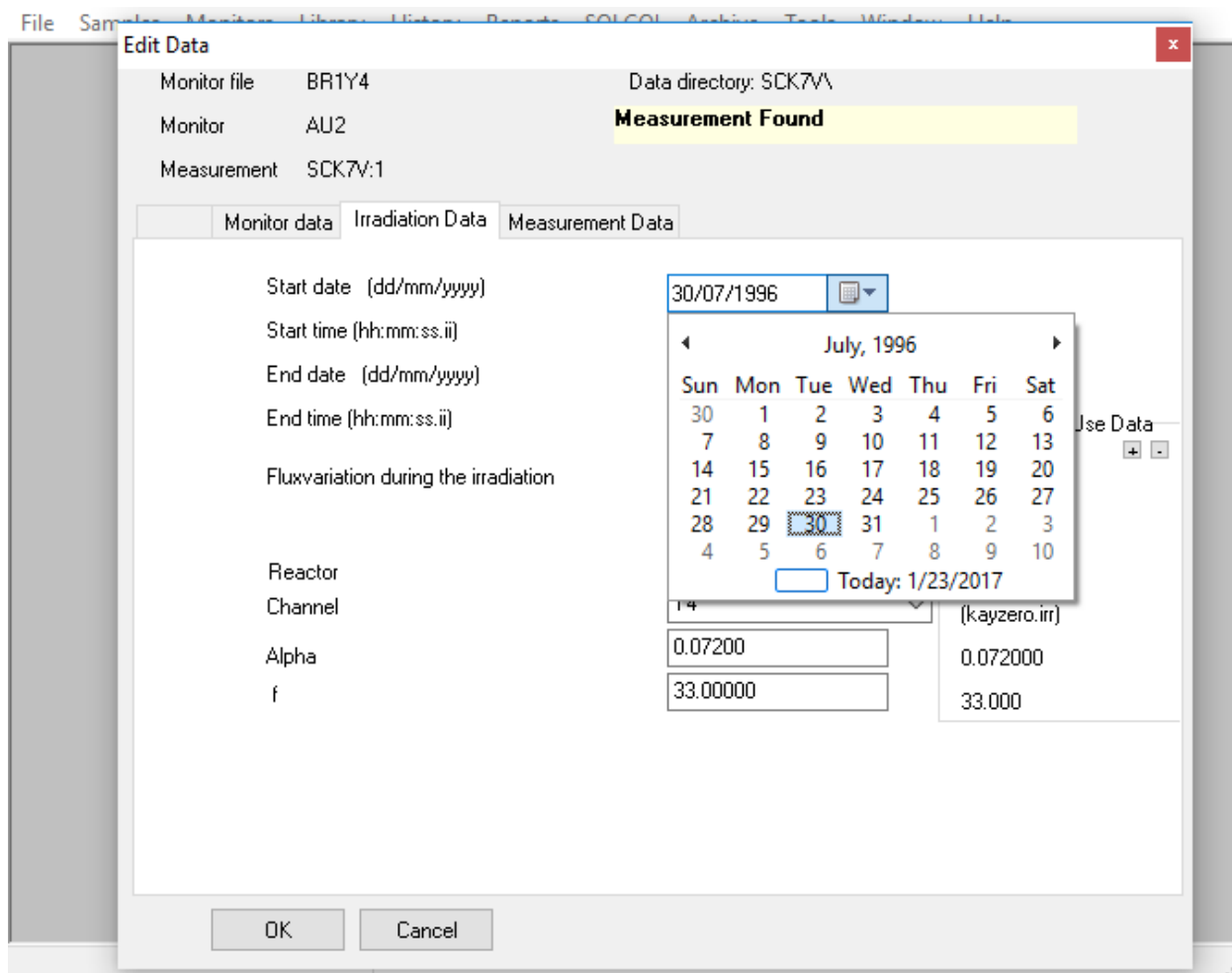


Figure 3.7: *Irradiation Data-tab.*

In the *Irradiation Data* tab the start and end date and time must be entered. The required formats are shown, see figure 3.7.

The reactor and channel can be picked from a list. The  $f$  and  $\alpha$  can be entered by clicking the "Click Here to Use Data" label on the right of the reactor edit field. The reactor and channel in which the irradiation took place have to be entered together with the corresponding  $f$  and  $\alpha$  values. You can select reactor and channel from a list. The  $f$  and  $\alpha$  are then be taken from a table stored on disk. The table is stored in the file 'KAYZERO.IRR' file in the Kayzero root directory, see Appendix 2.

The 'KAYZERO.IRR' file is an ASCII file. It can be updated using a file editor. Or you can enter and change the table by using the *File/Open* option, select for file type the 'Reactor Channels File'.

If you want to add new or change old data you can just click on the small "+" button at the top-right side of the panel and you will be prompted to confirm that you want to add or change the present data to the file. If you like to

delete data you just click the small “-“ button.

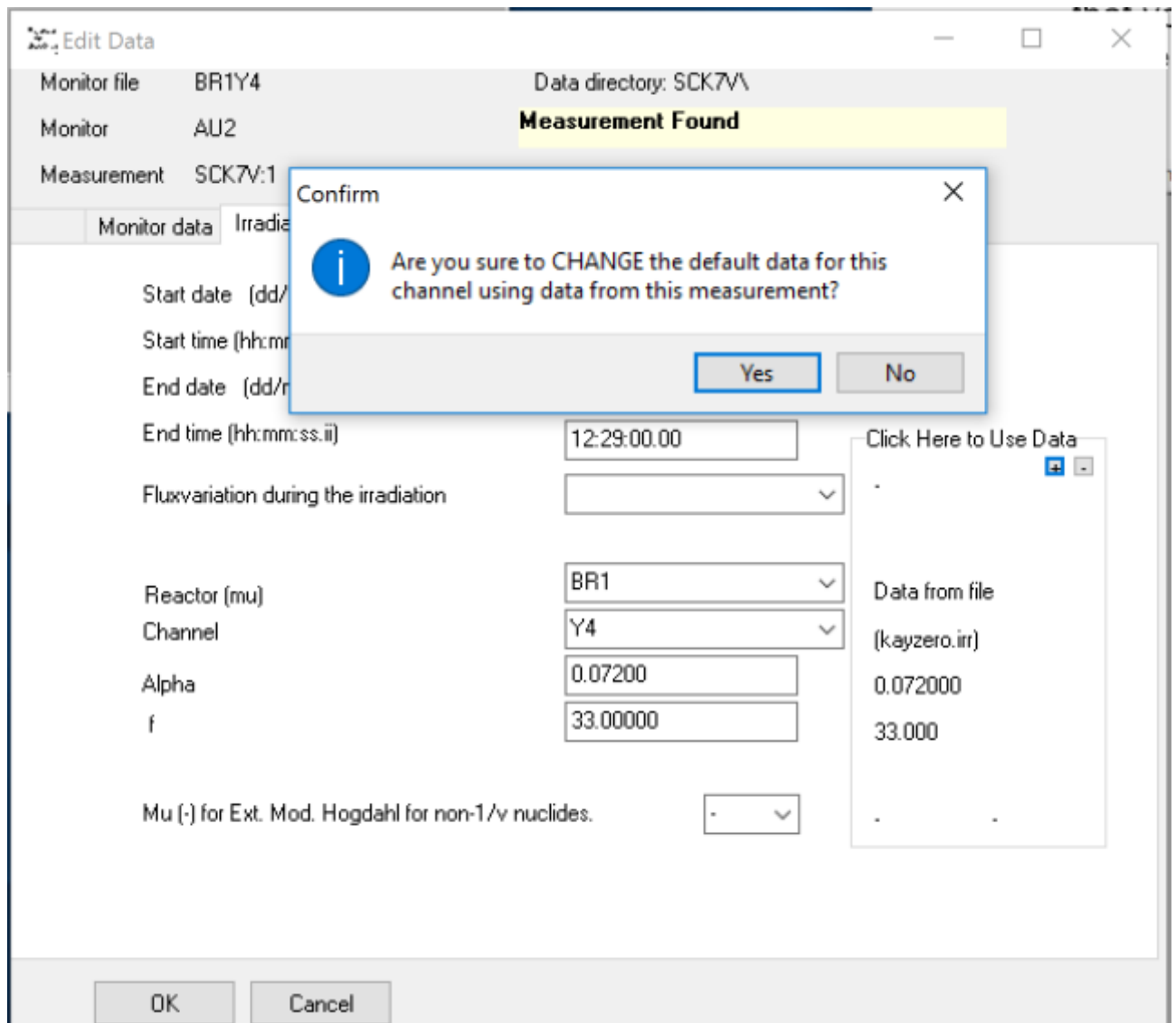


Figure 3.8 : Changing data in the Reactor and Channels list.

You can also use a ‘flux variation data file’ to correct for variations in the neutron flux during the irradiation. See chapter 6, Reference Guide.

The Comparator Factor  $F_c$  is not taken over because this is the value that is typically determined when irradiating a monitor. After the measurement and calculation of a monitor the reaction parameters are the result of the measurement depending the type of measurement only  $F_c$ ,  $T_N$ ,  $f_{fast}$  or  $f$  and  $\alpha$ .

The  $\mu$ -parameter is a reactor specific parameter and is needed to select the appropriate  $Q_0$  and  $E_r$  for the measurement of the neutron temperature. This temperature is needed in the activation reaction convention for non  $1/v$  nuclides. Lu-176 is the monitor to use. The  $\mu$  selected determines the reaction convention and its nuclear data. The original Westcott convention

was not used in Kayzero since it needed a totally different reactor calibration. Depending on the value entered, the simplified Westcott convention is used with a  $Q_0$  transferred from the  $s_0$  from literature, or the recently determined  $Q_0$ 's and  $E_r$ 's for the new Extended Modified Hogdahl convention is used.

$S_0$ 's especially the one of Lu-176 is temperature dependent. This is a minor effect however the new Extended Hogdahl method handles this without extra input, except for the  $\mu$ .

In the *Measurement Data*-tab you can enter the gamma spectrometric measurement data like spectrum and peak table file, and information for the determination of the efficiency, see Figure 3.8.

The screenshot shows the 'Edit Data' dialog box with the 'Measurement Data' tab selected. The 'Monitor file' is BR1Y4, 'Monitor' is AU2, and 'Measurement' is SCK7V:1. The 'Data directory' is SCK7V\.

**Measurement Found**

Detector: DSM2  
 Geometry: AU  
 Counting position: 3  
☐ Direct SOLCOI Calculation

Background spectrum PTF file: 2BG96.PTF  
 Deadtime (%): 0.00000  
 Peaktable file: ☐ Correct Hypermet 257V07.PTF  
 Start date (dd/mm/yyyy): 01/08/1996  
 Start time (hh:mm:ss.ii): 10:14:00.00  
 True Measuring Time (sec): 1954.00  
 Remarks:

**Info Panel:**  
 Non-Point Source  
 Geometry data Okay!  
 Volume: 0.020 ml  
 Density: 3.62 (2.7) g/ml  
 Mat: (Aluminum) : Okay  
 Click Here to Use Data 0.00  
 Sampo90 PTF (18 peaks)  
 01/08/1996  
 10:14:00.94  
 1954.00  
 SPE : 257V07.SPE

Buttons: OK, Cancel, SpectrumPlot, Peak Summation, Energy Calibration

Figure 3.8 : *Measurement Data*- tab.

In this screen the code name of the detector used, the counting vial type and the counting position have to be entered. In each of these inputs the validity is checked automatically. The 'info panel' on the right of the detector input field gives all relevant information as illustrated in Figure 3.8. In case of an error

the message is indicated here.

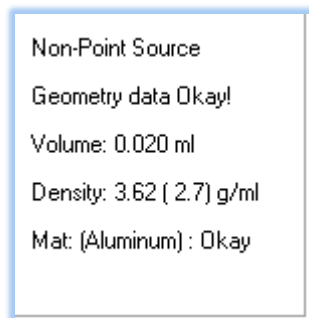


Figure 3.9 : Efficiency Info panel, for gold monitor AU on detector DSM2.

On this particular 'Info panel' Kayzero for Windows indicates with 'Geometry data Okay!' that it has found a SOLANG (effective solid angle, .SOL) file and a coincidence (.COI) file for the combination of the geometry AU and detector DSM2. And the reference efficiency file EFFDSM2.DAT and the corresponding SOLANG file DSM2.SOL for the reference position were found too. The panel indicates 'Non-Point Source' this means that the sample has a volume. The 'Direct SOLCOI Calculation' checkbox is visible, so the contents might be changed if you like and the necessary SOLCOI calculation will be performed when you calculate the measurement. This will cause some additional calculation time.

If background subtraction is to be performed, the relevant peak table file must be entered. This file must be located in the 'Efficiency Data'-directory.

#### Dead Time:

- Dead time from spectrum: enter a dead time of 0%;
- Dead-Time-Stabilizer (DTS): enter DTS preset dead time;
- Pulser: enter measured dead time
- Manual Pile-Up-rejection (PUR) correction: enter the corrected dead time
- Loss-free-counting: enter a dead time of 0%.
- ZDT: enter a dead time of 0%.

For the calculation of errors and detection limits when using the LFC-module the uncorrected spectrum should be collected as well. If the dual LFC spectrum option is used (this is advised) then there are several options to store the data and let Kayzero use it. Normally both spectra are stored in one file (Hypermet and Hyperlab can handle these spectra), Kayzero then normally detects automatically the uncorrected spectrum. The second uncorrected spectrum can also be stored in a file with the extension '.LFC', in this case Kayzero will also detect the Dual LFC Spectrum automatically.

If Kayzero has problems detecting the Dual LFC Spectrum automatically you should mark the Dual LFC Spectrum in the FWHMddddd.DAT file

(dddd=detector code) which is placed in the 'Efficiency Data'-directory, see Figure 3.10.

Correct calculation of errors and detection limits is not yet supported for Zero-Dead-Time units (please let us know if you need this).

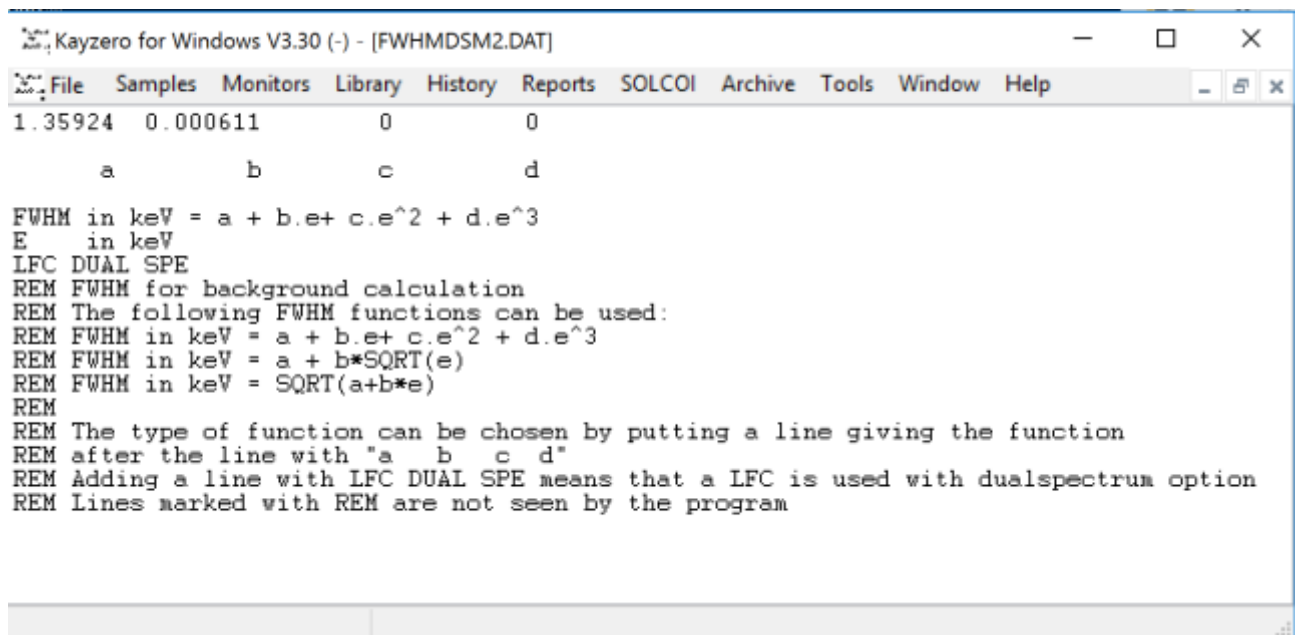


Figure 3.10 The FWHMDSM2.DAT file for a detector using the dual LFC spectrum option.

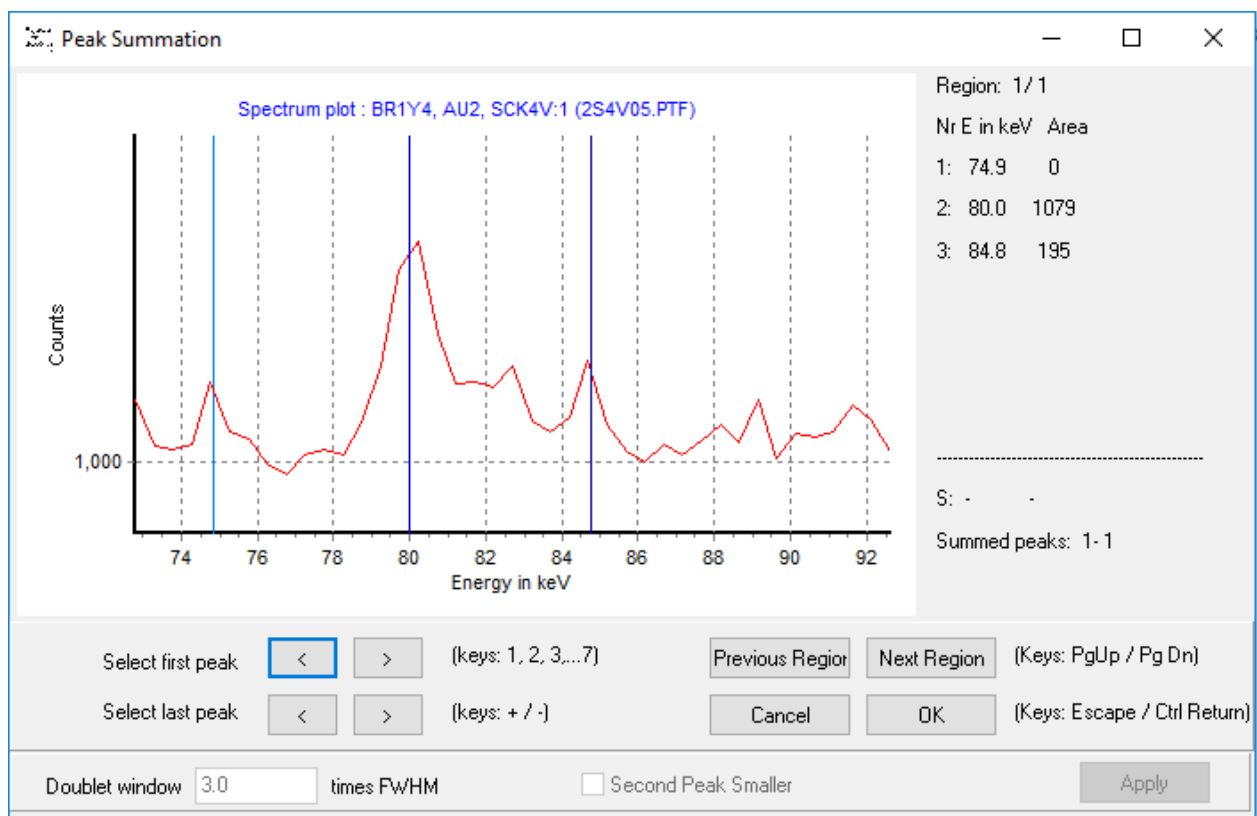
To select the correct peak table file use the pick-list to call up a table of files from which you can choose. Kayzero enters the relevant measurement data (start date and time and measuring time) if you double click on the info-panel on the right.

**Note:** Kayzero cannot automatically detect if during irradiation or decay the time was changed to day light savings time or changed to back normal. Please take care and correct yourself.

Now all the data of the first monitor have been entered. You can enter more monitor data by pressing the 'OK'-button or do an energy calibration or a peak summation.

### 3.3.3 Peak summation

Peaks are often not fitted perfectly when the spectrum is measured at (very) high count rates or in a period when the detector system is not well tuned. During the gamma spectrum deconvolution, using Sampo/HypermetPC or any other sophisticated software program, peaks might have to be inserted to fit the measured spectrum adequately.



Figur 3.11: *Peak Summation* Option (no summation needed)

Some of these peaks are more or less artificial and belong in fact to the main real gamma peak. The peak areas should be added to the main peak. This is essential because Kayzero can only use one peak area for one gamma line so if the artificial peaks are not added serious errors might occur. This is however easier said than done in most programs. In order to facilitate this problem an option was added to Kayzero. This is the *Peak Summation* option (see Figure 3.11) which you can find as a separate option in the *Samples* option or as part of *Measurement*-tab (see Figure 3.8). The program will automatically find peaks that are closer together then a given distance (expressed in x times the FWHM of the peak), see Figure 3.11. If there are peaks closer than this given interval the program will show the appropriate regions of the spectrum. You can click on the “Doublet Window” panel if you like to change the present values, press apply to see the result. The user will then have the opportunity to add peaks (<+>/<->). By using the <PgUp> and <PgDn> keys the regions can be selected.

**Note after a new ‘Peak Search’ in your ‘Gamma Spectrum Deconvolution’-program you need to re-do your *Peak Summation*!!!!!!**

The main peak to which all other smaller peaks should be added can be selected by typing the appropriate peak number (1-7, see Figure 3.11). All peaks at the right side of this main peak can be added by pressing the <+> key or deselected by using the <-> key. At the right of the screen the peaks

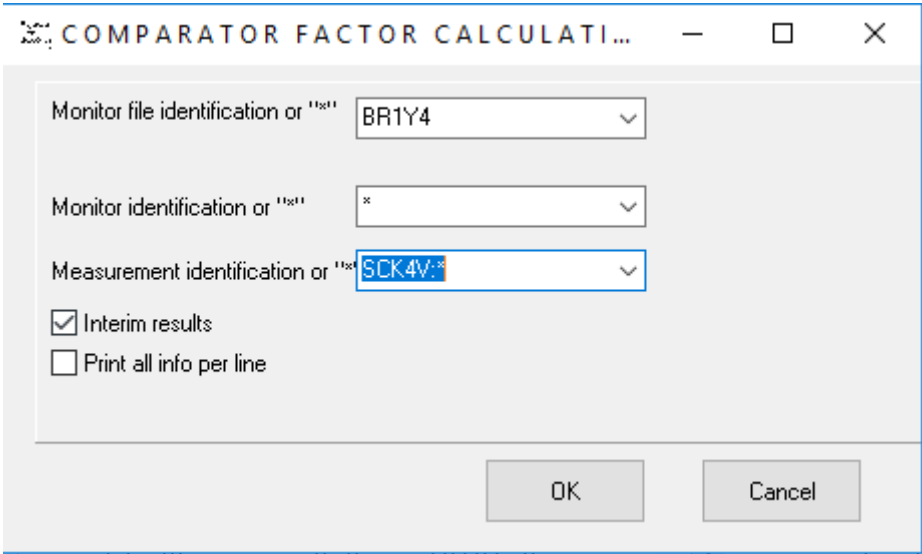
are given as well as the new combined peak. The new energy is the calculated as the weighed mean energy. The peak area is the sum of all peaks. The new standard deviation of the peak error is the calculated weighed error.

The results of the summed peaks can be viewed in the print of the PTF-file *Reports/Peak Table Data*. The calculated concentrations are based on the summed peak area, the added peaks are not used.

### 3.3.4 Calculating $F_c$

After entering the monitor data the comparator factor  $F_c$  can be calculated using *Monitors/Calculate Comparator Factor* (see Figure 3.12). In this option you have to enter the monitor file identification and the monitor identification. If you enter an asterisk (\*) here, the program will batch-wise calculate  $F_c$  data for all available monitors that have been entered.

So using the input in Figure 3.12 all data of monitors irradiated in BR1Y4 on directory 'SCK7V' will be calculated.



The screenshot shows a Windows-style dialog box titled "COMPARATOR FACTOR CALCULATI...". It has three dropdown menus for input: "Monitor file identification or """ set to "BR1Y4", "Monitor identification or """ set to "\*", and "Measurement identification or """ set to "SCK4V:". Below these are two checkboxes: "Interim results" (checked) and "Print all info per line" (unchecked). At the bottom right are "OK" and "Cancel" buttons.

Figure 3.12 : *Monitors/Calculate Comparator Factor* .

By creating a directory per irradiation day one can easily handle and find all data that is relevant after an long time irradiation or batch of short irradiations in a rabbit system.

While Kayzero for Windows is calculating the File name, monitor and measurement identification is displayed at the bottom of the program.

By marking the 'Interim results' checkbox you can print an output as given by SINGCOMP, the INW Gent program for  $k_0$ -NAA.

A burn-up correction procedure is built in; the correction factors are given when the 'Interim results' are printed. Burn-up correction for monitors and samples is performed using the data in 'KAYZERO.BUR' for the isotopes Eu-154, Ta-182, Au-198, Dy-165, Pm-149 and Rh-105. If this file is not present, burn-up correction is not performed.

### 3.3.5 Printing $F_c$

The calculated  $F_c$  can be printed using '*Monitors/Print  $F_c$ ,  $f$  and  $\alpha$* ' or '*Reports/Overview/ Monitors*'.

You can use the *Reports/Overview/ Monitors* option to print averaged  $F_c$ 's with expected and observed standard deviations (type of list 2 :irradiation data, see Figure 3.13). The output is shown in Figure 3.14.

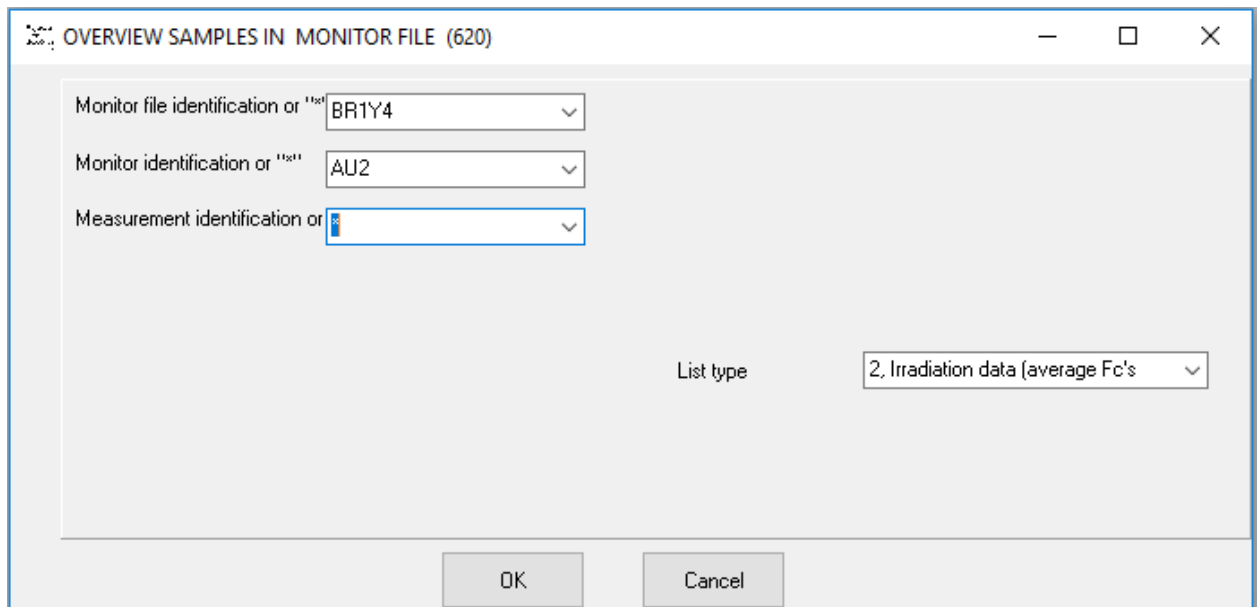


Figure 3.13 :  $F_c$  print option

You can use the data list provided by this option to check the entered data in order to detect input errors. You can do this before the calculations are performed.

The found value of  $F_c$  (which is proportional to the epithermal flux density) can be compared with the approximately known value, so input errors can also be detected.

Kayzero for Windows V3.30 (-) - [OVERVIEW SAMPLES IN MONITOR FILE (620) BR1Y4-AU2]

File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

Order : BR1Y4 List type : 2 (sorted on: id) BR1Y4|AU2|\*

Monit.#/Meas#	Irr.date	time t	irr.[s]	reactor/channel	f	alpha	Fc
AU2/SCK1V:1	03/06/96	09:00:00	4h	BR1/Y4	33.0	0.0720	3373.9
Fc =	3373.855	SD exp=	0.225 %	SD obs=	0.000 %		
AU2/SCK2V:1	24/06/96	08:55:00	4h	BR1/Y4	33.0	0.0720	3355.4
Fc =	3355.392	SD exp=	0.291 %	SD obs=	0.000 %		
AU2/SCK3V:1	25/06/96	08:57:00	4h	BR1/Y4	33.0	0.0720	3298.0
Fc =	3297.990	SD exp=	0.224 %	SD obs=	0.000 %		
AU2/SCK4V:1	27/06/96	08:59:00	4h	BR1/Y4	33.0	0.0720	3307.8
Fc =	3307.815	SD exp=	0.184 %	SD obs=	0.000 %		
AU2/SCK7V:1	30/07/96	08:29:00	4h	BR1/Y4	33.0	0.0720	3291.7
Fc =	3291.713	SD exp=	0.081 %	SD obs=	0.000 %		

Figure 3.14 : Result of  $F_c$  printout.

In this list the weighted mean comparator factor as well as the expected and observed standard deviations in the mean are given for the comparator isotope. Only gamma lines with k0 code = 1 are used for the calculation of the mean value.

By using the *Reporting/Results/Per gamma one measurement/Monitors* printing option (see figure 3.15) you can print  $F_c$  per measurement. Again the monitor file identification, the monitor identification and the measurement identification have to be specified.

REPORT - COMPARATOR FACTORS per MEASUREMENT (651)

Monitor file identification or "id" BR1Y4

Monitor identification or "id" AU2

Measurement identification or "x" \*

☐ Print Short Version

OK Cancel

Figure 3.15 : Another  $F_c$  Printout Option.

The result of this printing option is shown in Figure 3.16. If the irradiation of the monitor element results in more isotopes, the comparator factor for these isotopes will also be printed using this option. Attention must be paid to the fact that the self-absorption factor for epi-thermal neutrons (entered in

*Monitors/Measurement-Option* (Figure 3.6) is valid for the comparator isotope only.

Kayzero for Windows V3.30 (OPTION : 651)  
 REPORT: COMPARATOR FACTORS per MEASUREMENT  
 Filename : BR1Y4 Monitor id: AU2 Meas. id.: SCK7V:1

Element	Nuclide	Energy [keV]	Fc [-]	SD [%]	k0code	Interfer.nucl.
Au	Au-198	411.8	3.29171E+3	0.08	1	
Au	Au-198	675.9	3.32879E+3	1.06	3	

Gamma lines (P:3;N:I;dE0.70; k0-2015 : 03/07/2017)  
 Measured : 18  
 Explained : 16 88.9 % (explained by identified radionuclides)  
 Unexplained : 0 0.0 % (peak in library but unexplained)  
 Unknown : 2 11.1 % (gamma lines not in KAYZERO-library)  
 False peaks : 0 0.0 % (peak area is smaller than LD)

The unknown gamma-lines are (energy in keV): 83 1087

Figure 3.16 : Result of  $F_c$  printout *Reporting/Results/Per gamma one measurement/Monitors*. Only energies with k0 code=1 will be used for  $F_c$  calculation.

### 3.4 Determination of the Element Concentrations

All necessary options for the calculation of element concentrations after a NAA analysis are given in the *Sample Menu Options* (See Figure 3.17).

The measurement data of a neutron activation analysis are stored in a so-called order file. In this file data of up to 500 measurements can be stored. The order file identification is normally a number (like an order code). The order file can be linked to a client using the *Sample/Order Input*-option.

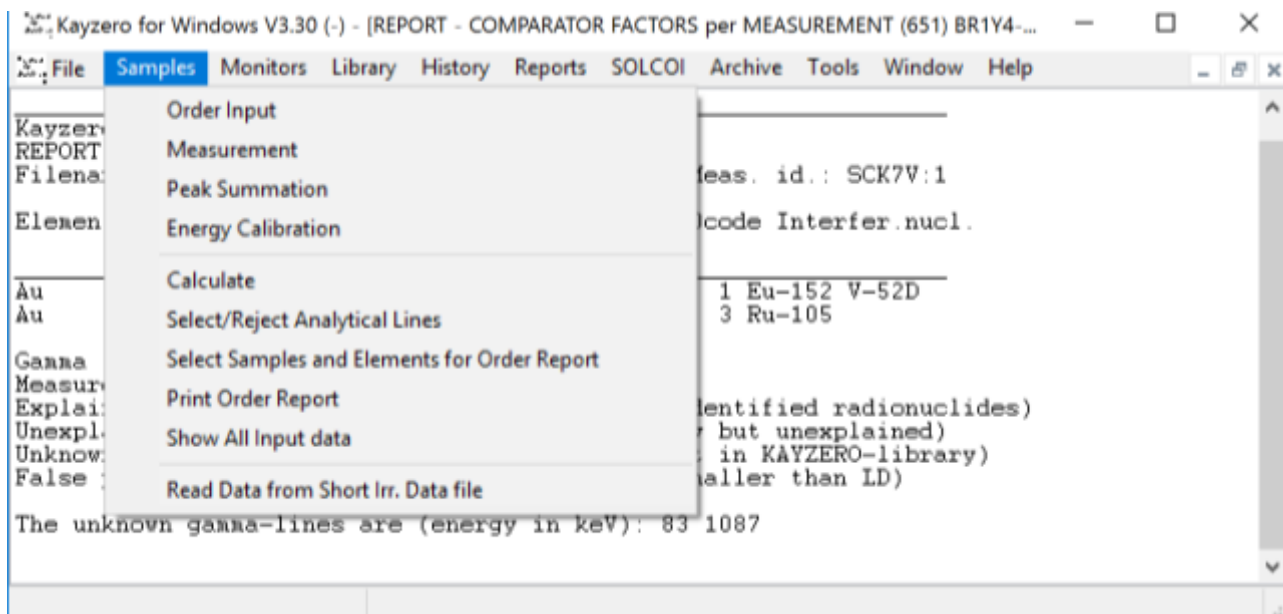


Figure 3.17 : *Sample-* options.

### 3.4.1 Order Input

By choosing the first option, *Order Input* (see Figure 3.17), you can enter general information about the analysis job (Figure 3.18), such as the name of the client and his/her department (and telephone number). In addition you enter some reference numbers or budget numbers, some information on the samples, the elements requested and the relevant dates. All this information can be used later to produce all sorts of different output. Even the analysis cost can be entered.

The order identification code, in this case 'DEMO', will be used to create two files : DEMO.DTA and DEMO.DDX. The order info is stored in the ORDERS.DIR file. These files are all located in the ORDER AND MONITOR FILES-subdirectory specified in *Tools/Options/Directories*.

Order Input Form : DEMO

Client: Vervecken

Institute: DSM Research

Telephone: 61421

Budget number: Eu-152

NAA number: 1

Sample Description: Data for demonstration purposes

Elements of Interest: ALL

Date order received: 01/01/1980

Date Results given: 04/06/1992

Date samples disposed: 01/01/1980

Total Analysis Cost: 0.00

OK Cancel

Figure 3.18 : Order Info.

### 3.4.2 Entering Measurement Data

Use *Samples/Measurement* to enter the sample data. All data will be stored in the file 'DEMO.DTA', so the order identification you have to enter is DEMO. KAYZERO for Windows then demands (see Figure 3.19) a sample identification (e.g. 1B). Again it is possible to enter letters and numerals.

The third input is the measurement identification. The measurement identification may be a number (e.g. 1) but can also be related to the subdirectory containing the data (the parent data directory is specified in *Tools/Options/Directories*). In the latter case the name should contain the name of the subdirectory followed by ':' and a measurement identification (e.g. SCK7V:1).

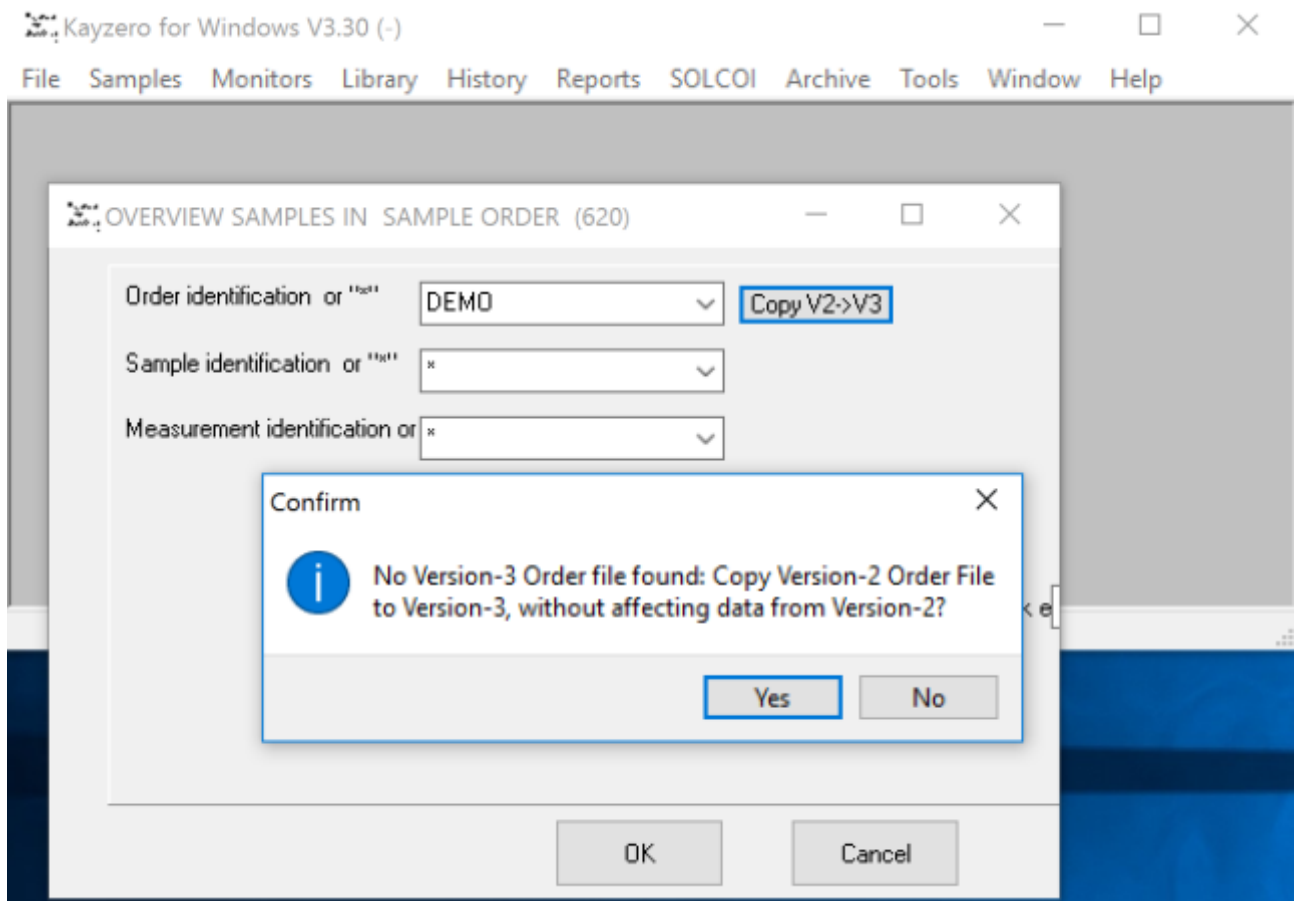


Figure 3.19 : Identification of a measurement and the update option in case a Version-2 order file exists.

If all spectra of a particular irradiation day are stored in a subdirectory, the measurement identification code can be used to select all data of that particular irradiation. In the example the irradiation was called 'SCK7V' and all measurement data was stored in the directory '....\SCK7V\'.

If you already worked with Kayzero for Windows then V3.30 and higher will ask you if you like to use the new file format. By choosing so you can continue working with the old software without being interfered with new data. Especially because V3.30 also used a new library that cannot be used by older versions of the software. It also allows you to compare the older and the newer version.

First the order index file is updated automatically. So you will be able to see all old orders. Later the order files can be updated separately. If an order file is not yet updated you will see the [Copy V2->V3](#)-button. By pressing you can start using all old information and preferably re-calculate.

The “Known” matrix information is the same for V2 and V3 data.

The order file name, the sample identification, the measurement identification, the measurement data directory and the order directory are displayed on each sample data input screen (see Figure 3.20 - 3.24).

On the tab sheet *Sample Data* (see figure 3.20) you have to enter the sample weight in grams. You can also enter a description and a label for the sample. The moisture content is used to calculate the dry-weight element concentration. The water content is not added automatically to the matrix composition.

**Edit Data** [Window Title Bar]

Order: DEMO      Data directory: SCK7V\

Sample: 1B      **Measurement Found**

Measurement: SCK7V:1

Sample data | Irradiation Data | Measurement Data | Short Input | Uncertainties

Sample Mass in gram: 4.739500

Moisture Content (m%): 0

Self absorption factor for thermal neutrons: 1.00000

Label: SCK7V\6

Irradiation Container for Blank Correction: R

Description of the sample:

Known Matrix

OK Cancel

Figure 3.20 : *Sample Data*-tab sheet.

In case of serious thermal neutron self absorption a correction factor can be entered. This factor can be calculated in the known Matrix screen (see Figure 3.6). The correction can best be done after the analysis when all components are known in the *Select Analytical Lines*-option. Epi-thermal self absorption is handled also in this option but now isotope specific.

If you measure your sample in the vial in which you irradiated the sample you might want to subtract blank concentration values. The file name of the blank

file can be entered under *Irradiation Container for Blank correction*. You can see a list of blank files.

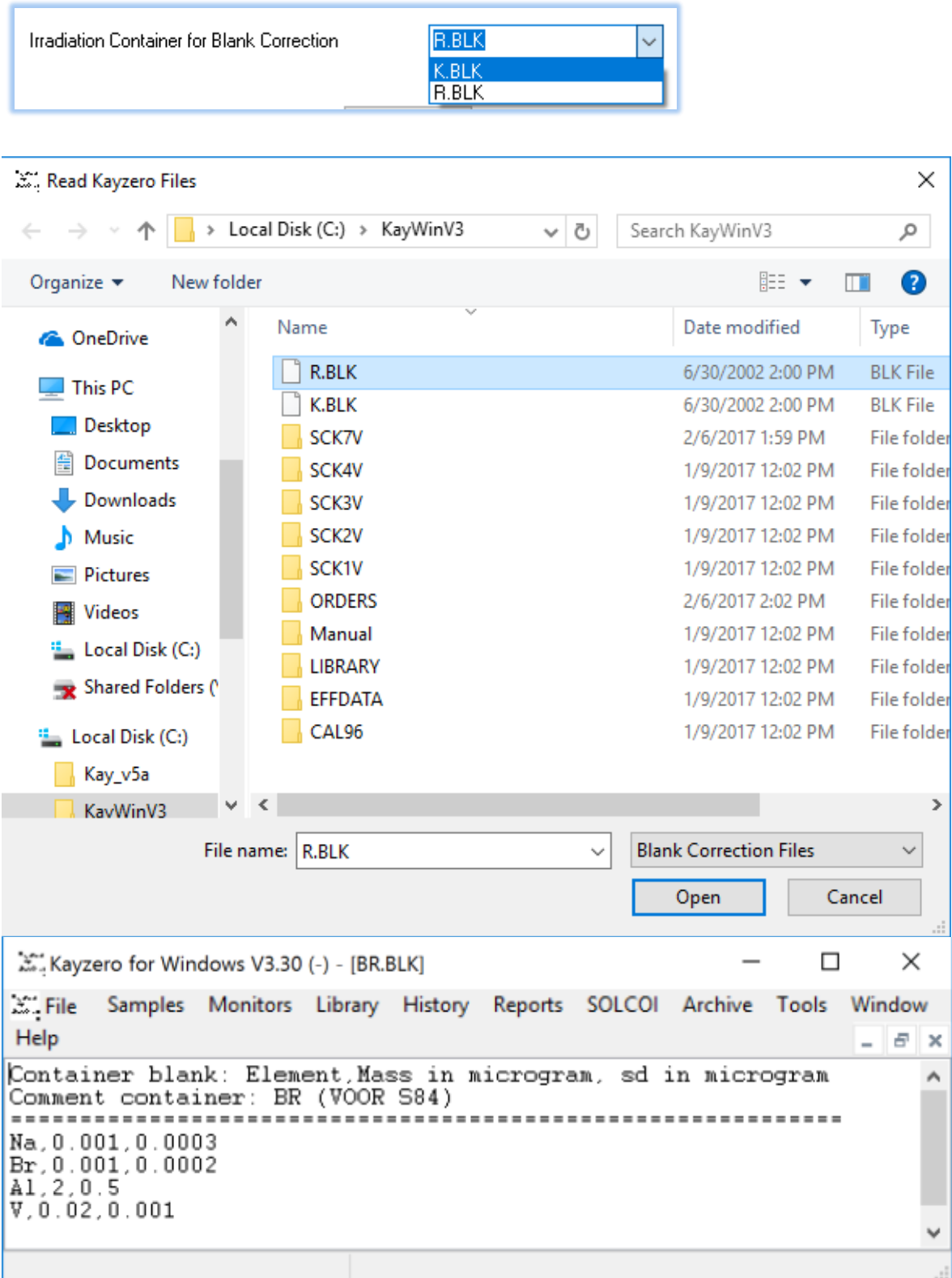


Figure 3.21: Selecting a *blank correction*-file using *File/Open* and typical *blank correction*-file format.

The blank files (.BLK) are stored in the root directory of the program. You can enter new blank values or create a blank file using the default blank files and the *File/Open/Blank Files*- option (see Figure 3.21A). Check an existing file

(e.g. 'R.BLK') to see the file format, See Figure 3.21B.

In the *Irradiation Data*-tab sheet you can enter the irradiation data (Figure 3.22). You should enter the start date and time of the irradiation. The formats are shown between brackets.

You also have to enter the codes of the reactor and channel in which the irradiation took place and the corresponding  $f$  and  $\alpha$  values. Also you have to enter the  $F_c$ -value, calculated in the previous chapter. The reactor information can be taken from the reactor-channel list as indicated previously for monitors.

**Edit Data** Data directory: SCK7V\

Order DEMO  
Sample 1B  
Measurement SCK7V:1

**Measurement Found**

Sample data Irradiation Data Measurement Data Short Input Uncertainties

Start date (dd/mm/yyyy) 30/07/1996  
Start time (hh:mm:ss.ii) 08:29:00.00  
End date (dd/mm/yyyy) 30/07/1996  
End time (hh:mm:ss.ii) 12:29:00.00  
Fluxvariation during the irradiation  
Reactor (mu) BR1  
Channel Y4  
Alpha 0.07200  
f 33.00000  
Comparator Factor 3291.10000  
Neutron Temperature (dC) / mu (-) -  
f fast (fast flux/epi-thermal flux) No Library

Click Here to Use Data

Data from file  
(kayzero.irr)  
0.072000  
33.000  
3300.0

OK Cancel

Figure 3.22: *Irradiation Data*-tab sheet.

If you select a Reactor/Channel (e.g. BR1/ xx) combination for which you never created a threshold reaction file Kayzero gives a message:

No threshold reaction correction file (D:\Kay\_v5a\BR1xx.PAR) found.

If you want to correct for threshold interferences please proceed as for the Blank-files mentioned in the previous page. Check an existing .PAR file and create your own and put it In the directory that is indicated on your screen, see Figure 3.37 for entering creating or changing this file.

The program will show hints when moving the mouse. Some on this input screen are shown in Figure 3.23

Figure 3.23 shows four screenshots of a software interface with various input fields and dropdown menus. Each screenshot has a red text box with a hint.

Hint 1: Mu for Extended Modified Hogdahl convention: 2.1 Water moderated, 3.7 Heavy water/Graphite moderated

Hint 2: Estimation of the neutron temperature (degree Celsius)

Hint 3: Uses User Threshold library in Rootdirectory : Kayzero.Trs

Hint 4: This file with extention '.REL' in the measurement data directory gives the element, isotope or energy specific Fc correction factors.

Hint 5: This file with extention '.FLX' in the measurement data directory gives the epithermal flux as function of time (hh:mm:ss).

Hint 6: In case of fluxfile, give the period at nominal flux.

Figure 3.23 Hints for entering reactor calibration options.

The hints should be self-explaining. Some are explained elsewhere.

The measurement data can be entered on the *Measurement Data*-tabsheet (Figure 3.24).

The detector that was used for the measurement, the counting vial type and the counting position have to be entered.

The detector name and vial type are chosen in *So/Coi*. A detector name has maximal 4 characters and a vial (source) maximal 3 characters. You can only use the detectors and sources defined in *So/Coi*.

**Edit Data** [Window Title]

Order: DEMO      Data directory: SCK7V\

Sample: 1B      **Measurement Found**

Measurement: SCK7V:1

Sample data   Irradiation Data   **Measurement Data**   Short Input   Uncertainties

Detector: **DSM2**      Matrix Interpolation

Geometry: **S**      Geometry data Okay!

Counting position: **2**      Volume: 10.799 ml

☐ Direct SOLCOI Calculation      Matrix Weight (gram) **4.739500**      Density: 0.44 ( 0.2- 8.0) g/ml

Matrix composition: **#C2H4**      Mat: (#SiO2) : Okay

Background spectrum PTF file: **2BG96.PTF**      Click Here to Use Data

Deadtime (%): **0.00000**      0.00

Peaktable file: ☐ Correct Hypermet      **2S7V01.PTF**      Sampo90 PTF (55 peaks)

Start date (dd/mm/yyyy): **30/07/1996**      30/07/1996

Start time (hh:mm:ss.ii): **16:24:04.00**      16:24:04.56

True Measuring Time (sec): **2473.00**      2473.00

Remarks:       SPE : 2S7V01.SPE (LFC-dual spe.)

OK   Cancel   SpectrumPlot   Peak Summation   Energy Calibration

Figure 3.24: *Measurement Data*-tabsheet.

There are two types of sources:

- point-sources (especially for calibration sources) and
- non-point sources.

For analysis purposes we use vials that are filled with the sample material. Because the solid-angle calculations were time-consuming, samples were standardized and the solid-angles and coincidence correction factors pre-

calculated.

## Matrix Interpolation

To add some flexibility in sample content composition and density the matrix interpolation technique was introduced (see Appendix 4 and 5). If a matrix interpolation dataset is found this will be marked in the info-box on the right of the detector field. You will have the possibility to enter the sample weight (for density calculation, the volume is known to the program) and (bulk) sample composition (see figure 3.25). If you enter a sample that is not covered by the matrix interpolation data set the program will warn you. The extra calculation time for calculating the correct solid angles and coincidence correction factors is negligible.

Detector	DSM2	Matrix Interpolation
Geometry	S	Geometry data Okay!
Counting position	2	Volume: 10.799 ml
<input type="checkbox"/> Direct SOLCOI Calculation	Matrix Weight (gram) <F4>=sample mass 4.739500 Matrix composition #C2H4	Density: 0.44 ( 0.2- 8.0) g/ml Mat: (#SiO2) : Okay

Detector	DSM2	Direct Solcoi Calculation
Geometry	S	
Counting position	2	Volume: 10.799 (10.799) ml
<input checked="" type="checkbox"/> Direct SOLCOI Calculation	Matrix Weight (gram) <F4>=sample mass 4.739500 Matrix composition #C2H4 Filling Height (mm) 10.400	Density: 0.44 (8.00) g/ml Mat: (#SiO2) (Vial Height: 10.40 mm)

Figure 3.25: Efficiency input data (matrix interpolation) and 'Direct Solcoi calculation'.

The volume of the container is 10.8 ml and the calculated density of the sample is 0.5 g/ml. The density is calculated using the matrix weight. The figures between brackets indicate that the matrix interpolation data set was calculated using densities from 0.2 to 8 g/ml, the matrix composition used was SiO<sub>2</sub>. The absorption data of the matrix composition of the sample (C<sub>2</sub>H<sub>4</sub>) and the calculated geometry (SiO<sub>2</sub>) are both known, so the matrix interpolation technique can be used (see Appendix 4/5).

## Direct Solcoi Calculation

If you select a non-point source you also have the option to do a 'Direct

SOLCOI Calculation' (see checkbox on the right side, only for non-point sources when the program finds the corresponding source file). If you mark this check box you do the Solcoi Calculation together with the normal calculations (*Sample/Calculate*) this will add some extra calculation time. You can enter the sample weight, composition but also the filling height in the vial (see figure 3.25B).

In the info-screen KAYZERO indicates if it has found all the SOLANG (effective solid-angle) and coincidence correction factor files for a matrix interpolation data set for the counting vial type S (5 densities) on detector DSM2.

### Summarizing efficiencies in Kayzero:

- all efficiencies are calculated using the Solid-Angle concept using SOLCOI
- **point sources** are typically pre-calculated (no sample information needed)
- **measurement vials** also called geometries need to be pre-entered
- measurement vials can contain all sorts of materials
  - o Matrix Interpolation using pre-calculated data, **fixed filling height**
  - o Direct Calculation using SOLCOI **variable filling height**, using material information from '**Known Matrix**' for special compositions.

### Gamma spectrometry

If background subtraction (optional) is performed, the relevant peak table file must be entered. This file must be located in the 'Efficiency Data'-directory.

The preset dead time has to be entered if a Dead-Time-Stabilizer (DTS) is used, otherwise the dead time as measured (with a pulser) has to be introduced.

If you enter a dead time of 0%, the dead time as measured by the multi-channel analyzer is taken from the spectrum data file.

In the case of an LFC the dead time entered should be 0%. If the dual LFC spectrum option is used (advised) then there are several options. The second uncorrected spectrum can be stored in a file with the extension '.LFC' the software will detect the Dual LFC Spectrum. If a dual spectrum is collected and stored in a single spectrum file the software can not automatically detect in all cases the uncorrected spectrum. To be sure that the dual spectrum is used, and this is important for a good calculation of errors and detection limits, the use of the Dual LFC Spectrum option should be marked in the FWHMdddd.DAT file (dddd=detector code) in the 'Efficiency Data'-directory, see Figure 3.10.

To select the correct peak table file use the picklist. KAYZERO automatically enters the relevant measurement data (start date and time, measuring time and MCA dead time) if you double-click on the info box on the right.

**Edit Data** [Minimize] [Maximize] [Close]

Order: DEMO      Data directory: SCK7V\

Sample: 1B      **Measurement Found**

Measurement: SCK7V:1

Sample data   Irradiation Data   **Measurement Data**   Short Input   Uncertainties

**Uncertainties**

Mass	<input type="text" value="0.02"/>	gram
Efficiency	<input type="text" value="1"/>	%
f	<input type="text" value="3"/>	%
alfa	<input type="text" value="0.03"/>	.
Fc	<input type="text" value="1"/>	%
Decay time	<input type="text" value="0.1"/>	s
Measurement duration	<input type="text" value="0.1"/>	s
Irradiation duration	<input type="text" value="0.1"/>	s

Figure 3.26 : Uncertainties of the entered data.

Kayzero can calculate 'Extended Uncertainties'. For this extra information is needed on the uncertainty in entered parameters, see Figure 3.26. The uncertainties of the nuclear data is taken from the latest k0-Scientific Committee database.

**This option is new and comments and improvements are welcome!!**

Now all the sample data for the measurement of the first sample have been entered. You can proceed with more measurements of this sample or enter the data for another sample. If you press the *Cancel Button* the data you have just entered will not be saved in the data file.

**Edit Data**

Order: DEMO      Data directory: SCK7V\

Sample: 1B      **Measurement Found**

Measurement: SCK7V:1

Sample data   Irradiation Data   Measurement Data   **Short Input**   Uncertainties

Detector: **DSM2**      Efficiency Data

Counting position (1-10): 2      Matrix Interpolation

Deadtime (%): 0.00000      Peak Table

Peaktable file: 2S7V01.PTF      0.00

Remark: If the Peak Table Name is changed, then the measurement time, the start date and time and the dead time will be updated automatically.

Comparator Factor: 3291.10000      Sampo90 PTF (55 peaks)

30/07/1996

16:24:04.56

2473.00

SPE : 2S7V01.SPE (LFC-dual spe.)

OK   Cancel   SpectrumPlot   Peak Summation   Energy Calibration

Figure 3.26: Short input in case of a second measurement of the same sample.

In case a sample is measurement twice or more the sample and irradiation information do not have to be entered again but the only the spectrum name is needed in principle, see Figure. 3.26.

### 3.4.3 Calculating the Element Concentrations

If the sample data have been correctly entered, the calculations of the element concentrations can be performed, see Figure 3.28 (*Samples/Calculate*). In this option the order identification, the sample identification and the measurement identification must be specified. If you enter an asterisk (\*) the system performs a batch-wise calculation of the element concentrations of all samples for the orders that have been entered.

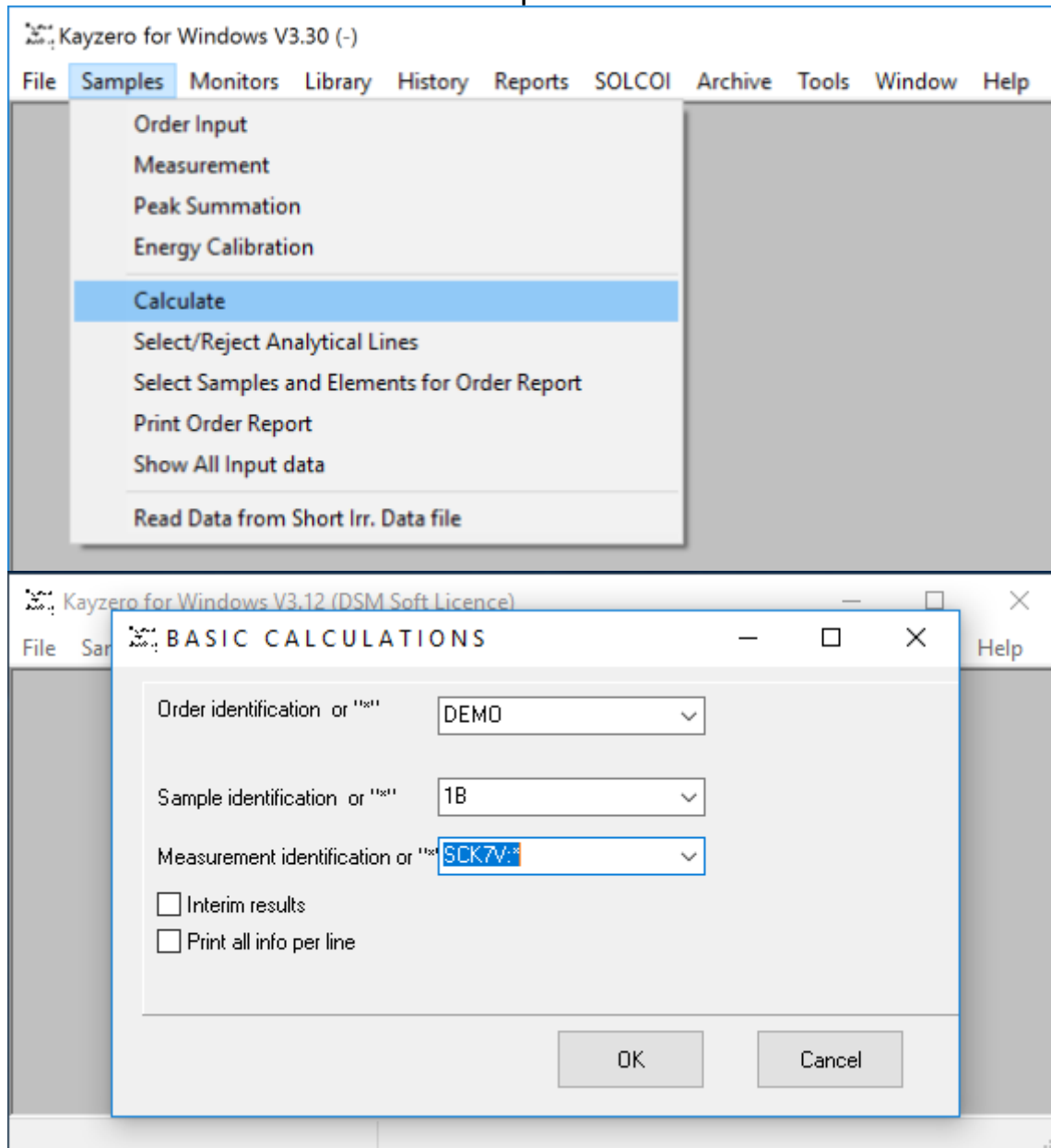
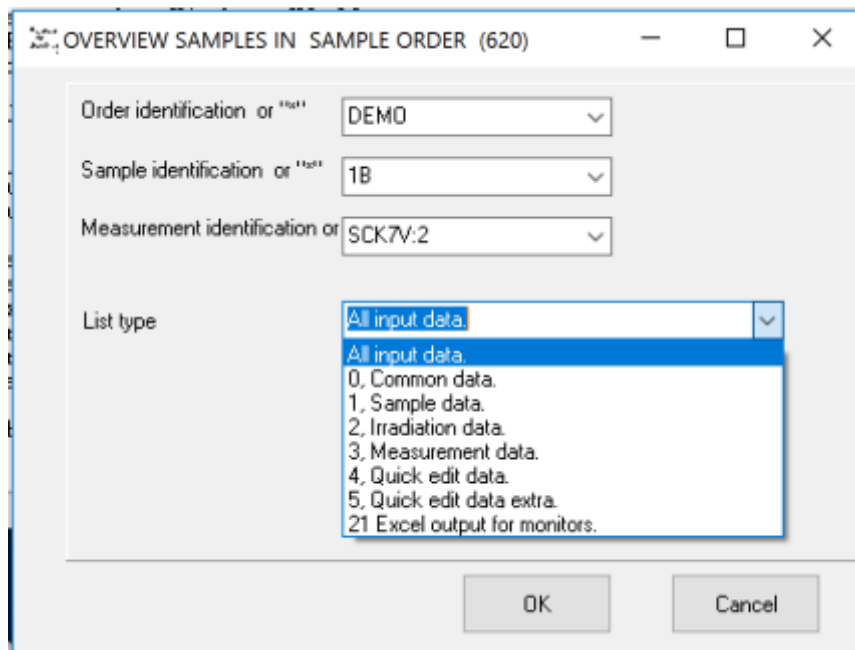


Figure 3.28 : *Calculate*-option in *Samples* menu and Selection of the measurements

While KAYZERO is calculating the sample measurement is displayed in the bar at the bottom of the program window.

The calculations have to be repeated whenever input data, spectra data, library or efficiency data have been changed. Calculation parameters can be edited, see Appendix 6. If you use the wildcards '\*'/'\*/'SCK7V\*' for the order, sample and measurement, respectively, only samples irradiated under code SCK7V will be calculated. Before starting the calculations the program will sort the measurements in order to minimize calculation times.



Kayzero for Windows V3.30 (-) - [OVERVIEW SAMPLES IN SAMPLE ORDER (620) DEMO]

File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

---

Kayzero for Windows V3.30 (OPTION : 620)

Order : DEMO from : Vervecken, DSM Research, 61421  
 Profilenr.: Eu-152 cost : fl. 0  
 Comment : Data for demonstration purposes  
 Elements : ALL

List type : 0 (sorted on: id) DEMO|\*|\*

Sample#/Meas#	Label	Description	Library
1B/SCK7V:1	SCK7V\6		k0-2015 : 03/
1B/SCK7V:2	SCK7V\6		k0-2015 : 03/
1B/SCK7V:3	SCK7V\6	imaginary sample	k0-2015 : 03/

---

Order : DEMO List type : 1 (sorted on: id) DEMO|\*|\*

Sample#/meas#	geom.	w.sample [g]	w. matrix [g]	matrix	height [mm]	moisture [%]	blank container
1B/SCK7V:1	S	4.73950	4.739500	#C2H4	-		R
1B/SCK7V:2	S	4.73950	4.739500	#C2H4	-		R
1B/SCK7V:3	S	4.73950	4.739500	#C2H4	-		R

---

Order : DEMO List type : 2 (sorted on: id) DEMO|\*|\*

Sample#/meas#	Irr.date	time t	irr.[s]	reactor/channel	f	alpha	Fc
1B/SCK7V:1	30/07/96 08:29:00		4h	BR1/Y4	33.0	0.0720	3291.1
1B/SCK7V:2	30/07/96 08:29:00		4h	BR1/Y4	33.0	0.0720	3291.1

Figure 3.29: List of all input data.

Before the calculations start you should check the input using *Reports/Overview/Samples* (List type: All Input Data) in order to avoid calculation errors (see Fig. 3.29). Interim results will give more information on the calculations and will show some values like efficiency, coincidence correction factors, burn-up correction factors etc. (see Fig. 3.30).

```

Kayzero for Windows V3.30 (-) - [BASIC CALCULATIONS DEMO:1B :Editable]
File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

K0 calculation 01/08/2017 11:48:35
Program version : V3.30 DSM
Z:\Downloads\KayWinV330\KayWinV33.exe 01/08/2017 08:00:00
DATA : Z:\Downloads\KAYWINV330\ORDERS\DEMO.ETA : 1B SCK7V:1
DATAFILES USED:
Z:\Downloads\KayWinV330\Kayzero.BUR 31/05/2016 16:00:02
Z:\Downloads\KayWinV330\Kayzero.DAT 01/08/2017 11:07:08
Z:\Downloads\KAYWINV330\LIBRARY\k0-2015.LB1 03/07/2017 23:06:06
Z:\Downloads\KAYWINV330\LIBRARY\k0-2015.LB2 03/07/2017 23:06:06
Z:\Downloads\KAYWINV330\EFFDATA\FWHMDSM2.DAT 15/06/2007 13:00:08
Z:\Downloads\KAYWINV330\EFFDATA\EFFDSM2.DAT 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\PTTDSM2.DAT 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\DSM2.SOL 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\1SDSM2.SOL 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\1SDSM2.COI 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\2SDSM2.SOL 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\2SDSM2.COI 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\3SDSM2.SOL 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\3SDSM2.COI 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\4SDSM2.SOL 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\4SDSM2.COI 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\5SDSM2.SOL 30/06/2002 14:00:00
Z:\Downloads\KAYWINV330\EFFDATA\5SDSM2.COI 30/06/2002 14:00:00
SPE : Z:\Downloads\KAYWINV330\SCK7V\2S7V01.SPE 01/08/2017 11:08:06
PTF : Z:\Downloads\KAYWINV330\SCK7V\2S7V01.PTF 30/06/2002 14:00:00
BGD SPE : Z:\Downloads\KAYWINV330\EFFDATA\2BG96.SPE 01/08/2017 11:08:04
BGD PTF : Z:\Downloads\KAYWINV330\EFFDATA\2BG96.PTF 26/02/2003 16:09:00

SAMPLE
4.739500 g
IRRADIATION PARAMETERS:
BRI/Y4 f = 33.0000 alpha = 0.0720 Fc = 3291.10
30/07/1996 08:29:00 ti= 14400 s
MEASUREMENT DATA:
2S7V01.PTF DSM2 S pos= 2 BGD : 2BG96.PTF
30/07/1996 16:24:04 tm= 2473 s DTS= 0.0 % td= 14104 s
Matrix = #C2H4 4.740 g

Isotope Library_energy[keV] Energy[keV] EnergyCorrection[keV] Area[cts] Error[%] CoiFactor
Na-24 1368.6 1368.4 0.0 9.57719E+3 1.13 0.9777 3.61081E+2 4.10096E-3 4.68000E-2 2.8
Na-24 1732.0 1731.8 0.0 4.87149E+2 8.82 1.0000 1.79578E+1 3.42373E-3 4.62000E-2 1.7
Na-24 2243.0 2242.7 0.0 5.69550E+2 5.92 1.0000 2.09953E+1 2.80993E-3 4.62000E-2 2.4
Na-24 2754.0 2754.0 0.0 5.01401E+2 1.42 0.9752 1.00555E+1 3.40330E-3 4.62000E-2 2.4

```

Figure 3.30: Interim Results.

A burn-up correction procedure is built in; the correction factors are given when the 'interim' results are printed. Burn-up correction for monitors and samples is performed using the data in 'KAYZERO.BUR' for the isotopes Eu-154, Ta-182, Au-198, Dy-165, Pm-149 and Rh-105. If this file is not present, burn-up correction is not performed.

### 3.4.4 Printing the Element Concentrations

When the calculations are finished you can print the calculated concentrations using *Reports/Results*, see Figure 3.31. You can change the output formats etc. using *Tools/Options* (see Appendix 6).

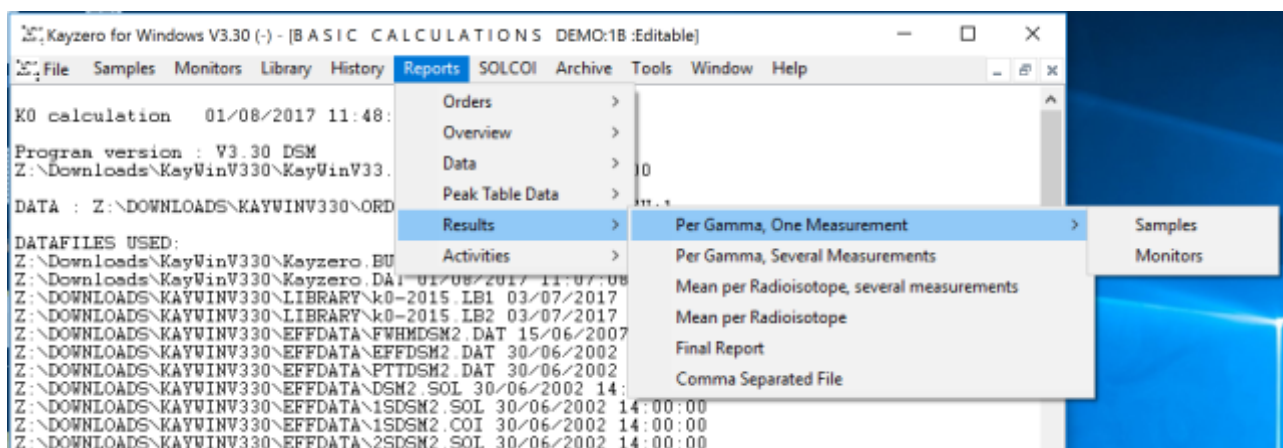


Figure 3.31 : Reports/Results menu

## NOTE

The concentration can be expressed in ng/g or mg/kg, and the format of the concentration figure can be scientific notation or a fixed notation with a number of decimal places, see Appendix 6: PRINT PARAMETERS or *Tools/Options*.

### Results/ Per gamma, One Measurement

Comparator factors and concentrations per gamma can be printed per measurement using this option. For this purpose an intermediate menu will appear enabling you to select *Samples* or *Monitors* (see Figure 3.32).

After selecting *Samples* you can enter the order identification, sample identification and measurement (or wildcards).

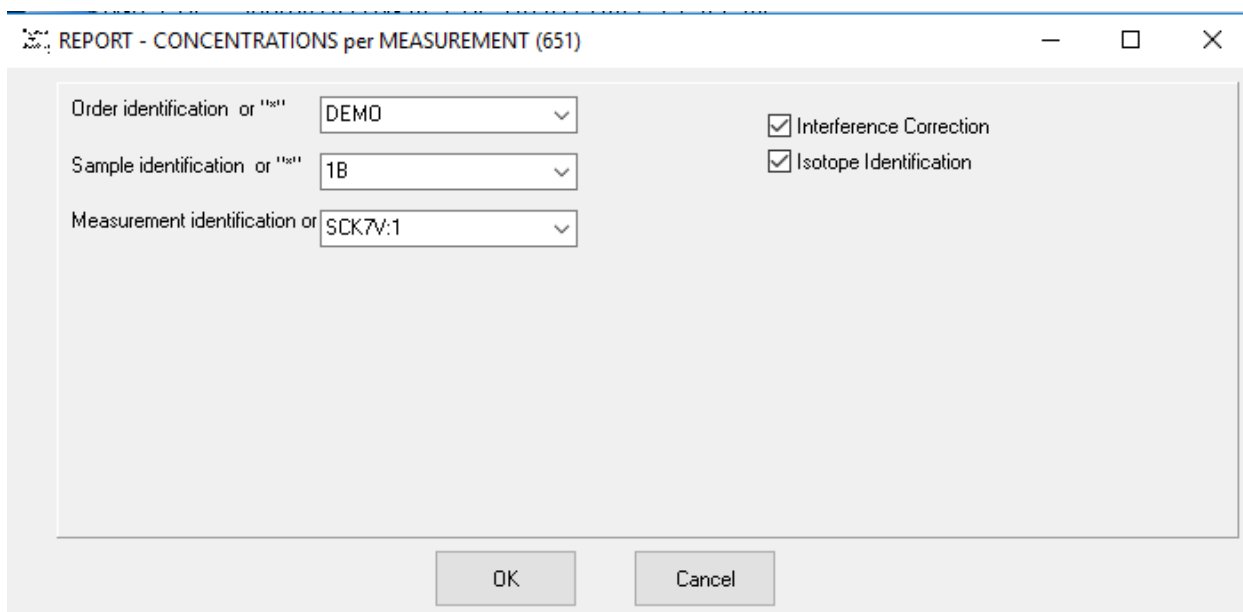


Figure 3.32 : Input for 'Reports/Results/Per Gamma, One Measurement/Samples'

The output of this option will be a list of measured gamma lines which the

system has been able to match with the KAYZERO Library (see Figure 3.33).

Kayzero for Windows V3.30 (-) - [REPORT - CONCENTRATIONS per MEASUREMENT (651) DEMO-1B]

File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

---

Kayzero for Windows V3.30  
 REPORT: CONCENTRATIONS per MEASUREMENT  
 Order id.: DEMO Sample id.: 1B Meas. id.: SCK7V:1

Element	Nuclide	Energy [keV]	Conc. [mg/kg]	SD [%]	Ext.UnC [%]	LD k0code [mg/kg]	Interfer.nucl.
Na	Na-24	1368.6	2.84564E-1	1.13	0.00	5.60834E-3	1
Na	Na-24	2754.0	2.58236E-1	1.43	0.00	2.17916E-3	1
Cl	Cl-38	1642.7	5.28289E+1	1.91	0.00	2.36815E+0	1
Cl	Cl-38	2167.4	5.02556E+1	1.62	0.00	1.08677E+0	1
Ar	Ar-41	1293.6	8.27435E-1	0.75	0.00	6.73417E-3	2 In-116m
	without interference corr.		8.42783E-1				
Mn	Mn-56	846.8	1.84584E-1	0.26	0.00	3.17052E-4	1
Mn	Mn-56	1810.7	1.79523E-1	0.71	0.00	1.27631E-3	1
Mn	Mn-56	2113.1	1.81256E-1	1.02	0.00	1.78482E-3	1 In-116m
Cu	Cu-64	511.0	8.64796E-2	2.18	0.00	6.08465E-3	2
Zn	Zn-65	1115.5	8.56849E+1	4.57	0.00	1.30891E+1	1
Zn	Zn-69m	438.6	8.58651E+1	0.41	0.00	5.18527E-1	1
Ga	Ga-72	479.2	2.69091E+0	40.39	0.00	4.35371E+0	3
Ga	Ga-72	834.0	1.38102E-2	8.10	0.00	4.14645E-3	1 Cu-64S
Ga	Ga-72	2201.7	2.00412E-2	13.93	0.00	9.74229E-3	1
Br	Br-80	616.6	1.50676E-1	11.46	0.00	6.72678E-2	1
Br	Br-82	554.3	1.42045E-1	3.33	0.00	1.64714E-2	1
Br	Br-82	619.1	1.47964E-1	5.93	0.00	3.29380E-2	1 Ba-131
Br	Br-82	698.4	1.48157E-1	7.15	0.00	3.93584E-2	1
Br	Br-82	776.5	1.41890E-1	2.77	0.00	1.21673E-2	1
Br	Br-82	827.8	1.63819E-1	7.28	0.00	4.36756E-2	1
Br	Br-82	1044.0	1.54960E-1	7.80	0.00	4.44258E-2	1
Br	Br-82	1317.5	1.62928E-1	7.02	0.00	4.00658E-2	1
Br	Br-82	1474.9	1.34344E-1	15.17	0.00	7.78869E-2	1
In	In-116m	416.9	5.88023E-4	33.82	0.00	7.95162E-4	1
In	In-116m	1097.3	6.50822E-4	17.62	0.00	4.45291E-4	1
In	In-116m	1293.5	3.57376E-2	0.67	0.00	2.85560E-4	1 Ar-41
	without interference corr.		3.57379E-2				
Sb	Sb-122	564.2	6.01884E-2	5.52	0.00	1.23081E-2	1
Ba	Ba-131	123.8	5.18049E+1	24.48	0.00	5.07035E+1	1
Ba	Ba-131	216.1	5.71389E+1	32.49	0.00	7.44162E+1	1
Ba	Ba-131	496.3	6.14210E+1	14.47	0.00	3.47952E+1	1
Ba	Ba-139	165.9	6.87920E+1	0.25	0.00	2.44477E-1	1
Ba	Ba-139	1420.5	6.30984E+1	13.35	0.00	3.18220E+1	3

Gamma lines (P:3;N:I;dE0.70; k0-2015 : 03/07/2017)

Measured	Explained	Unexplained	Unknown	False peaks
55	45	0	4	6
	81.8 %	0.0 %	7.3 %	10.9 %
	(explained by identified radionuclides)	(peak in library but unexplained)	(gamma lines not in KAYZERO-library)	(peak area is smaller than LD)

The unknown gamma-lines are (energy in keV): 2523 2657 2960 3370

Figure 3.33 : Output for 'Reports/Results/Per Gamma, One Measurement/Samples'

These gammas are called the explained gammas. This means a sensible concentration could be assigned to this line (<100% and >=LD). In the header, between brackets '(P:3;N:I;dE0.70; k0-2015 : 3/07/2017)', some codes are given. Using these codes you can trace how the output was computed and printed. P:3; means that only gammas were printed that had k0 code equal to or lower than 3. N; means that the nuclide identification algorithm was used. I; shows that interference correction was ON. The energy window was 0.7 keV (dE0.70;) and the library used was k0-2015, last

updated on 3/07/2017. It is possible to turn off nuclide identification and spectral interference correction.

Below the list of explained gamma lines the following extra information is given:

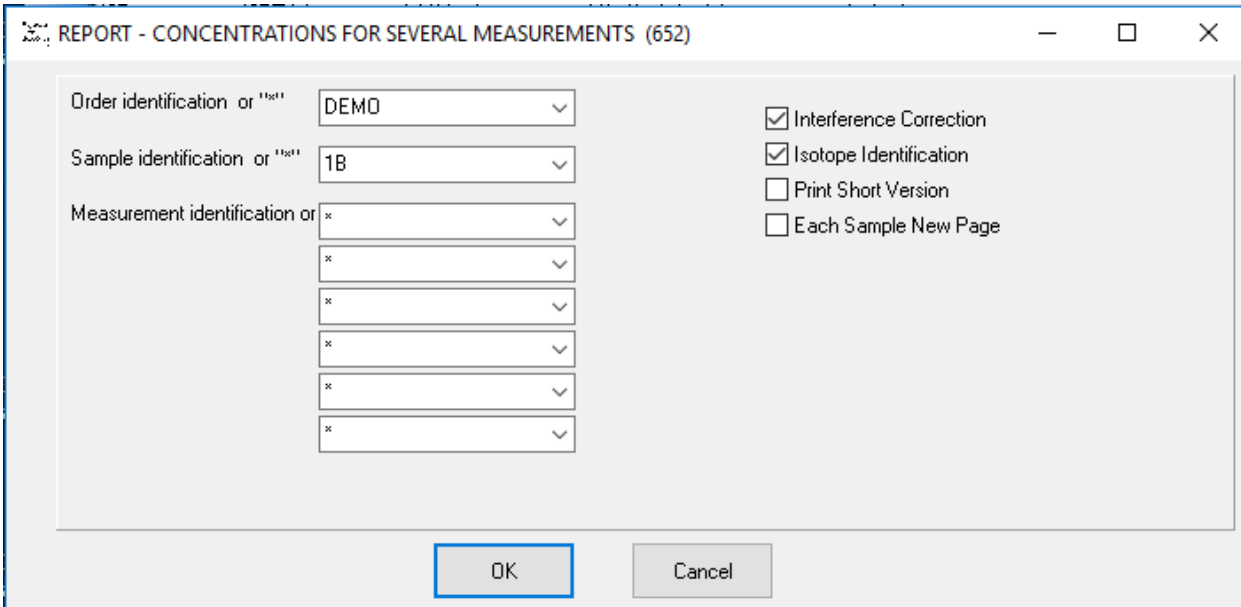
- the number of measured gamma rays,
- the number of unexplained gammas (found in the library, but not assigned to a radionuclide present in the sample),
- the number of unknown gammas (not found in the library),
- the number of false gammas (the peak area is smaller than the detection limit0,
- all unexplained gamma energies and
- all unknown measured gamma lines.

If you turn off isotope identification, all gammas will appear in the list of explained gammas.

### Reports: Results, Per gamma for several measurements

This option will give a list of all gamma lines found in several measurements. Per row the gamma line energy, the related element and radionuclide, and the found concentrations are given for up to six measurements.

The order identification, sample identification and up to 6 measurement identifications can be specified. Again, isotope identification and interference correction can be turned off, see figure 3.34.



REPORT - CONCENTRATIONS FOR SEVERAL MEASUREMENTS (652)

Order identification or "test" DEMO

Sample identification or "test" 1B

Measurement identification or "test" x

x

x

x

x

x

x

☒ Interference Correction

☒ Isotope Identification

☐ Print Short Version

☐ Each Sample New Page

OK Cancel

Figure 3.34 : Input for *Reports/Results/Per gamma, Several measurements*

An example of the output of this reporting option is not given in this manual but can be printed using the program. The gamma-lines that are not used for

the mean concentration calculation are marked with an '\*'. The mean is calculated using lines with the lowest k0 code. For instance, if there are gamma lines with a k0 code equal to one then only the lines with code one are used. If the lines have only codes higher than one then the mean is calculated using the gamma lines having a k0 code equal to two, and so on.

### **Report: Results, Mean per Radioisotope, Several Measurements**

The output as given using *Reports/Results/Per gamma, Several measurements* can be further reduced by reporting mean concentrations per radioisotope for all measurements. The input needed to obtain this report is identical with the previous report.

### **Report: Results, Mean per Radioisotope**

The mean concentrations of this are averaged per radioisotope over all selected measurements.

### **Report: Results, Final report**

This report will give the final result, with concentrations averaged over all gammas, all radioisotopes and all measurements. Whether or not elements are actually present in the sample are checked using the Element Identification algorithm (*Tools/Options/Special Parameters*).

In this option the nuclide identification and spectral interference correction are always turned ON.

### 3.5 Select/reject analytical gamma lines

This option '*Samples/Select/Reject analytical Lines*' is in practice the best way to handle the data. In combination with the options '*Select samples and Elements for Order Reports*' and '*Print Order Report*' the majority of analyses can be evaluated without extra handling.

The old way to handle the data using the previously mentioned options can still be used, but fission and reaction interfering correction, blank correction epi-thermal and thermal neutron self absorption correction and rejection of gamma lines can only be done using this option. Up to 6 irradiations/measurements per sample can be edited simultaneously, see figure 3.35.

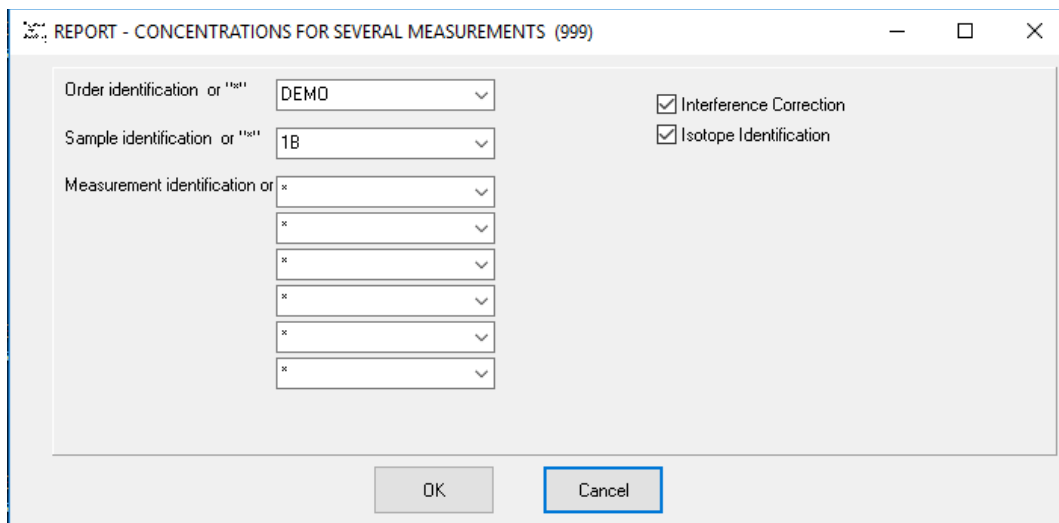


Figure 3.35: Input for '*Samples/Select/Reject analytical Lines*'.

After selecting the sample and the measurements the program will read the concentration data of all relevant measurements and combines them in a screen per element. In figure 3.36 the lines for Na-24 are given. In the header the sample and measurements are given. Below that one finds the element, nuclide, energy and the concentration found for each measurement. If a concentration is selected the space bar can be used to de-select or re-select the line. The averaged concentration for the measurement and the element average will change accordingly.

In this option all more sample related corrections are combined:

- blank correction,
- fission correction,
- interfering reaction correction,
- epi-thermal and thermal neutron self absorption correction,
- thermal self absorption correction.

In the case of Na-24 there is a possible threshold reaction interference. If the

sample matrix is Al then a serious interference will occur. In the case shown (Fig. 3.36) were no information on the Al content is available, the program provides a maximum interference of 1.4E+4 ng/g for an Al-content of 1.0E+9 ng/g (100m%). **By entering Al in the 'Known Matrix' this correction can be done.**

mg/kg	Energy	SCK7V:1	SCK7V:2	SCK7V:3
Na Na-24	1368.6 (1)	2.84564E-1	2.82455E-1	<2.1455E-1
-> without interfer. corr.				
	2754.0 (1)	2.58236E-1	2.70510E-1	-3.64767E-4
Threshold Reaction Interferences				
Al < 100%	Interference :	<1.40000E+4	<1.40000E+4	<1.40000E+4
Epi Thermal Self Absorption Correction				
Gepi : Na/Na-24		1.00000E+0	1.00000E+0	1.00000E+0
Nuclide Average				
Concentration :	2.77792E-1	2.73186E-1	2.77987E-1	-
Expected StnDev % :	1.75796E-1	8.86504E-1	1.79357E-1	-
Observed StnDev % :	1.31303E+0	4.77505E+0	2.08067E+0	-
Extended Uncer. % :	3.15806E+0	3.16190E+0	3.15790E+0	-
LD :	4.44306E-4	2.17916E-3	4.44306E-4	1.34919E-1
Blank Subtraction				
Container :		R	R	R
Blank correction :		-2.40992E-4	-2.40992E-4	-2.40992E-4
Element Average				
Concentration :	2.77792E-1	2.73186E-1	2.77987E-1	-
Expected StnDev % :	1.75796E-1	8.86504E-1	1.79357E-1	-
Observed StnDev % :	1.31303E+0	4.77505E+0	2.08067E+0	-
Extended Uncer. % :	3.15806E+0	3.16190E+0	3.15790E+0	-
LD element :	4.44306E-4	2.17916E-3	4.44306E-4	1.34919E-1

Figure 3.36: Input screen for selecting analytical gamma lines and performing corrections.

The threshold interference correction factors (see below for the definition) should be available in a file with the name "reactor"& "channel".par. This file is of course specific for each reactor channel. Per line the Nuclide, Element, interference correction factor and uncertainty is given (see Fig. 3.37B). The program will know from the irradiation data given which file to take. The file is stored in the start-up directory of the program (see Fig. 3.37A).

Fission interference will also be presented this way. The data is automatically generated.

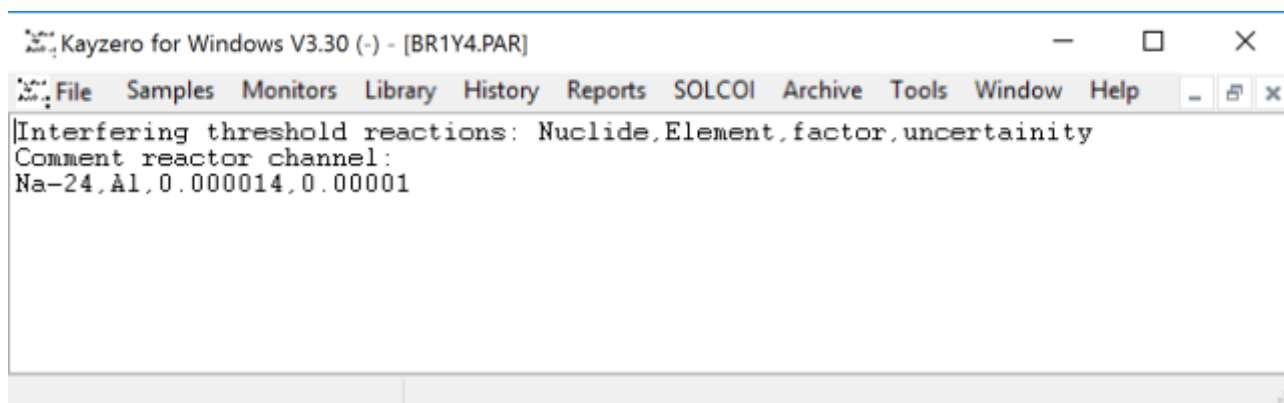
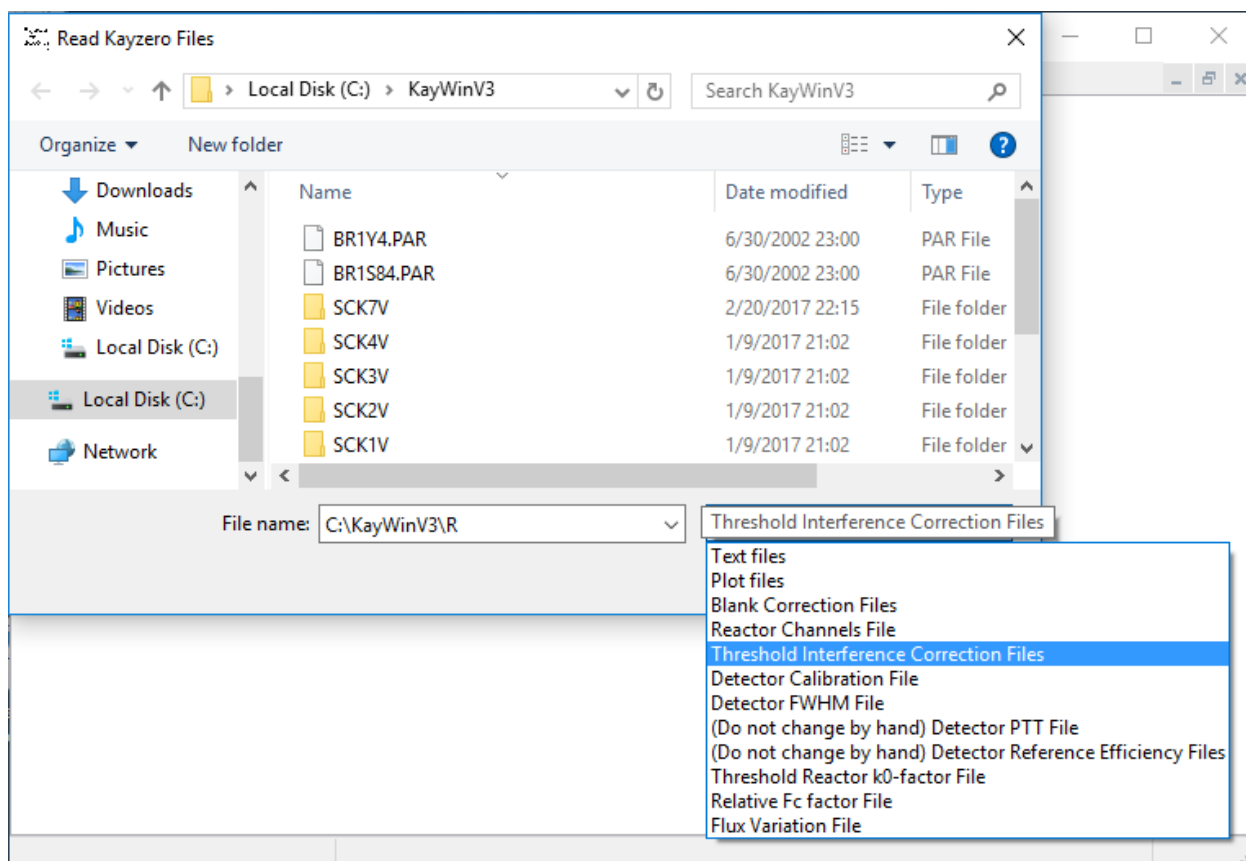


Figure 3.37: A: Selecting the Threshold Interference Correction File;  
B: Contents of a typical data file for threshold interference correction.

This interference correction factor is the apparent concentration of element 'x' based on the given nuclide divided by the concentration of the interfering element. In the case of the example of figure 3.37: if the matrix is 100% Al, the apparent Na concentration (based on Na-24) is 14 mg/kg (0.000014\*100%) with an uncertainty of 1 mg/kg. In this case the correction is significant even if only 0.1% of Al is present.

The gamma lines that can be selected are only the recommended lines (k0 code =1). In principle the other lines can be used as well. If there is an isotope with only tentative k0's (the element will be marked with an ‘\*’) and this element will also be shown.

In case the sample is irradiated and measured in the same sample vial then a blank correction might be needed. The irradiation container can be entered in the *Irradiation Data*- tab sheet. See Figure 3.23 for an example. In this case the sample was irradiated and measured in the same “Spronck”-vial (R). The polyethylene of this vial contains Cr. The blank mass of Cr in the vial was determined and entered in a file named “R.BLK”. These files are stored in the efficiency directory and can be edited using Kayzero (See Figure 3.37A). In figure 3.21 an example of the blank file is given.

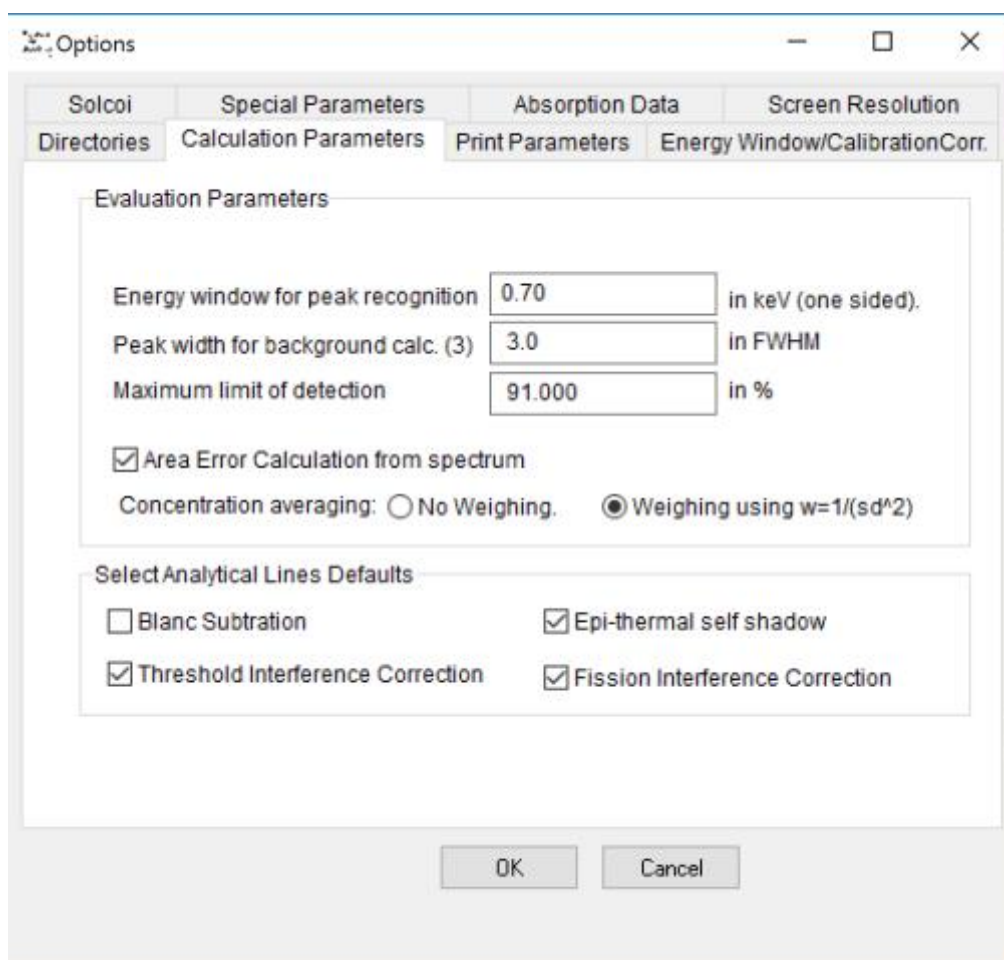


Figure 3.38: Default settings for corrections in the *Tools/Options* menu.

Order : DEMO Sample : 1B (P:3;N:E;dE0.70; k0-2015 : 03/07/2017)

OKCancelPrintPreviousNext

Br	Mo	In	Sb	Ba	La	Sm	Eu	W	End Check		
Na !	Cl !	Ar !	K !	Ca !	Cr !	Mn	Fe	Cu	Zn	Ga	As
mg/kg	Energy	SCK7V:1	SCK7V:2	SCK7V:3							
Cr Cr-51	320.1 (1)	<2.9317E+0	5.23137E-1	5.27379E-1							
Epi Thermal Self Absorption Correction											
Gepi :	Cr/Cr-51	-	1.00000E+0	1.00000E+0							
Nuclide Average											
Concentration :	5.26978E-1	-	5.23142E-1	5.27384E-1							
Expected StnDev % :	1.88159E+0	-	6.12914E+0	1.97705E+0							
Observed StnDev % :	2.36741E-1	-	-	-							
Extended Uncer. % :	3.11505E+0	-	3.11505E+0	3.11505E+0							
LD :	3.48266E-2	2.93173E+0	1.26249E-1	3.48266E-2							
Blank Subtraction											
Container :		-	R	R							
Blank correction :		-	2.10992E-1	-2.10992E-1							
Element Average											
Concentration :	5.12593E-1	-	3.12149E-1	5.27384E-1							
Expected StnDev % :	1.96296E+0	-	1.22964E+1	1.97705E+0							
Observed StnDev % :	1.06223E+1	-	-	-							
Extended Uncer. % :	3.11505E+0	-	3.11505E+0	3.11505E+0							
LD element :	3.48266E-2	2.93173E+0	1.26249E-1	3.48266E-2							

Expected Standard deviation larger than 10%

Figure 3.39: Input screen demonstrating blank subtraction.

The blank value is considerable and should be taken into account. In figure 3.39 the Cr –concentration for measurement SCK7V:3 was corrected and the other concentration was not corrected. This was done by selecting the blank mass (use the cursor keys or mouse) and selecting/deselecting the blank subtraction using the spacebar. A deselected is shown using the strikethrough font. One can clearly see the effect. Due to blank subtracting on the gamma lines the expected standard deviation on the remaining element concentration is larger than 10%, this is marked the blue colored font. Due to the subtraction for only one measurement the observed standard deviation is larger than three times the expected standard deviation, this is marked with a red font.

The program will also perform fission correction, this is based on a paper by F. De Corte (2000). The data is stored in a file named ("Kayzero.Fis"), the contents should not be changed. If the program detects a U-concentration one will have the possibility to perform a correction by selecting the correction value and pressing the spacebar.

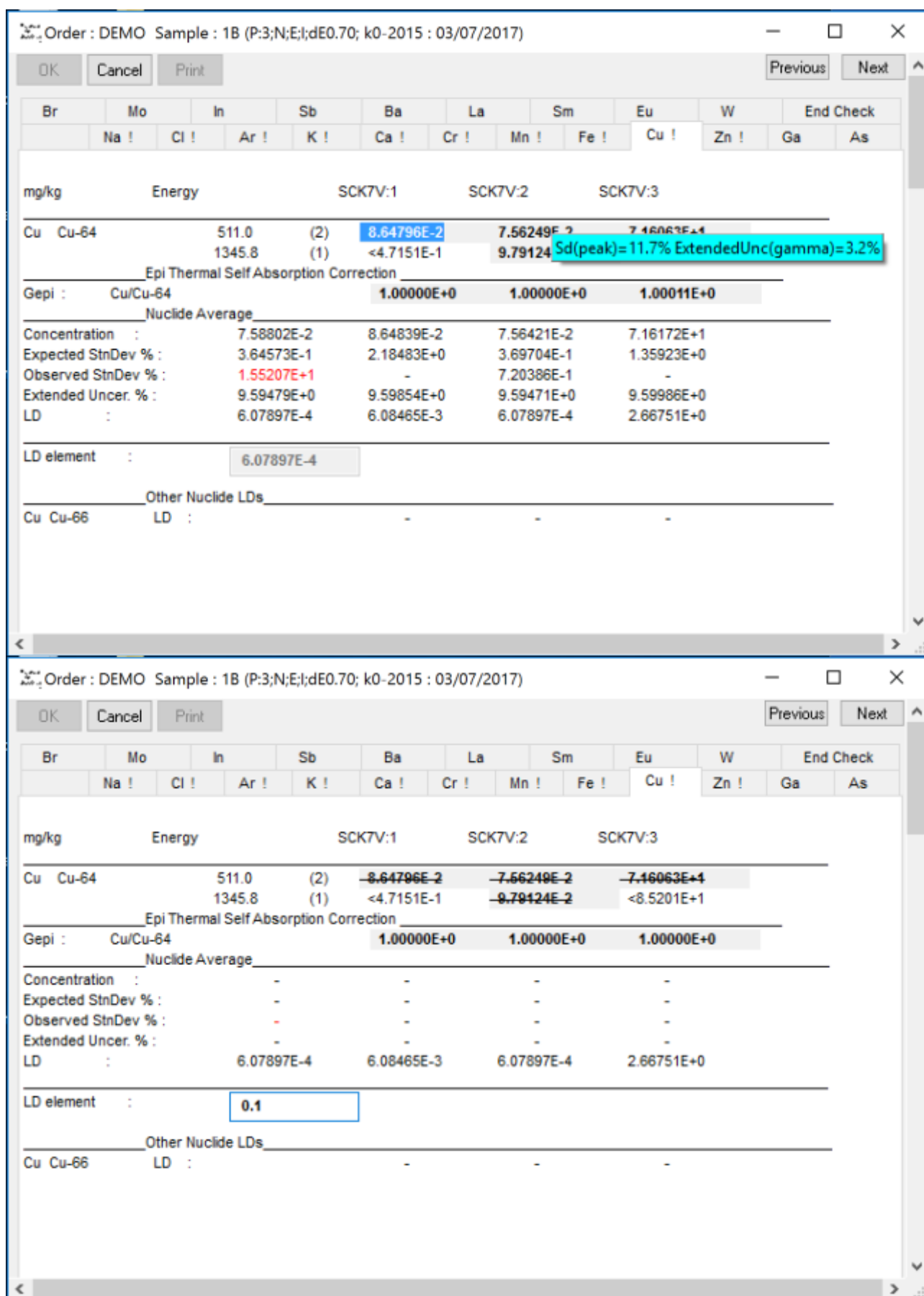


Figure 3.40: A:Before and B:after rejecting all results.

If one decides that no confident concentration value can be given based on

the found gamma-lines/concentrations it is possible to deselect all lines and give a detection limit. This is done by deselecting all lines using the spacebar and then entering a detection limit by hand. In this case 0.1 is chosen as the detection limit for copper based on Cu-64 (See Figure 3.40). There is a minimum concentration found at the 511 keV peak, thus the maximum concentration is lower than 0.1. If the detection limit entered is higher than 100%, then the element will not be printed in the output anymore.

The detection limits of other nuclides are always given in a short list. If there are problems identifying nuclides/elements this is very useful to check your results.

For fast selection of lines it is possible to use <CNTRL><Spacebar> to select and deselect all lines and to use <CNTRL><Tab> to go to the next element.

Order : DEMO Sample : 1B (P;3;N;E;l;dE0.70; k0-2015 : 03/07/2017)

OKCancelPrint

PreviousNext

	Na !	Cl !	Ar !	K !	Ca !	Cr !	Mn !	Fe !	Cu !	Zn !	Ga	As
Br !	Mo	In	Sb	Ba	La	Sm	Eu	W	End Check			

mg/kg	Energy	SCK7V:1	SCK7V:2	SCK7V:3
Br Br-80	616.6 (1)	1.50678E-1	<3.6001E-2	-
	665.8 (1)	<3.2817E-1	<1.9657E-1	-
Epi Thermal Self Absorption Correction				
Gepi : Br/Br-80		1.00000E+0	-	-
Nuclide Average				
Concentration :	1.50678E-1	1.50678E-1	-	-
Expected StnDev % :	1.14593E+1	1.14593E+1	-	-
Observed StnDev % :	-	-	-	-
Extended Uncer. % :	5.44214E+0	5.44214E+0	-	-
LD :	3.60018E-2	6.72678E-2	3.60018E-2	-

Br Br-82	554.3 (1)	1.42045E-1	1.12795E-1	1.09445E-1
	619.1 (1)	1.47964E-1	1.07249E-1	3.75871E-2
-> without interfer. corr.			1.11211E-1	1.99742E-1
	698.4 (1)	1.48157E-1	9.98580E-2	9.03074E-2
	776.5 (1)	1.41890E-1	1.13216E-1	1.10711E-1
	827.8 (1)	1.63819E-1	1.22413E-1	1.18178E-1
	1044.0 (1)	1.54960E-1	1.15268E-1	1.17445E-1
	1317.5 (1)	1.62928E-1	1.31507E-1	1.22478E-1
	1474.9 (1)	1.34344E-1	1.29344E-1	1.29926E-1
Epi Thermal Self Absorption Correction				
Gepi : Br/Br-82		1.00000E+0	1.00000E+0	1.00000E+0
Nuclide Average				
Concentration :	1.13726E-1	1.45293E-1	1.13801E-1	1.03425E-1
Expected StnDev % :	1.99093E-1	1.74587E+0	2.02992E-1	1.23675E+0
Observed StnDev % :	8.39214E-1	1.75920E+0	2.34677E+0	9.10205E+0
Extended Uncer. % :	4.92417E+0	4.92044E+0	4.92426E+0	4.92229E+0
LD :	7.51937E-4	1.21673E-2	7.51937E-4	6.50197E-3
Blank Subtraction				
Container :		R	R	R
Blank correction :		-2.10992E-4	-2.10992E-4	-2.10992E-4
Element Average				
Concentration :	1.13733E-1	1.45407E-1	1.13801E-1	1.03425E-1
Expected StnDev % :	1.99064E-1	1.72597E+0	2.02992E-1	1.23675E+0
Observed StnDev % :	6.44119E-1	6.43066E-1	8.86998E-1	3.44025E+0
Extended Uncer. % :	4.92425E+0	4.93147E+0	4.92426E+0	4.92229E+0
LD element :	7.51937E-4	1.21673E-2	7.51937E-4	6.50197E-3

Figure 3.40: Demonstration multiple nuclides for Br-80.

In Figure 3.40 one of the energies is printed in a green font.

This means that the interference correction for this line can be checked. By clicking at this figure with your mouse a special form will appear as shown in Figure 3.41. The standard interference correction is more or less qualitative and meant for only nuclide identification. This option will allow a much better correction and allows the user to check first the quality of the average concentration of the interfering elements.

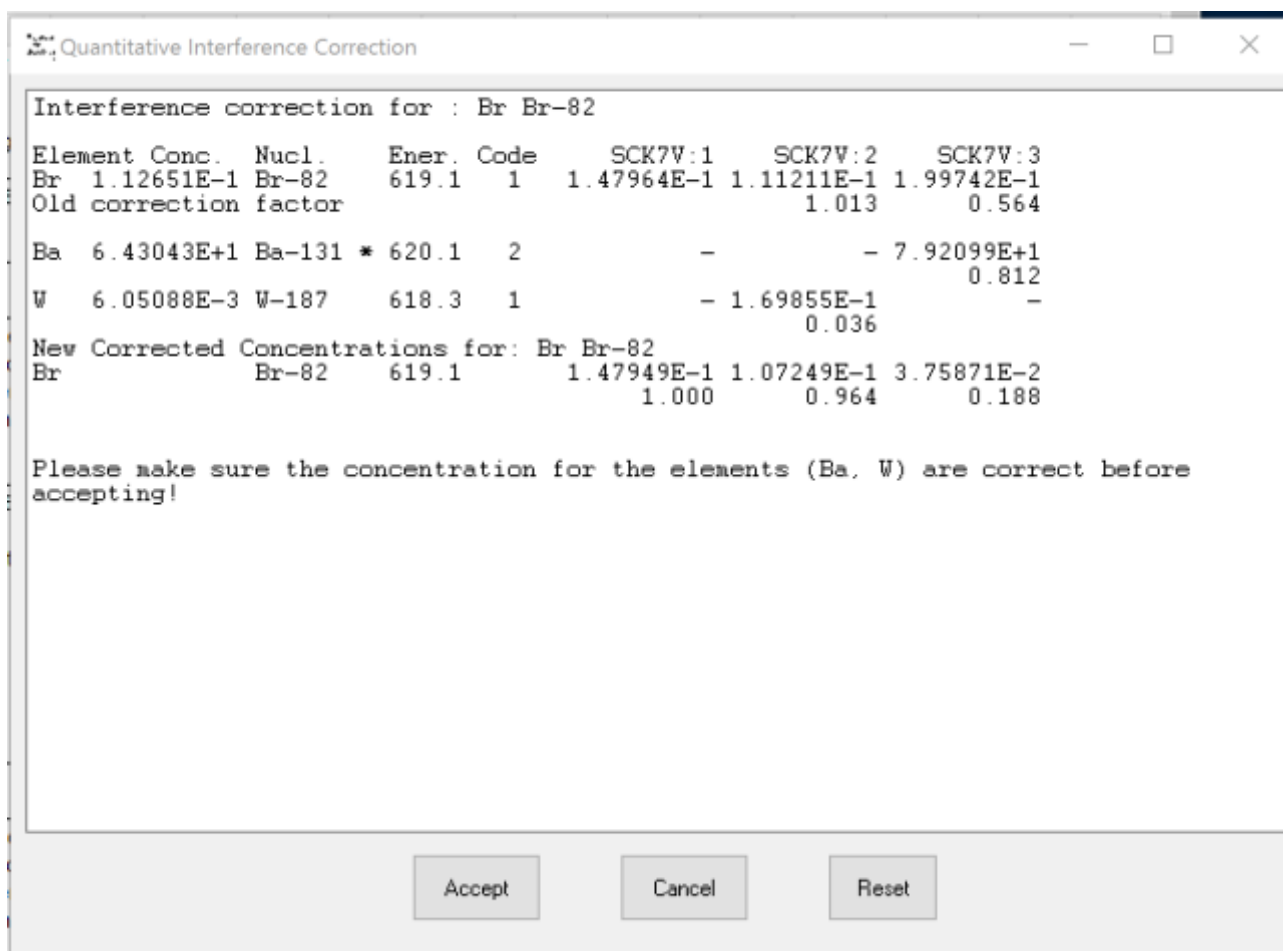


Figure 3.41: Quantitative interference correction.

You can accept the result or reset the old values. To make the best possible result you should check the results of all involved nuclides.

After the last element has been checked the screen given in Figure 3.42 will appear. Here the total spectrum count rate is given for each measurement as well as the total spectrum count rate for the background.

Order : DEMO Sample : 1B (P:3;N:E;l;dE0.70; k0-2015 : 03/07/2017)

OK Cancel Print Previous Next

Na !	Cl	Ar	K	Ca	Cr !	Mn !	Fe !	Cu !	Zn	Ga	As
Br !	Mo	In	Sb	Ba	La	Sm	Eu !	W	End Check		

Gth Correction ☒ Use only Measured Concentrations  
☐ Add non-measured con. Equi. to 100%  
☐ Add non-meas. elements abs. conc.

Order : DEMO Sample : 1B

	SCK7V:1	SCK7V:2	SCK7V:3	
Detector :	DSM2	DSM2	DSM2	
Position :	2	1	1	
Decay Time :	3h55m04s	19h45m24s	8d03h32m24s	
Measurement time :	41m13s	8h41m22s	15h18m49s	
Total cps SPECTRUM:	8.23994E+2	3.75750E+2	3.36408E+1	
Total cps BGD :	1.30227E+0	1.30227E+0	1.30227E+0	
Vial Radius mm :	0.000	0.000	0.000	
Vial Height mm :	0.000	0.000	0.000	
Neutron Temp C :	40.0	40.0	40.0	
Kth :	0.820	0.820	0.820	
Mass g :	4.739500	4.739500	4.739500	
Gth correction according to the original Kayzero-method.				
				Total Sum %.
Gth Initial :	1.000	1.000	1.000	0.033
Gth last run :	1.000	1.000	1.000	0.033

Figure 3.42: Final screen of option *Samples/Select/Reject analytical Lines*

If the difference between the spectrum and the background count rate is large then a new measurement after further decay might be sensible. A longer measurement time might perhaps a way to continue if decay will not help. You can also check the detector and the measurement position to see if you can improve the analysis results.

You always need to pass this last tab-sheet before ending this session.

The edited data can be stored and used later for the combined report. It is also possible to make a printout (or a .txt file) of the selections performed.

In this screen it is possible to do a correction for thermal neutron self absorption. All concentrations will be corrected. It is useful to do this a few times to see if  $G_{th}$  changes.

## 3.6 Order Report

### 3.6.1 Select Samples and Elements for Order Report

The final result of a neutron activation analysis is of course the report for the customer. In many cases the customer is only interested in a few elements. *Select Samples and Elements for Order Report* will give the operator the opportunity to select elements, samples and measurements (see Figure 3.43). The selection can be printed in the end result and an additional general systematical uncertainty can be added to the statistical measurement uncertainty (see *Tools/Options/Print Parameters*), or the extended uncertainty can be added to the normal standard deviation on the peak area's. The uncertainty can be given as a multiple of the combined standard deviation, this is also provided in the *Print Parameters*. The used uncertainty combination is printed per sample in the header of the table.

If needed the result can be prepared for an Excel file as well by choosing 'Excel' output. The elements can be selected using a drop down list. You can add more than one element or choose 'All'. If you do not want concentrations to be rounded off you can un-check the 'Round-off' checkbox.

REPORT - PREPARE RESULTS (900)

Order identification or "": DEMO

Sample identification or "": 1B

Measurement identification or "":

Interference Correction ☒

Isotope Identification ☒

Add Extended Uncertainty ☐

Add 3.5 % systematical error ☒

Excel Output ☐

Round off based on SD ☒

Elements of Interest: ALL

Ag, Al, ALL, Ar, As, Au, n-

OK Cancel

Figure 3.43: Input form for selection of samples and elements for an order output.

You can add several samples to the same report, even with different elements. Just don't rewrite the result file but append to it.

### 3.6.2 Print Order Report

The results of *Select Samples and Elements for Order Report* are written to a file. This file is read in the *Print Order Report* and converted to the desired output (Figure 3.44).

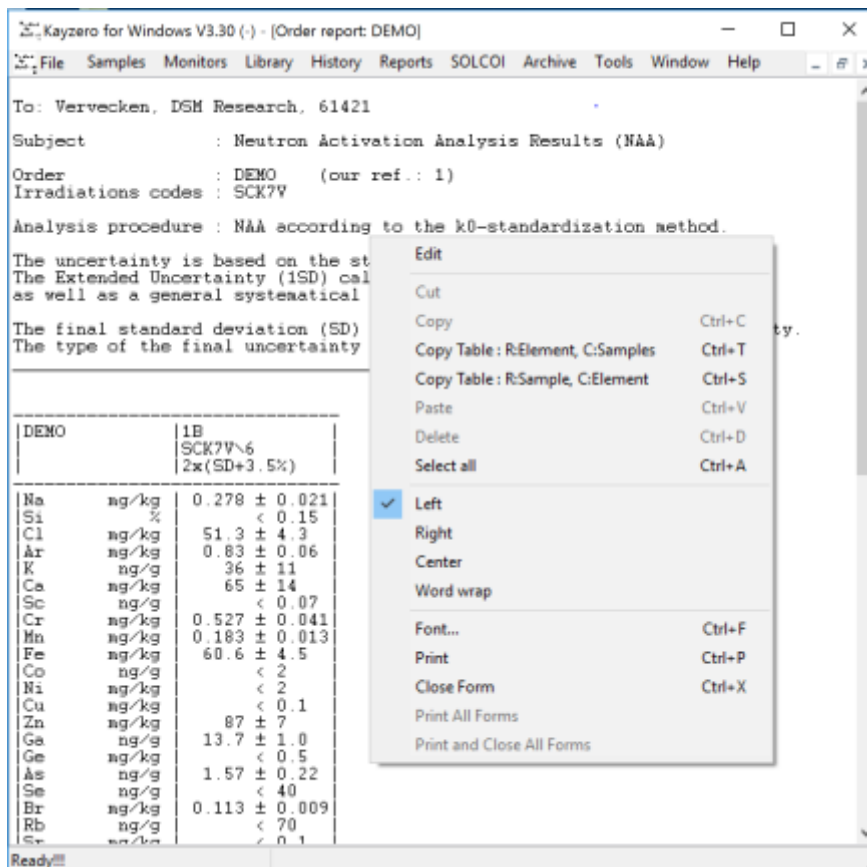


Figure 3.44: Report output

You can see in Figure 3.44 the report output after selecting the elements. The element and sample selection can be done multiple times.

By using the right mouse button a pop-up menu will appear. In this menu you see the options *Copy Table: R:Elements, C:Samples* and *Copy Table: R:Samples, C:Elements*. This will copy only the table from the report to the clipboard. This makes it possible to use the data in for instance a Word-document or an Excel sheet as a table.

The uncertainty is in this case equal to 2 times the combined standard deviation in the peak area's and a systematical 3.5% extended standard deviation, shown here as 2x(SD+3.5%).

## 4 SolCoi

---

SOLCOI is a part of Kayzero for Windows (originally: it was a separate software program) that helps the neutron activation analyst and the gamma-ray spectrometrists in determining efficiencies and coincidence correction factors. SOLCOI calculates effective solid angles and coincidence correction factors. The efficiency computation method involves extensive calculations resulting in effective solid angles which are stored in data files (**see Appendix 1**).

The SOLCOI user is expected to be familiar with the efficiency computation technique of the INW<sup>4</sup>. For a practical guideline in applying the efficiency computation method see the 'VADEMECUM FOR K<sub>0</sub> USERS' by De Corte and Simonits<sup>3</sup>. A short explanation is given in **Chapter 4.1**.

All steps needed for the calculation of effective solid angles and coincidence correction factors are given in **Chapter 4.2**.

In **Chapter 4.3** the fine-tuning of two detector dimensions is demonstrated and in **Chapter 4.4** the curve fitting of the reference detection efficiency  $\varepsilon_p$  and the peak-to-total (PTT) ratios is presented.

For extra help users can consult the **Appendix**, where detailed information is given on all algorithms and data file formats.

The detector calibration and fine tuning can be best done on measured data. However if a detector calibration has been done for k<sub>0</sub>-IAEA, this data can be used also. K<sub>0</sub>-IAEA has an output function for efficiencies on all positions including PPT-data.

### 4.1 General procedure

Before effective solid angles and coincidence correction factors can be calculated the reference detection efficiency  $\varepsilon_p$  and the peak-to-total (PTT) ratios have to be measured accurately. The reference efficiency has to be measured with calibrated point sources at the reference position at a minimum distance of 15 cm from the detector in order to avoid true coincidence effects. The PTT ratios have to be measured for every position using point sources. It is essential that all the efficiency calibration sources have the same 'calibration' geometry. If this is not the case, the efficiencies measured using the different geometries have to be converted using calculated effective solid angles.

This program can fit the detector calibration measurement data ( $\log \varepsilon_p$  or  $\log \text{PTT}$  vs  $\log E_\gamma$ ) and store the fit data in standard files for the fitted reference efficiency and the PTT ratios. Before starting the calculations the dead-layer and the vacuum gap of the detector have to be determined using measurements and the fine-tuning procedure.

If ready one can compute the detection efficiency for nearly any source using the reference efficiency curve and the effective solid angles for the calibration source geometry at the reference position and the effective solid angles for the source (see Vade Mecum and **Appendix 1**). The SolCoi-options for each of the above mentioned steps are shown in Figure 4.1.

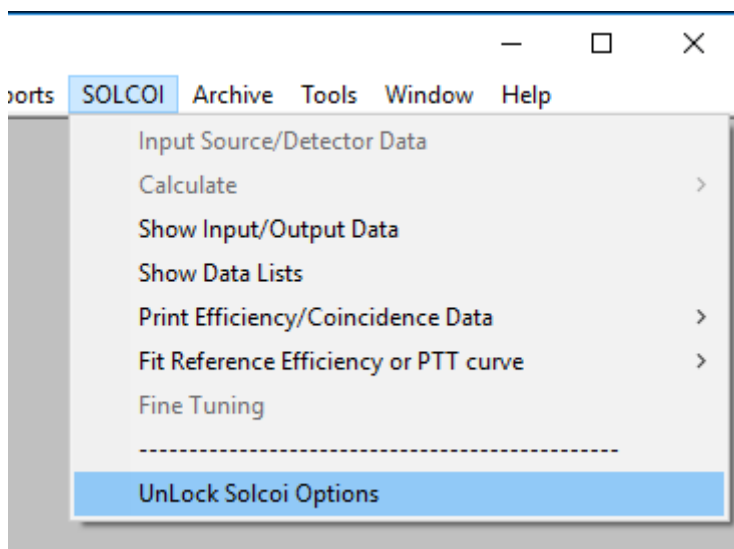
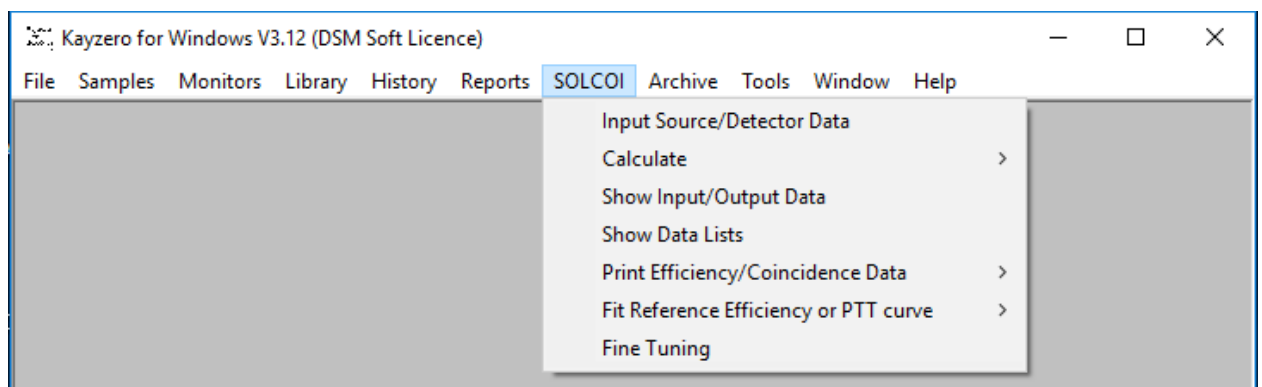


Figure 4.1: Main Menu of SOLCOI

For file locations and for file formats see **Appendix 2**. The data directory of SOLCOI can be checked/changed with *Tools/Options/SolCoi*. You can make this directory the same as the efficiency data directory of KAYZERO if you like or select a 'temporary' directory.

## 4.2 Effective Solid Angle and Coincidence Correction Factor Calculation

### 4.2.1 Data input and calculations

Data input and calculation options are grouped in the *Input Source/Detector Data*; this is the first option of the SOLCOI-menu (see Figure 4.1).

After entering the detector/source-holder data and the reference source geometry data you can calculate the reference effective solid angle data using *Calculate/Reference Effective Solid Angles* (see Figure 4.2). This is done only once after calibrating your detector.

For computing all the other effective solid angles you have to use *Calculate/Effective Solid Angles and Coincidence Factors*.

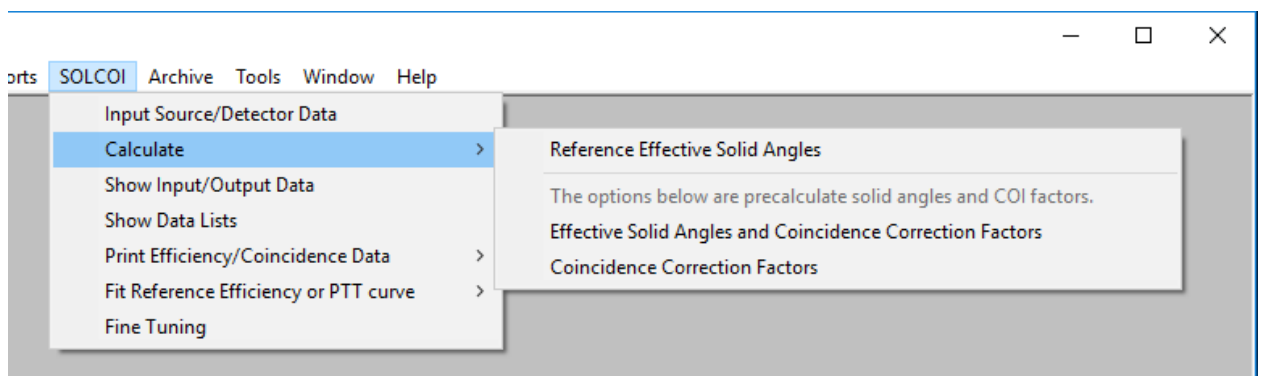


Figure 4.2: The *Calculate* menu.

The coincidence correction factors are calculated using the full-energy peak efficiency  $\epsilon_p$ ; the total efficiency ( $=\epsilon_p / \text{PTT}$ ) is calculated according to [3].

If you would like to calculate only the coincidence correction factors you can use : *Calculate/Coincidence Factors*.

## 4.2.2 Data input for a detector/source-holder combination.

Using *Input Source/Detector Data* (see Figure 4.2) you can enter all relevant detector and source-holder data. You can select detector data using the drop-down list or by typing the name of the detector (max. 4 characters).

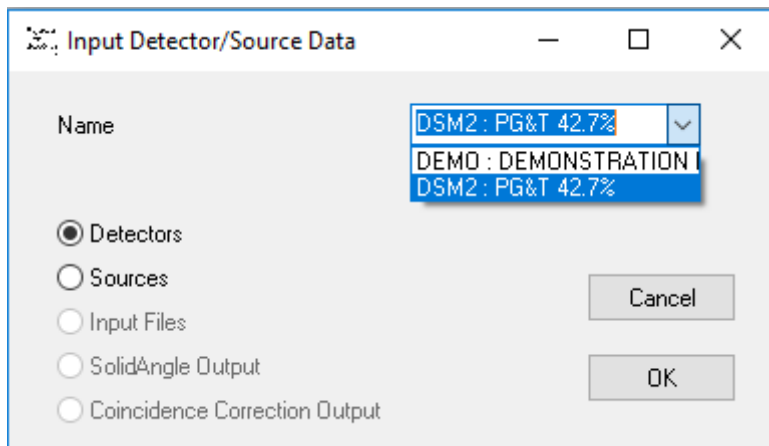


Figure 4.3: Detector data input, choosing a detector.

When you choose a new detector name the program will show a screen like the one in Figure 4.4. If you press <No> all detector data will be reset and if you press <Yes> the data of the detector last used (since the start of the program) will be used. Pressing <Cancel> will cancel this option.

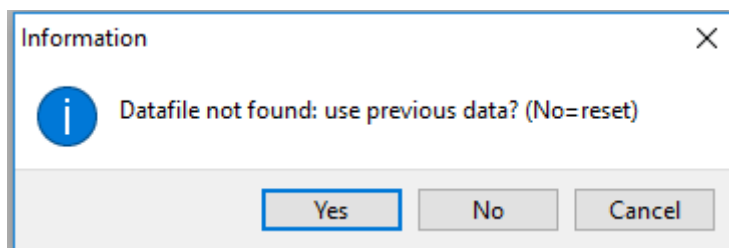


Figure 4.4: Input after selecting a new unknown detector.

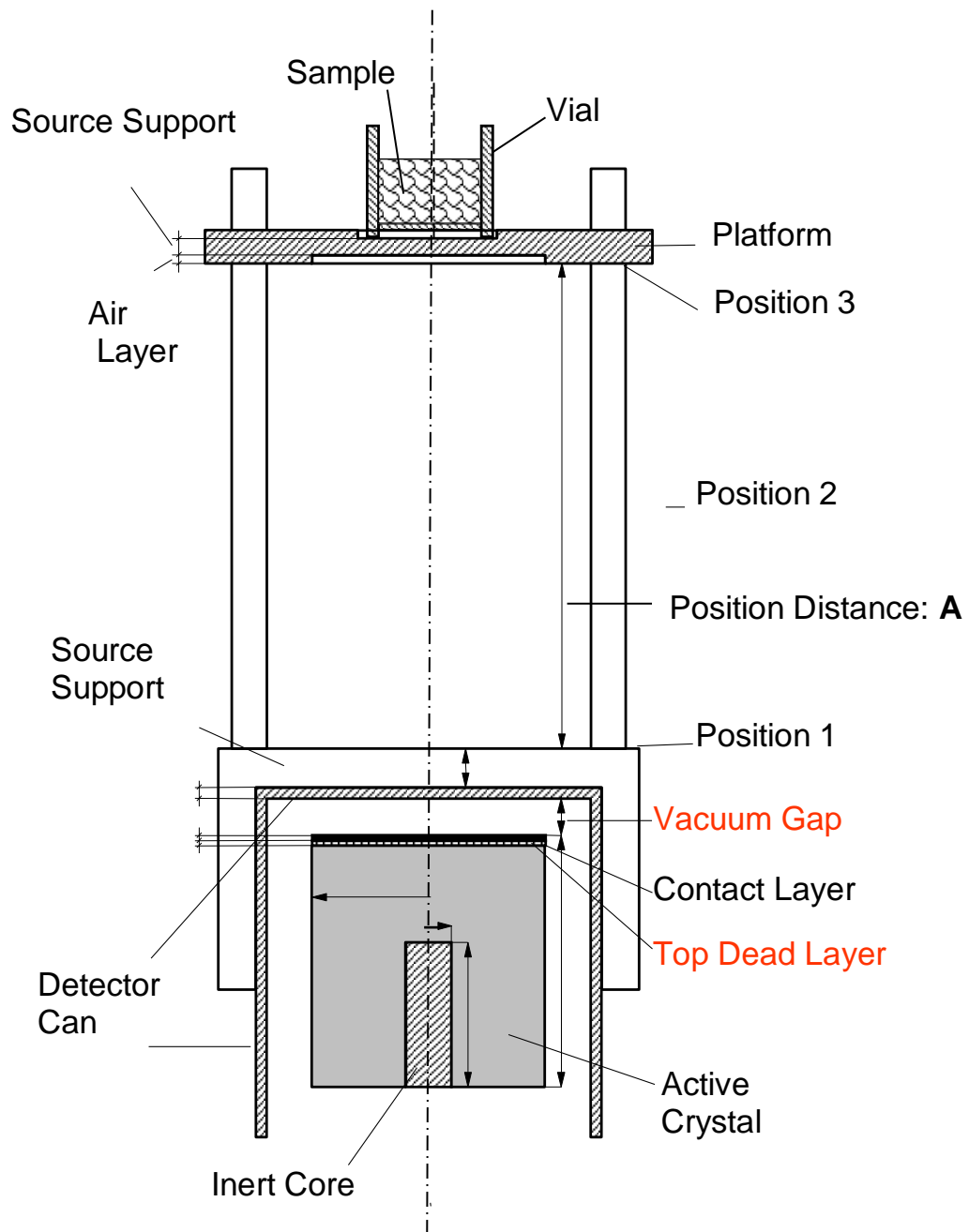


Figure 4.5: Detector Dimensions and explanation of descriptions used in fig. 4.6.

You can then enter the detector geometry, detector material and the source

holder geometry (see figure 4.5) using the screen given in figures 4.6. All units are SI units.

**Solang/Coincidence Detector Parameters**

**Detector Code** DSM2

**Comment** PG&T 42.7%

**User** Robbert van Sluijs

**Last Modification** 29/09/1996 17:40:27

**Detector Crystal**

Detector type 3: hyper pure with coaxial cavity

Crystal Material Germanium Density (kg/m3) 5350.000

Crystal Radius (mm) 30.810 Height (mm) 62.060

Cavity/Core Radius (mm) 4.000 Height (mm) 40.000

Vacuum Gap (mm) 5.280 Pulse Shaping (us) 4.000

**Absorbers**

	Material	Density (kg/m3)	Thickness (mm)
Contact Layer	-	0.000	0.000
Source Support	PMMA	1180.000	2.300
Detector Can	Copper	8920.000	0.500
Top Dead Layer	Germanium	5350.000	0.760
Other	Delrin	1410.000	1.000

**Platform**

Number of positions 5 Reference Position 0

Positions	1	2	3	4	5	6	7	8	9	10
Distance A (mm)	0.000	51.500	142.250	259.000	349.000	0.000	0.000	0.000	0.000	0.000

Air layer between can and top of the source platform (mm) 2.800

**Energies**

Number of Energies 17

Energy (keV)	40.0	50.0	60.0	80.0	100.0	150.0	200.0	300.0	400.0	500.0
	600.0	800.0	1000.0	1500.0	2000.0	3000.0	3500.0			

OK Cancel Print

Figure 4.6: Detector and source holder dimensions. Cavity/Inert core: the single open-ended detector (type 1) has a core and the hyper-pure detector (type 3) has a cavity with a contact layer.

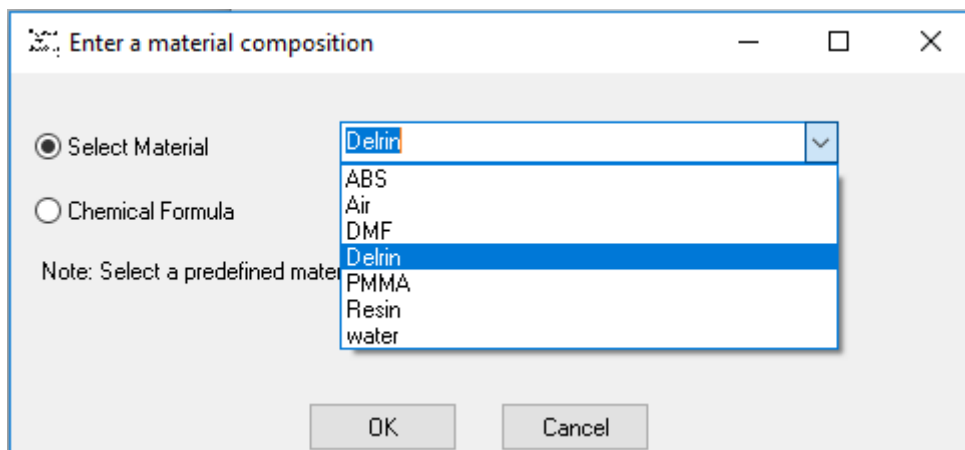


Figure 4.7: Material Composition Input, entering a predefined material, showing the drop-down list.

You have to enter the composition and density of the materials of which the detector, dead layer, detector can, etc. are made for the determination of the linear absorption coefficients. Mass-absorption coefficients of all elements are stored in data files<sup>5</sup>. If you click on the material input field a form like figure 4.7 will appear, if you click a drop down list with material will appear. Materials can be composed using *Tools/Material Compositions/Edit Materials*.

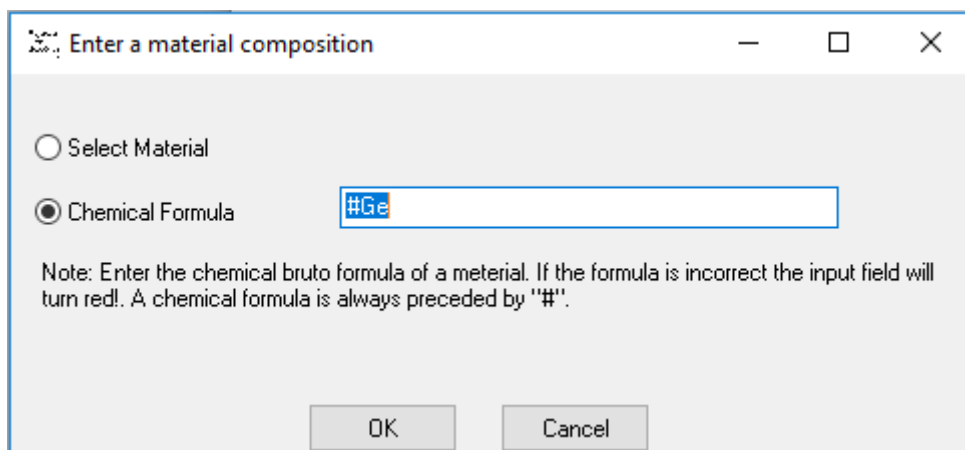


Figure 4.8: Entering a material composition by giving the brutto chemical formulae.

You can also enter a material composition by giving the brutto chemical formulae, see figure 4.8. The crystal radius and height is including the dead-layer thickness (see Figure 4.5).

The detector parameters include also the source holder parameters and the energy range. On the previous input screen (Figure 4.6) you can enter the number of energies and the number of source holder positions. Typical values for these parameters are 17 and 5 respectively. The maximum number of energies is 20 and the maximum number of positions is 10.

Distance A is the distance between the top of the source holder foot to the bottom of the platform (see figure 4.5).

Position 1 is considered to be the lowest position (closest to the detector). In this position the platform is on top of the source holder (see figure 4.5 and 4.6), and distance A is then zero. Any distance through air in this lowest position has to be entered also, see the next row.

You can print the input for your own archive by pressing <PRINT> and leave the screen by pressing <OK>.

This means that the date and time of modification will be changed and hence that all previously calculated effective solid angle data (solang data) are invalid and have to be recalculated when they are put in the list for batch-wise calculation *Solcoi/Calculate*. When a chosen detector and source combination are not modified the previously calculated SOLANG and COINCALC data will not be recalculated.

The detector and source parameters are independent of each other, so all source data files can be combined with all detector data files.

### 4.2.3 Data input for a source geometry

The combination of source geometry parameters has been chosen in such a manner that every source can be 'placed' on practically every detector/source-holder combination. Detector and source geometry parameters are completely independent.

Sample

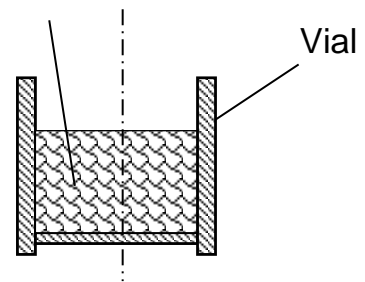


Figure 4.9: source.

The source dimensions are shown in Figure 4.9. A source name may contain up to 3 characters. The input of a source name is identical with the input of a detector name (see Figures 4.4). After selecting the source name the source parameters can be checked or edited. In Figure 4.10 the vial parameters, the source material and density are given.

A screenshot of a software dialog box titled 'Solang/Coincidence Source Parameters'. The dialog box contains several input fields and a checkbox. The fields are: 'Comment' (Au-Al-wire in spronckvial), 'User' (DV), 'Last Modification' (21/06/1993 13:45:46), 'Vial Wall Material' (#C2H4), 'Density (kg/m3)' (900.000), 'Inner Radius (mm)' (2.500), 'Inner Height (mm)' (1.000), 'Side Thickness (mm)' (0.750), 'Bottom Thickness (mm)' (0.650), 'Distance (mm)' (0.000), 'Matrix Interpolation' (unchecked), 'Vial Volume (ml)' (0.020), 'Source Material' (Aluminum), and 'Density 1 (kg/m3)' (2702.0). There are three buttons at the bottom: 'OK', 'Cancel', and 'Print'. A note at the bottom left says: 'Pay attention to the filling height when using matrix interpolation. Matrix interpolation can not be used for point sources.'

Figure 4.10: Input screen for vial/geometry parameters.

**Solang/Coincidence Source Parameters**

Comment: type S, 10 ml (polystyrene k0-sample vial)

User: RG RAS DSM Research

Last Modification: 03/10/1996 12:28:02

Vial Wall Material: #C2H4      Density (kg/m3): 1050.000

Inner Radius (mm): 18.180      Inner Height (mm): 10.400

Side Thickness (mm): 1.500      Bottom Thickness (mm): 1.000

Distance (mm): 0.000      (from vial bottom to platform)

☒ Matrix Interpolation      Vial Volume (ml): 10.799

Pay attention to the filling height when using matrix interpolation.  
Matrix interpolation can not be used for point sources.

Source Material: #SiO2

Density 1 (kg/m3): 200.0

Density 2 (kg/m3): 1000.0

Density 3 (kg/m3): 2000.0

Density 4 (kg/m3): 4000.0

Density 5 (kg/m3): 8000.0

OK      Cancel      Print

Figure 4.11: Material composition and density in the case of matrix interpolation for vial type S.

If you check the "matrix interpolation"-check box (Figure 4.10), you can enter more densities for the creation of a matrix interpolation dataset (see Figure 4.11). For an explanation of matrix interpolation see **Appendix 5**. This range of densities can be adjusted to the most commonly used source compositions and densities.

The source is in the case of matrix interpolation in fact a vial that can be filled with materials having, in principle, any composition and density. The only prerequisite is that the filling height (volume), in these standardized counting geometries, is always the same. If matrix interpolation is turned off (see Figure 4.10), the program calculates the standard effective solid-angles for the specified sample material and density.

## 4.2.4 Material composition input

The materials to be analyzed or the materials of construction of source holders or detectors may have complex compositions; rather than being composed of one single element, they may be mixtures of elements or compounds. For this reason SOLCOI offers the possibility to enter chemical formulas as input for material compositions. In the case of more complex chemical formulas or compositions of different compounds this is still difficult; for this reason SOLCOI contains an option for predefining materials. For data management of these materials you can use Option *Tools/Material Compositions/List of materials* and *Edit Materials* (see Figure 4.12).

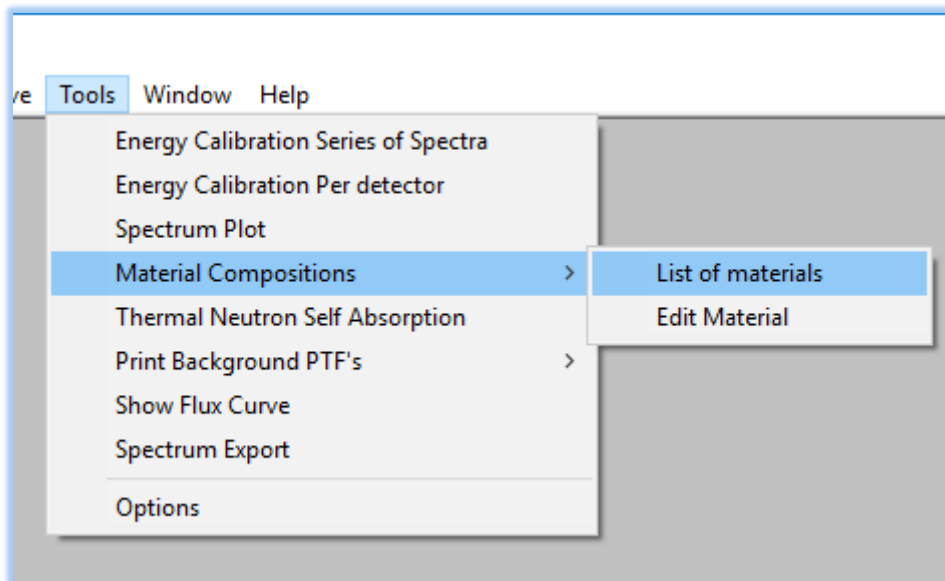
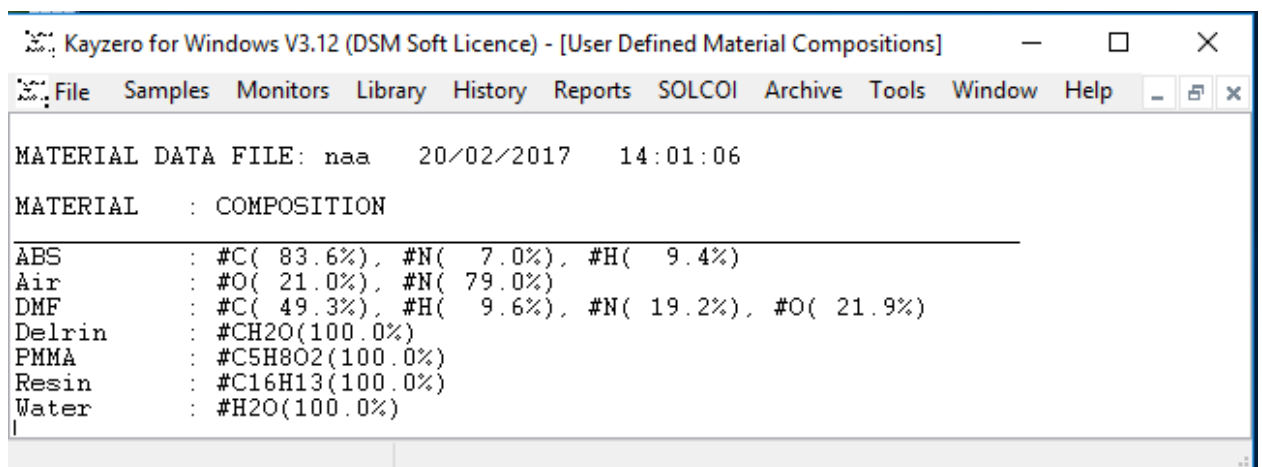


Figure 4.12: Material composition options.

To obtain a list of material compositions you can use Option *Tools/Material Compositions/List of materials*. This list contains all the material compositions available as well as the composition data (see Figure 4.13).



MATERIAL DATA FILE: naa 20/02/2017 14:01:06	
MATERIAL	COMPOSITION
ABS	: #C( 83.6%), #N( 7.0%), #H( 9.4%)
Air	: #O( 21.0%), #N( 79.0%)
DMF	: #C( 49.3%), #H( 9.6%), #N( 19.2%), #O( 21.9%)
Delrin	: #CH2O(100.0%)
PMMA	: #C5H8O2(100.0%)
Resin	: #C16H13(100.0%)
Water	: #H2O(100.0%)

Figure 4.13: Material compositions list.

Using *Tools/Material Compositions/Edit Materials* you can predefine materials and enter, modify, delete and print compositions. Material compositions that have to be entered or modified are chosen using the drop down list. The data input screen is given in Figure 4.14.

Chemical form / element	Weight fraction in %
#C	83.600
#N	7.000
#H	9.450
	0.000
	0.000
	0.000
	0.000
	0.000
	0.000
	0.000

Mass absorption Coefficient 1000 keV: 0.006958 m2/kg

OK Cancel Delete

Figure 4.14: Material composition input screen.

Material compositions can be deleted using the <Delete> button.

The material composition data are stored in a file. It is possible to make more than one data file. Change the material data filename and directory in option *Tools/Options/Absorption Data*. If you enter a new name then a new file is created.

## 4.2.5 Calculation of the effective solid angles for the reference position.

The reference efficiency is measured using a standardized source geometry, a so-called reference source geometry, which in most cases is a point source. All sources used for the measurement of the reference efficiency must have this same geometry. The measurement is performed using a specific position on a given source holder. The above definition gives all relevant information necessary for computing the reference SOLANG data. For the data that have to be entered, see Figure 4.15. The calculations can be performed batch-wise.

Calibration Source	Detector	Reference Position
PTB : PTB-reference sour	DSM2 : PG&T 42.7%	4
		1
		1
		1
		1
		1
		1
		1
		1

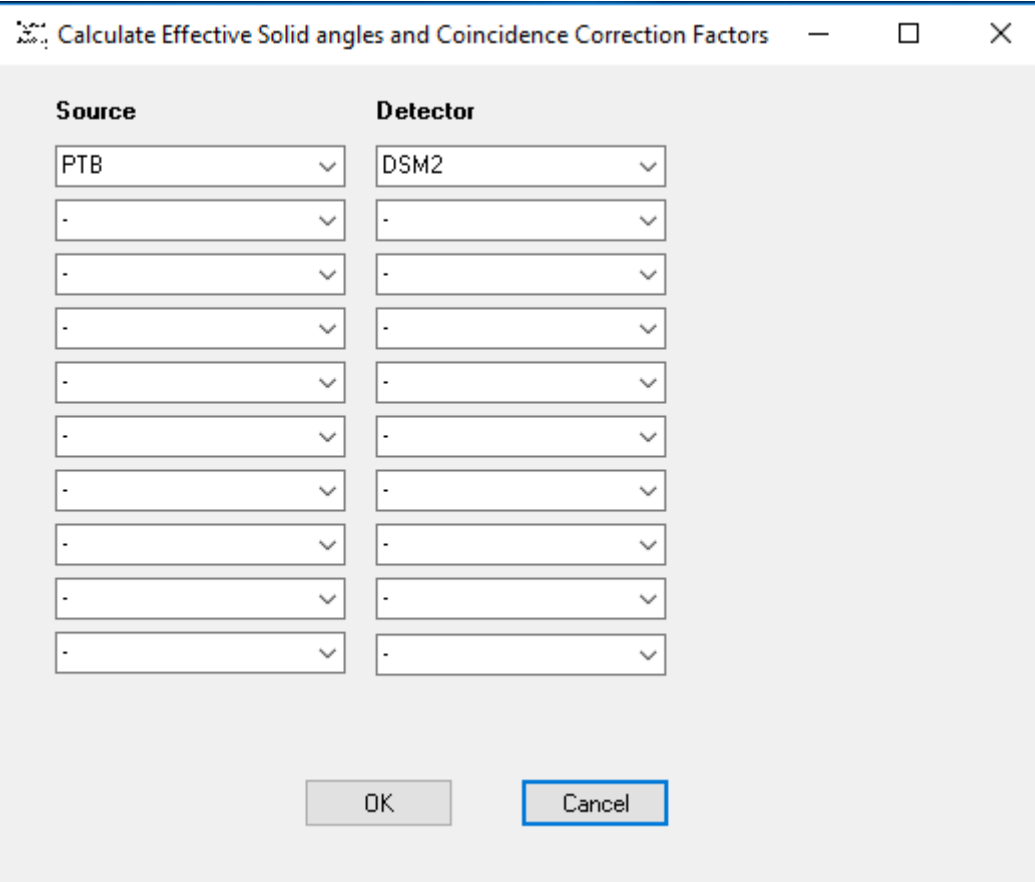
OK Cancel

Figure 4.15: Input screen for reference effective solid angle calculation.

Before the calculation is performed the estimated computation time is displayed. If a computation has already been performed it will only be recalculated if the data of the source or the detector have been modified.

## 4.2.6 Calculation of the effective solid angles and coincidence correction factors.

Using Option Calculate/ you can calculate effective solid angles and coincidence correction factors (Figure 4.16). If you enter detector names and source names the calculations can be performed. It is also possible to give a wildcard (“\*”) at the sources input field. Ten detector/source combinations can be entered. The expected calculation time will be displayed before the calculations are started. Cancelling the calculations is not possible, however you can quit the program (<Ctrl><Alt><Delete>) and the program will continue were it stopped if you restart the calculations.



Source	Detector
PTB	DSM2
-	-
-	-
-	-
-	-
-	-
-	-
-	-
-	-
-	-

OK Cancel

Figure 4.16: Input screen for effective solid angle and coincidence correction factor calculation.

If a computation has already been performed it will only be recalculated if the data of the source or the detector were modified.

## 4.2.7 Printing the input and result data

All input data for and results of the calculations can be displayed on screen or printed on a printer. The print data menu (see Figure 4.17) gives all the possibilities.

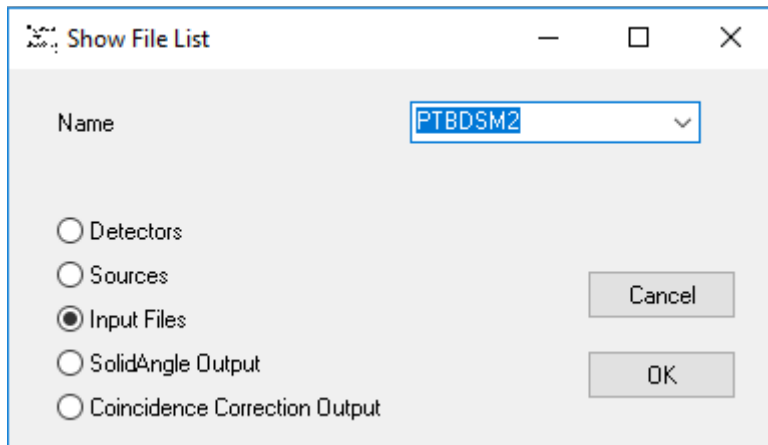


Figure 4.17: Print Data Input.

You can choose the name of the file to be printed using the drop down list. If all files should be printed, enter <\*>. If all matrix interpolation input files for source D on detector DSM2 should be printed, enter '?DDSM2'.

You can choose which kind of data file you want to print by checking the options on the left of the form.

For an explanation of the format of the files see the end of **Appendix 2**.

## 4.2.8 Efficiency curve and Coincidence correction factors

The effective solid angles in combination with the reference efficiency are meant for the computation of efficiencies by KAYZERO and NATACT. In order to investigate whether the calculation was correct the efficiency curves can be printed and plotted and coincidence correction factors can be printed, see Figure 4.17.

Using option *SOLCOI/Print Efficiency/Coincidence Data/Efficiencies* you can also calculate efficiencies for activity calculation programs. The detector calibration file format of Sampo/Sampo90 is supported.

Before making a plot or print of the efficiency curve you have to enter a detector, etc. using an input screen as in Figure 4.17.

Detector	Geometry	Position	Composition	Weight (gram)	Make Sampo (.CDF) Detector Calibration File	Energies (Column 1)	Energies (Column 2)
DSM2	D	All	#C2H4	0.70000	<input type="checkbox"/>	40.0	600.0
						50.0	800.0
						60.0	1000.0
						80.0	1500.0
						100.0	2000.0
						150.0	3000.0
						200.0	3500.0
						300.0	4000.0
						400.0	5000.0
						500.0	5000.0

Figure 4.18: Input screen for printing and plotting an efficiency curve.

If the input is not correct the program will give some remarks.

The printed outputs are given in Figures 4.19. The energy values for the printed efficiencies can be specified using the input screen of this option.

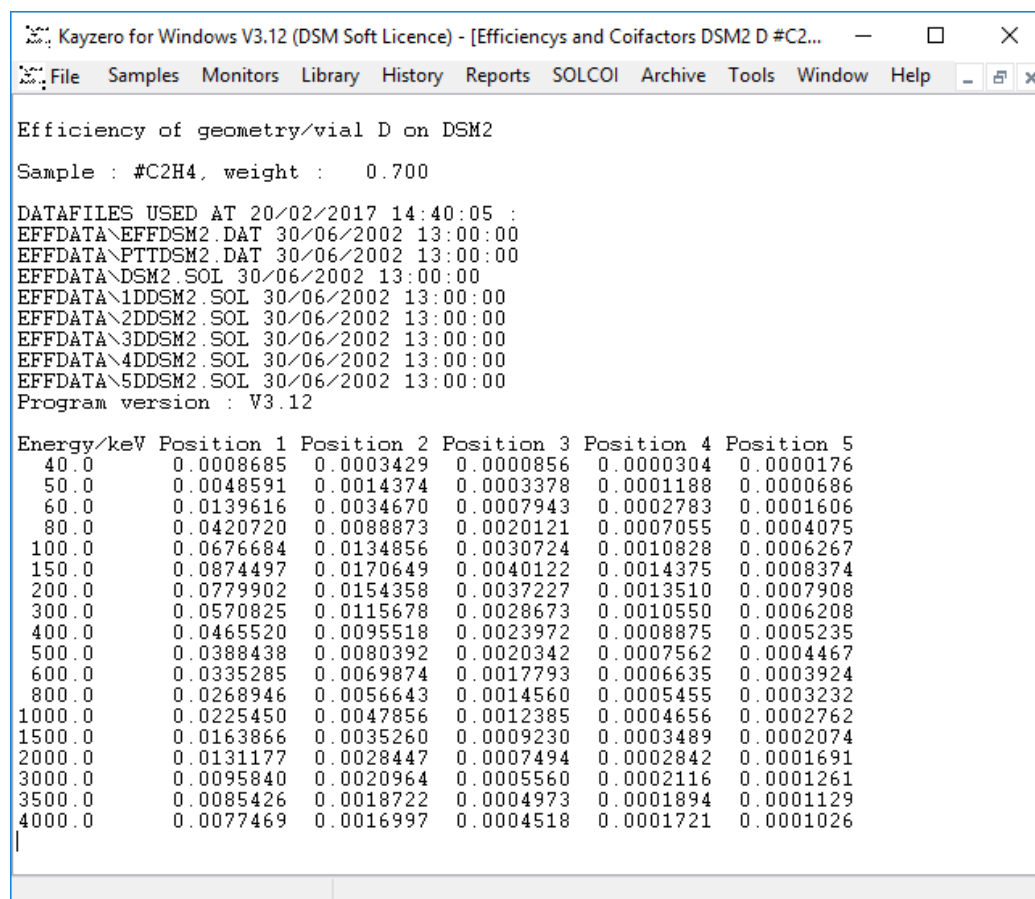


Figure 4.19: Printed efficiencies for vial D filled with 0.7 gram of #C2H4 (a resin) for all 5 positions of the source holder of detector DSM2.

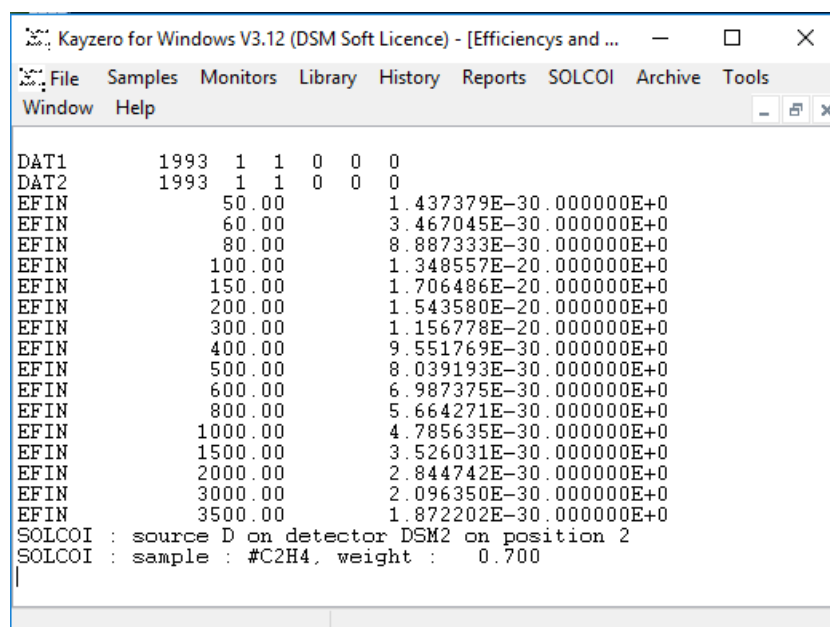
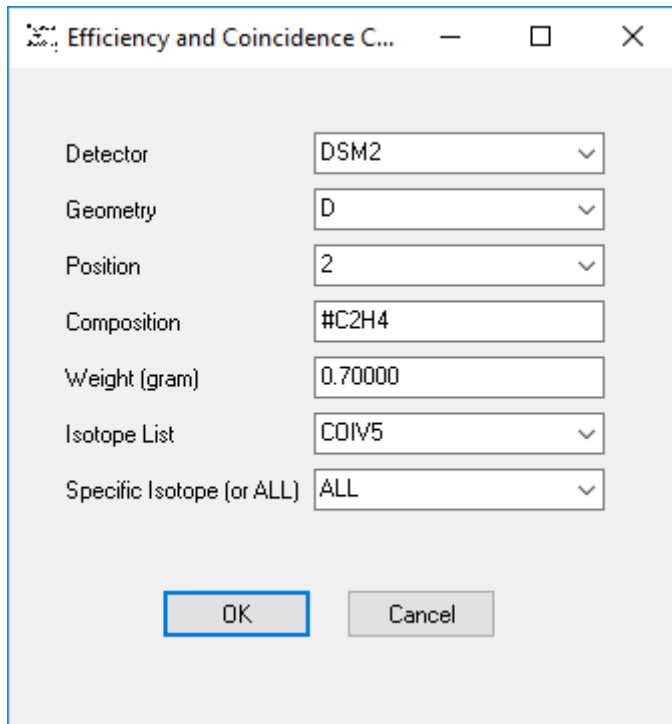


Figure 4.20: Detector calibration file for vial D filled with 0.7 gram of #C2H4 (a resin) at position 3 on the source holder of detector DSM2. The detector calibration (SAMPO efficiency calibration file) for the same source at position 2 is shown in Figure 4.20.

Coincidence correction factors can be printed using *SOLCOI/Print*

*Efficiency/Coincidence Data/Coincidence Correction and Efficiency.* The input is essentially the same as the input for efficiencies. The only difference is that a list of isotopes or one specific isotope has to be entered (see Figure 4.21) and no energies have to be selected.



The screenshot shows a Windows-style dialog box titled "Efficiency and Coincidence C...". It contains the following fields and values:

Field	Value
Detector	DSM2
Geometry	D
Position	2
Composition	#C2H4
Weight (gram)	0.70000
Isotope List	COIV5
Specific Isotope (or ALL)	ALL

At the bottom of the dialog are two buttons: "OK" and "Cancel".

Figure 4.21: Input screen for printing coincidence correction factors.

The isotope lists are located on the efficiency data directory ('EFFDATA') and may be modified. The coincidence correction-factors can only be printed for the isotopes and energies in the list COIV4.CLS. The efficiency is also given for the gamma energies of the isotope.

The output for Na-24 is given in Figure 4.22.

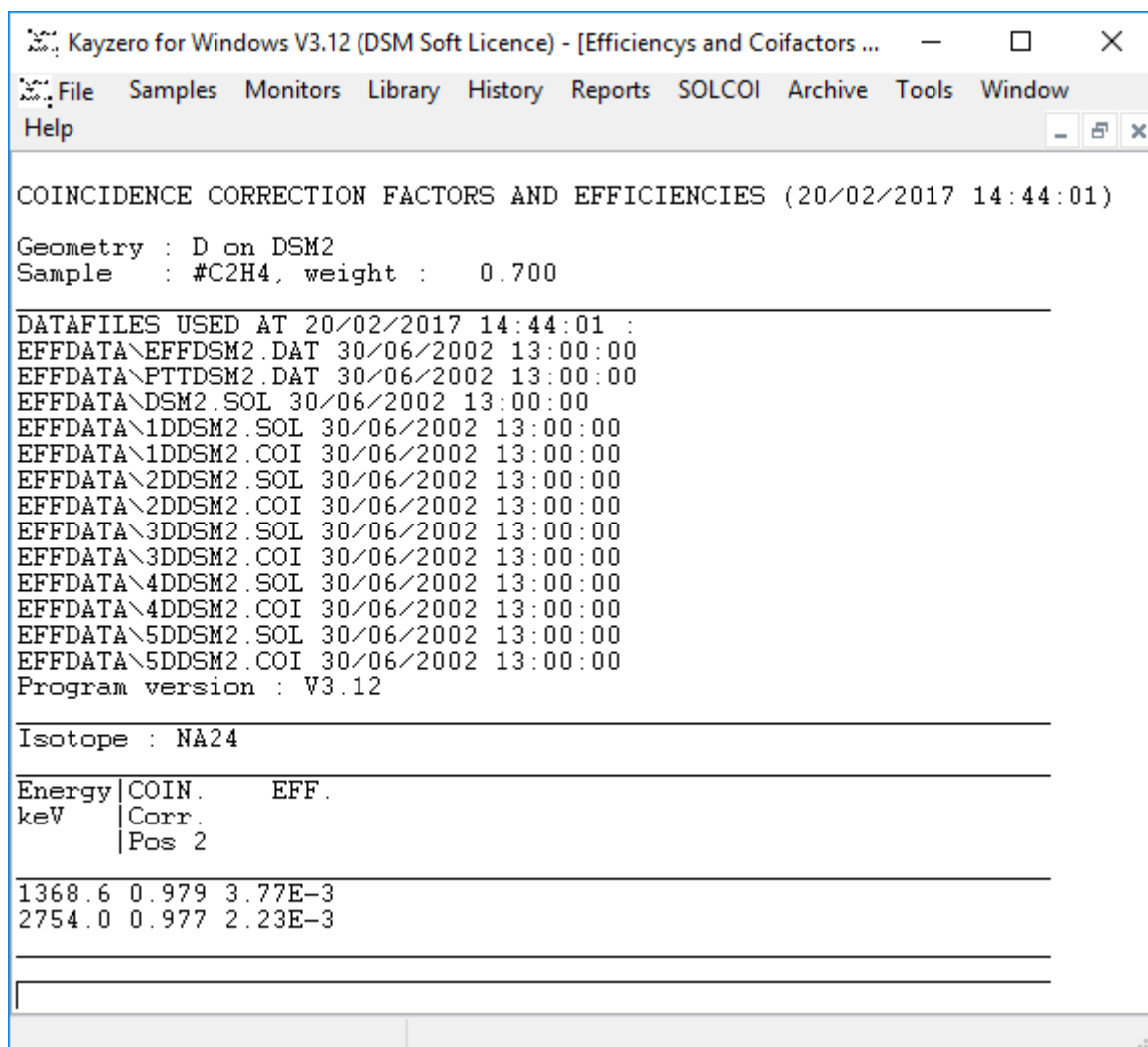


Figure 4.22: Coincidence correctionfactors and efficiencies for Na-24 for a sample in a type D vial at detector DSM2, position 2.

## 4.2.9 Showing all available input and result files

The Solcoi data files in the Solcoi directory can be listed using the *SolCoi/Show Data Lists* option. When selecting this option you can enter a wildcard or a name and select the type of data file list that you want to have (see Figure 4.23).

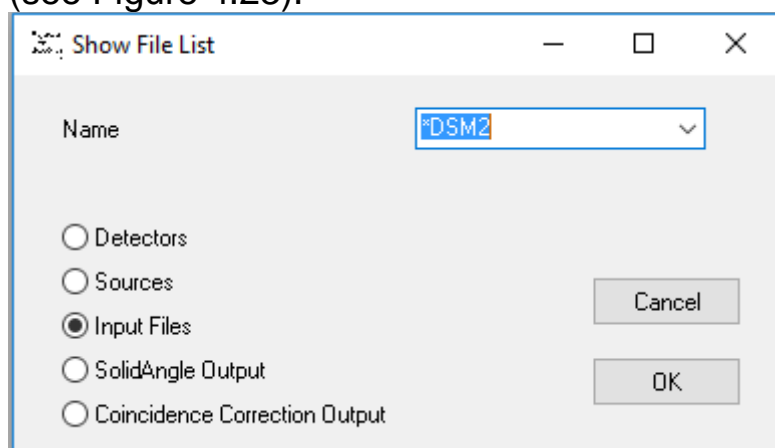


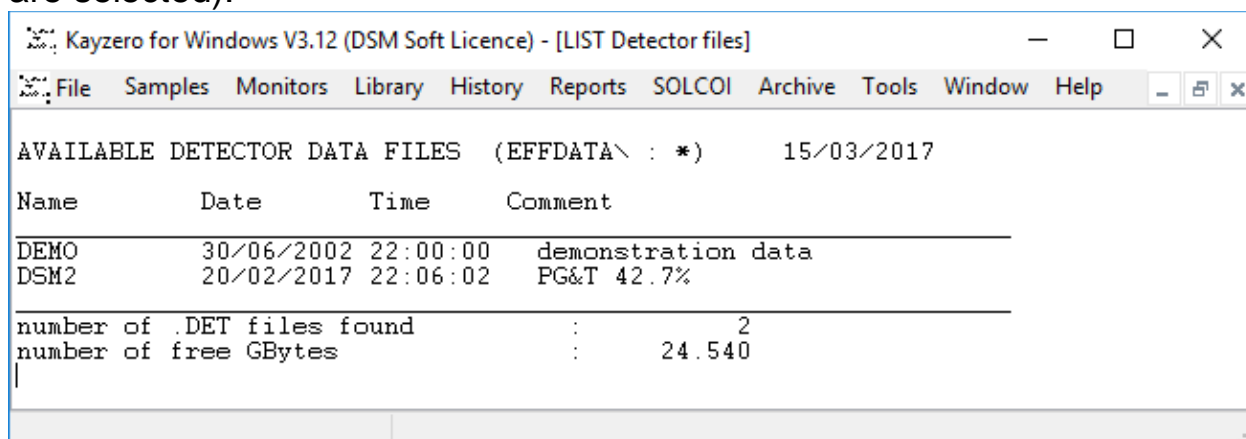
Figure 4.23: *Solcoi/Show Data Lists* option.

The file types are obvious however the Input Files need some explanation. The calculations are performed using the INW programs SOLANG and COINCALC. MS-Fortran programs need data files as input. These input files are made by SOLCOI. In the case of matrix interpolation five input files are made; one for each density (extension '.SIN'). A list of available input files is given in figure 4.24. Per input file it is shown whether or not the SOLANG / COINCALC calculations were performed; this is indicated using an S(OLANG) or C(OINCALC) between brackets after the comment. By entering 'DSM2' as a wildcard only all inputfiles related to detector DSM2 are listed.

Name	Date	Comment	
1DDSM2	30/06/2002	type D in R, SiO2	(SC)
1SDSM2	30/06/2002	type S, 10 ml (polystyrene k0-sample vial)	(SC)
2DDSM2	30/06/2002	type D in R, SiO2	(SC)
2SDSM2	30/06/2002	type S, 10 ml (polystyrene k0-sample vial)	(SC)
3DDSM2	30/06/2002	type D in R, SiO2	(SC)
3SDSM2	30/06/2002	type S, 10 ml (polystyrene k0-sample vial)	(SC)
4DDSM2	30/06/2002	type D in R, SiO2	(SC)
4SDSM2	30/06/2002	type S, 10 ml (polystyrene k0-sample vial)	(SC)
5DDSM2	30/06/2002	type D in R, SiO2	(SC)
5SDSM2	30/06/2002	type S, 10 ml (polystyrene k0-sample vial)	(SC)
AUDSM2	30/06/2002	Au-Al-wire in spronckvial	(SC)
DSM2	30/06/2002	reference solang	(S)
PTBDSM2	30/06/2002	PTB-reference source	(SC)
ZRDSM2	30/06/2002	Zirconium disc in spronckvial	(SC)
<hr/>			
number of .SIN files found		:	14
number of free GBytes		:	24.540

Figure 4.24: A list of available input files for SOLANG and COINCALC. S(olang) and/or C(oincalc) indicate that the calculations were performed.

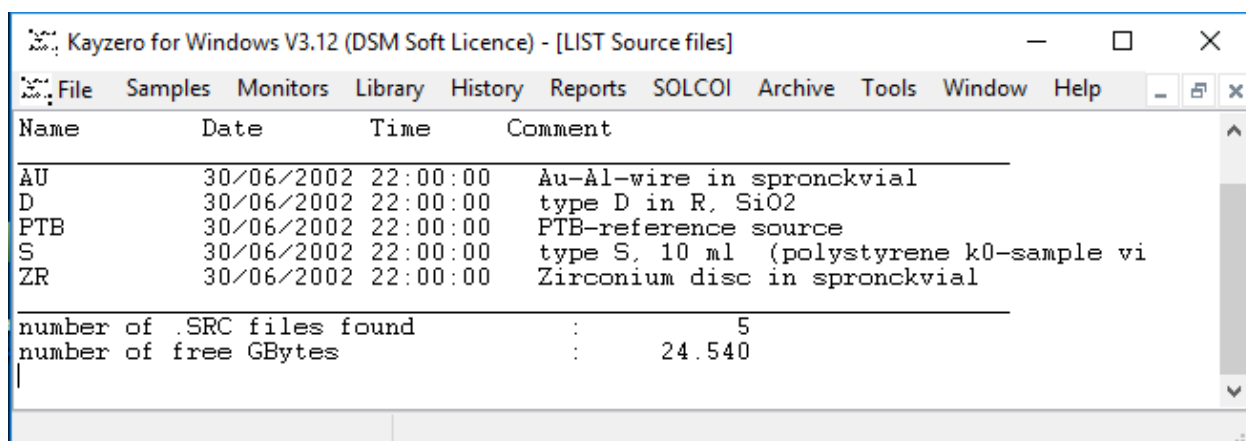
Other lists are those of available detector and source data files, Figures 4.25 and 4.26. All these lists can be filtered using the standard DOS filtering possibilities (e.g. DSM?). The standard filter is '\*' (using this means all files are selected).



Name	Date	Time	Comment
DEMO	30/06/2002	22:00:00	demonstration data
DSM2	20/02/2017	22:06:02	PG&T 42.7%

number of .DET files found : 2  
number of free GBytes : 24.540

Figure 4.25: List of available detector data files (.DET).



Name	Date	Time	Comment
AU	30/06/2002	22:00:00	Au-Al-wire in spronckvial
D	30/06/2002	22:00:00	type D in R, SiO2
PTB	30/06/2002	22:00:00	PTB-reference source
S	30/06/2002	22:00:00	type S, 10 ml (polystyrene k0-sample vi
ZR	30/06/2002	22:00:00	Zirconium disc in spronckvial

number of .SRC files found : 5  
number of free GBytes : 24.540

Figure 4.26: List of available source data files (.SRC).

When activating *Tools/Options/Solcoi* the results of the timing of the last calculations made on this computer (see Figure 4.27) are displayed. These data are used to predict the total calculation time before starting the actual calculations using *Solcoi/Calculate*. The calculation times for the effective solid angle calculations are given per position and per energy. They are in fact the calculation times needed for the calculation of single results. The coincidence correction factor calculation time is given for all nuclides and energies for one position.

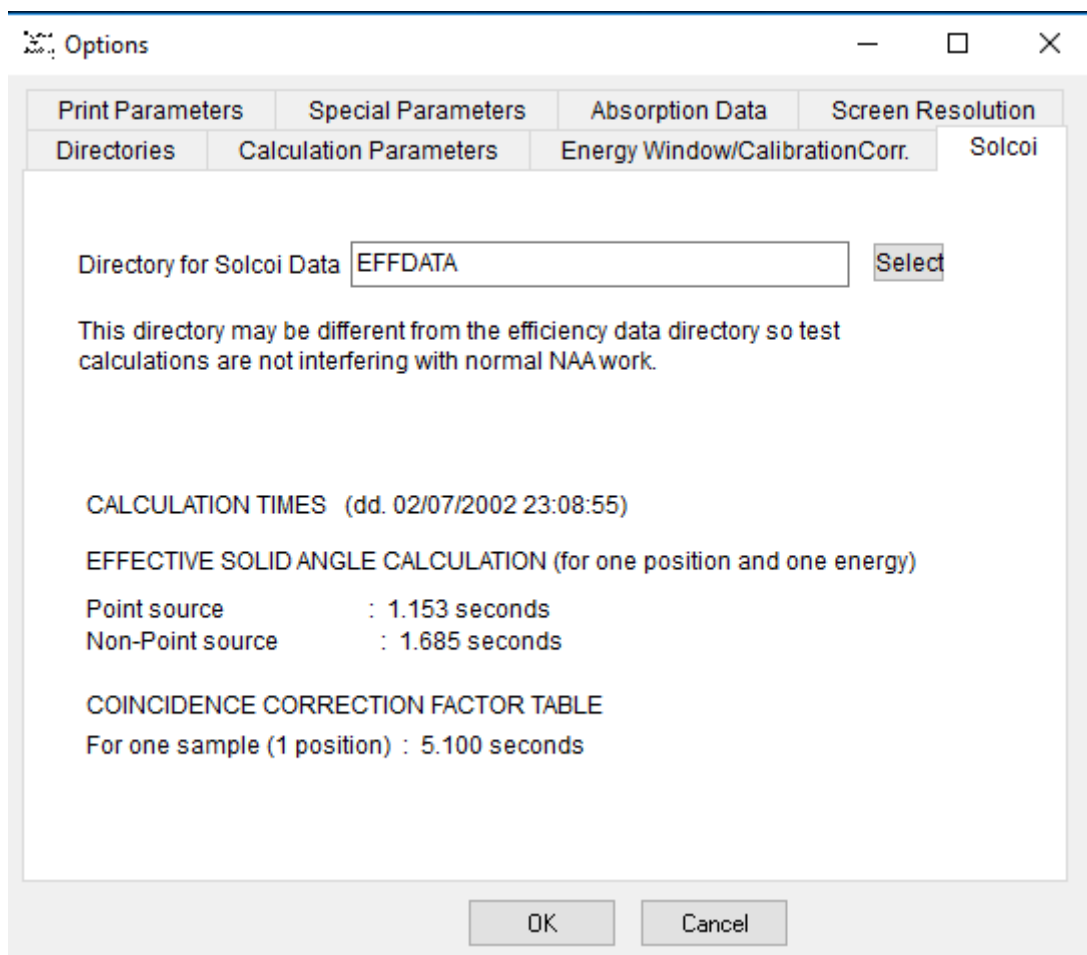


Figure 4.27: Calculation times (for an AMD 64 3000+).

## 4.3 Fine tuning

The experimental determination of the vacuum gap and the dead-layer thickness is essential for the use of the efficiency computation technique as explained in the 'VADEMECUM FOR K<sub>0</sub> USERS' (a part of this software package, see website [www.kayzero.com/download.html](http://www.kayzero.com/download.html)). The determination of these parameters is called 'fine tuning'. Fine tuning is performed by measuring several sources (with true coincidence free gamma lines) on the reference position and on positions closer to the detector. These sources do not need to be calibrated sources. The count-rate ratio of measurements on the reference position and a position closer to detector is used to check the efficiency conversion for different positions carried out by this program.

The deviations between measured and calculated ratios are mainly due to the fact that the vacuum gap and the dead-layer thickness are not well known.

The fine tuning in this program is performed after you have entered the dimensions of the sources used for measurements and the detector (see **Chapter 4.2**). First enter the measurement data. Either the measured count rate or the count-rate ratios should be entered, see Figure 4.28.

**Fine Tuning**

Detector: DEMO : demonstration data    Fine tuning : Measured Data    Existing Fine-Tuning data!

**Edit Measured Data and Calculate**

Energy	Source	Position 1	Position 2	Position 3	Position 4	Position 5
59.5	PTB	63.88330	28.26962	10.46278	3.96378	1.00000
122.1	PTB	65.38462	26.28205	9.87179	3.82692	1.00000
661.6	PTB	52.49110	21.70819	8.64769	3.50534	1.00000
1115.5	PTB	50.25641	20.79487	8.46154	3.56410	1.00000
0.0		0.00000	0.00000	0.00000	0.00000	0.00000
0.0		0.00000	0.00000	0.00000	0.00000	0.00000

Edit Measurement Data    Calculate

**Fine tune the values**

	User Data	Initial Data	Best Fit
Vacuum Gap [mm]	8.6806	8.6000	8.6806
Top Dead-Layer Thickness [mm]	0.3836	0.3800	0.3836

☐ Do not use data deviating more than 10%.

Print New Results

OK    Cancel    Small Form

Figure 4.28: Entering the fine tuning measurement values.

Based on the vacuum gap and dead-layer thickness supplied by the detector manufacturer a matrix is calculated for several vacuum gap and dead-layer thickness combinations. This may take a few minutes. Using this matrix of calculated points and the measured data points a best fit is computed for the desired parameters (see Figure 4.29).

Fine tune the values			
	User Data	Initial Data	Best Fit
Vacuum Gap [mm]	8.6806	8.6000	8.6806
Top Dead-Layer Thickness [mm]	0.3836	0.3800	0.3836

☐ Do not use data deviating more than 10%.

Print New Results

OK Cancel Small Form

Figure 4.29: Screen for changing the dead-layer thickness and vacuum gap.

If necessary you may change the values to find better suited values. Just enter in the 'User Data'-field your own guess for dead layer thickness and or vacuum gap and press the <Print New Results>-button. The results of these calculations are added to the automatically generated data given in Figure 4.30.

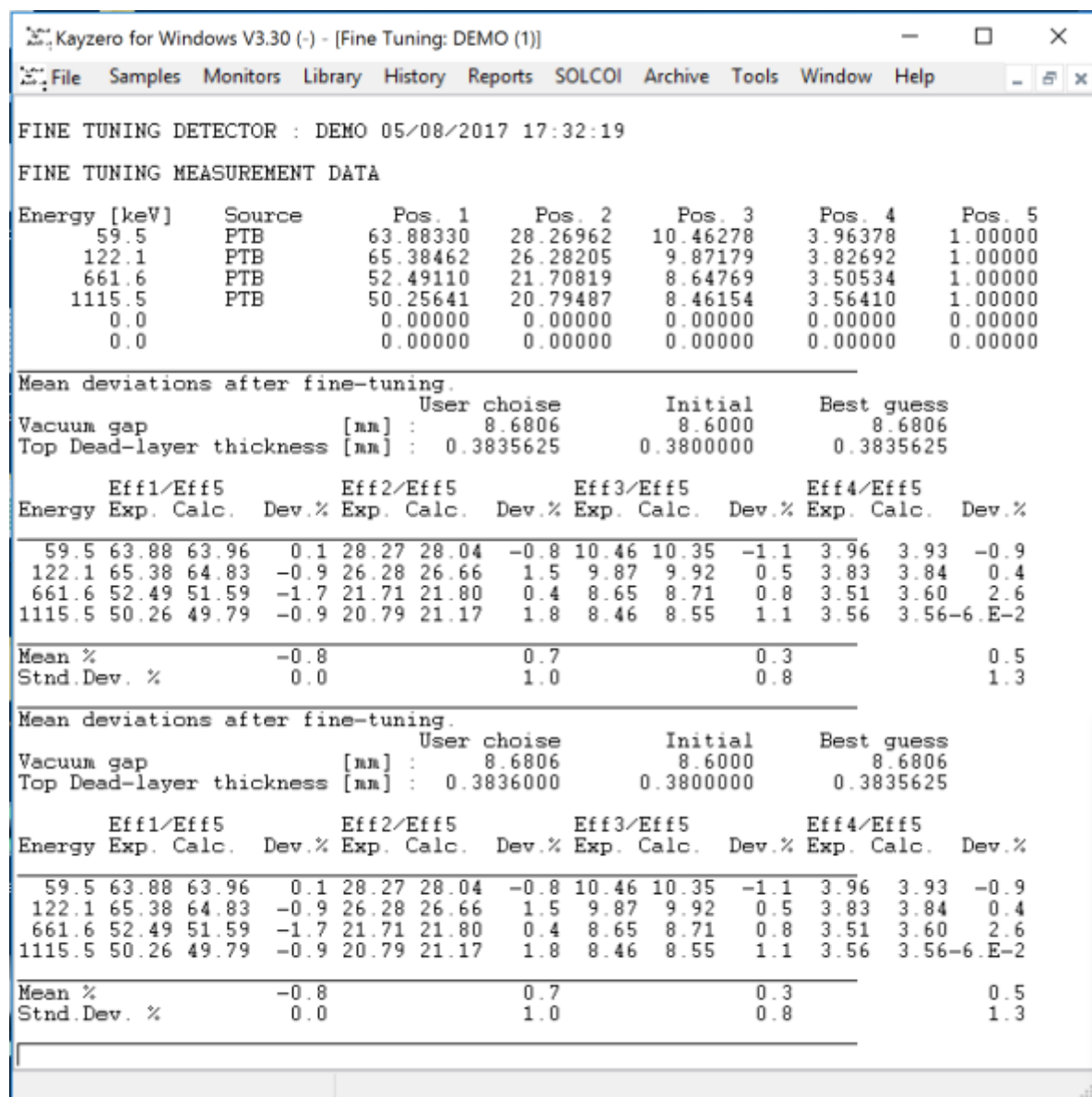


Figure 4.30 Fine tuning results for detector DEMO.

For every measured count-rate ratio a calculated ratio is given, as well as the difference between the two, expressed in %. The average difference (and the standard deviation in the average) is calculated per position. If necessary the deviations larger than 10% can be excluded from the average calculation (see Figure 4.29). It is obvious that the result of the fine-tuning in this example is very good.

The matrix data set is used to calculate results for the user values so these calculations are performed almost instantaneously.

The user selected 8 mm and 0.4 which is clearly not as good as the estimated best values.

## 4.4 Reference efficiency and peak-to-total ratio curve fitting

The photopeak efficiency on a reference position and the peak-to-total (PTT) ratio for all positions are determined using a large number of measurements. This information is necessary for the calculation of coincidence correction factors. In order to provide data for any energy the measurement data is fitted.

Using sub menu *SOLCOI/Fit Reference Efficiency or PTT curve* (See Figure 4.30) you can perform the fitting procedures and store the resulting data on disk.

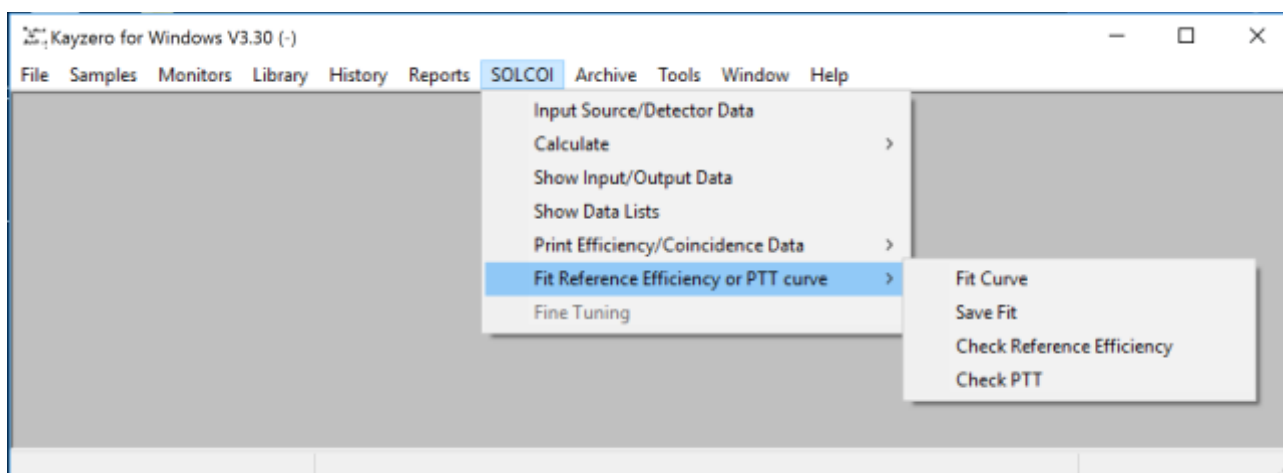


Figure 4.30: Reference Efficiency and PTT Fit menu.

### 4.4.1 Fit reference efficiency or PTT-curve

The reference efficiency and peak-to-total ratio curve fitting is performed in such a way that the coincidence correction program (SOLCOIN, a part of SOLCOI) and the NAA evaluation program (KAYZERO) or the activity calculation program (NATACT) can use this data.

Before starting the curve fitting the measurement data has to be stored in a comma separated ascii data file.

The extension of the file should be '.CAL' and for each measurement an energy, a reference efficiency or a Peak-to-total Ratio, a standard deviation of the measurement (optional) and a comment (optional) should be entered, see Figure 4.31 for an example of a PTT calibration data file.

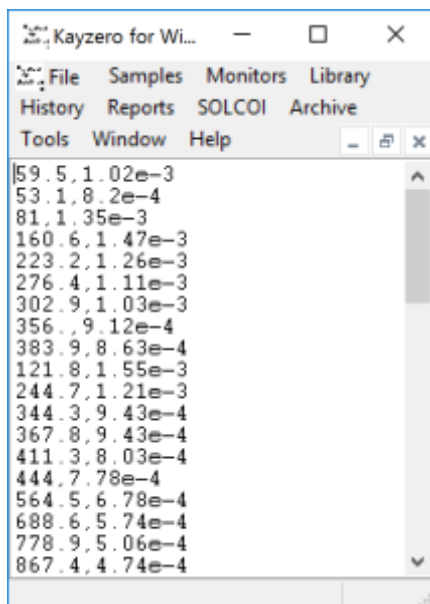


Figure 4.31 A Peak-to-total ratio measurement data file; only the energies and PTT-ratios are entered.

The program automatically determines whether an efficiency curve or a PTT curve is fitted by checking whether any of the measured values is higher than 0.2. It is assumed that absolute efficiencies of 20% are not possible for the reference efficiency and that the PTT curve will have at least one value above 0.2.

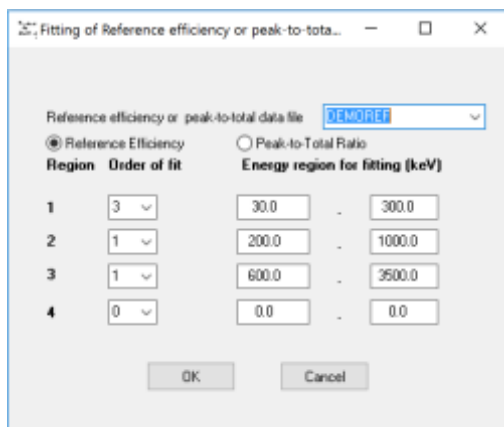


Figure 4.32: Reference Efficiency and PTT Fit Option.

You can choose from a list of available calibration data files before starting the fitting procedure, see figure 4.32. After selecting the measurement data set you should enter the fitting order of the polynomial per fitting region. You can use at most four fitting regions, the maximum fitting order being 3. An efficiency curve normally has a second order fit in the first region (20-300 keV), and one or two first order polynomials for the higher energies. A PTT curve has approximately the same shape but only one linear fit for the energies higher than 180 keV. Figure 4.34 Fitting output: Plot of PTT-ratio fit.

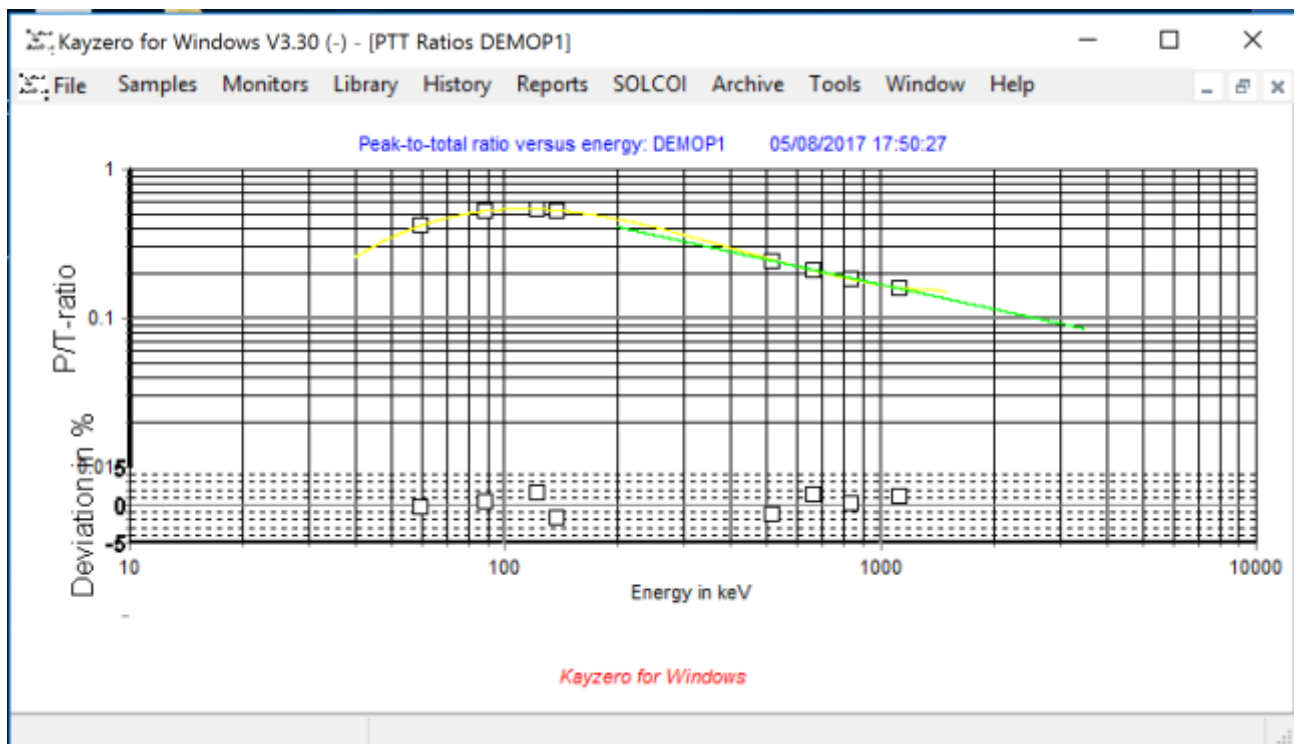


Figure 4.33 Fitting output: Plot of PTT-ratio fit.

When selecting the energy regions one should make sure that the energy regions overlap. The fitting is performed per energy region. After fitting the program automatically determines the borders of the regions by determining the crossing points of the curves determined. To ensure that the curves will cross or meet each other, the fitting regions should overlap. The fitting results are plotted (see Figure 4.33) and printed (see Figure 4.34).

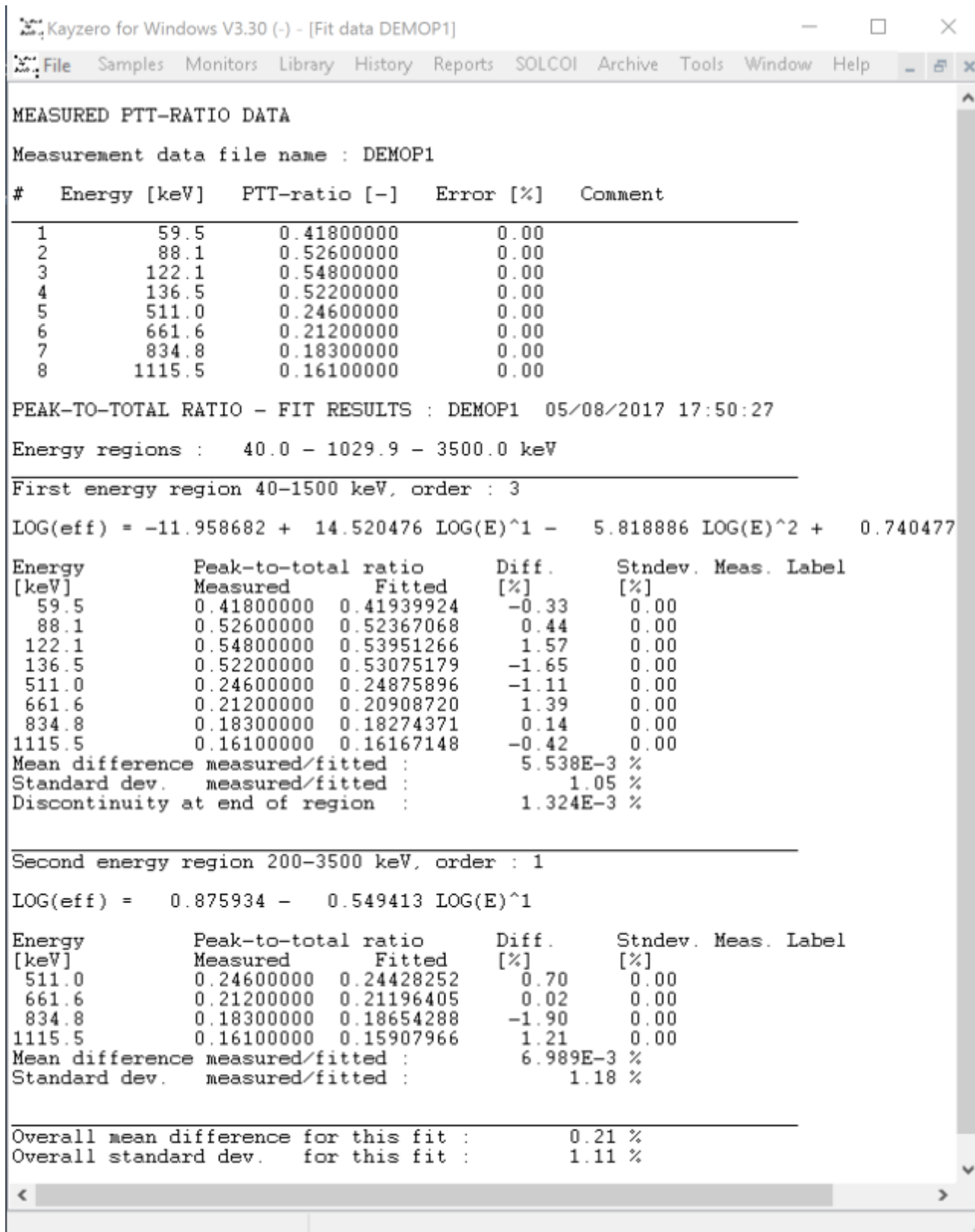


Figure 4.34 Fitting output: Measurement data and the results of the PTT-ratio fit.

## 4.4.2 Saving fitted data in KAYZERO data file

The results of the curve fitting can and should be stored in data files. You can use the *Save Fit* option, see Figure 4.30. The data is related to a detector so you should only enter a detector identification code. If the dimensions of the detector have already been entered you can the detector name from the list.

See Figure 4.35 for an example of saving a reference efficiency.

Store fit results in a PTT data file.

Detector: DEMO : demonstration data Position: 1

**Fit Data**

Energy Regions: 40.0 - 1030 - 3500

Eff = absolute efficiency E = energy in keV

1 LOG(eff) = -11.958682 + 14.520476 LOG(E) - 5.818886 LOG(E)<sup>2</sup> + 0.740477 LOG(E)<sup>3</sup>

2 LOG(eff) = 0.875934 - 0.549413 LOG(E)

OK Cancel

Figure 4.35. Storing of reference efficiency fit results.

The curve fitting data is shown and, after you select a detector code, stored in a data file. See **Appendix 2** for the name and format of this data file.

In case a PTT curve is stored the position has to be given as well.

First curve fit data of position 1 should be stored in an empty file and then all other positions can be stored successively.

#### 4.4.3 Comparing stored reference efficiency fit or peak-to-total ratio fit data with measured data.

The stored fitting results can be compared with the old measurement data points to confirm that the data files are still valid or to print out the old fitting results.

The program stores all fitting data in a file with extension '.FIT' so the fit can be retrieved at any time. If the fit was not carried out by this program, the program will ask for a data file name with the measurement data points.

The output is a print of the fit results and a plot (see Figure 4.36). In the case of a PTT-ratio fit this is done for all positions and an additional plot of all PTT curves is also given.

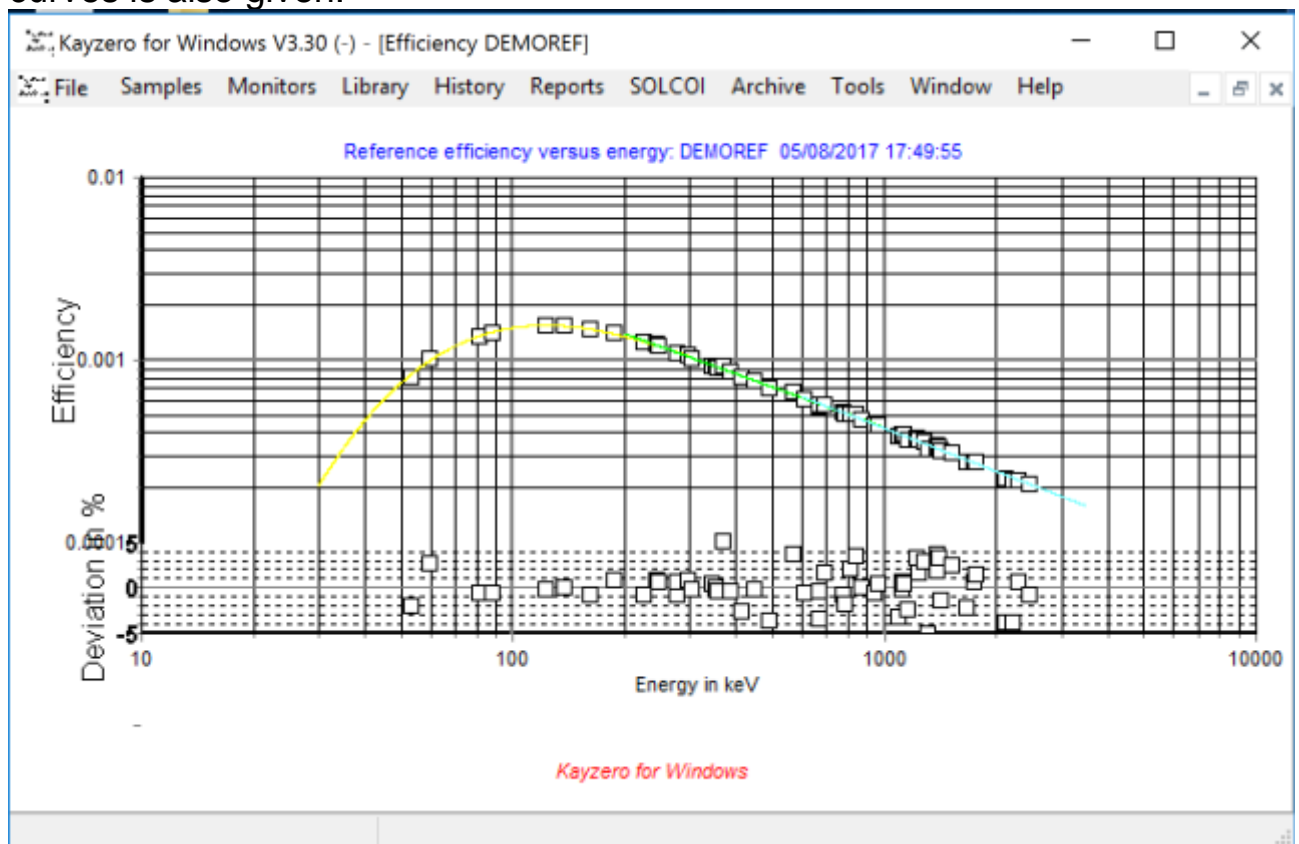


Figure 4.36 Comparison of measure efficiency data with the stored reference efficiency fit .

## 5 History of detector and reactor calibrations

---

The quality control options in KAYZERO for Windows concern the detector energy and efficiency calibration, the detector resolution and background and the reactor calibration (see Figure 5.1).

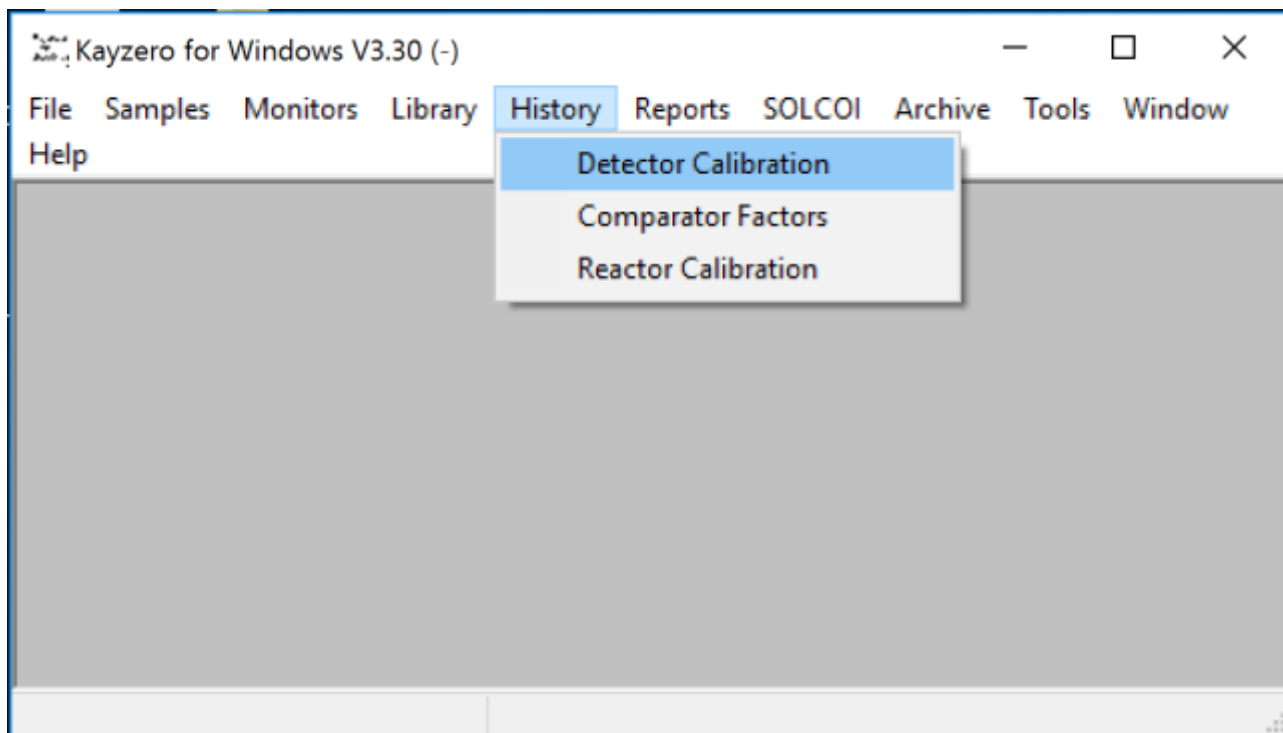


Figure 5.1: History of Detector and Reactor Calibrations Menu

### 5.1 Detector Calibration

Detector efficiency and energy calibration data can be monitored as a function of time by regularly measuring a reference source. The basic data of the source used have to be entered in KAYZERO. The detector calibration measurements are treated as NAA measurements so an order file has to be created first. A calibration order file can be recognized by the first three letters in its name : 'CAL'. In Figure 5.2 the input screen for entering calibration information is given. The source used for the calibrations should be a radionuclide that is present in the KAYZERO library.

The calibration source and the background should be measured regularly. The measurement data can be entered as a sample measurement using *Samples/Measurement*, see figure 5.3. In the example almost every week a measurement was performed and every two weeks a background was measured. The data were stored in a file named 'CAL96'. The measurement data (calibration and background spectra) were stored in the subdirectory

Calibration File Input Form : CAL96

Calibration Description: Energy calibration and eff. control, Eu-152 nr. 3 (1987)

Isotope: Eu-152

Half-life (days): 4934.528

Activity (kBq): 258.0000

Reference date: 01/01/1987

Energy 1 (keV): 121.80

Energy 2 (keV): 778.90

Energy 3 (keV): 1408.10

The 3 given gamma lines are used for efficiency, drift and FWHM monitoring.

Energy 4 (keV): 511.00

Energy 5 (keV): 1461.00

The last two gamma lines are used for background monitoring.

OK Cancel

Figure 5.2: Calibration file information input screen

The calibration measurements are performed weekly so the measurement identification and the spectrum name contains the week number: 'CAL96:01'. After entering the measurement data, the activities have to be calculated using the calculation option *Samples/Calculate*.

**Edit Data**

Order: CAL96      Data directory: CAL96\  
Sample: DET2      **Measurement Found**  
Measurement: CAL96:01

Measurement Data    Uncertainties

Detector: **DSM2**      Point Source  
Geometry: **PTB**      Geometry data Okay!  
Counting position: **3**

Background spectrum PTF file:       Click Here to Use Data  
Deadtime (%): **6.34828**      6.35  
Peaktable file: ☐ Correct Hypermet      2DET01.PTF      Sampo90 PTF (16 peaks)  
Start date (dd/mm/yyyy): **02/01/1996**      02/01/1996  
Start time (hh:mm:ss.ii): **10:57:08.00**      10:57:08  
True Measuring Time (sec): **6868.00**      6868.00  
Remarks:       SPE : 2DET01.SPE (LFC-dual spe.)

OK    Cancel    SpectrumPlot    Peak Summation    Energy Calibration

Figure 5.3: Calibration file information input screen

## Printing and plotting the calibration data.

The relative activity (measured activity divided by the reference activity), the energy shift (in channels), the energy resolution (FWHM) and the background of the detector can be printed and plotted.

Before printing and plotting the data, the plot wanted must be chosen, see figure 5.4. The printed output is given in figure 5.5 and the plotted output in figure 5.6.

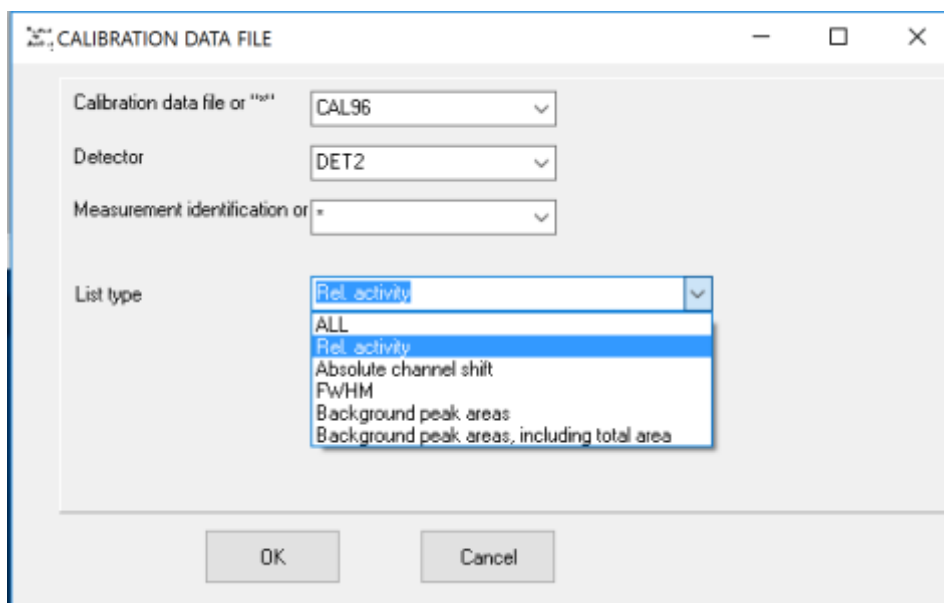


Figure 5.4: Selecting the type of detector calibration output.

Kayzero for Windows V3.30 (-) - [Detector Efficiency Data CAL96 DET2]

File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

DETECTOR EFFICIENCY DATA : CAL96 (Eu-152) 08/08/2017 21:23:00  
 DET21 For detector DET2  
 Eu-152, # = 121.80 keV,  $\sigma$  = 778.90 keV, \* = 1408.10 keV.  
 DETECTOR CODE DATE ACT.# ACT. $\sigma$  ACT.\*

DET2	CAL96:01	02/01/1996	1.01714E+0	1.03032E+0	1.04636E+0
DET2	CAL96:02	08/01/1996	1.02230E+0	1.03466E+0	1.04702E+0
DET2	CAL96:03	15/01/1996	1.01800E+0	1.02904E+0	1.04736E+0
DET2	CAL96:05	29/01/1996	1.02107E+0	1.02951E+0	1.04753E+0
DET2	CAL96:06	03/02/1996	1.01419E+0	1.03027E+0	1.05178E+0
DET2	CAL96:07	12/02/1996	1.02397E+0	1.03005E+0	1.04901E+0
DET2	CAL96:08	19/02/1996	1.02028E+0	1.03392E+0	1.05480E+0
DET2	CAL96:09	26/02/1996	1.01239E+0	1.02391E+0	1.05191E+0

AVERAGES for DETECTOR DET2

	ACT.#	ACT. $\sigma$	ACT.*
MEAN	1.01866E+0	1.03021E+0	1.04947E+0
STN. DEV.	3.74028E-3	3.06506E-3	2.82401E-3
STN. DEV. %	0.37	0.30	0.27
N	8	8	8

OVERALL STATISTICS

MEAN	1.01866E+0	1.03021E+0	1.04947E+0
STN. DEV.	3.74028E-3	3.06506E-3	2.82401E-3
STN. DEV. %	0.37	0.30	0.27
N	8	8	8
MAX	1.02397E+0	1.03466E+0	1.05480E+0
MIN	1.01239E+0	1.02391E+0	1.04636E+0
PERIOD	02/01/1996 - 26/02/1996		

Figure 5.5: The printed output of the relative activity of the detector calibration file CAL96 for DSM detector 2.

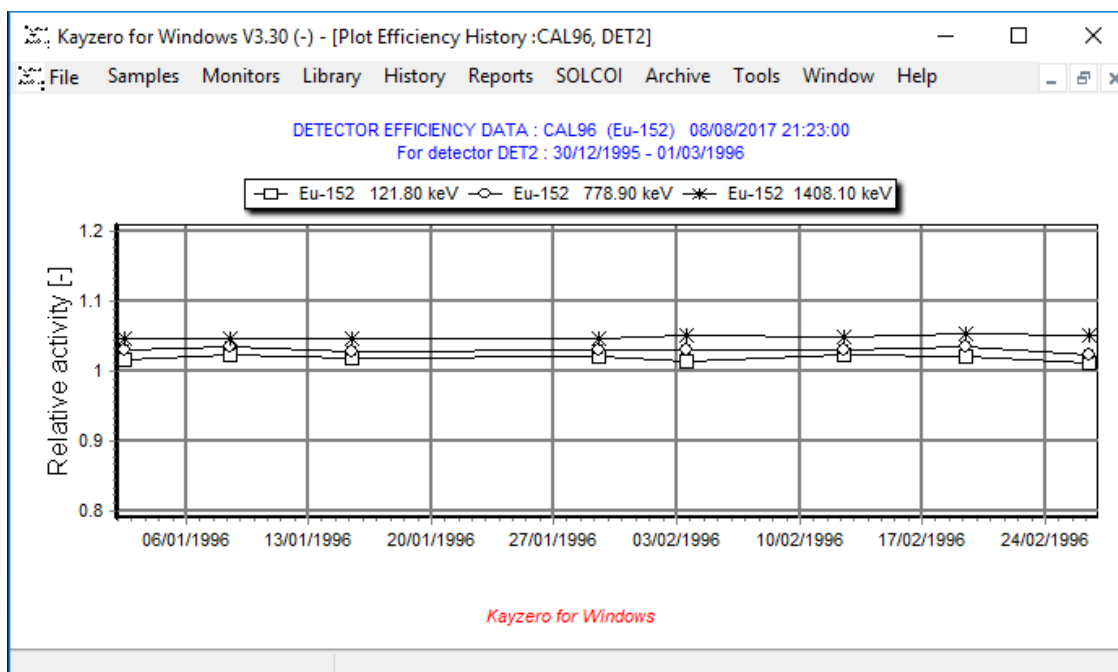


Figure 5.6: The plotted output of the relative activity of the detector calibration file CAL96 for DSM detector 2.

## 5.2 Comparator Factors

The comparator factor is a value proportional to the epithermal neutron flux and one of the three  $k_0$ -NAA reactor flux parameters.

All the comparator factor measurements that were stored in one monitor data file can be printed and plotted as a function of time using Option 52. If the monitors stored in one file were used in only one channel the data can be compared and plotted as a function of time.

By selecting a suitable filename (corresponding to the irradiation location) comparator factors can be printed/plotted per monitor type or per irradiation.

A mean comparator factor is calculated for every irradiation or subdirectory (in fact per measurement identification). You can select the comparator factors of any irradiation by entering a wildcard (\*) for the monitors and selecting a measurement identification code (SCK7V:\*). Another possibility is to select a monitor identification code (AU) and entering a wildcard for the measurements (\*).

An example is given in Figure 5.7. The resulting outputs are given in Figures 5.8 and 5.9.

MONITOR DATA FILE (722)

Monitor file identification or "\*\*\*"

Monitor identification or "\*\*\*"

Measurement identification or "\*"

OK Cancel

Figure 5.7: Input screen for *History/Comparator Factors*.

Kayzero for Windows V3.30 (-) - [MONITOR DATA BR1Y4 AU2]

File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

MONITOR DATA : BR1Y4 (06/08/2017 20:21:37)  
For monitor AU2 and irradiations \*

CODE	MONITOR	DATE	f	alpha	Fc
SCK1V	AU2	03/06/1996	3.30000E+1	7.20000E-2	3.39913E+3 09:00:00
SCK2V	AU2	24/06/1996	3.30000E+1	7.20000E-2	3.37012E+3 08:55:00
SCK3V	AU2	25/06/1996	3.30000E+1	7.20000E-2	3.31380E+3 08:57:00
SCK4V	AU2	27/06/1996	3.30000E+1	7.20000E-2	3.32911E+3 08:59:00
SCK7V	AU2	30/07/1996	3.30000E+1	7.20000E-2	3.32280E+3 08:29:00

OVERALL STATISTICS

MEAN	:	3.30000E+1	7.20000E-2	3.34699E+3
STN. DEV.	:	-	-	3.24345E+1
STN. DEV. %	:	-	-	0.97
N	:	5	5	5
MAX	:	3.30000E+1	7.20000E-2	3.39913E+3
MIN	:	3.30000E+1	7.20000E-2	3.31380E+3
PERIOD	:	03/06/1996 - 30/07/1996		

Figure 5.8: Printed output of *History/Comparator Factors*, monitors measured in BR1Y4.

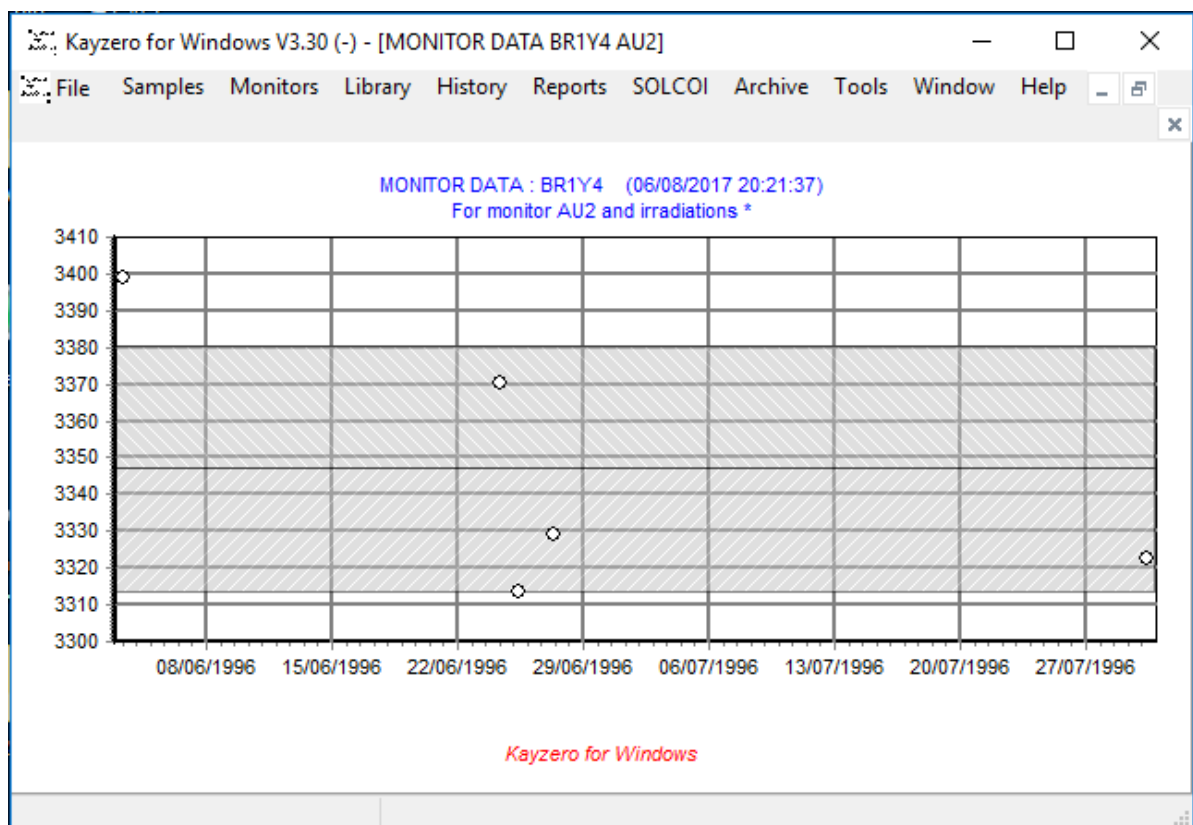


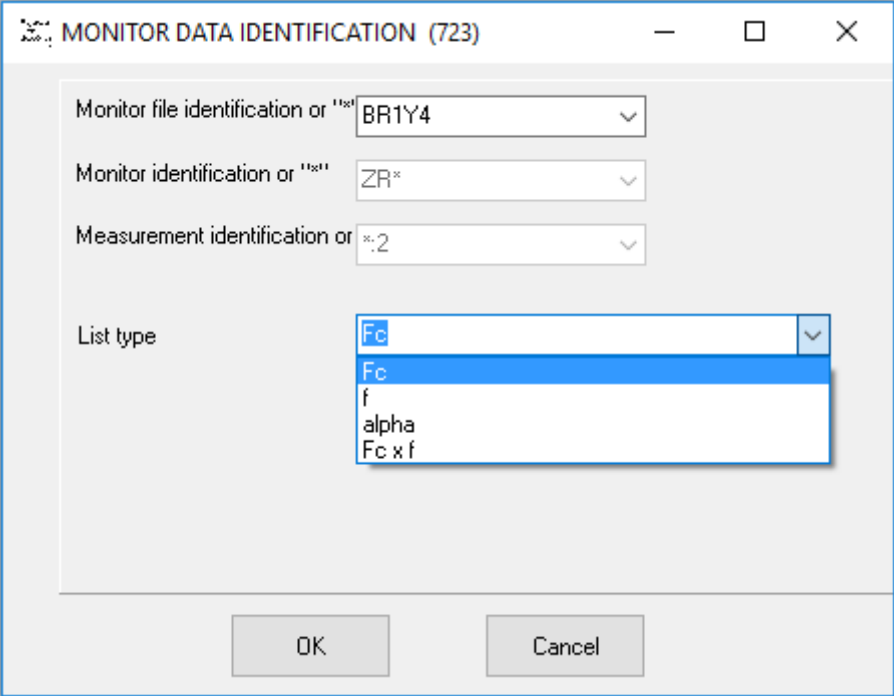
Figure 5.9: Plotted output of *History/Comparator Factors* for BR1Y4.

## 5.3 Reactor Calibration Data

The reactor flux parameters  $F_c$ ,  $f$  and  $\alpha$  can be determined by irradiating monitors. In this program the 'bare triple method' is used to calculate the reactor flux parameters. *History/Reactor Calibration*-option is based on the 'bare triple method' using the Au/Zr-monitor couple as described in the 'Vade Mecum'.

The reactor calibration parameters can be calculated by this program and are stored in the monitor file. For the benefit of the *History/Reactor Calibration*-option the reactor calibration data are stored in the data record of the second measurement of the Zr-monitor.

The reactor flux parameters can now be plotted and printed as a function of time. In figure 5.10 the necessary input screen is given.



MONITOR DATA IDENTIFICATION (723)

Monitor file identification or "id" BR1Y4

Monitor identification or "id" ZR\*

Measurement identification or "id" x.2

List type

- Fc
- f
- alpha
- Fc x f

OK Cancel

Figure 5.10: *History/Reactor Calibration*-option

## 6 Reference Guide

---

In this chapter some important additional options will be discussed.

### 6.1 Monitor Analysis Menu

Important options in this menu are the  $f$  and  $\alpha$  calculation using the 'Zirconium'-method and the 'Multi Monitors'-method.

The algorithm calculates all the neutron spectrum characterization parameters in terms of the Høgdahl convention. The results will be  $F_c$ ,  $f$  and  $\alpha$  values.

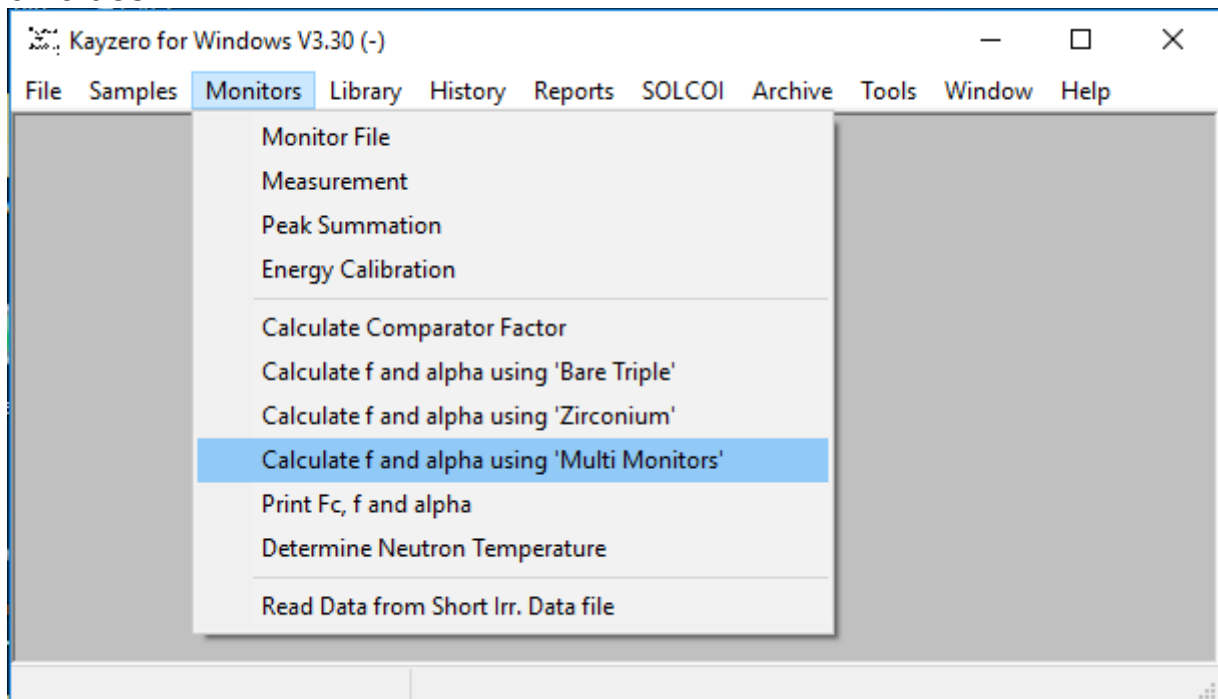


Figure 6.1: Monitor Analysis Menu.

#### 6.1.1 Calculate $f$ and $\alpha$ using the Zirconium-method

A special case of the 'Bare Triple' method is the use of a gold and a zirconium monitor couple. In this case, the gold-aluminum alloyed wire and a zirconium foil have to be irradiated simultaneously together with the sample. The day after the irradiation the gold monitor (Au-198) and the zirconium monitor (Nb-97m) should be measured briefly at the reference position. After another few days the zirconium foil should be measured a second time (for Zr-95) at a lower position, e.g. 1 or 2.

The screenshot shows a software window titled "f AND alpha CALCULATION using 'ZIRCONIUM'". It contains the following elements:

- Monitor file identification or "f":** A dropdown menu with "BR1Y4" selected.
- Gold Meas., Zr First Meas., Zr Second Meas.:** Three empty dropdown menus.
- Interim results:** An unchecked checkbox.
- Print all info per line:** An unchecked checkbox.
- Buttons:** "OK" and "Cancel" buttons at the bottom.

Figure 6.2: Zirconium-method calculation screen.

The data for these measurements should be entered using *Monitors/Measurement*-option and can then be used for  $f$  and  $\alpha$  calculation using this screen (see Figure 6.2). The result of the  $f$  and  $\alpha$  calculation will be displayed with the calculated values. They are stored in the data record of the second Zirconium measurement. The results can be printed using *Monitors/Print Fc, f and alpha* or plotted and printed using *History/Reactor Calibration*.

For an optimum use of the options we recommend using as monitor identification code AU or ZR combined with a number (AU1/ZR1) and using measurement identification codes consisting of simple numbers in combination with an irradiation code, e.g. SCK7V:1 and SCK7V:2.

### 6.1.2 Calculate $f$ and $\alpha$ using the 'Multi Monitor'-method

Multi Monitor method to calculate  $F_c$ ,  $f$  and  $\alpha$  can handle a set of maximal 12 monitors (radionuclides). These radionuclides must be well chosen with respect to their nuclear data (see the  $k_0$  standardization literature and Vade Mecum)<sup>1</sup>.

Enter the monitor measurements using the *Monitors/Measurements Data input* screen, enter the radionuclides as 'Comparator isotope'. When measuring a monitor under Cd you need to enter an  $f$  equal to 0. You can choose to use the Cd-ratio, Cd-covered or bare-method, see Figure 6.3.

Monitor File Identification: BR1Y4

	Monitor	Measurement Bare Monitor	Measurement Cd Covered
1	AU198	607:1	607:1CD
2	CO60	607:1	607:1CD
3	MN56	607:1	607:1CD
4	MD101	607:1	607:1CD
5	NP239	607:1	607:1CD
6	PA233	607:1	607:1CD
7		607:1	607:1CD
8	TC99M	607:1	607:1CD
9	ZN65	607:1	607:1CD
10			
11			
12			

☐ Interim results      Method: ☒ Cd-Ratio   ☐ Bare   ☐ Cd-Covered

OK   Cancel   Manual Input   S84   Y4   Load Set   Save Set

Figure 6.3: Multi-monitor method for f and alpha calculation.

Please check the Vade Mecum for the explanation of the multi-monitor method and the monitors to use.

The input needed for Figure 6.3 can be stored in a data file using the button <Save Set>, you can of course load the data using the <Load Set> button.

The 'Interim results' checkbox allows you determine your own averaged 'comparator factor' ratios from selected gamma-lines. Using the <Manual Input> you can enter these manually determined Cd-ratios if you like, see Figure 6.4.

Calculations Input form

Monitor File Identification: BR1

	Monitor	Measurement Bare Monitor	Measurement Cd Covered	Ratios	Std. Dev. (%)
1	AU198	607:1	607:1CD	3.653	0.533
2	CO60	607:1	607:1CD	25.503	0.454
3	MN56	607:1	607:1CD	43.830	1.920
4	MO101	607:1	607:1CD	4.263	2.000
5	NP239	607:1	607:1CD	1.448	4.000
6	PA233	607:1	607:1CD	5.189	0.220
7		607:1	607:1CD	0.000	0.000
8	TC99M	607:1	607:1CD	1.948	0.512
9	ZN65	607:1	607:1CD	29.907	0.504
10				0.000	0.000
11				0.000	0.000
12				0.000	0.000

☐ Interim results      Method: ☒ Cd-Ratio    ☐ Bare    ☐ Cd-Covered

BR1 Y4 June 2005

OK    Cancel    Automatic    S84    Y4    **Load Set**    Save Set

Figure 6.4: Entering manually determined Cd-ratios.

After pushing the <OK>-button  $f$  and  $\alpha$  are calculated resulting in a plot and a printed output (see Figure 6.5 and 6.6).

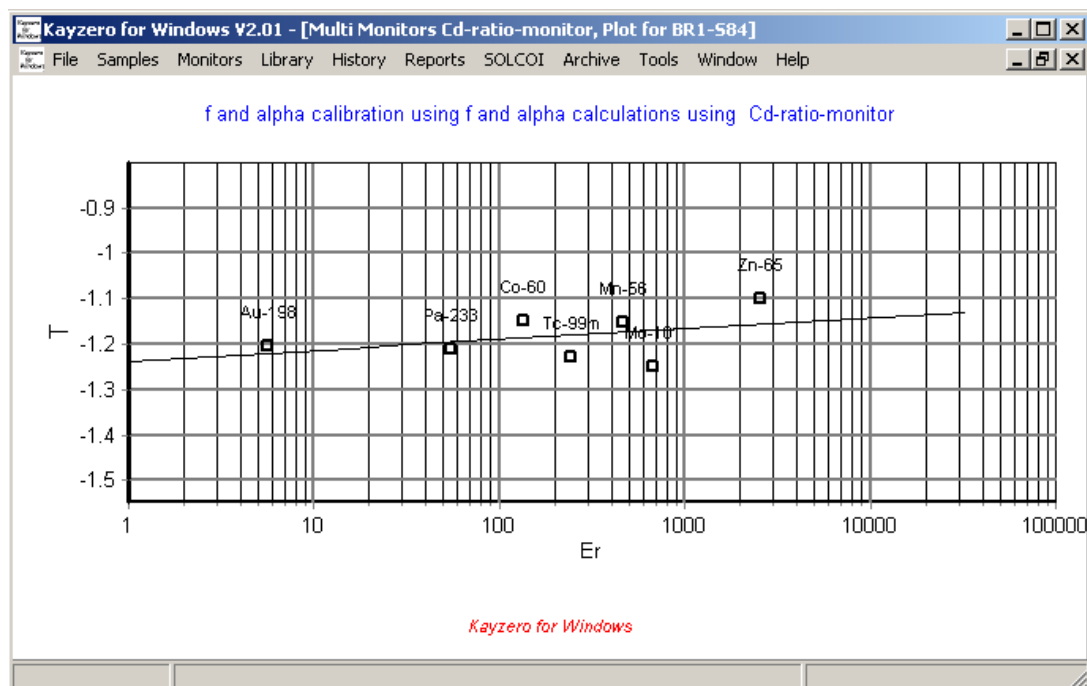


Figure 6.5: Plot of Cd-ratio multi monitor f and alpha determination result.

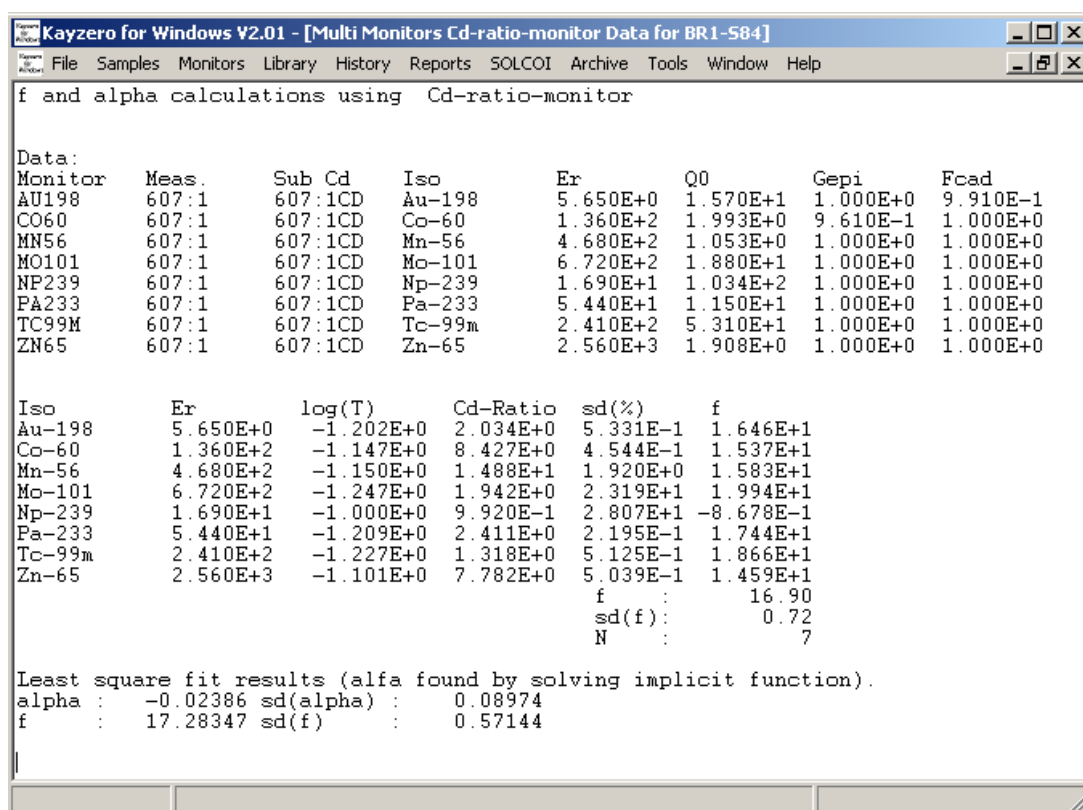


Figure 6.6: Print of Cd-ratio multi monitor f and alpha determination result.

## 6.2 Kayzero Library

In figure 6.7 the library options are given.

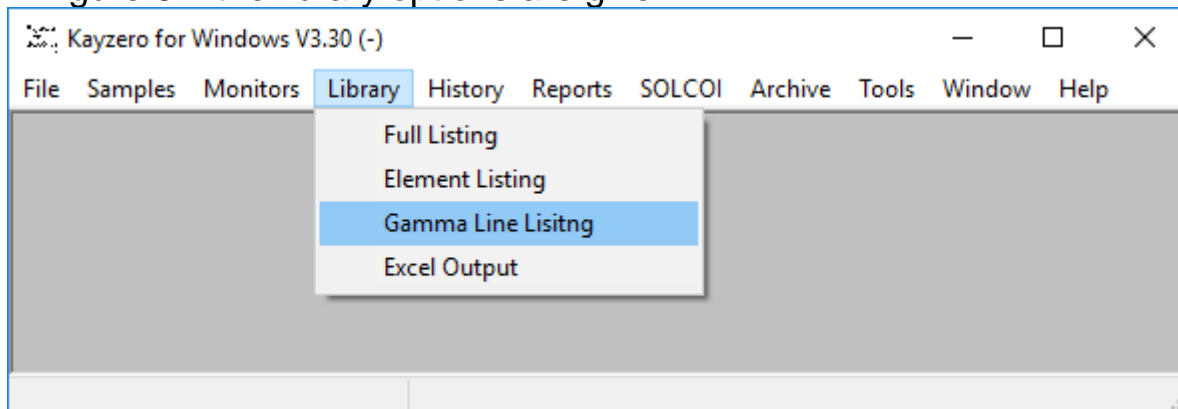


Figure 6.7: Kayzero Library menu.

### 6.2.1 Printing the Full Library

Notice that some elements are marked with an asterisk. These elements do not have gamma lines with a recommended  $k_0$  factor and should not be used for analysis. The data for these radionuclides have been added only for spectral interference correction and isotope/peak identification. For an explanation of the data, please check Appendix 7.

### 6.2.2 Printing data for a specific Element

Instead of printing the full library this output will print only data for selected elements.

### 6.2.3 Gamma Line Listing

Using this option the gamma lines in the library can be listed in order of increasing energy. This list can be used for spectrum evaluation and isotope identification, see Appendix 8.

### 6.2.4 Excel output

This option will make an Excel file with data in the library that looks similar to the k0-Database.

## 6.3 Reports Menu

All NAA results (typically concentrations) can be printed using the Reporting Menu: Reports see Figure 6.8. Most of these concentration reports are given in Section 3.6.

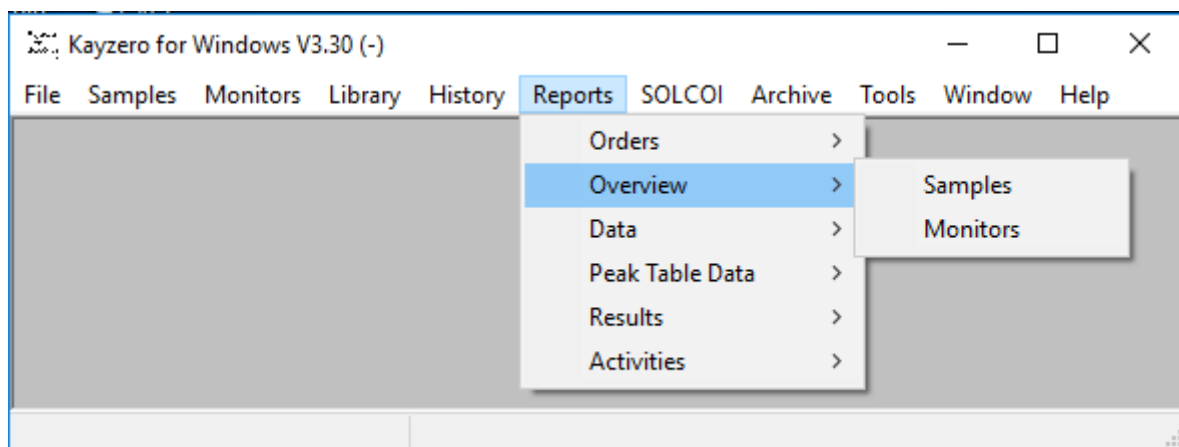


Figure 6.8: The Reports Menu

### 6.3.1 Print a list of Orders

Using Reports/Orders, you can list all orders and monitor files. You can make various types of order lists, depending on the selections you make in the screen shown in figure 6.9.

The image shows a screenshot of the 'Input for order list' dialog box. It features several input fields and checkboxes. On the left, there are four fields: 'Order identification' (with a dropdown arrow), 'Client' (with a dropdown arrow), 'Institute/Section' (with a dropdown arrow), and 'Budget number' (with a dropdown arrow). To the right of these fields are three checkboxes: 'Print Info', 'Print directories', and 'Sort to section+client name'. Below these fields and checkboxes is a section containing three rows of date range selectors. Each row has a date input field (defaulting to '01/01/1980'), a label (e.g., '<= date order received'), and another date input field (defaulting to '06/08/2017'). At the bottom of the dialog box are two buttons: 'OK' and 'Cancel'.

Figure 6.9: Input screen for printing lists of orders.

The lists can be sorted according to order identification or according to the combination institute/client (see the check boxes). The irradiation codes or the directories in which the measurement data are stored can also be printed.

## 6.3.2 Printing a list Measurements

Using the standard input selection screen a list of all measurements in an order can be made. This is the same option as is used in Chapter 3.

## 6.3.3 Printing a list Measurements

Per measurement a print can be made with all entered data, *Reports/Data*, see Figure 6.10.

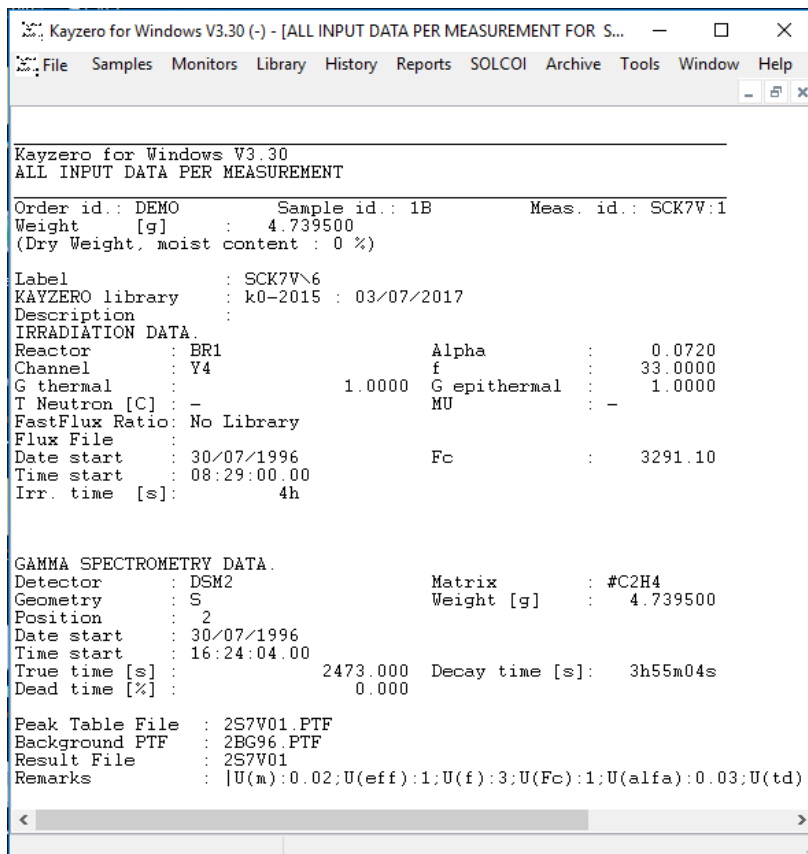


Figure 6.10: Printout of all measurement data for order: DEMO; sample: 1B; measurement SCK7V:1.

### 6.3.4 Printing the peak table file

The peak-table data file, including the parameters of the measured gamma-ray spectrum, can be printed using *Reports/Peak Table Data* (see Figure 6.11). You can print peak table files of the measurements of samples and monitors.

REPORT - PEAK DATA SAMPLE ORDER (640)

Order identification or "text"

Sample identification or "text"

Measurement identification or "text"

☒ Interference Correction

☒ Isotope Identification

Parameters for peak explanation.

Energy window in keV (one sided)

Figure 6.11: Input screen for printing the peak table file.

KAYZERO will recognize a peak in the measured spectrum if the KAYZERO Library contains a matching gamma line within the energy window (see Figure 6.12). If the measurement data have been previously calculated, it is possible to use only identified radionuclides for peak identification (see Figure 6.11).

If an LFC dual spectrum measurement is found, the weighing factor LFC-W is calculated. This is the ratio of the gross number of counts of a peak in the corrected spectrum and the gross number of counts in the same area in the uncorrected spectrum.

If the area of a peak was corrected for a peak in the detector background, the peak area without the background correction is also given ('without BS').

Kayzero for Windows V3.30 (-) - [REPORT - PEAK DATA SAMPLE ORDER (640) DEMO-1B]

File Samples Monitors Library History Reports SOLCOI Archive Tools Window Help

---

Kayzero for Windows V3.30  
 REPORT: PEAK DATA  
 Order id.: DEMO Sample id.: 1B Meas. id.: SCK7V:1

KAYZERO LIB. : k0-2015 : 03/07/2017 +/- 0.70 keV  
 Sample weight : 4.739500 g (Dry Weight, Moist content = 0 %)

IRRADIATION PARAMETERS:  
 BR1/Y4 f = 33.0000 Alpha= 0.0720 Fc = 3291.10  
 30/07/96 08:29:00 ti= 14400 s  
 Flux Correction file =  
 Neutron Temperature [C] = - MU = - FastFlux Ratio = No Lib

MEASUREMENT DATA:  
 2S7V01.PTF ( 55 peaks, 9- 4064 keV, 0.49594\*ch + 1.20261, N=8192 LFC)  
 Background interval = 3.00 \* FWHM in keV SD is calculated by KAYZERO.  
 FWHM = 1.359 + 6.1E-4 \* E + 0.000 \* E^2 + 0.000 \* E^3 (E in keV)  
 30/07/96 16:24:04 tm= 2473 DTS= 0.0 % td= 3h55m04s  
 DSM2 S pos= 2 matrix = #C2H4 4.740 g Background : 2BG96.PTF

Energy [keV]	Area [counts]	LFC-Backgr. [counts]	SD [%]	LFC-W [-]	Identification +/- 0.60 keV
51.29	0.0	10181.0	0.00	( 1.03)	Rh-104m*
124.12	710.4	14770.7	24.81	( 1.03)	Ba-131 Er-171
166.08	182068.7	12785.7	0.25	( 1.03)	Ba-139
216.17	506.6	13298.5	32.95	( 1.03)	Tb-160 Ru-97 Ba-131
268.29	592.4	10648.1	25.30	( 1.03)	Nd-149*
386.08	248.6	5926.4	44.85	( 1.03)	Eu-152D
417.24	308.7	5298.9	34.29	( 1.03)	In-116m
438.67	67171.2	4999.9	0.42	( 1.03)	Zn-69m
479.74	242.1	4659.5	40.90	( 1.03)	Ga-72 Y-90m W-187
487.23	363.2	4629.9	27.34	( 1.02)	La-140
492.26	157.9	4610.1	62.06	( 1.02)	Cd-115
496.30	686.6	4594.1	14.66	( 1.03)	Ba-131
511.00	5663.6	4824.1	2.22	( 1.03)	Mo-101D Cu-64 Zn-71
Without BS:	5688	4824	2.21		

Figure 6.12: A print of a peak table file

All reporting options related to concentrations are discussed in Chapter 3.  
 Printing all element concentrations are discussed in Chapter 3.

## 6.3.5 Printing Activities

The screenshot shows the Kayzero software interface. The top window is a dialog box titled "REPORT - ACTIVITIES SAMPLE ORDER (658)". It contains three dropdown menus for "Order identification or 'set'", "Sample identification or 'set'", and "Measurement identification or 'set'", with values "DEMO", "1B", and "SCK7V:1" respectively. There are checkboxes for "Interference Correction" and "Isotope Identification", both of which are checked. A "Minimum activity" field is set to "100 Bq". Below this, there are radio buttons for "2h", "3 months", and "1 year after end of irradiation", with "2h" selected. At the bottom are "OK" and "Cancel" buttons.

The bottom window is the main application window titled "Kayzero for Windows V3.30 (-) - [REPORT - ACTIVITIES SAMPLE ORDER (658) DEMO-1B]". It has a menu bar with "File", "Samples", "Monitors", "Library", "History", "Reports", "SOLCOI", "Archive", "Tools", "Window", and "Help". The main area displays the following text:

```
Kayzero for Windows V3.30
REPORT: ACTIVITIES

RE values are from user edittable file Kayzero.RE in program root directory, check 1
Activity after 2 hours after irradiation, higher than 100 Bq.
```

Below this text is a table with the following columns: Order, Sample, Measurement, Nuclide, Activity [kBq], SD [%], and RE [Sv].

Order	Sample	Measurement	Nuclide	Activity [kBq]	SD [%]	RE [Sv]
DEMO	1B	SCK7V:1	Na-24	1.0547E+0	1.13	2.130E-11
DEMO	1B	SCK7V:1	Cl-38	1.1742E+1	1.62	2.371E-10
DEMO	1B	SCK7V:1	Ar-41	1.3891E+2	0.75	2.8060E-9
DEMO	1B	SCK7V:1	Mn-56	1.7150E+1	0.26	3.464E-10
DEMO	1B	SCK7V:1	Zn-65	2.4416E-1	4.57	4.932E-12
DEMO	1B	SCK7V:1	Zn-69m	3.2052E+0	0.41	6.474E-11
DEMO	1B	SCK7V:1	Br-80	1.1241E+0	11.46	2.270E-11
DEMO	1B	SCK7V:1	Br-82	2.4517E-1	2.77	4.952E-12
DEMO	1B	SCK7V:1	In-116m	1.1972E+1	0.67	2.418E-10
DEMO	1B	SCK7V:1	Sb-122	1.4707E-1	5.52	2.970E-12
DEMO	1B	SCK7V:1	Ba-139	4.2936E+1	0.25	8.673E-10

Below the table, there is a section titled "Activity per Sample" with a horizontal bar chart showing the activity levels for each sample.

Figure 6.12A: Printing activities.

This option allows you to check the amount of activity produced directly (2 hrs) after irradiation, after the analysis (3 months) and after storage (1 year). All kinds of cross sections can be made.

## 6.4 Archive System

All NAA data are divided into sample data and monitor data. A group of (gamma spectrometric irradiation/measurements of) samples is combined into an order (data file). One order file may contain up to 500 sample measurements. Every measurement is unambiguously defined by:

- an order identification code (the name of the data file),
- a sample identification code and
- a measurement identification code.

It follows that an order file can comprise several samples. In a certain project X, for example, some samples may be irradiated and measured 4-6 times. The order file will then contain the data of the samples and the irradiations/measurements of these samples.

The same structure is used for monitors. The monitor data are combined into a monitor file where the monitors can be presented together in an overview.

For deleting, renaming etc. of measurement identification codes and other file maintenance operations the Archive menu can be used (see Figure 6.13).

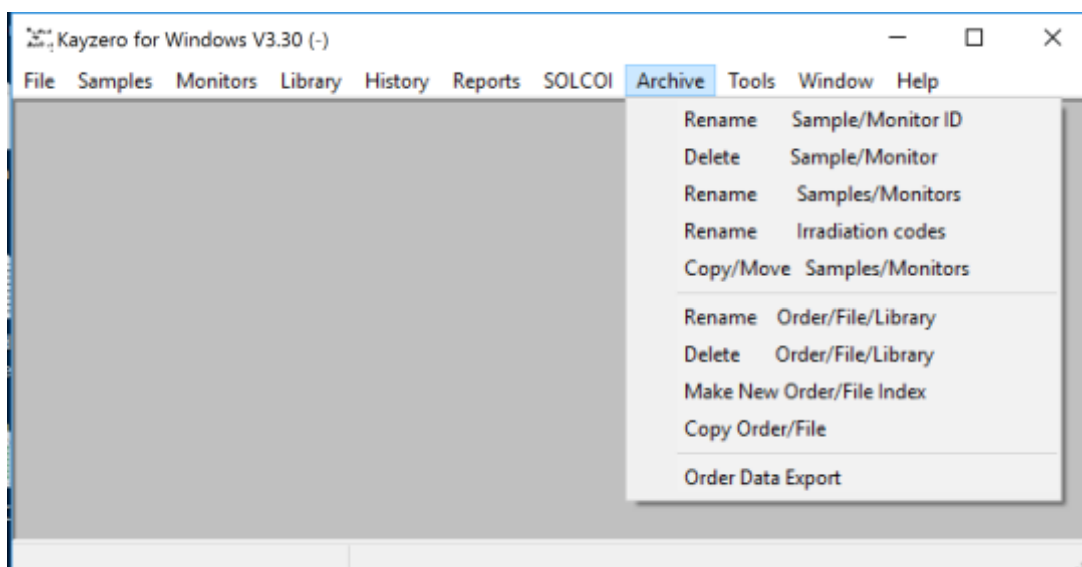


Figure 6.13: Archive menu.

# 6.5 Special Options Menu

The Special Options menu offers additional utilities (see figure 6.14).

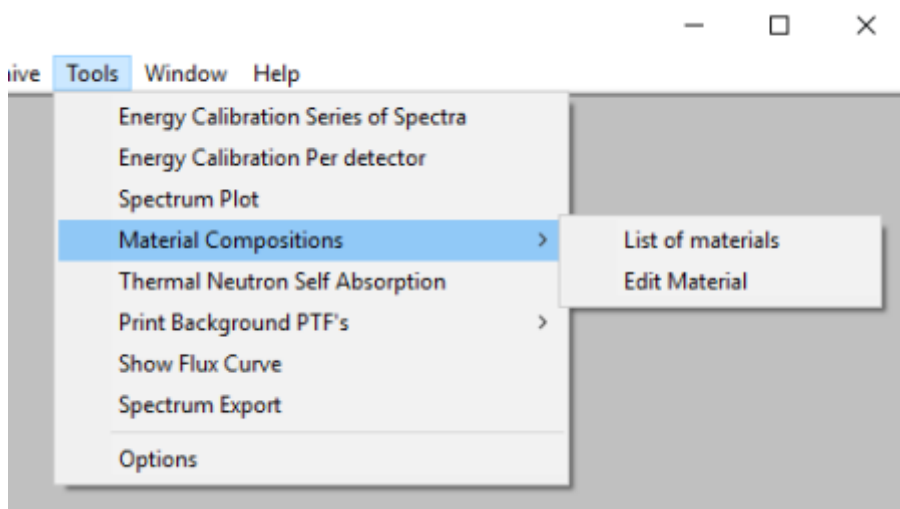


Figure 6.14: Tools

## 6.5.1 Energy Calibration (Series of Spectra)

The Energy Calibration option, can be very useful for performing an energy calibration based on the measured spectrum. The energy calibration is very important for proper program performance. Erroneous energy calibration may lead to unreliable results.

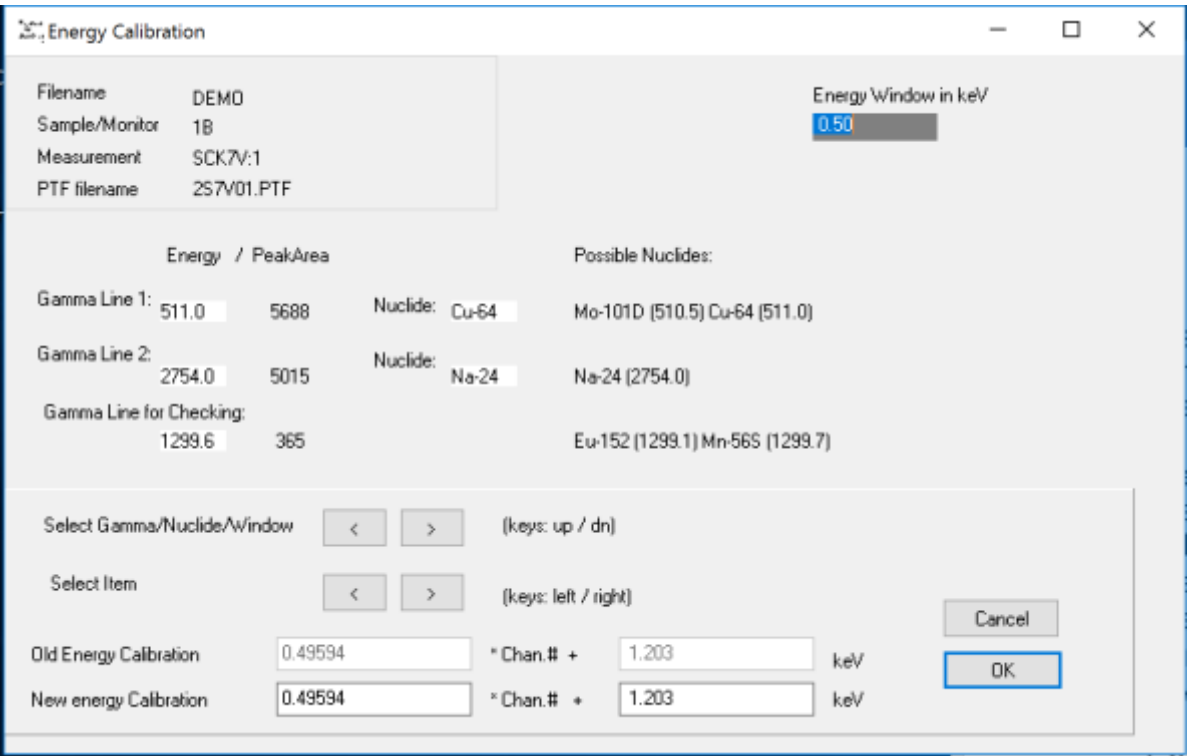


Figure 6.15: Energy calibration

It is advised to perform an energy calibration at least once a week or to perform an energy calibration on every spectrum using this option. For the energy calibration a first-order approximation ( $E = a \cdot Ch + b$ ) is used.

The energy calibration is performed by selecting for two gamma rays in the spectrum the corresponding radioisotopes (see Figure 6.15). The radioisotopes are found in the KAYZERO Library. The energy window can be changed in steps of 0.5 keV using  $\langle \uparrow \rangle$  and  $\langle \downarrow \rangle$ . If you press  $\langle \rightarrow \rangle$  the first energy is activated. By pressing  $\langle \uparrow \rangle$ , a higher energy can be selected. When a good peak is found, press  $\langle \rightarrow \rangle$  again; the corresponding radioisotope can then be selected from the list using  $\langle \uparrow \rangle$  and  $\langle \downarrow \rangle$ .

In short, to move to another field you should use  $\langle \leftarrow \rangle$  and  $\langle \rightarrow \rangle$  and to select another energy or isotope you should use  $\langle \uparrow \rangle$  and  $\langle \downarrow \rangle$ . The new energy calibration is also presented on this screen.

You can check the energy calibration again or even alter it by hand, see figure 6.15.

For energy calibration of a series of spectra a special option is available. The program will ask the directory where the spectra are located (See Figure 6.16). The  $\langle \text{Select Directory} \rangle$  button can be used to find a specific directory. The spectra to be calibrated can be selected using a wildcard. The new energy calibration can be given by hand or by performing a prior normal energy calibration, the found calibration will be shown here.

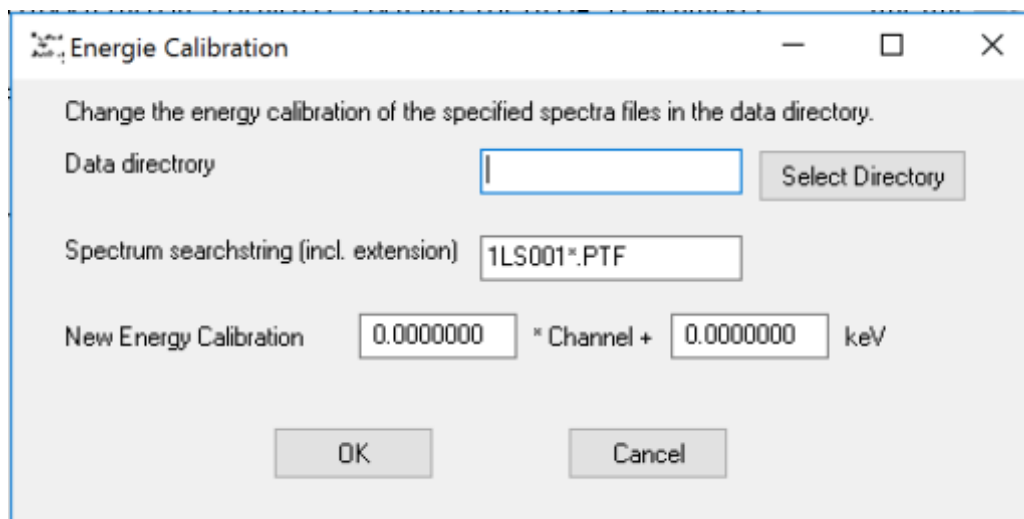


Figure 6.16: Energy Calibration for a series of samples screen.

Because the energy calibration is detector specific, it is also possible to change the energy calibration of all measurements in a series of measurements to be selected in Figure 6.16A on a specific detector.

**Change Energy Calibration**

Peak Table File: **257V01.PTF (1B/SCK7V:1)**

Old Energy Calibration:  \* Channel +  keV

New Energy Calibration:  \* Channel +  keV

Buttons: OK, Do not Change, Stop Batch

---

**Energy Calibration Per Detector**

Order identification or "":

Sample identification or "":

Measurement identification or "":

Detector:

Buttons: OK, Cancel

Figure 6.16A: Energy calibration of measurements within a series of measurements that were performed on a specific detector.

## 6.5.2 Spectrum Plot

The spectrum can be plotted using *Tools/Spectrum Plot*, see Figure 6.17. If an LFC dual spectrum was found, the ratio between the corrected and uncorrected spectrum (W) will be plotted below the corrected spectrum. If the count rates changed during the measurement, gamma lines showing serious decay will be visible in this plot.

By clicking the lines, you can print all found gamma peaks in the plot. Some gamma spectrum deconvolution programs might lose peaks. However, it is also nice to see how many peaks you have spread over the spectrum.

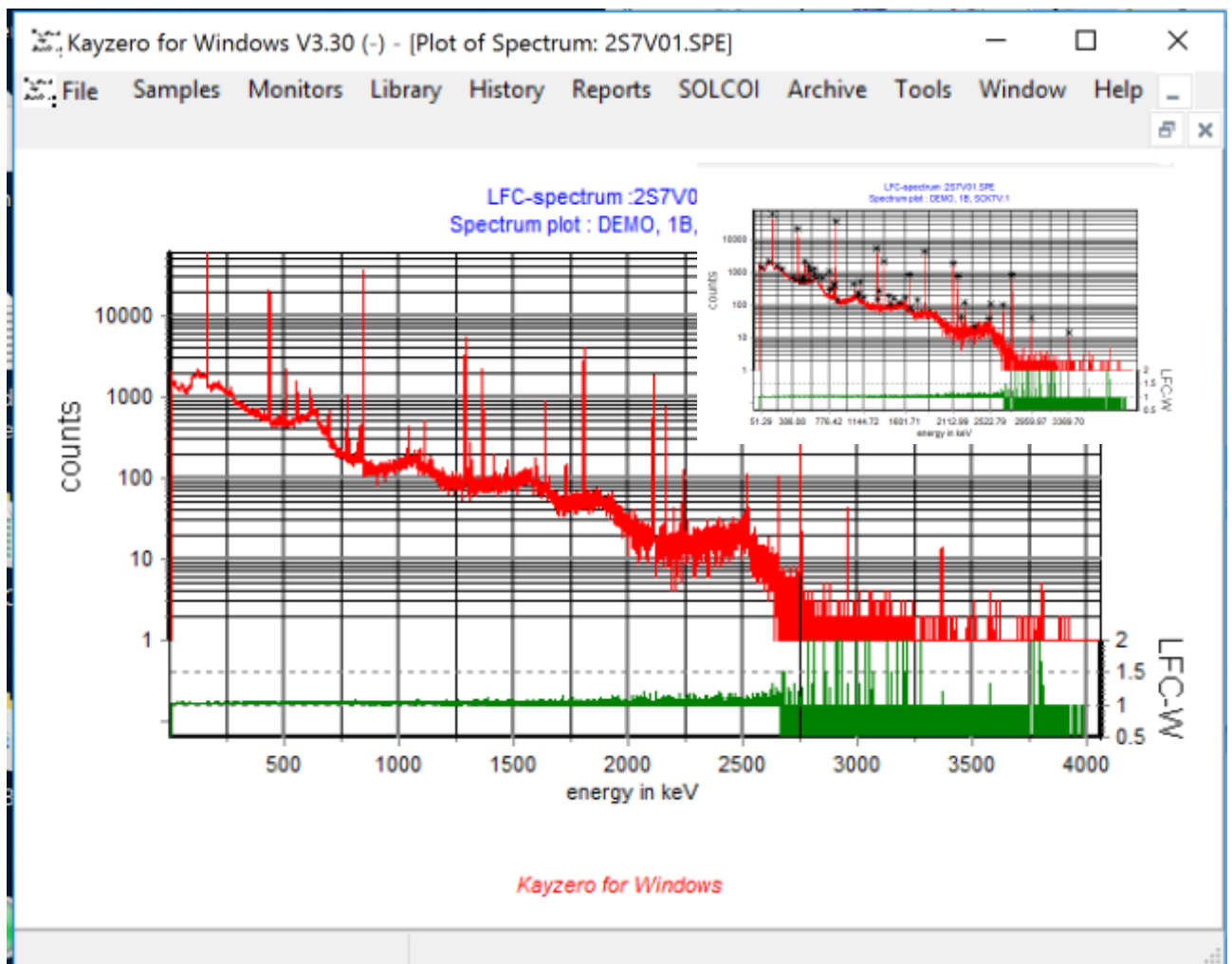


Figure 6.17: Spectrum plot ('In set': by clicking on the spectrum the found peaks are marked with an 'x').

## 6.5.3 Thermal neutron self-shielding

Thermal neutron self-shielding is handled in accordance with Erdtmann and Petri<sup>5</sup> and Chilians method, see also Figure 6.18. You can print a table for both methods if you like.

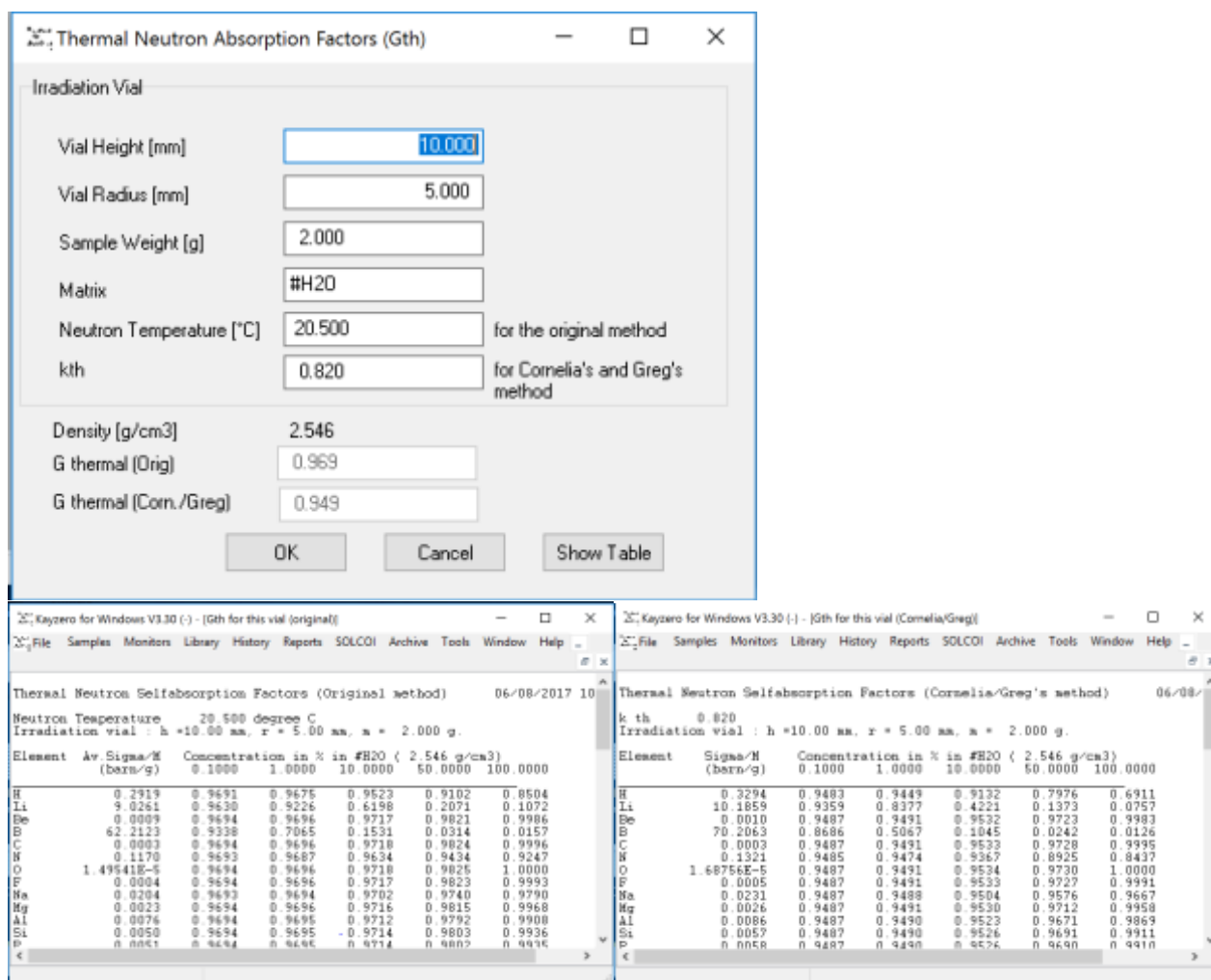


Figure 6.18: Neutron thermal self-shielding option, input and a part of both results.

## 6.5.4 Calculation Parameters

Some of the calculation and evaluation parameters can be changed using *Tools/Options*. These parameters are explained in Appendix 6. The algorithms used are explained in Appendix 4.

## 6.5.5 Directories

The relevant data used by KAYZERO are stored in several special directories. These directories can be changed using *Tools/Options/Directories*, if necessary (see Figure 6.19).

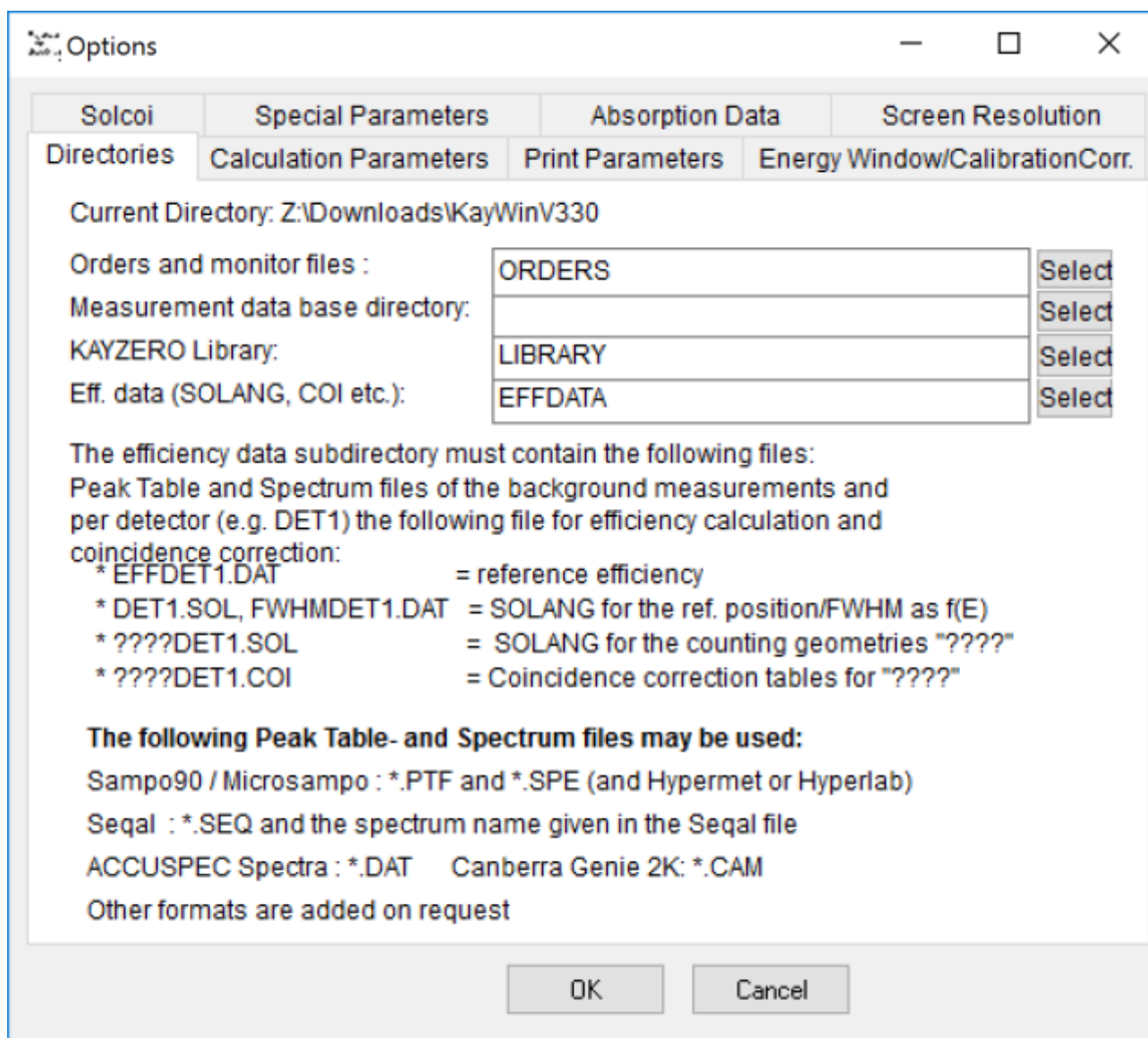


Figure 6.19: Data directories

When you indicate you want to change a directory the program checks whether the directory exists. If the directory is not valid there will be a beep and the cursor will not advance to the next field. Please check the directory or enter another directory.

“Orders and monitor files” directory

In this directory, the files are stored that are created for each order and each channel (data and index files). These files are administrated in a special file.

“Measurement data base” directory

One can use this directory to locate the directories in which all spectra and peak table files are stored. Consequently, the calculated concentration files (".ber") are stored in this directory.

The following Peak Table- and Spectrum files may be used:

Sampo90/MicroSampo	: *.PTF and *.SPE
Seqal	: *.SEQ and the spectrum name in the Seqal FILE
ACCUSPEC Spectra	: *.DAT
Genie2K	: *.CAM

Subdirectories can be indicated in the measurement names. As example: when the data base directory is ...\  
and the spectra are stored in ...\  
SCK7V, then the measurement identification in Kayzero (this is not the spectrum name) is SCK7V:1. ":1" indicates this is the first measurement of this sample on this directory.

In our case we have a code for each irradiation batch (e.g. SCK7V), all spectra of samples irradiated during this irradiation are stored in the corresponding directory. The irradiation batch is in our case a set of irradiations on one day in one channel.

A sample can be irradiated in several irradiation batches.

The above described method allows the combination of many measurements and irradiations. Up to six measurements can be combined in a result. The measurements can be selected by using wildcards like "SCK7V\*" or "\*:1".

"KAYZERO Library" directory :

This is the directory in which the library is stored.

"Efficiency data (SOLANG, COI etc.)" directory

The efficiency data subdirectory must contain the following files per detector (e.g. DET1):

- \* Peak Table and Spectrum files of the background measurements
- \* and files for efficiency calculation and coincidence correction:
  - EFFDET1.DAT = reference efficiency
  - DET1.SOL = SOLANG for the ref. position
  - FWHMDET1.DAT = FWHM as f(E)
  - ?????DET1.SOL = SOLANG for the counting geometries "????"
  - ?????DET1.COI = Coincidence correction tables for "????"

If one would like to convert an old system to the above described method (using subdirectories in a measurement base directory) the procedure for an

order is:

- copy the specific order files (.DTA) and index files (.DTX) to the orders directory
- change the directories according to the new method
- add the order to the system using option *Samples/Order Input*
- add the measurement subdirectory name to measurement name using option 851 in the DOS-Version.

All measurement data can stay on the original directory.

This procedure should be used for all subdirectories.

For monitors things are a little more difficult. Every irradiation/measurement should be added to the new, channel/reactor specific, monitor file.

# References

---

1. F. DE CORTE and A. SIMONITS, J. Radioanal. Nucl. Chem., 133 (1989) 3-41.
2. F. DE CORTE and A. SIMONITS, J. Radioanal. Nucl. Chem., 133 (1989) 43-130.
3. F. DE CORTE and A. SIMONITS, VADE MECUM FOR  $k_0$  - USERS (1994)
4. L. MOENS, J. DE DONDER, X. LIN, F. DE CORTE, A DE WISPELAERE, A. SIMONITS and J HOSTE, Nucl. Instrum. & Methods, 187 (1981) 451.
5. G. ERDTMANN and H. PETRI, Nuclear Activation Analysis: Fundamentals and techniques, from Treatise on Analytical Chemistry, Second Edition, Part 1, Volume 14, John Wiley and Sons Inc. New York (1986)
6. K. DEBERTIN and R.G. HELMER, GAMMA-AND X-RAY SPECTROMETRY WITH SEMICONDUCTOR DETECTORS, North Holland, Elsevier Science Publishing Company, Inc. Amsterdam, 1988.
7. E. STORM and H.I. ISRAEL, Photon Cross Sections from 0.001 to 100 MeV for Elements 1 through 100, Los Alamos Scientific Laboratory of the University of California, 1967.

# Appendix 1: Efficiency Calculation.

---

In view of the extensive calculations which must be done for efficiency determination and coincidence correction, counting geometries have to be standardized as much as possible. For these standardized geometries, SOLANG (effective solid angle,  $\Omega$ ) and COI (coincidence correction) tables are pre-calculated and stored in files which can be accessed by KAYZERO. Enter only the detector name, geometry and position.

Using the method described by Moens et al. in [Ref] the efficiency for bulky sources can be calculated from:

$$\varepsilon_p = \frac{\Omega}{\Omega_{\text{ref}}} * \varepsilon_{\text{ref}}$$

where  $\Omega$  and  $\Omega_{\text{ref}}$  are the effective solid angles, which are calculated using the SOLANG program developed at the Institute for Nuclear Science of the Gent University, Belgium for cylindrical samples on the detector axis and with a diameter smaller than the crystal.

[Ref]: L. Moens et al., Calculation of the absolute peak efficiency of gamma-ray detectors for different counting geometries, Nucl. Instr. and Meth., 187 (1981) 451-472.

# Appendix 2: Kayzero/SolCoi Files

---

## Description of Kayzero files

\*.EXE : executable files

\*.ABS : contains the name and location of mass absorption data and material composition data files. The material data filename and location can be edited using the appropriate option in KAYZERO or SOLCOI.

KAYWIN.EXE etc.

: programs.

SOLCOIS, SOLCOINA, SOLCOINB, SOLCOINC, SOLCOIND and SOLCOINE: the MS Fortran versions of the INW Gent programs SOLANG and COINCALC. COINCALE is split into five separate programs. The programs all use the same input file (\*.SIN) produced by SOLCOI and must be used in the given order. These programs are started from within Kayzero for Windows. For 32 bits and 64-bit Windows versions the latest SOLCOI programs (from 2006) have to be used.

KAYZERO.DAT and SOLCOI.STA

: are status program specific system files.

KAYZERO.IRR:

:  $f$ ,  $\alpha$  and  $F_c$  data of irradiation facilities. This file can be edited and extended using the DOS EDIT command.

KAYZERO.MON:

: monitor data. This file can be edited and extended using the DOS EDIT command.

KAYZERO.BUR:

: burn-up data for the most serious cases. If this file is not present burn-up correction is not performed.

KAYZERO.FIS:

: fission correction data. If this file is not present fission correction is not performed.

"reactor&channel".PAR:

: files containing the reaction interference correction factors for the specific channel. The name is a concatenation of the channel and reactor code used in KayWin. The length should not exceed 8 characters.

SOLCOI.TIM

: file containing the calculation times for effective angle and coincidence correction factor calculation; valid for the computer system on which SOLCOI was running.

SOLCOIS.DAT

: Gauss-Legendre interpolation constants for SOLCOIS.EXE

COIV4.DAT

: data file for the SOLCOINx.EXE files with all the radionuclides and energies for which the coincidence correction factors must or can be calculated.

SOL.TMP : this is an output file of SOLCOIS (SOLANG) produced during the last calculation of an 'effective solid angle' result file (.SOL file); SOL.TMP contains most of the given input.

MU-FIN.COE

: mass absorption data file

NAA.DAM

: material composition data file

List of the efficiency data needed for KAYZERO and SOLCOI, as well as the result and input files of SOLCOI in the directory KAYZERO\EFFDATA:

Special KAYZERO format

FWHMDSM2.DAT

- full-width at half maximum in keV as a function of energy in keV. This file is necessary for calculation of the Compton background in the spectrum. If no file is found, a constant FWHM of 2 keV is used.

- LFC dual spectrum on or off. It is impossible for the program to detect whether a dual LFC spectrum is recorded so it has to be indicated in this file for each detector.

\*.BLK- element content of the blank irradiation container (see fig 3.23)

Special SOLCOI format

DSM2.DET

- detector geometry parameters.

PTB.SRC

- PTB geometry (calibration source) parameters.

???.SRC

- source geometry parameters.

DSM2.FIT - fit parameters used to fit the efficiency curve.

ASCII files:

EFFDSM2.DAT

- reference efficiency for SOLANG (SOLCOIS).

PTTDSM2.DAT

- peak-to-total ratio for all positions.

DSM2.SOL

- calculated reference effective solid angles.

n???DSM2.SOL

- calculated effective solid angles.

n???DSM2.COI

- calculated coincidence correction factors.

Legends:

DSM2 is a detector/source-holder combination identifier.

??? is a possible standardized sample geometry.

PTB is the PTB calibration source geometry.

n is a number ranging from 1 to 5: used for matrix interpolation data files

# SolCoi Files in Efficiency Directory

## Special SolCoi format

DSM4.DET

- detector geometry parameters

PTB.SRC

- PTB geometry (calibration source) parameters

???.SRC

- source geometry parameters

## ASCII-files:

EFFDSM4.DAT

- reference efficiency for COINCALC

PTTDSM4.DAT

- peak-to-total ratio for all positions for COINCALC

DSM4.SOL

- calculated reference effective solid angles for COINCALC

n???DSM4.SOL

- calculated effective solid angles

n???DSM4.COI

- calculated coincidence correction factors

DSM4\*.CAL

- measured data for efficiency and PTT-ratio curve fitting

DSM4\*.FIT

- used parameters for efficiency and PTT-ratio curve fitting

DSM4.FIN

- measured data for the fine tuning

DSM4.RES

- interim results for the fine tuning

YOURLIST.CLS and COIV4.CLS

- energies and isotopes for coincidence and efficiency calculation

## Legends

DSM4 is a detector/source-holder combination identifier.

??? is a possible standardized sample geometry.

PTB is the PTB calibration source geometry.

n is a number ranging from 1 to 5: used for matrix interpolation data files.

# File Formats for SOLANG and COINCALC

**Reference efficiency:** ASCII-file  
(file name: EFF+'detector name'.DAT)

```

line    <position in file>
nr.      <11>
1:       ne
        <1-----10> <16-----25> <31-----40> <46-----55> <61-----70>>
2:       e0          e1          e2          ene
        <11>      <22>      <33>      <44>      <55>
3:       o1          o2          one
        <1-----10> <16-----25> <31-----40> <46-----55> <61-----70>>
4:       p1,0        p1,1        p1,2        p1,o1        p2,0
5:       p2,1        p2,2        p2,3        p2,n2        p3
6:       p3,1        p3,2        p3,3        p3,n3

```

where:

ne = number of energy regions (max. 4)  
e<sub>0...ne</sub> = energy of the beginning and/or end of a region  
o<sub>1...ne</sub> = order of the fits (max. 3)  
p<sub>i,j</sub> = parameter for region i and order j.

$$\text{For region } i: {}^{10}\log(\varepsilon) = \sum_{j=0}^{o_i} p_{i,j} \{ {}^{10}\log(E) \}^j$$

**Peak-to-total:** ASCII-file  
(file name: PTT+'detector name'+.DAT)

```

1:       ne          {position 1}
2:       e0          e1          e2          ene
3:       o1          o2          one
4:       p1,0        p1,1        p1,2        p1,o1        p2,0
5:       p2,1        p2,2        p2,3        p2,n2        p3,0
6:       p3,1        p3,2        p3,3        p3,n3
7:       ne          {position 2}
8:       etc.

```

This format is the same as that for the reference efficiency. This file contains the PTT for all positions on the source holder. For positions higher than the reference position PTT can be taken equal to that of the reference position.

## SOLANG and COINCALC input file: ASCII-file

(file name:'n'+source name+'detector name'+.SIN)

With n= 1..5 in case of a matrix interpolation source file.

{distance in cm, linear attenuation coefficient in 1/cm, energy in keV}

```
Type O in R en B                                     {comment}
RESEARCH\2ODSM4.SOL                                   {eff.solid angle file name}
RESEARCH\2ODSM4.COI                                   {coincidence corr. factor file
name}
RESEARCH\EFFDSM4.DAT                                   {ref. eff. data file name}
RESEARCH\PTTDSM4.DAT                                   {PTT data file name}
RESEARCH\DSM4.SOL                                       {ref. eff. solid angle data
file name}
COI.DAT                                                 {nuclide and gamma list file
name}
DSM4                                                     {detector data file
name (DSM4.DET) }
O                                                       {source data file name (O.SRC)}
  1.0000000000000000E+0000                             {density in g/cm3}
  7.21419629006732E-0002                             {volume of the vial/source in
cm3}
  2.5000000000000000E-0001                             {shaping time in us (for
COINCALC) }
#SiO2                                                  {matrix composition}
3                                                      {detector type}
  0.40500 0.14000 0.24000 0.2200017 5
{  r1      r2      r3      r4  ne np}
{r1=source radius; r2=height; r3=side wall thickness; r4=bot. wall
thickness;}
{ne=number of energies; np=number of positions;}
  1.10000 0.15000 0.03000 0.00000 3.04500 5.77000 0.45000 3.80000
{  s1      s2      s3      s4      s5      s6      s7      s8 }
{s1-s4=absorbers thickness; s5=crystal radius; s6=crystal height;}
{s7=inner core radius; s8=inner core height}
  0.00000                                     {contact layer thickness}
20202020                                     {number of integration points }
                                           {for non-point source}
20202020}
                                           {for disk source}
01242424}
                                           {for point source      01019696}
  40.00031.72550 0.00000 0.00000 0.00000
{ E      μ1      μ2      μ3      μ4 }
  0.000000000 0.000000000 1.27710000031.725500000 0.000000000
{  μ5      μ6      μ7      μ8      μ9 }
{μ: linear attenuation coefficient for E keV}
{μ1: detector crystal}
{μ2: source}
{μ3: vial wall}
{μ4: contact layer}
{μ5: Air}
{μ6-μ9: Absorbers 1-4}
```

```

50.00017.06650 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.83160000017.066500000 0.000000000
60.00010.16500 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.63990000010.165000000 0.000000000
80.000 4.70265 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.483300000 4.702650000 0.000000000
100.000 2.73385 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.421200000 2.733850000 0.000000000
150.000 1.35540 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.359509072 1.355400404 0.000000000
200.000 0.82390 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.321300000 0.823900000 0.000000000
300.000 0.56710 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.275400000 0.567100000 0.000000000
400.000 0.47936 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.247590000 0.479360000 0.000000000
500.000 0.42800 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.226530000 0.428000000 0.000000000
600.000 0.39055 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.209250000 0.390550000 0.000000000
800.000 0.33865 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.183870000 0.338650000 0.000000000
1000.000 0.30335 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.165240000 0.303345000 0.000000000
1500.000 0.24987 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.134598592 0.249866987 0.000000000
2000.000 0.21774 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.116370000 0.217745000 0.000000000
3000.000 0.18725 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.095850000 0.187250000 0.000000000
3500.000 0.18085 0.00000 0.00000 0.00000
0.000000000 0.000000000 0.089135188 0.180848259 0.000000000
{X}      {Y}      {X= distance from crystal to sample, Y=distance
through air}
2.12000 0.12000      {position 1}
4.12000 2.12000      {position 2}
8.12000 6.12000      {position 3}
15.1200013.12000{position 4}
25.1200023.12000{position 5}

{data used for the calculation of the above used linear
attenuation coeff.}
1000.0000#SiO2      {density in kg/m3 , material}
900.0000#C2H4
5350.0000Germanium
0.0000-
1180.0000PMMA
2700.0000Aluminium
5350.0000Germanium
0.0000-
DV      {user}
24/08/1992 08:10:37 {modification data & time}
0.00120000 {distance from platform to bottom of vial [m]}

```

**The typical size of a .SIN data file is 2,4 kBytes.**

## Effective solid angle: ASCII-file

(file name:'n'+source name+'detector name'+.SOL)

With n= 1..5 in case of a matrix interpolation source file.

```
line          <position in file>
nr            <11-15>   <26-30><31-----45><46-----60><61--->
  1:          n         p         volume      density      matrix
        <3-----15> <18-----30> <33-----45> <48-----60><63-----75>
  2:          e1         e2         e3         e4         e5
  3:          e6         e7         ...         ...
...
  4:          ...         en
  5:          sol1,1         sol1,2         sol1,3
sol1,4          sol1,5
  6:          ...         ...         ...         ...
  7:          sol1,n         sol2,1         sol2,2         ...
...
  8:          ...         ...         ...         ...
  9:          ...         sol2,n         ...         ...
...
 10:          ...         ...         ...         ...
 11:          ...         ...         ...         solp,n
where
```

n: number of energies,  
p: number of positions  
e: energy  
sol: effective solid angles

**The typical size for a '.SOL' file is 1.7 KByte.**

## Coincidence correction factors: ASCII-file

(file name:'N'+source name+'detector name'.COI)

With N= 1..5 in case of a matrix interpolation source file.

```
Volume vial          =      .87601   cm3
Number of positions  = 5
Coincidence factors for : type D in R, SiO2, 200 kg/m3
Detector DSM1
Pulse shaping time = 4.000 microsec.
Matrix material = #SiO2
Number of isotopes in data file : 160
NA24      2
 1368.6 keV      .94586      .98809      .99667      .99872
.99913
 2754.0 keV      .93892      .98708      .99644      .99861
.99910
MG27      3
 170.7 keV      .93331      .98632      .99628      .99854
.99908
 1014.4 keV      1.00239      1.00041      1.00010      1.00003
1.00002
AL28      1
SI31      1
S37      1
CL38      2
 1642.4 keV      .94369      .98775      .99659      .99868
```

**Appendix 2: KAYZERO/SOLCOI program, system and data files -A9-**

.99912				
2167.5 keV	.95635	.99066	.99741	.99900
.99934				
K42 2				
312.7 keV	.94011	.98724	.99647	.99863
.99910				
K43 10				
220.6 keV	.86143	.97243	.99267	.99707
.99825				
372.8 keV	.92676	.98536	.99607	.99844
.99904				
396.9 keV	.90148	.98055	.99483	.99794
.99876				
404.3 keV	.85631	.97091	.99221	.99689
.99812				
593.4 keV	.96897	.99368	.99821	.99923
.99954				
617.5 keV	.92028	.98461	.99592	.99837
.99903				
801.2 keV	.90148	.98055	.99483	.99794
.99876				
990.3 keV	13.29844	3.23029	1.55276	1.20258
1.11914				
1021.8 keV	.92068	.98471	.99595	.99838
.99903				
1394.6 keV	1.76175	1.13939	1.03475	1.01277
1.00752				
CA47 5				
489.2 keV	.93275	.98625	.99627	.99853
.99908				
530.4 keV	.93208	.98617	.99625	.99852
.99907				
767.0 keV	.96040	.99215	.99790	.99916
.99949				
807.9 keV	.92668	.98555	.99614	.99847
.99907				
1297.1 keV	1.00308	1.00057	1.00014	1.00005
1.00003				
SC47 1				
CA49 6				
143.2 keV	.93088	.98492	.99580	.99838
.99892				
856.1 keV	.94357	.98770	.99657	.99868
.99911				
987.3 keV	.94675	.98822	.99670	.99874
.99913				
1144.5 keV	.93728	.98649	.99627	.99857
.99904				
1408.9 keV	.94675	.98822	.99670	.99874
.99913				

This is only a part of the '.COI'-file, **the typical size is 40-45 kBytes.**

Some gamma rays have a coincidence correction factor of one or very close to one. Factors that differ less than 0.1% from one are not put in the file (Al28, Si31 etc.).

## Appendix 3: Algorithm and Data Evaluation

In the standardization step, intermediate results are produced by calculating a detection limit for every gamma line in the  $k_0$  library and, if there is a matching peak in the spectrum, calculating a concentration plus a standard deviation (see Figure A3.1). Depending on the measured spectrum, this results in a list of more than 600 detection limits -- one for every gamma line available in the  $k_0$  library -- and several concentration values.

The intermediate result is necessary for the evaluation steps:

- isotope identification,
- interference correction,
- mean element concentration calculation using the data from all measurements.

The evaluation steps are performed each time a result is printed.

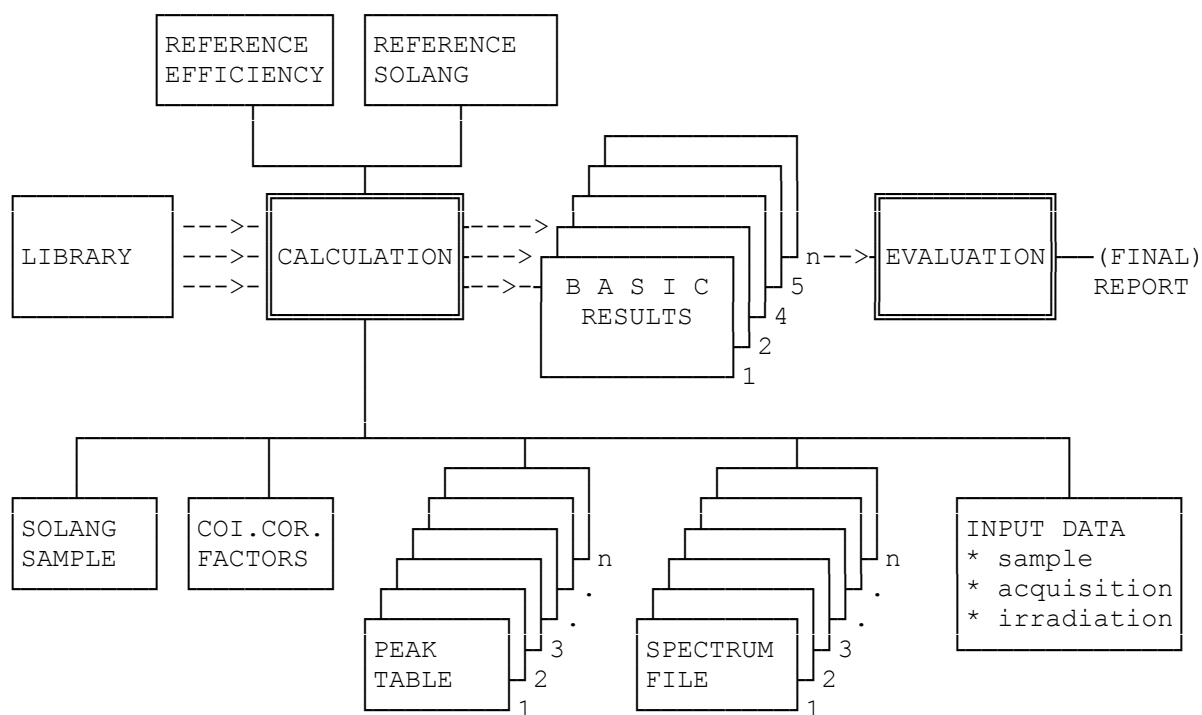


Figure A3.1: Schematic representation of the two main steps of the program and the necessary input data

## K<sub>0</sub> Standardization

$$\rho_a = \frac{\left[ \frac{N_p / t_m}{SDC \cdot W} \right]_a \cdot k_{0,Au}(m) (G_{th,m} \cdot f + G_{e,m} \cdot Q_{0,m}(\alpha)) \cdot \varepsilon_{p,m}}{\left[ \frac{N_p / t_m}{SDC \cdot w} \right]_m \cdot k_{0,Au}(a) (G_{th,a} \cdot f + G_{e,a} \cdot Q_{0,a}(\alpha)) \cdot \varepsilon_{p,a}} \cdot 10^6 \quad (1)$$

Using the k<sub>0</sub>-standardization method, an element concentration, -- ρ<sub>a</sub> in mg/kg -- can be calculated from the peak area of a single gamma line [ 1].  
where: N<sub>p</sub> is the net peak area of a gamma-line corrected for dead time and true coincidence losses (using the coincidence correction factor, see SOLCOI-manual); t<sub>m</sub> is the measuring time; S ,D and C are the saturation, decay and measuring factors respectively; W is the mass of the sample in grams; w is the mass of the monitor element in grams; G<sub>th</sub> and G<sub>e</sub> are correction factors for thermal and epithermal neutron self-absorption; Q<sub>0</sub> is the thermal-to-epithermal cross-section ratio; f and α are parameters describing the neutron flux distribution and ε<sub>p</sub> is the full-energy peak efficiency (see Figure A3.2). In this formula 'a' stands for analyte (the element analyzed) and 'm' stands for monitor. k<sub>0</sub>-values are taken from Ref. [2].

## Efficiency

In view of the extensive calculations which must be done for efficiency determination and coincidence correction, counting geometries should be standardized as much as possible. For these standardized geometries, SOLANG (effective solid angle, Ω) and COI (coincidence correction) tables are pre-calculated and stored in files which can be accessed by KAYZERO. You only need to enter the detector name, geometry and position. Using the method described by Moens et al. in [3] the efficiency for bulky sources can be calculated from:

$$\varepsilon_p = \frac{\Omega}{\Omega_{ref}} \cdot \varepsilon_{p,ref} \quad (2) \quad 2$$

where Ω and Ω<sub>ref</sub> are effective solid angles, which are calculated using the SOLANG program. In combination with KAYZERO, use is made of PC versions of the programs SOLANG and COINCALC (obtained from the Institute for Nuclear Sciences of the Gent University, Belgium) which are combined into SOLCOI.

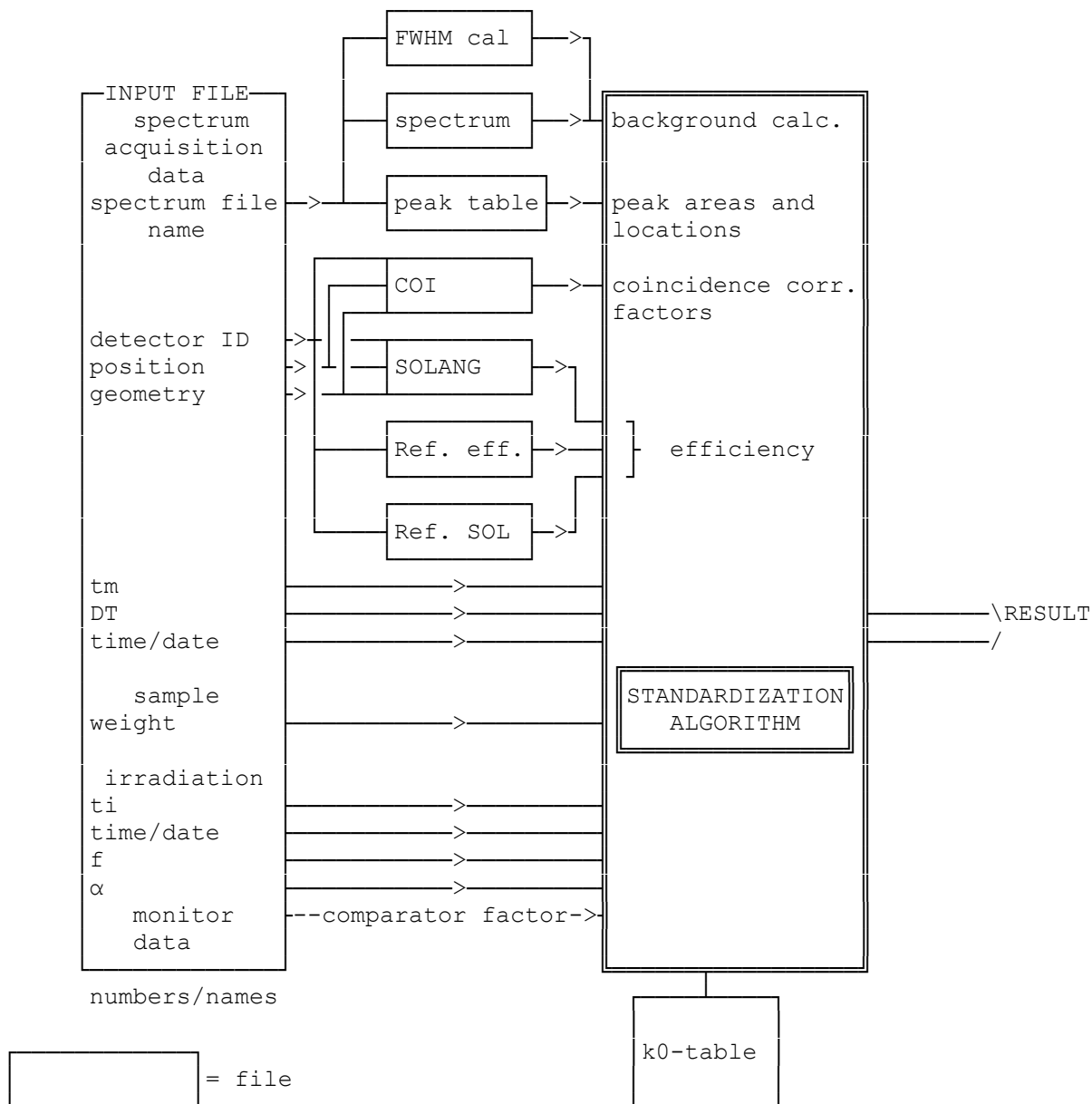


Figure A3.2: Input data for KAYZERO (f and  $\alpha$  are predetermined).

## Spectrum Deconvolution

The result of a spectrum deconvolution is stored in a peak table file which can be accessed by KAYZERO. Of this output file only the net peak areas and the peak location (in keV) are used. The standard deviation,  $\sigma_A$ , for the net peak area A is calculated using the formula:

$$\sigma_A = \sqrt{A + 2.B} \quad (3) \quad 3$$

where B is a summation of the counts in n channels of the expected peak width based on n/2 channels to the left and n/2 to the right of the peak.

The number n is calculated using the FWHM data (FWHM in keV as a function of energy,) stored in the FWHMDET1.DAT data file of the detector (e.g. DET1) system. The FWHM data are printed on the header of the PTF-printout.

For the computation of n, the FWHM is multiplied by a factor (see *Tools/Options/* see Appendix 4) and expressed in a number of channels using the energy calibration.

The detection limit, DL, in counts is calculated using Eq.(4):

$$DL = 2.706 + 4.653 \sqrt{B} \quad (4) \quad 4$$

In this formula, B (the background) is calculated in the energy region where the peak in question is supposed to be present.

## Comparator Factor

$$\rho_a = \frac{I \frac{N_p / t_m}{SDC \cdot W} J_a}{F_{c,Au} \cdot k_{0,Au}(a) (G_{th,a} \cdot f + G_{e,a} \cdot Q_{0,a}(\alpha)) \cdot \varepsilon_{p,a}} \quad (5) \quad 5$$

In Eq. 1 the nuclear data of a monitor isotope selected as the comparator can be compressed into the so-called comparator factor,  $F_{c,Au}$ . This reduces the  $k_0$ -formula to:

$$F_{c,Au} = \frac{I \frac{N_p / t_m}{SDC \cdot W} J_m 10^{-6}}{k_{0,Au}(m) (G_{th,m} \cdot f + G_{e,m} \cdot Q_{0,m}(\alpha)) \cdot \varepsilon_{p,m}} \quad 6$$

Here, the algorithm for calculation of the comparator factor is the same as that used for element concentrations. It can be shown from Eq. 5 and from the activation formula that the comparator factor is proportional to the epithermal neutron flux density (Eq. 6). This means that the comparator factor is a very useful parameter for checking input data and experimental conditions.

Thus, the approximate value of the comparator factor can be predicted using:

$$F_{c,Au} = \frac{N_{Av} \theta_{Au} \gamma_{Au} \sigma_{0,Au}}{M_{Au}} \phi_e 10^{-6} \cong \frac{\phi_e}{3.47 \cdot 10^6} \quad (6) \quad 7$$

with  $N_A$  - Avogadro's number,  $M$  - molar mass,  $\theta$  - isotopic abundance,  $\sigma_0$  - (n, $\gamma$ ) cross section at 2200 m/s neutron velocity and  $\gamma$  - absolute gamma intensity.

In case of co-irradiation of more than one monitor, a mean value for the comparator factor can be used. Then the comparator factors also directly indicate a gradient in epithermal flux density. KAYZERO contains several options for calculating the comparator factor,  $F_{c,Au}$ , as well as  $f$  and  $\alpha$ . For  $f$  and  $\alpha$  the 'Bare Triple Monitor' method is implemented in KAYZERO.

## Evaluation

In the evaluation step (when printing the results, Option 46) mean element concentrations must be calculated using the results of the standardization step. Evaluation is done using several successive data reduction steps:

- isotope identification: eliminating data of nuclides not measurable in the sample;
- gamma interference correction; and
- mean value calculation.

These three main data reduction options used for evaluation can easily be calculated by hand, making verification possible.

## Isotope/Element Identification

For isotope identification, a procedure is used which has been derived from a simple check of the concentration and detection limits of all gamma lines of a radioisotope.

If concentrations (peak areas) are found for gamma lines of a radioisotope, then the number of gamma lines found (X) is a measure of the probability that the radionuclide is present.

Of all concentrations found for X gamma lines of a given radionuclide, the lowest is considered. The higher the number of gamma lines (Y) for which no concentration is found (although the detection limit is lower than this lowest concentration) the less likely it is that the radionuclide concerned is present. Comparing these numbers (X and Y) provides an effective criterion for deciding whether or not a radionuclide is present. For obtaining acceptable results the following conditions are essential:

- energy calibration with an accuracy of better than 0.2 keV,
- good resolving power of the peak deconvolution algorithm,
- the peak finding algorithm in correspondence with the detection-limit definition used.

The isotope identification described above is performed for each measurement. The same procedure can also be done for all radioisotopes related to one element (one should then use element instead of radioisotope and radioisotope instead of gamma line). This so called 'element check' can be done for only one measurement (if there is more than one radioisotope related to an element) or for up to five measurements. This check is only applicable on the so called Final Result, Option 456; it is always switched on.

## Interference Correction

Gamma interference correction in KAYZERO is based on the use of calculated concentrations according to:

$$\rho_x = \rho'_x \left( 1 - \frac{\rho_y}{\rho'_y} \right)$$

where:

$\rho_x$  = concentration of element X (based on gamma line x) corrected for interference,

$\rho'_x$  = concentration of element X (based on gamma lines x + y) without correction for interference by gamma line y of element Y,

$\rho_y$  = concentration of element Y calculated from an interference-free gamma-line,

$\rho'_y$  = concentration of element Y (based on gamma lines x + y) without correction for interference by gamma line x of element X.

In a more general form and for n interfering radioisotopes, this leads to:

$$\rho = \rho' \left( 1 - \sum_{i=1}^n \frac{\rho_i}{\rho'_i} \right)$$

In KAYZERO an iterative method is used to calculate interference corrections. The method does not give an accurate result in all possible cases, but incorrect results can easily be corrected manually because all gamma peak areas are automatically converted to concentrations for all possible radionuclides during the standardization step.

## Weighted Mean Concentrations

Mean values give more reliable information about the concentration of an element in the sample under investigation. Since the counting statistics of all peak areas is not equally good, KAYZERO calculates a weighted mean using:

$$\rho = \frac{\sum \rho_i w_i}{\sum w_i} \quad 8$$

where  $w_i$  is the weighing factor. In KAYZERO Version 5,  $1/\sigma_i^2$  is used. The mean concentrations can be calculated per radionuclide or over all radionuclides related to one element.

$$\sigma_{obs} = \sqrt{\frac{\sum w_i (\rho - \rho_i)^2}{(n-1) \sum w_i}} \quad 9$$

The standard deviation of the mean concentration is calculated and presented as the observed uncertainty. Based on the standard deviation in the net peak area due to counting statistics, an expected uncertainty is calculated as well. One has:

$$\sigma_{exp} = \sqrt{\frac{\sum (w_i \sigma_i)^2}{(\sum w_i)^2}} \quad 10$$

The comparison of the expected and the observed uncertainty gives an idea about the quality of the result.

### References

1. F. DE CORTE and A. SIMONITS, J. Radioanal. Nucl. Chem., 133 (1989) 3-41.
2. F. DE CORTE and A. SIMONITS, J. Radioanal. Nucl. Chem., 133 (1989) 43-130.
3. Moens et al., Calculation of the absolute peak efficiency of gamma-ray detectors for different counting geometries, Nucl. Instr. and Meth., 187 (1981) 451-472.

## Appendix 4: Mass Absorption Coefficients

KAYZERO/SOLCOI uses a mass absorption coefficient data file (according to<sup>1</sup>). This data file contains mass absorption data (total minus coherent) for 80 elements from hydrogen to lead (except noble gases) and including radium, uranium and thorium, in the 1-5000 keV energy range. The K-edge discontinuity is included (see Figure A4.1).

All elements can be selected using their full name, or their symbol using a # in front. Chemical formulas can also be used, for instance #H2O for water.

More complex material compositions can be stored as a material composition (see Option 13 in SOLCOI). The coefficient for a certain energy is found using log-log 3-point interpolation.

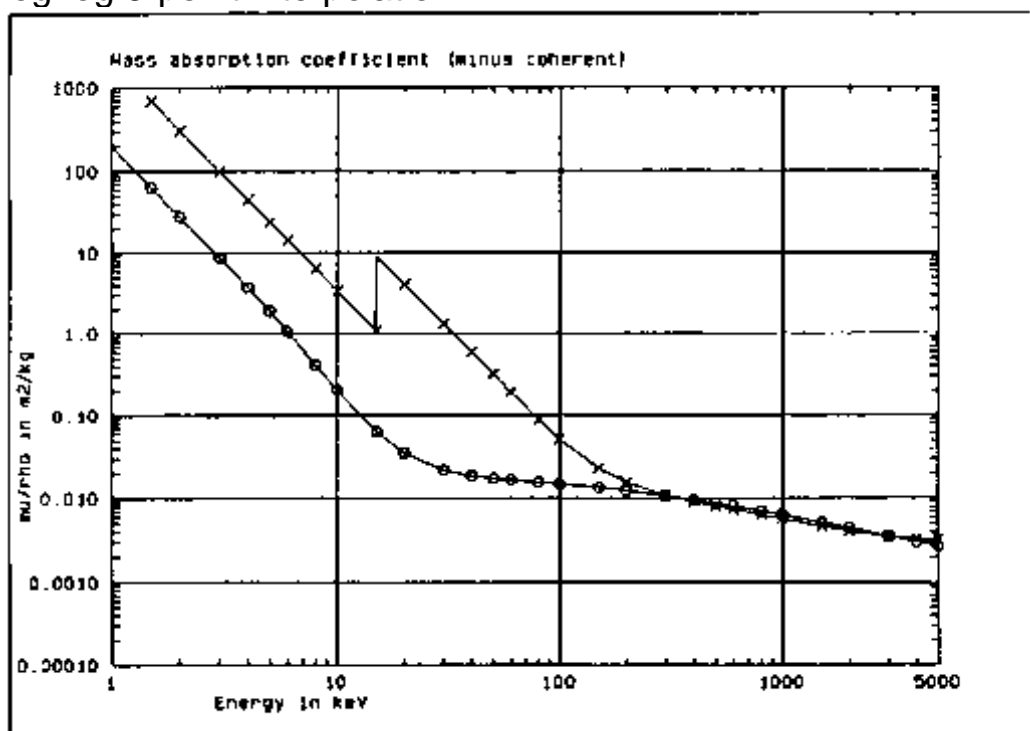


Figure A4.1: Mass absorption coefficients for carbon and germanium as a function of energy (o: carbon; x: germanium).

[1] E. STORM and H.I. Israel, Photon Cross Sections from 0.001 to 100 MeV for Elements 1 through 100, Los Alamos Scientific Laboratory of the University of California, 1967.

## Appendix 5: Matrix Interpolation / Vials

The calculation of a solid angle and a coincidence correction factor file for one position takes approximately 1.2 hours (for an 80386 processor). This is not too long compared to the measuring time but collecting the necessary data for the calculation (vial dimensions, wall thicknesses, vial material, sample composition and densities needed to calculate the linear absorption coefficients) takes time and may be a source of errors. These drawbacks can be avoided by using standard sample vials for counting. Then only the filling height, sample density and/or composition can vary. The filling height is a very important parameter in the standardization of sample vials and should also be standardized.

### Density Interpolation

In case the sample material and the sample vial is always the same but the filling density can vary, density interpolation can be used. By using pre-calculated data for several (standard) densities the solid angles and coincidence factors can be calculated by interpolation (\*) for a range of densities (see Figure A5.1). The lines in the plot are the results of interpolation using the calculation results for five densities given.

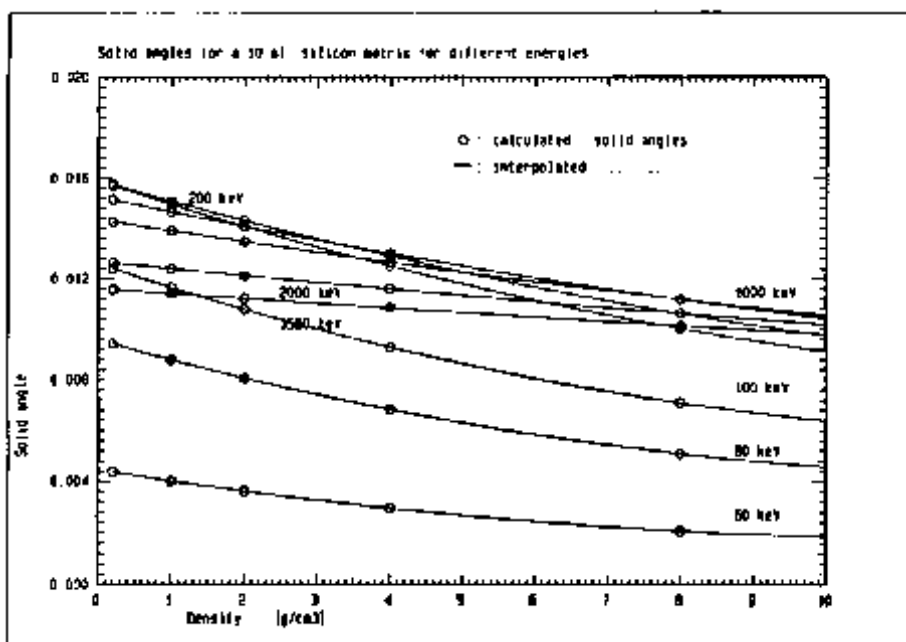


Figure A5.1: Density interpolation

(\*) log/log 3-point Aitkins interpolation is used in KAYZERO/SOLCOI

## Matrix Interpolation

The method of density interpolation described above is only applicable if the composition of the sample matrix is always the same. In the case of a wide range of sample matrices a more universal approach is necessary. After studying the effects of sample matrix and geometry on solid angles, a 'matrix interpolation' technique was implemented in the KAYZERO program for concentration calculation. Interpolation based on linear attenuation coefficients,  $\mu$  (or  $\rho.\mu/\rho$ ), instead of densities is a logical procedure considering the fact that the sample absorption data input for SOLANG is the  $\mu$ -value for different energies.

In Figure A5.2 the solid angles for different energies are given as a function of  $\mu$ . The points represent the calculated solid angles, the lines the results of interpolation (\*) between these points, and the dashed lines connect the points with equal density and matrix composition.

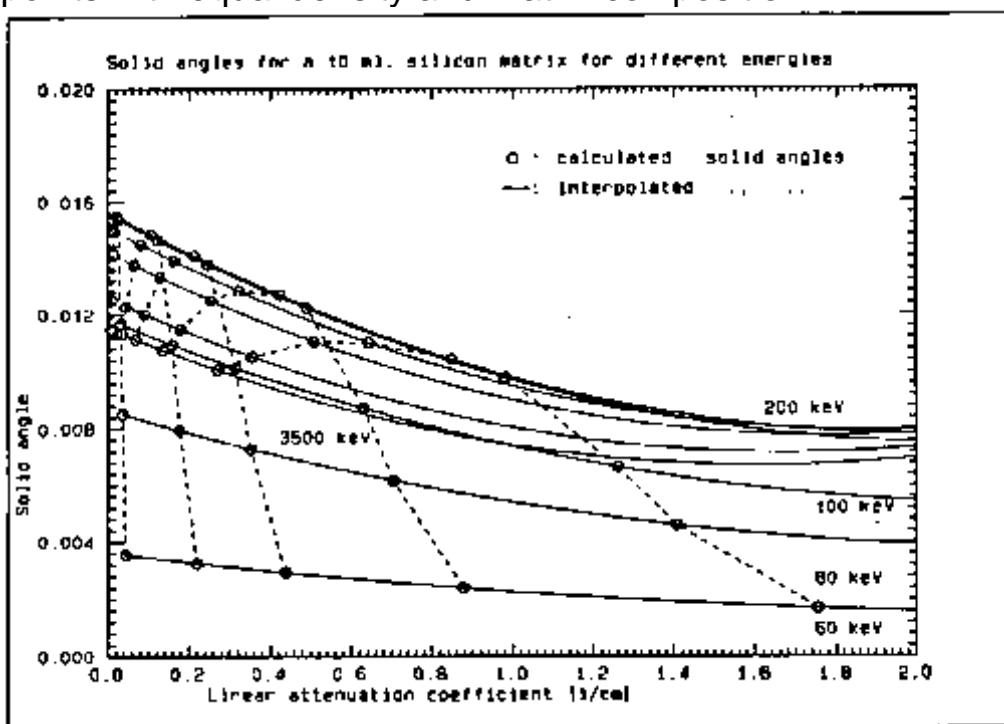


Figure A5.2: Matrix interpolation

(\*) log/log 3-point Aitkins interpolation is used in KAYZERO/SOLCOI

The differences between the calculated solid angles (using SOLCOI) and the interpolated solid angles are very small but the gain in efficiency and time is enormous. The inaccuracy of matrix interpolation can easily be checked by the user by comparison of matrix interpolation results with especially calculated values for different sample materials in the same vial.

# Appendix 6: Parameters.

## Calculation Parameters

The parameters for calculation (using the standardization formula), evaluation (see figure A6.1) and printing (see figure A6.2) of the results can be adjusted using *Tools/Options/Calculation Parameters*, <ALT><T><O>.

The screenshot shows the 'Options' dialog box with the 'Calculation Parameters' tab selected. The 'Evaluation Parameters' section contains the following settings:

- Energy window for peak recognition: 0.70 in keV (one sided).
- Peak width for background calc. (3): 3.0 in FWHM
- Maximum limit of detection: 91.000 in %
- ☒ Area Error Calculation from spectrum
- Concentration averaging: ☐ No Weighing. ☒ Weighing using  $w=1/(sd^2)$

The 'Select Analytical Lines Defaults' section contains the following settings:

- ☐ Blanc Subtraction
- ☒ Threshold Interference Correction
- ☒ Epi-thermal self shadow
- ☒ Fission Interference Correction

At the bottom are 'OK' and 'Cancel' buttons.

Figure A6.1: The *Calculation Parameters*-option.

Re. (1): The energy window for peak recognition can be adjusted if the energy calibration is not optimal. In this case it is best to adjust this calibration using *Energy Calibration*-Option. It is very important to have a good energy calibration and the energy window should be narrow enough to identify all radionuclides present in the spectrum. If there is more than one peak in the spectrum within the energy window, the spectrum peak will be assigned to the isotope with the nearest gamma line in the library.

Re. (2): For the determination of the detection limit, the Compton background is calculated by integration in the region where a gamma peak is supposed to be found. The width of the region is related to the FWHM for the gamma ray

energy. The integration boundary is the FWHM (expressed in channels) for the relevant energy multiplied by a conversion factor. This factor, a good value of which is three, can be entered as an answer to this question.

Re. (3): The selection of a maximum detection limit makes it possible to leave out peaks that are not interesting for analysis. For instance, in trace analysis it is not necessary to show detection limits higher than 5%.

Re. (4): The error in the net peak area can be calculated by KAYZERO using the peak area and the background under the peak. If not the error from the spectrum deconvolution program will be used.

Re. (5): The concentrations calculated for all gamma lines are averaged, the weighing factor is normally the standard deviation in the peak area. This can be turned off so all gammas are equally important.

Re. (6): In the option "Select analytical Lines" the corrections for blanc signal, epi-thermal self absorption, threshold interferences and fission interference can be done. For convenience, these options turned on or off by default.

# Print Parameters

See Figure A6.2

Options

Solcoi Special Parameters Absorption Data Screen Resolution  
Directories Calculation Parameters **Print Parameters** Energy Window/Calibration Corr.

Print concentration in: ☐ ng/g ☒ mg/kg

Concentration Notation ☒ scientific ☐ fixed Number of decimal place: 1

Time Period Notation ☐ seconds ☒ hh:mm:ss.nn

Print only gammas with k0code <=? (3) 3: including theoretically k0's

Order Reporting

Uncertainty given as 2.00 x sd

Systematical error 3.5 in % to be added to the final uncertainty in the element concentration

Font Courier (Size: 10)

OK Cancel

Figure A6.2: The *Print Parameters*-option.

Re. (1): The standard unit for the printed concentrations can be given in ng/g or mg/kg.

Re. (2): The concentrations can be printed in fixed or in scientific notation. If fixed notation is chosen the number of decimal digits can be set.

Re. (3): The time period can be printed in seconds or in time notation "hh:mm:ss"

Re. (4): When printing concentrations per gamma you may choose to print only gamma lines with a k0 code lower than or equal to a certain value. Printing all gamma lines up to k0 code 3 can be useful for manual interference correction. If you enter '0' only the gammas that are used for calculating the average concentration will be printed.

Re. (5): This is the systematical error added in option *Samples/Select Samples and Elements for Order Output* (<Alt><S><L>).

Re. (6): Uncertainty will be printed in the final report 2 times the standard deviation.

# Appendix 7: KAYZERO Library: Full listing

(the actual library might be different)

PRINT OF THE KAYZERO LIBRARY: k0-2015 (03/07/2017) 08/08/2017 - 1-

---

Isotope: F-20 Element: F MDrel: 1 [4 123 0]  
 Q0-1:  $2\,200 \pm 20.0\%$  Q0-2 : 0.000 Eres:  $44700.00 \pm 50.0\%$  eV  
 T1/2(2): 0.186 min  $\pm 0.07\%$   
 F1 : 0.000 F2 : 0.000 F3 : 0.000  
 F4 : 0.000 F Cd : 1.000 k0-nucl:  $9.980000\text{E-}4$   
 Energy k0factor code - interfering nuclides  
 1633.6  $9.980\text{E-}4 \pm 1.2\%$  1 -

---

Isotope: Na-24 Element: Na MDrel: 10 [0 3 1]  
 Q0-1:  $0\,590 \pm 20.0\%$  Q0-2 : 0.000 Eres:  $3380.00 \pm 11.0\%$  eV  
 T1/2(2):  $3.370000\text{E-}4$  min  $\pm 0.50\%$   
 T1/2(3): 897.600 min  $\pm 8.0\text{E-}3\%$   
 F1 : 0.000 F2 : 0.000 F3 : 0.000  
 F4 : 0.000 F Cd : 1.000 k0-nucl:  $4.680000\text{E-}2$   
 Energy k0factor code - interfering nuclides  
 346.6  $4.680\text{E-}2 \pm 50.0\%$  5 - H-181  
 857.6  $4.680\text{E-}2 \pm 50.0\%$  4 -  
 1368.6  $4.680\text{E-}2 \pm 0.6\%$  1 - Sb-124  
 1732.0  $4.620\text{E-}2 \pm 50.0\%$  5 -  
 2243.0  $4.620\text{E-}2 \pm 50.0\%$  4 -  
 2754.0  $4.620\text{E-}2 \pm 0.9\%$  1 -

---

Isotope: Mg-27 Element: Mg MDrel: 1 [0 4 2]  
 Q0-1:  $0\,640 \pm 20.0\%$  Q0-2 : 0.000 Eres:  $2.570\text{E+}5 \pm 13.0\%$  eV  
 T1/2(2): 9.462 min  $\pm 0.12\%$   
 F1 : 0.000 F2 : 0.000 F3 : 0.000  
 F4 : 0.000 F Cd : 1.000 k0-nucl:  $3.524000\text{E-}4$   
 Energy k0factor code - interfering nuclides  
 170.7  $3.020\text{E-}6 \pm 1.0\%$  1 - Ge-77\*D  
 843.8  $2.530\text{E-}4 \pm 0.5\%$  1 -  
 1014.4  $9.800\text{E-}5 \pm 0.2\%$  1 - K-42S

---

Isotope: Al-28 Element: Al MDrel: 1 [0 5 3]  
 Q0-1:  $0\,710 \pm 20.0\%$  Q0-2 : 0.000 Eres:  $11800.00 \pm 5.9\%$  eV  
 T1/2(2): 2.241 min  $\pm 0.05\%$   
 F1 : 0.000 F2 : 0.000 F3 : 0.000  
 F4 : 0.000 F Cd : 1.000 k0-nucl:  $1.750000\text{E-}2$   
 Energy k0factor code - interfering nuclides  
 756.9  $1.750\text{E-}2 \pm 50.0\%$  5 - Zr-95 Eu-154  
 1267.9  $1.750\text{E-}2 \pm 50.0\%$  4 -  
 1778.9  $1.750\text{E-}2 \pm 0.8\%$  1 - Rb-88

---

Isotope: Si-31 Element: Si MDrel: 1 [0 6 4]  
 Q0-1:  $1\,110 \pm 6.0\%$  Q0-2 : 0.000 Eres:  $2280.00 \pm 0.4\%$  eV  
 T1/2(2): 157.320 min  $\pm 11.44\%$   
 F1 : 0.000 F2 : 0.000 F3 : 0.000  
 F4 : 0.000 F Cd : 1.000 k0-nucl:  $2.070000\text{E-}4$   
 Energy k0factor code - interfering nuclides  
 1266.2  $1.450\text{E-}7 \pm 0.7\%$  1 -

---

Isotope: Lu-176m Element: Lu MDrel: 1 [Q 104, 120]  
 Q0-1: 34.800 ± 3.1% Q0-2 : 0.000 Fres: 16.10 ± 5.0% eV  
 T1/2(2): 218.100 min ± 0.08 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 1.944000E-1  
 Energy k0 factor code - interfering nuclides  
 88.4 1.730E-2 ± 1.5% 1 - Ag-109m\* Hf-175 Cd-117

---

Isotope: Lu-177 Element: Lu MDrel: 1 [Q 105, 121]  
 Q0-1: 1.909 ± 20.0% Q0-2 : 0.000 Fres: 0.16 ± 50.0% eV

---- Non-1/v Nuclide-----  
 Use Extended Modified Hgdaahl by choosing mu in "Irradiation data"  
 For mu=2.1 Fres : 0.13 eV Qextended: 3.45  
 For mu=3.7 Fres : 0.13 eV Qextended: 3.09 @0 dC to 2.31 @100 dC Fres : 0.13 eV

---

T1/2(2): 9691.200 min ± 0.15 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 1.238000E-1  
 Energy k0 factor code - interfering nuclides  
 112.9 4.150E-2 ± 10.0% 2 - H-171 Ga-72 Ta-182 Yb-175  
 208.4 7.140E-2 ± 10.0% 2 - Nd-149\* Au-199 Pm-151\* Ta-182D

---

Isotope: Eu-152 Element: Eu MDrel: 1 [Q 90, 105]  
 Q0-1: 1.537 ± 20.0% Q0-2 : 0.000 Fres: 0.45 ± 50.0% eV

---- Non-1/v Nuclide-----  
 Use Extended Modified Hgdaahl by choosing mu in "Irradiation data"  
 For mu=2.1 Fres : 1.3 eV Qextended: 0.7  
 For mu=3.7 Fres : 0.29 eV Qextended: 0.7

---

T1/2(2): 7121498.400 min ± 0.04 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 4.504000E+1  
 Energy k0 factor code - interfering nuclides  
 90.1 6.070E+0 ± 50.0% 5 - H-175 Cd-117 Nd-147  
 121.8 1.280E+1 ± 0.8% 1 - Nd-147 Se-75 Zn-71 Eu-152m Re-186 Yb-177 Eu-154  
 244.7 3.440E+0 ± 0.3% 1 - Sm-155  
 344.3 1.190E+1 ± 0.9% 1 - H-175 Eu-152m Cd-117 Pm-151\*  
 386.0 9.360E+0 ± 50.0% 5 -  
 411.1 9.900E-1 ± 20.0% 3 - Au-198 V-52D  
 444.0 1.390E+0 ± 1.2% 1 - I-128 H-180m Nd-149\* Sb-124  
 482.3 1.220E-2 ± 20.0% 3 - H-181 Ag-110mD  
 564.5 2.690E-1 ± 20.0% 3 - Cs-134 As-76 Sb-122 Cd-117m\*  
 601.1 6.070E+0 ± 50.0% 4 - Ga-72 Zr-97\*  
 778.9 5.700E+0 ± 0.8% 1 - Mo-99  
 867.4 1.880E+0 ± 0.9% 1 - As-76 La-140  
 897.0 9.360E+0 ± 50.0% 4 - Rb-88  
 964.1 6.460E+0 ± 0.4% 1 - Eu-152m Br-82S Tb-160X  
 1085.9 4.570E+0 ± 0.4% 1 - Ge-77\* La-140S  
 1089.7 7.590E-1 ± 20.0% 3 - Sn-125\* In-116mD  
 1112.1 6.070E+0 ± 0.8% 1 -  
 1213.0 6.310E-1 ± 20.0% 3 - As-76  
 1299.1 7.220E-1 ± 20.0% 3 - Mn-56S  
 1408.0 9.360E+0 ± 0.6% 1 - Ca-49

---

Isotope: Eu-152m Element: Eu MDrel: 1 [Q 89, 106]  
 Q0-1: 1.492 ± 20.0% Q0-2 : 0.000 Fres: 0.45 ± 50.0% eV

---- Non-1/v Nuclide-----  
 Use Extended Modified Hgdaahl by choosing mu in "Irradiation data"  
 For mu=2.1 Fres : 1.3 eV Qextended: 0.7  
 For mu=3.7 Fres : 0.29 eV Qextended: 0.7

T1/2(2): 558.720 min  $\pm$  0.11 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 2.068000E+1  
 Energy k0 factor code - interfering nuclides  
 121.8 1.480E+0  $\pm$  10.0% 2 - Nd-147 Se-75 Zn-71 Eu-152 Re-186 Yb-177 Eu-154  
 344.2 4.980E-1  $\pm$  10.0% 2 - H-175 Eu-152 Cd-117 Pm-151\*  
 562.9 4.910E-2  $\pm$  20.0% 3 - Cs-134 As-76 Sb-122  
 841.6 3.020E+0  $\pm$  10.0% 2 -  
 963.3 2.490E+0  $\pm$  10.0% 2 - Tb-160 Br-82S Eu-152  
 1314.7 2.080E-1  $\pm$  20.0% 3 -  
 1389.0 1.670E-1  $\pm$  20.0% 3 -

---

Isotope: Eu-154 Element: Eu MDrel: 10 [0.91, 107]  
 Q0-1: 5.660  $\pm$  20.0% Q0-2 : 0.000 Fres: 5.80  $\pm$  4.0% eV  
 T1/2(2): 46.000 min  $\pm$  0.50 %  
 T1/2(3): 4519574.280 min  $\pm$  0.05 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 2.203000E+0

Energy k0 factor code - interfering nuclides  
 123.1 8.935E-1  $\pm$  20.0% 3 - Eu-152 Eu-152m Re-186 Yb-177 Ba-131 Er-171  
 248.0 1.550E-1  $\pm$  10.0% 2 - Ba-131  
 252.4 7.770E-1  $\pm$  50.0% 5 - Os-193  
 591.8 1.080E-1  $\pm$  1.5% 1 - Os-185  
 692.4 3.830E-2  $\pm$  20.0% 3 - Sb-122  
 723.3 4.460E-1  $\pm$  1.5% 1 - Ce-143 Sb-124 Zr-95 Ru-105  
 756.9 1.080E-1  $\pm$  10.0% 2 - Zr-95 A-28D  
 763.4 7.770E-1  $\pm$  50.0% 4 - Cd-117m\* Ag-110m  
 873.2 2.720E-1  $\pm$  1.4% 1 - Ag-110mS  
 996.4 2.300E-1  $\pm$  10.0% 2 - In-116mS  
 1004.7 3.944E-1  $\pm$  20.0% 3 -  
 1274.4 7.770E-1  $\pm$  1.1% 1 -  
 1596.5 3.944E-2  $\pm$  20.0% 3 - La-140 Ca-72

---

Isotope: Yb-169 Element: Yb MDrel: 10 [0.101, 117]  
 Q0-1: 4.833  $\pm$  20.0% Q0-2 : 0.000 Fres: 0.61  $\pm$  50.0% eV

---- Non-1/v Nuclide-----

Use Extended Modified Hogdahl by choosing mu in "Irradiation data"

For mu=2.1 Fres : 0.53 eV Q0extended : 10.8

For mu=3.7 Fres : 0.53 eV Q0extended : 10.8

---

T1/2(2): 0.767 min  $\pm$  0.50 %  
 T1/2(3): 46123.200 min  $\pm$  0.02 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 4.614000E-2  
 Energy k0 factor code - interfering nuclides  
 63.1 2.040E-2  $\pm$  10.0% 2 - Re-188m  
 93.6 1.180E-3  $\pm$  20.0% 3 - Re-188m Hf-180m N-65D Zn-65D Dy-165 Pa-233  
 109.8 7.790E-3  $\pm$  10.0% 2 -  
 118.2 8.490E-4  $\pm$  20.0% 3 -  
 130.5 5.170E-3  $\pm$  10.0% 2 - Os-191 Rh-105m Ru-105  
 177.2 1.040E-2  $\pm$  10.0% 2 - Ga-70\* Pm-151\*  
 198.0 1.640E-2  $\pm$  10.0% 2 - Nd-147 Tb-160 Ta-182 Se-75 Ge-75\* Nd-149\* Ta-182D  
 307.7 4.340E-3  $\pm$  10.0% 2 - Tc-101 Er-171 Ir-192 Pd-109

---

Isotope: Yb-175 Element: Yb MDrel: 10 [0.102, 118]  
 Q0-1: 0.460  $\pm$  20.0% Q0-2 : 0.000 Fres: 602.00  $\pm$  8.0% eV  
 T1/2(2): 0.001 min  $\pm$  0.50 %  
 T1/2(3): 6026.400 min  $\pm$  0.02 %  
 F4 : 0.000 F Cd : 1.000 k0-nucl: 4.875000E-1  
 Energy k0 factor code - interfering nuclides  
 113.8 9.420E-3  $\pm$  1.3% 1 - Ga-72 Lu-177 Ta-182 Nd-149\* Pa-233  
 137.7 5.690E-4  $\pm$  0.6% 1 - Hf-181 Re-186 Br-82 In-116m Os-193 Os-193X  
 144.9 1.590E-3  $\pm$  1.5% 1 - Ce-141  
 282.5 1.460E-2  $\pm$  0.3% 1 - Cd-161\*

396.3 3.120E-2 ± 0.6% 1 -

---

Isotope: Yb-177 Element: Yb MDrel: 10 [Q 103, 119]  
Q0-1: 2.500 ± 1.8% Q0-2 : 0.000 Pres: 412.00 ± 5.1% eV  
T1/2(2): 0.107 min ± 0.50 %  
T1/2(3): 114.660 min ± 0.16 %  
F4 : 0.000 F Cd : 1.000 k0-nucl: 4.410000E-3  
Energy k0 factor code - interfering nuclides  
122.7 1.640E-4 ± 10.0% 2 - Zn-71 Eu-152 Eu-152m Re-186 Eu-154 Ba-131 H-171  
139.3 6.480E-5 ± 10.0% 2 - In-116m Os-193 Os-193 X Ge-75m Tc-99m  
150.6 8.940E-4 ± 10.0% 2 - Co-60 D Sr-85m\*  
898.9 3.120E-5 ± 10.0% 2 - Rb-88  
941.8 4.870E-5 ± 10.0% 2 -  
1028.1 2.940E-5 ± 10.0% 2 - Cd-117m\*  
1080.2 2.680E-4 ± 10.0% 2 - B-82  
1119.7 2.740E-5 ± 10.0% 2 - Sc-46  
1149.8 2.960E-5 ± 10.0% 2 - Ir-194  
1241.2 1.620E-4 ± 10.0% 2 -

---

for more radionuclides see the listing made by the program

## Explanation of some of the data in the KAYZERO Library M/D (mother/daughter) relations and factor F1-F5

k0codes:

=====

- 1: recommended  $k_0$ -factor
- 2: tentative (measured in only one laboratory)
- 3: theoretical  $k_0$ -factor (for interference correction purposes only)
- 4: single escape peaks, with  $k_0$ -factor of original peak (added according<sup>1</sup>)
- 5: double escape peaks, with  $k_0$ -factor of original peak (added according<sup>1</sup>)
- 7: effective energy with recommended  $k_0$ -factor
- 8: effective energy with non-recommended  $k_0$ -factor

Eres :

=====

The mean resonance energy; if Eres is zero KAYZERO will use Q0-1 instead of  $Q_0(\alpha)$ .

Mother/Daughter relations:

=====

The M/D relations are in the KAYZERO Library numbered from 1 to 19. These number correspond to the roman numbers in the  $k_0$ -standardization literature of De Corte and Simonits<sup>2</sup>. In Table A7.1 these numbers and the factors F1-F5 given in the library are explained.

Half-lives are given in minutes

=====

$k_0$  factors/  $k_0$ codes point of attention

=====

Some  $k_0$  factors are only defined for an artificial effective gamma peak (in fact a combination of two gamma lines close together). These gamma lines are given in table A7.2. There are two types:

- A: The lines can be separated using modern gamma-ray spectrometers and deconvolution software. In this case the two separate  $k_0$  factors are given as well as the  $k_0$  factor for the summation. In the latter case the  $k_0$  code is 7 or 8.
- B: The lines cannot be separated.

## References

=====

1. G. ERDTMANN and W. SOYKA, The Gamma Rays of the Radionuclides, Topical Presentations in Nuclear Chemistry, Kernchemie in Einzeldarstellungen, Volume 7. Verlag Chemie, Weinheim New York, 1979.
2. F. DE CORTE and A. SIMONITS, J. Radioanal. Nucl. Chem., 133 (1989) 43-130.

M/D rel. KAYZERO	M/D code ref.[2]	F1-F5
1	I	-
2	II/a	-
3	II/b	-
4	II/c	-
5	II/d	$F1=\gamma_2/(F_2.\gamma_3)$
6	III/a	$F2=F_{24}/(F_2.F_3)$
7	III/b	-
8	III/c	-
9	IV/a	$F3=F_2.\sigma_0^m/\sigma_0^g$
10	IV/b	-
11	IV/c	-
12	V/a	$F3=k_0^m/k_0^g$
13	V/b	-
14	V/c	-
15	VI	-
16	VII/a	$F1=F_{24}.\sigma_0^m/(\sigma_0^g.F_3); F3=F_2.\sigma_0^m/\sigma_0^g$
17	VII/b	$F1=F_{24}.\sigma_0^m/(\sigma_0^g.F_3)$
18	VIII	$F1=F_{35}/(F_3.F_4); F2=F_{25}/F_4; F4=F_{24}; F5=\lambda_5$
19	IV/d	$F1=\gamma_2/(F_2.\gamma_3); F2=F2; F3=\sigma_0^m/\sigma_0^g$
20	V/d	-

Table A7.1: Explanation of mother/daughter relations and factors F1-F5.

Isotope	Eff. energy in keV (k0code)	Energy 1 in keV (k0 code)	Energy 2 in keV (k0 code)
Ga-72	2501.7 (7)	2491.0 (1)	2507.9 (1) [2507.8 + 2515.0]
As-76	559.2 (7)	557.1 (1)	563.2 (2)
As-76	1215.2 (7)	1212.9 (1)	1216.1 (1)
Mo-101	192.4 (7)	191.9 (1)	195.9 (1)
Mo-101	1012.4 (7)	1011.1 (2)	1012.5 (1)
Ru-105	469.4 (7)	469.4 (1)	470.1
Pd-109	311.1 (7)	309.1 (3)	311.4 (1)
Sn-117m	158.5 (7)	156.0 (1)	158.6 (1)
Tb-160	965.1 (7)	962.3 (2)	966.2 (2)
Hf-181	133.5 (7)	133.0 (1)	136.4 (2) [136.3 + 136.9]
Re-188	633.2 (7)	633.0 (1)	635.0 (1)
Os-193	139.0 (7)	138.9 (1)	142.1 (1)
Os-193	557.9 (7)	557.4 (1) [556.0 + 557.4]	559.3 (1) [559.3 + 560.0]
Np-239	228.1 (7)	226.4 (3)	228.2 (1) [227.8 + 228.2]

Table A7.2A: Isotopes and k<sub>0</sub>'s with effective energies and effective k<sub>0</sub>-factors: lines that can be separated using modern gamma-ray spectroscopy.

Isotope	Eff. energy in keV (k0code)	Energy 1 in keV (rel.y intensity)	Energy 2 in keV (rel.y intensity)
Ga-72	2507.9 (1)	2507.8 (13)	2515.0 (0.2)
Mo-101	505.9 (1)	505.1 (20)	505.9 (638)
Mo-101	590.1 (1)	590.1 (300)	590.1 (870)
Mo-101	870.9 (2)	869.7 (18)	871.1 (96)
Mo-101	934.1 (2)	933.3 (40)	934.2 (181)
Mo-101	1251.0 (2)	1249.4 (14)	1251.1 (245)
Pd-109	414.4 (3)	413.0 (27)	415.2 (44)
Ag-110m	706.8 (7)	706.7 (17.4)	708.1 (0.29)
Sn-125	1088.9 (2)	1087.7 (12.3)	1089.2 (47.3)
Nd-149	97.0 (2)	96.9 (0.13)	97.0 (5.6)
Nd-149	155.9 (2)	155.1 (0.13)	155.9 (22.9)
Nd-149	198.9 (2)	198.0 (0.19)	198.9 (5.37)
Nd-149	349.1 (2)	347.8 (0.62)	349.2 (5.31)
Nd-149	423.7 (2)	423.6 (28.7)	425.2 (1.05)
Nd-149	556.4 (3)	555.9 (2.26)	556.8 (1.68)
Pm-151	163.3 (3)	162.9 (3.9)	163.6 (6.9)
Pm-151	167.8 (3)	167.8 (37)	168.4 (4.1)
Pm-151	177.0 (3)	176.5 (3.8)	177.2 (17)
Eu-152	444.0 (1)	444.0 (1.22)	444.0 (10.54)
Eu-152	564.5 (3)	564.0 (23.6)	566.4 (6.2)
Eu-152	964.1 (1)	963.4 (0.50)	964.1 (54.6)
Eu-152	1085.9 (1)	1084.0 (11.7)	1085.9 (475)
Yb-169	118.2 (3)	117.4 (0.11)	118.2 (5.22)
Er-171	210.6 (2)	210.1 (0.07)	210.6 (6.42)
Hf-181	136.4 (2)	136.3 (7.27)	136.9 (1.07)
Ta-182	1157.5 (3)	1157.3 (1.7)	1158.1 (1.15)
Os-193	180.9 (2)	180.0 (4.6)	181.8 (4.9)
Os-193	219.1 (2)	219.1 (7.0)	219.0 (0.22)
Os-193	557.4 (1)	556.0 (0.08)	557.4 (33)
Os-193	559.3 (1)	559.3 (12.3)	560.0 (0.07)

Table A7.2B: Isotopes and  $k_0$ 's with effective energies and effective  $k_0$ -factors: lines that cannot be separated using modern gamma-ray spectroscopy.

# Appendix 8: KAYZERO Library: Gamma line listing

(example, might be different in the actual library)

PRINT OF THE GAMMA-LINES IN THE KAYZERO LIBRARY : VER4\_0  
3/12/2001

T 1/2 : 0.0 > T 1/2 > 100000000000. minutes

Energy keV	Isotope	Element	T 1/2 min.	yield %	k0-code
---------------	---------	---------	---------------	------------	---------

58.6	Co-60m	Co*	10.5	2.089	2
63.1	Yb-169	Yb*	46117.4	44.213	2
63.6	Re-188m	Re	18.6	22.583	3
67.8	Ta-182	Ta	164779.0	41.217	2
69.7	Sm-153	Sm	2776.2	4.312	1
70.4	Pd-111m	Pd*	330.0	30.641	3
74.7	U-239	U	23.5	48.101	1
75.4	Pa-233	Th	38832.5	1.408	3
80.2	I-131	Te	11549.8	2.331	2
80.6	Ho-166	Ho	1609.8	6.330	1
80.9	Mo-101	Mo	14.6	4.771	2
84.3	Tm-170	Tm	185184.0	3.260	1
86.8	Pa-233	Th	38832.5	1.991	3
86.8	Tb-160	Tb	104112.0	13.380	1
88.0	Ag-109m	Pd*	822.1	3.610	2
88.4	Lu-176m	Lu	218.1	8.899	1
89.4	Hf-175	Hf	100800.0	2.354	3
89.7	Cd-117	Cd	149.4	4.071	2
90.1	Eu-152	Eu*	7122670.0	13.477	(double
escape peak)					
91.1	Nd-147	Nd	15811.2	27.899	1
92.2	Br-82	Br	2118.0	0.760	3
92.4	Re-188m	Re	18.6	5.606	1
93.3	Hf-180m	Hf	330.0	17.311	1
93.5	Ni-65	Ni	151.0	15.119	(double
escape peak)					
93.5	Zn-65	Zn	351734.4	50.619	(double
escape peak)					
93.6	Yb-169	Yb*	46117.4	2.557	3
94.7	Pa-233	Th	38832.5	10.997	3
94.7	Dy-165	Dy	140.0	3.580	1
96.7	Se-75	Se	172481.8	3.440	3
97.0	Nd-149	Nd*	103.7	1.635	2
97.1	Rh-104m	Rh*	4.3	2.985	3
97.4	Gd-153	Gd	347904.0	30.206	1
98.5	Sc-46	Sc	120658.0	100.000	(double
escape peak)					
99.3	Ta-182	Ta	164779.0	37.540	(double

escape peak)					
100.0	Pm-151	Nd*	1704.0	2.536	3
100.1	Ta-182	Ta	164779.0	14.435	2
101.9	Pm-151	Nd*	1704.0	1.282	3
102.3	Gd-161	Gd*	3.7	17.395	2
103.2	Sm-153	Sm	2776.2	28.298	1
103.2	Gd-153	Gd	347904.0	21.701	1
103.7	Np-239	U	3393.4	19.975	3
104.0	Pa-233	Th	38832.5	0.881	3
104.3	Sm-155	Sm	22.3	74.570	3

for more lines see the listing by the program.