Kayzero for Windows

for reactor neutron activation analysis (NAA)
using
the k_0 standardization method

Version 2

User's Manual
Version 1.00
November 2005

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 2

Distribution and support :

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1 Introduction

Kayzero for Windows is a program that helps the Neutron Activation Analyst in evaluating 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[1,2]. The method involves extensive calculations and the use of large data files. The Kayzero for Windows user is expected to be familiar with gammaspectroscopy, NAA and the k_0 method. For practical guidelines regarding this method see the 'VADEMECUM FOR k_0 USERS' by De Corte and Simonits[3].

The installation and the use of Kayzero for Windows are explained in Chapter 2, Installation and User Interface.

All steps needed for the evaluation of an analysis are given in Chapter 3, Analysis Evaluation, which explains step by step how to proceed after all measurements have been performed. All efficiency calibration and calculation procedures, from the former SolCoi Program, are handled in chapter 4 SolCoi. 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.

Kayzero for Windows is the successor of Kayzero/Solcoi version 5A. Solcoi and Kayzero are now integrated. The user interface is developed under Windows. Many new features such as direct efficiency calculation, f and alpha using the Cd-ratio method and reactor flux variation correction are added.

The updated version 5, June 2002 contains new correction methods for reaction interference, fission products and irradiation blank concentration correction. From version 5 it is was also possible to select the analytical gamma lines to be used for the final order result. The final order result is used to give the data for the selected elements for all selected samples.

2 Installation and User Interface

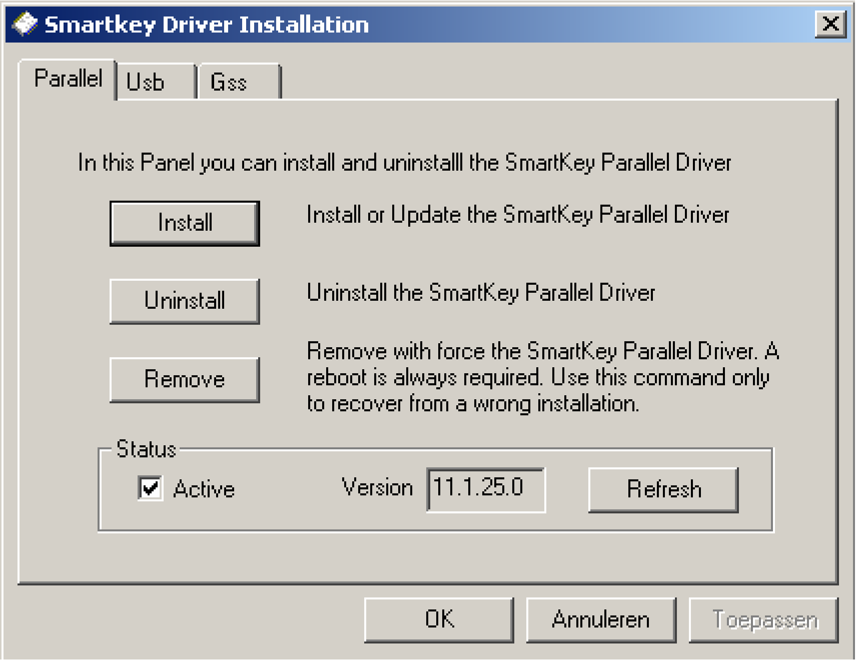
2.1 Installation

Kayzero for windows can be installed on a Personal Computer running under Windows (98SE and higher) with a free USB port needed for the copy protection key (parallel port key is optional). If you only use the program for demonstration you can skip the section however you will have limited features.

Before running the software you have to install the copy protection key software. Warning: Do not connect the USB-key to the computer before running the SDI-software and wait until the software asks you to connect it.

The program can be downloaded from the website 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 to.

Run (double click on the) the program 'USB Key Setup.exe'. The following screen will appear:



In this Panel you can install and uninstalll the SmartKey Parallel Driver

Install or Update the SmartKey Parallel Driver

Uninstall the SmartKey Parallel Driver

Remove with force the SmartKey Parallel Driver. A reboot is always required. Use this command only to recover from a wrong installation.

Status

☑ Active

Version 11.1.25.0

Figure 2.1: Screen of 'USB Key Setup.exe'

Select your Key-type and click on Install. Wait until you are asked to connect the key.

2.1.1 New user of Kayzero

The software is installed by copying the KAY_V5A directory downloaded from the 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 Kayzero/Solcoi Version 4

Do as mentioned under 2.1.1

Copy the following files from your current Kayzero/Solcoi directory to the new Kayzero for Windows directory:

Kayzero.Dat
Kayzero.Sys
Solcoi.Tim
Kayzero.Irr
Kayzero.Mon
*.Sta
Kayzero.Abs
*.Dam

2.1.3 Upgrade from Kayzero/Solcoi Version 5

Do as mentioned under 2.1.2 but copy the following files too:

*.Par *.Cls *.Blk

2.1.4 Upgrade from Kayzero/Solcoi Version 5A

Store the downloaded ‘KayWin.Exe’-program to your Kayzero directory.

2.2 Run The Program

Run the Kayzero for Windows – software: ‘KayWin.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 replaces the Help.

2.3.1 The ‘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.

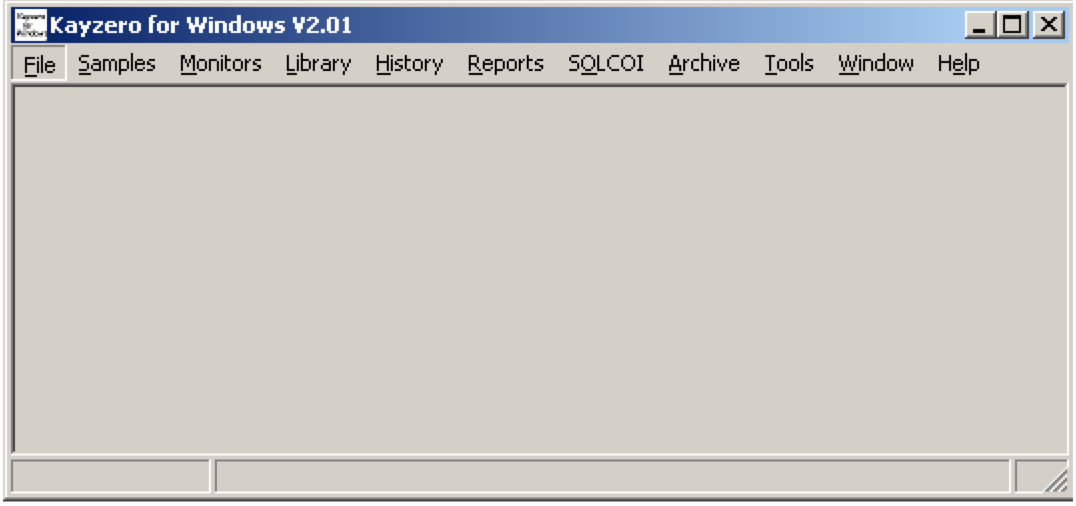
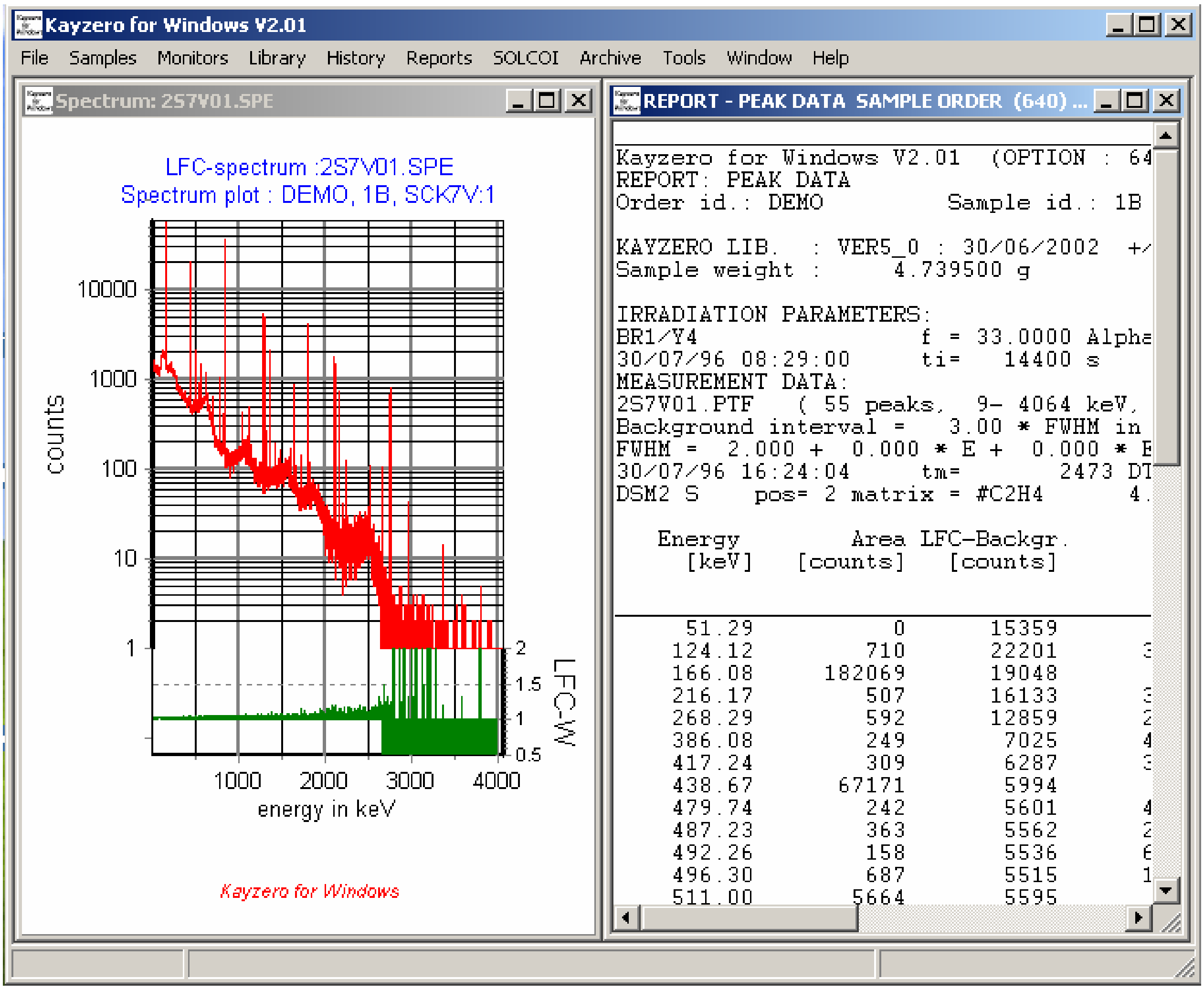


Figure 2.2: Main screen of Kayzero for Windows

2.3.2 Program 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.

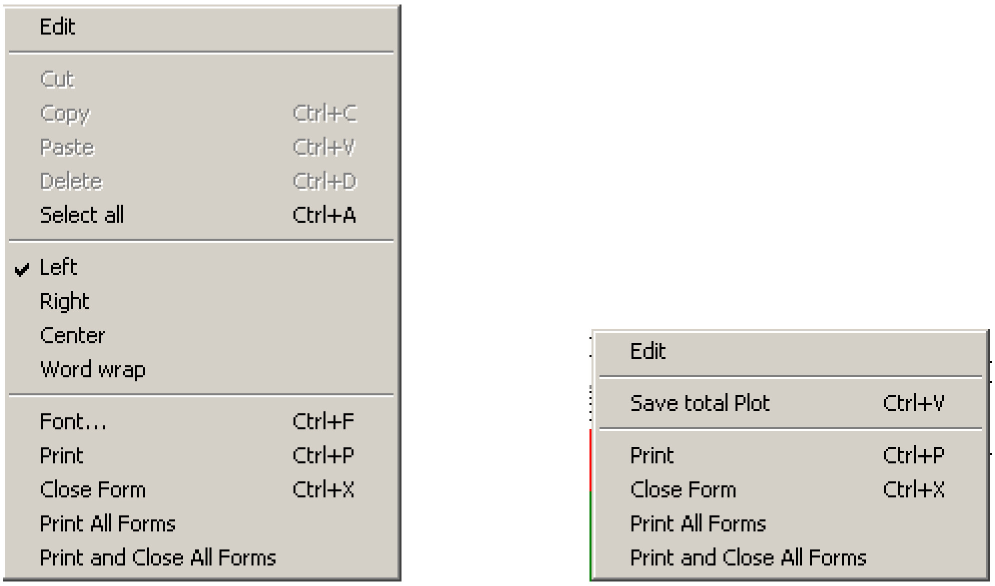


```
Kayzero for Windows V2.01   (OPTION  : 64
REPORT: PEAK DATA
Order id.: DEMO            Sample id.: 1B

KAYZERO LIB.   : VER5_0 : 30/06/2002   +/
Sample weight  :      4.739500 g

IRRADIATION PARAMETERS:
BR1/Y4                   f  = 33.0000 Alph
30/07/96 08:29:00        ti=   14400 s
MEASUREMENT DATA:
2S7V01.PTF    ( 55 peaks,   9- 4064 keV,
Background interval =    3.00 * FWHM in
FWHM =  2.000 +  0.000 * E +  0.000 * E
30/07/96 16:24:04        tm=        2473 DT
DSM2 S     pos= 2 matrix = #C2H4       4.

   Energy          Area LFC-Backgr.
    [keV]    [counts]    [counts]

     51.29           0      15359
    124.12         710      22201        3
    166.08      182069      19048
    216.17         507      16133        3
    268.29         592      12859        2
    386.08         249       7025        4
    417.24         309       6287        3
    438.67       67171       5994
    479.74         242       5601        4
    487.23         363       5562        2
    492.26         158       5536        6
    496.30         687       5515        1
    511.00        5664       5595
```

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

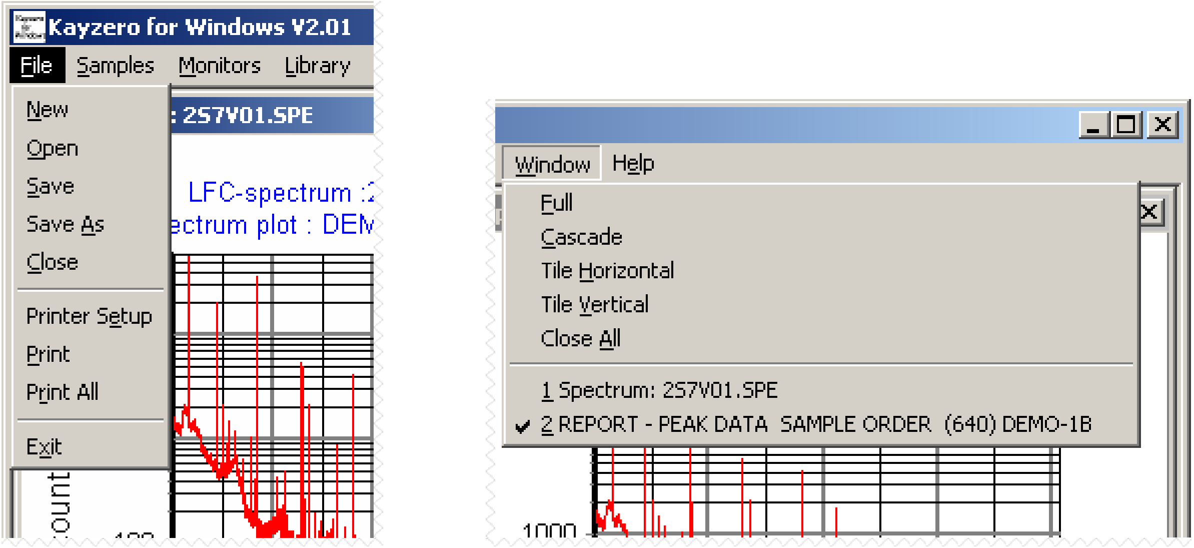
When pressing the right mouse button, a pop-up menu opens (see Figure 2.4). This pop-up menu is specific for each type of output.

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’).



A: Text output pop-up B: Graph output pop-up

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.

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.

2.3.3 (File)names

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

Orders, spectrum, samples, reactor, channel names should not exceed 8 characters. Directory names should not exceed 60 characters, sources 3 characters and detectors 4 characters.

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>+<R> . 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.

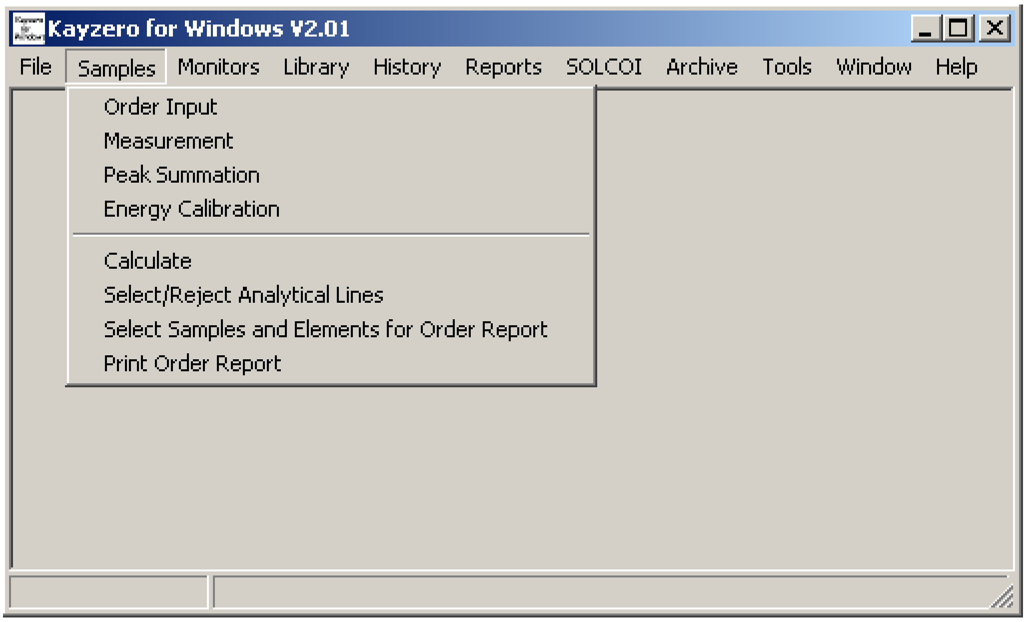


Figure 3.1 : Main screen of Kayzero for Windows.

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, enter and edit the data of a measured spectrum and start the calculations. It is also possible to do peak summation, energy calibration, select the analytical lines that you want to use and to print the result of the analysis for selected elements and samples.

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 and results.
All output is directed to the main form of the program and can be printed or plotted from here.

SolCoi The SOLCOI program is integrated in Kayzero for Windows.

Tools
This submenu contains the following options: performing a new energy calibration based on measured spectra; plotting the compton background and the spectrum of a sample or monitor; and changing the calculation parameter settings, directories and the material composition data.

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

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_0-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 α, for channel Y4 of the BR1 were predetermined and are assumed to be constant over time.

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).

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

- enter the measurement data of the monitor(s) in KAYZERO;
- check the spectra for split-up peaks (new option: Peak summation);
- to determine F_c, calculate the flux parameters, f and α (using a gold/ zirconium monitor) or use predefined values of f and α and e.g. a gold monitor for determination of F_c (only if the parameters f and α can be considered to be constant);
- print the flux parameters;
- enter the measurement data of the sample and the flux parameters in KAYZERO;
- calculate the element concentrations;
- check and correct (for blank concentrations, reaction interferences and outliers) the results (new option);
- print the element concentrations.

3.3 Monitor Data

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

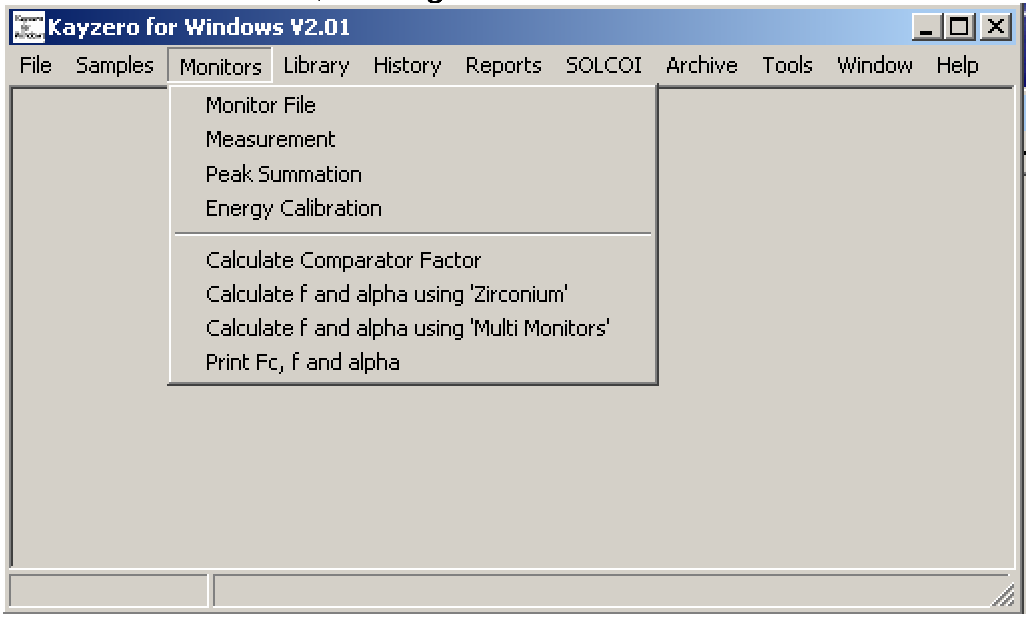


Figure 3.2: *Monitor* menu

The monitor-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.

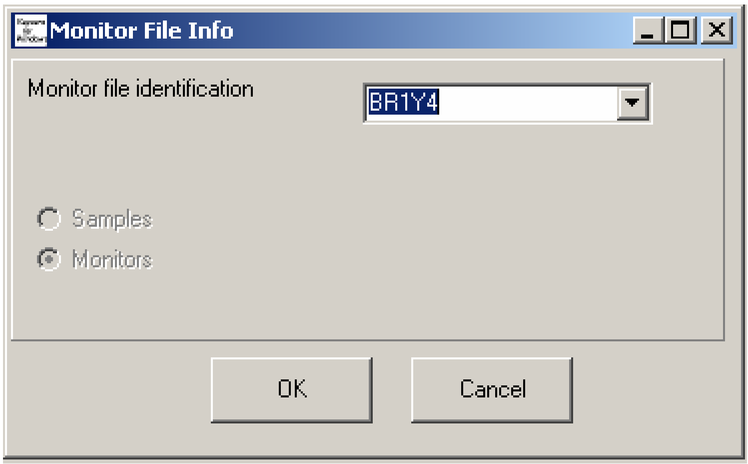
When three monitors are irradiated a full flux parameter set (F_c, f and α) can be determined using ‘Calculate f and alpha using Multi Monitors’ however three is the absolute minimum and results in high uncertainties for f and α. Better is to use an Au/Zr monitor couple, using the special optimized Au/Zr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

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 α 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).

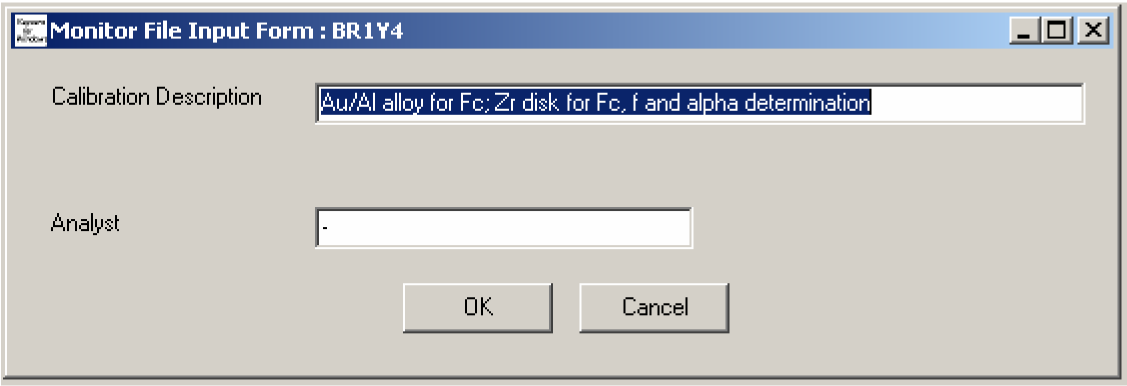


Monitor File Info

Monitor file identification: BR1Y4

○ Samples
● Monitors

Figure 3.3A: Select Monitor filename.



Monitor File Input Form : BR1Y4

Calibration Description: Au/Al alloy for Fc; Zr disk for Fc, f and alpha determination

Analyst: -

Figure 3.3B: Monitor file info.

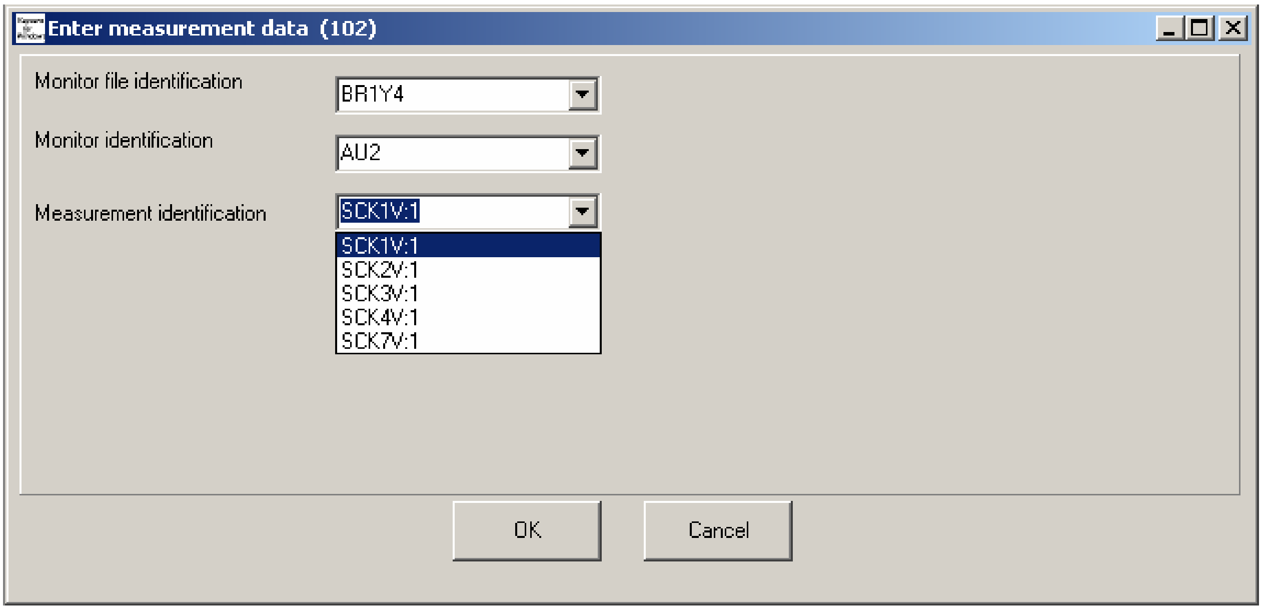
3.3.2 Entering Monitor Data

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 it may also 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 semicolumn (e.g. SCK7V:1 were '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).

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



Monitor file identification: BR1Y4

Monitor identification: AU2

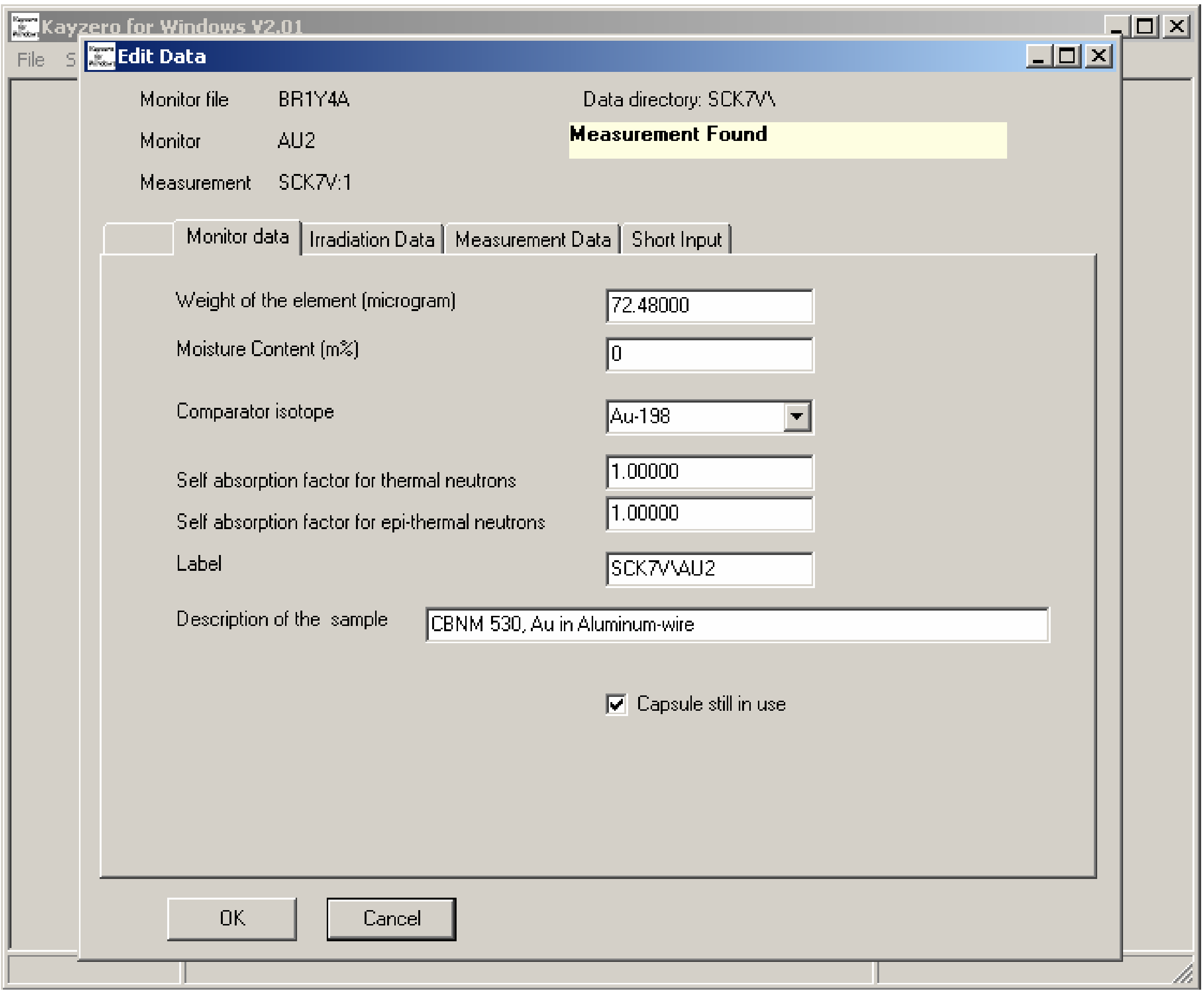
Measurement identification: SCK1V:1

- SCK1V:1
- SCK2V:1
- SCK3V:1
- SCK4V:1
- SCK7V:1

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 µg (72.48 mg * 0.1 % = 72.48 µg). 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.



Monitor file BR1Y4A

Monitor AU2

Measurement SCK7V:1

Data directory: SCK7V\

Measurement Found

Weight of the element (microgram) 72.48000

Moisture Content (m%) 0

Comparator isotope Au-198

Self absorption factor for thermal neutrons 1.00000

Self absorption factor for epi-thermal neutrons 1.00000

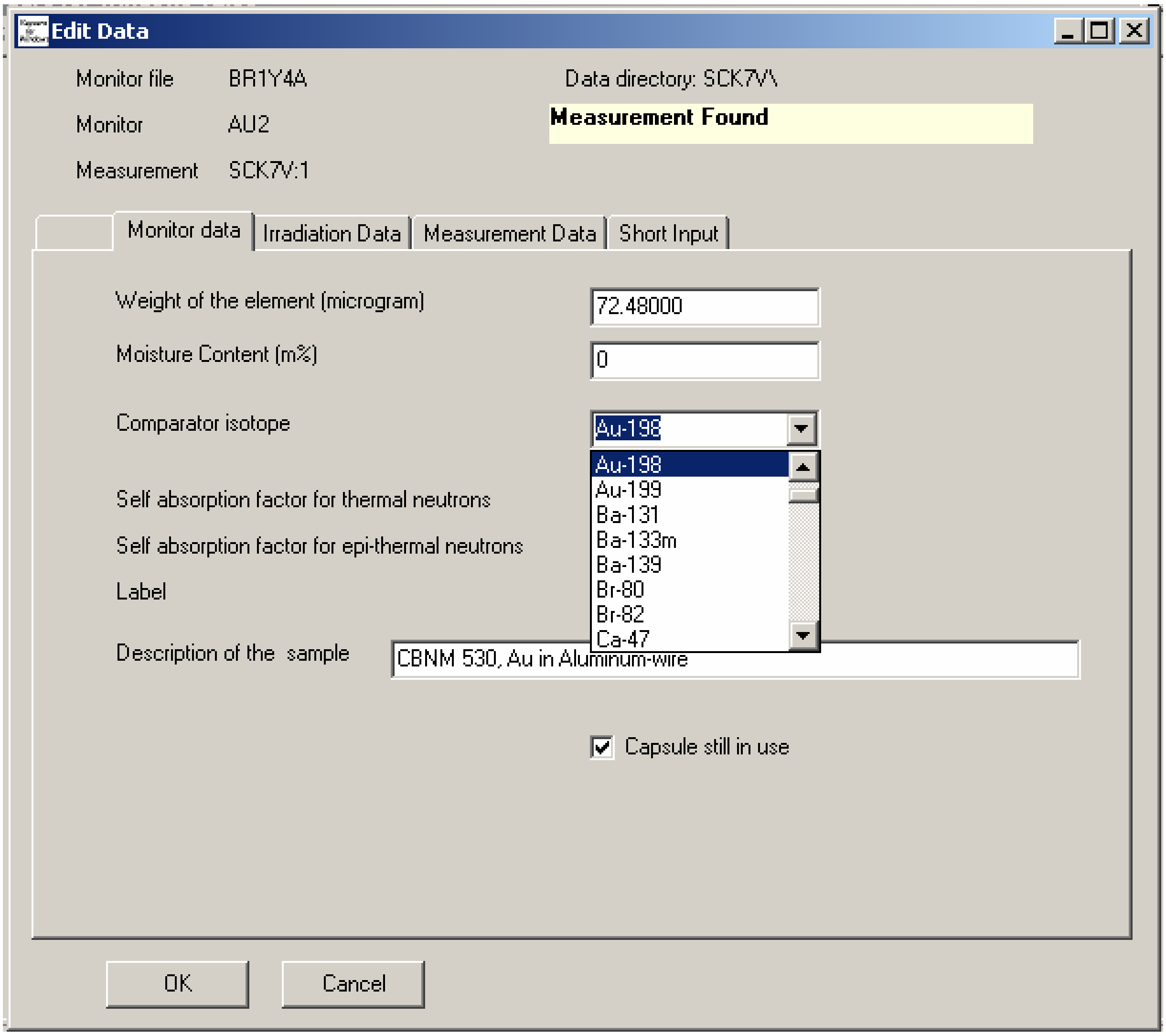
Label SCK7V\AU2

Description of the sample CBNM 530, Au in Aluminum-wire

☑ Capsule still in use

Figure 3.5: Monitor data input.

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



Monitor file BR1Y4A
Monitor AU2
Measurement SCK7V:1
Data directory: SCK7V\
Measurement Found

Weight of the element (microgram) 72.48000
Moisture Content (m%) 0
Comparator isotope Au-198

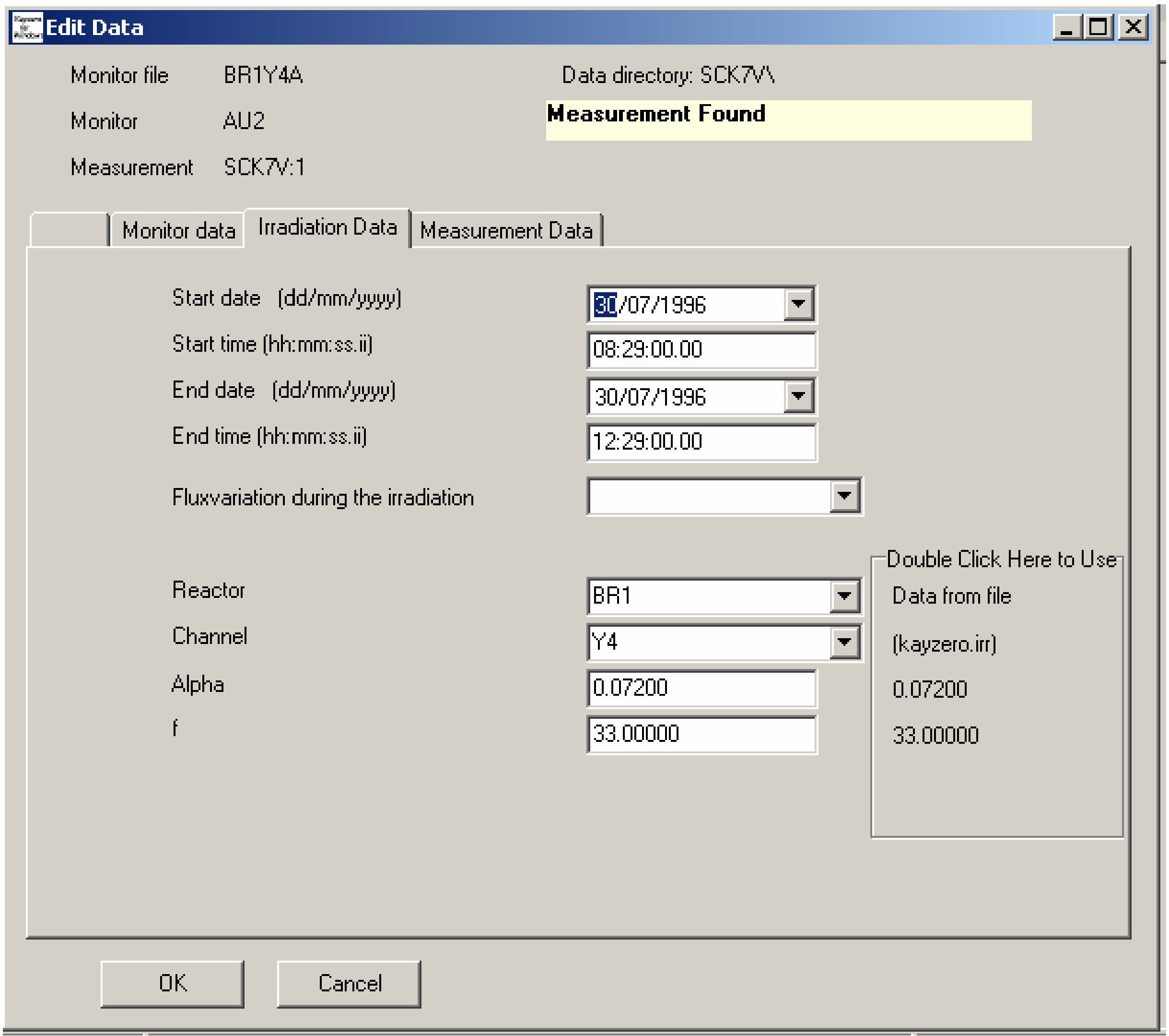
- Au-198
- Au-199
- Ba-131
- Ba-133m
- Ba-139
- Br-80
- Br-82
- Ca-47

Self absorption factor for thermal neutrons
Self absorption factor for epi-thermal neutrons
Label
Description of the sample CBNM 530, Au in Aluminum-wire

☑ Capsule still in use

Figure 3.6: *Monitor Data*-tab with a list of possible comparator radioisotopes.

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



Monitor file BR1Y4A
Monitor AU2
Measurement SCK7V:1
Data directory: SCK7V\
Measurement Found

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

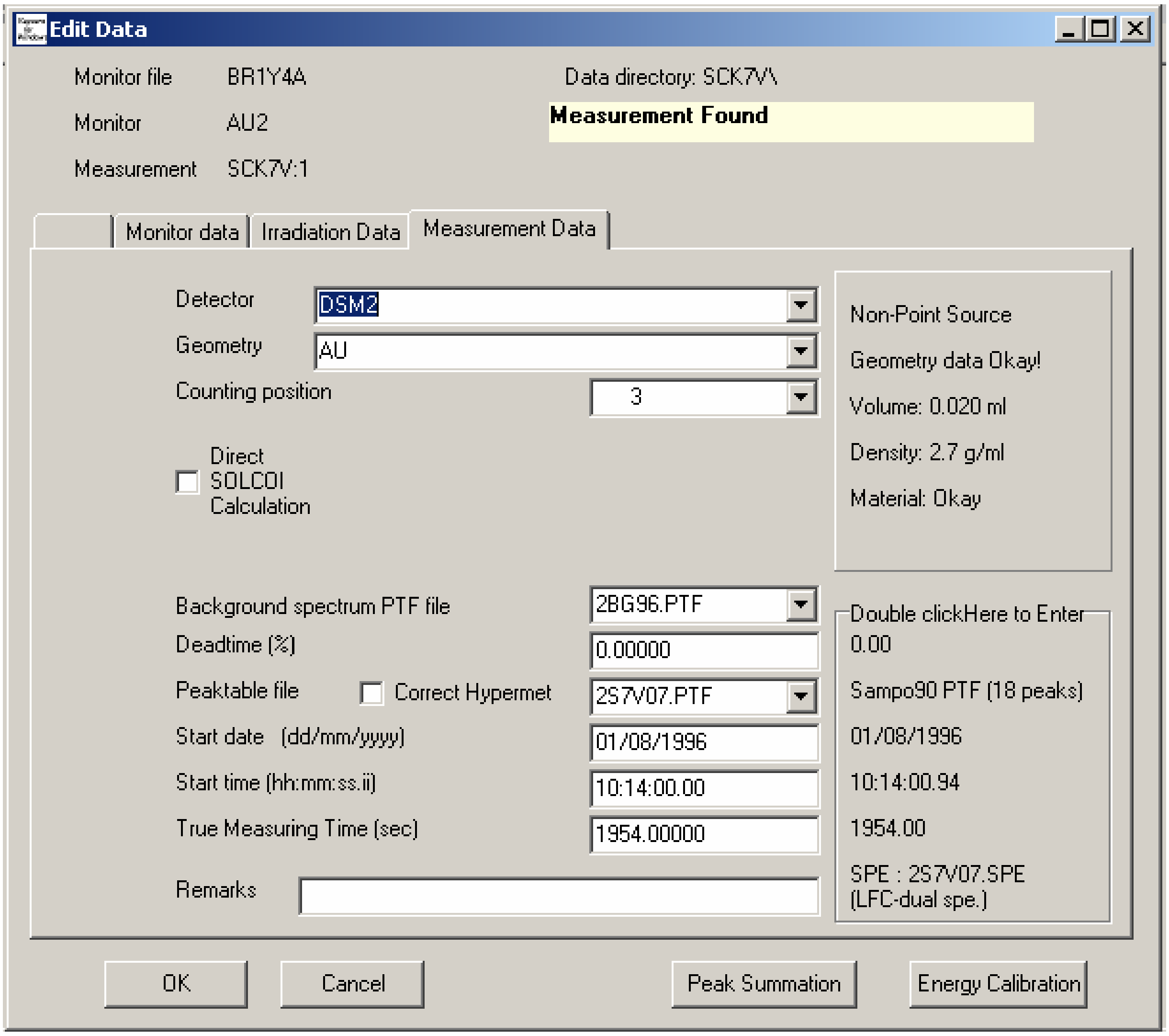
Reactor BR1
Channel Y4
Alpha 0.07200
f 33.00000

Data from file
(kayzero.irr)
0.07200
33.00000

Figure 3.7: *Irradiation Data-tab*. The reactor and channel can be picked from a list. The f and α can be entered by clicking the panel name 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 α values. You can select reactor and channel from a list. The f and α can 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’. For editing this file you need to use the right mouse button and enter ‘ok’ as password. In the *Measurement Data*-tab you can enter the measurement data, see Figure 3.8. 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.



Monitor file BR1Y4A

Monitor AU2

Measurement SCK7V:1

Data directory: SCK7V\

Measurement Found

Detector DSM2

Geometry AU

Counting position 3

☐ Direct SOLCOI Calculation

Non-Point Source

Geometry data Okay!

Volume: 0.020 ml

Density: 2.7 g/ml

Material: Okay

Background spectrum PTF file 2BG96.PTF

Deadtime (%) 0.00000

Peaktable file ☐ Correct Hypermet 2S7V07.PTF

Start date (dd/mm/yyyy) 01/08/1996

Start time (hh:mm:ss.ii) 10:14:00.00

True Measuring Time (sec) 1954.00000

Remarks

Double clickHere to Enter

0.00

Sampo90 PTF (18 peaks)

01/08/1996

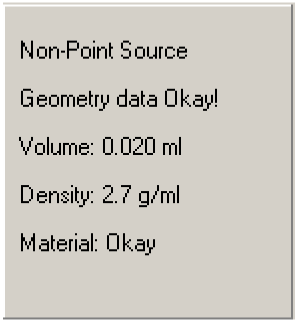
10:14:00.94

1954.00

SPE : 2S7V07.SPE
(LFC-dual spe.)

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.



Non-Point Source

Geometry data Okay!

Volume: 0.020 ml

Density: 2.7 g/ml

Material: Okay

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.

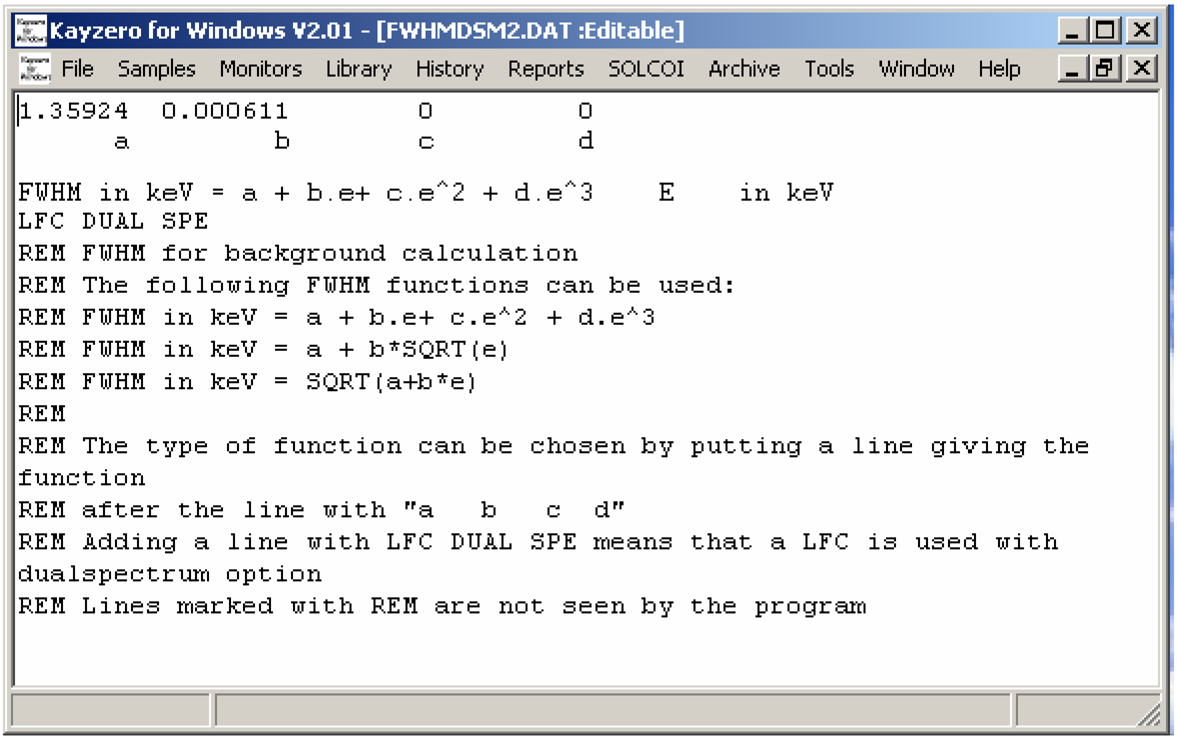
If background subtraction is to be performed, the relevant peak table file must be entered. This file must be located in the ‘Efficiency Data’-directory.

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 FWHMdddd.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).



```
1.35924  0.000611        0          0
      a          b         c          d

FWHM in keV = a + b.e+ c.e^2 + d.e^3    E    in keV
LFC DUAL SPE
REM FWHM for background calculation
REM The following FWHM functions can be used:
REM FWHM in keV = a + b.e+ c.e^2 + d.e^3
REM FWHM in keV = a + b*SQRT(e)
REM FWHM in keV = SQRT(a+b*e)
REM
REM The type of function can be chosen by putting a line giving the
function
REM after the line with "a   b   c  d"
REM Adding a line with LFC DUAL SPE means that a LFC is used with
dualspectrum option
REM Lines marked with REM are not seen by the program
```

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

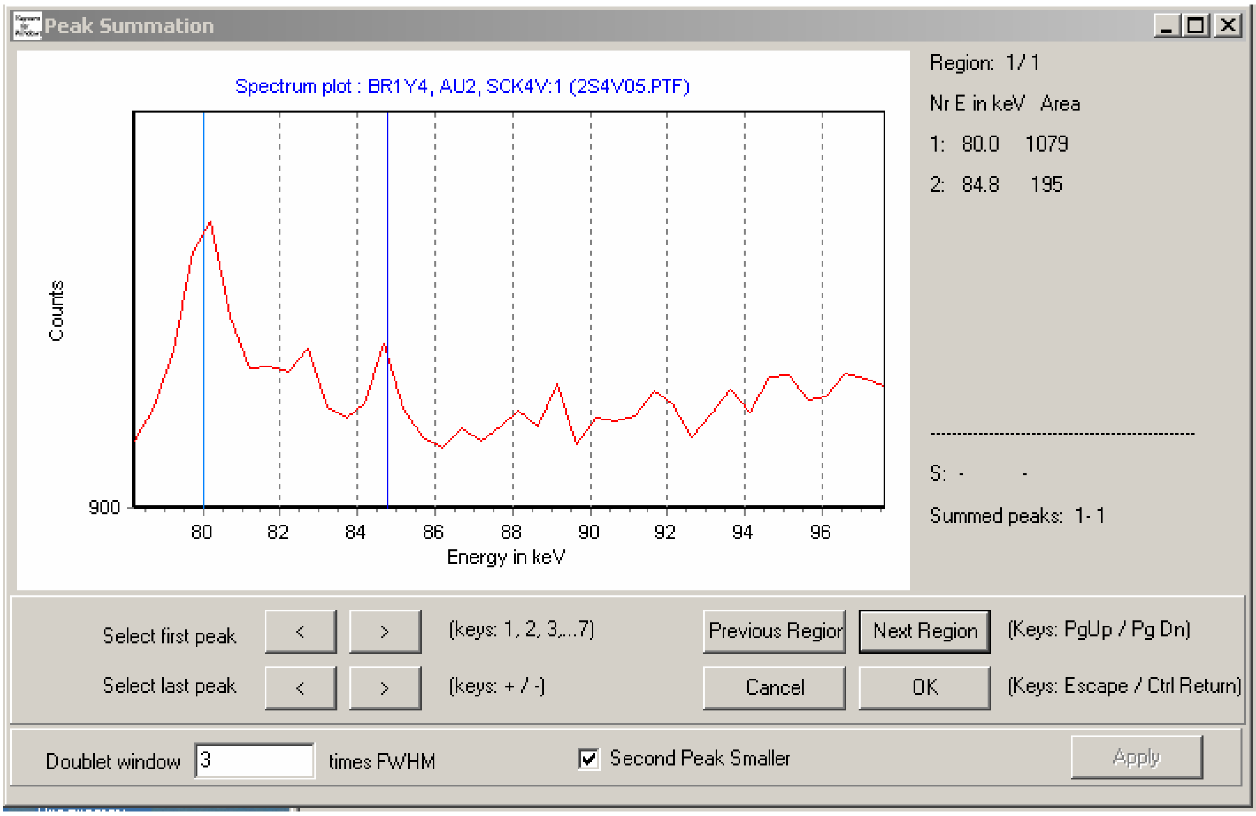
To select the correct peak table file use the pick-list to call up a table of files from which you can choose. Kayzero enters the relevant measurement data (start date and time and measuring time) if you double click on the info-panel on the right.

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



```
Region:  1/1
Nr E in keV   Area
1:  80.0    1079
2:  84.8     195
S:  -        -
Summed peaks:  1-1
```

Doublet window 3 times FWHM

☑ Second Peak Smaller

Figuur 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 then done in most programs. In order to facilitate this problem a new 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* (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*!!!!!!

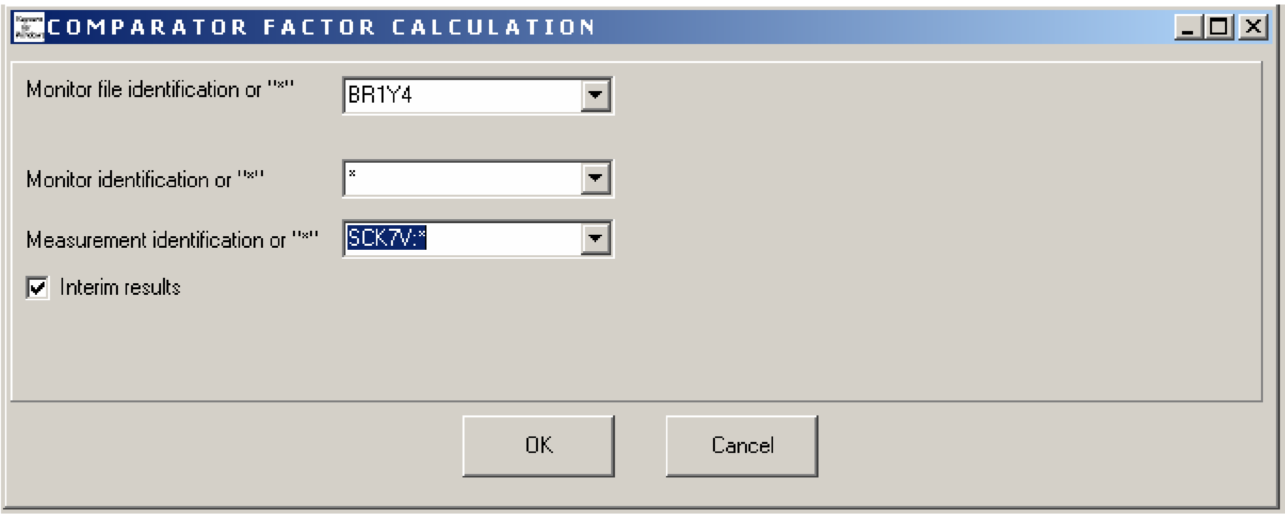
The main peak to which all other smaller peaks should be added can be selected by typing the appropriate peak number (1-7, see Figure 3.11). All peaks at the right side of this main peak can be added by pressing the <+> key or deselected by using the <-> key. At the right of the screen the peaks are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



Monitor file identification or "*" BR1Y4

Monitor identification or "*" *

Measurement identification or "*" SCK7V:*

☑ Interim results

Figure 3.12 : *Monitors/Calculate Comparator Factor* .

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.

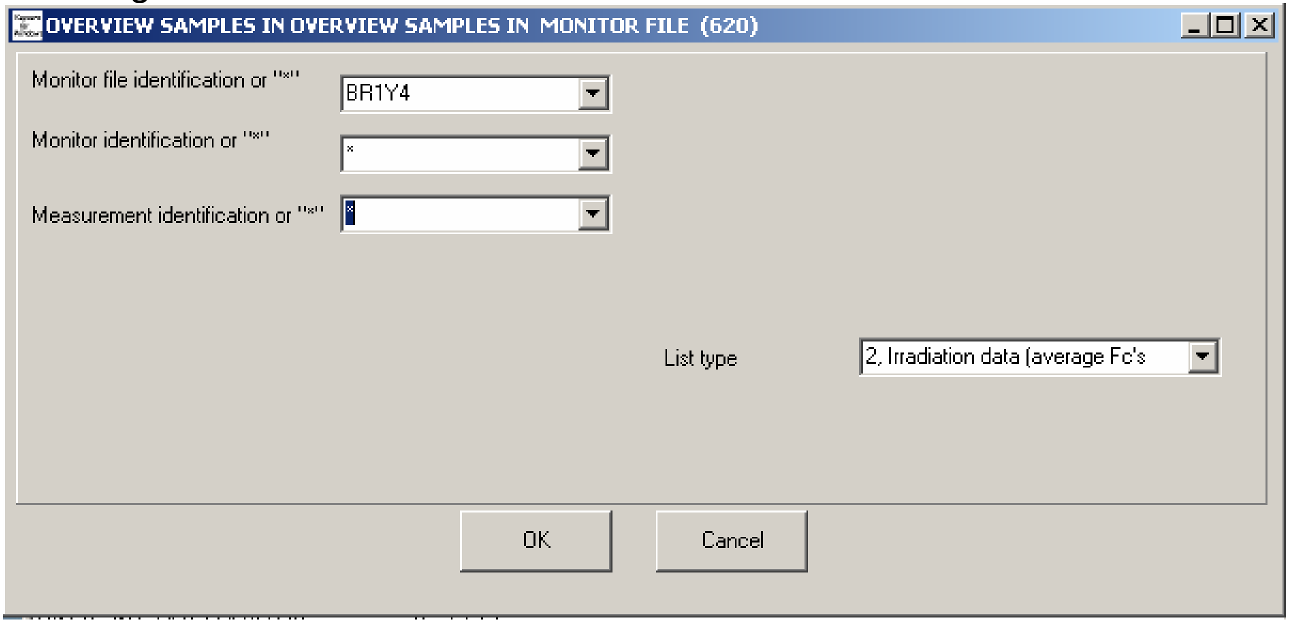
A burn-up correction procedure is built in; the correction factors are given when the 'Interim results' are printed. Burn-up correction for monitors and samples is performed using the data in 'KAYZERO.BUR' for the isotopes Eu-154, Ta-182, Au-198, Dy-165, Pm-149 and Rh-105. If this file is not present,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

3.3.5 Printing F_c

The calculated F_c can be printed using '*Monitors/Print Fc, 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.

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. However, the value of F_c (which is proportional to the epithermal flux density) can be estimated, so input errors can also be detected by checking the calculated values.


OVERVIEW SAMPLES IN OVERVIEW SAMPLES IN MONITOR FILE (620)

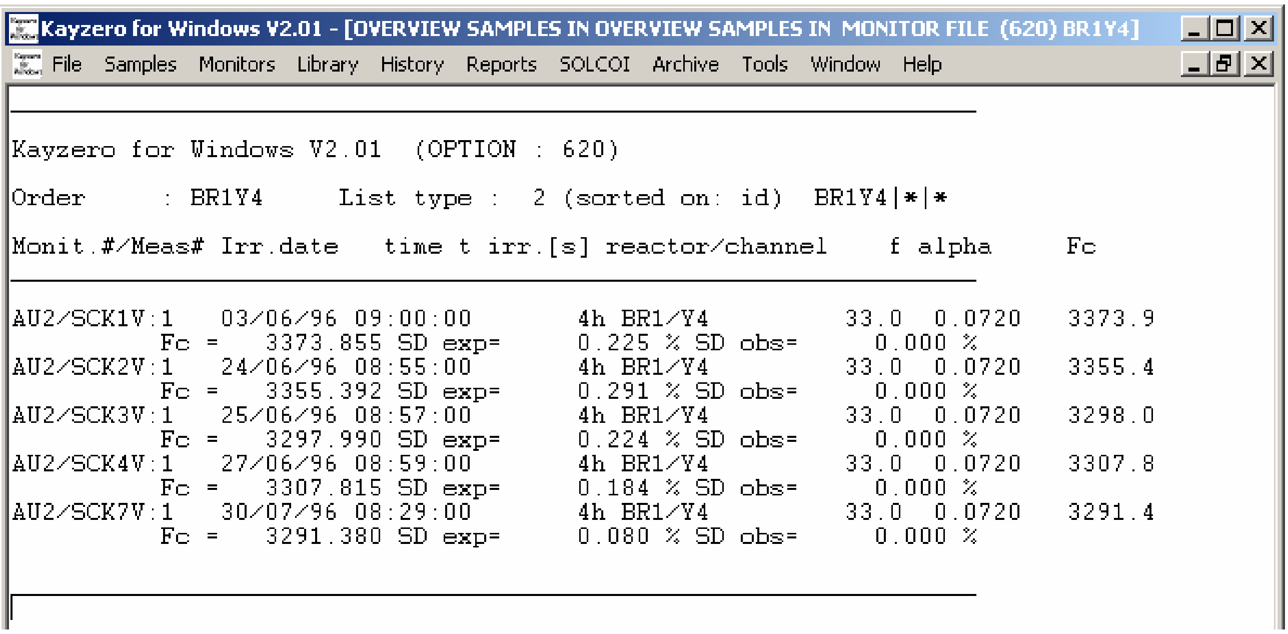
Monitor file identification or "*": BR1Y4

Monitor identification or "*": *

Measurement identification or "*": *

List type: 2. Irradiation data (average Fc's

Figure 3.13 : F_c print option

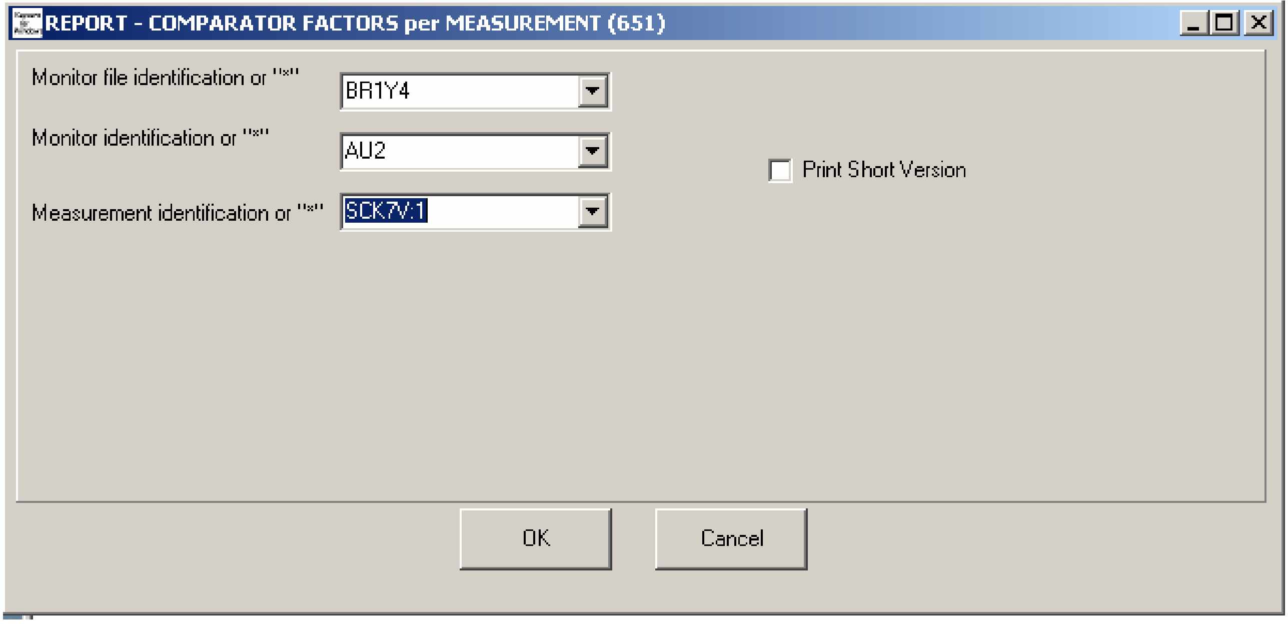


```
Kayzero for Windows V2.01  (OPTION : 620)

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

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   3291.4
          Fc =   3291.380 SD exp=     0.080 % 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.



Monitor file identification or "*" BR1Y4

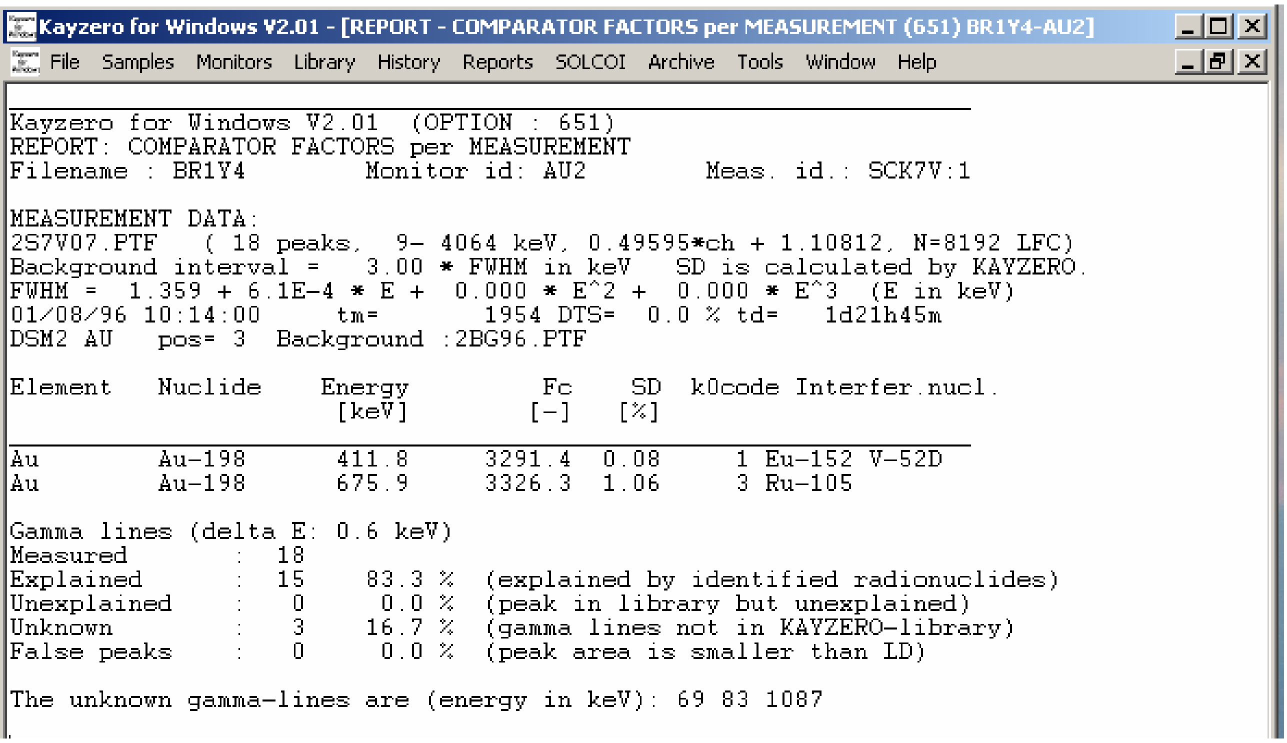
Monitor identification or "*" AU2

Measurement identification or "*" SCK7V:1

☐ Print Short Version

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 V2.01  (OPTION : 651)
REPORT: COMPARATOR FACTORS per MEASUREMENT
Filename : BR1Y4        Monitor id: AU2        Meas. id.: SCK7V:1

MEASUREMENT DATA:
2S7V07.PTF   ( 18 peaks,  9- 4064 keV, 0.49595*ch + 1.10812, 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)
01/08/96 10:14:00     tm=       1954 DTS=  0.0 % td=   1d21h45m
DSM2 AU   pos= 3  Background :2BG96.PTF

Element   Nuclide    Energy         Fc     SD  k0code Interfer.nucl.
                      [keV]        [-]    [%]
Au        Au-198      411.8     3291.4  0.08      1 Eu-152 V-52D
Au        Au-198      675.9     3326.3  1.06      3 Ru-105

Gamma lines (delta E: 0.6 keV)
Measured        :  18
Explained       :  15     83.3 %  (explained by identified radionuclides)
Unexplained     :   0      0.0 %  (peak in library but unexplained)
Unknown         :   3     16.7 %  (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): 69 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. The order file can be linked to a client using the *Sample/Order Input*-option.

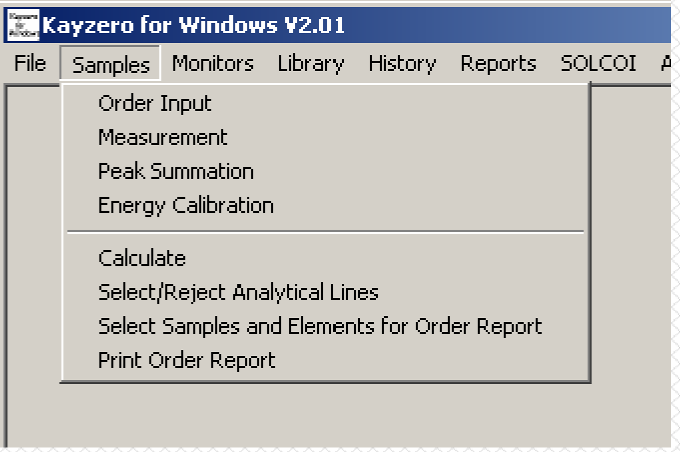
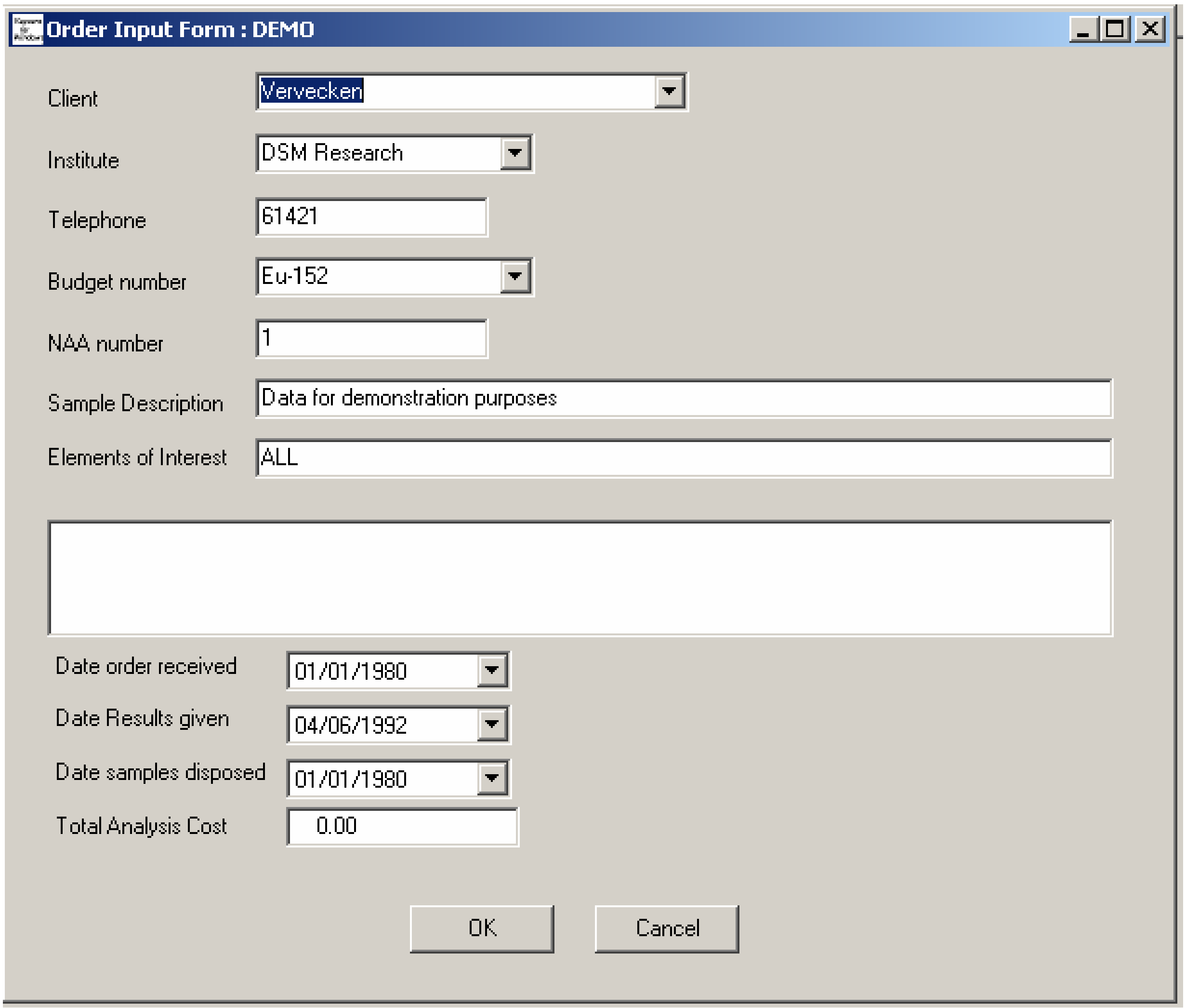


Figure 3.17 : *Sample*- options.

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*.



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

Figure 3.18 : Order Info.

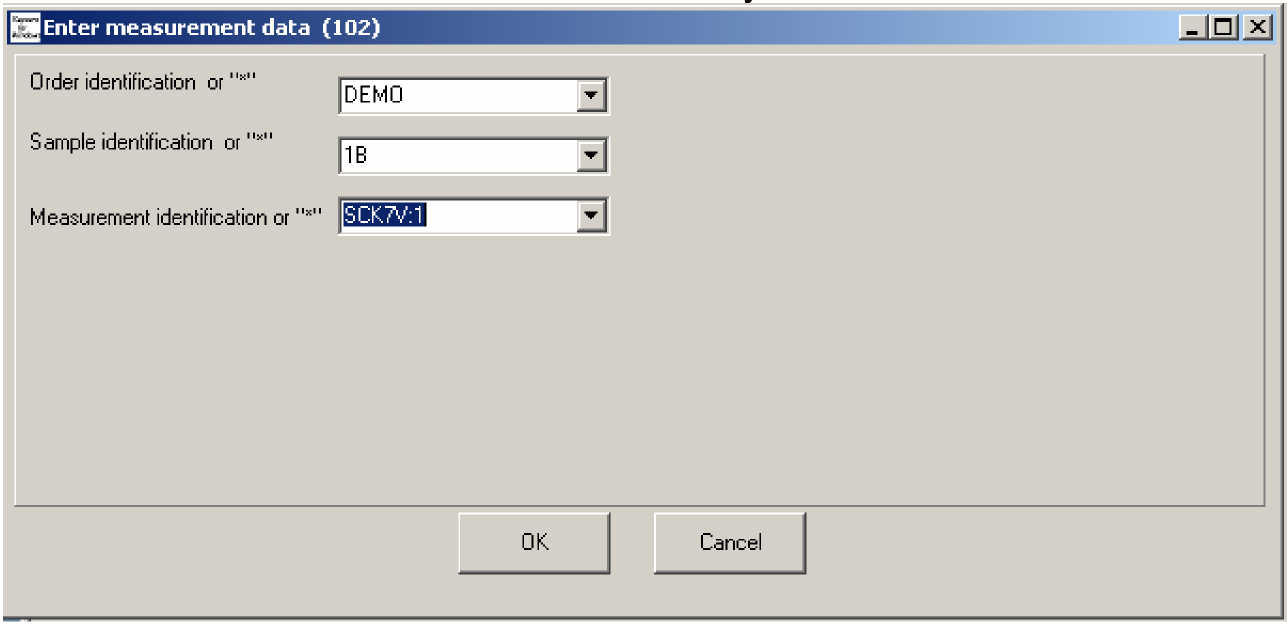
3.4.2 Entering Measurement Data

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).

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).

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\'.



Order identification or "*" DEMO

Sample identification or "*" 1B

Measurement identification or "*" SCK7V:1

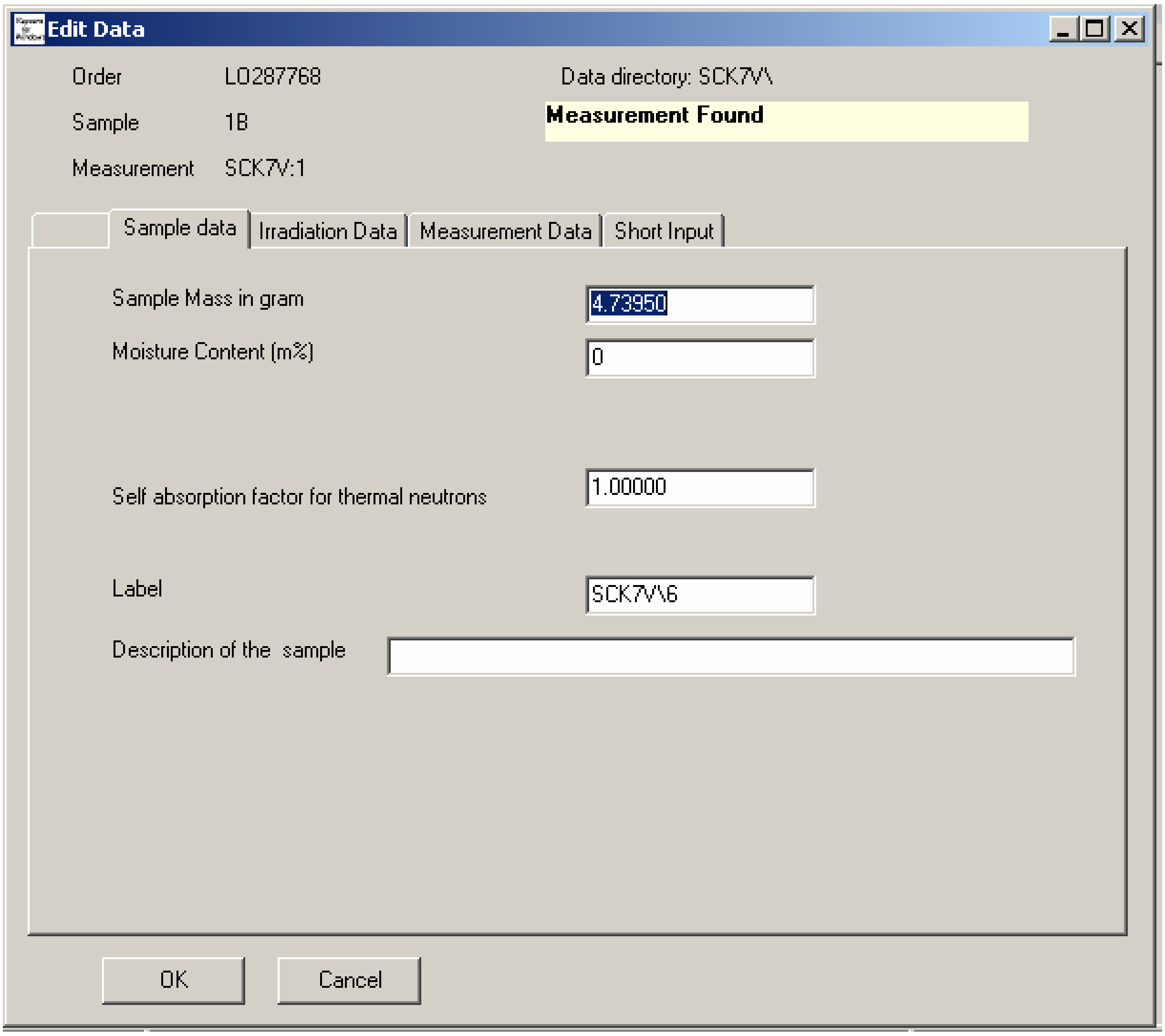
Figure 3.19 : Identification of a measurement.

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.

You can calculate the self-absorption factor for thermal neutrons for the irradiated sample using the*Tools/Thermal Neutron Self Absorption*-Option and then enter it.

In case of serious epithermal self-shielding, you should calculate or measure a correction factor and apply it to the end result for every individual isotope manually.

In the *Irradiation Data*-tab sheet you can enter the irradiation data (Figure 3.21). You should enter the start date and time of the irradiation. The formats are shown between brackets.



Order L0287768

Sample 1B

Measurement SCK7V:1

Data directory: SCK7V\

Measurement Found

Sample Mass in gram: 4.73950

Moisture Content (m%): 0

Self absorption factor for thermal neutrons: 1.00000

Label: SCK7V\6

Description of the sample:

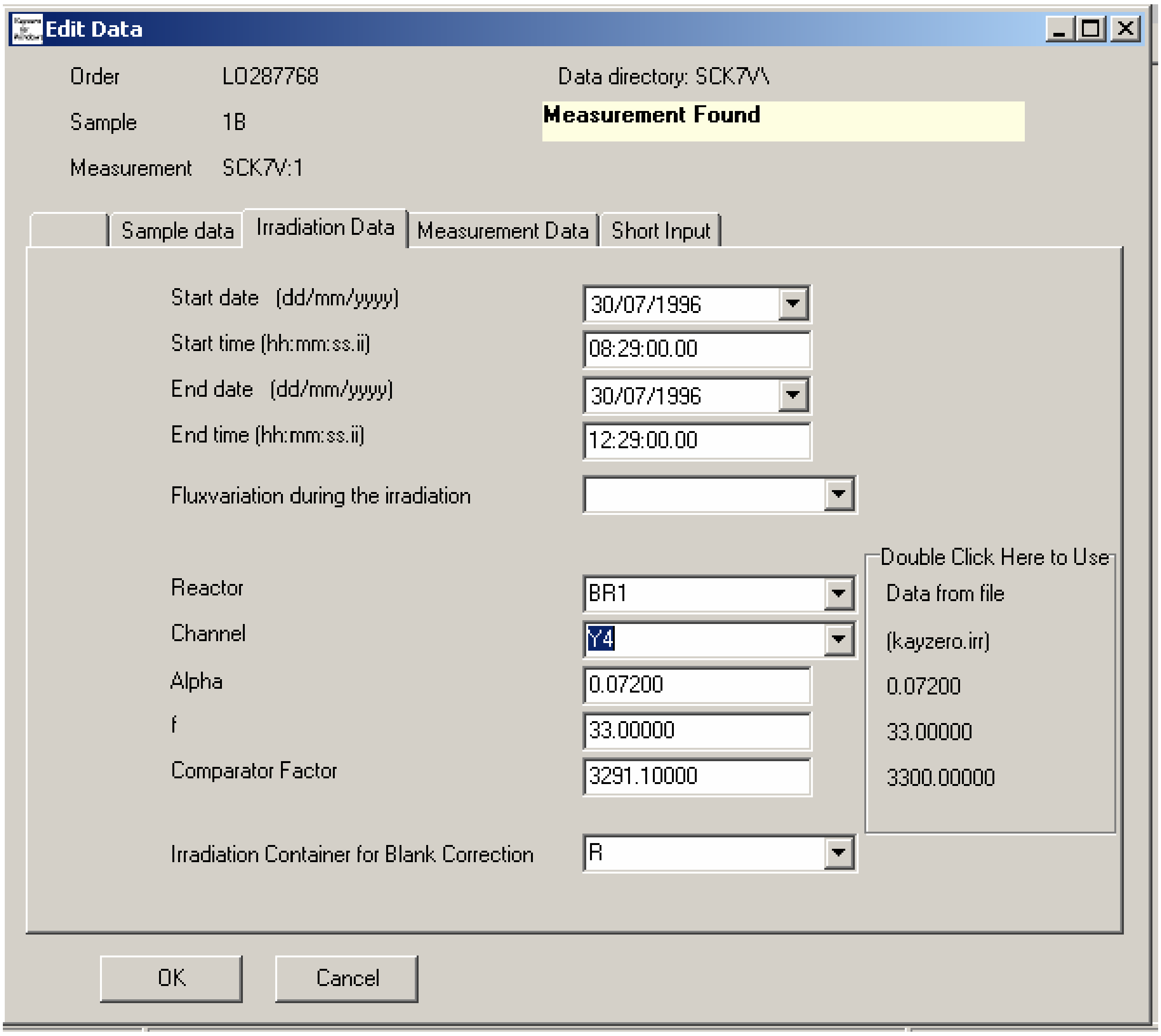
Figure 3.20 : *Sample Data*-tab sheet.

You also have to enter the codes of the reactor and channel in which the irradiation took place and the corresponding f and α values. Also you have to enter the F_c-value, calculated in the previous chapter.

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 next page. Check an existing .PAR file and create you own.



Order L0287768

Sample 1B

Measurement SCK7V:1

Data directory: SCK7V\

Measurement Found

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 BR1

Channel Y4

Alpha 0.07200

f 33.00000

Comparator Factor 3291.10000

Double Click Here to Use Data from file (kayzero.irr)

0.07200

33.00000

3300.00000

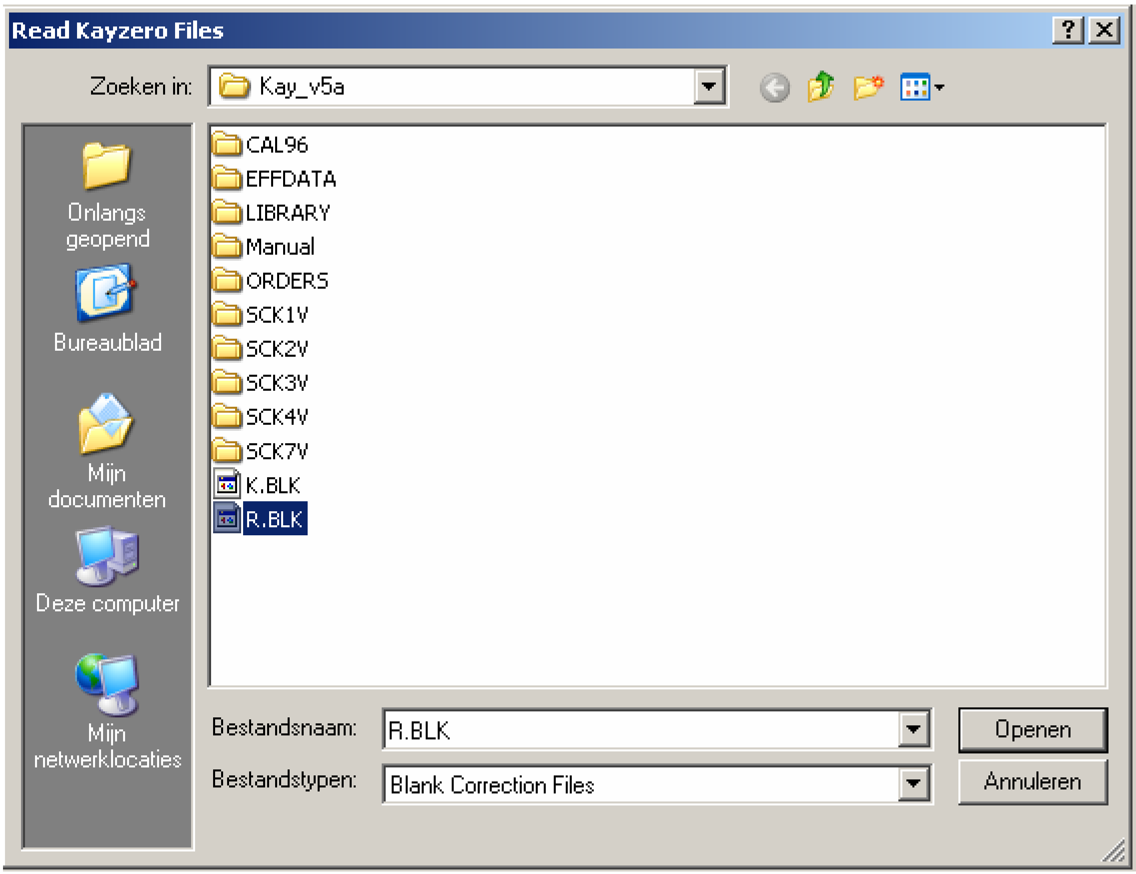
Irradiation Container for Blank Correction R

Figure 3.21: *Irradiation Data*-tab sheet.

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.

Irradiation Container for Blank Correction R

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 3.22). Check an existing file (e.g. ‘R.BLK’) to see the file format, See Figure 3.23.

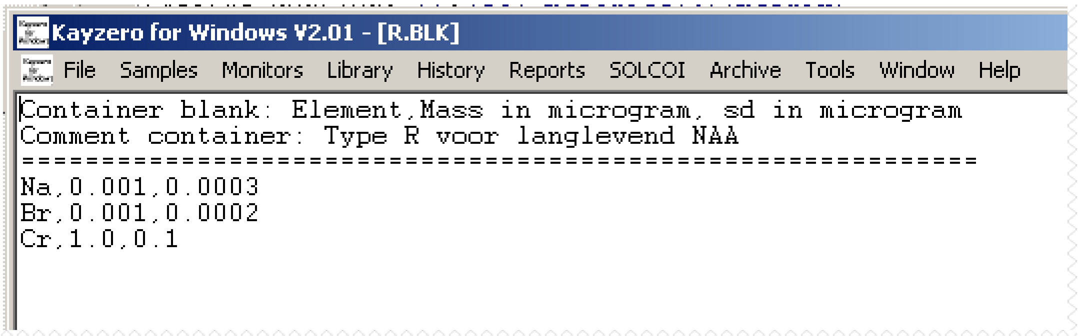


Zoeken in: Kay_v5a

Bestandsnaam: R.BLK

Bestandstypen: Blank Correction Files

Figure 3.22: Selecting a *blank correction*-file using *File/Open*.



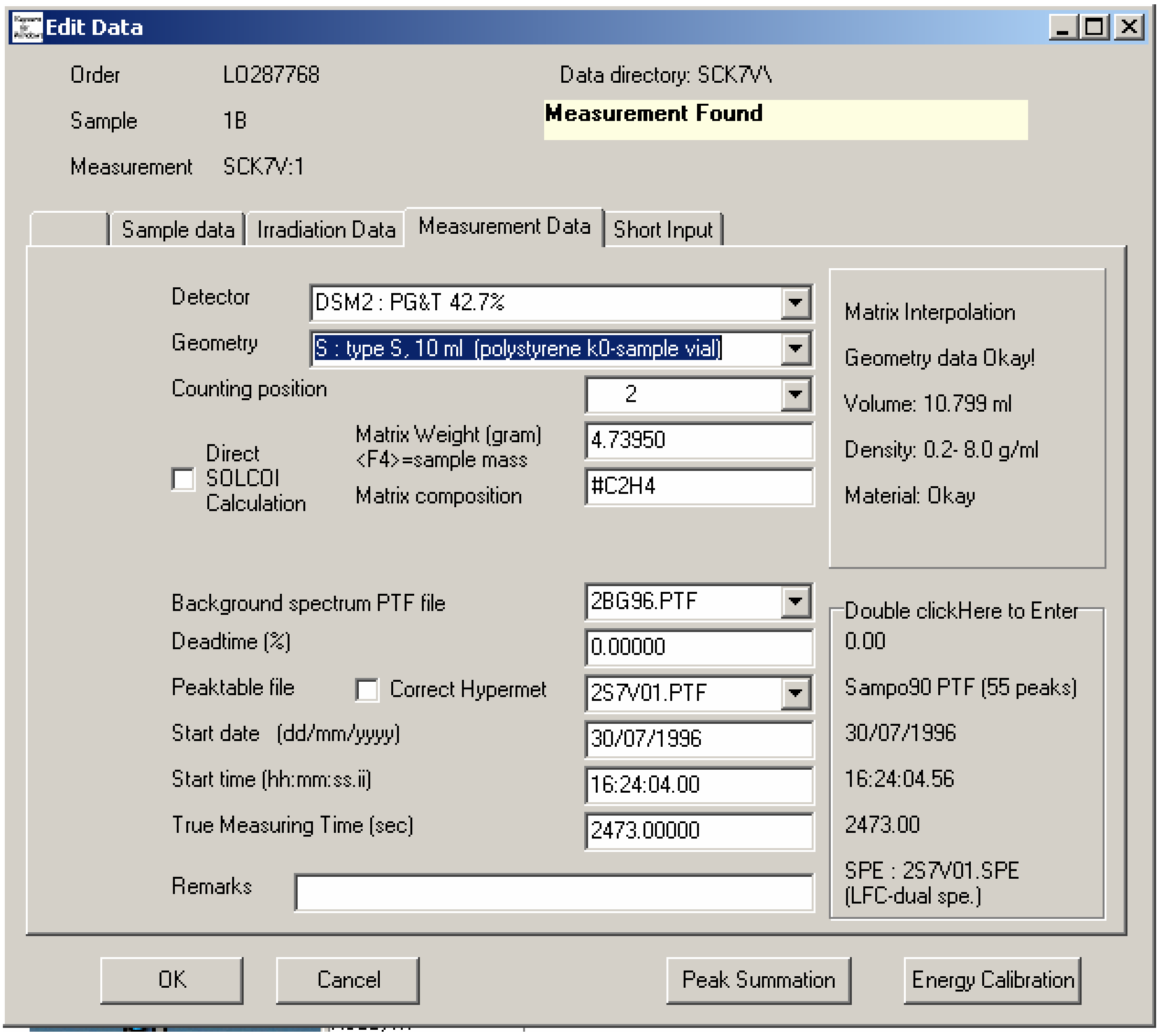
```
Container blank: Element,Mass in microgram, sd in microgram
Comment container: Type R voor langlevend NAA
============================================================
Na,0.001,0.0003
Br,0.001,0.0002
Cr,1.0,0.1
```

Figure 3.23: The typical *blank correction*-file format.

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 *SolCoi*. A detector name has maximal 4 characters and a vial (source) maximal 3 characters. You can only use the detectors and sources defined in *SolCoi*.



Order L0287768

Sample 1B

Measurement SCK7V:1

Data directory: SCK7V\

Measurement Found

Detector: DSM2 : PG&T 42.7%

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

Counting position: 2

☐ Direct SOLCOI Calculation

Matrix Weight (gram) <F4>=sample mass: 4.73950

Matrix composition: #C2H4

Background spectrum PTF file: 2BG96.PTF

Deadtime (%): 0.00000

Peaktable file: ☐ Correct Hypermet: 2S7V01.PTF

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

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

True Measuring Time (sec): 2473.00000

Remarks:

Matrix Interpolation

Geometry data Okay!

Volume: 10.799 ml

Density: 0.2- 8.0 g/ml

Material: Okay

Double clickHere to Enter

0.00

Sampo90 PTF (55 peaks)

30/07/1996

16:24:04.56

2473.00

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

Figure 3.24: *Measurement Data*-tabsheet.

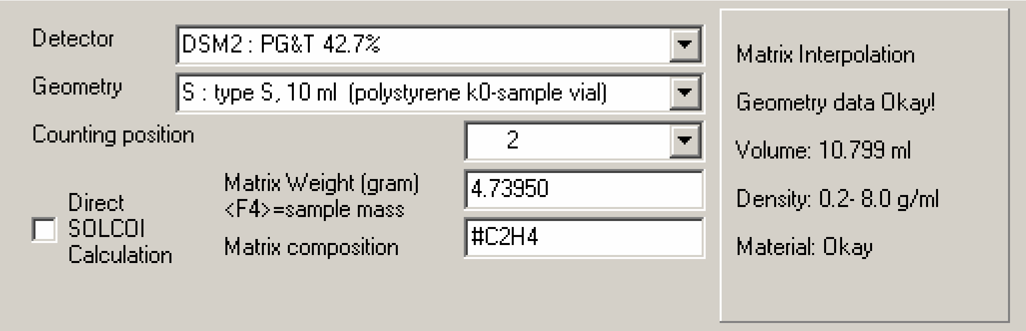
There are two types of sources:

- point-sources (especially for calibration sources (like the PTB-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 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 knows 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 : PG&T 42.7%
Geometry: S : type S, 10 ml (polystyrene k0-sample vial)
Counting position: 2
☐ Direct SOLCOI Calculation
Matrix Weight (gram) <F4>=sample mass: 4.73950
Matrix composition: #C2H4

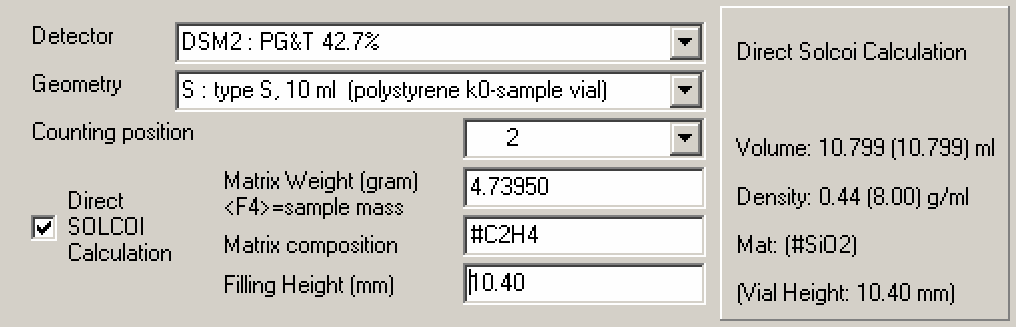
Matrix Interpolation
Geometry data Okay!
Volume: 10.799 ml
Density: 0.2- 8.0 g/ml
Material: Okay

Figure 3.25: Efficiency input data (matrix interpolation).

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_2. The absorption data of the matrix composition of the sample (C_2H_4) and the calculated geometry (SiO_2) 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 3.26).



Detector: DSM2 : PG&T 42.7%

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

Counting position: 2

☑ Direct SOLCOI Calculation

Matrix Weight (gram) <F4>=sample mass: 4.73950

Matrix composition: #C2H4

Filling Height (mm): 10.40

Direct Solcoi Calculation

Volume: 10.799 (10.799) ml

Density: 0.44 (8.00) g/ml

Mat: (#SiO2)

(Vial Height: 10.40 mm)

Figure 3.26: Efficiency input data (Direct Solcoi Calculation marked).

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.

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.

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.

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 3.27 (*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.

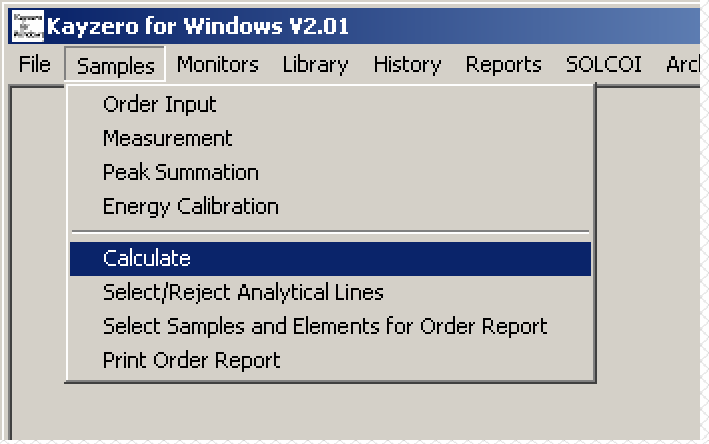
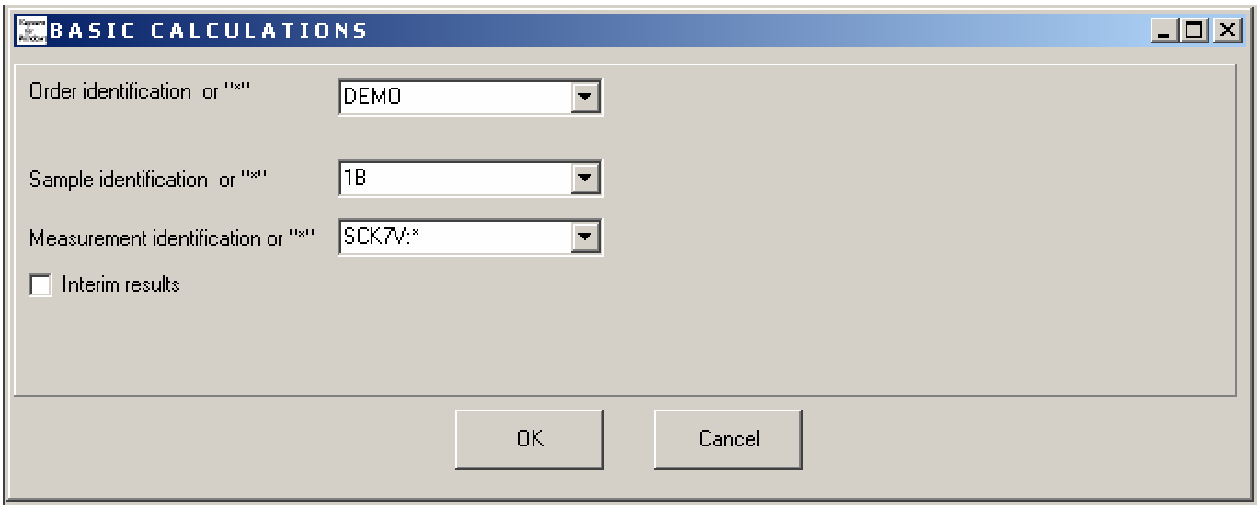


Figure 3.27 : Calculate-option in Samples menu



Order identification or "*": DEMO

Sample identification or "*": 1B

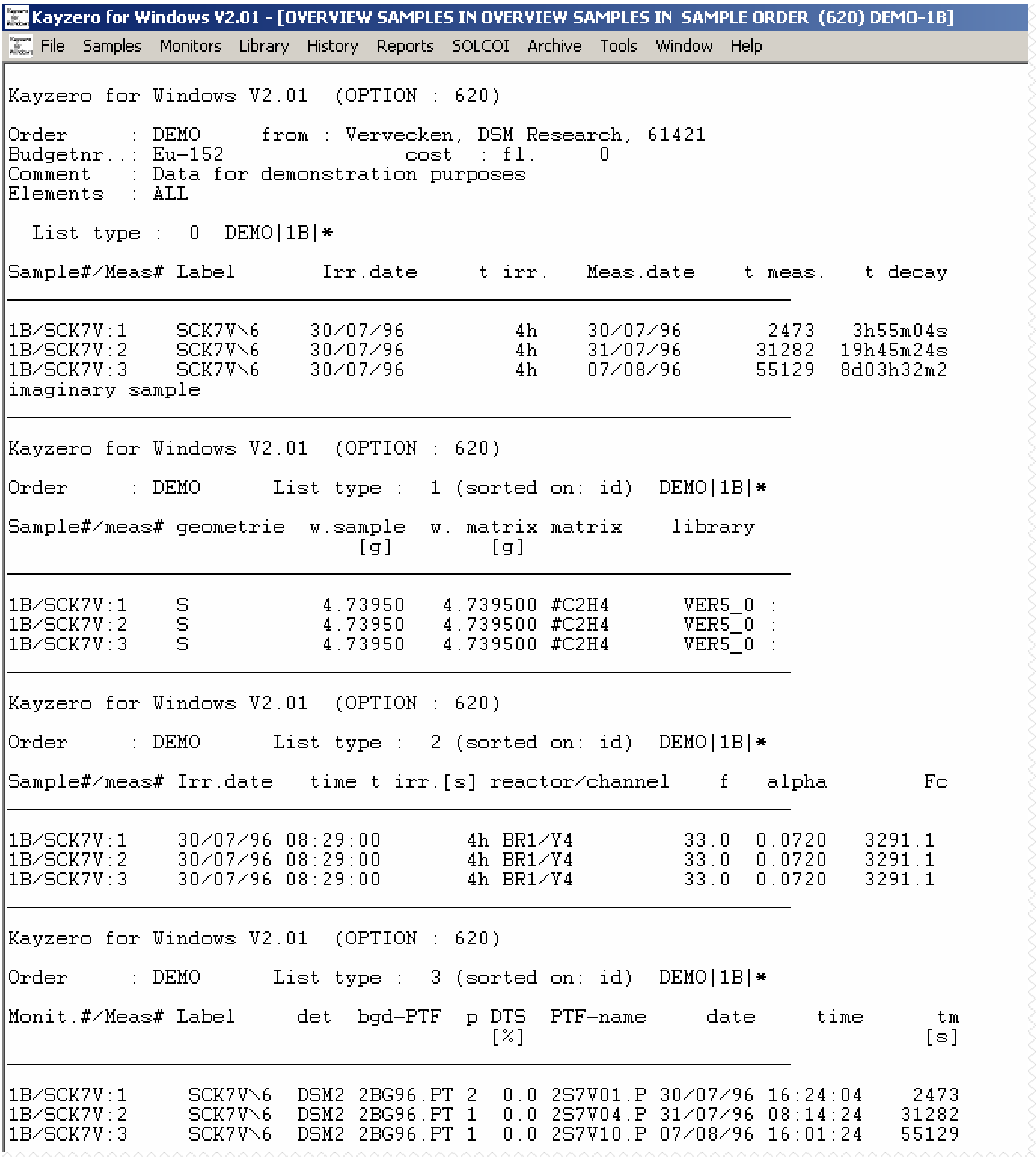
Measurement identification or "*": SCK7V:*

☐ Interim results

Figure 3.28 : Selecting the measurements

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

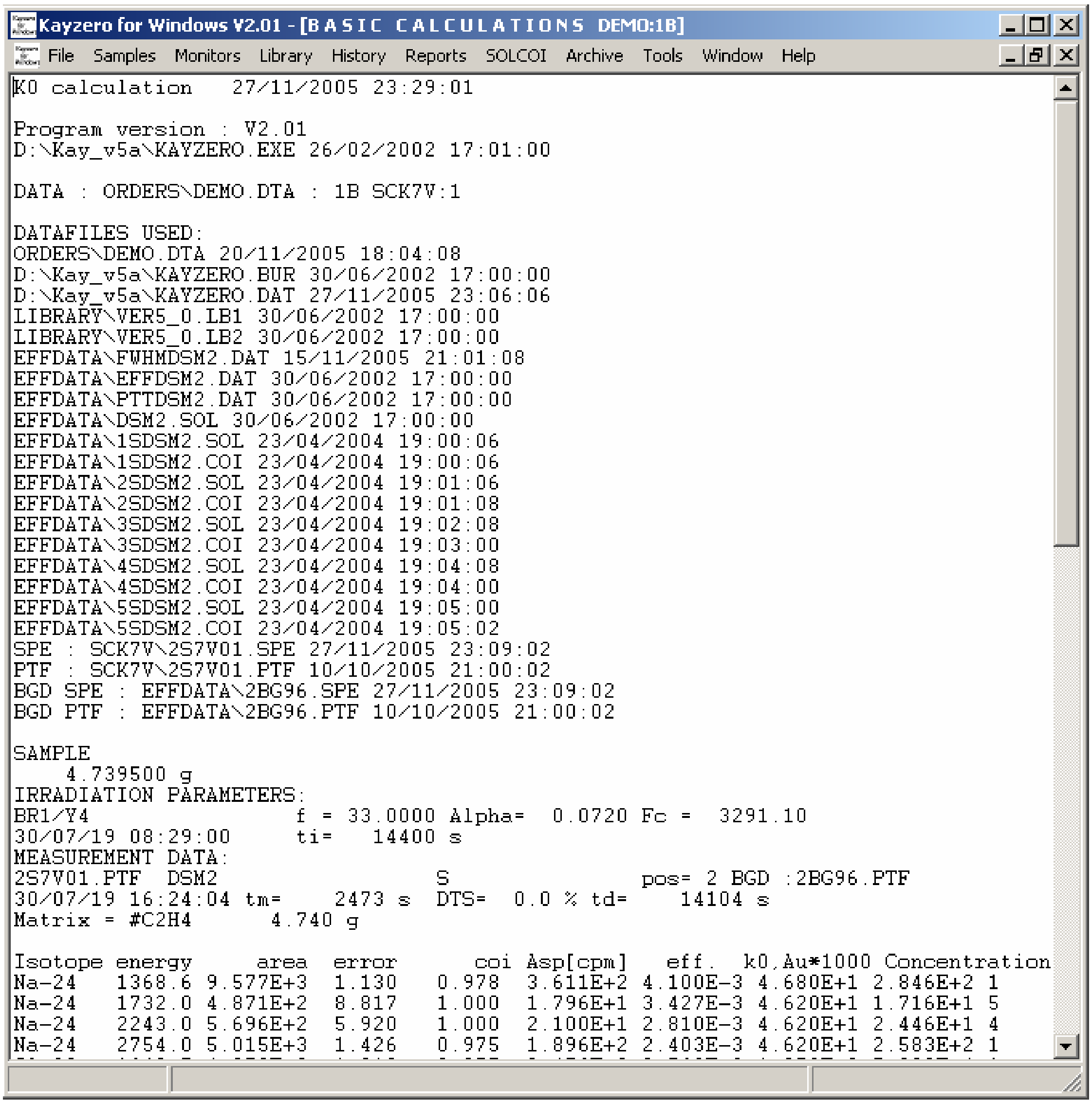
The calculations have to be repeated whenever input data, spectra data, library or efficiency data have been changed. Calculation parameters can be edited, see Appendix 6. If you use the wildcards '*'/ '*'/'SCK7V*' for the order, sample and measurement, respectively, only samples irradiated under code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



```
Kayzero for Windows V2.01  (OPTION : 620)

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

  List type :   0  DEMO|1B|*

Sample#/Meas# Label        Irr.date      t irr.   Meas.date     t meas.   t decay
________________________________________________________________________________

1B/SCK7V:1    SCK7V\6     30/07/96         4h     30/07/96        2473   3h55m04s
1B/SCK7V:2    SCK7V\6     30/07/96         4h     31/07/96       31282  19h45m24s
1B/SCK7V:3    SCK7V\6     30/07/96         4h     07/08/96       55129  8d03h32m2
imaginary sample
________________________________________________________________

Kayzero for Windows V2.01  (OPTION : 620)

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

Sample#/meas# geometrie  w.sample   w. matrix matrix     library
                            [g]         [g]
________________________________________________________________

1B/SCK7V:1     S           4.73950   4.739500 #C2H4      VER5_0  :
1B/SCK7V:2     S           4.73950   4.739500 #C2H4      VER5_0  :
1B/SCK7V:3     S           4.73950   4.739500 #C2H4      VER5_0  :
________________________________________________________________

Kayzero for Windows V2.01  (OPTION : 620)

Order      : DEMO      List type :   2 (sorted on: id)  DEMO|1B|*

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
1B/SCK7V:3    30/07/96 08:29:00       4h BR1/Y4           33.0  0.0720   3291.1
________________________________________________________________

Kayzero for Windows V2.01  (OPTION : 620)

Order      : DEMO      List type :   3 (sorted on: id)  DEMO|1B|*

Monit.#/Meas# Label      det   bgd-PTF   p DTS  PTF-name     date      time       tm
                                           [%]                                    [s]
________________________________________________________________

1B/SCK7V:1     SCK7V\6   DSM2 2BG96.PT 2  0.0 2S7V01.P 30/07/96 16:24:04    2473
1B/SCK7V:2     SCK7V\6   DSM2 2BG96.PT 1  0.0 2S7V04.P 31/07/96 08:14:24   31282
1B/SCK7V:3     SCK7V\6   DSM2 2BG96.PT 1  0.0 2S7V10.P 07/08/96 16:01:24   55129
```

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).



```
K0 calculation    27/11/2005 23:29:01

Program version : V2.01
D:\Kay_v5a\KAYZERO.EXE 26/02/2002 17:01:00

DATA : ORDERS\DEMO.DTA : 1B SCK7V:1

DATAFILES USED:
ORDERS\DEMO.DTA 20/11/2005 18:04:08
D:\Kay_v5a\KAYZERO.BUR 30/06/2002 17:00:00
D:\Kay_v5a\KAYZERO.DAT 27/11/2005 23:06:06
LIBRARY\VER5_0.LB1 30/06/2002 17:00:00
LIBRARY\VER5_0.LB2 30/06/2002 17:00:00
EFFDATA\FWHMDSM2.DAT 15/11/2005 21:01:08
EFFDATA\EFFDSM2.DAT 30/06/2002 17:00:00
EFFDATA\PTTDSM2.DAT 30/06/2002 17:00:00
EFFDATA\DSM2.SOL 30/06/2002 17:00:00
EFFDATA\1SDSM2.SOL 23/04/2004 19:00:06
EFFDATA\1SDSM2.COI 23/04/2004 19:00:06
EFFDATA\2SDSM2.SOL 23/04/2004 19:01:06
EFFDATA\2SDSM2.COI 23/04/2004 19:01:08
EFFDATA\3SDSM2.SOL 23/04/2004 19:02:08
EFFDATA\3SDSM2.COI 23/04/2004 19:03:00
EFFDATA\4SDSM2.SOL 23/04/2004 19:04:08
EFFDATA\4SDSM2.COI 23/04/2004 19:04:00
EFFDATA\5SDSM2.SOL 23/04/2004 19:05:00
EFFDATA\5SDSM2.COI 23/04/2004 19:05:02
SPE : SCK7V\2S7V01.SPE 27/11/2005 23:09:02
PTF : SCK7V\2S7V01.PTF 10/10/2005 21:00:02
BGD SPE : EFFDATA\2BG96.SPE 27/11/2005 23:09:02
BGD PTF : EFFDATA\2BG96.PTF 10/10/2005 21:00:02

SAMPLE
    4.739500 g
IRRADIATION PARAMETERS:
BR1/Y4                f = 33.0000 Alpha=  0.0720 Fc =  3291.10
30/07/19 08:29:00     ti=   14400 s
MEASUREMENT DATA:
2S7V01.PTF  DSM2                 S                 pos= 2 BGD :2BG96.PTF
30/07/19 16:24:04 tm=    2473 s  DTS=  0.0 % td=    14104 s
Matrix = #C2H4       4.740 g

Isotope energy     area  error      coi Asp[cpm]   eff.  k0,Au*1000 Concentration
Na-24   1368.6 9.577E+3  1.130   0.978  3.611E+2 4.100E-3 4.680E+1 2.846E+2 1
Na-24   1732.0 4.871E+2  8.817   1.000  1.796E+1 3.427E-3 4.620E+1 1.716E+1 5
Na-24   2243.0 5.696E+2  5.920   1.000  2.100E+1 2.810E-3 4.620E+1 2.446E+1 4
Na-24   2754.0 5.015E+3  1.426   0.975  1.896E+2 2.403E-3 4.620E+1 2.583E+2 1
```

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).

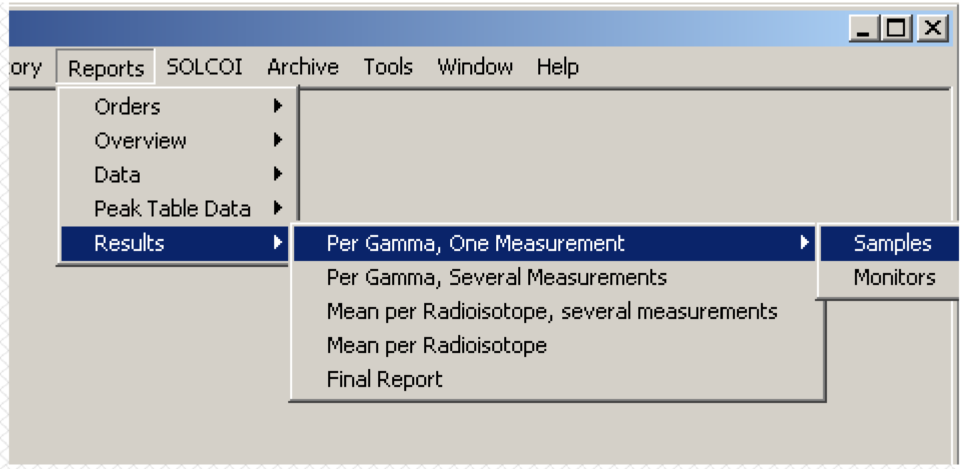


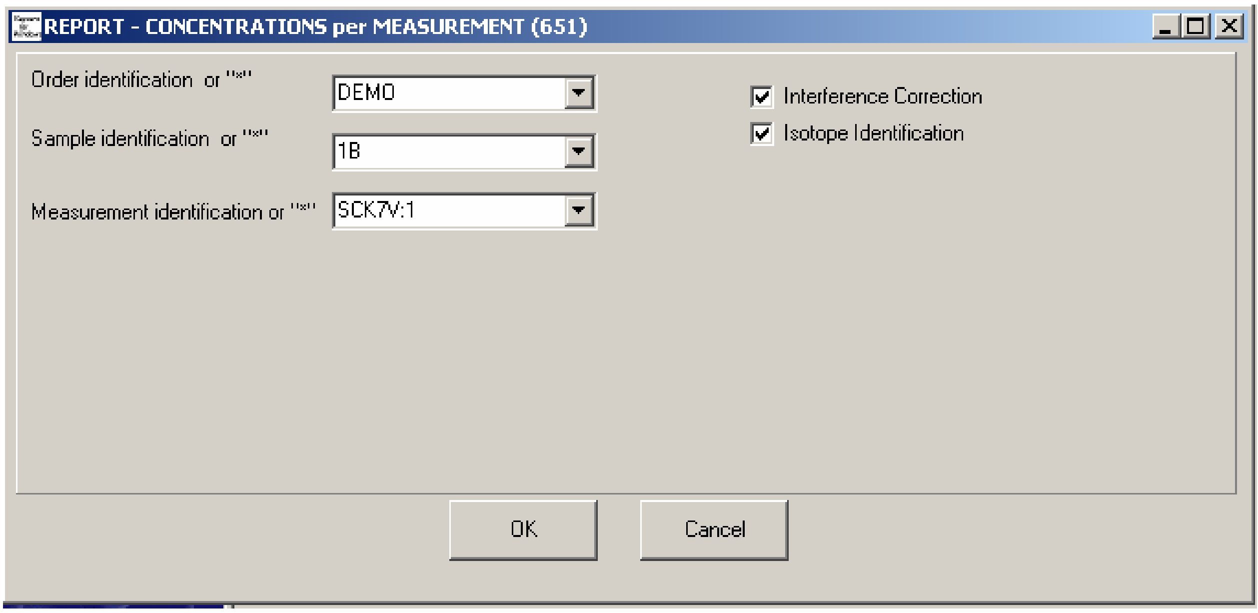
Figure 3.31 : *Reports/Results* menu

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).



REPORT - CONCENTRATIONS per MEASUREMENT (651)

Order identification or "*" DEMO

Sample identification or "*" 1B

Measurement identification or "*" SCK7V:1

☑ Interference Correction

☑ Isotope Identification

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

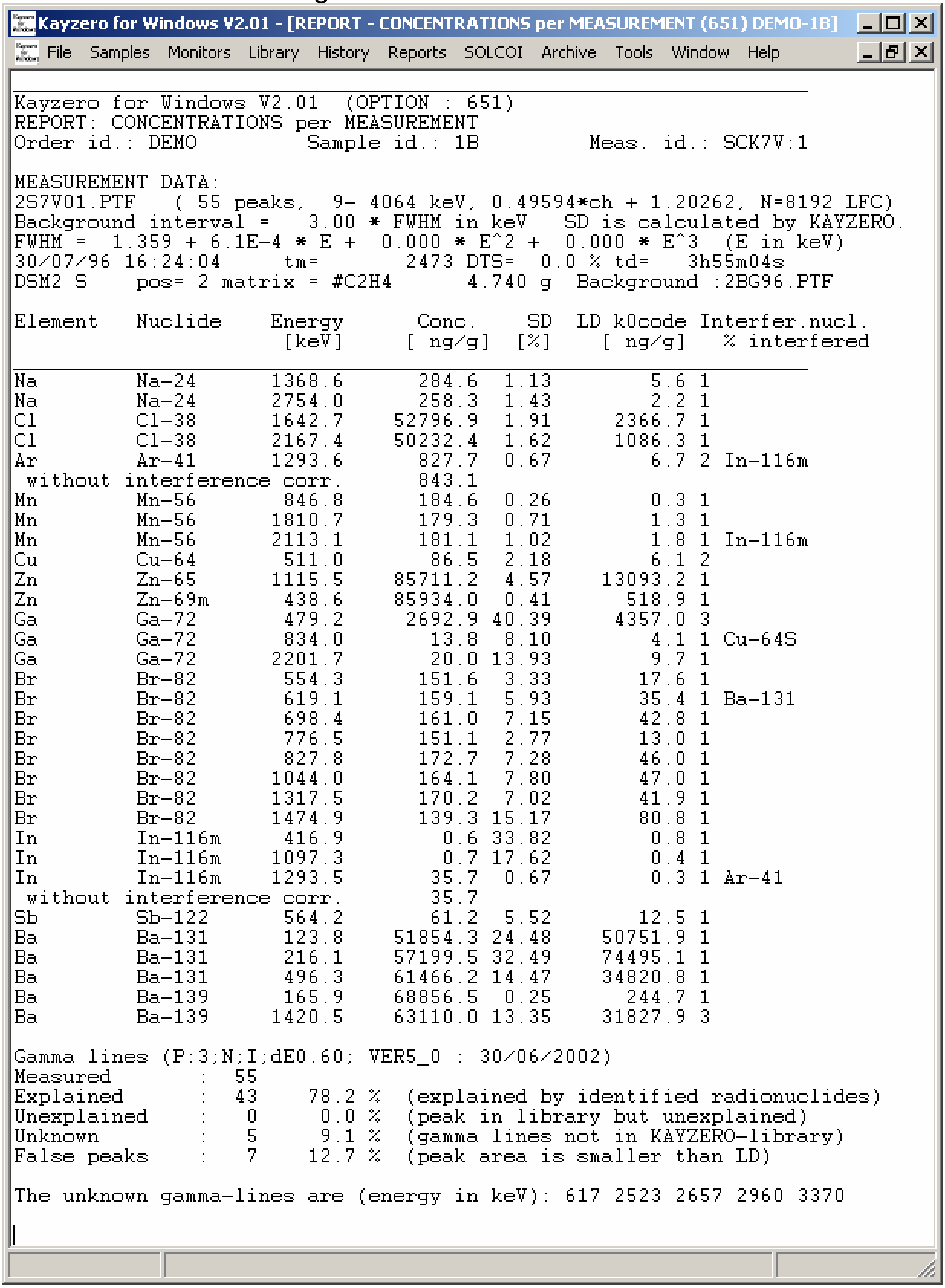
The output of this option will be a list of measured gamma lines which the system has been able to match with the KAYZERO Library (see Figure 3.33).

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;dE0.60; VER5_0 : 30/06/2002)', 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 0.6 keV (dE0.60;) and the library used was VER5_0, last updated on 30/06/2002. 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 (gamma lines, found in the KAYZERO-library, that cannot be assigned to a radionuclide present in the sample),
- the number of unknown gammas (gammas not found in the library),
- the number of false gammas: the peak area is smaller than the detection limit,
- all unexplained gamma energies and

- all unknown measured gamma lines.



```
Kayzero for Windows V2.01  (OPTION : 651)
REPORT: CONCENTRATIONS per MEASUREMENT
Order id.: DEMO         Sample id.: 1B         Meas. id.: SCK7V:1

MEASUREMENT DATA:
2S7V01.PTF   ( 55 peaks,  9- 4064 keV, 0.49594*ch + 1.20262, 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

Element   Nuclide    Energy      Conc.    SD  LD k0code Interfer.nucl.
                      [keV]     [ ng/g]  [%]    [ ng/g]   % interfered

Na        Na-24      1368.6      284.6  1.13        5.6 1
Na        Na-24      2754.0      258.3  1.43        2.2 1
Cl        Cl-38      1642.7    52796.9  1.91     2366.7 1
Cl        Cl-38      2167.4    50232.4  1.62     1086.3 1
Ar        Ar-41      1293.6      827.7  0.67        6.7 2 In-116m
 without interference corr.      843.1
Mn        Mn-56       846.8      184.6  0.26        0.3 1
Mn        Mn-56      1810.7      179.3  0.71        1.3 1
Mn        Mn-56      2113.1      181.1  1.02        1.8 1 In-116m
Cu        Cu-64       511.0       86.5  2.18        6.1 2
Zn        Zn-65      1115.5    85711.2  4.57    13093.2 1
Zn        Zn-69m      438.6    85934.0  0.41      518.9 1
Ga        Ga-72       479.2     2692.9 40.39     4357.0 3
Ga        Ga-72       834.0       13.8  8.10        4.1 1 Cu-64S
Ga        Ga-72      2201.7       20.0 13.93        9.7 1
Br        Br-82       554.3      151.6  3.33       17.6 1
Br        Br-82       619.1      159.1  5.93       35.4 1 Ba-131
Br        Br-82       698.4      161.0  7.15       42.8 1
Br        Br-82       776.5      151.1  2.77       13.0 1
Br        Br-82       827.8      172.7  7.28       46.0 1
Br        Br-82      1044.0      164.1  7.80       47.0 1
Br        Br-82      1317.5      170.2  7.02       41.9 1
Br        Br-82      1474.9      139.3 15.17       80.8 1
In        In-116m     416.9        0.6 33.82        0.8 1
In        In-116m    1097.3        0.7 17.62        0.4 1
In        In-116m    1293.5       35.7  0.67        0.3 1 Ar-41
 without interference corr.       35.7
Sb        Sb-122      564.2       61.2  5.52       12.5 1
Ba        Ba-131      123.8    51854.3 24.48    50751.9 1
Ba        Ba-131      216.1    57199.5 32.49    74495.1 1
Ba        Ba-131      496.3    61466.2 14.47    34820.8 1
Ba        Ba-139      165.9    68856.5  0.25      244.7 1
Ba        Ba-139     1420.5    63110.0 13.35    31827.9 3

Gamma lines (P:3;N;I;dE0.60; VER5_0 : 30/06/2002)
Measured       :  55
Explained      :  43    78.2 %  (explained by identified radionuclides)
Unexplained    :   0     0.0 %  (peak in library but unexplained)
Unknown        :   5     9.1 %  (gamma lines not in KAYZERO-library)
False peaks    :   7    12.7 %  (peak area is smaller than LD)

The unknown gamma-lines are (energy in keV): 617 2523 2657 2960 3370
```

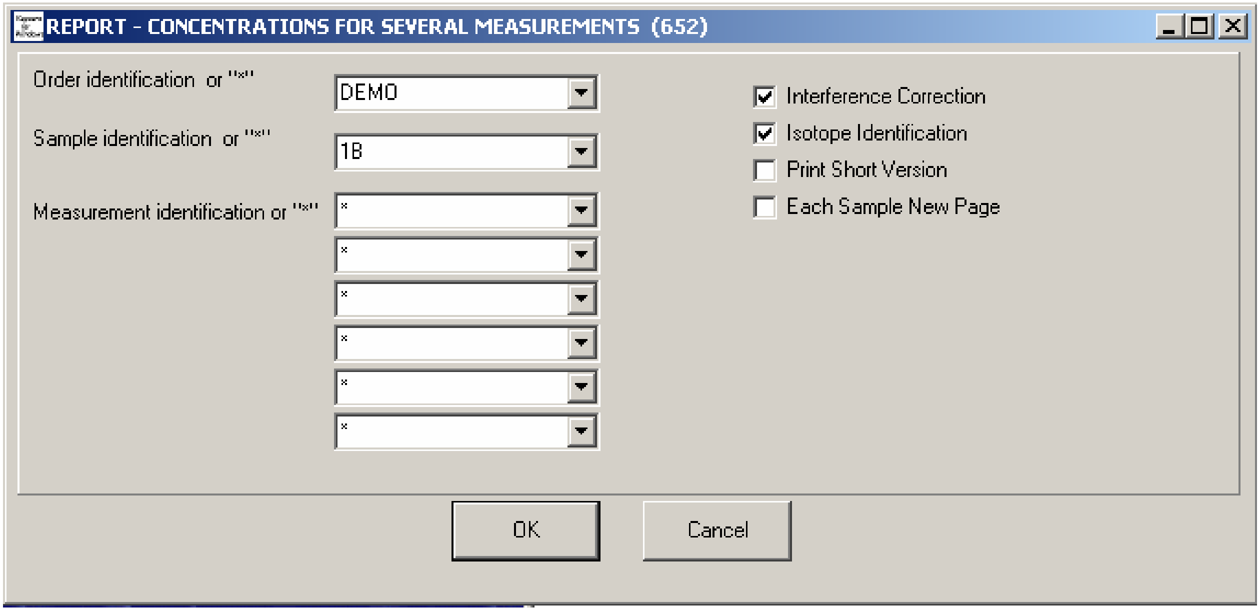
Figure 3.33 : Output for '*Reports/Results/Per Gamma, One Measurement/Samples*'

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.



Order identification or "*": DEMO

Sample identification or "*": 1B

Measurement identification or "*":
*
*
*
*
*
*

☑ Interference Correction
☑ Isotope Identification
☐ Print Short Version
☐ Each Sample New Page

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.

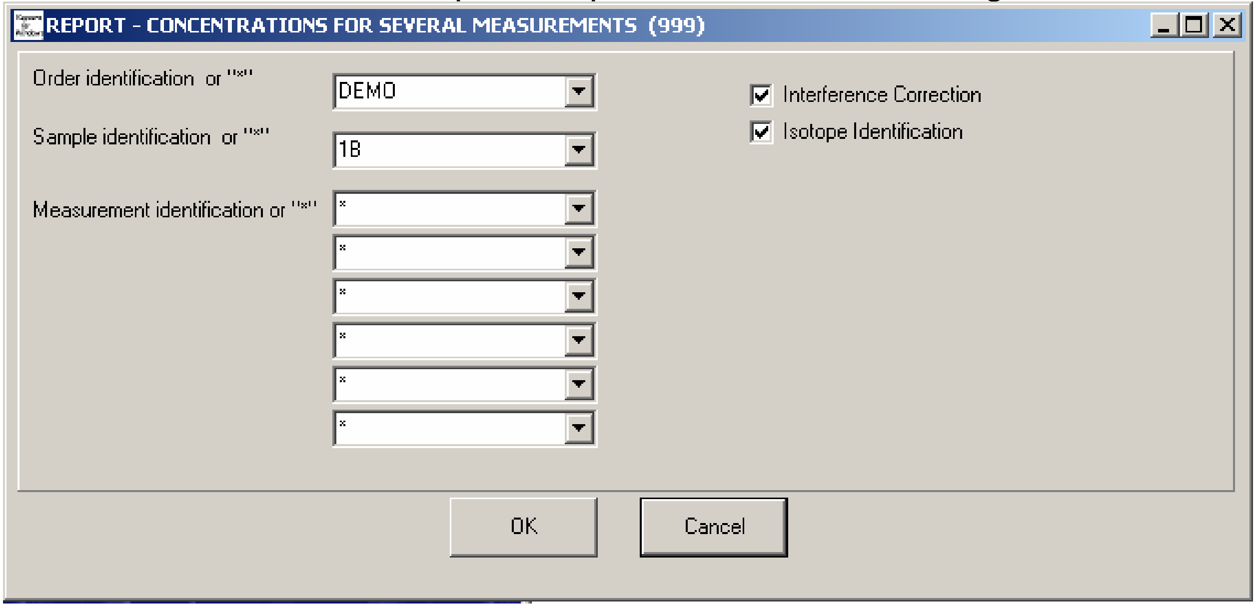
Report: Results, Final report

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, blank correction, fission correction and reaction interfering correction.

This option *'Samples/Select/Reject analytical Lines'* was new in the V5 version and 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 handled.
The old way to handle the data using the previously mentioned options can still be used, but fission and reaction interfering correction, blank correction and rejection of gamma lines is not performed. Up to 6 irradiations/measurements per sample can be edited, see figure 3.35.


REPORT - CONCENTRATIONS FOR SEVERAL MEASUREMENTS (999)

Order identification or "*": DEMO

Sample identification or "*": 1B

Measurement identification or "*": *

*

*

*

*

*

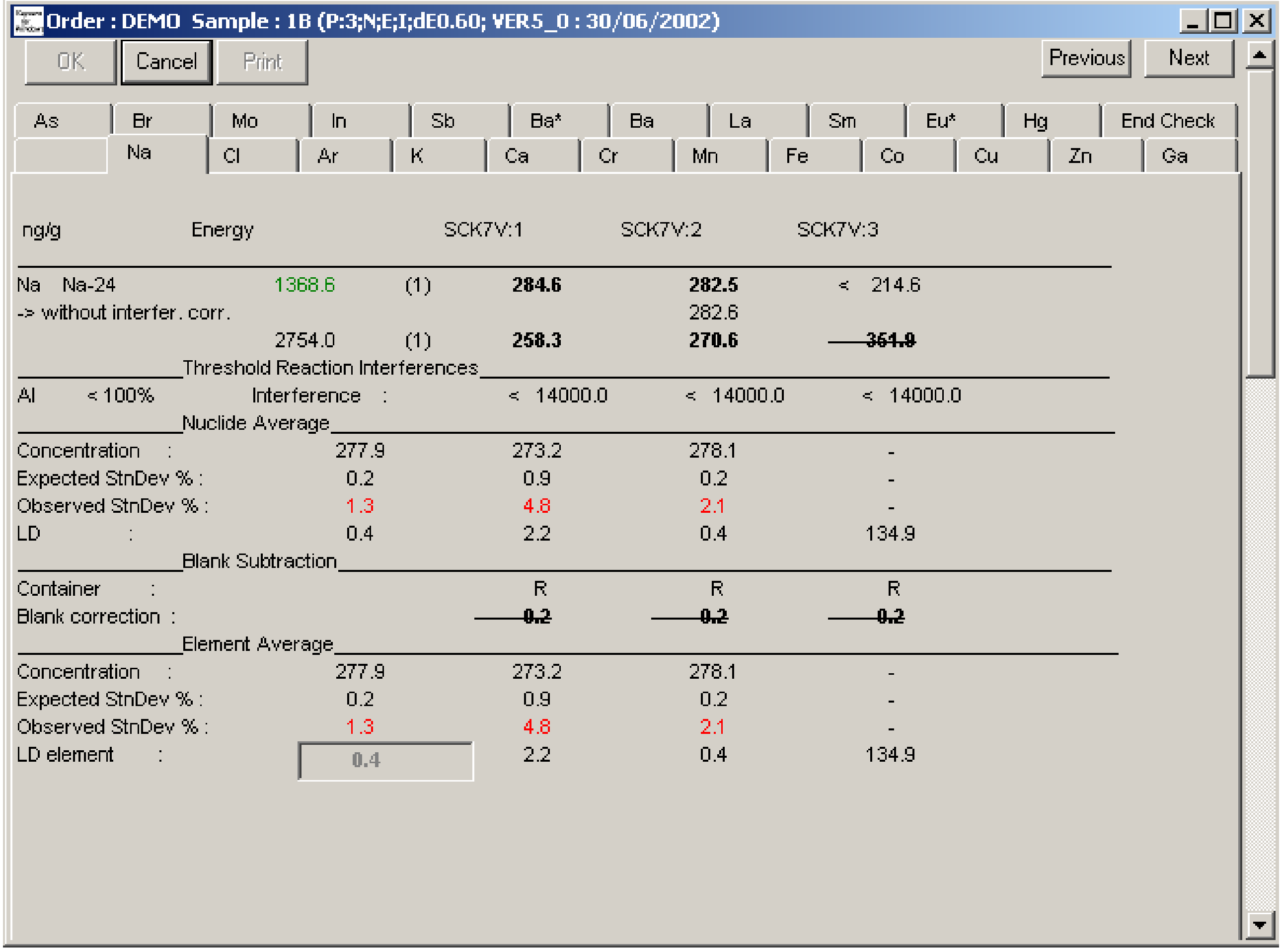
☑ Interference Correction

☑ Isotope Identification

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 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%).

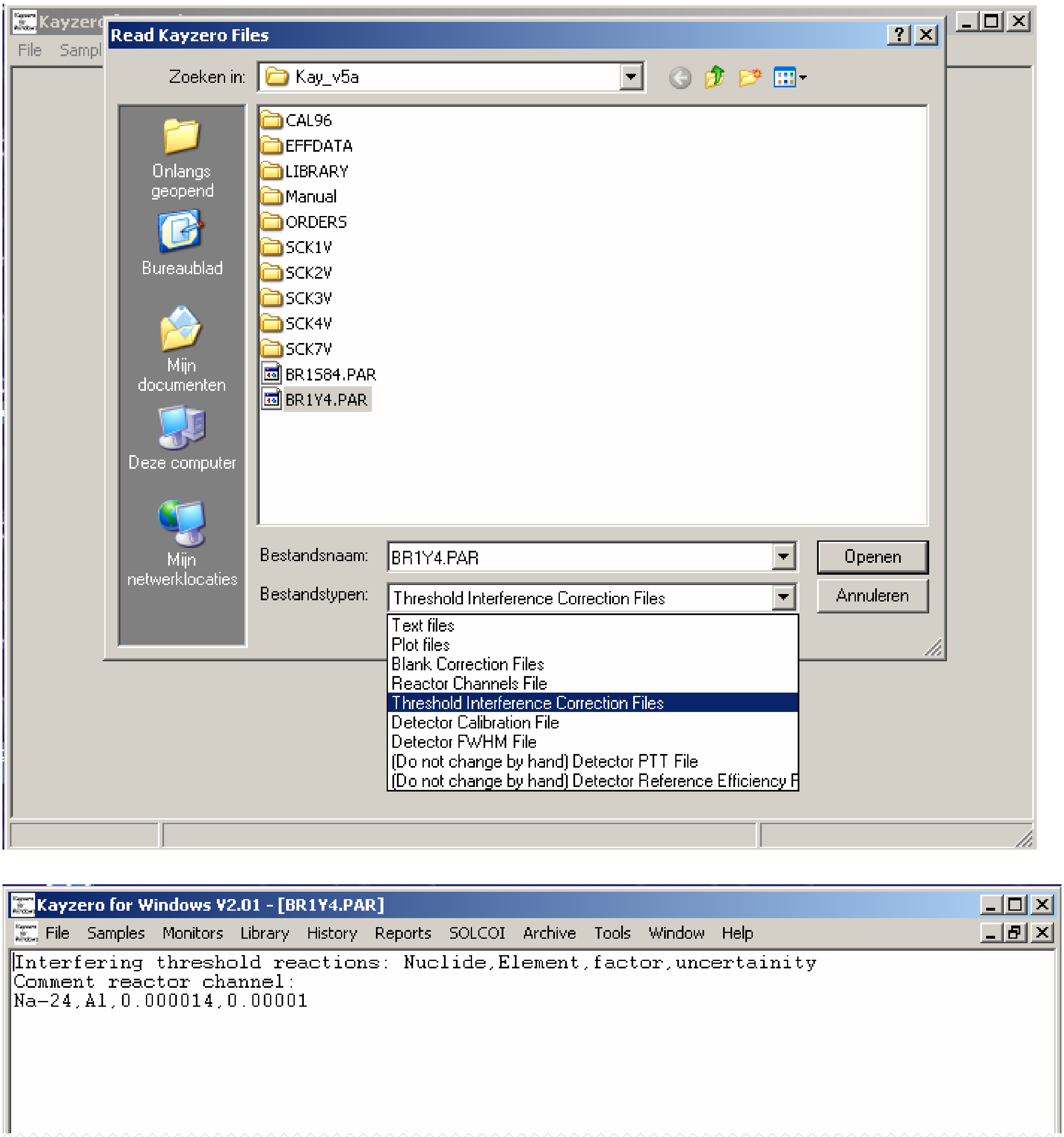


```
ng/g              Energy              SCK7V:1        SCK7V:2        SCK7V:3

Na   Na-24              1368.6   (1)     284.6          282.5       <  214.6
-> without interfer. corr.                              282.6
                        2754.0   (1)     258.3          270.6          ~~364.9~~
_______________Threshold Reaction Interferences_______________________________
Al      < 100%        Interference   :   <  14000.0     <  14000.0     <  14000.0
_______________Nuclide Average________________________________________________
Concentration   :          277.9         273.2          278.1            -
Expected StnDev % :        0.2           0.9            0.2              -
Observed StnDev % :        1.3           4.8            2.1              -
LD              :          0.4           2.2            0.4            134.9
_______________Blank Subtraction______________________________________________
Container       :                        R              R                R
Blank correction :                       ~~0.2~~        ~~0.2~~          ~~0.2~~
_______________Element Average________________________________________________
Concentration   :          277.9         273.2          278.1            -
Expected StnDev % :        0.2           0.9            0.2              -
Observed StnDev % :        1.3           4.8            2.1              -
LD element      :          0.4           2.2            0.4            134.9
```

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.



Zoeken in: Kay_v5a

Bestandsnaam: BR1Y4.PAR

Bestandstypen: Threshold Interference Correction Files

```
Interfering threshold reactions: Nuclide,Element,factor,uncertainity
Comment reactor channel:
Na-24,Al,0.000014,0.00001
```

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

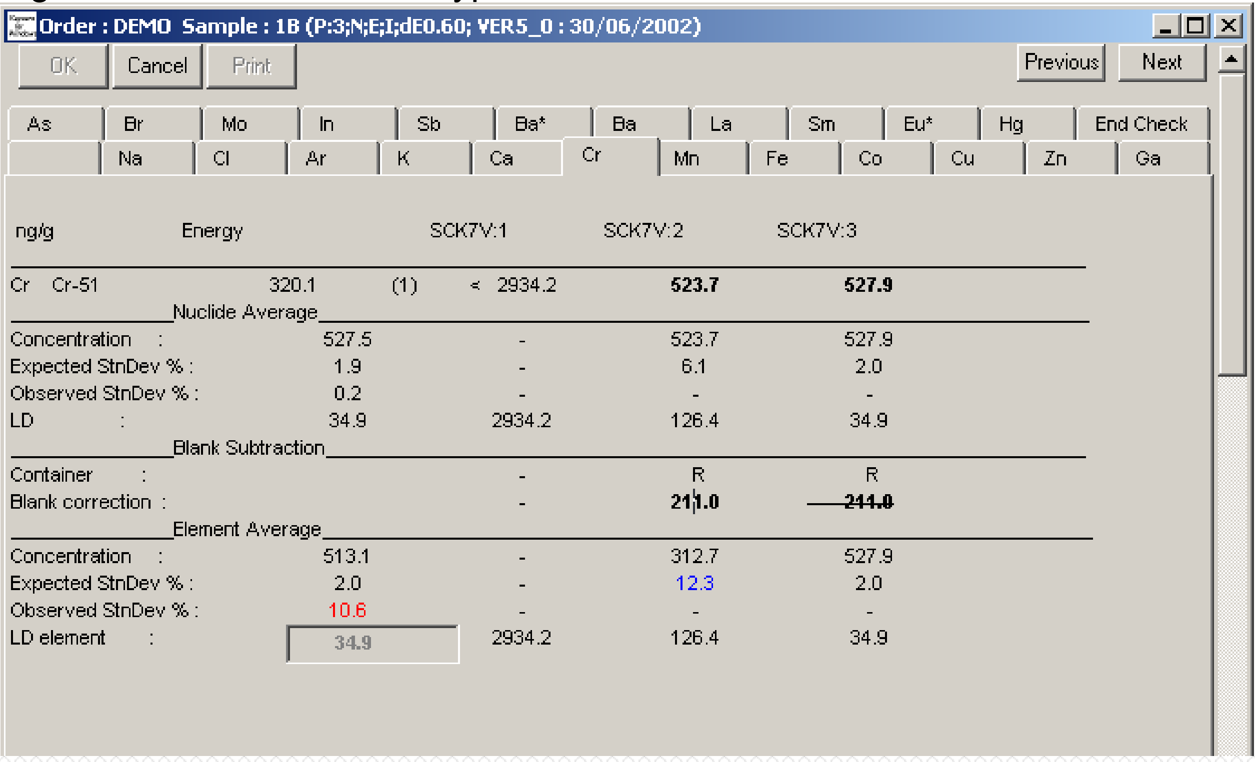
This interference correction factor is the apparent concentration of element ‘x’ based on the given nuclide divided by the concentration of the interfering element. In the case of the example of figure 3.37: if the matrix is 100% Al, the apparent Na concentration (based on Na-24) is 14 mg/kg (0.000014*100%) 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*- tabsheet. 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 3.38 an example of the blank file is given.

```
Container blank: Element,Mass in microgram, sd in microgram
Comment container: Type R voor langlevend NAA
============================================================
Na,0.001,0.0003
Br,0.001,0.0002
Cr,1.0,0.1
```

Figure 3.38: Contents of a typical data file for blank correction.

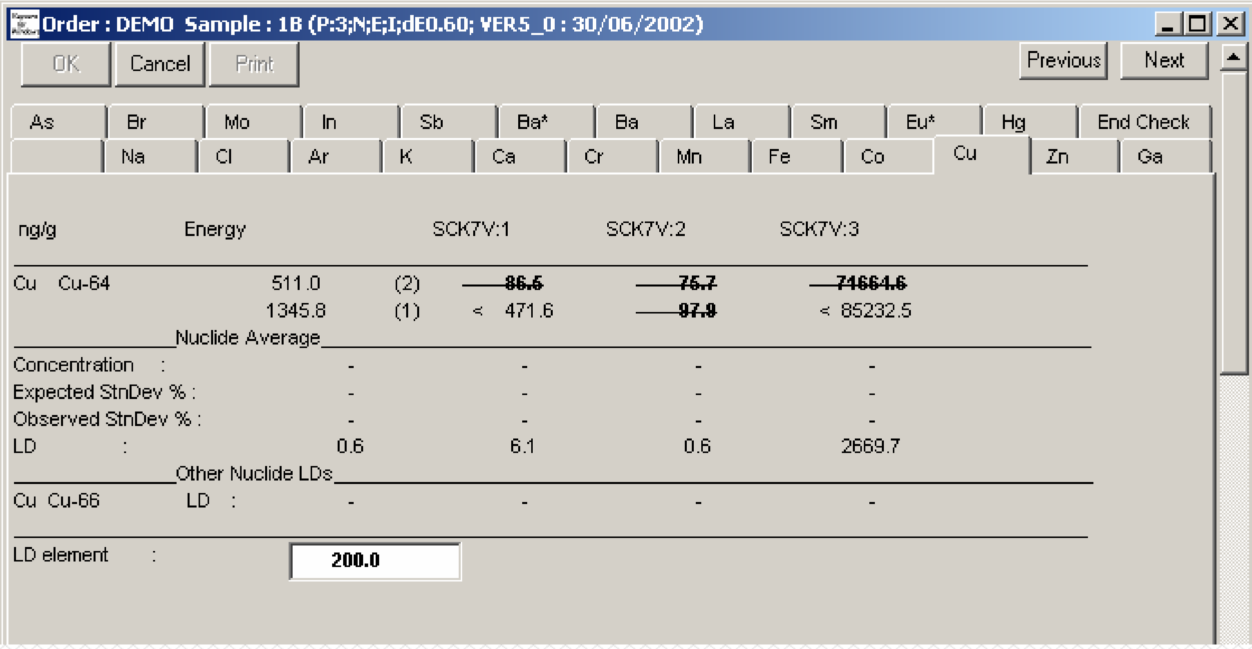


```
ng/g              Energy                  SCK7V:1          SCK7V:2          SCK7V:3

Cr   Cr-51              320.1      (1)   <  2934.2         523.7            527.9
________________Nuclide Average______________________________________________________
Concentration    :            527.5          -             523.7            527.9
Expected StnDev % :             1.9          -               6.1              2.0
Observed StnDev % :             0.2          -                 -                -
LD            :                34.9       2934.2           126.4             34.9
________________Blank Subtraction____________________________________________________
Container        :                           -                 R                R
Blank correction  :                          -             211.0        ~~211.0~~
________________Element Average______________________________________________________
Concentration    :            513.1          -             312.7            527.9
Expected StnDev % :             2.0          -              12.3              2.0
Observed StnDev % :            10.6          -                 -                -
LD element     :               34.9       2934.2           126.4             34.9
```

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 recent paper by F. De Corte (2000). The data are 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.



Order : DEMO Sample : 1B (P:3;N;E;I;dE0.60; VER5_0 : 30/06/2002)

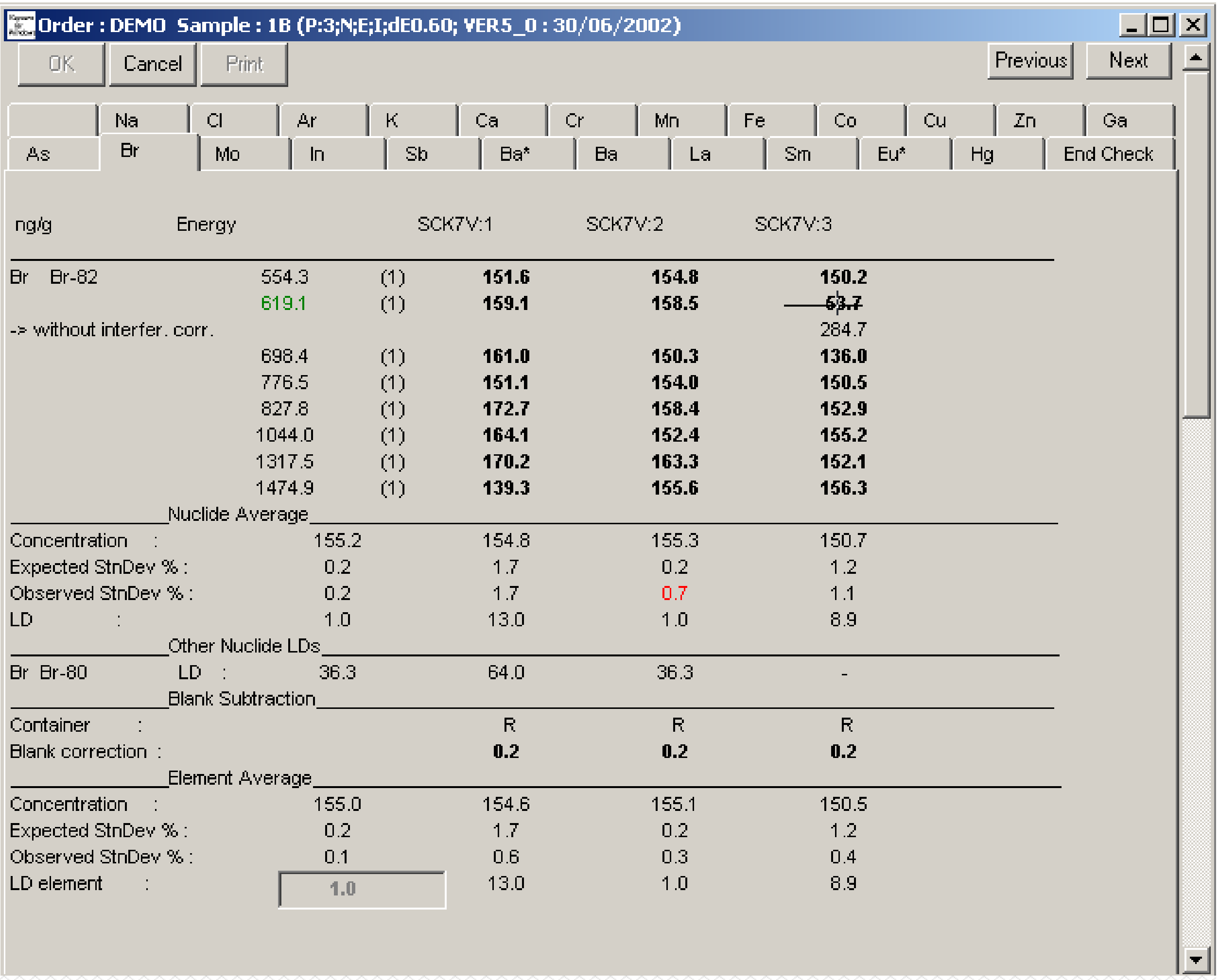
ng/g	Energy		SCK7V:1	SCK7V:2	SCK7V:3
Cu Cu-64	511.0	(2)	~~86.6~~	~~75.7~~	~~71664.6~~
	1345.8	(1)	< 471.6	~~97.9~~	< 85232.5
Nuclide Average					
Concentration :		-	-	-	-
Expected StnDev % :		-	-	-	-
Observed StnDev % :		-	-	-	-
LD :		0.6	6.1	0.6	2669.7
Other Nuclide LDs					
Cu Cu-66	LD :	-	-	-	-

LD element : 200.0

Figure 3.40: Input screen demonstrating rejection of all data and giving a detection limit.

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 200 is chosen as the detection limit for copper based on Cu-64 (See Figure 3.39). There is a minimum concentration found at the 511 keV peak, thus the maximum concentration is lower than 200. 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. See for example figure 3.40.



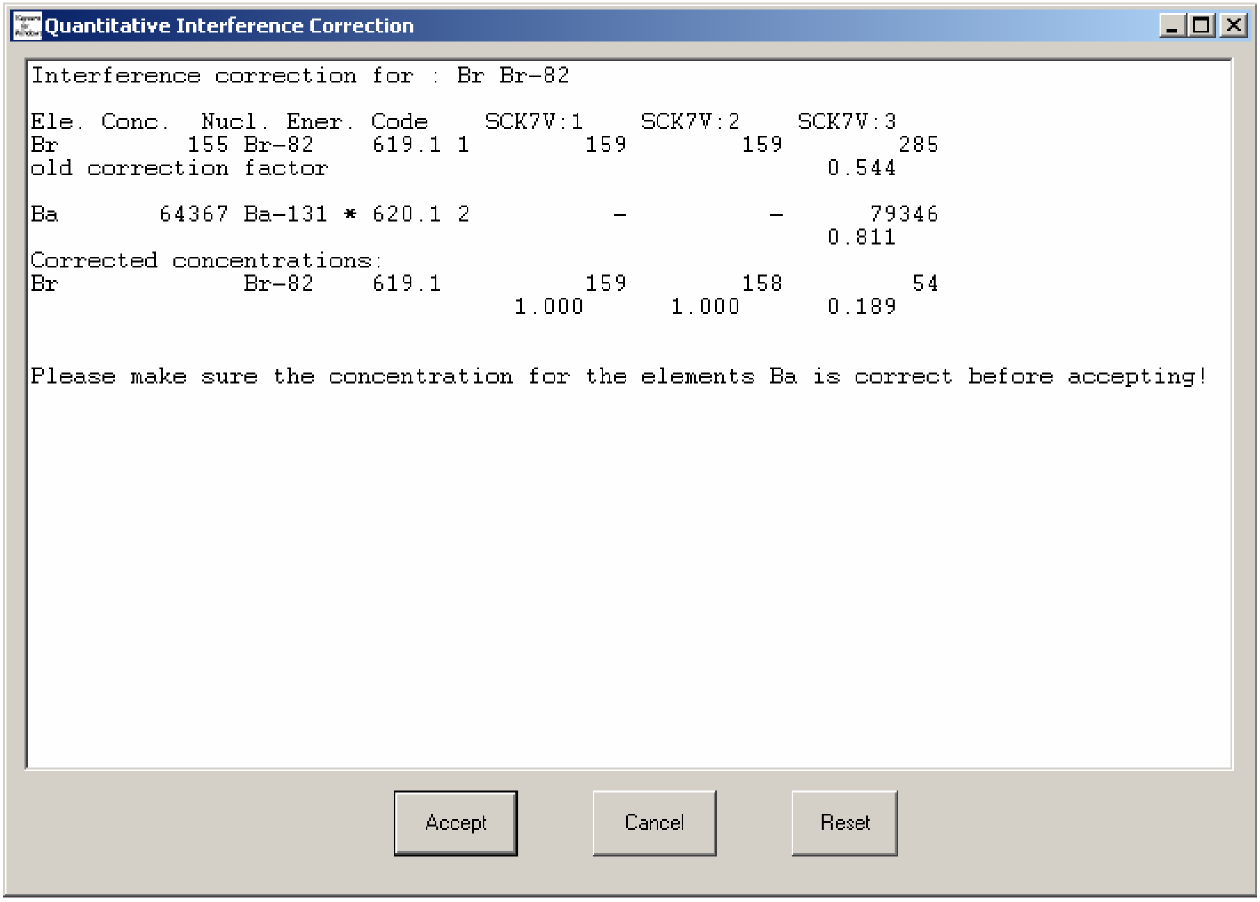
```
ng/g              Energy              SCK7V:1        SCK7V:2        SCK7V:3
_________________________________________________________________________________
Br   Br-82              554.3    (1)    151.6          154.8          150.2
                        619.1    (1)    159.1          158.5          63.7
-> without interfer. corr.                                            284.7
                        698.4    (1)    161.0          150.3          136.0
                        776.5    (1)    151.1          154.0          150.5
                        827.8    (1)    172.7          158.4          152.9
                       1044.0    (1)    164.1          152.4          155.2
                       1317.5    (1)    170.2          163.3          152.1
                       1474.9    (1)    139.3          155.6          156.3
_____________Nuclide Average______________________________________________________
Concentration    :            155.2     154.8          155.3          150.7
Expected StnDev % :             0.2       1.7            0.2            1.2
Observed StnDev % :             0.2       1.7            0.7            1.1
LD             :                1.0      13.0            1.0            8.9
_____________Other Nuclide LDs____________________________________________________
Br  Br-80          LD   :      36.3      64.0           36.3            -
_____________Blank Subtraction____________________________________________________
Container      :                          R              R              R
Blank correction :                        0.2            0.2            0.2
_____________Element Average______________________________________________________
Concentration    :            155.0     154.6          155.1          150.5
Expected StnDev % :             0.2       1.7            0.2            1.2
Observed StnDev % :             0.1       0.6            0.3            0.4
LD element      :             [  1.0  ]  13.0            1.0            8.9
```

Figure 3.40: Demonstration of incompatible limits of detection for Br-80.

The detection limit of Br-80 in Figure 3.40 shows that there might be something wrong. The Br-80 concentration is lower than 40 ng/g while the Br-80 is not present in the list.

Looking more closer at the peak-table file and other reports is becomes clear why Br-80 is not found. The highest peak of Br-80 is very close to a high peak of Br-82 and is therefore not found.

In this 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.

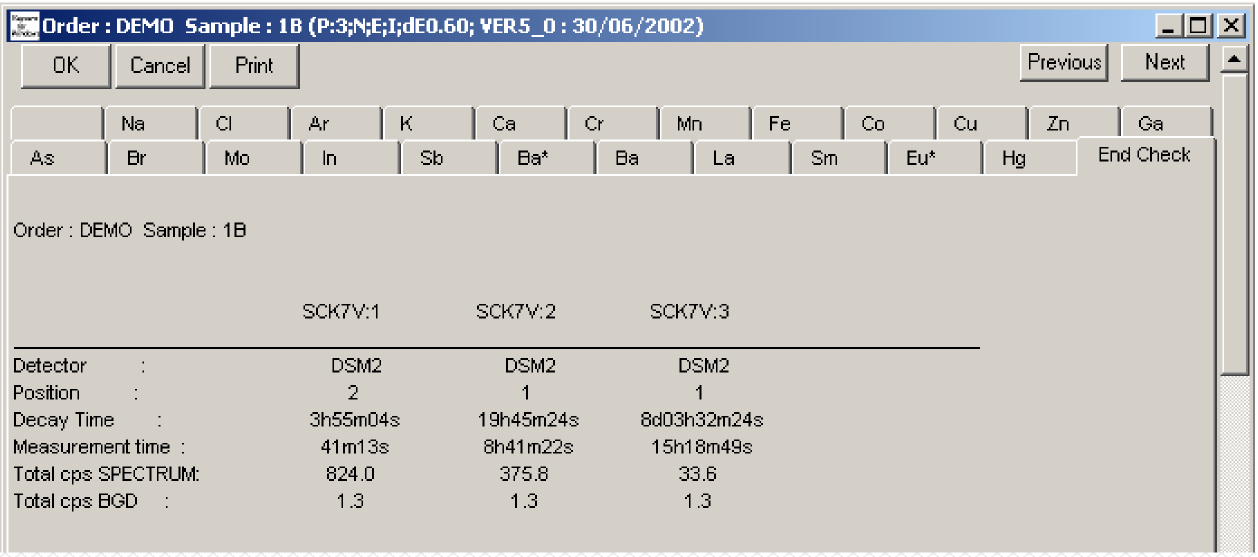


```
Interference correction for : Br Br-82

Ele. Conc.  Nucl. Ener. Code    SCK7V:1    SCK7V:2    SCK7V:3
Br         155 Br-82    619.1 1        159        159        285
old correction factor                                   0.544

Ba       64367 Ba-131 * 620.1 2          -          -      79346
                                                        0.811
Corrected concentrations:
Br             Br-82    619.1          159        158         54
                                  1.000      1.000      0.189


Please make sure the concentration for the elements Ba is correct before accepting!
```

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. In this particular case the correction is not really necessary and also not very good, so de-selection of the bromine line (in figure 3.40) is a better and simpler action.

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



```
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:             824.0            375.8            33.6
Total cps BGD     :              1.3              1.3              1.3
```

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.

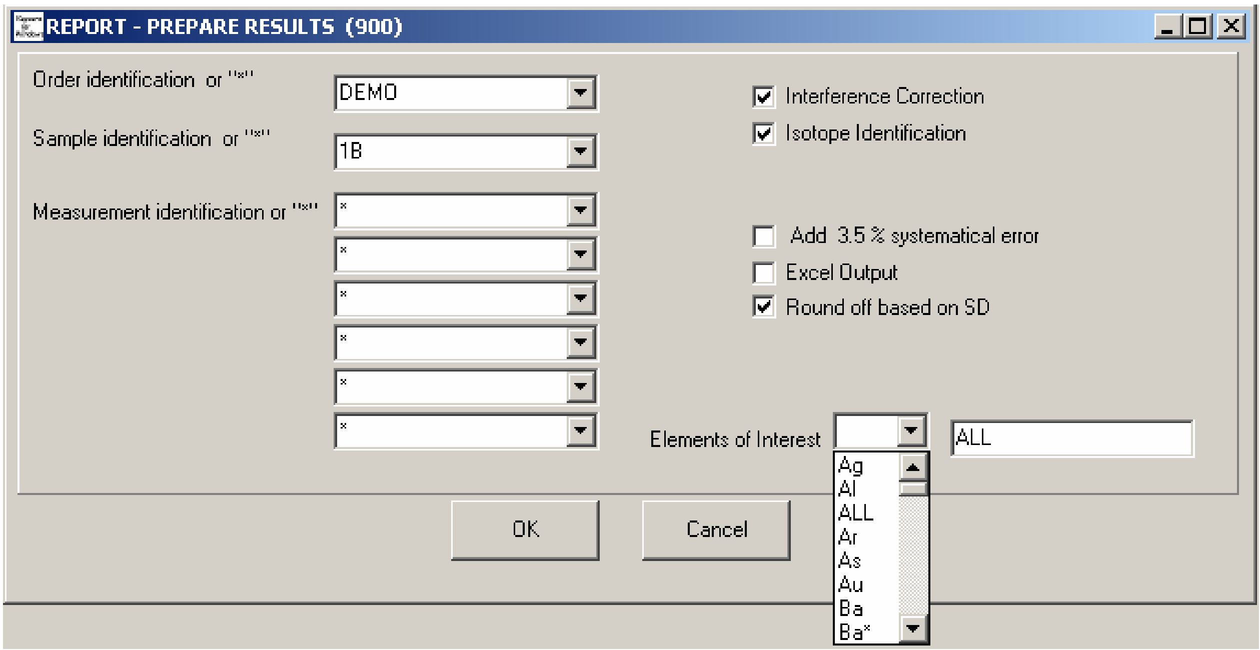
You always need to pass this last tab-sheet before ending this session.

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.

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 error can be added to the statistical measurement uncertainty (see *Tools/Options/Print Parameters*). 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 3.5 % systematical error

☐ Excel Output

☑ Round off based on SD

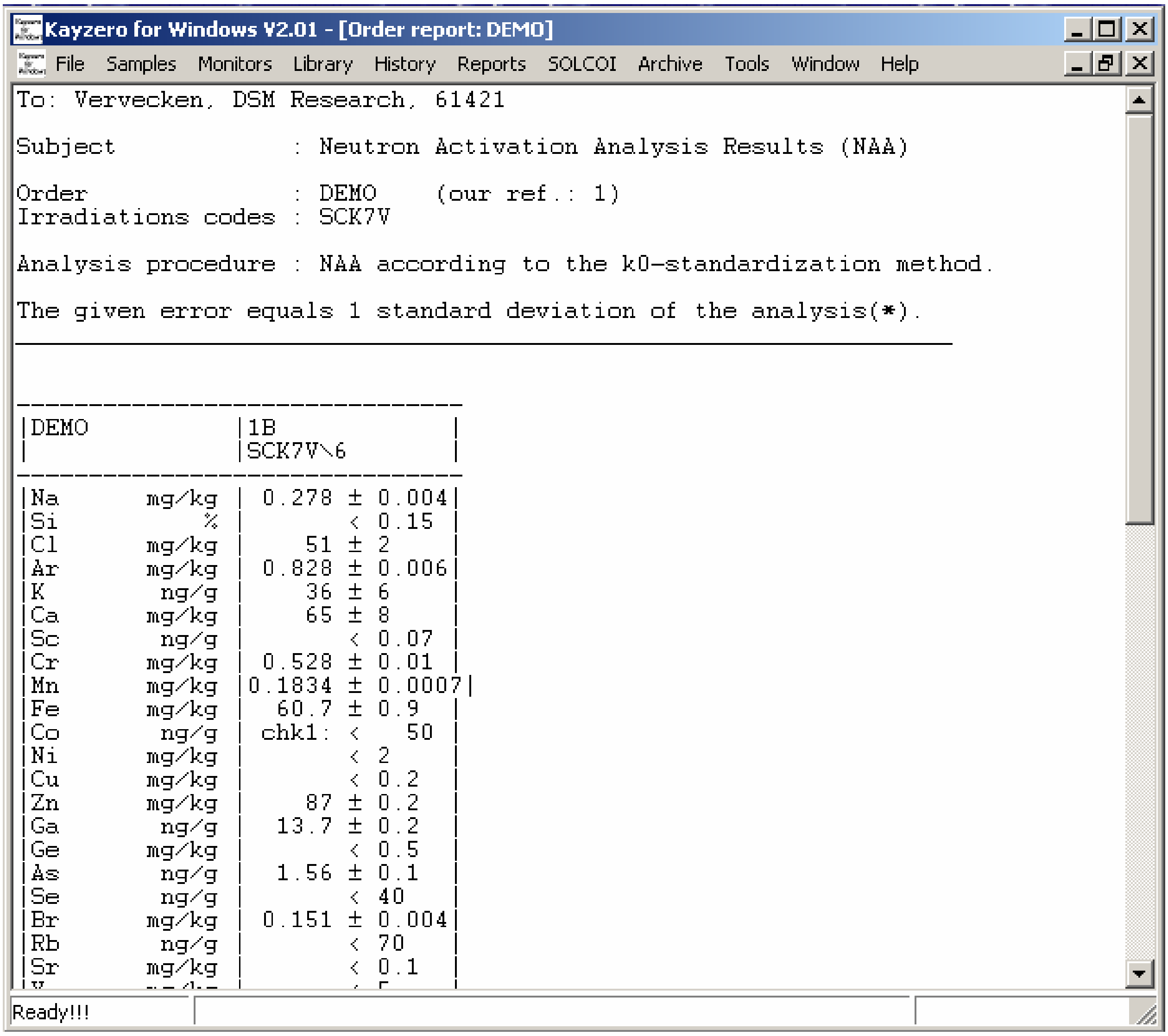
Elements of Interest ALL

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.

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).



```
To: Vervecken, DSM Research, 61421

Subject                : Neutron Activation Analysis Results (NAA)

Order                  : DEMO    (our ref.: 1)
Irradiations codes     : SCK7V

Analysis procedure     : NAA according to the k0-standardization method.

The given error equals 1 standard deviation of the analysis(*).
_________________________________________________________________


-------------------------------
|DEMO          |1B            |
|              |SCK7V\6       |
-------------------------------
|Na      mg/kg |  0.278 ± 0.004|
|Si          % |        < 0.15 |
|Cl      mg/kg |     51 ± 2    |
|Ar      mg/kg |  0.828 ± 0.006|
|K       ng/g  |     36 ± 6    |
|Ca      mg/kg |     65 ± 8    |
|Sc      ng/g  |        < 0.07 |
|Cr      mg/kg |  0.528 ± 0.01 |
|Mn      mg/kg |0.1834 ± 0.0007|
|Fe      mg/kg |   60.7 ± 0.9  |
|Co      ng/g  |  chk1: <   50 |
|Ni      mg/kg |        < 2    |
|Cu      mg/kg |        < 0.2  |
|Zn      mg/kg |     87 ± 0.2  |
|Ga      ng/g  |   13.7 ± 0.2  |
|Ge      mg/kg |        < 0.5  |
|As      ng/g  |   1.56 ± 0.1  |
|Se      ng/g  |        < 40   |
|Br      mg/kg |  0.151 ± 0.004|
|Rb      ng/g  |        < 70   |
|Sr      mg/kg |        < 0.1  |
```

Figure 3.44: Report output

You can see in figure 3.44 that Kayzero for Windows marked the concentration for Co with ‘chk1’. This means that the observed standard deviation was very high (larger than 30%), normally a concentration with a standard deviation this high is lower than the detection limit. If you check the results in *Samples/Select/Reject analytical Lines* you will see why (Co is not present, Br has sum-peaks on 1173 and 1333).

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 spectrometrist 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[4]. For a practical guideline in applying the efficiency computation method see the 'VADEMECUM FOR K_0 USERS' by De Corte and Simonits [3]. 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 ε_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 majority of improvements in version 5 can be found in the algorithms for the calculation of coincidence correction factors. New is the option for the separate calculation of coincidence correction factors. You can now also give a wildcard for the calculation of all or specific sources.

4.1 General procedure

Before effective solid angles and coincidence correction factors can be calculated the reference detection efficiency ε_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 ε_p or log PTT vs log E_γ) 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.

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.

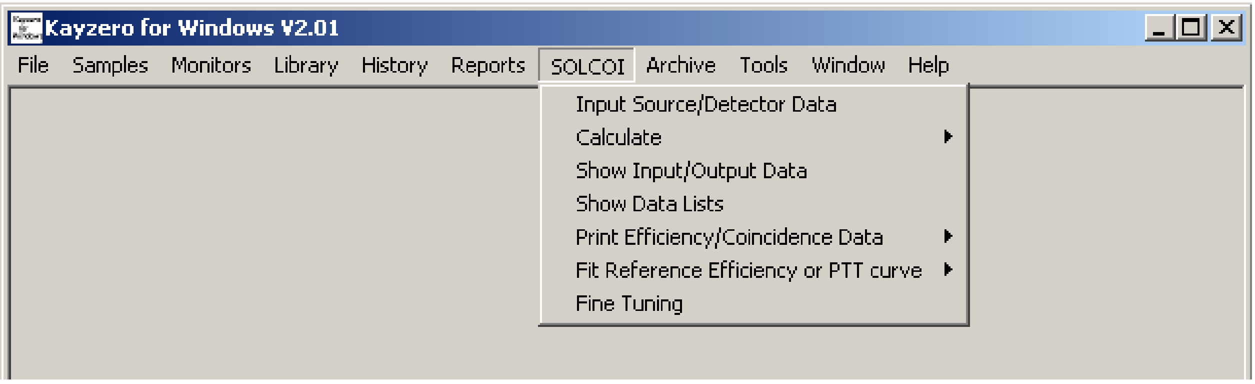


Figure 4.1: Main Menu of SOLCOI

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.*

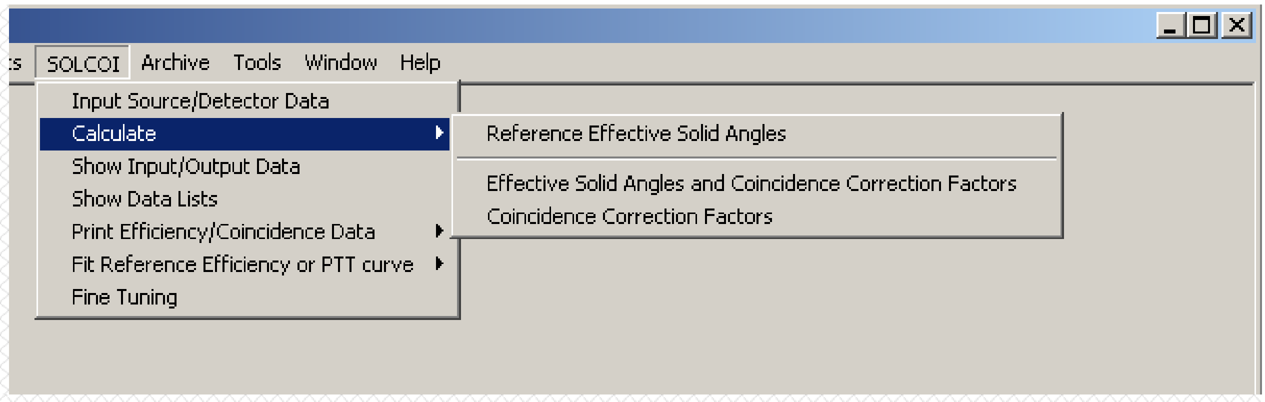


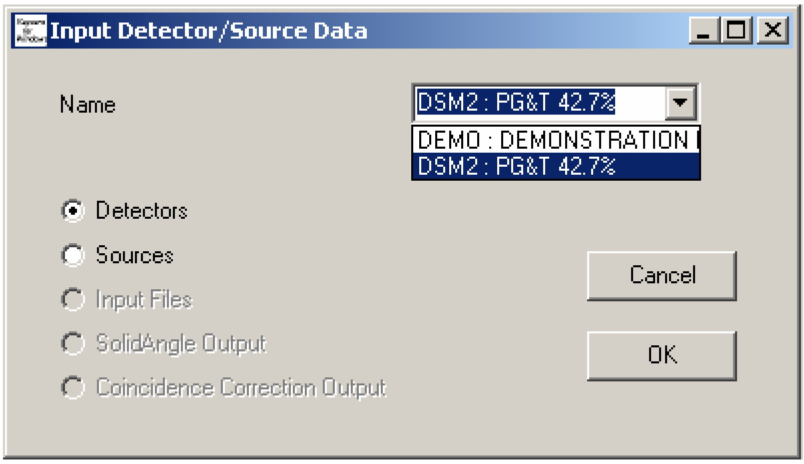
Figure 4.2: The *Calculate* menu.

The coincidence correction factors are calculated using the full-energy peak efficiency ε_p; the total efficiency (=ε_p / 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).



Input Detector/Source Data

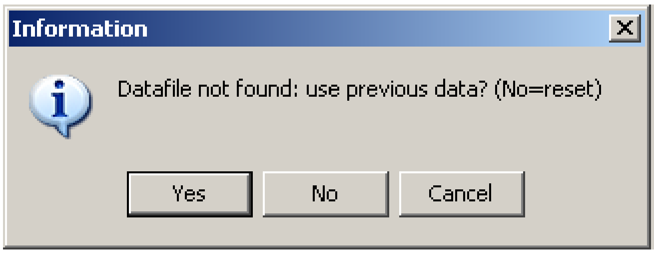
Name: DSM2 : PG&T 42.7%

DEMO : DEMONSTRATION
DSM2 : PG&T 42.7%

● Detectors
○ Sources
○ Input Files
○ SolidAngle Output
○ Coincidence Correction Output

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.



Information

Datafile not found: use previous data? (No=reset)

Figure 4.4: Input after selecting a new unknown detector.

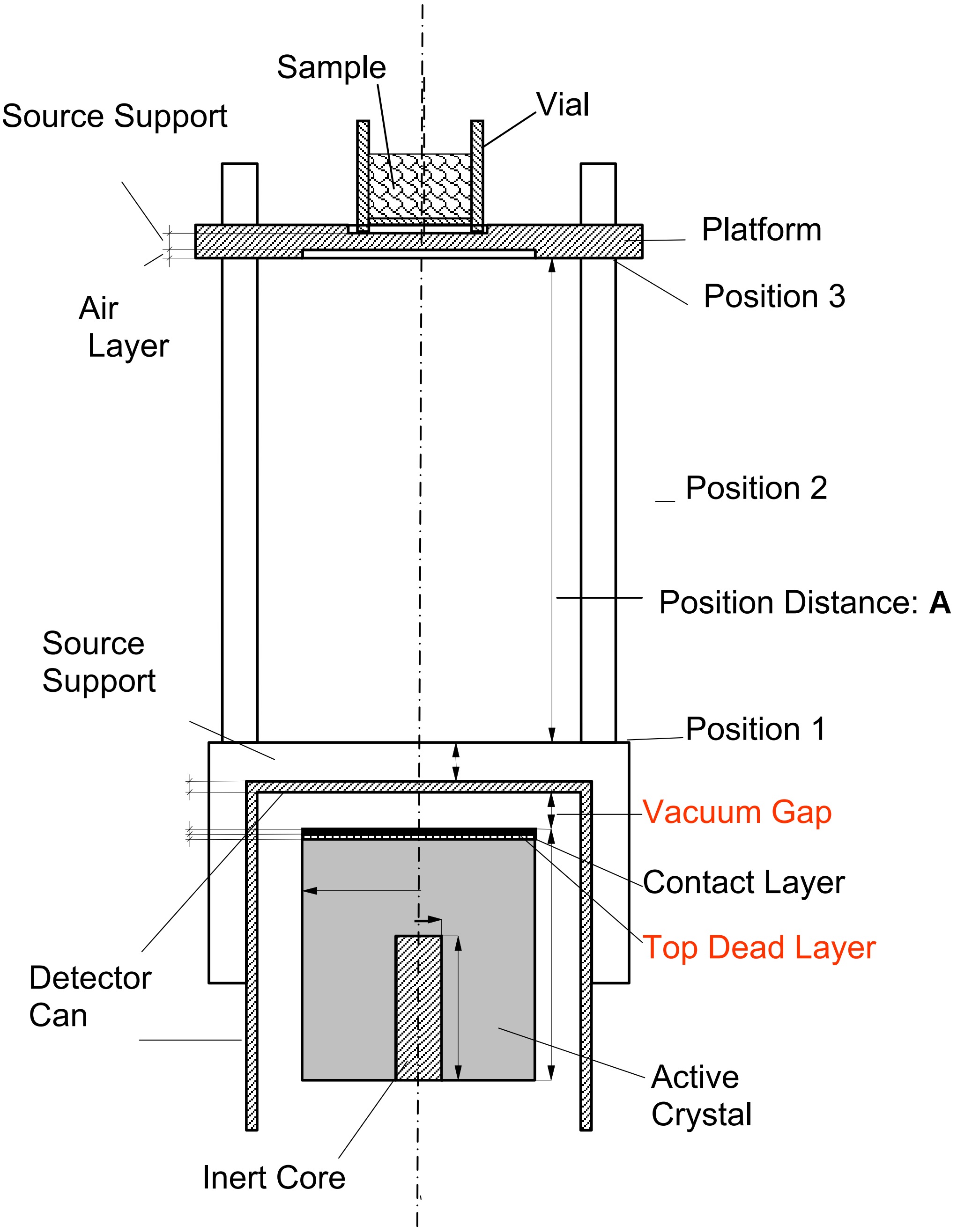
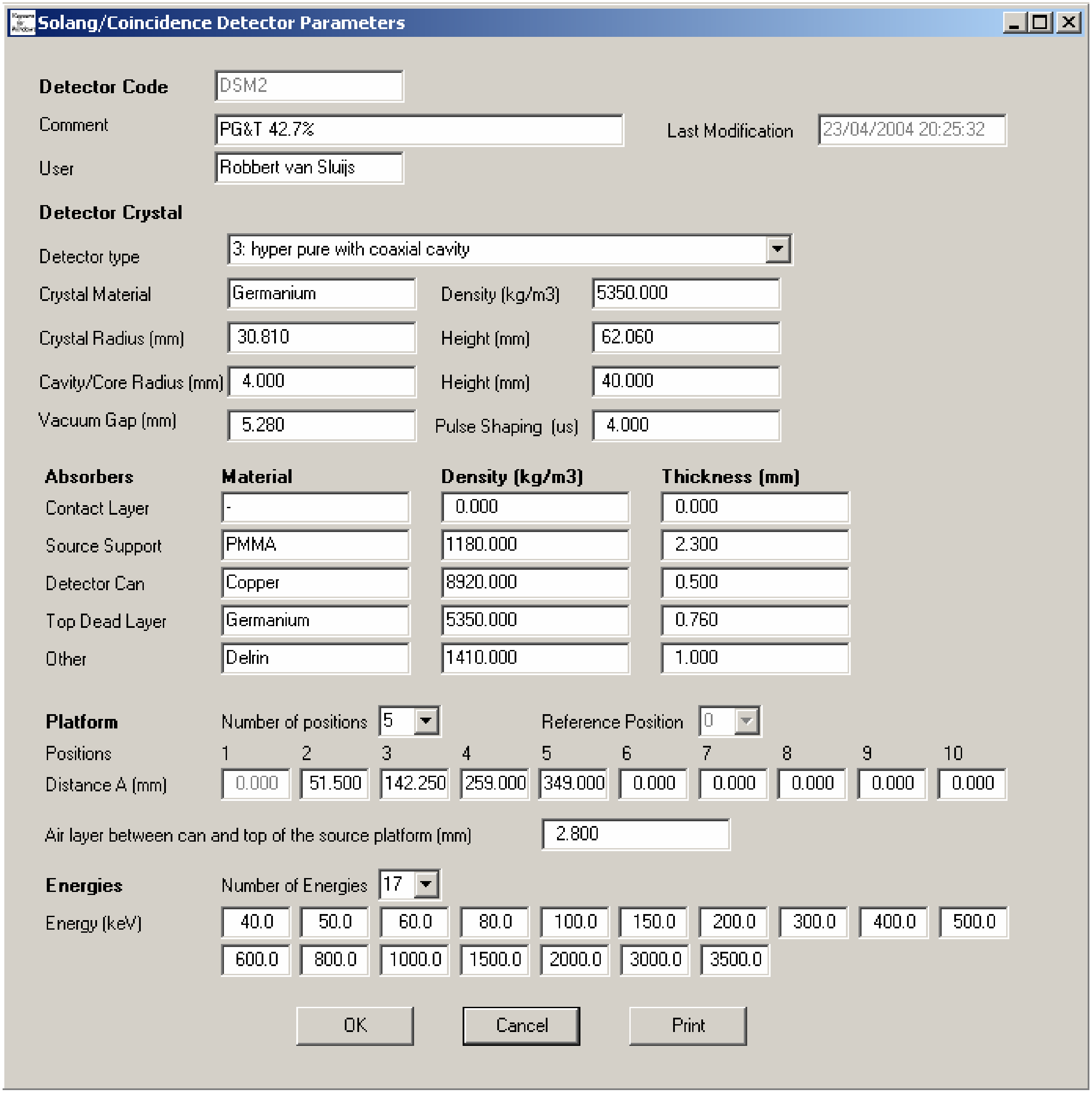


Figure 4.5: Detector Dimensions and explanation of descriptions used in fig. 4.6.

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.



Detector Code DSM2

Comment PG&T 42.7%

Last Modification 23/04/2004 20:25:32

User Robbert van Sluijs

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

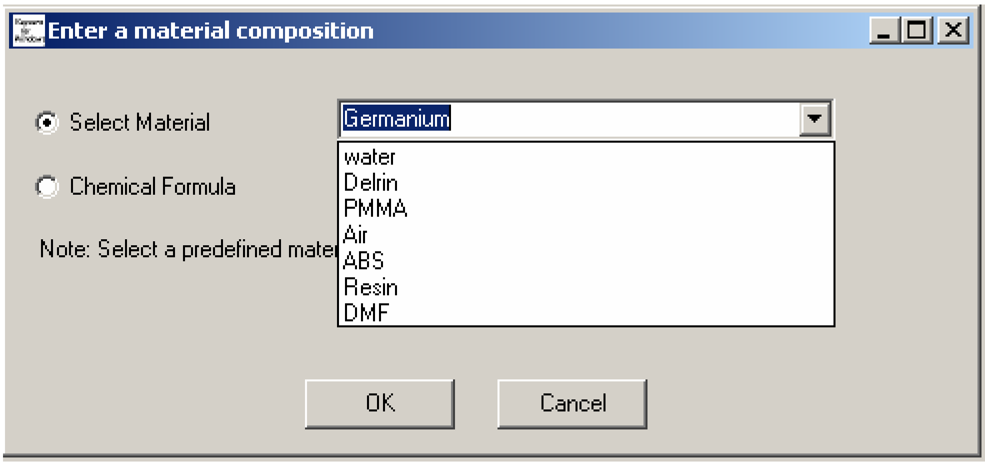
Positions	1	2	3	4	5	6	7	8	9	10
Distance A (mm)	0.000	51.500	142.250	259.000	349.000	0.000	0.000	0.000	0.000	0.000

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			

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



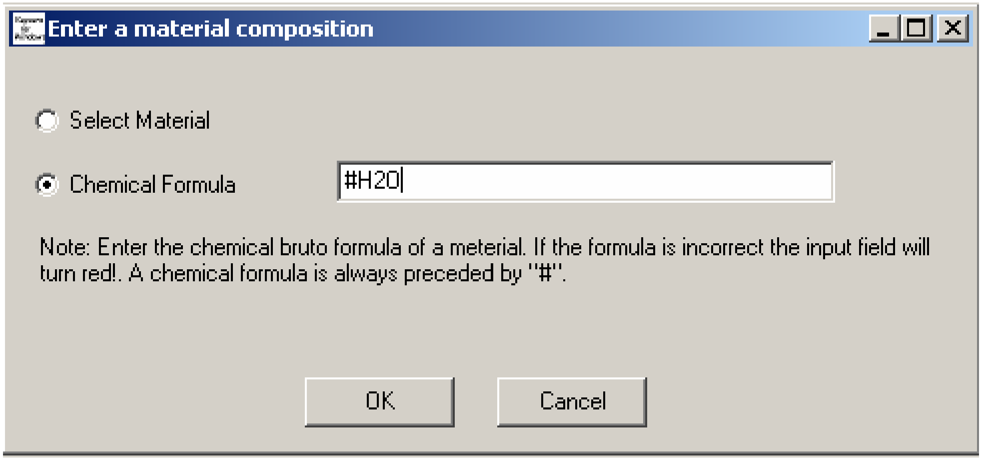
● Select Material: Germanium

○ Chemical Formula

Note: Select a predefined mate

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[5]. 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*.



○ Select Material

● Chemical Formula: #H20

Note: Enter the chemical bruto formula of a meterial. If the formula is incorrect the input field will turn red!. A chemical formula is always preceded by "#".

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

You can also enter a material composition by giving the bruto 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.

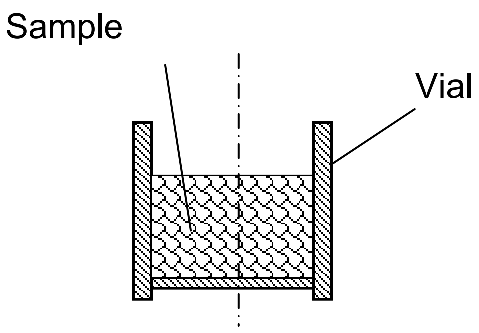
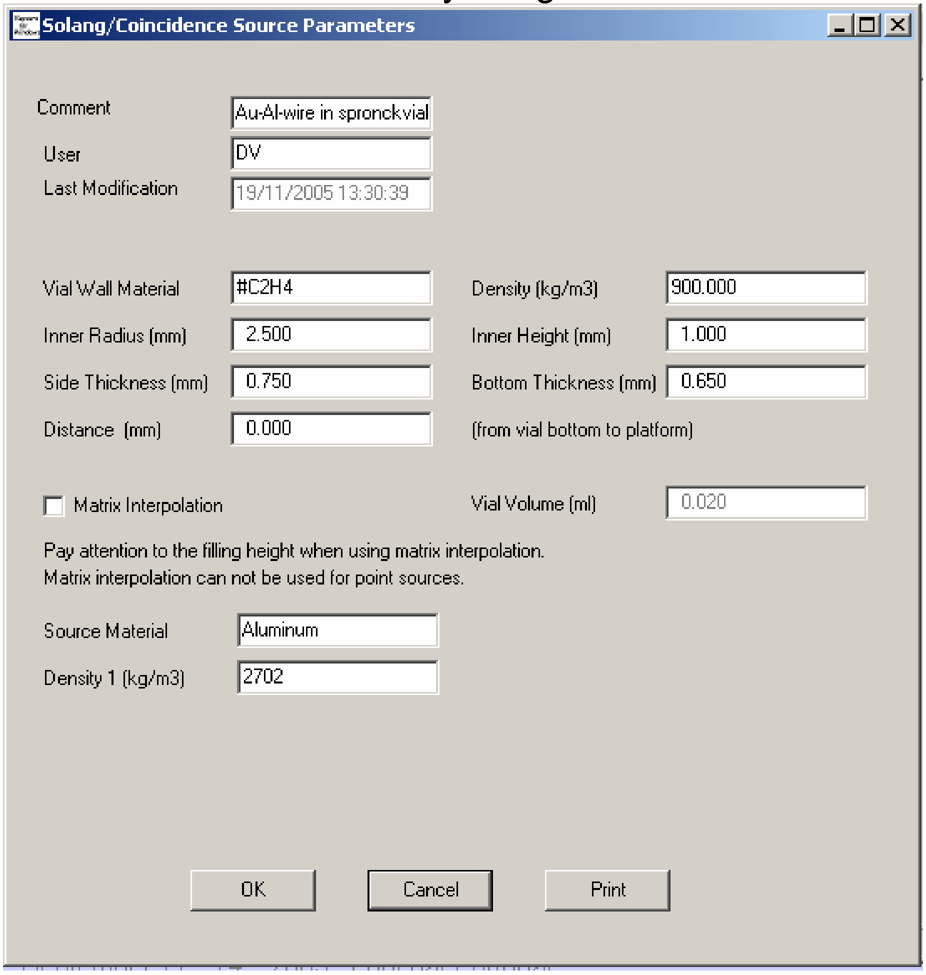


Figure 4.9: source.

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.

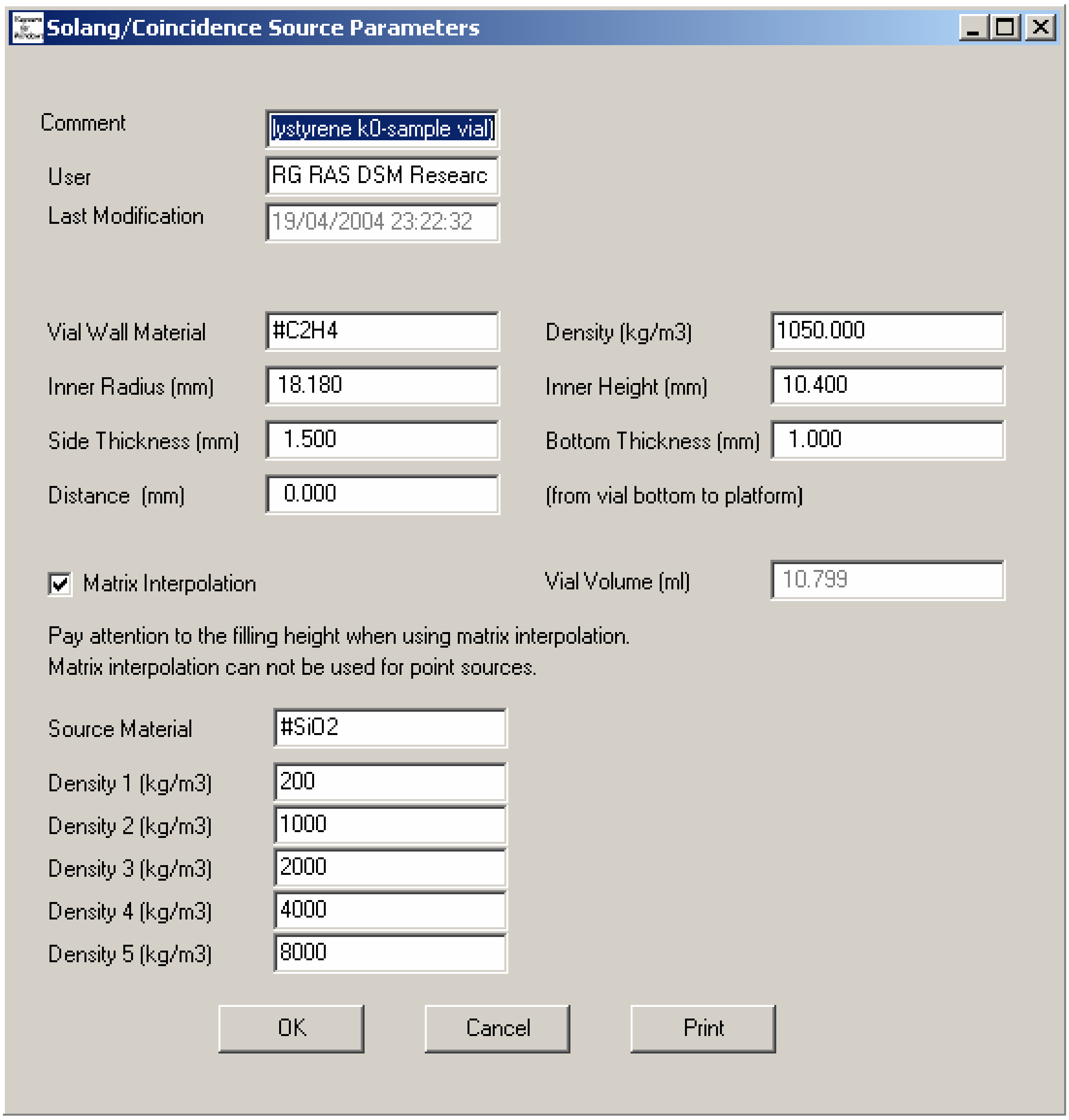


Comment	Au-Al-wire in spronckvial		
User	DV		
Last Modification	19/11/2005 13:30:39		
Vial Wall Material	#C2H4	Density (kg/m3)	900.000
Inner Radius (mm)	2.500	Inner Height (mm)	1.000
Side Thickness (mm)	0.750	Bottom Thickness (mm)	0.650
Distance (mm)	0.000	(from vial bottom to platform)	
☐ Matrix Interpolation		Vial Volume (ml)	0.020

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

Source Material	Aluminum
Density 1 (kg/m3)	2702

Figure 4.10: Input screen for vial/geometry parameters.



Comment	lystyrene k0-sample vial)		
User	RG RAS DSM Researc		
Last Modification	19/04/2004 23:22:32		
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
Density 2 (kg/m3)	1000
Density 3 (kg/m3)	2000
Density 4 (kg/m3)	4000
Density 5 (kg/m3)	8000

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).

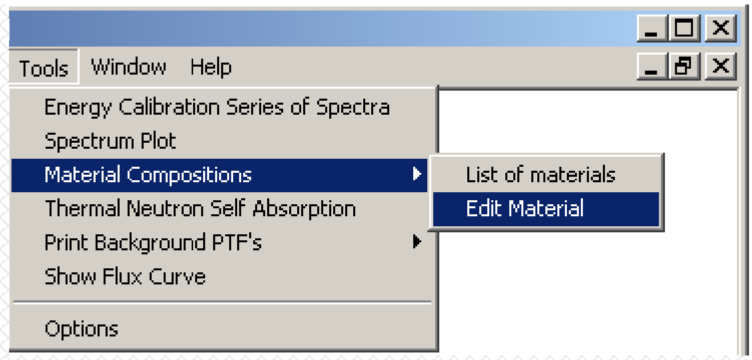
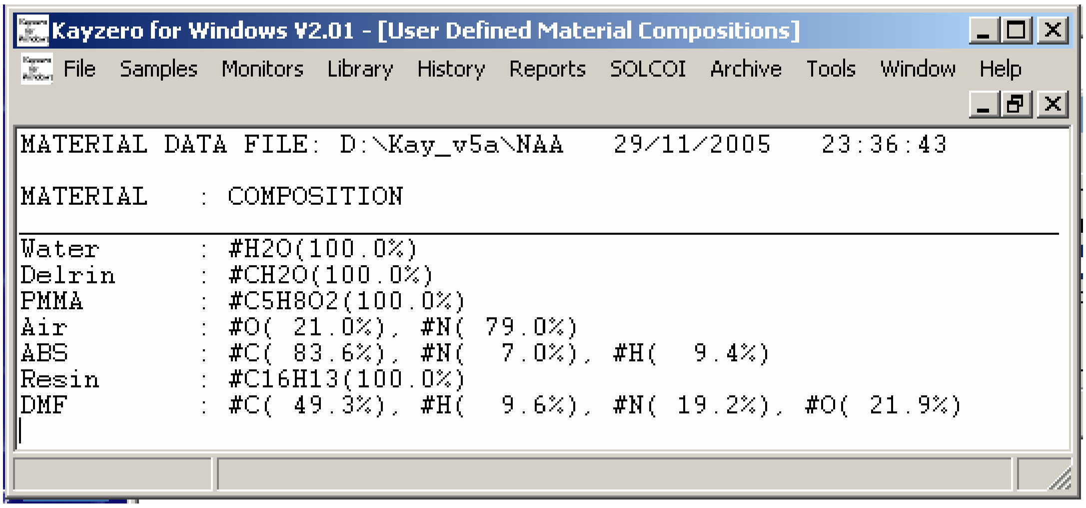


Figure 4.12: Material composition options.

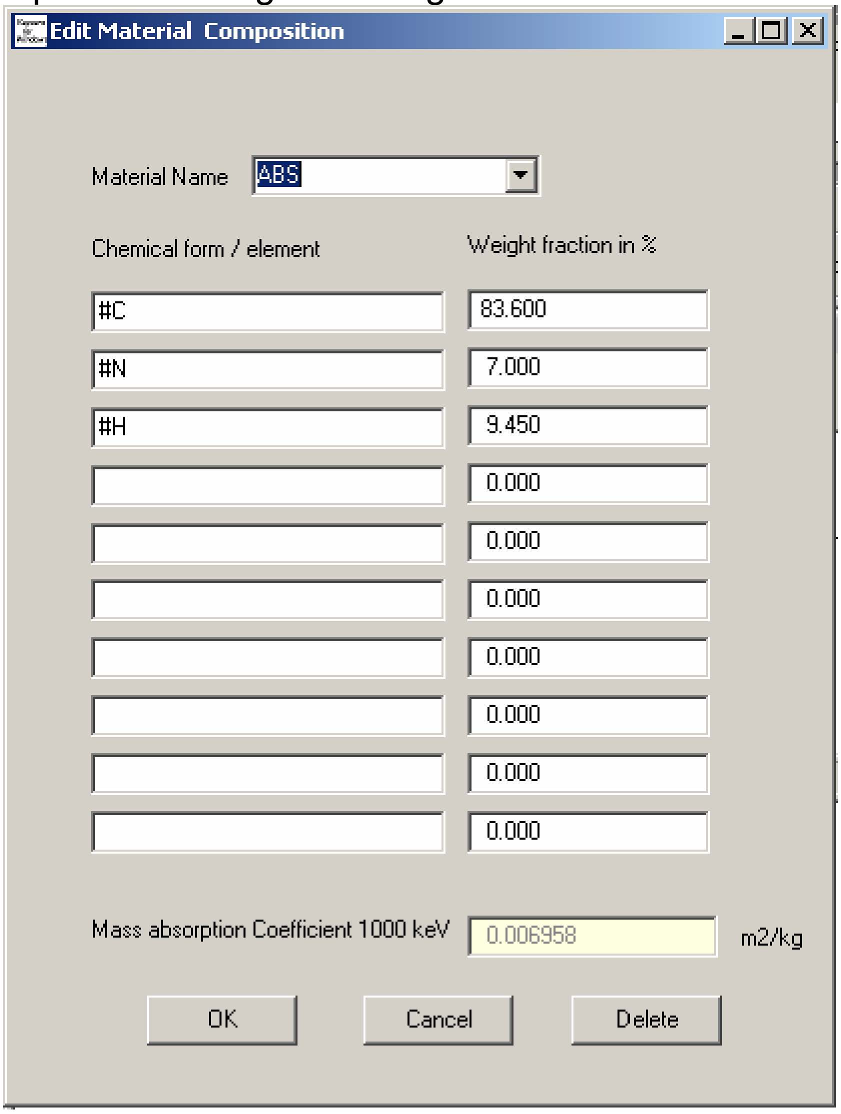
To obtain a list of material compositions you can use Option *Tools/Material Compositions/List of materials*. This list contains all the material compositions available as well as the composition data (see Figure 4.13).



```
MATERIAL DATA FILE: D:\Kay_v5a\NAA    29/11/2005    23:36:43

MATERIAL    : COMPOSITION
______________________________________________________________________
Water       : #H2O(100.0%)
Delrin      : #CH2O(100.0%)
PMMA        : #C5H8O2(100.0%)
Air         : #O( 21.0%), #N( 79.0%)
ABS         : #C( 83.6%), #N(  7.0%), #H(  9.4%)
Resin       : #C16H13(100.0%)
DMF         : #C( 49.3%), #H(  9.6%), #N( 19.2%), #O( 21.9%)
```

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.



Material Name: ABS

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

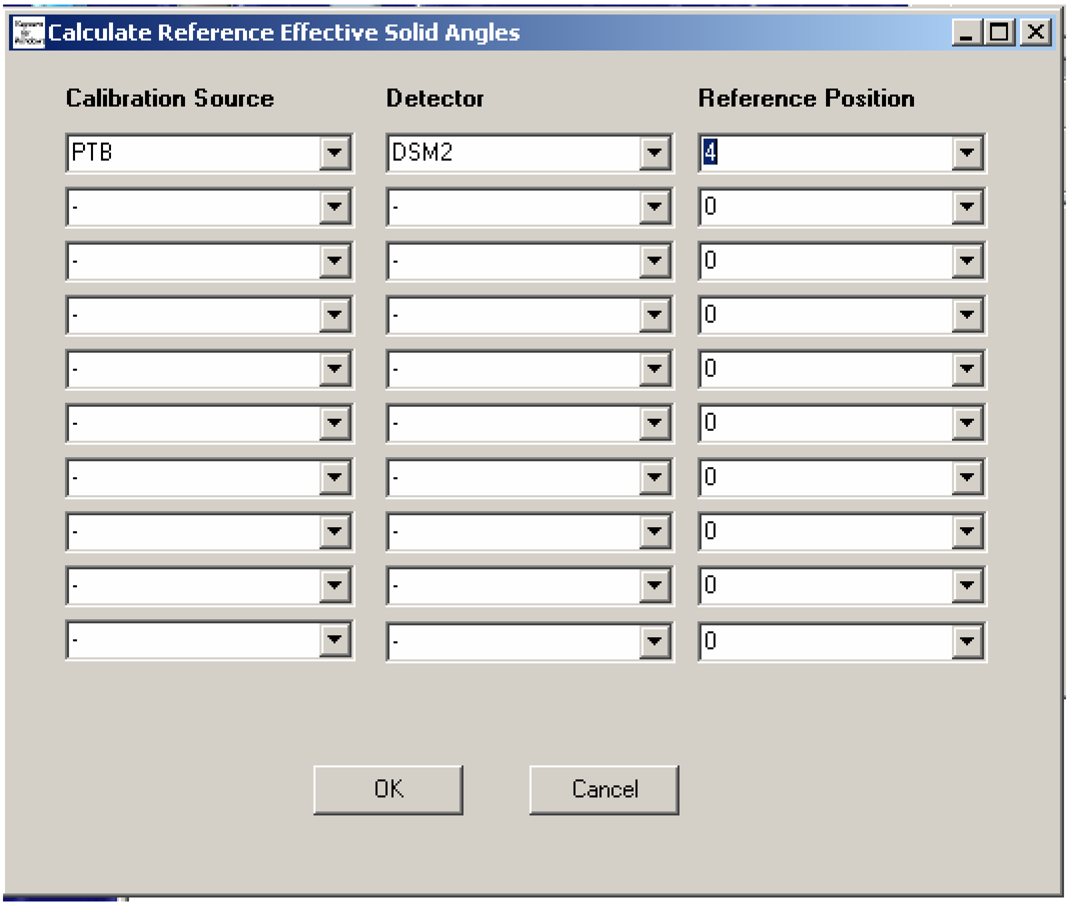
Figure 4.14: Material composition input screen.

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.



Calculate Reference Effective Solid Angles

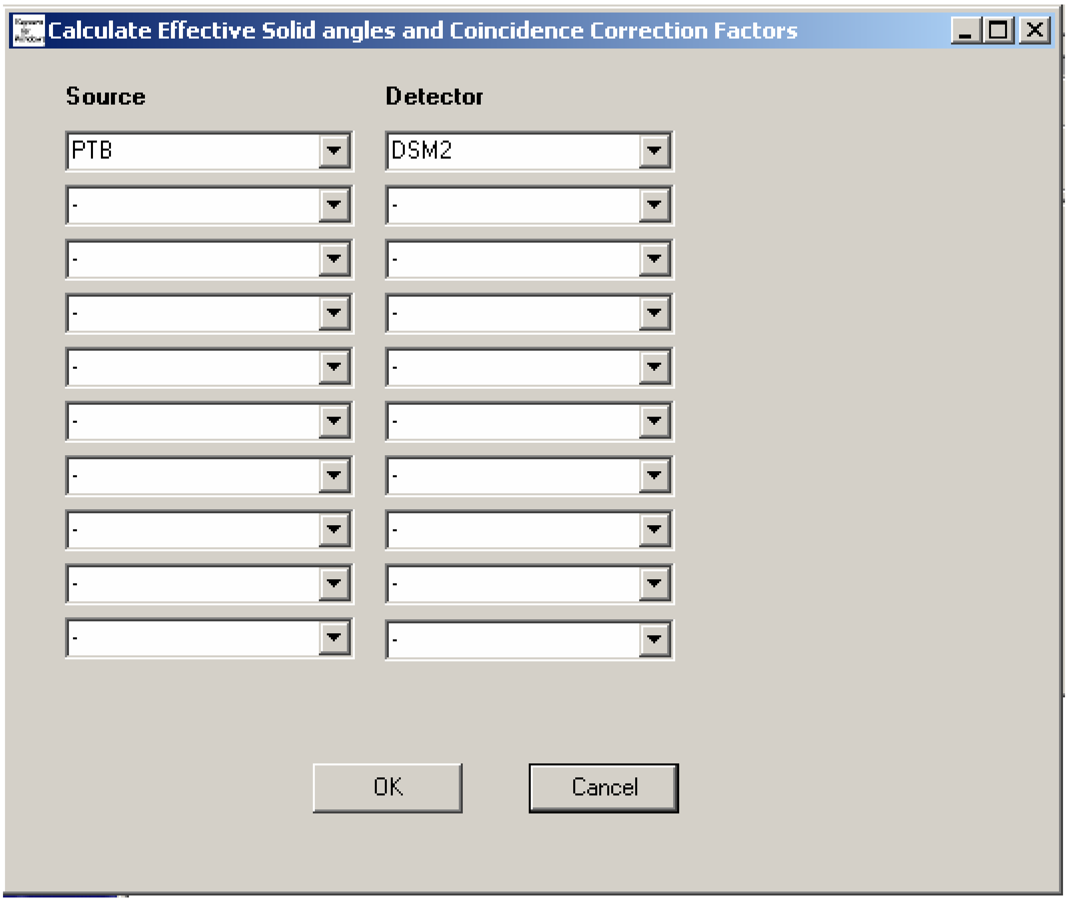
Calibration Source	Detector	Reference Position
PTB	DSM2	4
-	-	0
-	-	0
-	-	0
-	-	0
-	-	0
-	-	0
-	-	0
-	-	0
-	-	0

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.



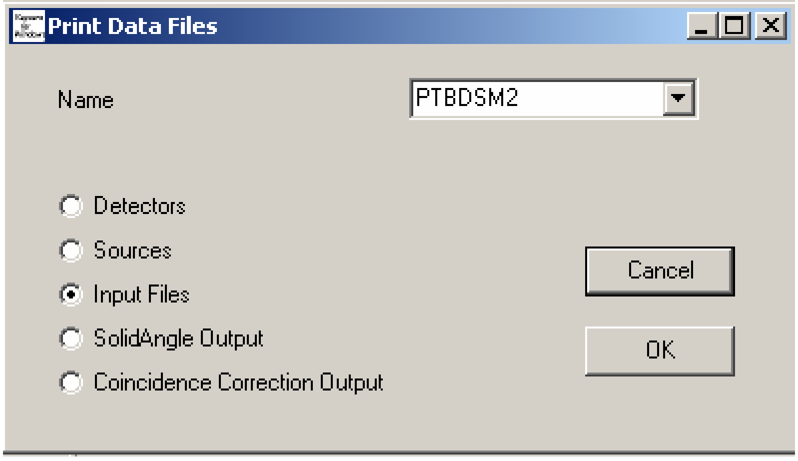
Source: PTB
Detector: DSM2

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.



Print Data Files

Name PTBDSM2

○ Detectors
○ Sources
● Input Files
○ SolidAngle Output
○ Coincidence Correction Output

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.

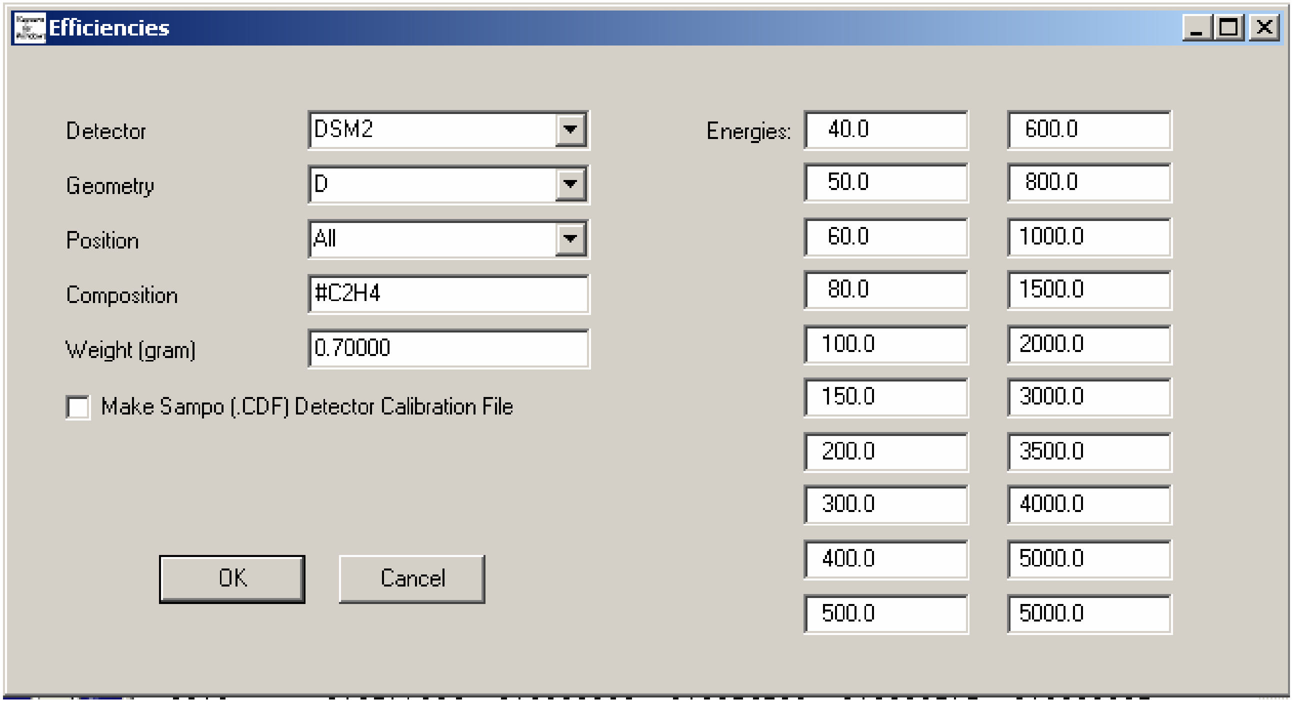
For an explanation of the format of the files see the end of **Appendix 2**.

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.

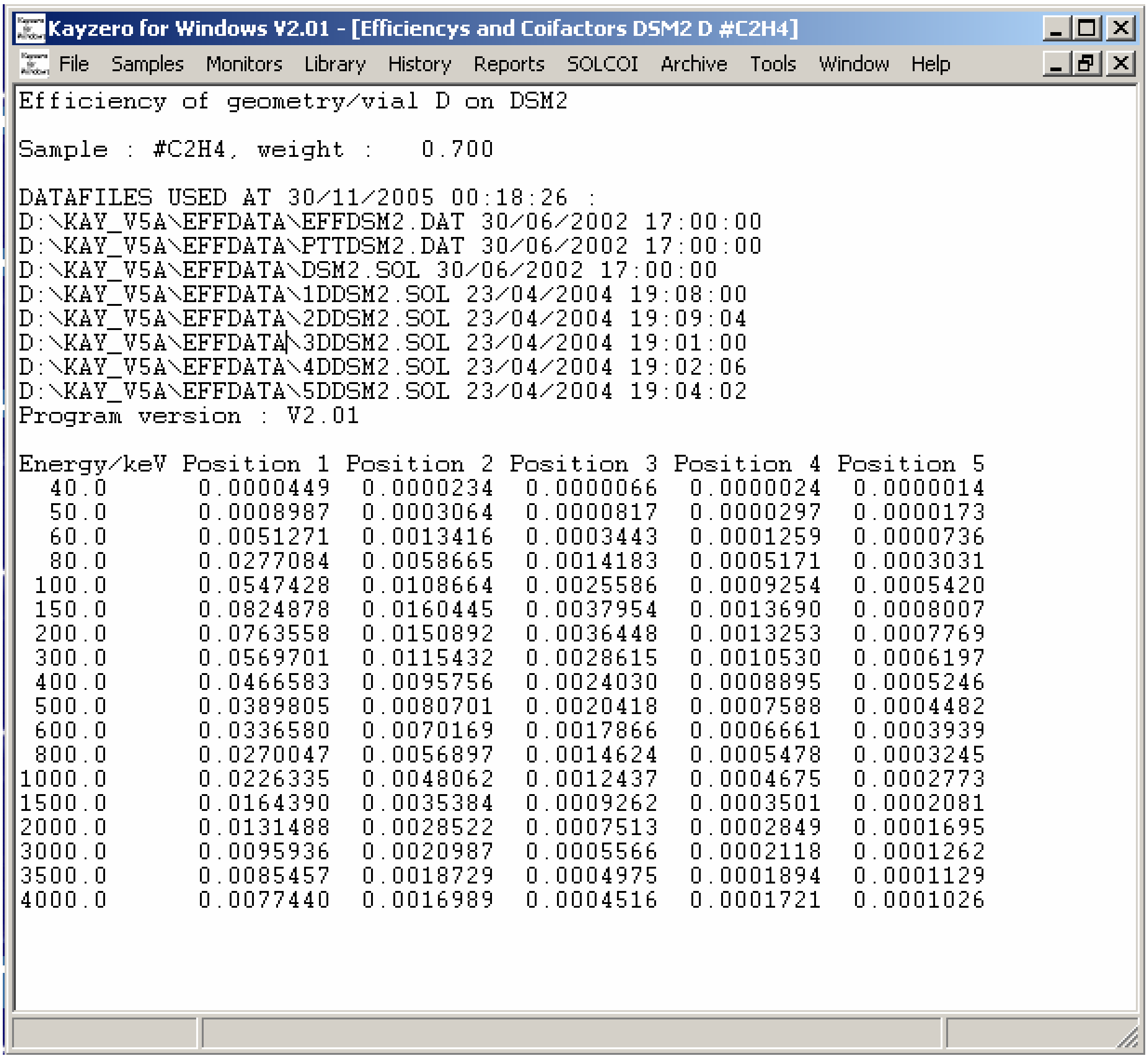


Detector: DSM2
Geometry: D
Position: All
Composition: #C2H4
Weight (gram): 0.70000
☐ Make Sampo (.CDF) Detector Calibration File

Energies:
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
4000.0
5000.0
5000.0

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

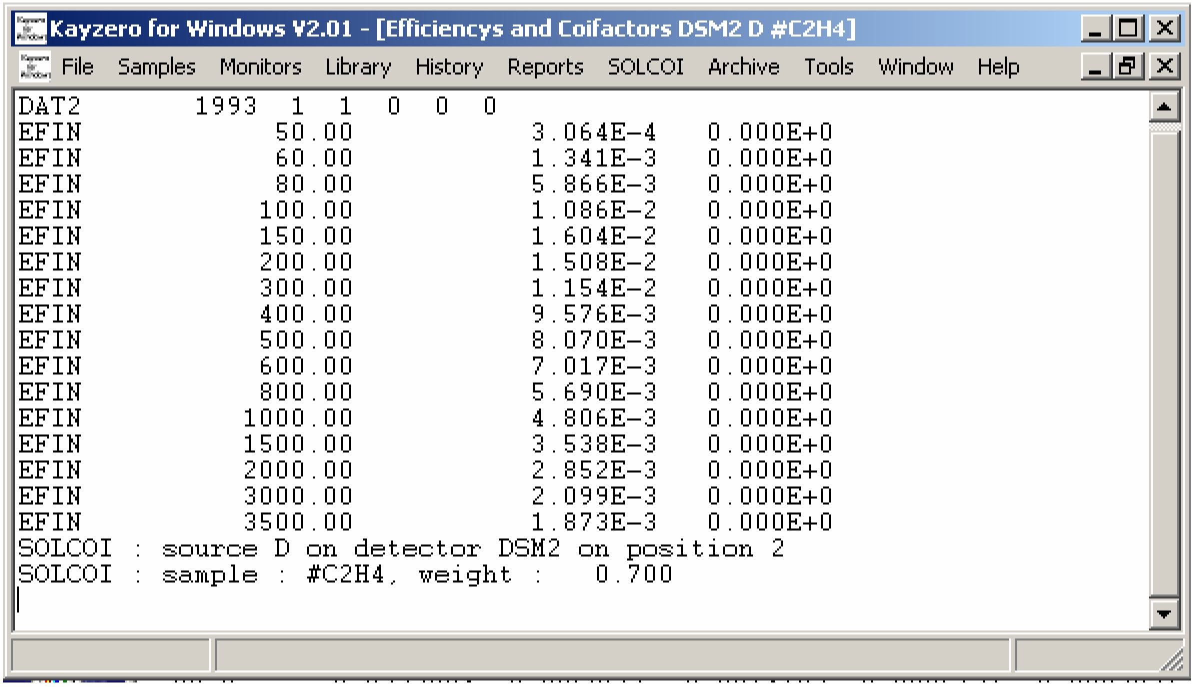
If the input is not correct the program will give some remarks.
The printed outputs are given in Figures 4.19. The energy values for the printed efficiencies can be specified using the input screen of this option.



```
Efficiency of geometry/vial D on DSM2

Sample : #C2H4, weight :   0.700

DATAFILES USED AT 30/11/2005 00:18:26 :
D:\KAY_V5A\EFFDATA\EFFDSM2.DAT 30/06/2002 17:00:00
D:\KAY_V5A\EFFDATA\PTTDSM2.DAT 30/06/2002 17:00:00
D:\KAY_V5A\EFFDATA\DSM2.SOL 30/06/2002 17:00:00
D:\KAY_V5A\EFFDATA\1DDSM2.SOL 23/04/2004 19:08:00
D:\KAY_V5A\EFFDATA\2DDSM2.SOL 23/04/2004 19:09:04
D:\KAY_V5A\EFFDATA\3DDSM2.SOL 23/04/2004 19:01:00
D:\KAY_V5A\EFFDATA\4DDSM2.SOL 23/04/2004 19:02:06
D:\KAY_V5A\EFFDATA\5DDSM2.SOL 23/04/2004 19:04:02
Program version : V2.01

Energy/keV Position 1 Position 2 Position 3 Position 4 Position 5
  40.0      0.0000449  0.0000234  0.0000066  0.0000024  0.0000014
  50.0      0.0008987  0.0003064  0.0000817  0.0000297  0.0000173
  60.0      0.0051271  0.0013416  0.0003443  0.0001259  0.0000736
  80.0      0.0277084  0.0058665  0.0014183  0.0005171  0.0003031
 100.0      0.0547428  0.0108664  0.0025586  0.0009254  0.0005420
 150.0      0.0824878  0.0160445  0.0037954  0.0013690  0.0008007
 200.0      0.0763558  0.0150892  0.0036448  0.0013253  0.0007769
 300.0      0.0569701  0.0115432  0.0028615  0.0010530  0.0006197
 400.0      0.0466583  0.0095756  0.0024030  0.0008895  0.0005246
 500.0      0.0389805  0.0080701  0.0020418  0.0007588  0.0004482
 600.0      0.0336580  0.0070169  0.0017866  0.0006661  0.0003939
 800.0      0.0270047  0.0056897  0.0014624  0.0005478  0.0003245
1000.0      0.0226335  0.0048062  0.0012437  0.0004675  0.0002773
1500.0      0.0164390  0.0035384  0.0009262  0.0003501  0.0002081
2000.0      0.0131488  0.0028522  0.0007513  0.0002849  0.0001695
3000.0      0.0095936  0.0020987  0.0005566  0.0002118  0.0001262
3500.0      0.0085457  0.0018729  0.0004975  0.0001894  0.0001129
4000.0      0.0077440  0.0016989  0.0004516  0.0001721  0.0001026
```

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.

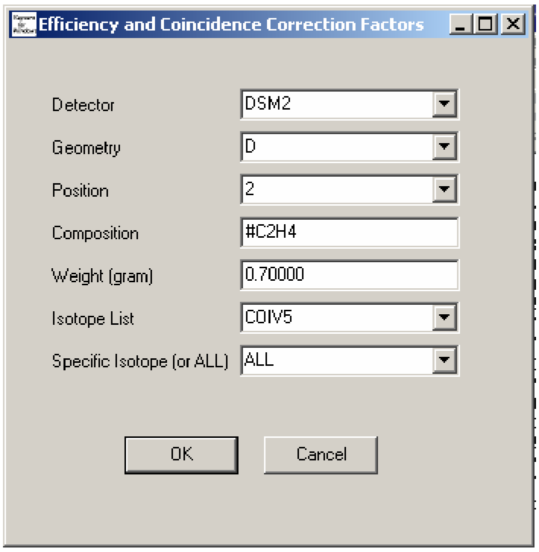
The detector calibration (SAMPO efficiency calibration file) for the same source at position 2 is shown in Figure 4.20.



```
DAT2        1993   1   1   0   0   0
EFIN             50.00            3.064E-4   0.000E+0
EFIN             60.00            1.341E-3   0.000E+0
EFIN             80.00            5.866E-3   0.000E+0
EFIN            100.00            1.086E-2   0.000E+0
EFIN            150.00            1.604E-2   0.000E+0
EFIN            200.00            1.508E-2   0.000E+0
EFIN            300.00            1.154E-2   0.000E+0
EFIN            400.00            9.576E-3   0.000E+0
EFIN            500.00            8.070E-3   0.000E+0
EFIN            600.00            7.017E-3   0.000E+0
EFIN            800.00            5.690E-3   0.000E+0
EFIN           1000.00            4.806E-3   0.000E+0
EFIN           1500.00            3.538E-3   0.000E+0
EFIN           2000.00            2.852E-3   0.000E+0
EFIN           3000.00            2.099E-3   0.000E+0
EFIN           3500.00            1.873E-3   0.000E+0
SOLCOI : source D on detector DSM2 on position 2
SOLCOI : sample : #C2H4, weight :   0.700
```

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.

Coincidence correction factors can be printed using *SOLCOI/Print Efficiency/Coincidence Data/Coincidence Correction and Efficiencie*. 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.

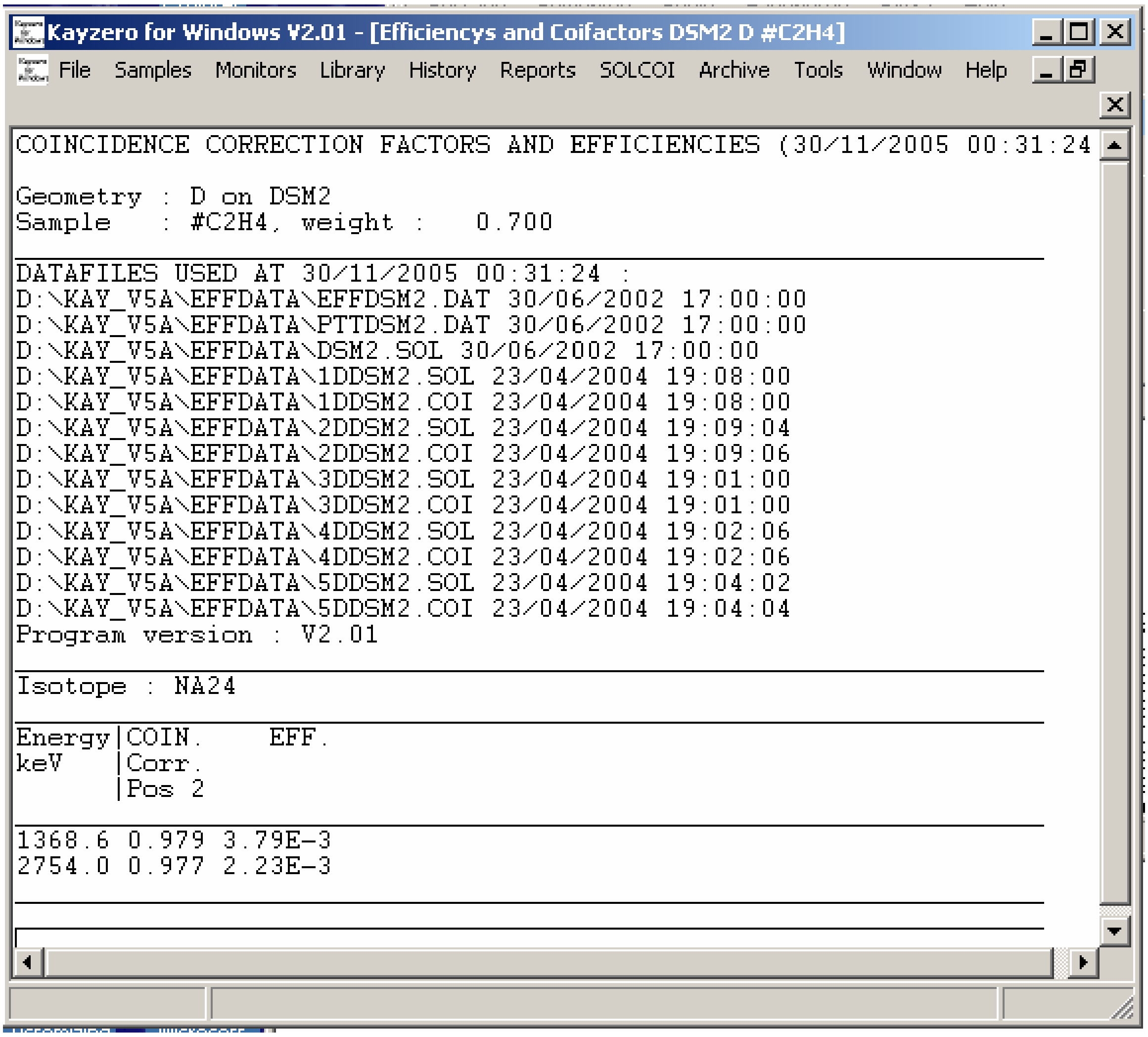


Detector: DSM2
Geometry: D
Position: 2
Composition: #C2H4
Weight (gram): 0.70000
Isotope List: COIV5
Specific Isotope (or ALL): ALL

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.

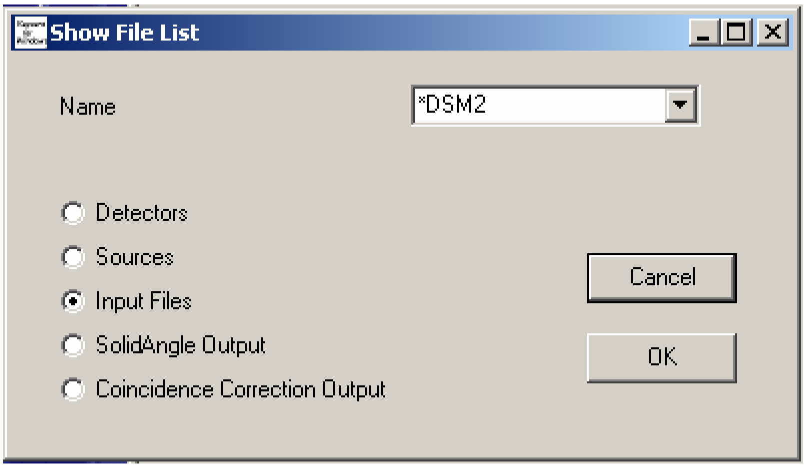


```
COINCIDENCE CORRECTION FACTORS AND EFFICIENCIES (30/11/2005 00:31:24

Geometry : D on DSM2
Sample   : #C2H4, weight :   0.700

DATAFILES USED AT 30/11/2005 00:31:24 :
D:\KAY_V5A\EFFDATA\EFFDSM2.DAT 30/06/2002 17:00:00
D:\KAY_V5A\EFFDATA\PTTDSM2.DAT 30/06/2002 17:00:00
D:\KAY_V5A\EFFDATA\DSM2.SOL 30/06/2002 17:00:00
D:\KAY_V5A\EFFDATA\1DDSM2.SOL 23/04/2004 19:08:00
D:\KAY_V5A\EFFDATA\1DDSM2.COI 23/04/2004 19:08:00
D:\KAY_V5A\EFFDATA\2DDSM2.SOL 23/04/2004 19:09:04
D:\KAY_V5A\EFFDATA\2DDSM2.COI 23/04/2004 19:09:06
D:\KAY_V5A\EFFDATA\3DDSM2.SOL 23/04/2004 19:01:00
D:\KAY_V5A\EFFDATA\3DDSM2.COI 23/04/2004 19:01:00
D:\KAY_V5A\EFFDATA\4DDSM2.SOL 23/04/2004 19:02:06
D:\KAY_V5A\EFFDATA\4DDSM2.COI 23/04/2004 19:02:06
D:\KAY_V5A\EFFDATA\5DDSM2.SOL 23/04/2004 19:04:02
D:\KAY_V5A\EFFDATA\5DDSM2.COI 23/04/2004 19:04:04
Program version : V2.01

Isotope : NA24

Energy|COIN.    EFF.
keV   |Corr.
      |Pos 2

1368.6 0.979 3.79E-3
2754.0 0.977 2.23E-3
```

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).

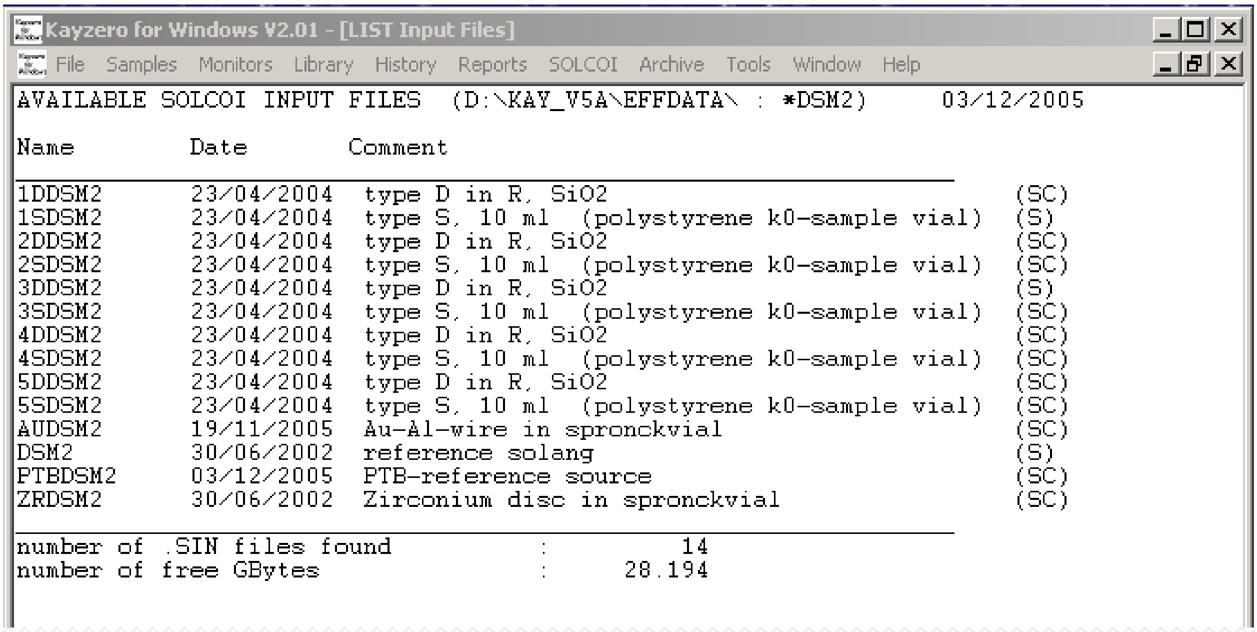


Name: *DSM2

○ Detectors
○ Sources
● Input Files
○ SolidAngle Output
○ Coincidence Correction Output

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

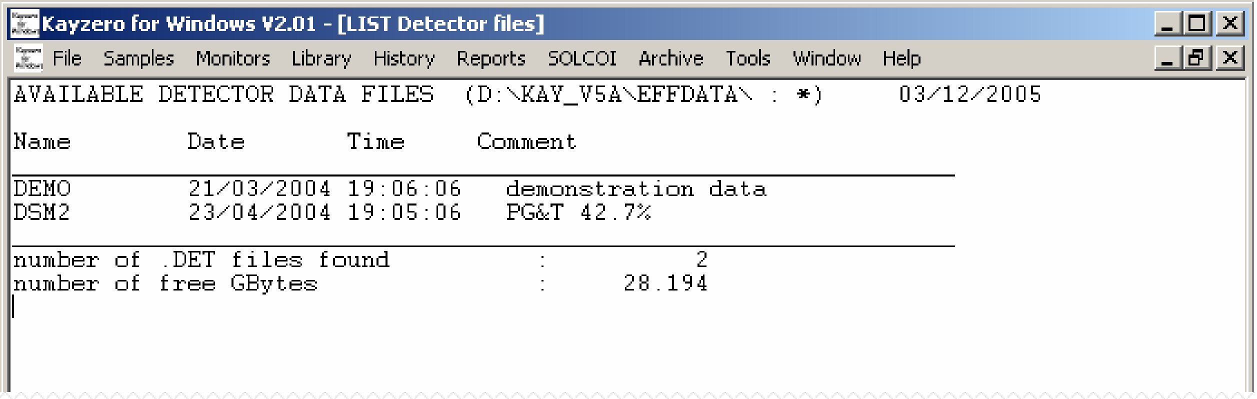
The file types are obvious however the Input Files need some explanation. The calculations are performed using the INW programs SOLANG and COINCALC. MS-Fortran programs need data files as input. These input files are made by SOLCOI. In the case of matrix interpolation five input files are made; one for 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.



```
AVAILABLE SOLCOI INPUT FILES  (D:\KAY_V5A\EFFDATA\ : *DSM2)     03/12/2005

Name         Date        Comment

1DDSM2       23/04/2004  type D in R, SiO2                                (SC)
1SDSM2       23/04/2004  type S, 10 ml  (polystyrene k0-sample vial)    (S)
2DDSM2       23/04/2004  type D in R, SiO2                                (SC)
2SDSM2       23/04/2004  type S, 10 ml  (polystyrene k0-sample vial)    (SC)
3DDSM2       23/04/2004  type D in R, SiO2                                (S)
3SDSM2       23/04/2004  type S, 10 ml  (polystyrene k0-sample vial)    (SC)
4DDSM2       23/04/2004  type D in R, SiO2                                (SC)
4SDSM2       23/04/2004  type S, 10 ml  (polystyrene k0-sample vial)    (SC)
5DDSM2       23/04/2004  type D in R, SiO2                                (SC)
5SDSM2       23/04/2004  type S, 10 ml  (polystyrene k0-sample vial)    (SC)
AUDSM2       19/11/2005  Au-Al-wire in spronckvial                        (SC)
DSM2         30/06/2002  reference solang                                 (S)
PTBDSM2      03/12/2005  PTB-reference source                             (SC)
ZRDSM2       30/06/2002  Zirconium disc in spronckvial                    (SC)

number of .SIN files found          :          14
number of free GBytes               :      28.194
```

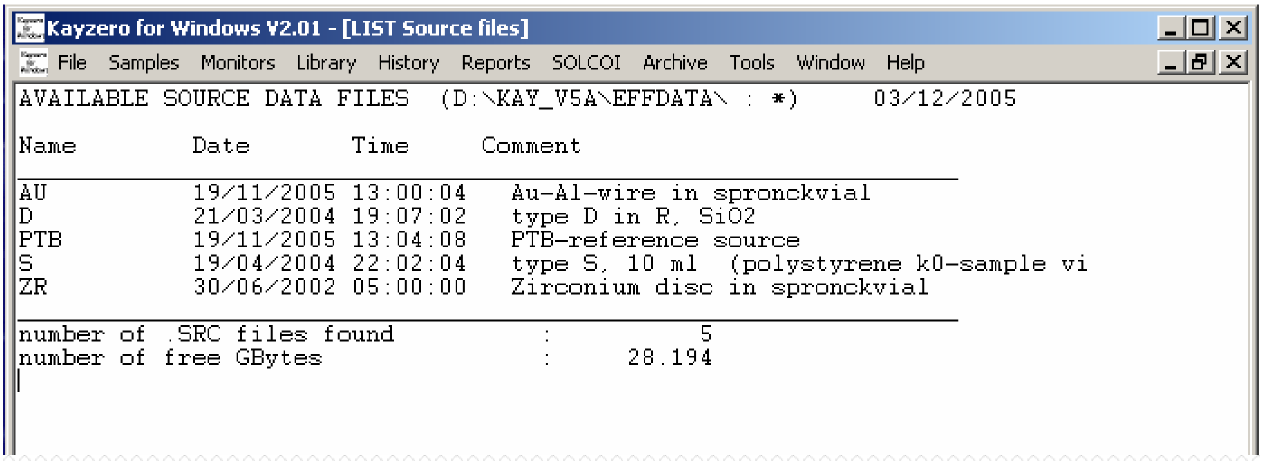
Figure 4.24: A list of available input files for SOLANG and COINCALC. S(olang) and/or C(oincalc) indicate that the calculations were performed.

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).



```
AVAILABLE DETECTOR DATA FILES  (D:\KAY_V5A\EFFDATA\ : *)     03/12/2005

Name         Date        Time      Comment
------------------------------------------------------------------
DEMO         21/03/2004 19:06:06   demonstration data
DSM2         23/04/2004 19:05:06   PG&T 42.7%
------------------------------------------------------------------
number of .DET files found          :          2
number of free GBytes               :     28.194
```

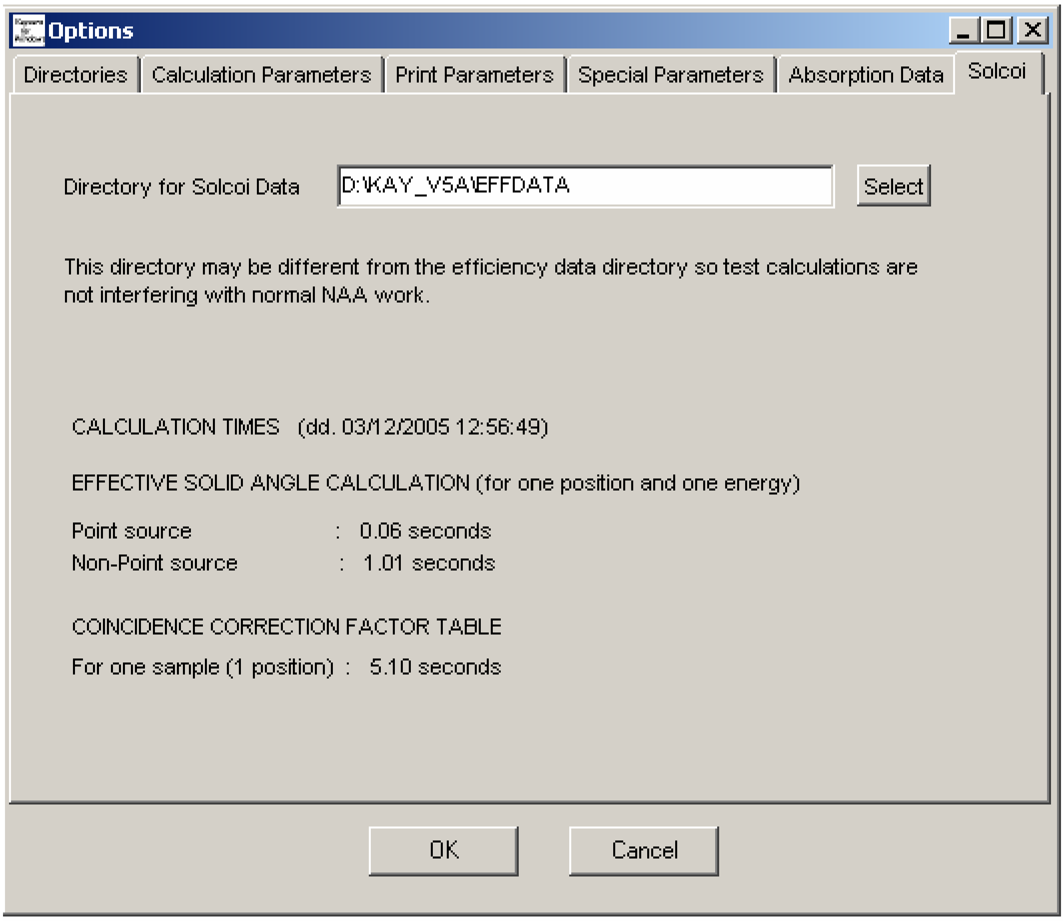
Figure 4.25: List of available detector data files (.DET).



```
AVAILABLE SOURCE DATA FILES  (D:\KAY_V5A\EFFDATA\ : *)     03/12/2005

Name         Date        Time      Comment
------------------------------------------------------------------
AU           19/11/2005 13:00:04   Au-Al-wire in spronckvial
D            21/03/2004 19:07:02   type D in R, SiO2
PTB          19/11/2005 13:04:08   PTB-reference source
S            19/04/2004 22:02:04   type S, 10 ml  (polystyrene k0-sample vi
ZR           30/06/2002 05:00:00   Zirconium disc in spronckvial
------------------------------------------------------------------
number of .SRC files found          :          5
number of free GBytes               :     28.194
```

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.



Directory for Solcoi Data D:\KAY_V5A\EFFDATA

This directory may be different from the efficiency data directory so test calculations are not interfering with normal NAA work.

CALCULATION TIMES (dd. 03/12/2005 12:56:49)

EFFECTIVE SOLID ANGLE CALCULATION (for one position and one energy)

Point source : 0.06 seconds
Non-Point source : 1.01 seconds

COINCIDENCE CORRECTION FACTOR TABLE

For one sample (1 position) : 5.10 seconds

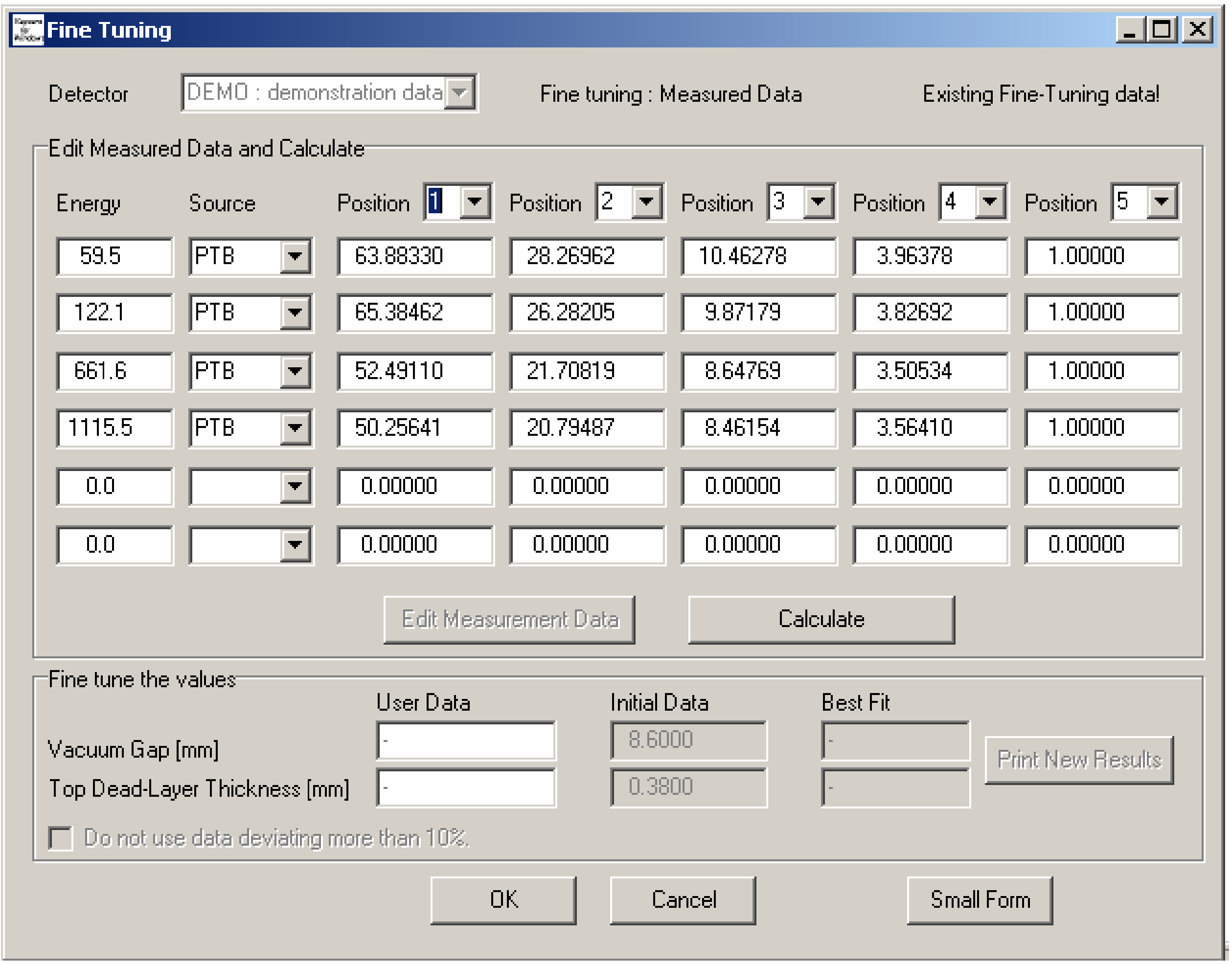
Figure 4.27: Calculation times (for an AMD 64 3000+).

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_0 USERS' (a part of this software package, see website 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.



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

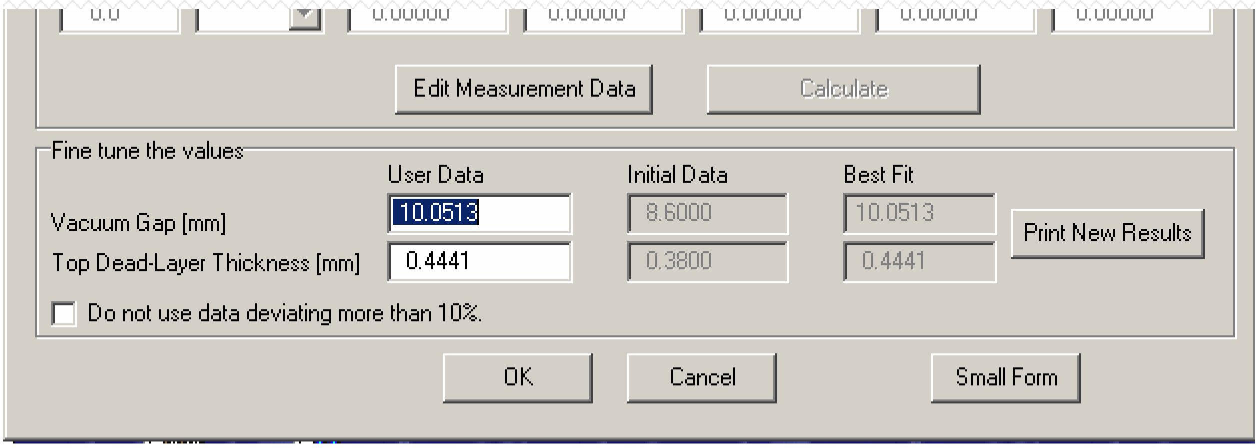
Fine tune the values

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

☐ Do not use data deviating more than 10%.

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).



0.0		0.00000	0.00000	0.00000	0.00000	0.00000

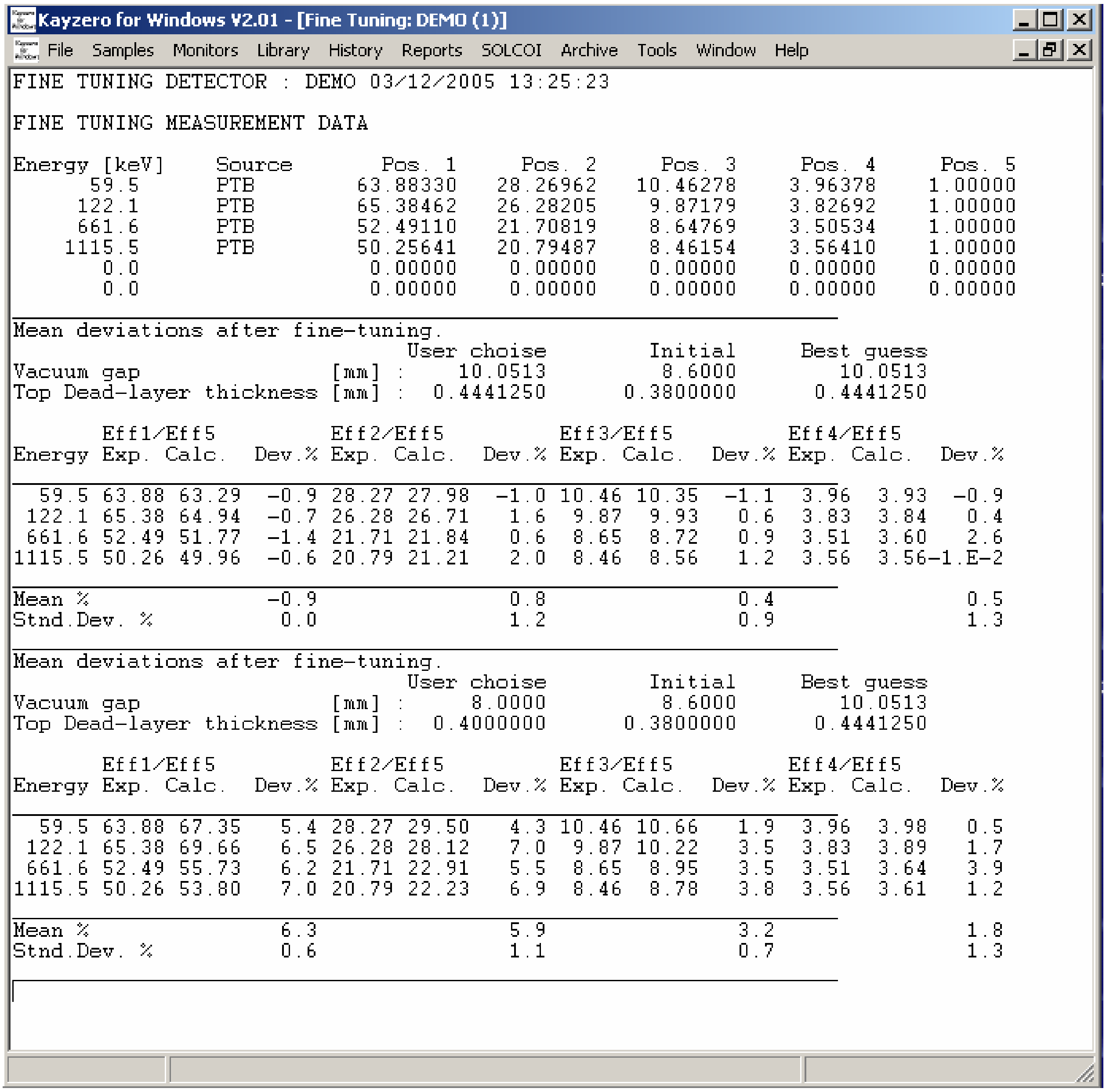
Fine tune the values

	User Data	Initial Data	Best Fit
Vacuum Gap [mm]	10.0513	8.6000	10.0513
Top Dead-Layer Thickness [mm]	0.4441	0.3800	0.4441

☐ Do not use data deviating more than 10%.

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 deadlayer 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.



```
FINE TUNING DETECTOR : DEMO 03/12/2005 13:25:23

FINE TUNING MEASUREMENT DATA

Energy [keV]    Source       Pos. 1     Pos. 2     Pos. 3     Pos. 4     Pos. 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

Mean deviations after fine-tuning.
                               User choise        Initial     Best guess
Vacuum gap               [mm] :    10.0513         8.6000        10.0513
Top Dead-layer thickness [mm] :  0.4441250      0.3800000      0.4441250

       Eff1/Eff5         Eff2/Eff5         Eff3/Eff5         Eff4/Eff5
Energy Exp. Calc.  Dev.% Exp. Calc.  Dev.% Exp. Calc.  Dev.% Exp. Calc.  Dev.%

  59.5 63.88 63.29  -0.9 28.27 27.98  -1.0 10.46 10.35  -1.1  3.96  3.93  -0.9
 122.1 65.38 64.94  -0.7 26.28 26.71   1.6  9.87  9.93   0.6  3.83  3.84   0.4
 661.6 52.49 51.77  -1.4 21.71 21.84   0.6  8.65  8.72   0.9  3.51  3.60   2.6
1115.5 50.26 49.96  -0.6 20.79 21.21   2.0  8.46  8.56   1.2  3.56  3.56-1.E-2

Mean %              -0.9               0.8               0.4               0.5
Stnd.Dev. %          0.0               1.2               0.9               1.3

Mean deviations after fine-tuning.
                               User choise        Initial     Best guess
Vacuum gap               [mm] :     8.0000         8.6000        10.0513
Top Dead-layer thickness [mm] :  0.4000000      0.3800000      0.4441250

       Eff1/Eff5         Eff2/Eff5         Eff3/Eff5         Eff4/Eff5
Energy Exp. Calc.  Dev.% Exp. Calc.  Dev.% Exp. Calc.  Dev.% Exp. Calc.  Dev.%

  59.5 63.88 67.35   5.4 28.27 29.50   4.3 10.46 10.66   1.9  3.96  3.98   0.5
 122.1 65.38 69.66   6.5 26.28 28.12   7.0  9.87 10.22   3.5  3.83  3.89   1.7
 661.6 52.49 55.73   6.2 21.71 22.91   5.5  8.65  8.95   3.5  3.51  3.64   3.9
1115.5 50.26 53.80   7.0 20.79 22.23   6.9  8.46  8.78   3.8  3.56  3.61   1.2

Mean %               6.3               5.9               3.2               1.8
Stnd.Dev. %          0.6               1.1               0.7               1.3
```

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.

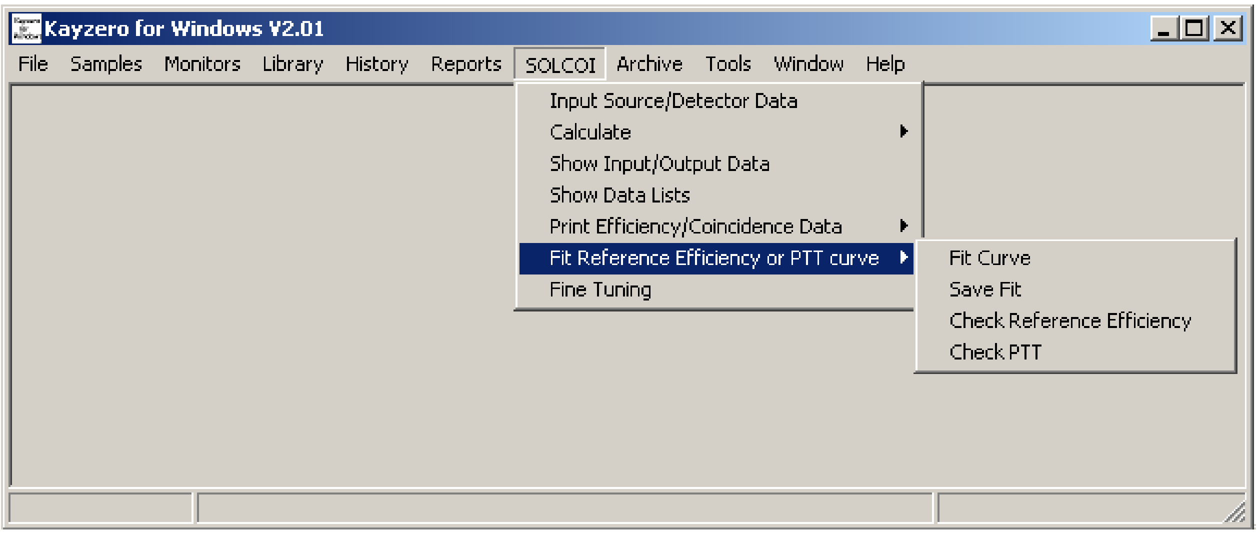


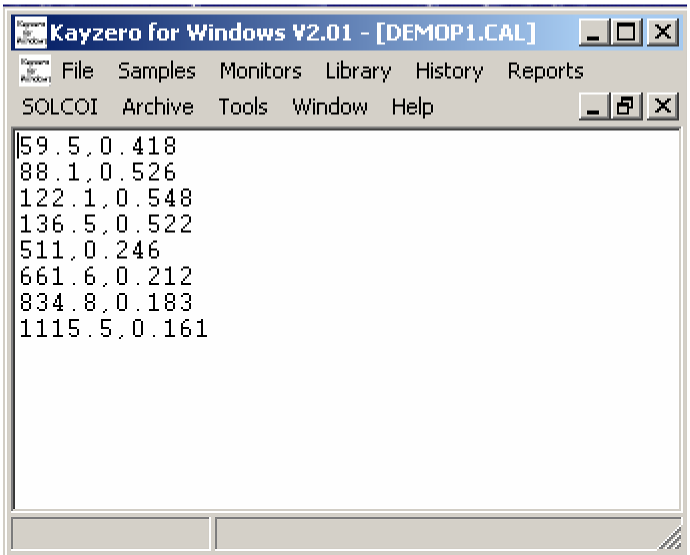
Figure 4.30: Reference Efficiency and PTT Fit menu.

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

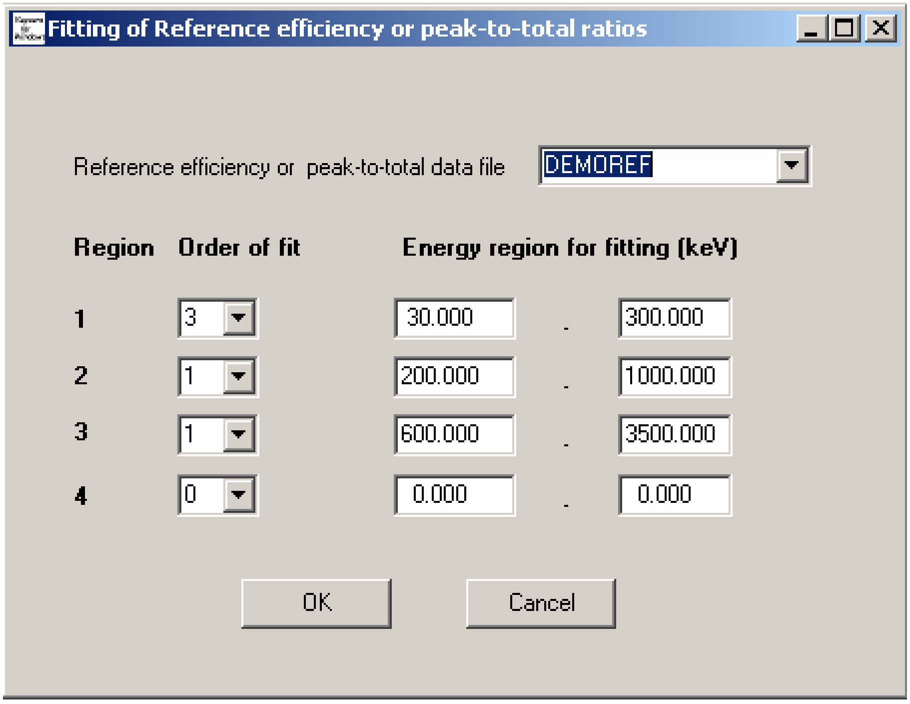
Figure 4.31 for an example of a PTT calibration data file.



```
59.5,0.418
88.1,0.526
122.1,0.548
136.5,0.522
511,0.246
661.6,0.212
834.8,0.183
1115.5,0.161
```

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.



Reference efficiency or peak-to-total data file: DEMOREF

Region	Order of fit	Energy region for fitting (keV)	
1	3	30.000	300.000
2	1	200.000	1000.000
3	1	600.000	3500.000
4	0	0.000	0.000

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.

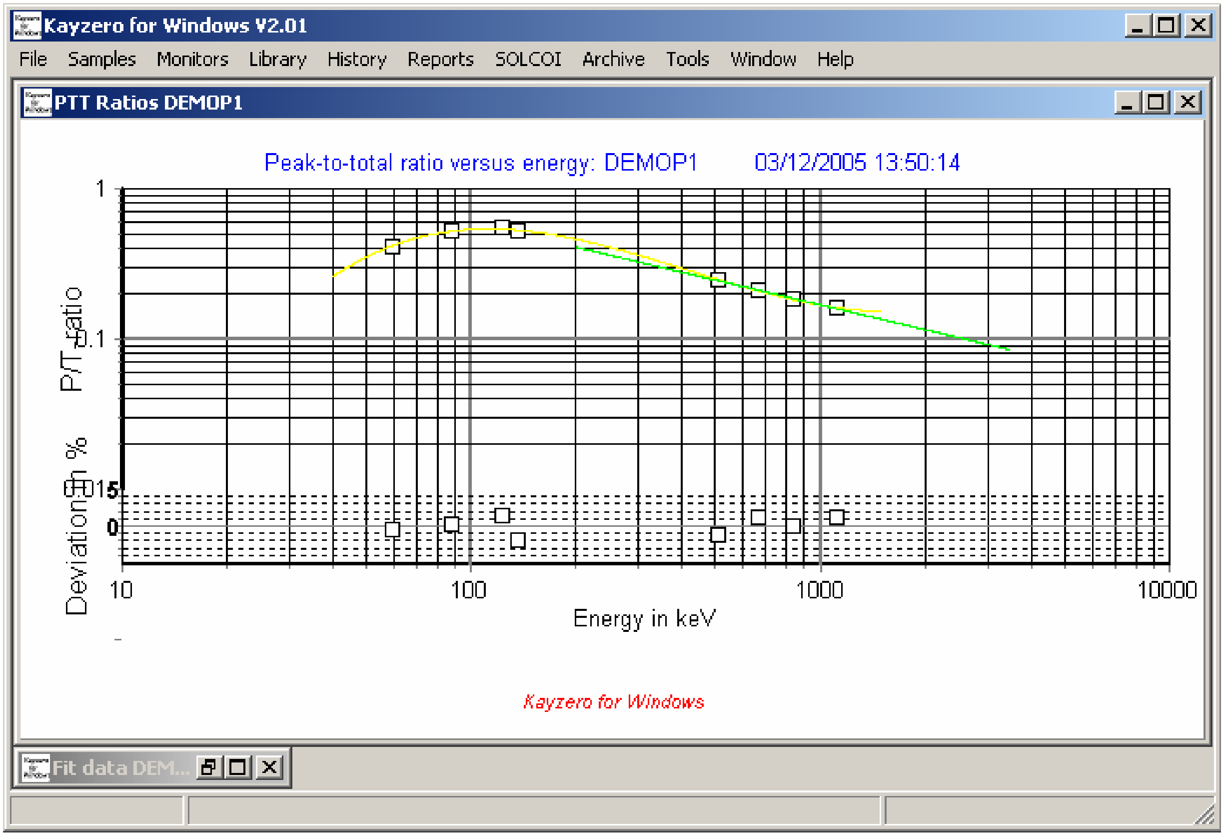
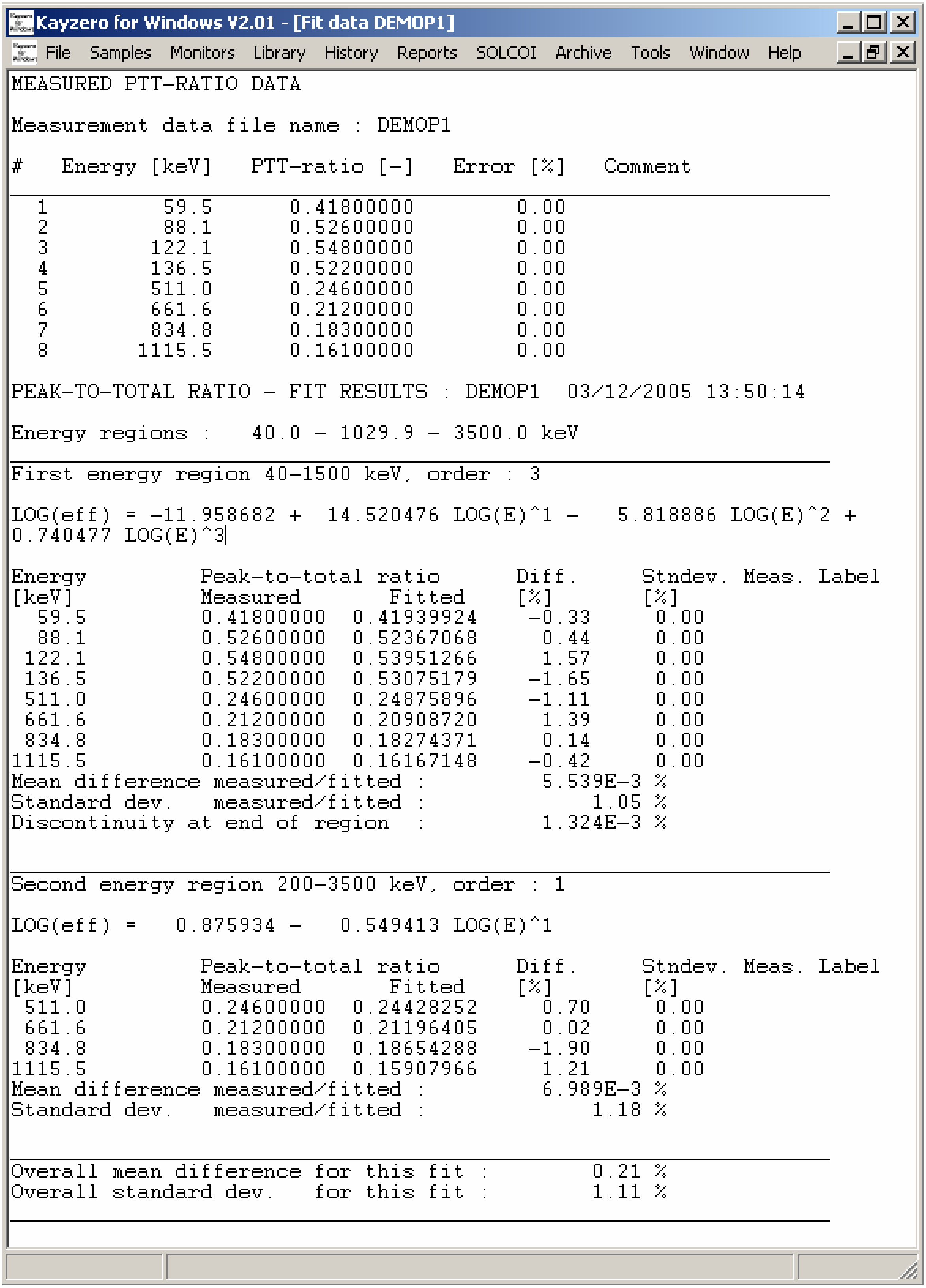


Figure 4.33 Fitting output: Plot of PTT-ratio fit.

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).



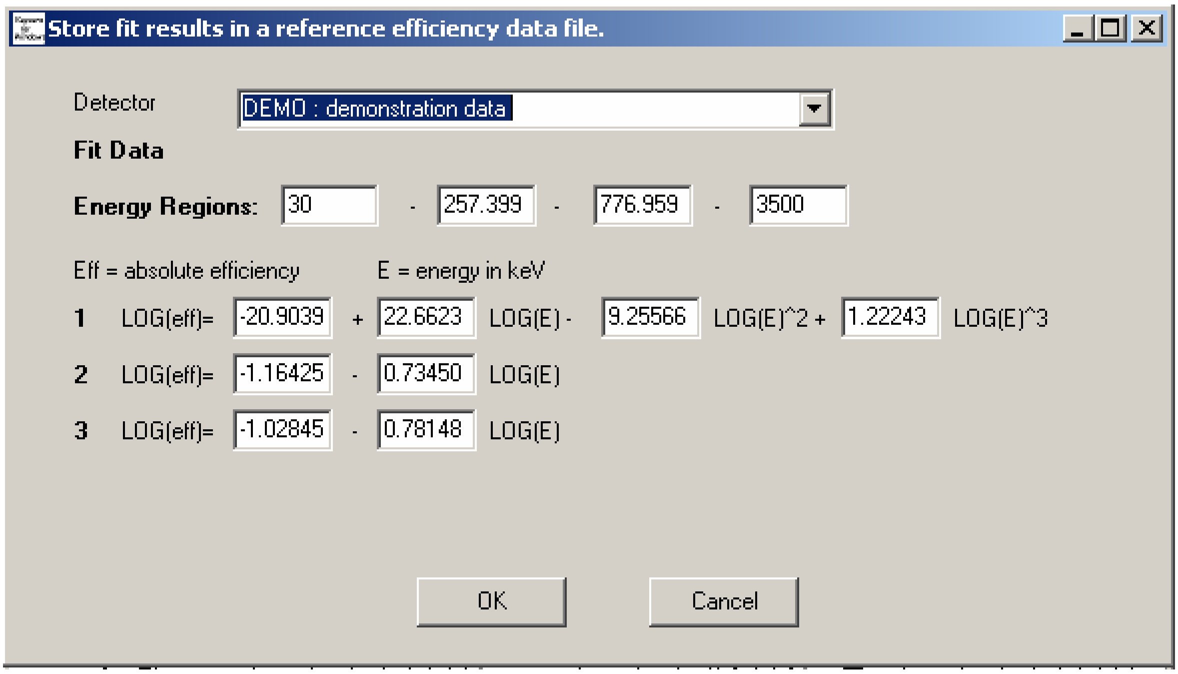
```
MEASURED PTT-RATIO DATA

Measurement data file name : DEMOP1

#   Energy [keV]   PTT-ratio [-]   Error [%]   Comment

-----------------------------------------------------------------
  1         59.5      0.41800000       0.00
  2         88.1      0.52600000       0.00
  3        122.1      0.54800000       0.00
  4        136.5      0.52200000       0.00
  5        511.0      0.24600000       0.00
  6        661.6      0.21200000       0.00
  7        834.8      0.18300000       0.00
  8       1115.5      0.16100000       0.00

PEAK-TO-TOTAL RATIO - FIT RESULTS : DEMOP1  03/12/2005 13:50:14

Energy regions :   40.0 - 1029.9 - 3500.0 keV
-----------------------------------------------------------------
First energy region 40-1500 keV, order : 3

LOG(eff) = -11.958682 +  14.520476 LOG(E)^1 -   5.818886 LOG(E)^2 +
0.740477 LOG(E)^3

Energy         Peak-to-total ratio      Diff.     Stndev. Meas. Label
[keV]          Measured       Fitted    [%]       [%]
  59.5         0.41800000  0.41939924    -0.33      0.00
  88.1         0.52600000  0.52367068     0.44      0.00
 122.1         0.54800000  0.53951266     1.57      0.00
 136.5         0.52200000  0.53075179    -1.65      0.00
 511.0         0.24600000  0.24875896    -1.11      0.00
 661.6         0.21200000  0.20908720     1.39      0.00
 834.8         0.18300000  0.18274371     0.14      0.00
1115.5         0.16100000  0.16167148    -0.42      0.00
Mean difference measured/fitted :         5.539E-3 %
Standard dev.    measured/fitted :             1.05 %
Discontinuity at end of region   :        1.324E-3 %

-----------------------------------------------------------------
Second energy region 200-3500 keV, order : 1

LOG(eff) =   0.875934 -   0.549413 LOG(E)^1

Energy         Peak-to-total ratio      Diff.     Stndev. Meas. Label
[keV]          Measured       Fitted    [%]       [%]
 511.0         0.24600000  0.24428252     0.70      0.00
 661.6         0.21200000  0.21196405     0.02      0.00
 834.8         0.18300000  0.18654288    -1.90      0.00
1115.5         0.16100000  0.15907966     1.21      0.00
Mean difference measured/fitted :         6.989E-3 %
Standard dev.    measured/fitted :             1.18 %

-----------------------------------------------------------------
Overall mean difference for this fit :        0.21 %
Overall standard dev.   for this fit :        1.11 %
-----------------------------------------------------------------
```

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 reference efficiency data file.

Detector DEMO : demonstration data

Fit Data

Energy Regions: 30 - 257.399 - 776.959 - 3500

Eff = absolute efficiency E = energy in keV

1 LOG(eff)= -20.9039 + 22.6623 LOG(E) - 9.25566 LOG(E)^2 + 1.22243 LOG(E)^3

2 LOG(eff)= -1.16425 - 0.73450 LOG(E)

3 LOG(eff)= -1.02845 - 0.78148 LOG(E)

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.

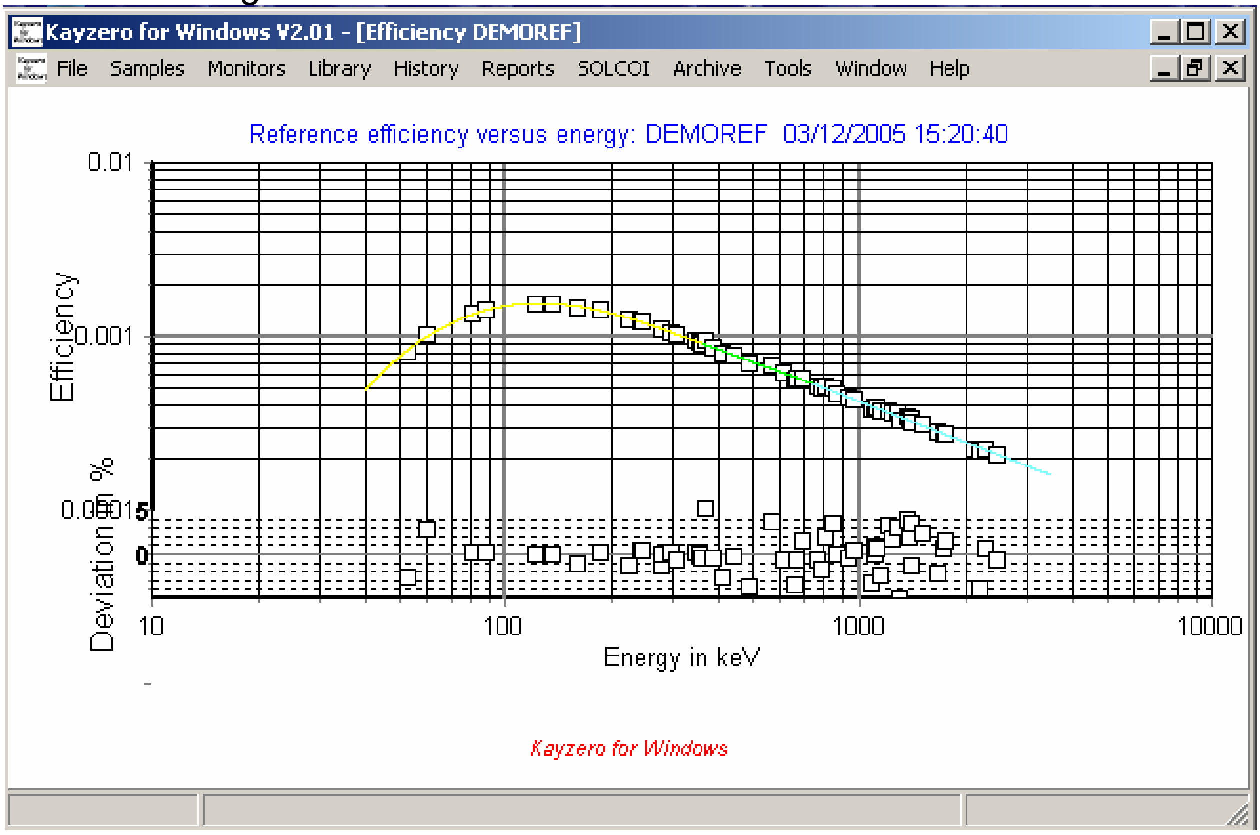


Figure 4.36 Comparison of measure efficiency data with the stored reference efficiency fit .

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).

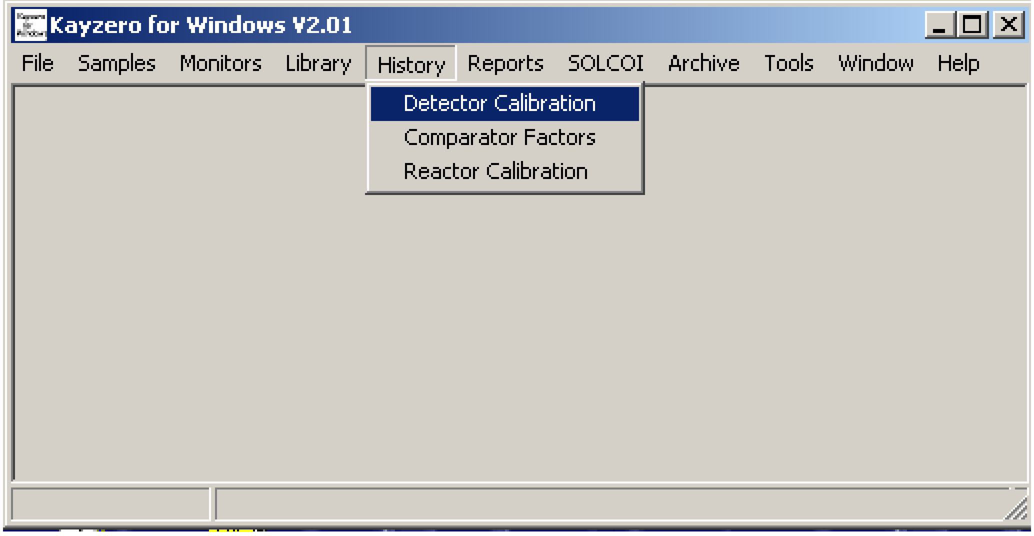
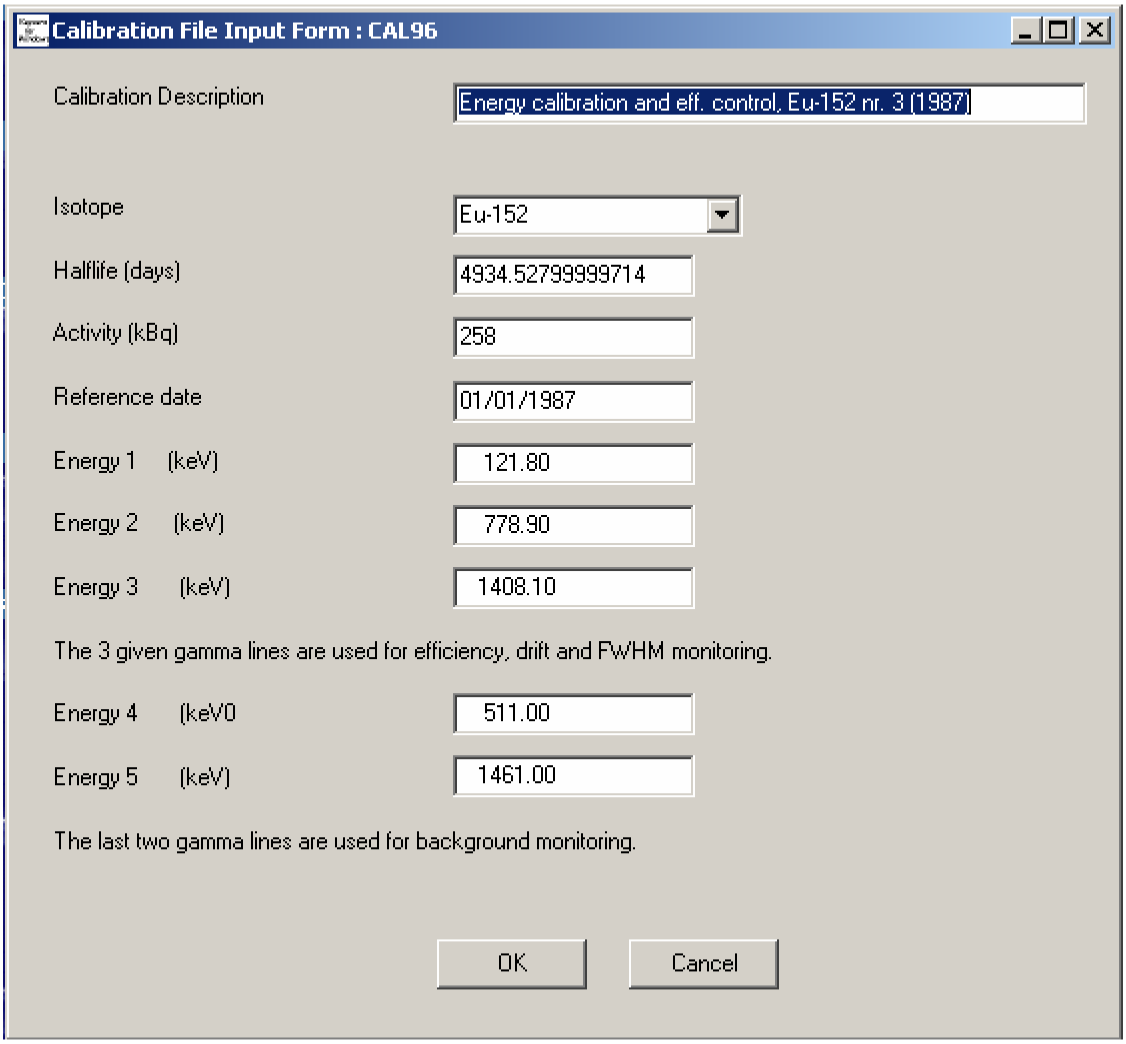


Figure 5.1: History of Detector and Reactor Calibrations Menu

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 CAL96.



Calibration File Input Form : CAL96

Calibration Description	Energy calibration and eff. control, Eu-152 nr. 3 (1987)
Isotope	Eu-152
Halflife (days)	4934.52799999714
Activity (kBq)	258
Reference date	01/01/1987
Energy 1 (keV)	121.80
Energy 2 (keV)	778.90
Energy 3 (keV)	1408.10

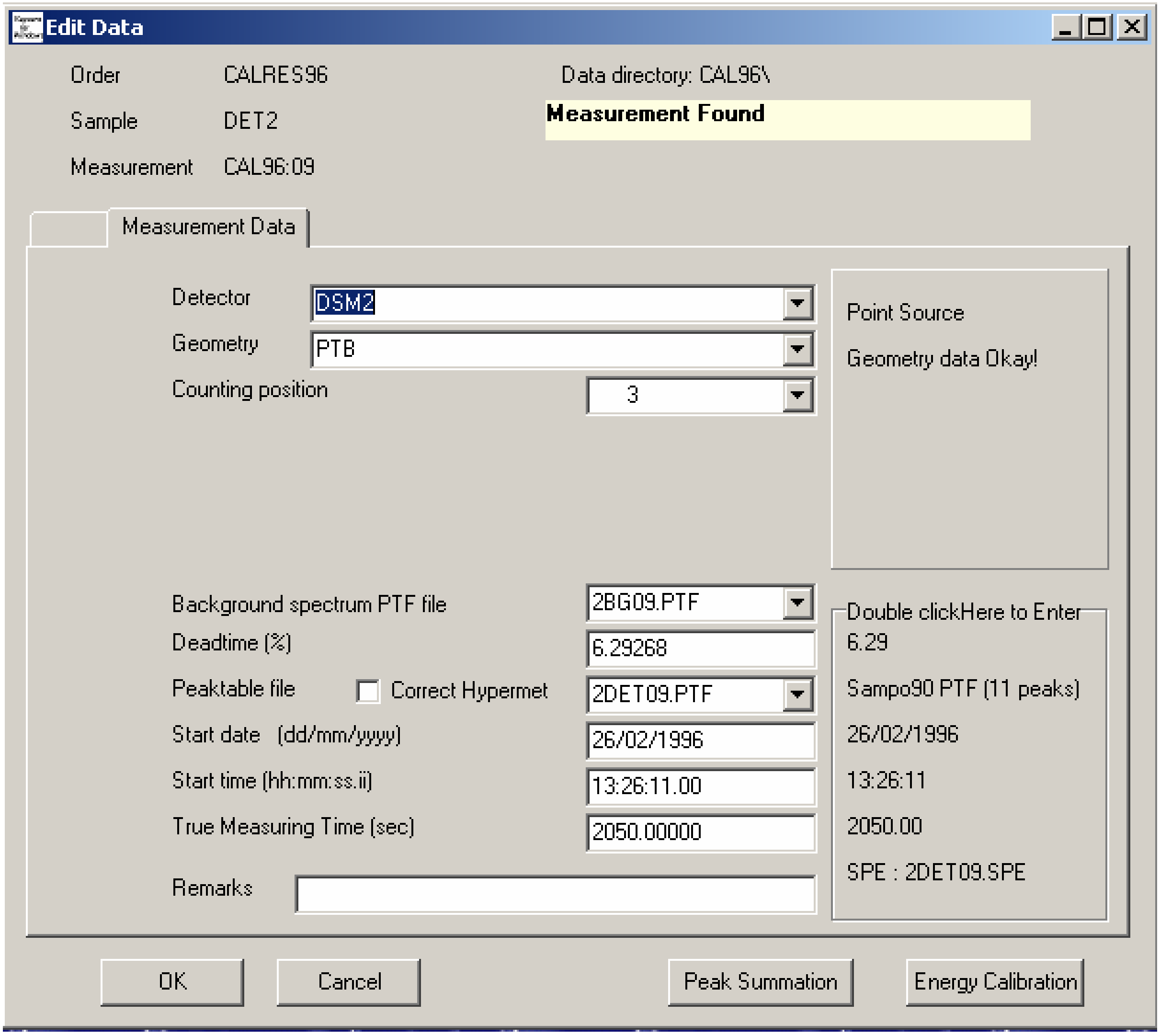
The 3 given gamma lines are used for efficiency, drift and FWHM monitoring.

Energy 4 (keV0	511.00
Energy 5 (keV)	1461.00

The last two gamma lines are used for background monitoring.

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*.



Order CALRES96

Sample DET2

Measurement CAL96:09

Data directory: CAL96\

Measurement Found

Detector: DSM2

Geometry: PTB

Counting position: 3

Point Source

Geometry data Okay!

Background spectrum PTF file: 2BG09.PTF

Deadtime (%): 6.29268

Peaktable file ☐ Correct Hypermet: 2DET09.PTF

Start date (dd/mm/yyyy): 26/02/1996

Start time (hh:mm:ss.ii): 13:26:11.00

True Measuring Time (sec): 2050.00000

Remarks:

Double clickHere to Enter

6.29

Sampo90 PTF (11 peaks)

26/02/1996

13:26:11

2050.00

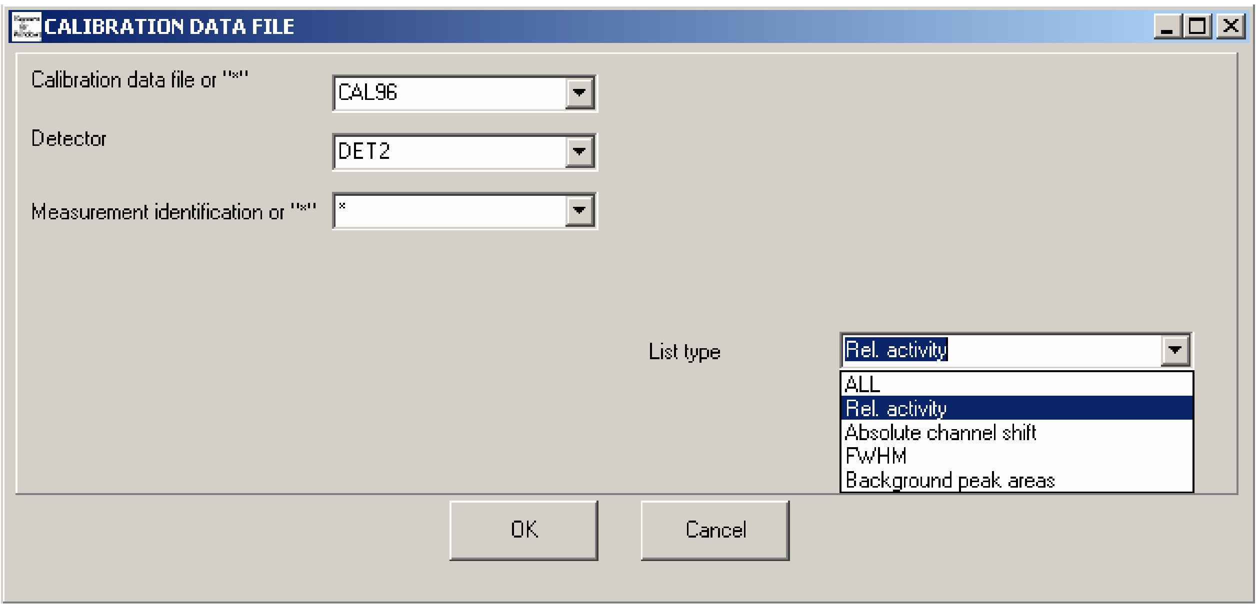
SPE : 2DET09.SPE

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.



Calibration data file or "*": CAL96

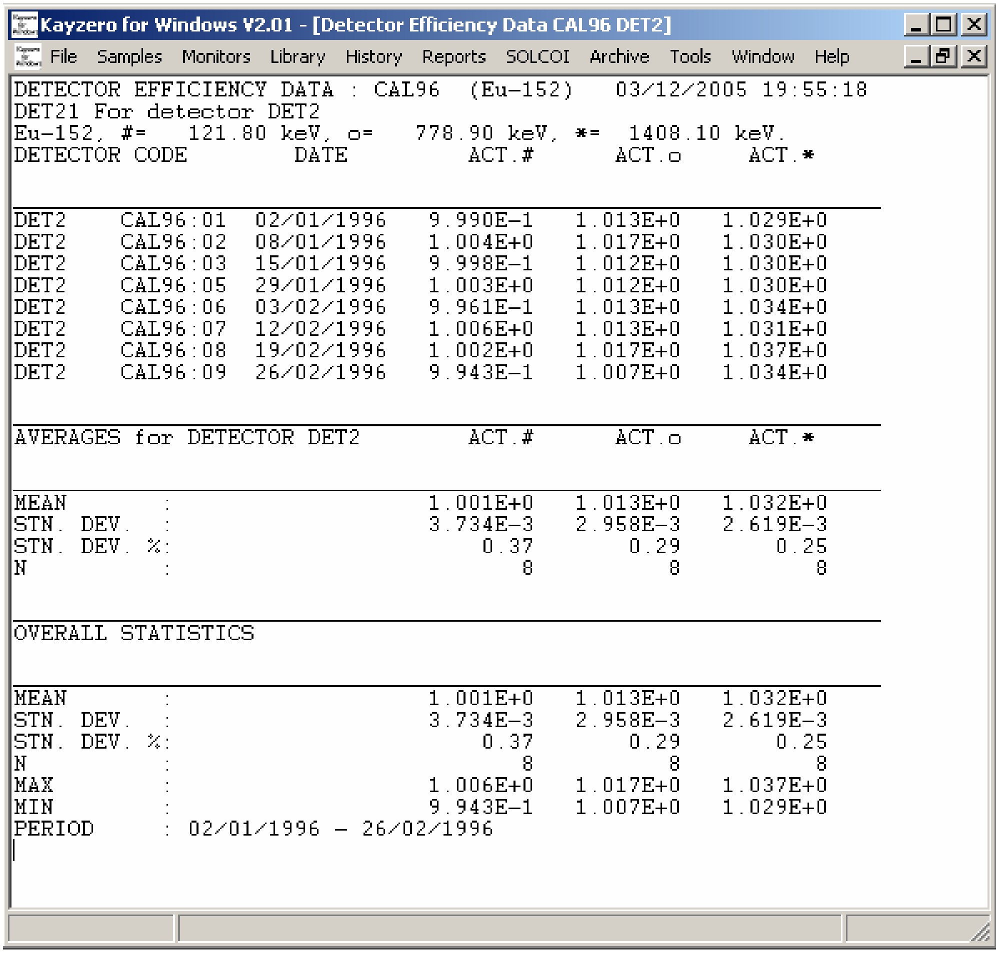
Detector: DET2

Measurement identification or "*": *

List type: Rel. activity

- ALL
- Rel. activity
- Absolute channel shift
- FWHM
- Background peak areas

Figure 5.4: Selecting the type of detector calibration output.



```
DETECTOR EFFICIENCY DATA : CAL96  (Eu-152)   03/12/2005 19:55:18
DET21 For detector DET2
Eu-152, #=   121.80 keV, o=   778.90 keV, *=  1408.10 keV.
DETECTOR CODE        DATE         ACT.#      ACT.o     ACT.*


DET2    CAL96:01  02/01/1996   9.990E-1   1.013E+0   1.029E+0
DET2    CAL96:02  08/01/1996   1.004E+0   1.017E+0   1.030E+0
DET2    CAL96:03  15/01/1996   9.998E-1   1.012E+0   1.030E+0
DET2    CAL96:05  29/01/1996   1.003E+0   1.012E+0   1.030E+0
DET2    CAL96:06  03/02/1996   9.961E-1   1.013E+0   1.034E+0
DET2    CAL96:07  12/02/1996   1.006E+0   1.013E+0   1.031E+0
DET2    CAL96:08  19/02/1996   1.002E+0   1.017E+0   1.037E+0
DET2    CAL96:09  26/02/1996   9.943E-1   1.007E+0   1.034E+0


AVERAGES for DETECTOR DET2        ACT.#      ACT.o     ACT.*


MEAN       :                   1.001E+0   1.013E+0   1.032E+0
STN. DEV.  :                   3.734E-3   2.958E-3   2.619E-3
STN. DEV. %:                       0.37       0.29       0.25
N          :                          8          8          8


OVERALL STATISTICS


MEAN       :                   1.001E+0   1.013E+0   1.032E+0
STN. DEV.  :                   3.734E-3   2.958E-3   2.619E-3
STN. DEV. %:                       0.37       0.29       0.25
N          :                          8          8          8
MAX        :                   1.006E+0   1.017E+0   1.037E+0
MIN        :                   9.943E-1   1.007E+0   1.029E+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.

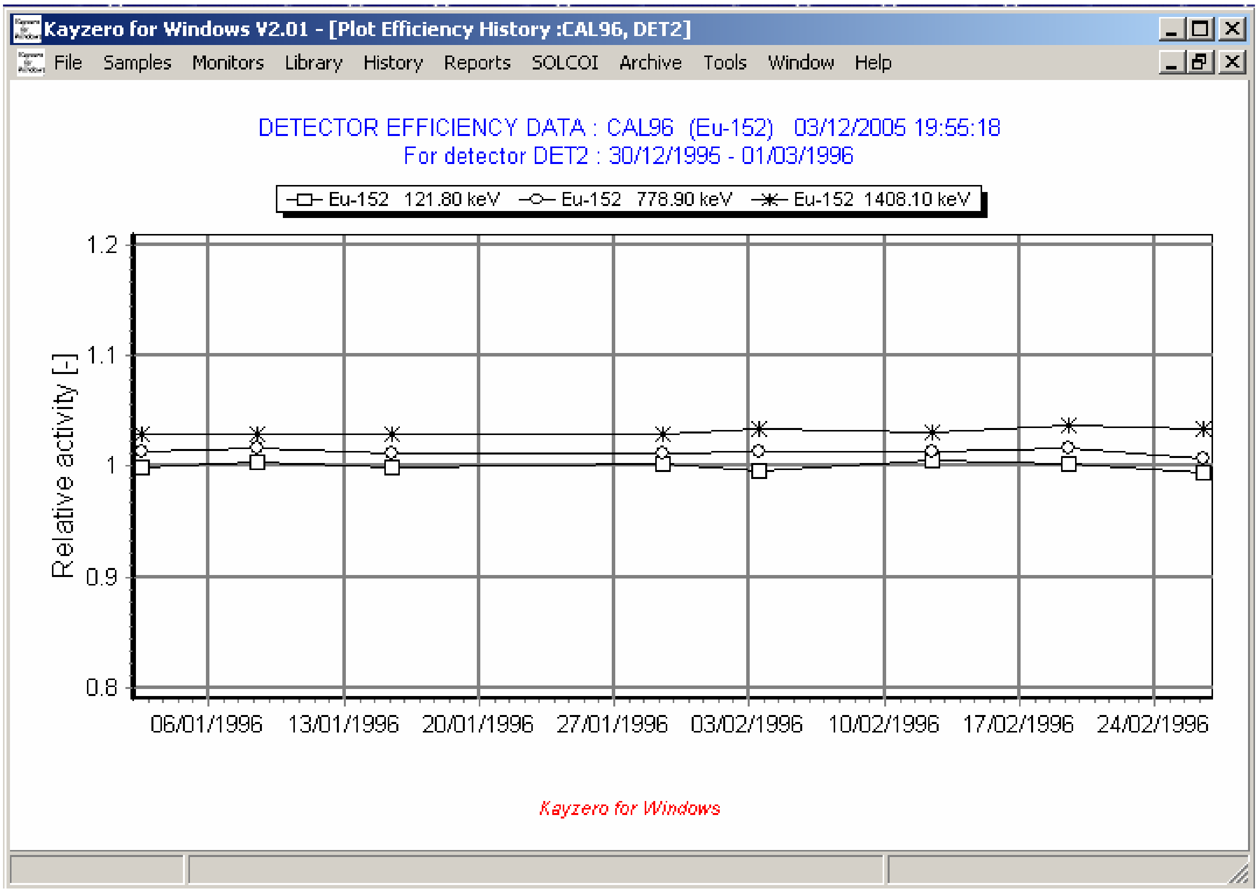


Figure 5.6: The plotted output of the relative activity of the detector calibration file CAL96 for DSM detector 2.

5.2 Comparator Factors

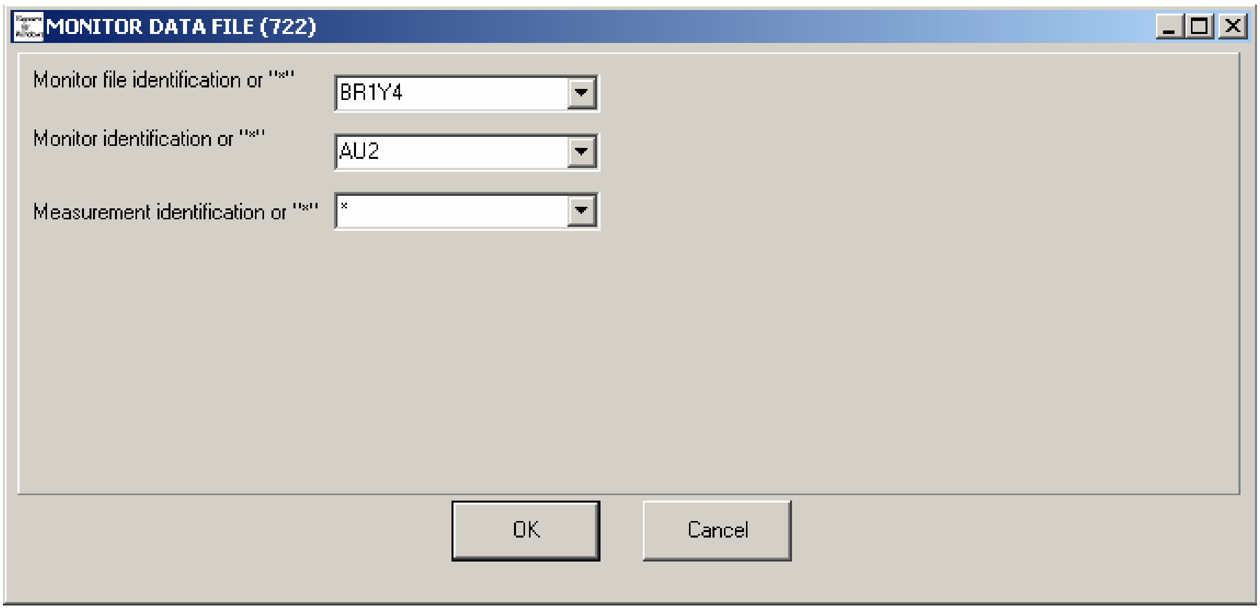
The comparator factor is a value proportional to the epithermal neutron flux and one of the three k_0-NAA reactor flux parameters.

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.

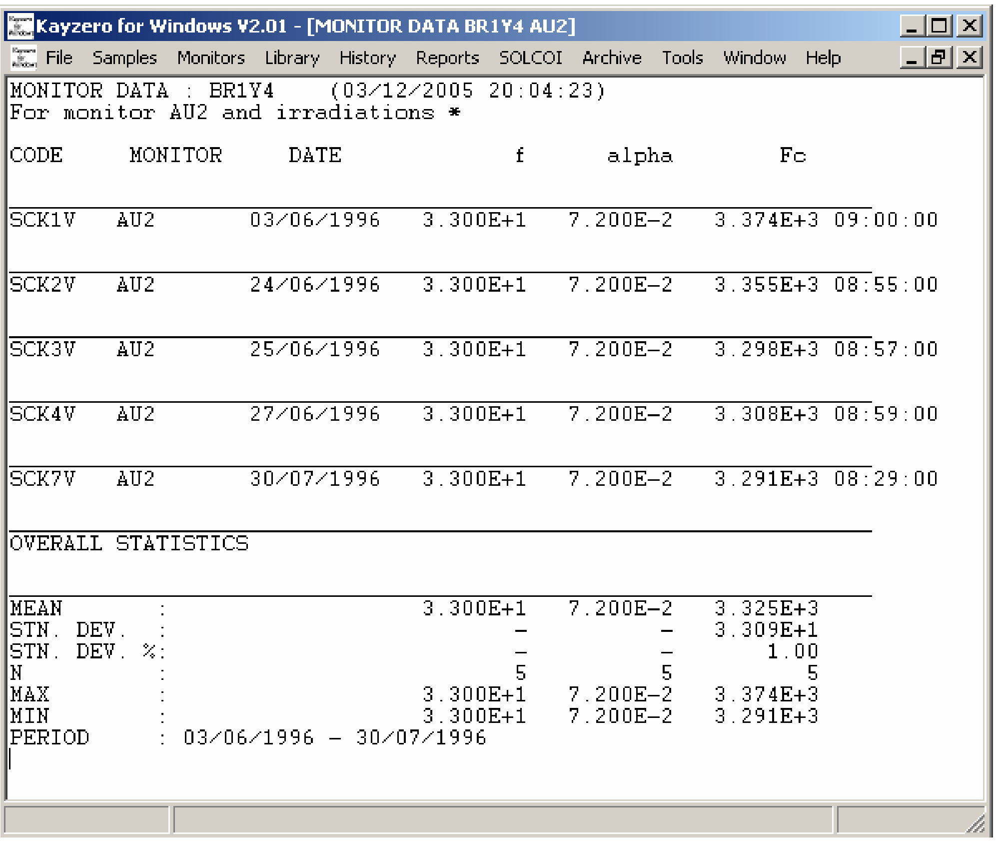


Monitor file identification or "*" BR1Y4

Monitor identification or "*" AU2

Measurement identification or "*" *

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



```
MONITOR DATA : BR1Y4     (03/12/2005 20:04:23)
For monitor AU2 and irradiations *

CODE      MONITOR      DATE              f        alpha          Fc

SCK1V    AU2         03/06/1996    3.300E+1    7.200E-2    3.374E+3 09:00:00

SCK2V    AU2         24/06/1996    3.300E+1    7.200E-2    3.355E+3 08:55:00

SCK3V    AU2         25/06/1996    3.300E+1    7.200E-2    3.298E+3 08:57:00

SCK4V    AU2         27/06/1996    3.300E+1    7.200E-2    3.308E+3 08:59:00

SCK7V    AU2         30/07/1996    3.300E+1    7.200E-2    3.291E+3 08:29:00

OVERALL STATISTICS

MEAN          :                    3.300E+1    7.200E-2    3.325E+3
STN. DEV.     :                           -           -    3.309E+1
STN. DEV. %:                              -           -        1.00
N             :                           5           5           5
MAX           :                    3.300E+1    7.200E-2    3.374E+3
MIN           :                    3.300E+1    7.200E-2    3.291E+3
PERIOD        :  03/06/1996 - 30/07/1996
```

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

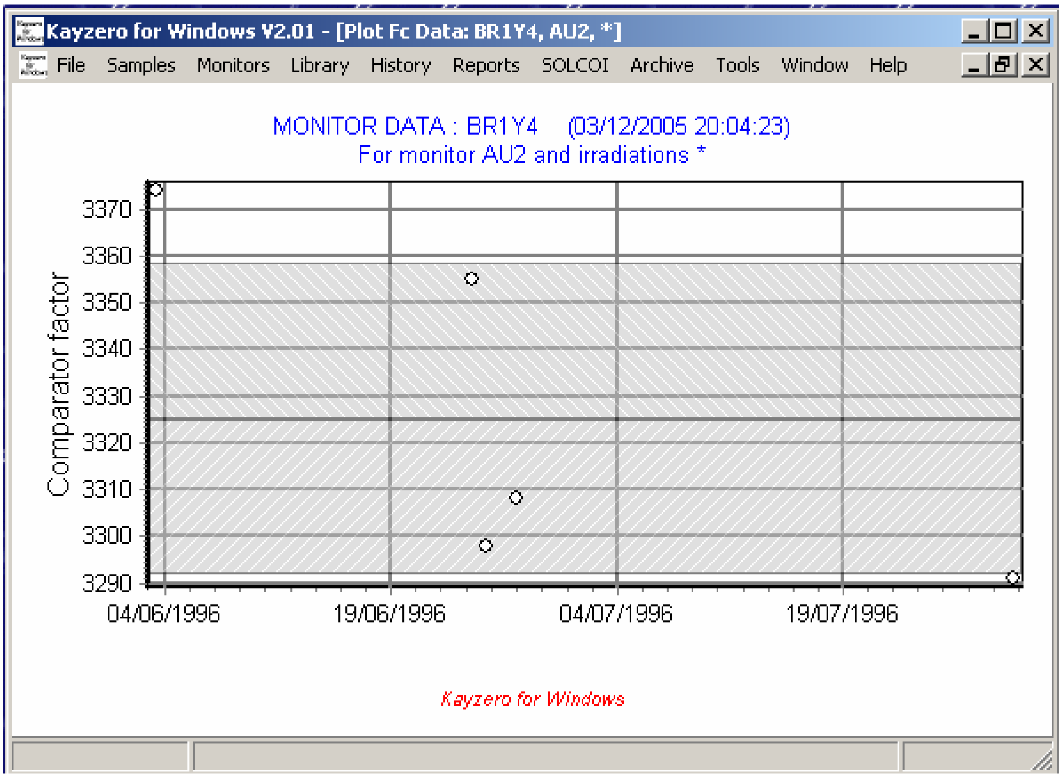


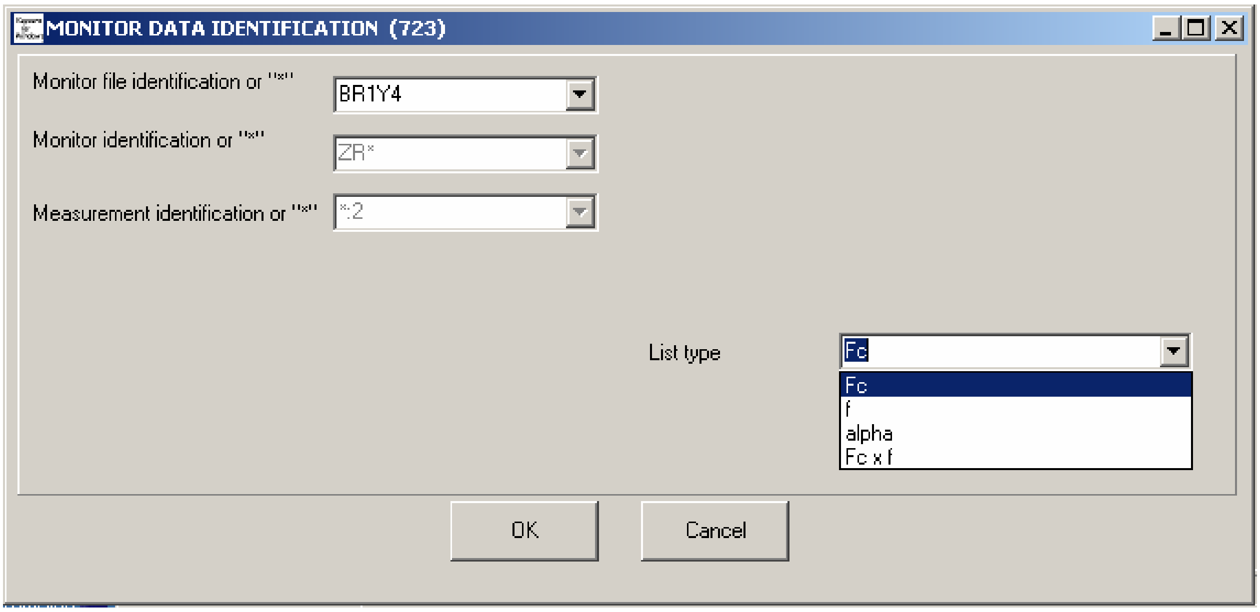
Figure 5.9: Plotted output of *History/Comparator Factors* for BR1Y4.

5.3 Reactor Calibration Data

The reactor flux parameters Fc, f and α 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 "*": BR1Y4

Monitor identification or "*": ZR*

Measurement identification or "*": *:2

List type: Fc

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 α 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 Fc, f and α values.

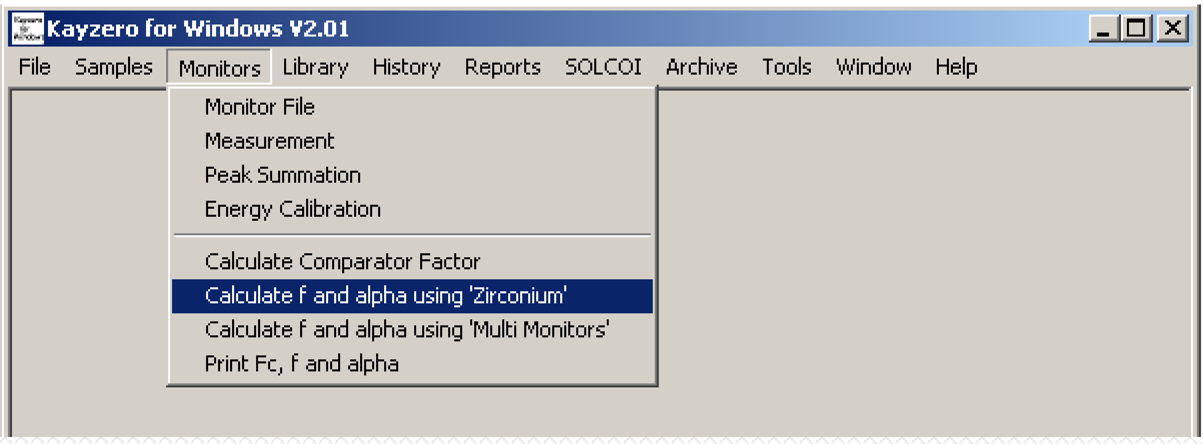
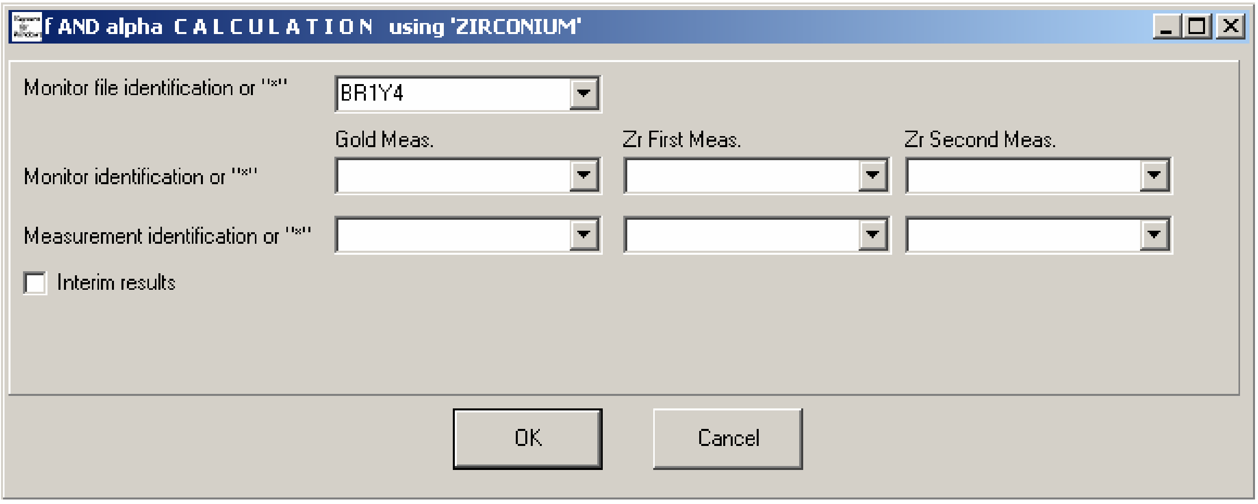


Figure 6.1: Monitor Analysis Menu.

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.



Monitor file identification or "*": BR1Y4

Gold Meas.

Zr First Meas.

Zr Second Meas.

Monitor identification or "*"

Measurement identification or "*"

☐ Interim results

Figure 6.2: Zirconium-method calculation screen.

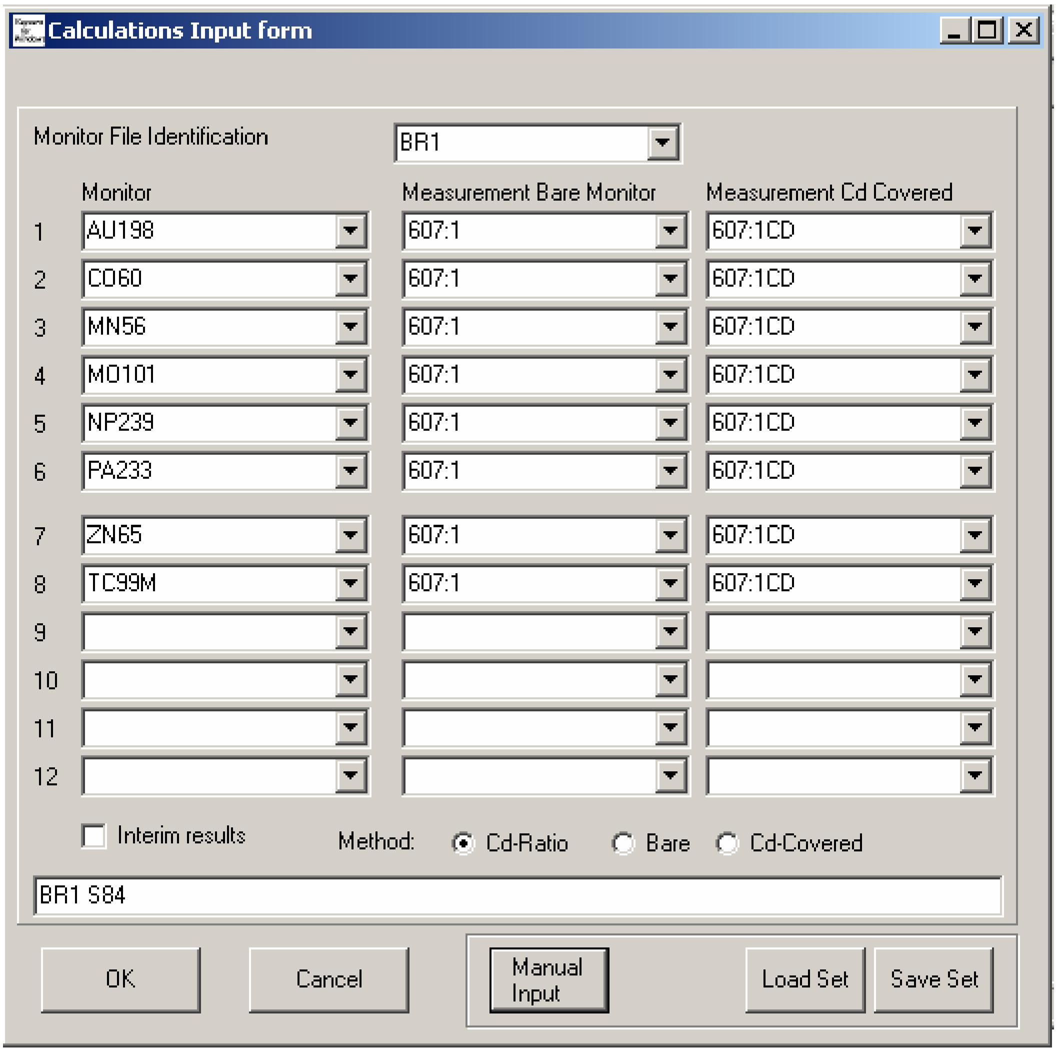
The data for these measurements should be entered using *Monitors/Measurement*-option and can then be used for f and α calculation using this screen (see Figure 6.2). The result of the f and α calculation will be displayed with the calculated values. They are stored in the data record of the second Zirconium 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 Fc, f and α 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)[1].

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: BR1

	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	MO101	607:1	607:1CD
5	NP239	607:1	607:1CD
6	PA233	607:1	607:1CD
7	ZN65	607:1	607:1CD
8	TC99M	607:1	607:1CD
9			
10			
11			
12			

☐ Interim results

Method: ● Cd-Ratio ○ Bare ○ Cd-Covered

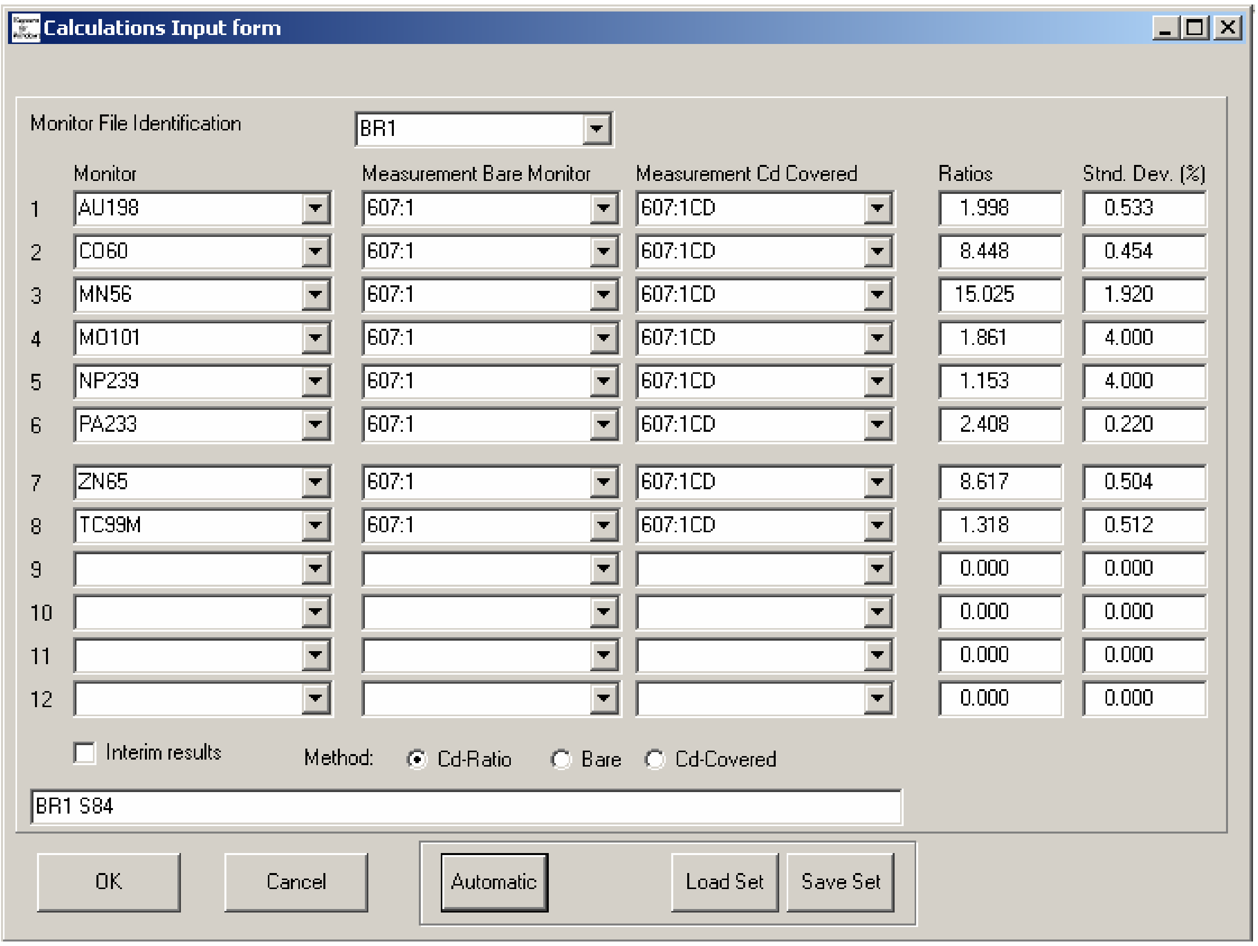
BR1 S84

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.



Monitor File Identification: BR1

	Monitor	Measurement Bare Monitor	Measurement Cd Covered	Ratios	Stnd. Dev. (%)
1	AU198	607:1	607:1CD	1.998	0.533
2	CO60	607:1	607:1CD	8.448	0.454
3	MN56	607:1	607:1CD	15.025	1.920
4	MO101	607:1	607:1CD	1.861	4.000
5	NP239	607:1	607:1CD	1.153	4.000
6	PA233	607:1	607:1CD	2.408	0.220
7	ZN65	607:1	607:1CD	8.617	0.504
8	TC99M	607:1	607:1CD	1.318	0.512
9				0.000	0.000
10				0.000	0.000
11				0.000	0.000
12				0.000	0.000

☐ Interim results

Method: ● Cd-Ratio ○ Bare ○ Cd-Covered

BR1 S84

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).

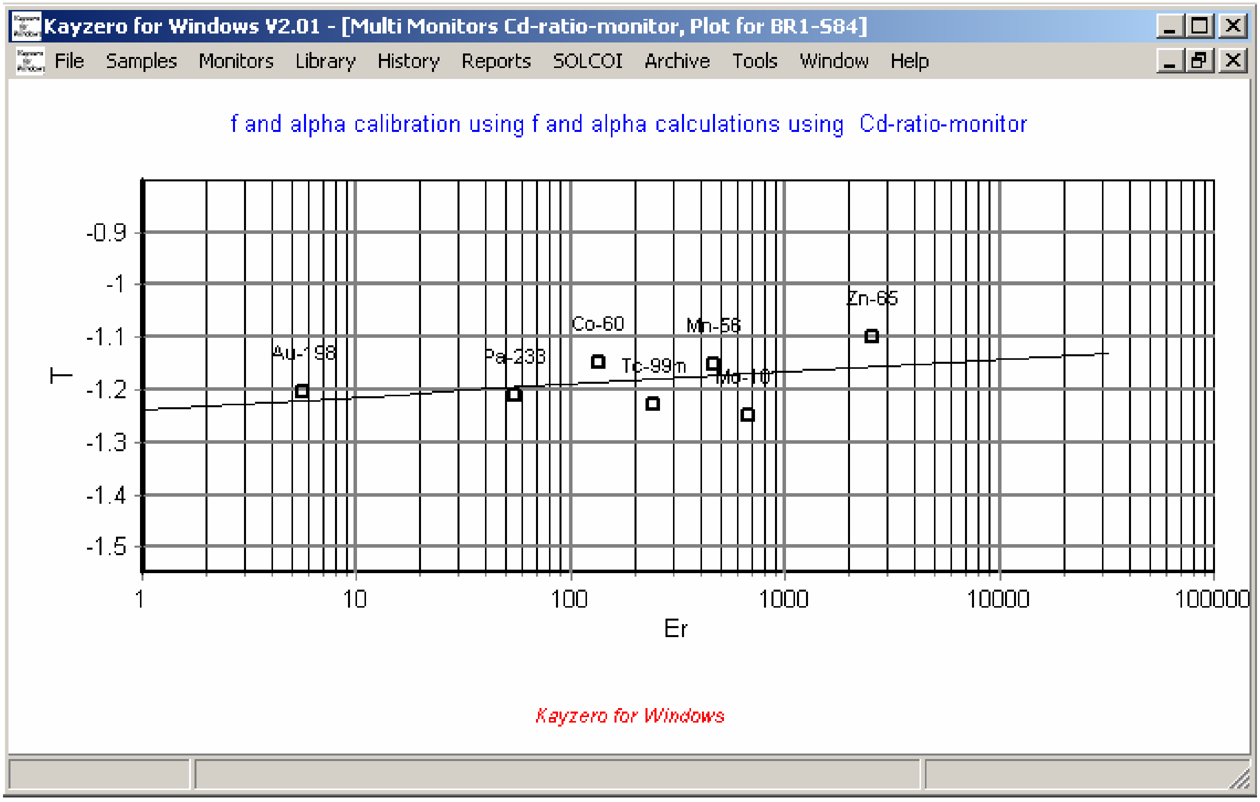
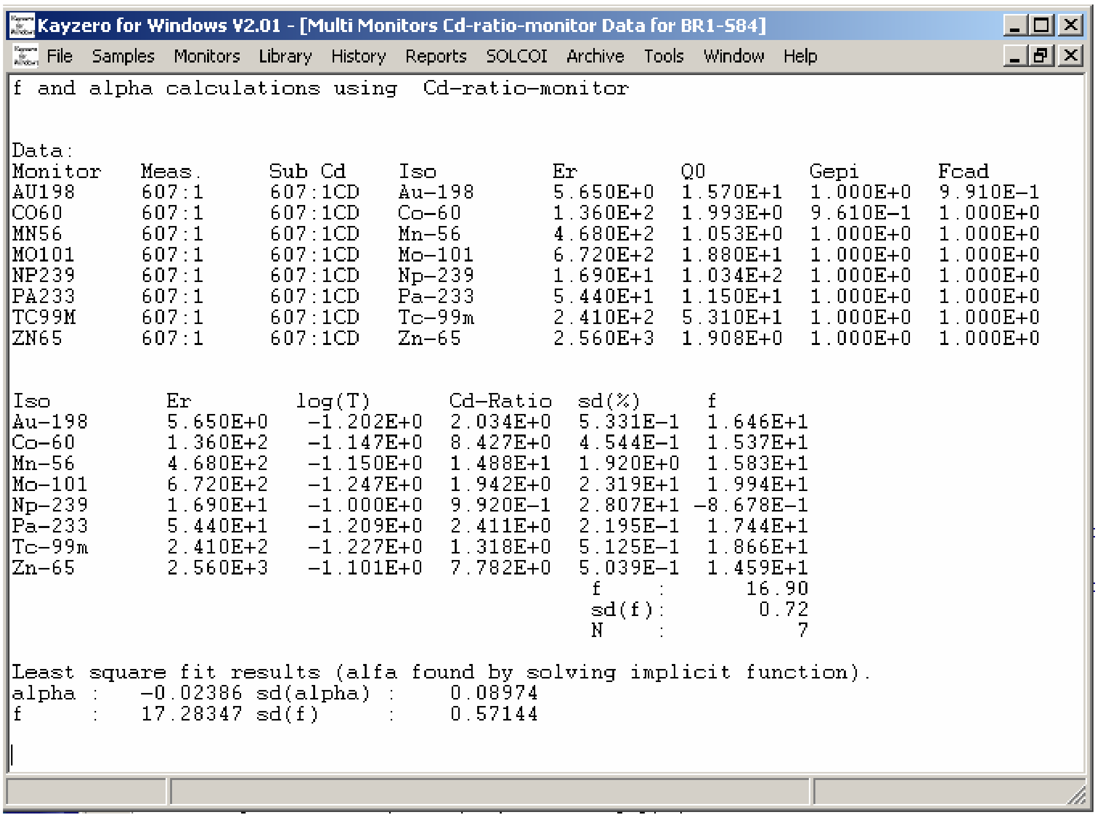


Figure 6.5: Plot of Cd-ratio multi monitor f and alpha determination result.



```
f and alpha calculations using  Cd-ratio-monitor


Data:
Monitor     Meas.       Sub Cd      Iso          Er          Q0          Gepi        Fcad
AU198       607:1       607:1CD     Au-198       5.650E+0    1.570E+1    1.000E+0    9.910E-1
CO60        607:1       607:1CD     Co-60        1.360E+2    1.993E+0    9.610E-1    1.000E+0
MN56        607:1       607:1CD     Mn-56        4.680E+2    1.053E+0    1.000E+0    1.000E+0
MO101       607:1       607:1CD     Mo-101       6.720E+2    1.880E+1    1.000E+0    1.000E+0
NP239       607:1       607:1CD     Np-239       1.690E+1    1.034E+2    1.000E+0    1.000E+0
PA233       607:1       607:1CD     Pa-233       5.440E+1    1.150E+1    1.000E+0    1.000E+0
TC99M       607:1       607:1CD     Tc-99m       2.410E+2    5.310E+1    1.000E+0    1.000E+0
ZN65        607:1       607:1CD     Zn-65        2.560E+3    1.908E+0    1.000E+0    1.000E+0


Iso          Er          log(T)      Cd-Ratio   sd(%)       f
Au-198       5.650E+0     -1.202E+0  2.034E+0   5.331E-1    1.646E+1
Co-60        1.360E+2     -1.147E+0  8.427E+0   4.544E-1    1.537E+1
Mn-56        4.680E+2     -1.150E+0  1.488E+1   1.920E+0    1.583E+1
Mo-101       6.720E+2     -1.247E+0  1.942E+0   2.319E+1    1.994E+1
Np-239       1.690E+1     -1.000E+0  9.920E-1   2.807E+1   -8.678E-1
Pa-233       5.440E+1     -1.209E+0  2.411E+0   2.195E-1    1.744E+1
Tc-99m       2.410E+2     -1.227E+0  1.318E+0   5.125E-1    1.866E+1
Zn-65        2.560E+3     -1.101E+0  7.782E+0   5.039E-1    1.459E+1
                                                 f     :       16.90
                                                 sd(f):         0.72
                                                 N     :           7

Least square fit results (alfa found by solving implicit function).
alpha  :    -0.02386 sd(alpha)  :     0.08974
f      :    17.28347 sd(f)      :     0.57144
```

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.

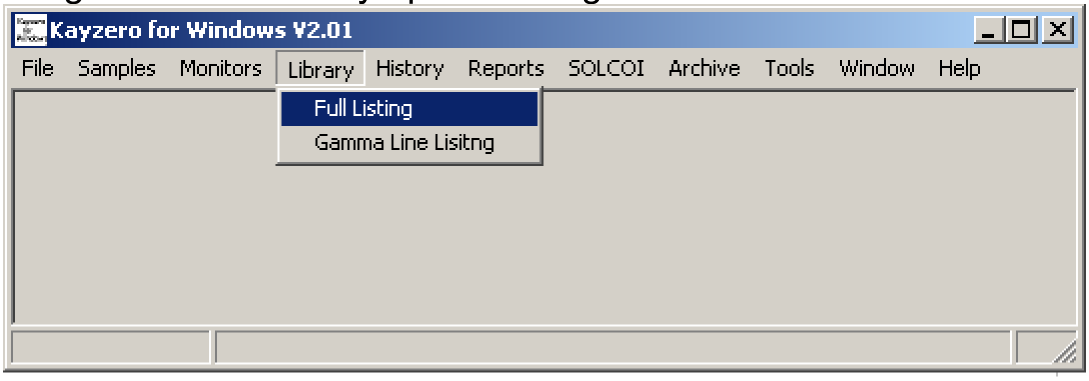


Figure 6.7: Kayzero Library menu.

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 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).

6.3 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.

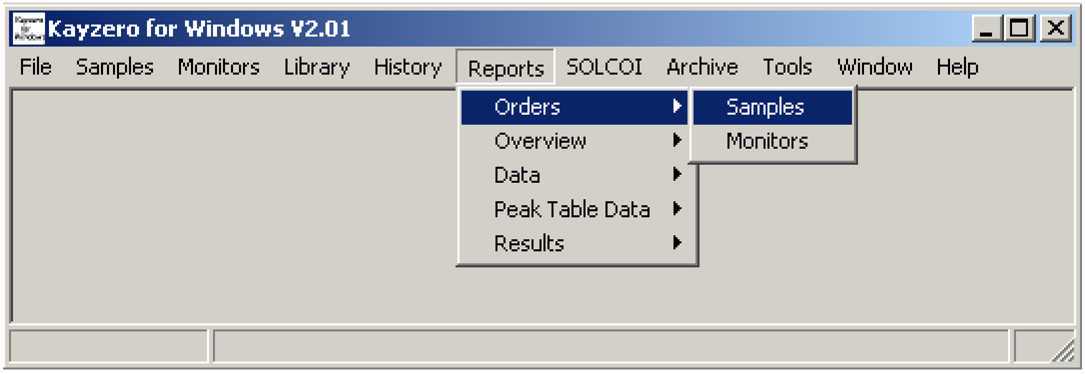
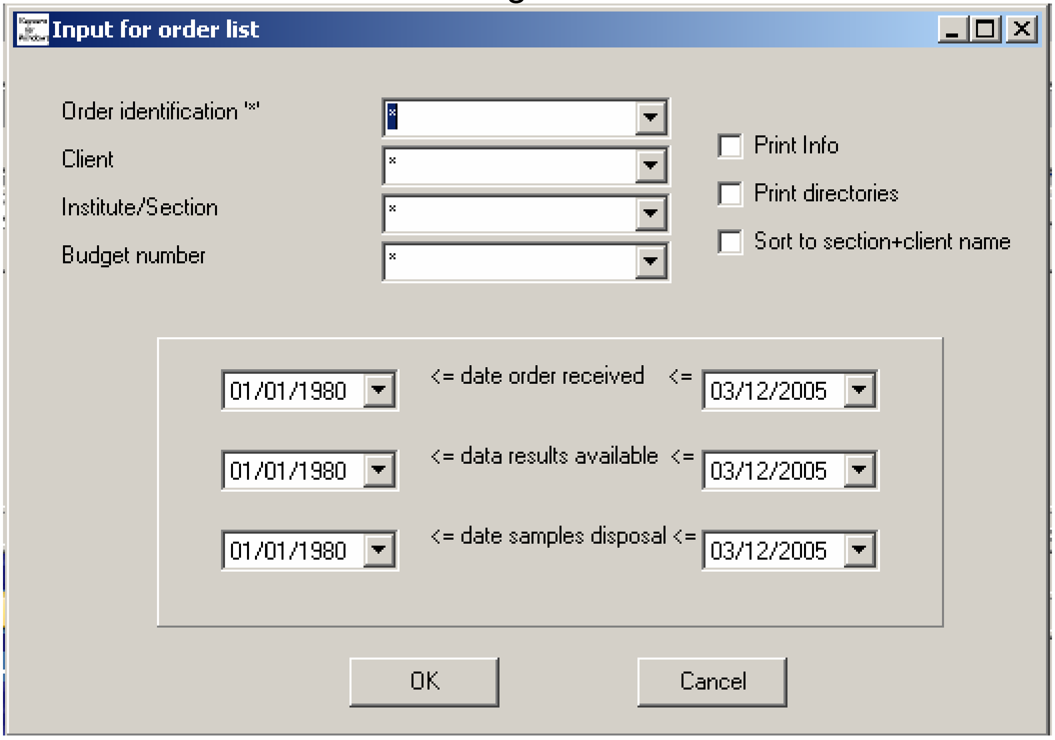


Figure 6.8: The Reports Menu

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.



Order identification "*" *
Client *
Institute/Section *
Budget number *

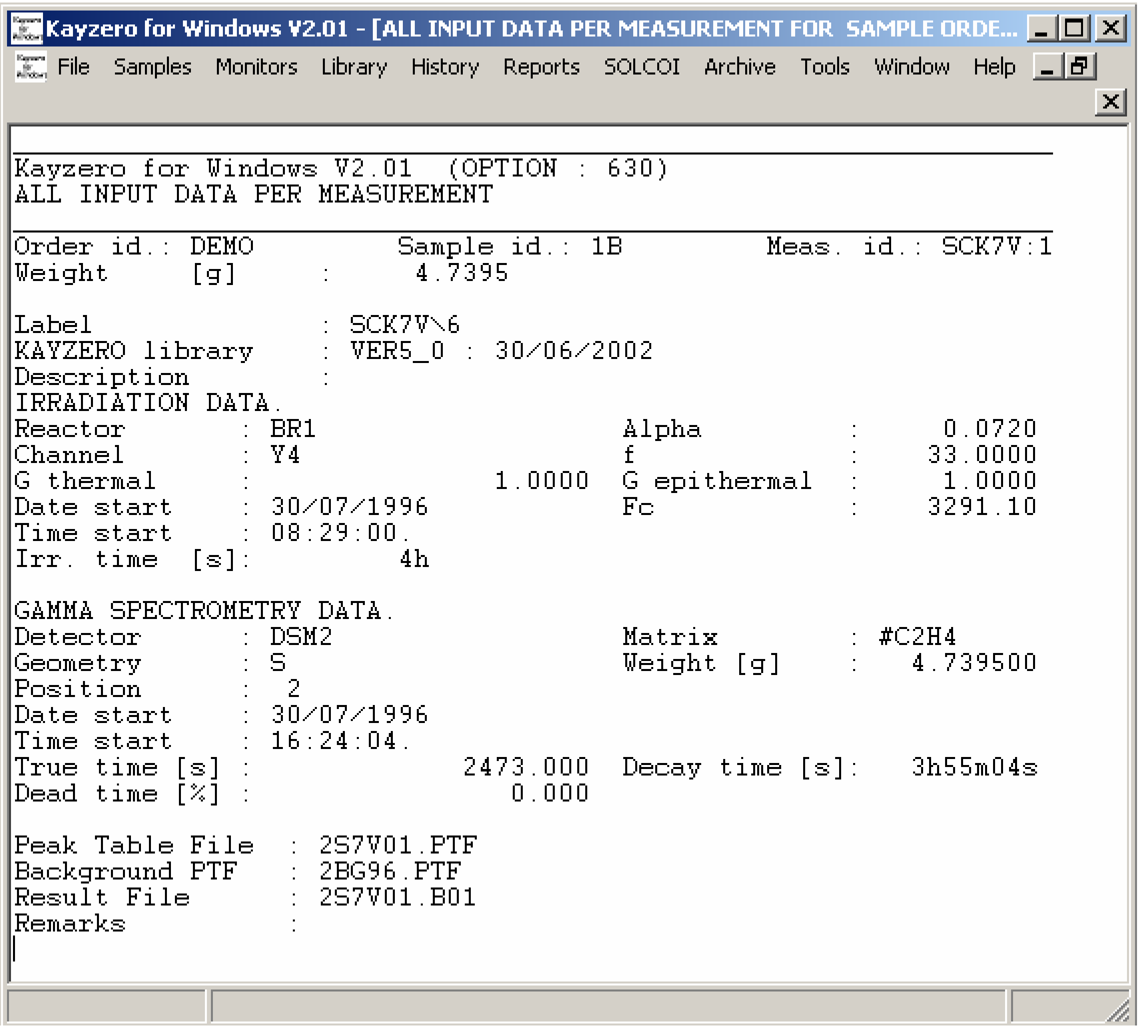
☐ Print Info
☐ Print directories
☐ Sort to section+client name

01/01/1980 <= date order received <= 03/12/2005
01/01/1980 <= data results available <= 03/12/2005
01/01/1980 <= date samples disposal <= 03/12/2005

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.

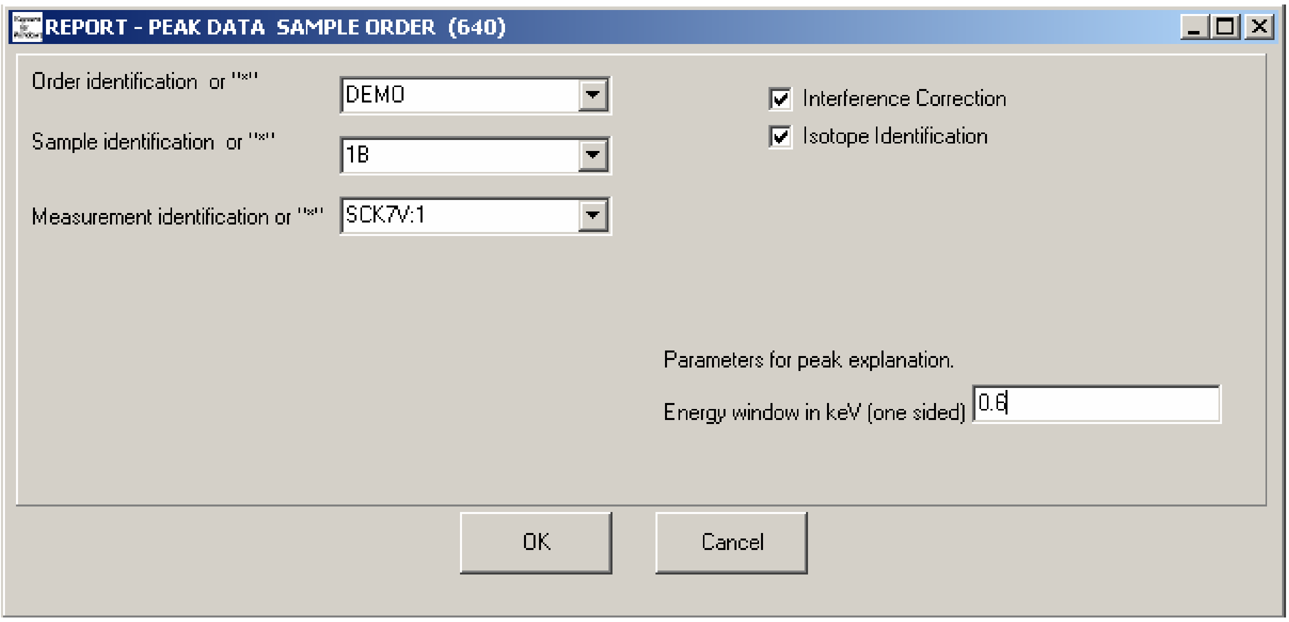
Per measurement a print can be made with all entered data, *Reports/Data*, see Figure 6.10.



```
Kayzero for Windows V2.01  (OPTION : 630)
ALL INPUT DATA PER MEASUREMENT

Order id.: DEMO          Sample id.: 1B          Meas. id.: SCK7V:1
Weight     [g]      :      4.7395

Label               : SCK7V\6
KAYZERO library     : VER5_0 : 30/06/2002
Description         :
IRRADIATION DATA.
Reactor        : BR1                     Alpha          :      0.0720
Channel        : Y4                      f              :     33.0000
G thermal      :                1.0000   G epithermal   :      1.0000
Date start     : 30/07/1996              Fc             :     3291.10
Time start     : 08:29:00.
Irr. time  [s]:         4h

GAMMA SPECTROMETRY DATA.
Detector       : DSM2                    Matrix         : #C2H4
Geometry       : S                       Weight  [g]    :    4.739500
Position       :  2
Date start     : 30/07/1996
Time start     : 16:24:04.
True time [s]  :              2473.000   Decay time [s]:    3h55m04s
Dead time [%]  :                 0.000

Peak Table File   : 2S7V01.PTF
Background PTF    : 2BG96.PTF
Result File       : 2S7V01.B01
Remarks           :
```

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

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.



Order identification or "*" DEMO

Sample identification or "*" 1B

Measurement identification or "*" SCK7V:1

☑ Interference Correction

☑ Isotope Identification

Parameters for peak explanation.

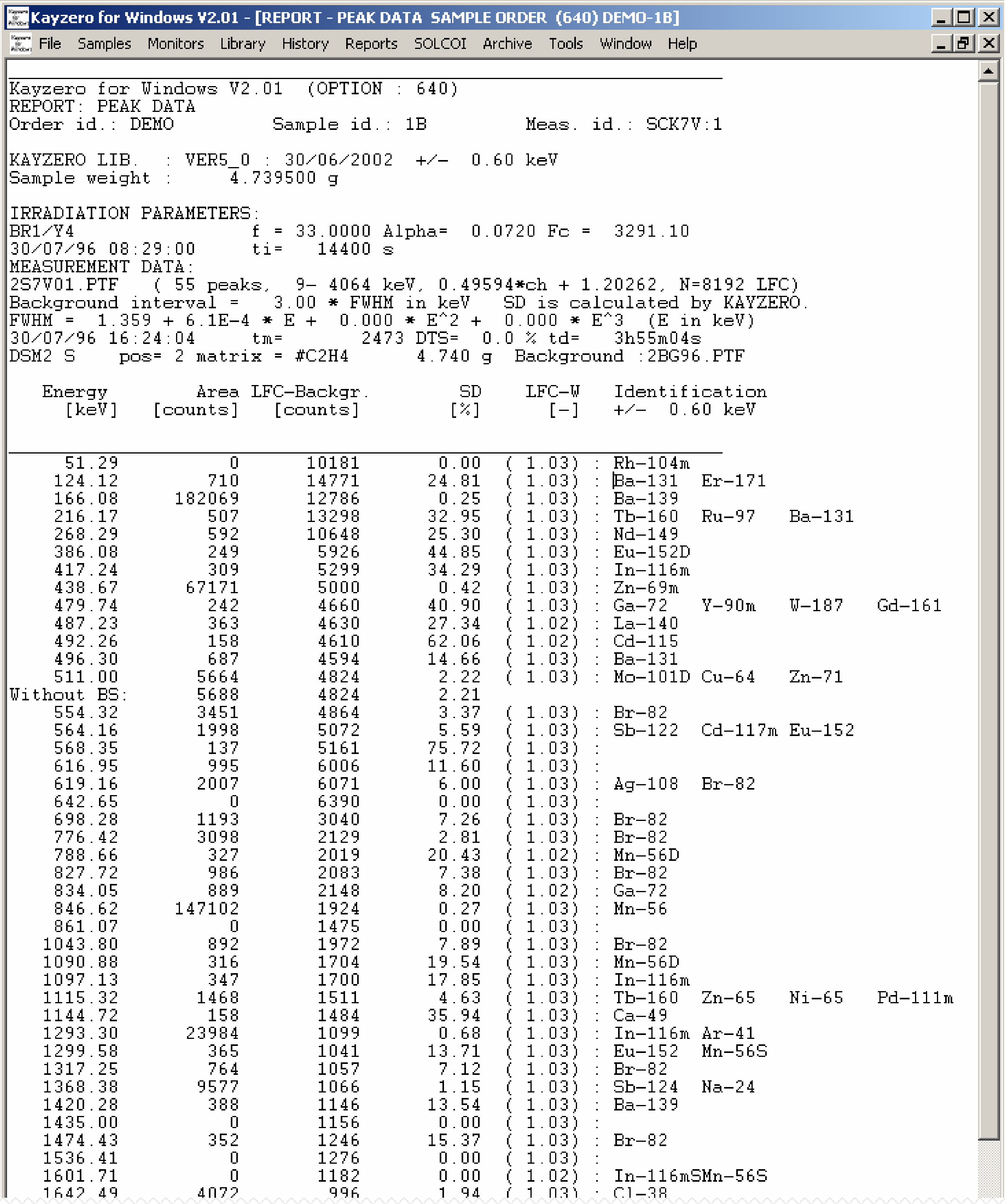
Energy window in keV (one sided) 0.6

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 V2.01  (OPTION : 640)
REPORT: PEAK DATA
Order id.: DEMO         Sample id.: 1B         Meas. id.: SCK7V:1

KAYZERO LIB.  : VER5_0 : 30/06/2002  +/-  0.60 keV
Sample weight :      4.739500 g

IRRADIATION PARAMETERS:
BR1/Y4                 f = 33.0000 Alpha=  0.0720 Fc =  3291.10
30/07/96 08:29:00      ti=   14400 s
MEASUREMENT DATA:
2S7V01.PTF   ( 55 peaks,  9- 4064 keV, 0.49594*ch + 1.20262, 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        Area LFC-Backgr.        SD    LFC-W   Identification
     [keV]   [counts]   [counts]        [%]      [-]   +/-  0.60 keV

     51.29          0      10181       0.00  ( 1.03) : Rh-104m
    124.12        710      14771      24.81  ( 1.03) : Ba-131  Er-171
    166.08     182069      12786       0.25  ( 1.03) : Ba-139
    216.17        507      13298      32.95  ( 1.03) : Tb-160  Ru-97   Ba-131
    268.29        592      10648      25.30  ( 1.03) : Nd-149
    386.08        249       5926      44.85  ( 1.03) : Eu-152D
    417.24        309       5299      34.29  ( 1.03) : In-116m
    438.67      67171       5000       0.42  ( 1.03) : Zn-69m
    479.74        242       4660      40.90  ( 1.03) : Ga-72   Y-90m   W-187   Gd-161
    487.23        363       4630      27.34  ( 1.02) : La-140
    492.26        158       4610      62.06  ( 1.02) : Cd-115
    496.30        687       4594      14.66  ( 1.03) : Ba-131
    511.00       5664       4824       2.22  ( 1.03) : Mo-101D Cu-64   Zn-71
Without BS:      5688       4824       2.21
    554.32       3451       4864       3.37  ( 1.03) : Br-82
    564.16       1998       5072       5.59  ( 1.03) : Sb-122  Cd-117m Eu-152
    568.35        137       5161      75.72  ( 1.03) :
    616.95        995       6006      11.60  ( 1.03) :
    619.16       2007       6071       6.00  ( 1.03) : Ag-108  Br-82
    642.65          0       6390       0.00  ( 1.03) :
    698.28       1193       3040       7.26  ( 1.03) : Br-82
    776.42       3098       2129       2.81  ( 1.03) : Br-82
    788.66        327       2019      20.43  ( 1.02) : Mn-56D
    827.72        986       2083       7.38  ( 1.03) : Br-82
    834.05        889       2148       8.20  ( 1.02) : Ga-72
    846.62     147102       1924       0.27  ( 1.03) : Mn-56
    861.07          0       1475       0.00  ( 1.03) :
   1043.80        892       1972       7.89  ( 1.03) : Br-82
   1090.88        316       1704      19.54  ( 1.03) : Mn-56D
   1097.13        347       1700      17.85  ( 1.03) : In-116m
   1115.32       1468       1511       4.63  ( 1.03) : Tb-160  Zn-65   Ni-65   Pd-111m
   1144.72        158       1484      35.94  ( 1.03) : Ca-49
   1293.30      23984       1099       0.68  ( 1.03) : In-116m Ar-41
   1299.58        365       1041      13.71  ( 1.03) : Eu-152  Mn-56S
   1317.25        764       1057       7.12  ( 1.03) : Br-82
   1368.38       9577       1066       1.15  ( 1.03) : Sb-124  Na-24
   1420.28        388       1146      13.54  ( 1.03) : Ba-139
   1435.00          0       1156       0.00  ( 1.03) :
   1474.43        352       1246      15.37  ( 1.03) : Br-82
   1536.41          0       1276       0.00  ( 1.03) :
   1601.71          0       1182       0.00  ( 1.02) : In-116mSMn-56S
   1642.49       4072        996       1.94  ( 1.03) : Cl-38
```

Figure 6.12: A print of a peak table file

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).

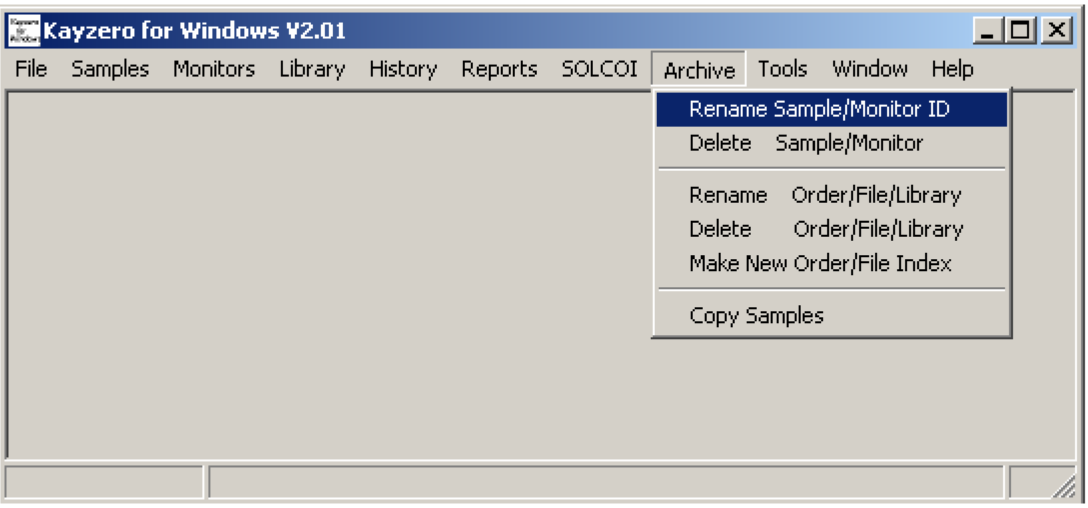


Figure 6.13: Archive menu.

6.5 Special Options Menu

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

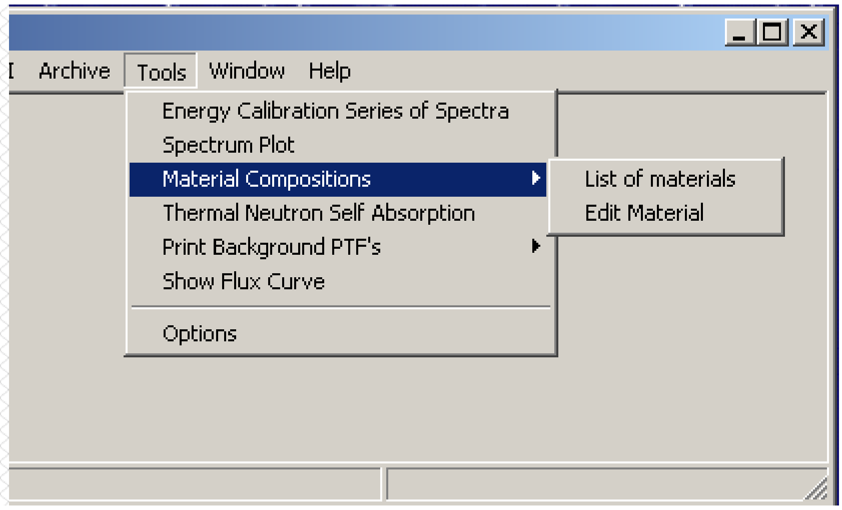
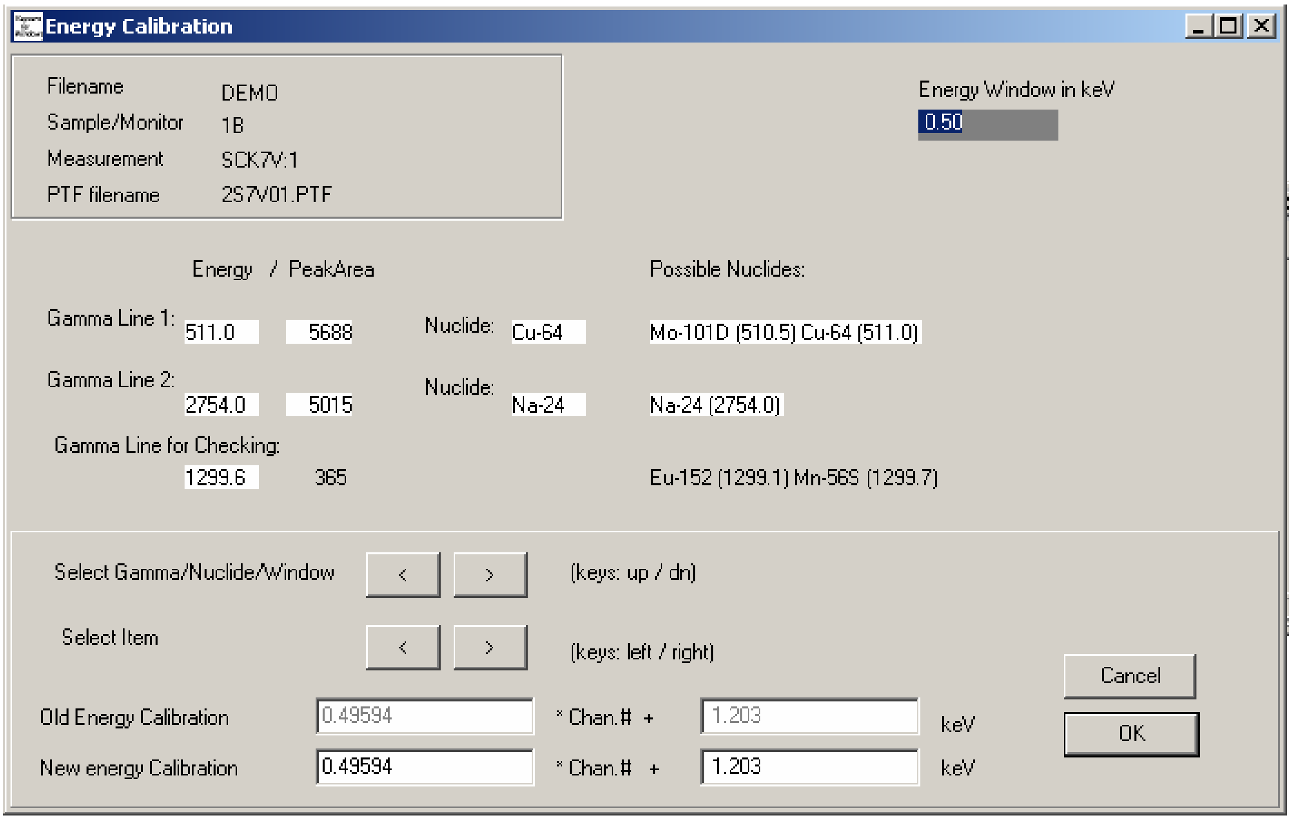


Figure 6.14: Tools

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.



Filename DEMO
Sample/Monitor 1B
Measurement SCK7V:1
PTF filename 2S7V01.PTF

Energy Window in keV 0.50

	Energy	PeakArea	Nuclide:	Possible Nuclides:
Gamma Line 1:	511.0	5688	Cu-64	Mo-101D (510.5) Cu-64 (511.0)
Gamma Line 2:	2754.0	5015	Na-24	Na-24 (2754.0)
Gamma Line for Checking:	1299.6	365		Eu-152 (1299.1) Mn-56S (1299.7)

Old Energy Calibration 0.49594 * Chan.# + 1.203 keV
New energy Calibration 0.49594 * Chan.# + 1.203 keV

Figure 6.15: Energy calibration

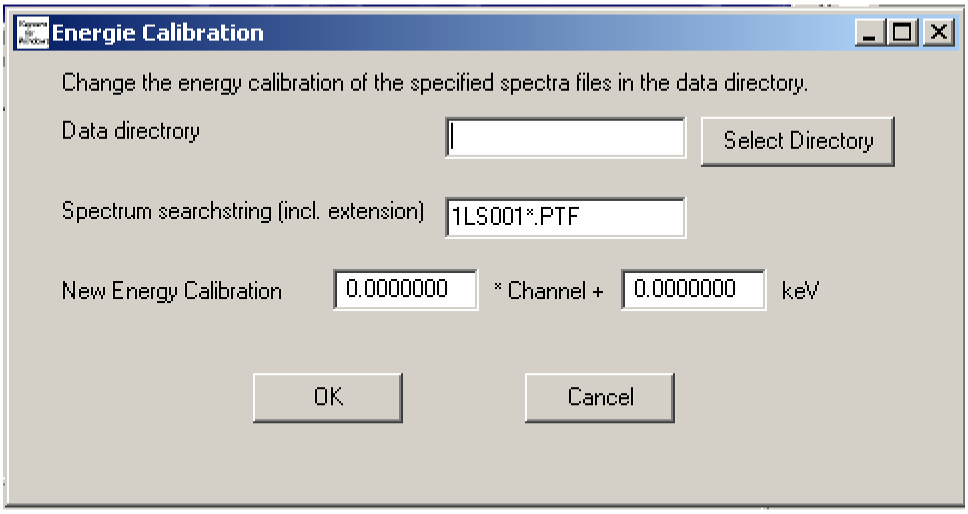
It is advised to perform an energy calibration at least once a week or to perform an energy calibration on every spectrum using this option. For the energy calibration a first-order approximation (E = a.Ch+b) is used.

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 <↑> and <↓> . If you press <→> the first energy is activated. By pressing <↑>, a higher energy can be selected. When a good peak is found, press <→> again; the corresponding radioisotope can then be selected from the list using <↑> and <↓>.

In short, to move to another field you should use <←> and <→> and to select another energy or isotope you should use <↑> and <↓>. 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 <Select Directory> can be used to find a specific directorie. 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.


Change the energy calibration of the specified spectra files in the data directory.

Data directory

Spectrum searchstring (incl. extension) 1LS001*.PTF

New Energy Calibration 0.0000000 * Channel + 0.0000000 keV

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

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 loose peaks. However it is also nice to see how many peaks you have spread over the spectrum.

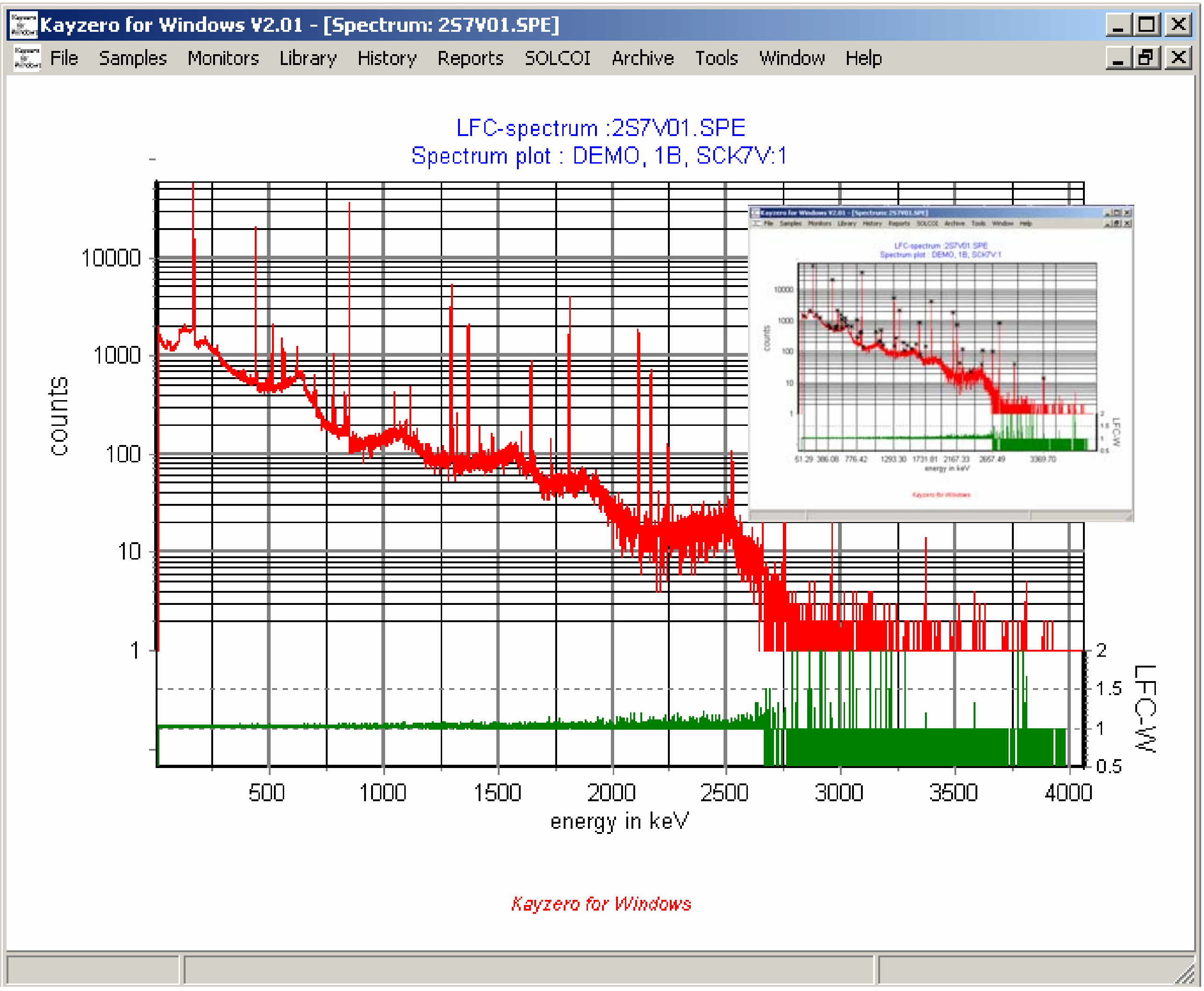
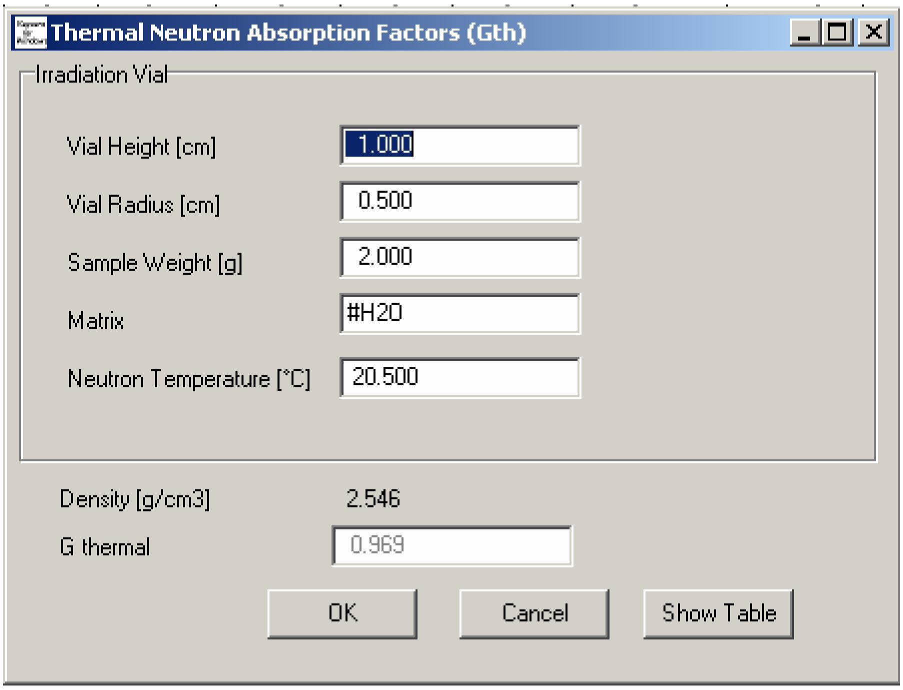


Figure 6.17: Spectrum plot (‘In set’: by clicking on the spectrum the found peaks are marked with an ‘x’).

6.5.3 Thermal neutron self-shielding

Thermal neutron self-shielding is handled in accordance with Erdtmann and Petri[5], see also figure 6.18. You can print a table if you like.



Vial Height [cm] 1.000
Vial Radius [cm] 0.500
Sample Weight [g] 2.000
Matrix #H2O
Neutron Temperature [°C] 20.500
Density [g/cm3] 2.546
G thermal 0.969

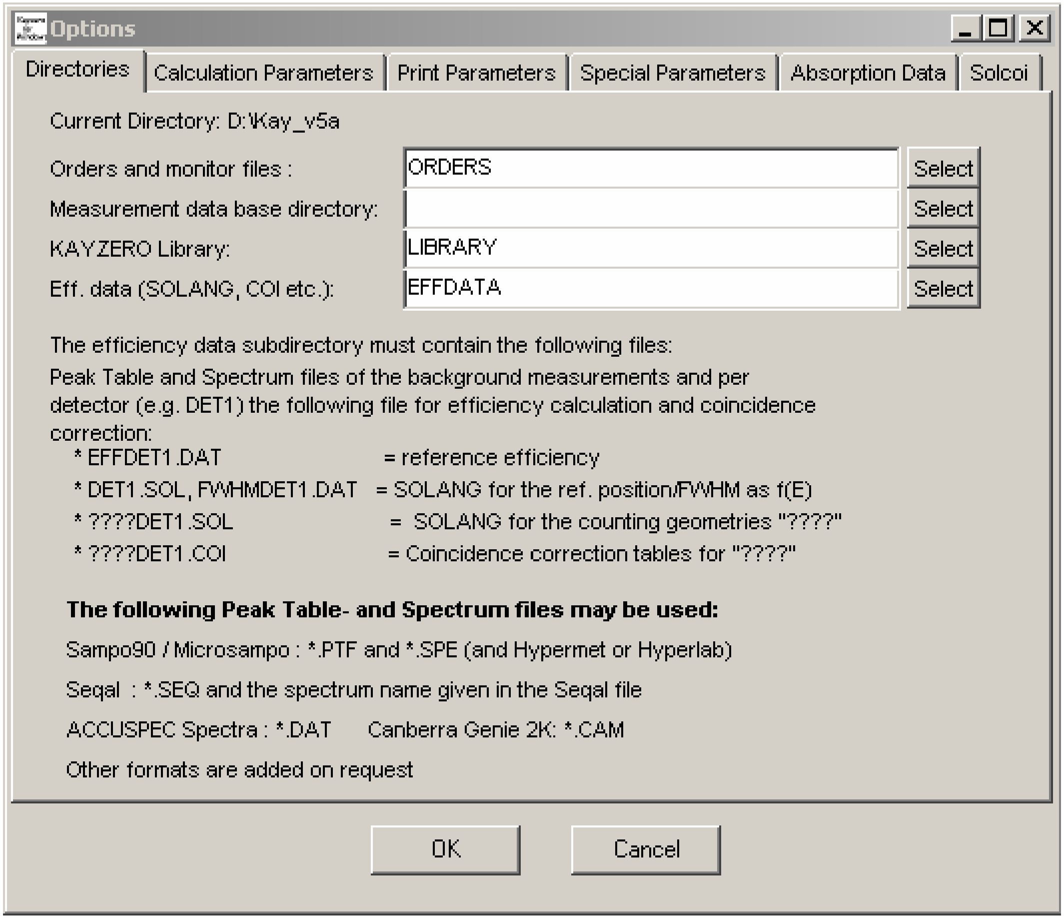
Figure 6.18 : Neutron thermal self-shielding option, input and result.

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).



Current Directory: D:\Kay_v5a

Orders and monitor files : ORDERS
Measurement data base directory:
KAYZERO Library: LIBRARY
Eff. data (SOLANG, COI etc.): EFFDATA

The efficiency data subdirectory must contain the following files:
Peak Table and Spectrum files of the background measurements and per detector (e.g. DET1) the following file for efficiency calculation and coincidence correction:

* EFFDET1.DAT = reference efficiency
* DET1.SOL, FWHMDET1.DAT = SOLANG for the ref. position/FWHM as f(E)
* ????DET1.SOL = SOLANG for the counting geometries "????"
* ????DET1.COI = Coincidence correction tables for "????"

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

Sampo90 / Microsampo : *.PTF and *.SPE (and Hypermet or Hyperlab)

Seqal : *.SEQ and the spectrum name given in the Seqal file

ACCUSPEC Spectra : *.DAT Canberra Genie 2K: *.CAM

Other formats are added on request

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

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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, Ω) and COI (coincidence correction) tables are precalculated 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:

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

where Ω and Ω_{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.

KAYZERO.DAT and SOLCOI.STA
: are status program specific system files.
KAYZERO.IRR:
: f, α 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
: Gaus-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: e_0 e_1 e_2 e_{ne}
<11> <22> <33> <44> <55>
3: o_1 o_2 o_{ne}
<1-----10> <16-----25> <31-----40> <46-----55> <61-----70>>
4: $p_{1,0}$ $p_{1,1}$ $p_{1,2}$ $p_{1,o1}$ $p_{2,0}$
5: $p_{2,1}$ $p_{2,2}$ $p_{2,3}$ $p_{2,n2}$ p_3
6: $p_{3,1}$ $p_{3,2}$ $p_{3,3}$ $p_{3,n3}$

where:
ne = number of energy regions (max. 4)
$e_{0...ne}$ = energy of the beginning and/or end of a region
$o_{1..ne}$ = order of the fits (max. 3)
$p_{i,j}$ = parameter for region i and order j.

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: e_0 e_1 e_2 e_{ne}
3: o_1 o_2 o_{ne}
4: $p_{1,0}$ $p_{1,1}$ $p_{1,2}$ $p_{1,o1}$ $p_{2,0}$
5: $p_{2,1}$ $p_{2,2}$ $p_{2,3}$ $p_{2,n2}$ $p_{3,0}$
6: $p_{3,1}$ $p_{3,2}$ $p_{3,3}$ $p_{3,n3}$
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)}
 1.00000000000000E+0000                {density in g/cm3}
 7.21419629006732E-0002                {volume of the vial/source in
cm3}
 2.50000000000000E-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 0.338655000 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:      e_1       e_2         e_3          e_4            e_5
 3:      e_6        e_7                   ...       ...
  ...
 4:    ...       e_n
 5:    sol_{1,1}          sol_{1,2}                sol_{1,3}
  sol_{1,4}   sol_{1,5}
 6:    ...       ...         ...          ...       ...
 7:    sol_{1,n}     sol_{2,1}            sol_{2,2}     ...
  ...
 8:    ...       ...         ...          ...       ...
 9:    ...               sol_{2,n}        ...       ...
  ...
10:    ...       ...         ...          ...       ...
11:    ...       ...                      ...              sol_{p,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
 .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 DataEvaluation

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.

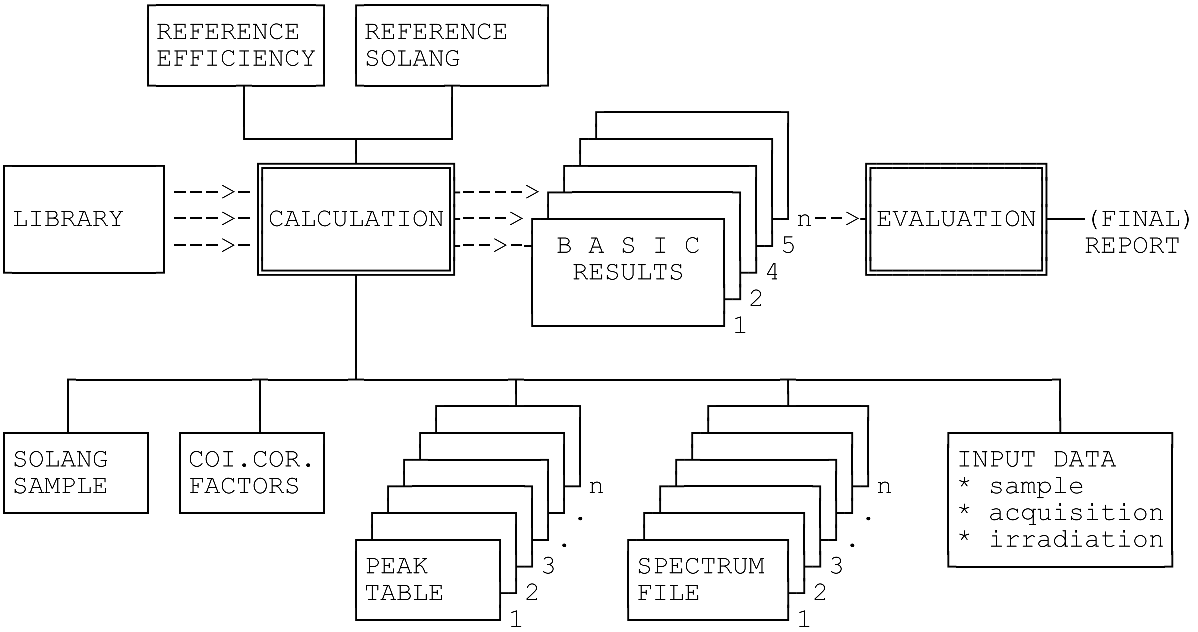


Figure A3.1: Schematic representation of the two main steps of the program and the necessary input data

K_0 Standardization

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

Using the k_0-standardization method, an element concentration, -- ρ_a in mg/kg -- can be calculated from the peak area of a single gamma line [1].
where: N_p 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_m 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_{th} and G_e are correction factors for thermal and epithermal neutron self absorption; Q_0 is the thermal-to-epithermal cross-section ratio; f and α are parameters describing the neutron flux distribution and ε_p 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_0-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 standardised as much as possible. For these standardised 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:

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

where Ω and Ω_{ref} 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.

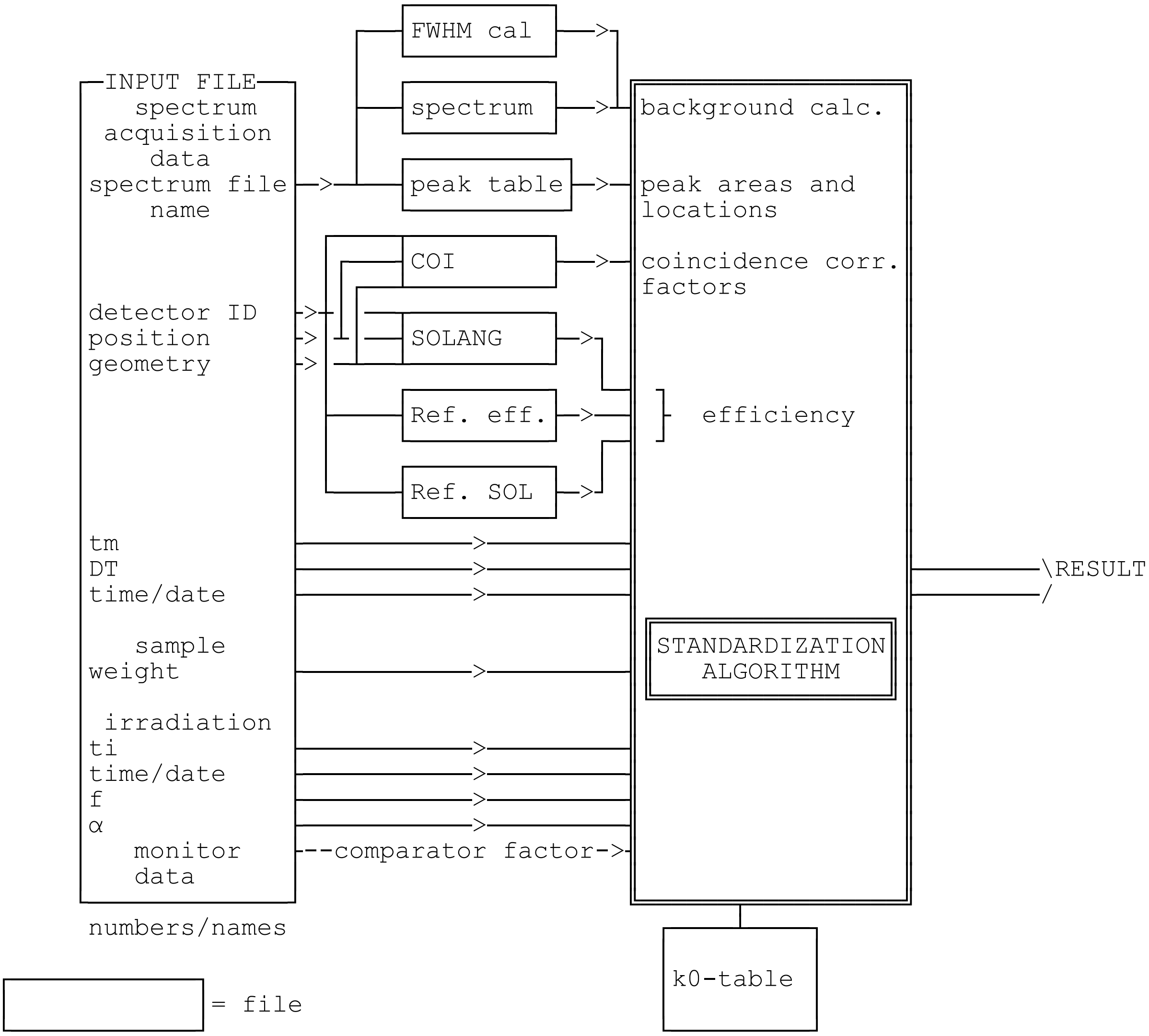


Figure A3.2: Input data for KAYZERO (f and α are predetermined).

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, σ_A, for the net peak area A is calculated using the formula:

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

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):

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

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

Comparator Factor

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

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:

$$F_{c,Au} = \frac{[\frac{N_p / t_m}{SDC.w}]_m \cdot 10^{-6}}{k_{0,Au}(m)(G_{th,m} \cdot f + G_{e,m} \cdot Q_{0,m}(\alpha)).\varepsilon_{p,m}} \qquad 6$$

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:

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

with N_A - Avogadro's number, M - molar mass, θ - isotopic abundance, $\sigma_{0\,,}$- (n,γ) cross section at 2200 m/s neutron velocity and γ - 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 α. For f and α 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 standardisation 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:

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

ρ'_X= concentration of element X (based on gamma lines x + y) without correction for interference by gamma line y of element Y,

ρ_Y = concentration of element Y calculated from an interference-free gamma-line,

ρ'_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:

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

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:

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

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

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

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:

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

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[1]). 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.

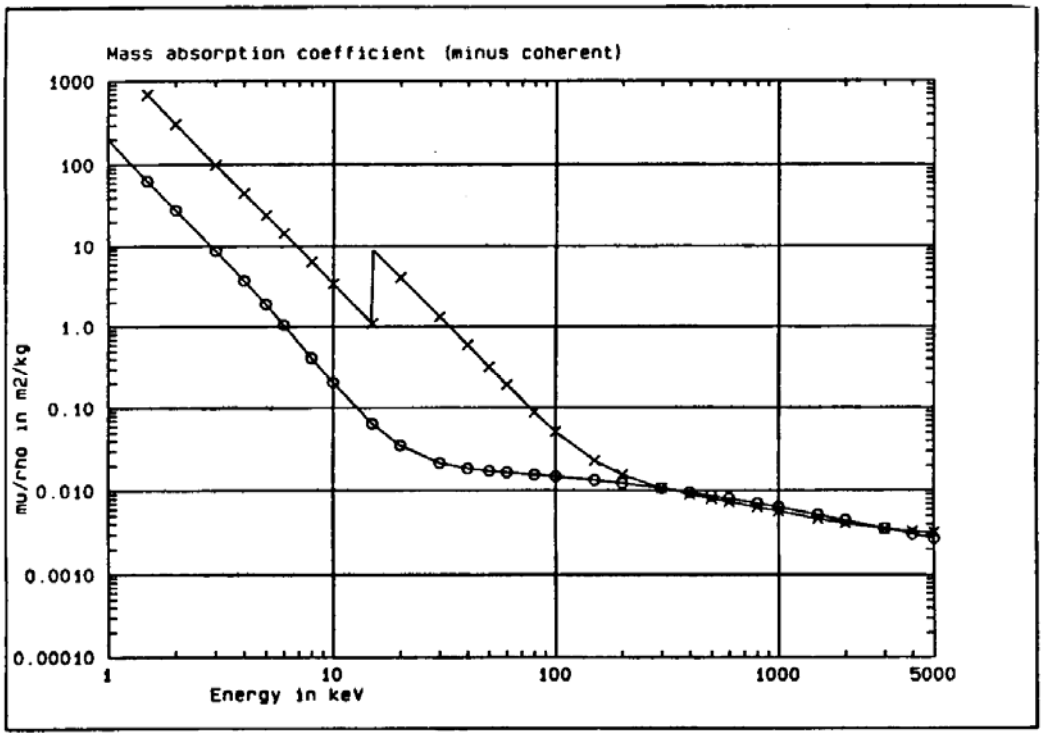


Figure A4.1: Mass absorption coefficients for carbon and germanium as a function of energy (o : carbon; x : germanium).

[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 a 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 precalculated 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.

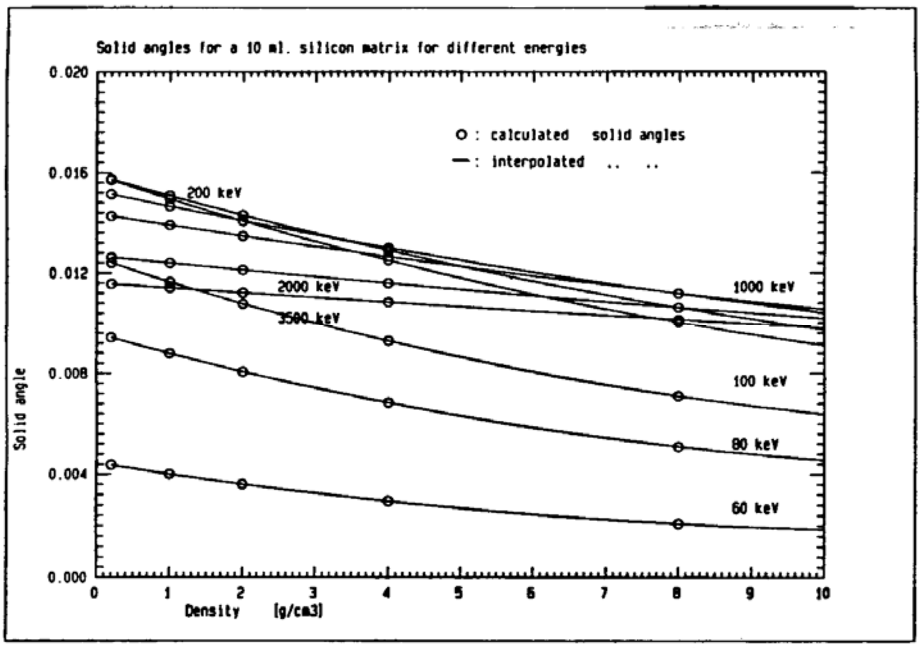


Figure A5.1: Density interpolation

(*) 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, μ (or ρ.μ/ρ), instead of densities is a logical procedure considering the fact that the sample absorption data input for SOLANG is the μ-value for different energies.
In Figure A5.2 the solid angles for different energies are given as a function of μ. 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.

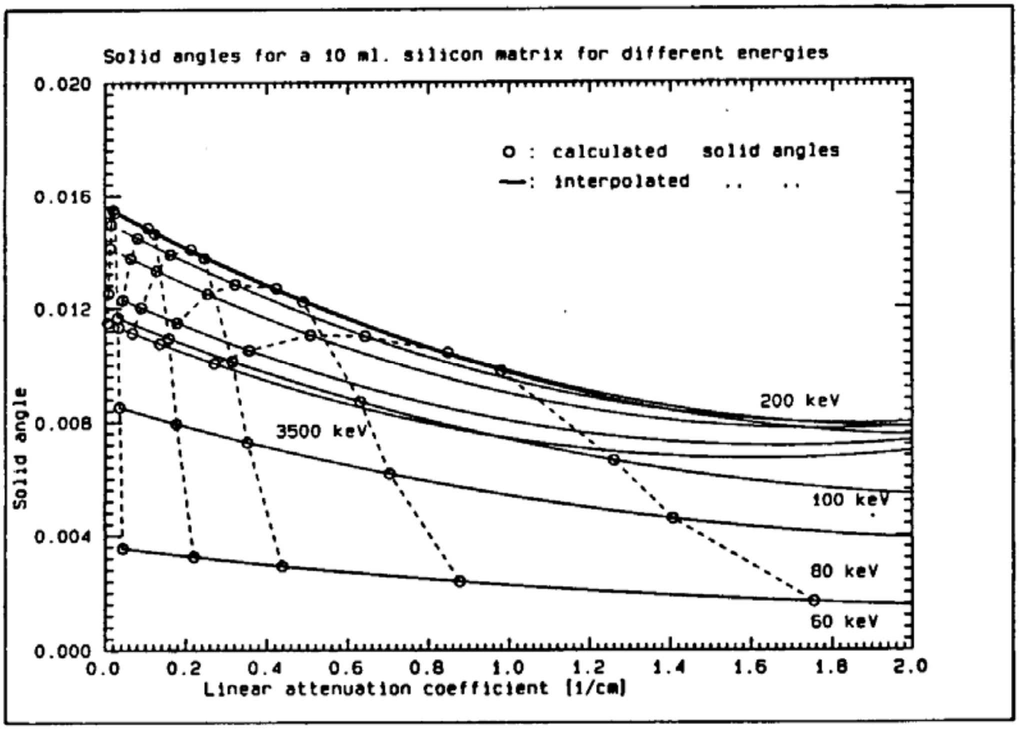


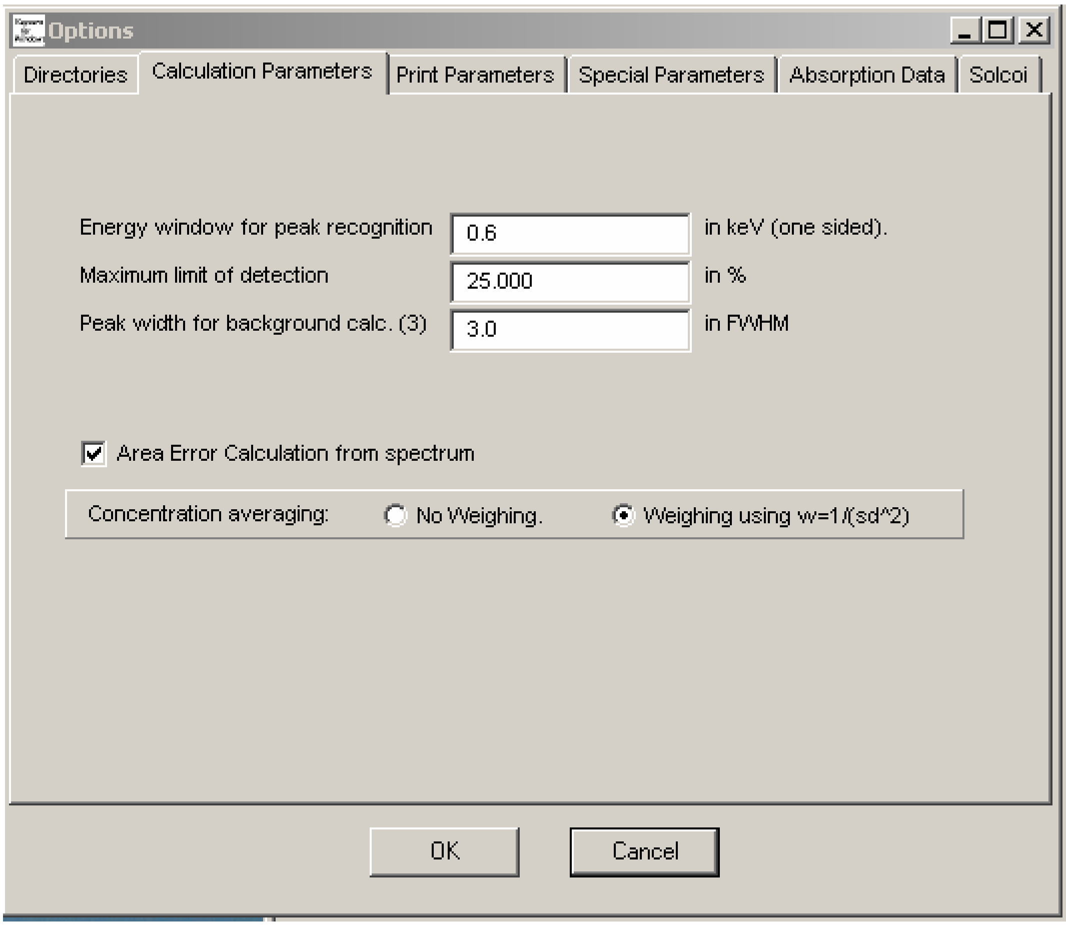
Figure A5.2: Matrix interpolation

(*) 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.

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> .



Energy window for peak recognition 0.6 in keV (one sided).
Maximum limit of detection 25.000 in %
Peak width for background calc. (3) 3.0 in FWHM

☑ Area Error Calculation from spectrum

Concentration averaging: ○ No Weighing. ● Weighing using w=1/(sd^2)

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

Calculation Parameters

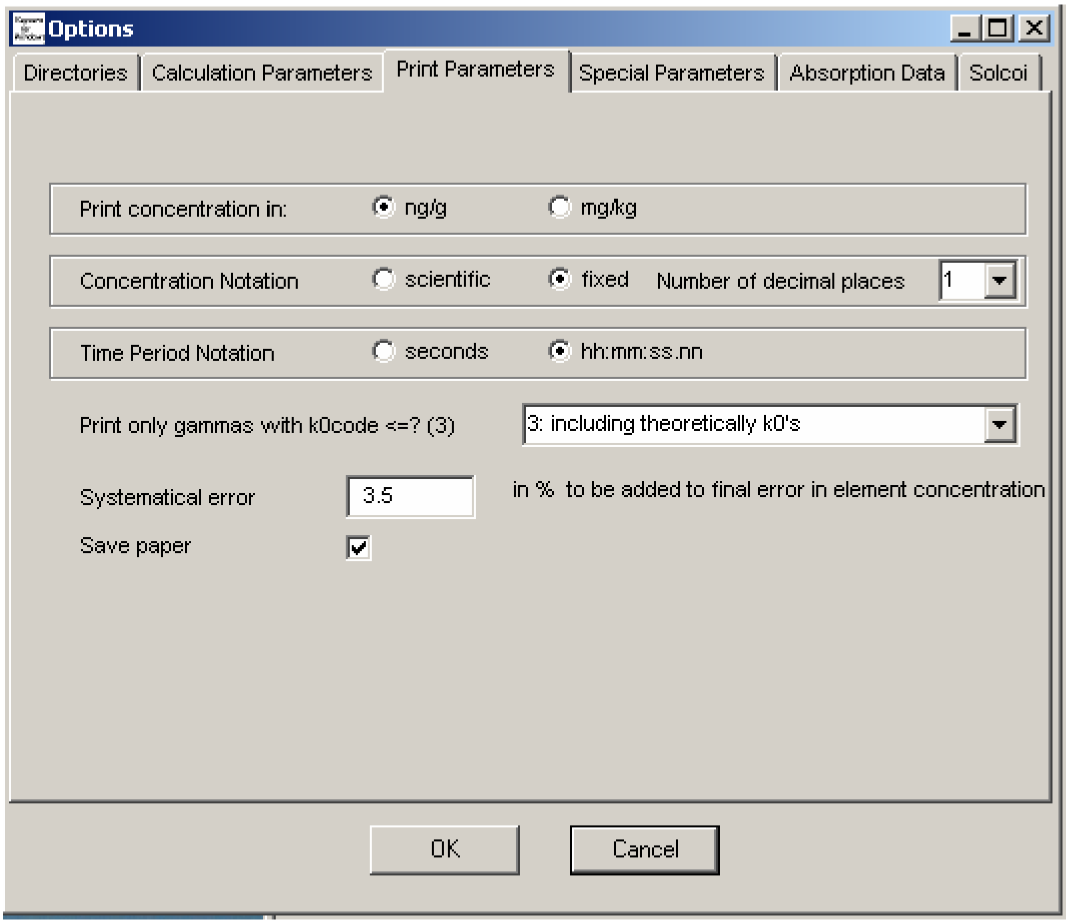
Re. (1): The energy window for peak recognition can be adjusted if the energy calibration is not optimal. In this case it is best to adjust this calibration using *Energy Calibration*-Option. It is very important to have a good energy calibration and the energy window should be narrow enough to identify 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): 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. (3): 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. (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 of so all gamma's are equally important.



Print concentration in: ● ng/g ○ mg/kg

Concentration Notation ○ scientific ● fixed Number of decimal places 1

Time Period Notation ○ seconds ● hh:mm:ss.nn

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

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

Save paper ☑

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

Print Parameters

See Figure A6.2.

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): In most cases when the spectra do not contain many peaks it can be useful to print more information on a page. Sometimes it may be convenient to separate all lists (by a page break); in such cases you should uncheck the box.

Appendix 7: KAYZERO Library: Full listing

(the actual library might be different)

```
PRINT OF THE KAYZERO LIBRARY : VER4_0 (3/12/2001)      3/12/2001
- 1-

_________________________________________________________________
Isotope: F-20        Element: F*         M/D rel:  1
Q0-1   :        1.500 Q0-2   :        0.000 Eres   : 44700.0 eV
T1/2(2):        0.183 T1/2(3):        0.000 T1/2(4):        0.000
[min]
F1     :        0.000 F2     :        0.000 F3     :        0.000
F4     :        0.000 F5     :        0.000
Energy     k0 factor    code - interfering nuclides
 1633.6      1.010E-3    2   -
_________________________________________________________________
Isotope: Na-24       Element: Na         M/D rel: 10
Q0-1   :        0.590 Q0-2   :        0.000 Eres   :  3380.0 eV
T1/2(2):     3.370E-4 T1/2(3):      897.540 T1/2(4):        0.000
[min]
F1     :        0.000 F2     :        0.000 F3     :        0.000
F4     :        0.000 F5     :        0.000
Energy     k0 factor    code - interfering nuclides
  346.6      4.680E-2    5   -
  857.6      4.680E-2    4   -
 1368.6      4.680E-2    1   - Sb-124
 1732.0      4.620E-2    5   -
 2243.0      4.620E-2    4   -
 2754.0      4.620E-2    1   -
_________________________________________________________________
Isotope: Mg-27       Element: Mg         M/D rel:  1
Q0-1   :        0.640 Q0-2   :        0.000 Eres   : 2.57E+5 eV
T1/2(2):        9.458 T1/2(3):        0.000 T1/2(4):        0.000
[min]
F1     :        0.000 F2     :        0.000 F3     :        0.000
F4     :        0.000 F5     :        0.000
Energy     k0 factor    code - interfering nuclides
  170.7      3.020E-6    1   -
  843.8      2.530E-4    1   -
 1014.4      9.800E-5    1   -
_________________________________________________________________
Isotope: Al-28       Element: Al         M/D rel:  1
Q0-1   :        0.710 Q0-2   :        0.000 Eres   : 11800.0 eV
T1/2(2):        2.241 T1/2(3):        0.000 T1/2(4):        0.000
[min]
F1     :        0.000 F2     :        0.000 F3     :        0.000
F4     :        0.000 F5     :        0.000
Energy     k0 factor    code - interfering nuclides
  756.9      1.750E-2    5   - Zr-95 Eu-154
 1267.9      1.750E-2    4   -
 1778.9      1.750E-2    1   -
```

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[1])
5: double escape peaks, with k_0-factor of original peak (added according[1])
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[2] . In Table A7.1 these numbers and the factors F1-F5 given in the library are explained.

Half-lifes 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 7or 8.
B: The lines can not 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_0's with effective energies and effective k_0-factors: lines that can be separated using modern gamma-ray spectroscopy.

Isotope	Eff. energy in keV (k0code)	Energy 1 in keV (rel.γ intensity)	Energy 2 in keV (rel.γ 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 can not 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 > 10000000000. minutes
Energy    Isotope    Element              T 1/2   yield  k0-code
   keV                                     min.       %
_________________________________________________________________
    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.