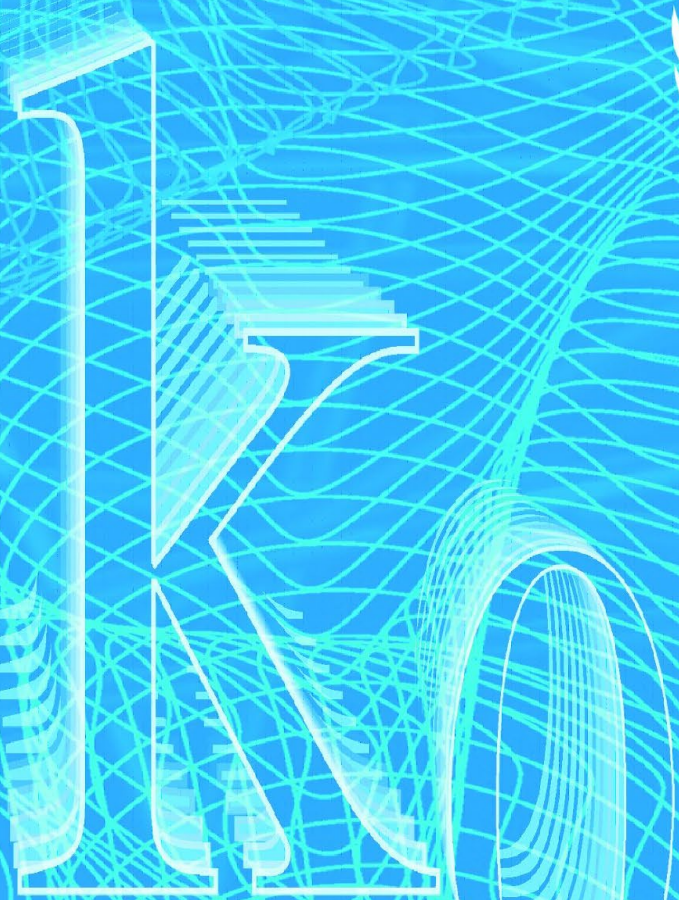
sofware for single-comparator instrumental neutron activation analysis



IAEA

The k_0-IAEA program manual for version 10.20

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The k_0-IAEA program manual for version 10.2

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Basics

In this chapter, the basic philosophy and the way the k0-IAEA program works are described. To get the best results with the program, it is recommended to read this chapter entirely. In addition, a tutorial with how-to instruction videos is available.

Introduction to instrumental neutron activation analysis (INAA)

Theory

Instrumental Neutron Activation Analysis (INAA) is a nuclear technique used to determine element concentrations in any kind of sample. Most elements in the periodic system can be determined at very low levels, i.e. mg/kg in samples that weigh something in the order of 100 mg.

The sample is irradiated with neutrons, usually generated with a research reactor. All atomic nuclei in the sample have a probability of capturing a neutron. This probability is expressed in units of area and called the neutron capture cross section. For thermal neutrons, the thermal neutron capture cross section is a widely published entity, e.g. in the Chart of the Nuclides. The intensity of the neutron radiation is expressed as intensity: per unit area per unit time. Nuclei with the same number of protons but different numbers of neutrons are isotopes of each other, i.e. belong to the same element. The fraction of nuclei of a certain element that have a particular number of neutrons is the isotopic abundance. After capturing a neutron, the nucleus may have become unstable, i.e. radioactive. The level of induced radioactivity depends on the number of generated unstable nuclei and the half-life of the radionuclide. When decaying at a later time to a stable form, it may emit gamma rays, each with a particular probability. The emitted gamma rays can be detected with a semiconductor detector with a very high energy resolution. In the resulting gamma-ray spectrum, the energy of a detected peak indicates what element was present in the sample, and the area of the detected peak allows for the quantitative determination of the amount of the element present in the sample.

In practice

Different institutes have slightly different methods of applying INAA. Here, the routine method applied at the Interfaculty Reactor Institute is very briefly described.

A small amount of sample material, i.e. 1 mg to 1 g, is weighed in a polyethylene capsule. Together with samples of known composition (standards or flux monitors), the sample is irradiated for up to 4 hours in a pneumatic rabbit facility. Depending on the half-lives of the radionuclides generated from the elements of interest, the sample and the standards are measured with a semiconductor detector after selected waiting times. All relevant information, i.e. irradiation, cooling and counting time, sample weights and compositions of standards are made available to a computer that interprets the gamma-ray spectrum in terms of element concentrations. In some materials, more than 40 elements can thus be determined simultaneously.

The total turn-around time depends on the half-lives of the relevant radionuclides. For aluminum or selenium, for example, concentrations can be obtained in minutes. For other elements, waiting times between irradiation and measurement of several weeks may be required.

Advantages as compared to some other trace element analysis techniques.

INAA is non-destructive: The sample need not be dissolved, and the probability of contamination is therefore low. In some cases, the residual radioactivity in the sample is low enough for the client to get his sample back unharmed.

INAA is nuclear: The method is independent of the chemical and physical state of the sample.

INAA is insensitive to low-Z elements: Other elements in low-Z matrices can be determined with high sensitivities. A typical example is geological material.

INAA is linear: After calibration at only one concentration level, the technique is accurate no matter whether ppm's of percentages close to 100 % are to be determined.

Introduction to k_0-INAA

The k_0-method is a single-comparator standardization protocol for Instrumental Neutron Activation Analysis (INAA). Comparator and flux monitor are synonymous in the k_0 method. The rate of production of radioactive atoms from stable atoms of interest (as observed with a gamma-ray detector) is related to the activation rate of gold through the so-called k_0 constant. This relative production rate depends on the specific irradiation facilities and gamma-ray detectors used. The method therefore also prescribes how to determine the required characteristics of the irradiation facility and the detector. The k_0 constant is defined for the simplest activation-decay type as

$$k_0 = \frac{M_c \theta_a \sigma_a \gamma_a}{M_a \theta_c \sigma_c \gamma_c}$$

where a and c denote analyte and comparator, resp., and

M = atomic mass [g.mol^{-1}]
σ = thermal neutron cross-section [m^2]
θ = isotopic abundance
γ = absolute gamma-ray abundance

This constant represents the relative production rate, or rather the part of that rate that is independent of irradiation facility and detector, and plays an essential part in the computation of concentrations in k_0 INAA. The constituents of the constant could be found in literature separately, but in some cases with poor reliability. The k_0 constants were therefore measured directly in some specialized institutes: At the Institute for Nuclear Sciences in Gent, at the KFKI institute in Budapest and at Riso in Denmark.

The same definition also applies to prompt gamma rays.

Knowing the k_0 constants, once the irradiation facility and the detector have been characterized, each sample needs to be co-irradiated with a gold comparator only, rather than with as many comparators (or standards) as there are elements to be determined in the sample. Errors in standard preparation are thus excluded. In exchange, systematic errors in the k_0 constants will affect all results obtained. These errors have been shown to be small, however. The general agreement is that the errors in the constants are smaller than 3.5 %.

Sample and gold comparator may have different shapes, neutron and gamma absorption characteristics. Correction procedures for these differences are also considered to be integral parts of the k_0-method.

The irradiation facility is characterized with a few parameters that define the neutron spectrum, i.e. f, alpha and T. The detector is characterized with two efficiency curves.

The interested reader is referred to the classical k_0 paper by Simonits and De Corte [1], and to Frans De Corte's thesis on the topic [2].

Comparators and flux parameters

Four flux parameters are required in the k_0 method to characterize an irradiation facility and the (n, gamma) reaction rates achieved in it.

The second parameter is the thermal-to-epithermal ratio named *f*. The better the thermalization, the higher the value of *f*.

The third parameter is alpha, which describes the deviation from the perfect 1/E epithermal neutron spectrum.

The fourth parameter is the temperature of the Maxwell-Boltzmann velocity distribution that describes the thermal component of the neutron spectrum.

In the k0-IAEA program, there is a fifth flux parameter, the fast flux. Also, the meaning of some of the other parameters is slightly different than in the original k_0 method.

Irradiation facility characterization strategies - choice of comparator

It can be assumed that the fast flux and the thermal flux are proportional to each other in an irradiation container - both can vary quite a bit from day to day and from point in space to point in space, but in the same way. Also, it can be assumed that *f* and alpha do not vary at all in an irradiation container, and not even from day to day. This means that it is pretty safe to only determine *f*, alpha

and the fast-to-thermal ratio once in a while. The thermal flux however must be determined every time, with comparators on each side of the sample to be analyzed.

A suitable comparator for complete neutron spectrum characterization needs to contain a number of isotopes. A classical mixture contains Au, Zr, Lu and Fe. To determine the thermal flux alone, any element can be used that yields a suitable radionuclide. Au, Zn and Fe are popular in this respect.

Efficiency conversion calculations

Considered an integral part of the k_0 method is the conversion of the efficiency curve measured in one counting geometry to the curve required for another geometry. This was necessary in the early days because it was not considered possible to extract an efficiency curve from gamma-ray spectra measured in a counting geometry close to the detector, because of coincidence summing. So the calibration measurements were performed at a large distance from the detector. Even though we now can measure efficiency curves in any geometry, with the k0-IAAE program that is, the approach is still useful because calibration sources typically are point sources, and INAA samples are not.

In the original k_0 method, this conversion of efficiencies from one geometry to the other was developed by Luc Moens and the method is still known under his name. His implementation was a numerical integration over the source and detector volumes, in the two geometries to be related to each other, yielding a series of conversion factors for different gamma-ray energies.

In the k0-IAEA program, the numerical integration is not performed, but instead a Monte Carlo calculation is used. Because of the low-level source code being very simple and applicable in all sorts of conditions, this was considered the safest method.

The k0-IAEA methods

The thermal flux, f, alpha and T

Originally, the k_0 method was based on the Høgdahl convention. Blaauw adapted this convention to remove all references to the cadmium cut-off energy from the k_0 formulas. It is therefore also applicable to (n,gamma)-reactions that are not well-behaved in the energy range near the Cd cut-ff energy. In this adapted Høgdahl convention [ref 6], the capture probability per atom per unit time is treated as the sum of the integral of the Maxwell-Boltzmann spectrum times the 1/v part of the cross section, plus the integral over the epithermal spectrum times the resonances.

$$p = \Phi_t \sigma_0 + \Phi_e I_0'(\alpha) = \Phi_t \left(\sigma_0 + I_0'(\alpha) \Big/ f \right) \tag{1}$$

where

$$\Phi_t = v_0 n = v_0 \int_0^\infty \Phi \frac{1}{v} \frac{2v^3}{v_0^4} e^{-\left(v/v_0\right)^2} dv \tag{2}$$

This approach is valid only if the capture cross section is indeed 1/v in the thermal region, say below 0.65 eV.

If that is not the case, the so-called Westcott g-factor is to be applied to the thermal cross section. This factor is a function of the temperature T of the neutron velocity distribution.

$$p = \Phi_t g(T) \sigma_0 + \Phi_e I_0'(\alpha) \tag{3}$$

The g(T) factor is defined by

$$g(T) = \frac{1}{\Phi_t \sigma_0} \int_0^\infty \sigma(v) \Phi \frac{2v^3}{v_T^4} e^{-\left(v/v_T\right)^2} dv \tag{4}$$

or, after combining Eqs 2 and 4, by

$$g(T) = \frac{1}{\sigma_0 v_0} \frac{\int_0^\infty \sigma(v) \Phi \frac{2v^3}{v_T^4} e^{-\left(v/v_T\right)^2} dv}{\int_0^\infty \frac{1}{v} \frac{2v^3}{v_T^4} e^{-\left(v/v_T\right)^2} dv} \tag{5}$$

and *sigma(v)* in turn can be calculated with the Breit-Wigner expression and the known resonance parameters. The integral in the numerator can be evaluated numerically to obtain *g(T)* as a function of v_T, which is directly related to *T* by

$$v_T = v_0 \sqrt{T / T_0} \tag{6}$$

where v_0 is 2200 m/s, and T_0 is 293.6 K.
So we get

$$\left(v / v_T\right)^2 = \frac{v^2 T_0}{v_0^2 T} \tag{7}$$

and

$$g(T) = \frac{1}{\sigma_0 v_0} \frac{\int_0^\infty \sigma(v) \frac{2v^3 T_0^2}{v_0^4 T^2} e^{-\frac{v^2 T_0}{v_0^2 T}} dv}{\int_0^\infty \frac{1}{v} \frac{2v^3 T_0^2}{v_0^4 T^2} e^{-\frac{v^2 T_0}{v_0^2 T}} dv} = \frac{1}{\sigma_0 v_0} \frac{\int_0^\infty \sigma(v) \frac{2v^3}{v_0^4} e^{-\frac{v^2 T_0}{v_0^2 T}} dv}{\int_0^\infty \frac{1}{v} \frac{2v^3}{v_0^4} e^{-\frac{v^2 T_0}{v_0^2 T}} dv} \tag{8}$$

The integral in the denominator has an analytical solution

$$\int_0^\infty \frac{1}{v}\frac{2v^3}{v_T^4} e^{-\left(v/v_T\right)^2} dv = \frac{\sqrt{\pi}}{2v_T} \tag{9}$$

so

$$g(T) = \frac{2}{\sigma_0\sqrt{\pi}}\sqrt{T/T_0}\int_0^\infty \sigma(v)\frac{2v^3}{v_0^4} e^{-\frac{v^2T_0}{v_0^2T}} dv \tag{10}$$

and sigma(v) can be modeled with a Lorentzian superposed on a 1/v relationship:

$$\sigma(E) = \frac{\sigma_0\sqrt{E_0}}{\sqrt{E}} + \frac{\sigma_r w}{\pi}\frac{1}{w^2 + (E_r - E)^2} \tag{11}$$

where E_r is the resonance energy, w is the FWHM of the resonance and σ_r is the magnitude of the resonance. However, the fact that the velocity distribution of the absorbing nuclei must be taken into account by integration makes the integral a double one and rather time consuming to compute when fitting a T to observed capture rates. So it was decided to enter g(T) values directly in the catalogue of nuclear data, taken from ref 7. The program interpolates between the tabulated values.

The special activation-decay cases

The definition of the k_0 constant is not the same for all activation-decay cases. One might define the k_0 constant for a given gamma-ray energy of a given radionuclide obtained by activation of the element as the number of gamma-rays of that energy that will eventually be emitted by that radionuclide, per gram of element and per second irradiation time in a purely thermal neutron flux – relative to the number of 411 keV gamma-rays emitted by Au-198 when gold is activated. This definition applies to most activation-decay cases, but not all.

In all the exceptional cases, addition information is needed to use the k_0.

For each element-radionuclide pair, this additional number is now given in the databases of the k0-IAEA program and made visible in the list of k_0 values. The value of the number is closely related to additional numbers as specified in [DECORTE2003]. It can be interpreted as the ratio of the k_0 that you would get if the definition of the k_0 was made to be applicable to all activation-decay cases as described above, and the k_0 as defined by De Corte *et al.* The following table lists all the exceptional cases, even if no examples of such cases can be found in [DECORTE2003].

Table 1: Additional compound constant definitions for the exceptional cases

case	k_0-IAEA additional number definition	number specified in [DECORTE2003]
IIIa	$1 + \frac{F_{24}}{F_2F_3}$	$\frac{F_{24}}{F_2F_3}$
IVa	$1 + F_2\frac{\sigma_0^m}{\sigma_0^g}$	$F_2\frac{\sigma_0^m}{\sigma_0^g}$
IVc	$1 + \frac{\sigma_0^g}{F_2\sigma_0^m}$	$\frac{\sigma_0^g}{F_2\sigma_0^m}$
Va	$1 + F_2\frac{\sigma_0^m}{\sigma_0^g}$	$F_2\frac{\sigma_0^m}{\sigma_0^g}$
VIIa	$1 + \frac{\sigma_0^m(F_{24} + F_2F_3)}{\sigma_0^gF_3}$	$\frac{\sigma_0^m(F_{24} + F_2F_3)}{\sigma_0^gF_3}$
VIIb	$1 + \frac{\sigma_0^mF_{24}}{\sigma_0^gF_3}$	$\frac{\sigma_0^mF_{24}}{\sigma_0^gF_3}$
VIII	$1 + \frac{\sigma_0^gF_{35} + \sigma_0^m(F_{25} + F_{24}F_4)}{\sigma_0^gF_3F_4}$	$\frac{\sigma_0^gF_{35} + \sigma_0^m(F_{25} + F_{24}F_4)}{\sigma_0^gF_3F_4}$

The fast flux

The above convention describes (n,gamma) reactions, including uranium fission reactions. However, there is another class of reactions call threshold reactions. These reactions occur only if the neutron energy is higher than a certain threshold level. Typically, MeV energies are required, and only unmoderated neutrons are fast enough. In the k0-IAEA program, these reactions are taken into account using a specific cross section and a parameter characterizing the fast flux.

Detector characterization

Just like in the original k_0 method, a detector is characterized with a full-energy peak efficiency curve, that gives the probability of a photon depositing all of its energy in the active part of the detector crystal as a function of photon energy, and a peak-to-total curve, that indirectly yields the probability of the photon depositing any part of its energy in the active part of the detector. However, the way the curves are determined is much simpler in the k0-IAEA program than in the original k_0 method.

Thermal and epithermal neutron self-shielding

Thermal neutron self-shielding is performed by the "De Corte" methods, based on the matrix composition and sample shapes specified by the user.
Epithermal neutron self-shielding is performed using a method developed by Andrej Trkov. What follows is his description:
Self-shielding factors are interpolated from tables generated by NJOY in three-group structure. Self-shielding factors for the second energy group with boundaries at 0.55 eV and 2 MeV are included. Self-shielding factors are tabulated in terms of the Bondarenko dilution cross section, which is defined for a resonance absorber as the macroscopic potential cross section of the surrounding nuclei per absorber atom. The macroscopic dilution cross section is given by

$$\Sigma_b = \Sigma_{gb} \sum_i n_i \sigma_{pi} \tag{12}$$

where the n_j are the number densities of the surrounding nuclei (i) and the σ_{pj} are their potential scattering cross sections.
According to the equivalence theory the geometrical self- shielding is equivalent to material self-shielding through a suitably defined geometrical component contribution Σ_{gb}, which is given by

$$\Sigma_{gb} = \frac{a^*}{l} \text{ and } l = \frac{4V}{S} = \frac{dh}{h + d/2} \tag{13}$$

where the mean chord length *l* is proportional to the volume- to-surface ratio defined by the diameter "d" and foil thickness or wire length "h".
The value 1.16 is assumed for the Bell factor a*.
The microscopic Bondarenko dilution cross section is given by the relation

$$\sigma_b = \Sigma_b / n \tag{14}$$

where *n* is the number density of the absorber nuclei.

The code is an extension of the MATCMP code by A. Trkov, Institute J. Stefan, Ljubljana, Slovenia (1992)

Prompt gamma activation analysis with k0-IAEA

As of version 3.00, PGNAA spectra can be interpreted with the k0-IAEA program.

The principle of operation is as follows. If a measurement and irradiation overlap in time, in the history of the sample, the software assumes that prompt gamma rays were being detected in that time span. In those cases where a radionuclide is produced, the decay gamma-rays of that radionuclide as well as the prompt gamma's due to its formation are expected in the gamma-ray spectrum and used for interpretation. In practice, this means that the software expects to see gamma-rays from short-lived radionuclides in the prompt spectrum, besides the prompt gamma-rays themselves.

In reality, the radionuclide just produced may capture neutrons itself and produce yet another radionuclide (like in the ^{197}Au -> ^{198}Au -> ^{199}Au case). This double capture is disregarded in prompt-gamma mode, even though the program knows, understands and corrects for this process when a

sample is activated and measured for INAA, that is without overlapping measurement and irradiation. In other words, it is assumed that neutron fluxes as used for PGNAA are much smaller than those used for INAA, so that double capture can be ignored.

A sample denoted to be a comparator will yield a neutron flux when interpreted, in INAA experiments as well as in PGNAA.

In the PGNAA implementation, no provisions have been made for the “Liz Mackey” effect: Neutron scattering, neutron self-shielding and gamma-ray self-absorption are *not* yet corrected for in PGNAA measurements. This implies that sample and flux monitors must be matched with respect to geometry – internal standardization being the best solution of all. Also, no coincidence-summing corrections are performed for any gamma lines in prompt gamma-ray spectra. In those cases where Q0 values are available, they have been introduced in the databases and will be used, even though in most cases, there are very few epithermal neutrons in a neutron beam as used for PGNAA.

Internal standardization can be performed (in INAA as well as PGNAA) by creating two samples in the series database, identical in all respects except that one is denoted comparator and has a known concentration in it of at least one element, and the other is denoted as ordinary. The sample histories of the two must also be identical, and the gamma-ray spectrum is the same file (no two copies of the spectrum files are required). When the comparator is interpreted, the average neutron flux during irradiation is calculated, and when the sample is interpreted next (after “mapping” the fluxes), all the concentrations are calculated.

PGNAA and INAA spectra related to the same sample can be interpreted simultaneously.

The data used for the k_0 PGNAA gamma rays were taken from tables 2 and 4 in G.L.Molnar, “New prompt gamma-ray data” in “Development of a Database for Prompt gamma-ray Neutron Activation Analysis”, International Nuclear Data Committee INDC(NDS)-443, page 69-91. As of version 10.00, the complete IAEA database of prompt gamma-rays was included with the program, as found at (https://www-nds.iaea.org/pgaa).

Efficiency calibrations

Efficiency curve fitting to a measured spectrum. This action is performed when a calibration sample is interpreted. If the certificate specifies only one radionuclide, and if that one radionuclide is Cs-137, Sn-113, Mn-54, or Hg-203, the p/t ratio curve will be calculated. If the composition of the calibration source is anything else, the full-energy peak efficiency curve will be fitted to the spectrum. The p/t curve must be determined first. The p/t curve is considered to be independent of sample-detector distance, so it needs to be determined only once for each detector. The same applies to the escape ratio curves. The full-energy peak efficiency curve is stored with the distance it was measured at, after conversion by the solid angle method to the efficiency of a point source at that distance.

One detector at one distance can have only one efficiency curve. Overwriting a curve that was determined earlier is only possible after disabling the earlier curve. If the detector has changed somehow, for example if the crystal has moved inside the cryostat, or if it has been etched again as a repair, it is advisable to give the entire detector a new name and treat it as if it were entirely new.

It is possible and even advisable to measure efficiency curves for each commonly used sample geometry. When interpreting sample spectra, the efficiency curve with the distance that matches the sample-detector distance the best is used. This way, the correction factors that translate the calibration geometry to the sample geometry stay close to unity assuring optimum accuracy.

In the preliminary meetings about k0-IAEA, it was discussed how the efficiency calibration should be performed in the k0-IAEA package. It was decided to adopt a mixture of a method proposed by De Felice et al. [5], where one measurement of e.g. Cs-137 would be employed to determine the peak-to-total curve in its entirely, and then the Delft approach [4] would be used for the efficiency curve fit, knowing the peak-to-total and taking coincidence summing into account. This procedure was expected to be stable and applicable in all or most counting geometries used in INAA.

After further investigation, however, it transpired that De Felice's method sets the peak-to-total ratio equal to unity for all energies below 160 keV, so the (160,1) datapoint is a given and then uses one more parameter to determine the slope on an original scale of p/t versus $E\ \mu_f/\mu_t$, where the μ are the photoelectric and total linear attenuation coefficients of Ge. The more widely accepted approach where the p/t ratio is a linear function on a log-log scale of the photon energy could also be restricted to one degree of freedom by setting the (160,1) datapoint, however, from practical experience this appears to be way too high a value, and instead the (90,1) datapoint was taken. In the implementation, the user is offered the choice of using one or more sources for the p/t calibration, all of them necessarily being single photon emitters (meaning that Zn-65 and Co-57 are not allowed). If the user employs more than one, he will need to use the 'import' feature and the (90,1) datapoint is not used. After that, he can use any mixture of radionuclides with known activity for the full-energy peak efficiency calibration.

The full-energy peak efficiency curve fit will fail if less than 6 datapoints are available. The p/t fit will fail if no datapoints are available (but in that case, the default is taken). The escape ratio curve fits will fail if less than 3 datapoints are available (but in that case, a reasonable default is taken).

Please note that if the symmetry axis of a cylindrical sample is perpendicular to the detector, the distance to be specified between detector and sample is the distance between the central axis of the sample container and the end cap of the detector. Otherwise, the distance between the surface supporting the outer sample capsule (or other recipient, if present) and the end cap of the detector must be given.

The k0-IAEA program has no facility to deal with absorbers in between the sample and the detector. That means that if an absorber is to be used, the efficiency calibration must be performed with the absorber in place. If the detector is also sometimes used without an absorber, the solution is to give the detector two names in the system, where one name refers to the detector without the absorber, and the other name to the detector with the absorber.

If all the counting on some detector is performed with the samples in their capsules inside e.g. test tubes or some other outer container, one could perform the efficiency calibration with the calibration source in the same configuration. Only containers and objects that are present during sample measurement, but not during calibration source measurement, need to be specified in the k_0 method, because of the renormalization to the measured reference efficiency curve.

The holistic interpretation method

The holistic analysis of gamma-ray spectra in instrumental neutron activation analysis was developed in the early 1990's by Blaauw and was published in 1994 [8].

The measured peak areas in a gamma-ray spectrum are considered to be the linear sums of the contributions of the individual components of the sample. These components normally are radionuclides, but in the case of INAA, the elements constituting the sample can be regarded as such. A single element may yield more than one radionuclide upon irradiation, but if the neutron capture cross-section for each reaction is known, the relation between the contributions of such radionuclides is also known and need not be established in the interpretation process. The interpretation problem can therefore be written as

$$\vec{a} = M\vec{c}$$

where

a_i = the area of the ith observed peak area,

M_{ij} = the area of the ith observed peak computed assuming that the concentration of element j is unity,

c_j = the concentration of element j,

If as many peak areas as concentrations are involved, the set of equations can simply be solved by

$$\vec{c} = M^{-1}\vec{a}$$

where M^{-1} is the inverse of the square matrix M. If more entities are involved than independent peak areas, no unique solution can be found. This situation can usually be avoided by identifying the indistinguishable entities and removing all but one of them from the set of equations. If more peak areas than entities are involved, linear least squares (LLS) methods are used to find the optimal solution for the set of equations. If only the a_i have known uncertainties, the LLS solution is given by

$$\vec{c} = (M^t W M)^{-1} M^t W \vec{a}$$

where M^t is the transpose of M, and W is a diagonal matrix containing the uncertainties in the a_i. The uncertainties σ_j in the resulting c_j are given by

$$\sigma_j^{\,2} = (M^t W M)_{jj}^{-1}$$

The interpretation problem can only be solved this way if all the M_{ij} and a_i are known. The M_{ij} for all the spectra involved are computed from the sample weight, the sample history and the neutron fluxes using the k_1 method. The k_1 method is a version of the k_0 method allowing for the use of threshold- and fission reactions as well as the for the interpretation of sum peaks caused by cascade summing, implemented in the k0-IAEA program.

The ai are mostly determined by conventional fitting techniques of the peaks in the measured gamma-ray spectra. Afterwards, the peaks indicated by the Mij are compared to the peaks actually observed.

A concentration is computed for each element from each predicted peak. If the peak was not observed in a spectrum, a maximum area is estimated from the characteristics of the peak-search algorithm and the continuum in the measured spectrum, and the corresponding concentration is calculated. If the peak was detected, the maximum concentration is calculated from the measured peak area + 2 x the uncertainty in the area. The lowest concentration thus calculated for each element, from all of its peaks, is taken as the "maximum concentration" present in the sample, to be used in the later interpretation steps. If this "maximum concentration" exceeds 100 %, then 100 % is taken instead. If it exceeds the concentration specified in the matrix composition of the sample, that concentration will be taken instead.

Next, each peak that was predicted but not observed is either eliminated from the M_{ij} matrix, or inserted in the a_i vector if the concentration computed from the maximum area of the unobserved peak is lower than the maximum concentration computed from other peaks that were really observed. The peak area to be inserted is take to be zero, but its uncertainty is obtained from the characteristics of the peak-search algorithm and the continuum in the measured spectrum.

To reduce the size of the system of equations to be solved, insignificant contributions of elements to peaks are eliminated. A contribution is considered insignificant if the maximum contribution, as resulting from the "maximum concentration" determined earlier, is smaller than 1 % of the peak area, or smaller than the uncertainty in the measured peak area.

Now that the M_{ij} and the a_i match, the matrix is checked for the presence of indistinguishable element spectra. If such a pair is found, one of them is removed from the matrix and the two will later be reported as indistinguishable.

A first LLS solution is obtained as described above. This solution is used to propagate the uncertainties of the M_{ij} to the a_i. The second solution obtained using the enlarged uncertainties of the a_i is considered to be final. The uncertainties of the c_j obtained in the first solution result from counting statistics only, in the second solution they cover uncertainties in catalogued peak intensities, capture cross-sections and isotopic abundances as well. For peaks for which a k_0 constant is known, the associated uncertainty is used to this end. For all other peaks, a 10 % uncertainty is used.

If the final concentration obtained exceeds the intermediate “maximum” concentration, a warning message is popped up to inform the user.

Peak shape and the parameters

The peak itself is represented by a Gaussian function, mostly characterized by its area and width. The width is expressed in terms of FWHM, that is 2.355 times the standard deviation of the Gaussian function.

Then, there are the two tails. The low-energy tail, representing imperfect charge collection in the detector crystal, is parametrized by a single number, being the number of standard deviations from the centroid of the Gaussian where the tail begins. The tail itself is an increasing exponential function, joined smoothly to the Gaussian.

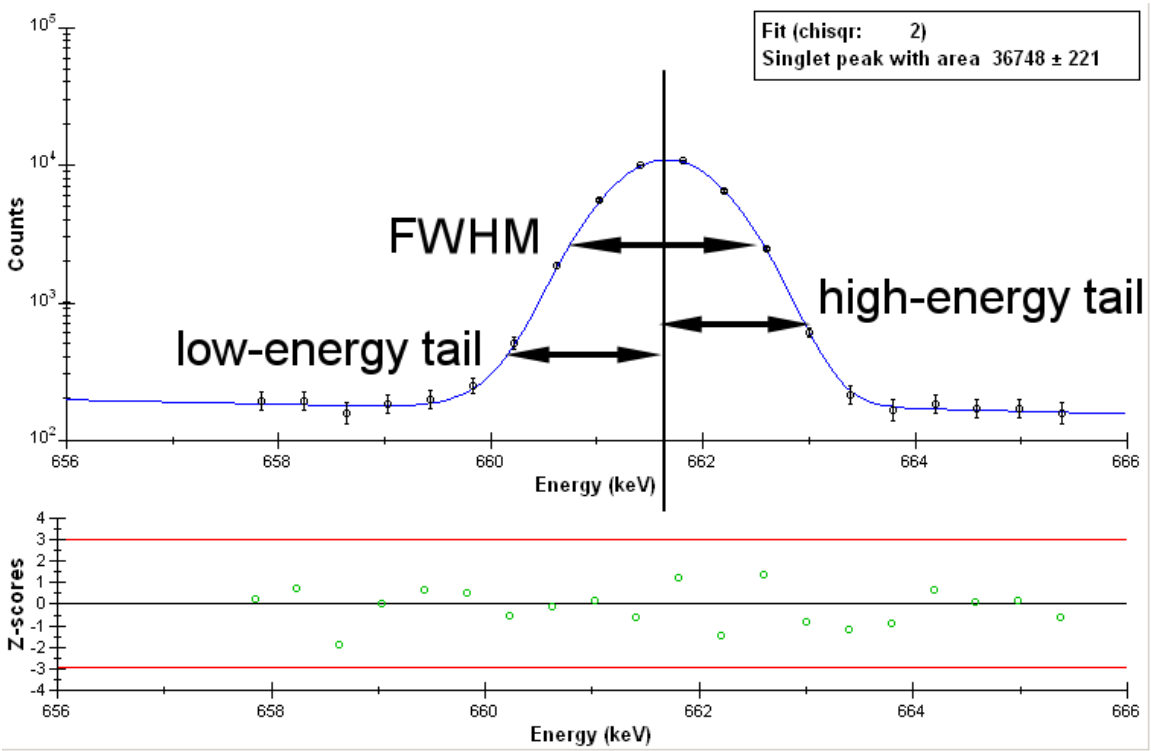
The high-energy tail, representing pile-up, is also parametrized by a single number, being the number of standard deviations from the centroid of the Gaussian where the tail begins. The tail itself is a decreasing exponential function, joined smoothly to the Gaussian.

Underneath the peak is the continuum. This is modelled as a parabolic shape.

Forward scattering in materials between the detector crystal and the sample may result in the so-called Compton step. The shape of it is the error function, being the primitive of the Gaussian, so it is characterized by the width of the Gaussian and a height, which is expressed as a fraction of the peak area.

Single and double escape peaks may have negative Compton steps due to small energy losses of the escaping photons in the detector crystal, all other peaks should have positive or zero Compton steps.

The peak shape and the parameters are illustrated here:



Determining peak areas and energies

Peak areas and energies are determined from the measured channel contents in a mostly standard way. The logic is as follows.

To determine reliably position and area of the components of a multiplet in a realistic spectrum as obtained in INAA, the software attempting the feat must know in advance what the widths and other shape parameters of the peaks are. So it must have a shape calibration available.

In order to perform a shape calibration correctly, the program must be aware of the fact that the 511 keV peak is Doppler-broadened. It can only use this knowledge if an energy calibration is available. So the energy calibration must be made before the shape calibration.

Peak areas must be corrected for background before they can be interpreted in terms of neutron fluxes or element concentrations. So a background spectrum, in terms of a list of peak energies and count rates, must be available to use for the correction.

Dead-time correction can be based on the use of an electronically generated pulser peak that should contain a known number of pulses in a measurement with 0 deadtime. In Delft, for example, the pulser peak frequency is exactly 25 Hz, so by looking at the measured pulser peak area, it becomes clear what the dead time in the measurement has been.

The previous paragraphs explain why the calibration of the software for peak area determination proceeds as it does: First, the energy calibration is made, next the shape calibration, and finally a background spectrum is analyzed. All these are stored in the permanent database, labelled with detector identification and time of spectrum acquisition.

The energy calibration is performed as follows.

Highly significant, free-standing peaks are detected in the spectrum using a rough estimate of peak width entered by the user. A gaussian shape is fitted to the channel contents to pinpoint the peak positions. The user assigns photon energies to the peak positions, and a linear or quadratic curve is fitted to the datapoints. This curve represents the energy calibration.

The shape calibration is performed as follows.

Highly significant, free-standing peaks are detected in the spectrum using a rough estimate of peak width entered by the user. A gaussian shape with two tails is fitted to the channel contents. If the 511 keV peak is present in the spectrum, the parameters of this peak are stored separately. Next, an attempt is made to fit a square root relation to the peak FWHMs as a function of peak energy. Then, each peak in turn is thrown out to see what peak has the largest impact on the chisqr of the fit. If that peak is much narrower than it should be according to the fit, and the user has indicated the presence of a pulser peak, the program assumes this peak to be the pulser peak, and the parameters thereof are also stored separately. The program proceeds to throw out peaks that are outliers until the chisqr no longer decreases.

All datapoints are kept and shown in the graphs so the user can assess the quality of the result.

The low-energy tail and high-energy tail parameter curves are fitted to the datapoints that were left over after the FWHM onslaught.

The analyzed background spectrum is stored in terms of count rates in the peaks. The count rate of the pulser peak should be equal to the known pulser frequency, if all is well. To this end, the dead time of the background spectrum is considered to be 0 % by the software.

Once the calibrations are present, the analysis of an unknown spectrum is performed as follows.

The program detects the peaks using the smoothed 2nd derivative of the channel contents. The width of the filter used to this end is tuned to the widths of the peaks in the spectrum using the shape calibration. For each detected peak, the position, area, and continuum underneath are estimated from the channel contents. The shape parameters are taken from the calibration.

The program then determines which peaks overlap, that is, which peaks contribute significantly to the channels where the other peak dominates. If peaks overlap mutually, a doublet or multiplet has been established.

The peaks are ordered in a list of multiplets, where a multiplet can contain any number of peaks from unity up.

The multiplets are sorted on total area. Then, the multiplets are fitted to the spectrum starting with the one with the largest area. The contributions of neighboring multiplets are subtracted from the channel contents of the current multiplet before attempting to fit.

When fitting singlet peaks with good statistics, the program will allow the shape parameters to vary in the fit, otherwise it will keep them constant.

The user is allowed to manipulate the estimate that is made before the fitting starts - sometimes the user knows best. The user can also choose to integrate a multiplet as a whole, instead of attempting to determine the areas of the individual components.

When all is well, the program calculates the total area of the peaks, that is including the areas under the tails, as well as the width of the region where the peak contributes significantly to the channel contents. This width, rather than the confidence interval of the peak position, will be used in the end when matching measured to expected gamma-ray energies.

If a peak has been integrated, the start- and stop channels of the integration are used to this end.

The peak positions are converted to energies using the energy calibration, corrected for dead time based on the data in the spectrum file, or on the count rate in the pulser peak if a pulser peak is present.

Peak search, detection limits, unobserved peaks

Any peak search algorithm can and will overlook peaks in a gamma-ray spectrum depending on how noisy the spectrum is at the peak position, on the peak width and the peak areas. Most analysis programs these days perform the peak search by calculating a smoothed second derivative of the spectrum, dividing each resulting channel content by its own uncertainty due to Poisson counting statistics, and by searching for channels where the content is minimal and smaller than some threshold. Often, 3 is used as the threshold, meaning that the probability of a peak being detected where there is no peak is less than 0.5 %. The higher the threshold, the smaller the probability of seeing peaks where there are none, but the larger a peak needs to be to be reliably detectable.

k0-IAEA takes lists of peak energies and areas as input. Its native file format is the IAEA .gsr format. But to interpret a spectrum as well as possible, it also needs to know what peak areas would have been easily overlooked in the spectrum. For this, it needs to know the continuum level and the threshold of the peak search algorithm. It assumes that the peak search of the analysis program used falls in the general category described above. Then, it can assume upper levels for peak areas of undetected peaks, leading to upper levels of element concentrations of elements that were never detected in the spectra. Such an upper level is a kind of detection limit and is reported by k0-IAEA in the end. If the element was detected, the program can still pretend that it wasn't and calculate upper levels of peak areas that would have made them easy to overlook.

There are quite a few definitions of detection limits around, and few apply to gamma-ray spectrometry. The detection limits and/or upper limits reported by k0-IAEA are defined as published by Blaauw [3].

To specify the peak search threshold used for the peak analysis, nothing needs to be done in Canberra's GeniePC. But when using other software, a fragment as in the following example must be added to the peak analysis results file (.gsr format):

```
$THRESHOLD:
3
```

If no information is there, the program will assume that the threshold 2.0 was used. This threshold level is known to be a good value for k0-IAEA to work with.

Uncertainty propagation

The k0-IAEA program propagates a number of sources of uncertainties to the final results. Two kinds of uncertainties are distinguished: random and systematic. The 'precision' of the final result is calculated from the random uncertainties only, and some might prefer to call it 'reproducibility' for that reason. The 'accuracy' contains the systematic sources as well and corresponds to the GUM uncertainty with coverage factor 1.

As you will see, however, some known sources of uncertainty are not propagated to the final result. The reason for this is that we have not been able to observe the effect of these uncertainties on the final results in Delft.

Some sources could be systematic or random, depending on your procedures. For example, if you would determine *f* and alpha for each sample, they would be a random source between samples,

but systematic within a sample. If you would determine *f* and alpha once a year, it would be a systematic source. The following table was put together assuming typical routine procedures.

Propagated are

Source of uncertainty	propagated to result	treated as type
Peak area	flux, concentration, efficiency	random
Efficiency	not propagated	
Efficiency conversion	not propagated	
k_0 constant	flux, concentration	systematic
Q_0 constant	not propagated	systematic
E_r	not propagated	systematic
Neutron flux	concentration	random
f ratio	flux, concentration	systematic
alpha	flux, concentration	systematic
decay scheme data	not propagated	systematic
sample mass	flux, concentration	random
dry/wet ratio	flux, concentration	random
thermal self-shielding	not propagated	systematic
epithermal self-shielding	not performed	
gradients in time	not performed	
gradients in space	concentrations	random
conflicting peaks	concentrations, fluxes	systematic

A special note about *f* and alpha uncertainty propagation: these parameters have a strong negative correlation. All the concentrations in the sample are calculated twice: Once with the best values for *f* and alpha, and once with *f* increased with its uncertainty and alpha decreased with its uncertainty. The resulting uncertainty due to *f* and alpha in any concentration is then the difference between the two results.

Literature

Only the most essential references are given here, that explain aspects of the k0_IAEA program. Some of these can be found as .pdf files in the “k0_iaea_documentation” folder on the installation CD.

1 A.Simonits, F.de Corte, “Single comparator methods in reactor neutron activation analysis”, J.Hoste, J. Radioanal. Chem., 24 (1975) 31-46

2 F. de Corte, The k_0 Standardization Method - a Move to the Optimization of NAA, thesis, Rijksuniversiteit Ghent, Ghent, Belgium, 1987.

3 M.Blaauw, ‘Statistical Properties of a Peaksearch Algorithm for Gamma-Ray Spectrometry as related to Currie’s Detection Limits’, Nucl.Instr.Meth. A336 (1993) 273-277

4 M.Blaauw, ‘The Use of Sources Emitting Coincident γ-Rays for Determination of Absolute Efficiency Curves of Highly Efficient Ge Detectors’, Nucl.Instr.Meth. A332 (1993) 493-500

5 M. Blaauw, ‘The accuracy of k1-standardized INAA applied to a gold-lined well-type detector’, J.Radioanal.Nucl.Chem., 245 (2000) 185-188

6 R. Gunnink, A.L. Prindle, ‘Non-conventional ways for accurately calibrating germanium detectors’, J.Radioanal.Nucl.Chem. 160 (1992) 305-314

7 P. De Felice, P. Angelini, A. Fazio, R. Biagini, ‘Fast procedures for coincidence-summing correction in gamma-ray spectrometry’, Appl. Radiat.Isot. 52 (2000) 745-752

8 M.Blaauw, P.Bode, M. de Bruin, ‘An alternative convention describing the (n,γ)-reaction rate suited for use in the k_0 method of NAA’, J.Radioanal.Nucl.Chem. 152 (1991) 435-445

9 N.E. Holden, ‘Temperature dependence of the Westcott g-factor for Neutron Capture Reactions in ENDF/B-VI’, presented at the 36th IUPAC general assembly, Aug 7-15 1991, Germany, BNL-46465

10 M. Blaauw, ‘The holistic analysis of gamma-ray spectra in instrumental neutron activation analysis’, Nucl.Instr.Meth A353 (1994) 269-271

Web links

The most important link for k_0 INAA is to the official k0 website (www.k0naa.org). The IAEA has also dedicated a web page to the program: http://www-naweb.iaea.org/napc/iachem/K0-IAEA.html.

Getting started

To install the software on your computer, please refer to the README.TXT files in the installation package. The how-to videos in the tutorial that comes with it will be of assistance in using the program.

Before even thinking of beginning to use the program, one needs to be familiar with the basics of INAA and k_0 INAA. Some help on these topics is provided in this manual, but it is advisable to also read the early papers on the topic.

Then, one needs to understand a little of the information organization in the program and in the associated files, as given in this chapter.

When designing the program, it was recognized that there are several kinds of information involved, and each kind is stored in its own way.

Some information is not supposed to change ever. Like radionuclide half-lives, decay schemes and k_0 constants. These data are all stored in the k0_IAEA\catalogs folder. The IAEA will see to it that these files are updated periodically, and new versions can be made available. If you have registered as a user (by sending an email to the responsible officer at the Agency, see the IAEA website to find the current person in charge), you will be notified when new versions are made available.

Some information is specific to the experimental facilities used, like detector geometries, irradiation facilities and calibrations thereof. Also, certificates with known compositions of materials and calibration sources are best maintained at the local level. All this information is stored in \k0_IAEA\permanent_data.k0i. It is a wise precaution to make backups of the \k0_IAEA folder in its entirety, so you will be able to reproduce old results.

The permanent database can be edited with the Edit/Permanent database command.

Some information is specific to a batch of samples, possibly all irradiated together, possibly considered to be a group because they all belong to one investigation, or because they are to end up in one report, or because of any other reason: it is up to the user to group the samples in batches that are called 'series' in the k0_IAEA program. A series normally will consist of unknown samples to be analyzed, comparator samples, a blank and one or more reference materials. Together with the associated spectra, all information associated to a series of samples should be stored in a single folder with the same name as the series. The information that is specific to a series can be entered or edited with the Edit/Series database command.

The first step when starting to use the program is to edit the permanent database and enter the detectors (that means entering detector dimensions from the manufacturer's specifications) and irradiation facilities you are going to use. The sample capsules you use also need to be defined and the shape, size and composition stored. You will find that you may also have to enter some material compositions.

The known compositions of comparators and reference materials to be used are also to be entered. And the certified activities of calibration sources. Be sure to think of a consistent way of naming all these materials and items, in order to avoid confusion later on. (For example, always call NIST reference materials NIST-something, and IAEA materials IAEA-something, so that later on, when the lists of these materials tends to get quite long, you can still find what you are looking for.

The second step is to calibrate the detector with respect to energy vs. channel number, and peak width versus photon energy, so that peak areas can be determined from raw channel contents. Closely related is the determination of the background count rates. In the c:\k0_iaea\examples folder, the series BG_Ecal can be inspected to see how it's done. The \k0_IAEA\Examples\iaea1995 example series contains the 1995 IAEA test spectra for gamma-ray spectrometry and can be used to practice the peak area determination process."

The third step is to calibrate the efficiency of the detector. In the c:\k0_IAEA\Examples folder, the series Eu-152PTB can be inspected to see how it's done.

The fourth step is to characterize the irradiation facilities.

The fifth step is to analyze samples and report them.

The second through fifth step all involve series of samples and associated spectra, so you will need to use the Edit/Series database command to create series and samples every time.

Analyzing spectra

A spectrum is analyzed in a few steps.

The detector must have been defined in the permanent database first of all.

Energy and shape calibrations must be present before all the peak energies and areas can be determined.

These calibrations can be stored in the permanent database, and if present there, used for the analysis of a selected spectrum of a selected sample.

Energy calibration

Open a series and select a suitable spectrum.

Next, select the Spectrum analysis/Calibration/Fit calibration peaks option. This determines the positions and shapes of all nice, free-standing peaks in the spectrum, and resets the list of energy calibration points. Now, use the Spectrum analysis/Calibration/Energy calibration option to see and modify the list of calibration points. Afterwards, the results of the fit can be viewed with the View/Curves for the spectra/Energy option. If needed, the list of calibration points can be improved on at this point by repeating the Spectrum analysis/Calibration/Energy calibration option, until the curve and the fit to the datapoints look good.

The curve can now be stored in the permanent database with the Detector/Energy calibrations/Store current calibration option. The curve gets stored with a timestamp, so that when spectra measured on the same detector are retrieved in the future, the proper energy calibration can be found in the permanent database.

Shape calibration

The energy calibration must have been performed first. Now, select the Spectrum analysis/Calibration/Fit calibration peaks option. This determines the positions and shapes of all nice, free-standing peaks in the spectrum. Now, use the Spectrum analysis/Calibration/FWHM calibration option. If your spectrometer has a pulser connected, answer “yes” to the corresponding question, if not the answer must be “no”. Afterwards, the results of the fit can be viewed with the View/Curves for the spectra/FWHM option. Use the Detector/Shape calibrations/Store current calibration option to save the curves in the permanent database.

Peak area determination

Open a series and select the spectrum to be analyzed. Energy and shape calibrations must have been performed already.

Now, select the Spectrum analysis/Analyze all peaks option. Use View/Raw (or fitted) spectra and fix the problems indicated in the bottom graph by zooming in and right-clicking on the problems. At any point, the results can be saved with the Spectrum analysis/Write peak areas to file option. But this option is available only after a background spectrum has been analyzed and stored, so the first analysis result that is stored, for each detector, must be the background spectrum.

Background and deadtime

The first spectrum to be analyzed is the background spectrum. Once all peaks have been fitted and their areas have been determined – please do this one with great care – the background is stored with the Detector/Background spectra/Store background spectrum option. If the spectrometer has a pulser installed, the background spectrum with pulser will allow for dead time correction of all spectra acquired later. If the system has no pulser, make sure you answered “no” to the corresponding question when you made the shape calibration.

Best routine procedure

Perform a new energy calibration and shape calibration every week. The program will always select the youngest calibration that predates the actual spectrum to analyze it, so new calibrations will not interfere with reproducing old results.

Calibrate the efficiency of a detector.

Requirements

In order to calibrate the efficiency a detector, edit the permanent database first and enter the detector and its dimensions. Also enter the certificates of the calibration sources. You will need two or three spectra: a spectrum from a source containing only Cs-137 or one of the other radionuclides that emit only one gamma-ray at a time, i.e. Mn-54, Sn-113, Sr-85 or Hg-203. Cs-137 is the best one for the purpose. The second spectrum should be of a standard mixed radionuclide calibration source containing for example all of the nuclides already mentioned, plus Co-57, Cd-109, Co-60 and Y-88. Eu-152 is also a good candidate. The optional third spectrum should be of a source containing Na-24. The activities of the Cs-137 and Na-24 sources do not need to be known.

The spectra must be measured with the detector, long enough so that the peak statistics in each main peak of each radionuclide are better than 0.5 %. The Cs-137 and Na-24 sources should be measured at about 10 cm, but the precise position is not very important. The mixed source must be counted at a precisely known distance from the detector. If the detector is to be used with an absorber in place, it makes sense to have the absorber also present during the calibration measurements.

Now, a series of samples containing only these three samples can be created. Store the spectrum files in the series folder and use the Edit/Series database command to inform the software about the existence of the two spectra.

Peak-to-total ratio and Full-energy peak efficiency curve determination

Now interpret the single-radionuclide Cs-137 sample. A peak-to-total curve is calculated. Store the curve in the permanent database with Detector/Efficiency curve/Store efficiency curve. Next, interpret the other sample, and a full-energy peak efficiency curve will be calculated. You can take a look at the fitted efficiency curves with View/Fitted efficiency curve. You can store the curve at this time, or postpone doing that until you have also determined the escape ratio curves.

Escape-ratio efficiency curves determination

Gamma-ray with energies above 1022 keV may be detected through pair production in the detector crystal. A positron is created that will deposit its kinetic energy within the crystal, and then annihilate, producing two 511 keV photons. These photons have a significant probability of escaping from the crystal, leading to artificial peaks in the gamma-ray spectrum at energies of 511 and 1022 keV below the original peak energy. Single escape peaks are 511 keV below the main gamma-ray energy and Doppler-broadened, double-escape peaks are 1022 keV below the main gamma-ray energy and not broadened. The escape peaks are not often used to determine concentrations with in INAA, but they can potentially interfere with original gamma-rays coming from other radionuclides, so it is worthwhile to characterize the detector in this respect.

The ratio of the probabilities of obtaining a count in an escape peak over the original peak is called the escape ratio, and it strongly depends on the original gamma-ray energy and detector crystal size. Kai Heydorn published equations for the escape ratio curves in Trans. Am. Nucl. Soc. 60 (1989), 3 that were implemented in k0-IAEA. It is safe to assume that the escape ratios do not depend on the sample counting geometry, since they are basically detector crystal properties.

To determine and store the escape ratio curves, you will need to do the following.
First, determine the peak areas of the main peaks (2754 keV and 1368 keV for Na-24) as well as of the escape peaks (for Na-24, the single escape peaks at 2243 keV and 857 keV, double escape peaks at 1732 keV and 346 keV). The single escape peaks will most likely require manual integration to get a good peak area.
Next, calculate the escape ratios and their uncertainties due to Poisson statistics (the examples here are for Na-24):

single escape ratio at 2754 keV = area at 2243 keV / area at 2754 keV
single escape ratio at 1368 keV = area at 857 keV / area at 1368 keV
double escape ratio at 2754 keV = area at 1732 keV / area at 2754 keV
double escape ratio at 1368 keV = area at 346 keV / area at 1368 keV

Select series, select a sample and use menu option “View/select spectrum of interest” to point out the detector you determined the escape ratios for. It could be the Na-24 spectrum you just used, for example.

Use the menu option “Detector/Efficiency curves/Export reference efficiency curves” to save the curves to a text file with a .k0e extension, in any location you like.

Open the file you just saved with Notepad or some such text editor and append the escape ratios you calculated at the end of the list. When reading this file as input, k0-IAEA will ignore efficiency values set to 0.0. The datapoint at 1023 keV is added to force the escape ratio curves into a physically correct shape. Save the file.

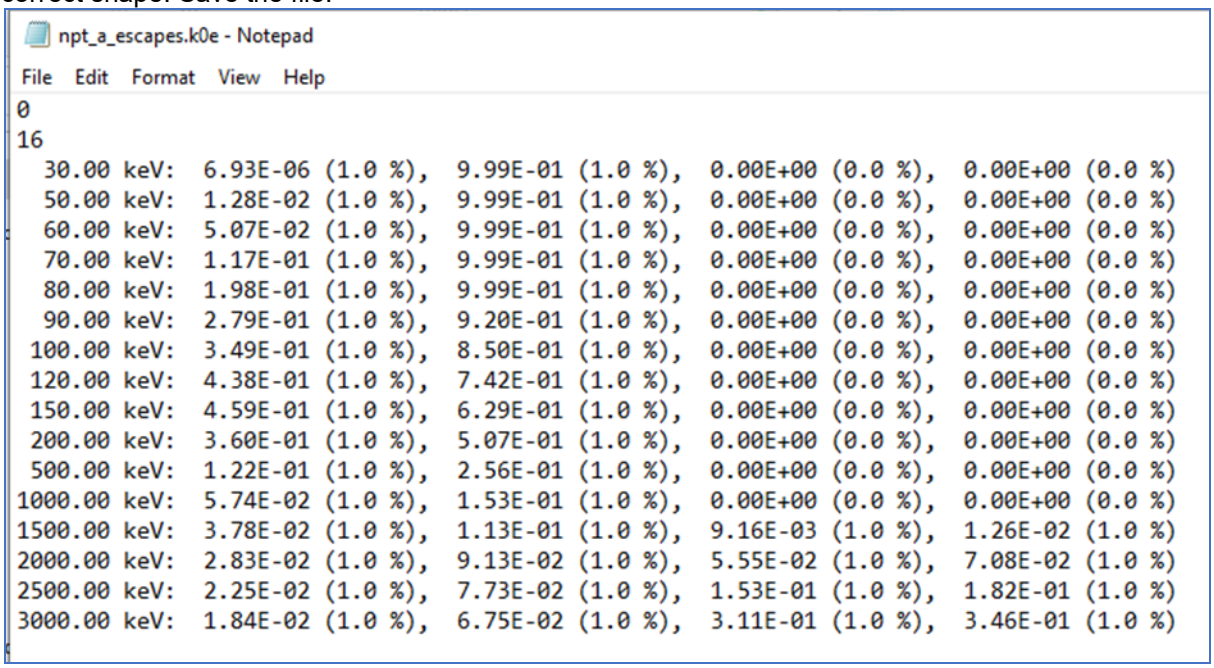


Figure 1: before adding the measured escape ratios. The escape ratios in the two last columns are theoretical estimates for an ordinary detector.

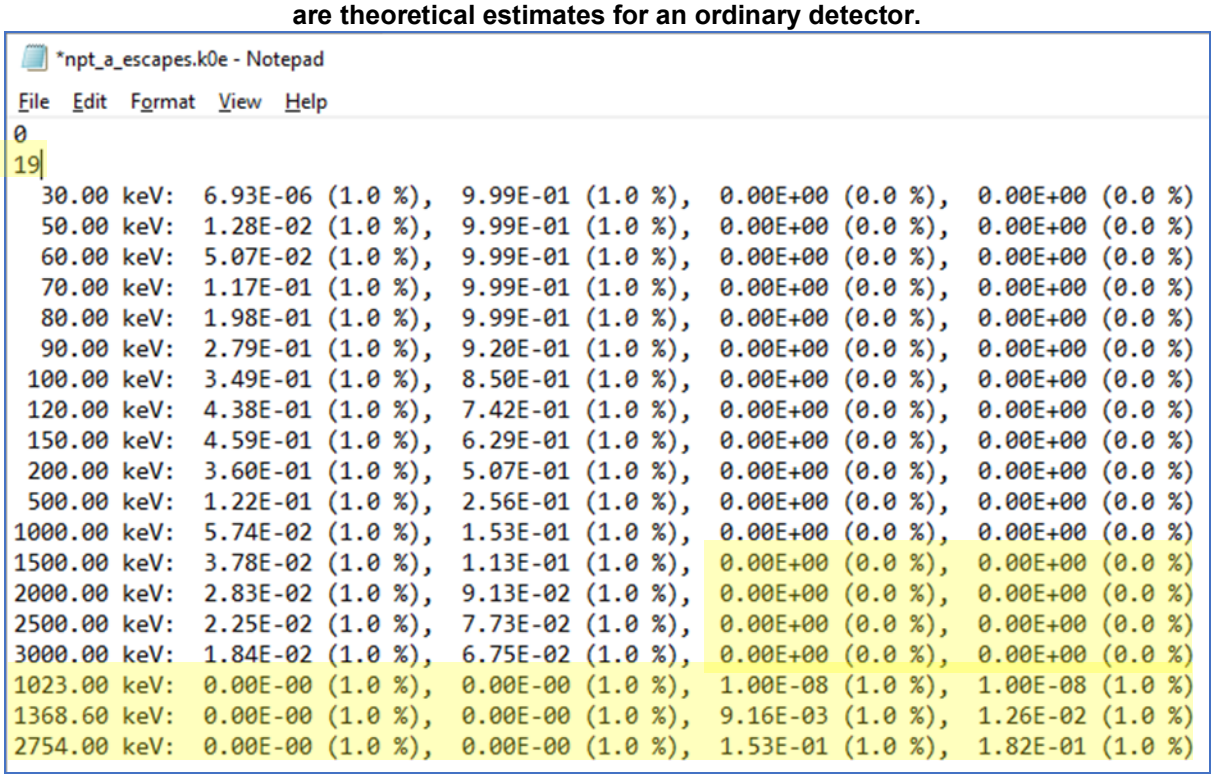


Figure 2: After adding the measured escape ratios. Modified and inserted values are highlighted. The escape ratios and their uncertainties should be your measured ones, not the values with the 1% values shown here as example.

Now use the menu option “Detector/Efficiencies/Import efficiencies from file”. The k0-IAEA program will pop up a dialogue window that allows you to tinker with the efficiency values from the *.k0e file you just selected, but there should be no need to do that. Just click “OK”.

The k0-IAEA program will proceed by asking you if you want to fit each of the efficiency curves to the imported data. In the current situation, the answer is “no” for the Full-energy peak curve.

It then asks if you want to keep the curve you already had, the answer is “yes” for the Full-energy peak curve.

The same answers apply to the peak-to-total curve. But next, it asks if you want to fit the single escape (“Escape 1 ratio curve”) and now the answer is “yes”, same as for the “Escape 2 ratio curve”.

The program will now fit the two escape ratio curves to the data and show you the quality of the fit in numerical terms.

The quality will be perfect since the fits have two degrees of freedom and we only supplied two real datapoints for each curve (at 1368 and 2754 keV).

Now, you can take a look at the fitted efficiency curves with View/Fitted efficiency curve and they should look like this:

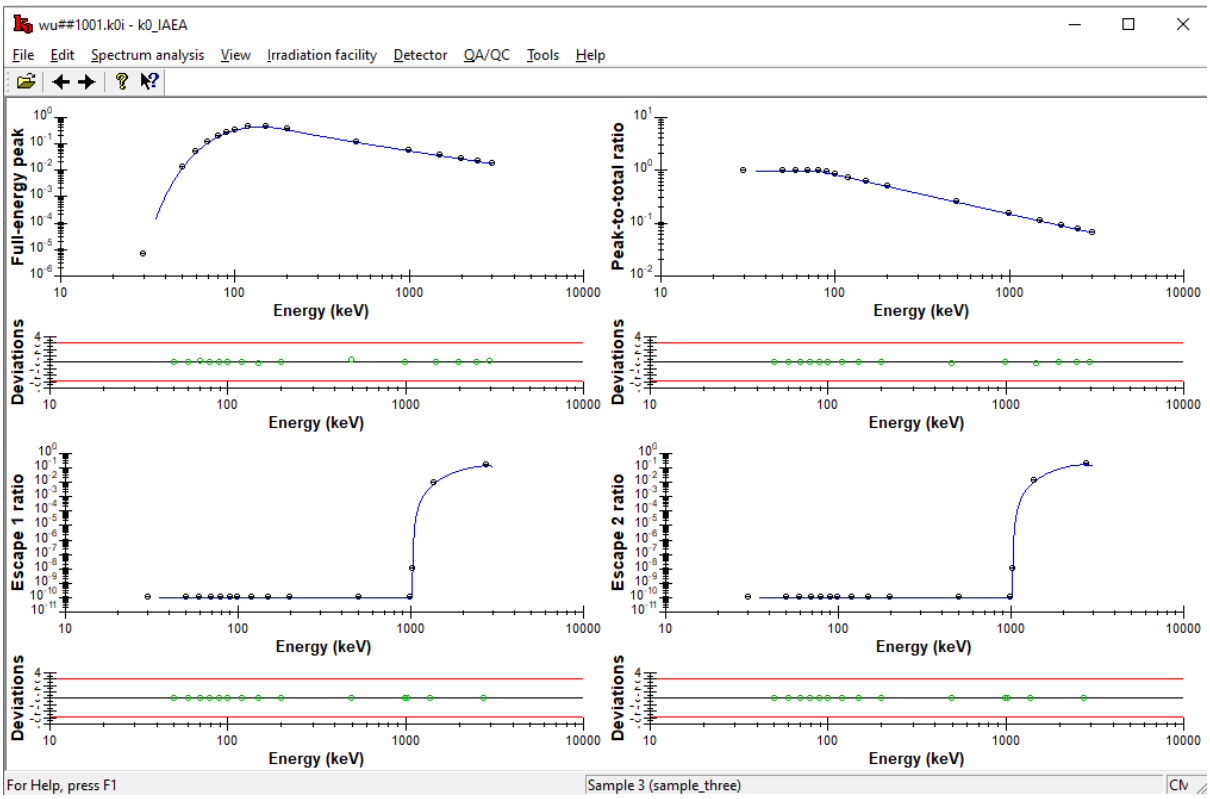


Figure 3: The fitted efficiency curves. All "deviations" should be 0 because the peak-to-total and full-energy curves were not really fitted, and the escape ratio curves had as many degrees of freedom as they had datapoints.

The results of these calculations can be inspected in various ways using the View menu. They must explicitly be stored in the permanent database with the Detector/Efficiency curves/Store efficiency curves command. You may get an error message stating that an efficiency curve has already been stored for this detector and counting geometry if you made previous attempts. The reason is that the software will only accept one “active” efficiency curve for a given detector and counting geometry. In that case, you must disable the old curve in the permanent database before you can store the new set of curves.

Final efficiency calibration remarks

At this point, your Ge detector is fully calibrated and ready for use.

If the calibration samples have been counted on various detectors and in various geometries, it is ok to have all those measurements stored in one single series. Just point out which spectrum you wish to interpret before interpreting. The program will know where to store the result. It is a rather good idea

to count the mixed radionuclide source at all distances from the detector that you will be using in the future and determine full-energy peak efficiency curves from each spectrum, to minimize the loss of accuracy that is unavoidable when efficiency curves are converted from one geometry to the other.

Alternatively, it is possible to create a text file with old efficiency data, import it in k0-IAEA and fit the curves to those data. To do this, use toe Detector/Import option in the main program. The program will then prompt for the detector and distance when the curves are stored in the permanent database. The data must have been obtained with point sources for this purpose.

Characterize an irradiation facility.

It will be necessary to calibrate a detector first. Then, create a series that contains lots of comparators that each will allow for the determination of the neutron spectrum. Interpret all the comparators with the Interpret all samples command, make a map of all the results in the irradiation container space with the Edit/Map fluxes command, and use the Irradiation facility/Store flux parameters command to store the average values in the permanent database. These values will be used for all subsequent irradiations in the same facility, until a new characterization is performed of course. All sets of parameters and their time of determination are kept, so that in future interpretations of samples, the right set will be selected by k0_IAEA.

Since the comparators that have the right composition for this step are expensive and/or difficult to prepare, they can be re-used. Simply irradiate and count them again, in a different facility or at a later time in the same facility and store the information about that in the same series as the first time. Point out for which irradiation to store the average parameters before storing them with the Irradiation facility/Irradiation of interest... command. Of course, flux monitors need some time to decay before they can be used again. One half-life of the longest-lived radionuclide in the mix will be long enough for that: k0_IAEA corrects for previous irradiations as long as all the information is contained in a single series.

One way to create suitable flux monitors is by inserting different pieces of material in a single sample capsule, for example Al-Au wire, Fe foil, Zr-foil and a little Lu_2O_3 powder in a tiny bag. One may wish to separate these components again after irradiation and count them separately, after different decay times. This is possible: In the interpretation of such a (set of) samples, it will be necessary to deselect the peaks of the elements not present in the spectrum under observation. This needs to be done only once for the set of samples, since deselected peaks are remembered and reapplied on a per-spectrum basis.

Create a series of samples and associated spectra.

A series is created with the File/New command. Next, it is edited with the Edit/Series database command to enter the samples, sample classification information, sample packaging information, irradiations and measurements.

Edit series database.

The dialogue-based editor for this purpose should be self-explanatory – the tutorial videos will show you how to do things.

The packing/unpacking actions are a part of the sample history. One could package an amount of sample material in some recipient, irradiate it, unpack it, repackage it in another recipient, losing some mass in the process, and measure it. Or one could put the original recipient (e.g. a polyethylene capsule) in a second recipient (e.g. a test tube) of a sample changer before counting.

The first event in the sample history is a packaging event, since at this point the sample shape and mass are defined. And usually, the associated unpacking time is far in the future. The software expects the sample to be packaged in the innermost recipient first, and in the outermost recipient last. Unpacking must take place in the reverse order.

The software allows for a maximum of five recipients wrapping around each other. Absorbers in between the sample and the detector can also be introduced as a (wide) recipient of which only the bottom dimension is important. The side-looking counting geometry cannot be used in this case. The solution is then to consider the absorber to be an integral part of the detector and measure the detector efficiency in the presence of the absorber.

Edit permanent database.

The dialogue-based editor for this purpose should be self-explanatory explanatory – the tutorial videos will show you how to do things.

Neutron Spectrum data

When creating a new irradiation channel, make sure that an initial estimate is present for all the Neutron Spectrum parameters. Give this first estimate a date that precedes all your activities, for example Jan 1, 1900. Suitable numbers are :Thermal: 4E16, Ratio: 40, Alpha: 0.05, Fast: 2E17, Temperature: 300 K. If you have already characterized the facility in the past with the k_0-method, then use the numbers you obtained.

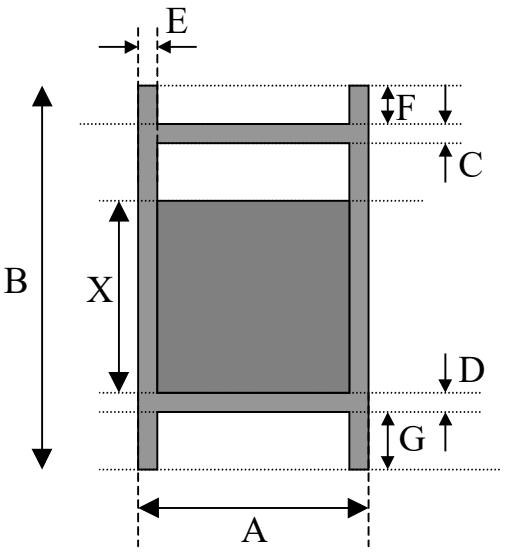
To create a new facility, click on the triangle-labelled part of the 'Add' button and then select 'facility'. Fill out the form and then repeat, but this time click on 'characterization'.

Recipient dimensions:

All recipients are defined as cylinders. The figure explains what's what:

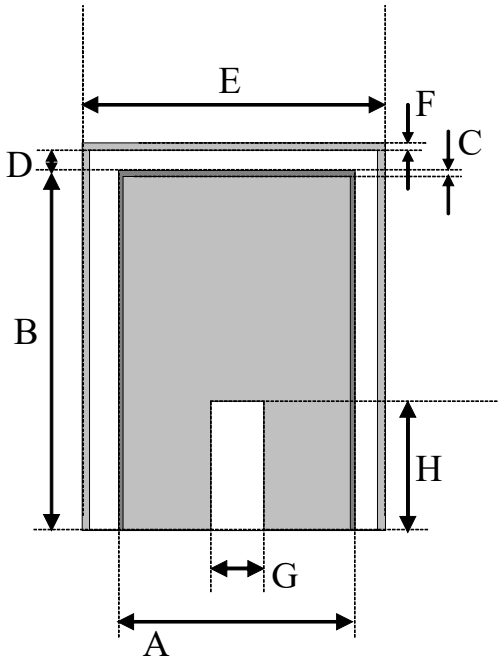
A: outer diameter
B: outer height
C: Top thickness
D: Bottom thickness
E: Side thickness
F: Top empty space
G: Bottom empty space

X: Sample height (entered as filling height in the packaging record with the series database editor). This height is interpreted as wire diameter if the sample is a wire, and as a slab thickness if the sample is a slab of material. A powder or liquid sample is treated as a slab for the purposes of thermal self-shielding calculations.



Detector dimensions

The dimensions requested by the program are indicated in the following drawing and table:



Detector type	coaxial	well-type
A	Crystal diameter	Crystal diameter
B	Crystal length	Crystal length
C	Dead layer thickness	Not used
D	End cap to crystal	Not used
E	Top cover diameter	Not used
F	Top cover thickness	Cover thickness
G	Core diameter	Well diameter
H	Core height	Well depth

Analyze samples.

Simply select the sample and interpret it with the Edit/Interpret selected sample command, or with the Edit/Interpret all samples command.

Report the results.

Use the File/Report command.

Menus and commands

In this section, all menus, command and options are discussed. Since some commands and setting can be approached by various routes, the order in which the subjects are presented was made as logical as possible, but it does not always reflect the menu structure of the program.

This section will be of use especially to those readers who have already studied the “Basics” and “How to” sections.

File menu commands

The File menu offers the following commands:

New	Creates a new series.
Open	Opens an existing series.
Report	Creates and saves the report on the current series. Reporting is performed only for ordinary samples, blanks and reference materials.
Close	Closes an opened series.
Exit	Exits k0_IAEA.

Please note that there is no File/Save command: The database files are being saved continuously by the Windows™ operating system.

New command (File menu)

Use this command to create a new series in k0_IAEA. A series consists of a folder and data files in that folder. Select the parent folder and type the name of the new series folder in the Choose parent folder and name of new series dialog box. The series database file will be created automatically and the default deselected_peaks file copied.

You can open an existing series with the Open command.

File New dialog box

This is a standard Windows dialog. You are to select the folder the new series is to be created in, and to specify the name of the new series. After that, the program will prompt for the name of the analyst and a description of the series with the Create Series dialog.

Open command (File menu)

Use this command to open an existing series with the File open dialog box. If a series is already open, it will be saved and closed automatically before opening the new series.

You can create new series with the New command.

Shortcuts
Keys: CTRL+O

File Open dialog box

The following options allow you to specify which file to open:

Look in

Specify the folder the series’ .k0i file resides in. This folder will have the name of the series.

File Name

Type or select the series filename you want to open. This box lists files with the extension you select in the List Files of Type box.

List Files of Type

Select the type of file you want to open: Only .k0i files can be opened.

Report command (File menu)

Use this command to create a report on the analysis results of the current series. First, you will be prompted to select a report template file, next the report file with the Choose folder and report filename dialog box.

Close command (File menu)

Use this command to save and close the current series.

1, 2, 3, 4 command (File menu)

Use the numbers and filenames listed at the bottom of the File menu to open the last four documents you closed. Choose the number that corresponds with the document you want to open.

Exit command (File menu)

Use this command to end your k0_IAEA session. You can also use the Close command on the application Control menu. k0_IAEA prompts you to save documents with unsaved changes.

Shortcuts
Keys: ALT+F4

Report dialog box

Use this dialog to select in which folder and under what name to save the report file. The report is always saved in the standard .txt format.

Create Series dialog.

The dialog allows one to choose the analyst of the series and enter a short description text.

Edit menu commands.

The Edit menu offers the following commands:

Series database	Call the external Series database editor program
permanent Database	Call the external Permanent database editor program
Read series data from tab-separated text file...	Instead of using the external Series database editor program, read series data from tab-separated text file. This allows for time specification in terms of milliseconds.
Select sample	Select the sample of interest
Next sample	Select the next sample in the series as the sample of interest
Previous sample	Select the previous sample in the series as the sample of interest
Fit peaks in spectrum	Opens a pop-up menu described below
Options for interpretation	Set a few choices that affect the interpretation process
Map fluxes	Map the flux parameters in the irradiation container, determine the fluxes for the samples from the fluxes observed with the comparators
Interpret selected sample	Interpret the select sample. If the sample is ordinary, a reference material or a blank, elemental concentrations will be calculated. If the sample is a comparator, flux parameters will be determined. If the sample is a calibration source, an efficiency curve will be determined.
Interpret all samples	All samples are interpreted. Firstly the comparators are interpreted, then the flux map is made, and then the remaining samples are interpreted. If necessary, the peak areas in the spectra are determined first.

Read series data from tab-separated file.

The option can be selected only after a series has been created.
When selected, a dialog box opens up that allows you to choose the tab-separated text file.
In this file, first of all the samples must be defined. Next, the events that happened will be specified.

The text file refers to reference materials, materials, detectors etc. by name. All these must have been defined in the permanent database first.

The input file can be best prepared in Excel, and then exported to a tab separated .txt file. Examples are available ("wu##1002 series data.xls" and "wu##1002 series data.txt")

Select sample of command (Edit menu)

A dialog box opens up that allows you to choose the sample of interest from a list. This sample and its spectra or other associated data will be shown, depending on the choices made in the View menu.

When a sample is selected, the program attempts to gather all the information needed to interpret the sample. It is at this point that the spectrum files are read. If no filename is present, the user is prompted to select one for the raw spectrum.

The raw spectrum is read, and the acquisition date and time compared to the times in the series database. If it is the first time that the spectrum is associated with the sample, the times from the raw spectrum are copied to the series database. (This is the most convenient way of entering the information in the database. If a discrepancy is found at a later time, the user is warned and asked what to do: Copy the times to the series database or not. If not, the sample cannot be interpreted, and the user will have to modify the raw spectrum file.

If no filename is present in the series database yet, the program makes a guess at the name of the file with the peak areas and energies. If it fails, the user is prompted to select one.

Next sample command (Edit menu)

This sample is selected and its spectra or other associated data will be shown, depending on the choices made in the View menu.

Previous sample command (Edit menu)

The previous sample in the series is selected as the sample of interest. This sample and its spectra or other associated data will be shown, depending on the choices made in the View menu.

Interpretation options command (Edit menu)

This dialogue allows you to control the interpretation process in a few respects. Most of the settings are stored in the registry so they will not be reset when the program exits or the computer reboots. Some have to do with the peak fitting (peak area determination), others with the interpretation process that comes after the peak areas have been established.

Spectrum analysis options for all samples

Search-for-peaks threshold

Not all spectrum analysis programs specify their peak search threshold in the output files. And sometimes what they put there is not what it seems to be. K0_iaea will show negative residuals if peaks are expected by the program but not detected by the peak analysis software. If this happens too often, raising this parameter to a higher value should help. It can also help when interpreting high-count rate loss-free or zero deadtime spectra.

The threshold selected is used as default for spectra newly read into the program. If it is to be used no matter what information is given in the spectrum files, the Override threshold box should be ticked.

In version 2.0 and up, this parameter sets the sensitivity of k0-IAEA's own peak search. If the value is set to 2, for example, peak with areas that are at least twice as large as the uncertainty in the area are to be detected.

FWHM estimate for peak search.

Not all spectrum analysis programs specify their peak widths in the output files.

The FWHM specified here is used as default for spectra newly read into the program. In version 2.0 and up, this parameter sets the width for k0-IAEA's own peak search, to be used when searching for calibration peaks. If the value is set to 2, for example, peak with areas that are at least twice as large as the uncertainty in the area are to be detected.

External peak fitting program

Ticking this box tells the program that you use an external program to determine peak areas and energies. The next two boxes are relevant if this is the case.

Override spectrum file search-for-peaks threshold

When this box is ticked, the Search-for-peaks-threshold will be used in the interpretation of the spectra, that is in the estimation of detection limits and upper limits, instead of the threshold possibly stated in the output files of the external peak fitting program. This option is only relevant if external peak fitting software has been used.

Correct for dead time.

If externally determined peak areas in the input files have not been corrected for dead time and pile up, ticking this box will correct for that using the real time / live time information in the series database. The measured peak areas are not corrected, but instead, the expected peak areas are. These expected areas are normally calculated assuming zero dead time.

Not selecting this option means that the continuum channels in the raw spectrum data file will need to be corrected for dead time before they can be used for detection limit estimation.

In any case the sample must be reselected after this option has been changed, so that the spectrum files will be read again and treated consistently afterwards. This option is only relevant if external peak fitting software has been used.

Interpretation options for all kinds of samples

Intermediate results in log file of interpretation

Ticking this box tells the program to write intermediate results to a log file in the series folder. The name of the log file is the sample number, followed by log.txt. These files can get pretty large. The file format is explained here

All Asp in log file of interpretation

Ticking this box tells the program to report on expected and assigned peaks, with specific count rates Asp, (as defined in the k0 literature) results to a log file in the series folder. The name of the log file is log#.txt, where # is the sample number. These files can get pretty large. The file format is explained here. To make it smaller, when trying to figure out what's going on with a specific element, you can set the element of interest with View/Options for plot/views.

Use threshold and Fission reactions.

When this option is selected, the program will include fission- and threshold reactions for neutron spectrum characterization and element concentration determinations.

Use all (not only k0) peaks for upper limits.

When this option is selected, the program will use peaks that do not have assigned k0-values, like escape peaks and peaks resulting from threshold capture reactions, to determine detection limits and concentrations from. Such concentrations will have large associated accuracies, as compared to the reproducibility expected from the counting statistics, due to the fact that the k0-data have never been determined within the framework of the k0-method.

No adjustment of efficiencies

Ticking this box tells the program not to use the routine that converts efficiencies from the reference values to the values for the actual sample. This should only be done if it is absolutely certain that the calibration geometry and the sample geometry are identical.

Precision for efficiency transfer

Here you can select the precision for the efficiency conversion. The conversion is performed at some 16 energy values, and the curve is fitted with only 6 parameters, so the precision in final concentrations is about a factor of three better than the value selected here. A value of 1 % is recommended as a good compromise between computation time and precision of the final results. Only relevant if the "No adjustment of efficiencies" box has **not** been ticked.

Insignificance threshold

In the holistic interpretation method, each peak area is supposed to be the linear sum of the contributions of all elements in the sample. Contributions below this threshold level are disregarded, which speeds up calculations. 1 % is a safe value, since the k0-method supposedly has inherent uncertainties up to 2.5 %. Contributions smaller than the statistical uncertainty in a peak area are always disregarded.

Lower energy threshold

If your efficiency curve is bad below a certain energy, or you don't trust low-energy peaks for some other reason, you can set the threshold for that here, to a value between 0 and 90 keV. Peaks below the ADC-threshold of each spectrum are ignored as well, no matter what you choose here.

Edit list of deselected peaks.

Clicking this button allows one to see and/or edit the list of deselected peaks for the current spectrum. Note that this list is applied in the subsequent interpretation of all samples in the series. Assuming that all samples have been measured an equal number of times, one list is used for each first measurement, one for each second measurement, etc.

Interpretation options for comparators specifically

Thermal flux to be calculated only.

The program will only attempt to determine all the flux parameters from comparators with a suitable composition. However, if you would like to force the program to determine only the thermal flux from a comparator with a complex composition, this is the box to tick. Go here to read more about comparators in the k0-method for INAA.

If this box is not ticked, the program will calculate a fast flux from the threshold reactions, if present. It will also attempt to determine f, alpha and T, by fitting the thermal flux, if successful the thermal flux and f, if successful the thermal flux and f and alpha, and if successful finally the thermal flux and f and alpha and T to the observed activation rates.

Force reinterpretation

Comparators can be used more than once in different irradiations. This is not recommended practice. The program will warn you when to tell it to reinterpret comparators that were already interpreted in the past, unless you tick this box.

Interpretation options for efficiency calibration sources only

Anti-Compton system present (not yet active)

If an anti-Compton system is present, the normal definition of the peak-to-total ratio as used in coincidence summing correction calculations does not apply. The only way to determine it is by measuring a spectrum that shows coincidence summing – like a Eu-152 spectrum. Tick this box and the p/t ratio curve will be fitted to the measured spectrum along with the full-energy efficiency curve.

The default setting for this option is that there is no anti-Compton system present, and the setting is not remembered by the program either: It only needs to be ticked when the efficiency curve is being calculated by the interpretation of a calibration source spectrum.

This option is inactive because we have not been able to make it work yet…

Map fluxes command (Edit menu)

This option becomes useful when the comparators in the series have been interpreted. Using the information on the locations of the samples and comparators in the irradiation container in the series database, the program fits quadratic polynomials to the determined flux parameters as a function of row position for each column. The resulting polynomials can be plotted using the View/Select flux parameter to view and the View/Map of flux parameter options.

The flux parameter value that will be employed for the current sample is also indicated in these graphs. The flux parameters determined for the samples are entered in the sample histories.

It is possible to assign the same position, (rabbit, column and row) to any number of flux monitors. The same position can also be assigned to a sample. In that case, the weighted average of the flux parameters measured with the comparators will be applied to the sample.

The program identifies irradiations using the time, rabbit and facility. For each point in time, each rabbit and each facility, a flux map as described above is made.

If a sample has not been co-irradiated with a comparator, it must have been irradiated after the comparator, in the same facility, and in the same rabbit. The program will find the previous irradiation in the same facility and rabbit, and it will use the flux map made for that point in time for the current sample. To this end, the comparators that were used to make the map, with the interpretation results, must be present in the same series as the samples.

If no comparator in the series has been irradiated in the same rabbit and facility at a time preceding the sample irradiation, the program will issue a warning and apply the flux parameters as stored in the permanent database.

Interpret selected sample command (Edit menu)

The selected sample is interpreted.

If the sample is a **calibration source**, efficiency curves will be fitted as described here. The resulting curves can be inspected using the View/Fitted efficiency curve option. The same fit, represented by showing how well the new efficiency curve reproduces the measured calibration spectrum, can be inspected using the View/Graphical results. After the fitting, the fitted curve is converted to a curve for a point source located at the center of mass of the calibration sample (if the counting geometry was specified to be side-looking) or at the center of the surface supporting the sample (if the sample's symmetry axis was parallel to the detector's). This conversion is performed at a 0.5 % precision for 15 energies which may take some time. The difference between the curve for the actual geometry and the reference, point-source geometry can be seen using the View/Efficiency curves for the spectra option. Finally, there's information on the process and its results to be found in the logfile and the View/Numerical results.

If the sample is a **comparator**, flux parameters will be calculated depending in the Interpret Options settings. If the comparator is being reinterpreted, the results will NOT be transferred to the maps of flux parameters or the sample histories unless the Edit/Map fluxes option is used after interpreting the comparator. Only then, the flux parameters to be used for the interpretation of the samples in the series are calculated.

If the sample is an **ordinary sample**, a **blank** or a **reference material**, all spectra of the sample will be interpreted simultaneously. The flux parameters determined with the Edit/Map fluxes command will be used. The interpretation is performed in a number of steps:

First comes the conversion of efficiency curves. Using Monte Carlo techniques optimized for cylindrically symmetric counting geometries, the actual efficiencies for the current sample are calculated as described here. The precision for this is determined with the Interpret Options settings.

Knowing the detector efficiencies, the sample history, the k0-constants, radionuclide half-lives and the radionuclide decay-schemes, the program calculates what peak energies and areas are expected from each element.

The program proceeds by checking the presence of each and every peak in the measured spectra. No matter whether the peak is observed or not, an upper limit for the amount of the element in question in the sample is calculated (if a peak was not observed, the upper limit is estimated from the continuum in the spectrum at the peak location according to Blaauw's method [1], and automatically also is the detection limit). (Normally, only peaks with "official" k0-values are used for that. In the Edit/Options for interpretation dialogue, the user can choose to also use non-k0 peaks to this end.)

Knowing these upper limits, every peak is checked again to see whether the element in question could have contributed to that peak significantly or not. A contribution is considered insignificant if it is smaller than the uncertainty in the observed peak area. Such insignificant contributions to peaks are dropped.

What remains after all that is a system of linear equations, where the element concentrations are the unknowns, and each peak represents an equation. This system of equations is solved by linear least squares methods as described in [8]. Not all equations are linked by shared peaks: Each subset is solved separately. If the log-file option was switched on in the Interpret Options, the complete set of equations is written to file.

The preceding steps are performed twice: Once with the thermal/epithermal ratio f set to its optimum value minus the uncertainty and the epithermal shape parameter alpha set to its optimum value plus its uncertainty, and once with both parameters set to their optimum values. All this is done to propagate the uncertainties in these strongly correlated parameters.

If there is something very wrong with the spectra (energy calibration for example) or with the neutron spectrum parameters (like a bad fast flux giving bad expectations for threshold reactions), the finally calculated concentration can become much larger than the maximum amount calculated earlier. If this happens, the program issues a warning that stops automated interpretation - the user has to click on *OK* to proceed. The problem needs to be found and solved, or the concentration for the element(s) in question may be way off. The quickest solution usually is to deselect the peak that gives rise to the erroneous maximum amount.

Afterwards (again when the log-file option is switched on) the program reports possible contributions to each relevant peak, observed or not, in the log file. A peak is considered relevant even if it was not observed, when it would have been expected to be easily observable at the upper level of the element concentration calculated earlier.

Almost all of the data in the log file can also be accesses using the View/Graphical results option.

Interpretation status / Efficiency calibration status dialogs

During the interpretation, a dialog box shows what stage the interpretation process is in.

Interpret all samples command (Edit menu)

This command tells the program to interpret all samples in the current series. If comparators are present, these will be interpreted first. Then, the maps of the flux parameters are made. Finally, the ordinary samples, reference materials and blanks are interpreted.

If any spectrum of any sample has not been analyzed, that is, the peak area file was not found, the spectra will be analyzed just before the sample is interpreted. The peak areas are written to a .k0p file for later inspection. Intermediate fitting parameters are also stored. This automated procedure will only work if energy and shape calibrations have been performed for the detectors used, and if a background spectrum has been stored for each detector as well.

Check out the help on the Analyze all -peaks and Interpret selected sample options for more detailed information.

Spectrum analysis menu

None of the options in this menu can be selected if no specific spectrum has been selected with View/Select spectrum of interest.

Perform peak search	Performs peak search, using the settings in the Edit/Options for interpretation dialogue.
List of peaks	The list of detected peaks can be edited, for example to throw single escape peaks or unrecognized doublets out.
Calibration	A pop-up menu appears for energy and shape calibration.
Analyze all peaks	All peak energies and areas in the spectrum are determined. A peak search is performed first if it had not been done already. To see the results, use the View/Raw spectra option and right-click on the peak of interest.
Modify estimates and fits	The list of fit regions and peak estimates is offered for inspection and modification. After this, the peaks are fitted again using the new estimates. Estimates and fits can also be modified by right-clicking on the peak while viewing the graph of the estimate or the fit. After selecting the parameter to be modified, you can modify the estimated value using the mouse scroll wheel or the '+' and '-' keys on the numeric keypad. It is advised to this while viewing the estimate so you can see the immediate effect. Once the estimate looks OK, the fit will typically also be good.
Reanalyze all peaks	The current fit results replace the estimates, and the fitting is repeated.
Write peak areas to file	The peak areas are corrected for background and deadtime, and the results written to file. Intermediate fit results, such as shape parameters and manual fits, are stored as well. There is no need to do this in order for the new fit results to be used for interpretation, but it would be a shame to forget to do it, because then you will have to repeat steps the next time you open this series.

Calibration pop-up menu

With the options in thus menu, the energy- and shape calibrations of the detector can be performed. (The efficiency calibration is performed by interpreting a sample of the *source* type. See the help on the Edit/Interpret option.)

Fit calibration peaks	The nice, free-standing peaks are fitted to be used in the energy and/or shape calibration steps coming next. A peak search is performed first if it had not been done already.
Energy calibration	A list of energy calibration points is put together and the calibration performed. The result can be inspected with View/Curves for the spectra/Energy
Save current energy calibration	The current energy calibration is stored in the permanent database for the current detector, with a timestamp that comes from the current gamma-ray spectrum.
FWHM calibration	The peak shape calibration is performed. The results can be inspected with View/Curves for the spectra/FWHM. The left and right tail parameters are calibrated as well. More on peak shape in the Basics chapter.
Write current shape calibration	The current shape calibration is stored in the permanent database for the current detector, with a timestamp that comes from the current gamma-ray spectrum.

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########$K####################KK123#####k######

Perform peak search.

The peaks are detected using a 'Mexican hat filter', which itself is the 2nd derivative of a Gaussian with a width matched to the width of the peaks in the spectrum. This filter determines the smoothed 2nd derivative of the spectrum channel contents, and then finds the minima that occur at the peak positions. For uncalibrated detectors, the width of the filter is determined by the 'FWHM for smoothing' set with the Edit/Options for interpretation' dialogue. For detectors with a shape calibration in the permanent database, the width of the filter is taken from the shape calibration and adjusted as the width of peaks increases from low energy to high energy.

Edit list of peaks

The list of detected peaks is one of the standard lists of items that the program maintains. Like all other lists, it is edited with the 'Edit list' dialogue.

If a peak is to be inserted or edited, the 'Peak search record' dialogue pops up.

Peak search record dialogue

In this dialogue, the peak position (in terms of energy) and significance can be set.

The significance is the ratio of peak area to uncertainty, for example, a peak with 100 counts on zero background would have a significance of 100/√100 = 10.

The significance of the peak must be larger than 5 in order for the peak to be fitted and used in the shape calibration.

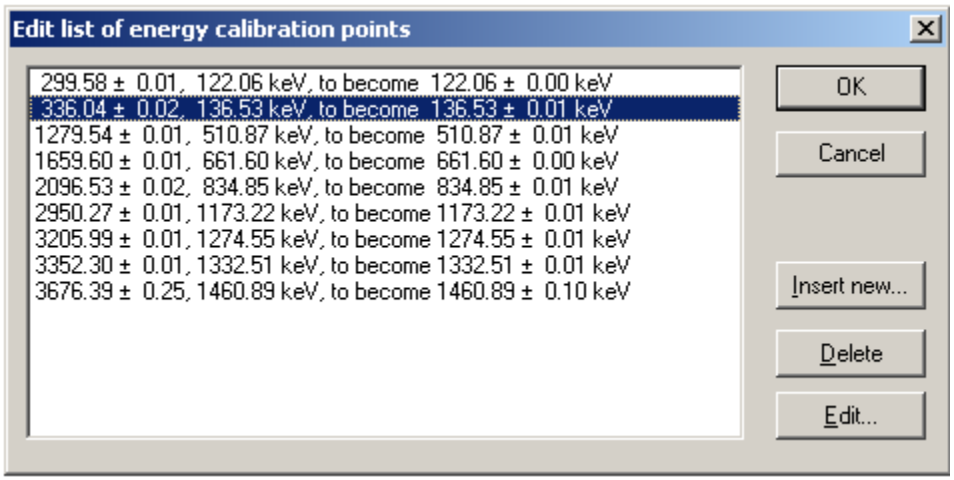
Fit calibration peaks

The peaks with significance larger than 5 and not overlapping with other peaks are fitted, with all shape parameters determined in the fit. More on peak shape in the Basics chapter.

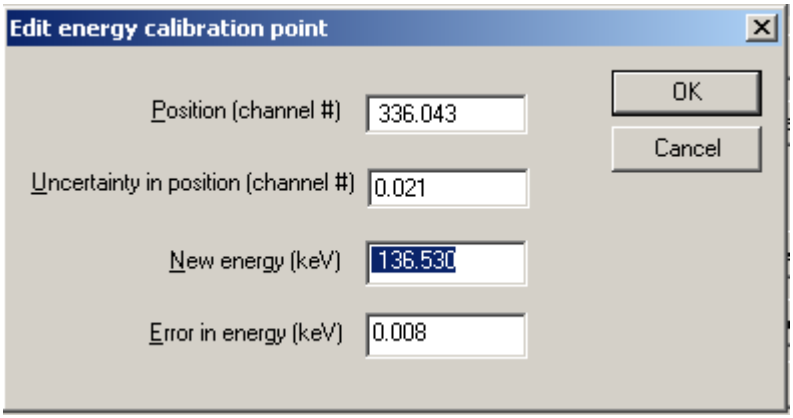
Energy calibration

Usually, an energy calibration is present in the system somehow. The spectrum file may contain an energy calibration, the peak area file may contain one (which then overrules the calibration in the spectrum file), and there may be one in the permanent database. When the last one is not identical to the one stored with the spectrum or with the peak areas, the user is asked what to do. If all these are not present, a unity calibration is used where channel number translates directly to energy in keV.

So, one way or the other, some energy calibration is always present. When the Energy calibration option is selected, the program takes all fitted calibration peaks and puts them in a list for the user. This list is one of the standard lists maintained by the program and is edited like all the others. The first dialogue that pops up shown looks like this:



and when a specific entry is to be inserted or edited, the dialogue that pops up looks like this:



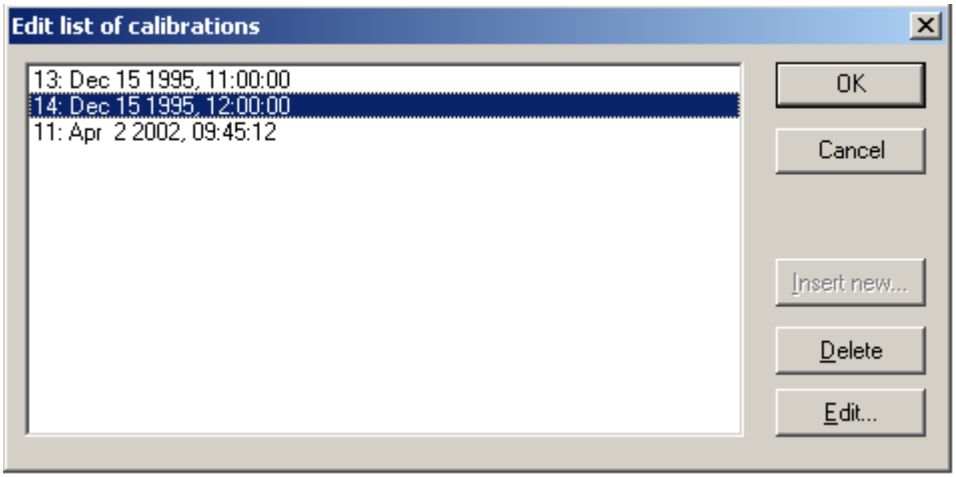
The use is to select a few peaks (five or more is recommended) and enter the correct associated photon energies. When exiting from the list edit dialogue, the calibration is performed. The program attempts to fit the energy data points with a straight line first, and then with a quadratic polynomial, and keeps what yields the best fit. The resulting calibration curve can be inspected with View/Curves for the spectra/Energy.

Save current energy calibration.

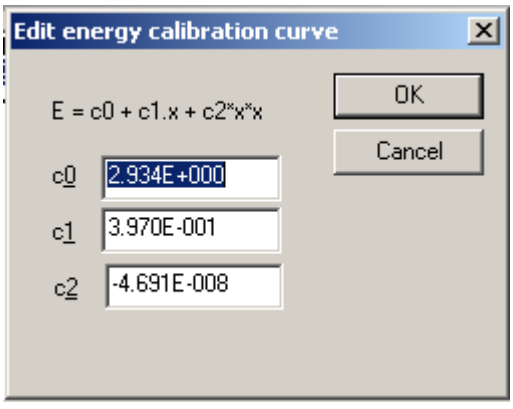
The current energy calibration is stored in the permanent database. In that database, the energy calibrations are stored according to detector used and the acquisition time of the spectrum. The polynomial coefficients can be inspected and even modified through the Detector/Energy Calibrations/List of energy calibrations option.

Edit energy calibrations.

Energy calibration entries can be deleted, inserted and edited. The list of energy calibrations is a standard list, edited like the others in the system. The list is offered to the user like this:



Each entry can be edited with the dialogue shown here:



FWHM calibration

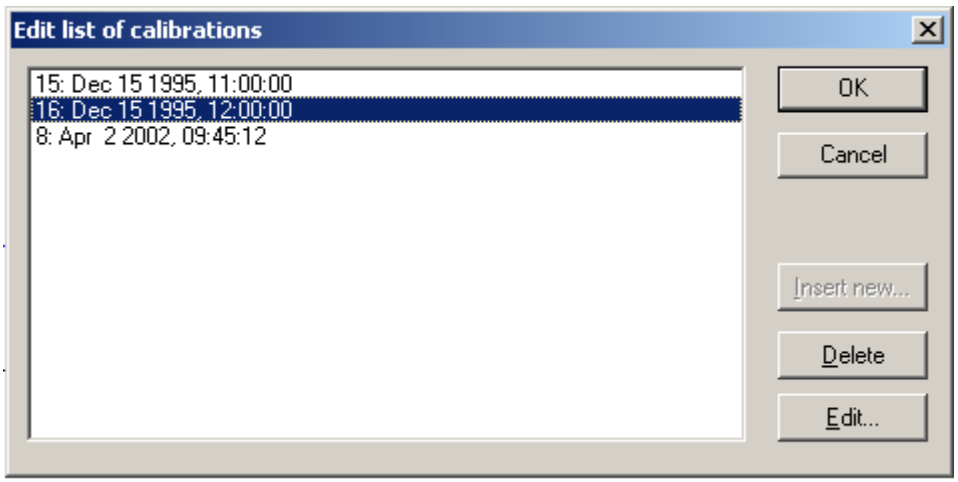
The FWHM calibration can be performed after the Spectrum analysis/Calibration/Fit calibration peaks option has een used. The program asks whether a pulser peak is present in the spectrum, which is than recognized because of its narrow shape. Make sure you answer “no” to that question if you don’t have a pulser, because if you answer “yes”, incorrect dead-time corrections and missing element concentrations will result. A square root relation is used to relate peak width to energy, and straight lines to associate the low-energy and high-energy tail parameters to the peak energies. An exception is made for the Doppler-broadened 511 keV peak, and also for the pulser peak if present. The resulting curves can be inspected with View/Curves for the spectra.

Write current shape calibration.

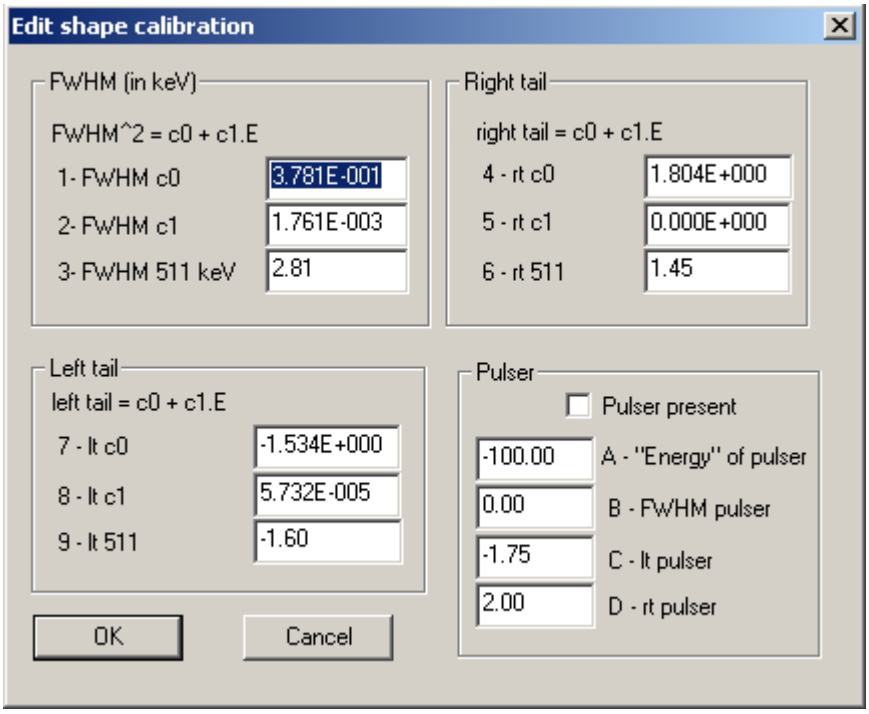
The current FWHM and tail-parameter calibration is stored in the permanent database. In that database, the calibrations are stored according to detector used and the acquisition time of the spectrum. The polynomial coefficients can be inspected and even modified through the Detector/Shape Calibrations/List of shape calibrations option.

Edit shape calibrations.

Shape or FWHM calibration entries can be deleted, inserted and edited. The list of shape calibrations is a standard list, edited like the others in the system. The list is offered to the user looking like this:



Each entry can be edited with the dialogue shown here:



Analyze all peaks.

All peaks in the spectrum are detected and fitted as describes in the Basics section.

Reanalyze all peaks.

The current estimates are replaced by the fit results and the fit is repeated. This may be helpful when dealing with pairs of peaks that are contributing to each other's fitting regions, when the first estimates are much worse than the fit results.

Write peak areas to file.

The peak energies and areas are written the a .k0p file, in the same folder as where the original spectrum resides. This should be the series folder. The contents of the .k0p file are the ones used for interpretation of the sample. Also, a .k0b file is written that stores the intermediate fit results, including the user's actions and manipulations.

View menu commands

The View menu offers the following commands. The view shown is always updated according to the current status of the sample. The selected view has no influence on the actions performed with the options in the Edit menu.

History	Show the history of the sample of interest
Raw spectra	Show the raw spectra of the sample of interest
Curves for the spectra	A menu pops up with available curves.
Peak fit views	A menu pops up with available views of fitted regions in the spectrum.
Efficiency curves for the spectra	Show the efficiency curves for the spectra of the sample of interest
Flux parameter to view	Choose which flux parameter is to be shown in the plot of the flux parameter map
Map of flux parameter	Show a plot of the flux parameter map relevant for the current sample
Graphical results	Show the interpretation results in graphical form (works for all kinds of samples)
Fitted efficiency curve	Show the interpretation result in the form of fitted efficiency curves (calibration sources only)
Numerical results	Show the interpretation results as text
Select spectrum of interest	Select which spectrum to see specifically in the Graphical results
Options for plot/views	Make a few choices that determine how the graphs look, and how peak positions are represented (energy of channel)
Zoom in mode	When set, the left mouse button zooms in, in spectrum plots
Zoom out mode	When set, the left mouse button zooms out, in spectrum plots.
Toolbar	Shows or hides the toolbar.
Status Bar	Shows or hides the status bar.

History command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the history of the current sample, that is, the times of packaging, irradiation and measurement, and the irradiation flux if known.

Raw spectra command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the raw spectra of the current sample. Like all spectrum plots, the graph is interactive. By right-clicking on a peak, a variety of information can be obtained, as explained here.. When viewing a peak fit, estimate or the parameters, the previous or next region can be selected with the left and right arrow keys.

Multiplet pop-up menu

This menu appears when right-clicking on a peak when viewing raw spectra. The options shown are the following:

Assignment of peak	This option is available after interpretation only. The constituents of the peak as determined in the interpretation step are shown.
Estimate View	The plot is shown of the estimated peaks in the fitted region. Once this is shown, the estimate can be modified.
Fit view	The plot is shown of the fitted peaks in the fitted region. Once this is shown, the estimated parameters can be modified and the fit repeated.
Integration view	The plot is shown where the user can determine the peak area by integration.
Values of parameters	The values of the estimated and fitted parameters are shown for all the peaks in the region. More on peak shape in the Basics chapter.
Spectrum view	The view switches to what can also be selected with the View/Raw spectra option

Peak pop-up menu

This menu pops up when right-clicking on a peak when viewing the fit or the estimate.

Assignment of peak	This option is available after interpretation only. The constituents of the peak as determined in the interpretation step are shown.
New peak here	A new peak is inserted in the estimate at the clicked-on location.
Delete peak here	The peak closest to the clicked-on position is deleted from the estimate.
Estimate View	The plot is shown of the estimated peaks in the fitted region. Once this is shown, the estimate can be modified.
Modify estimate	The parameters of the estimate for the region can be modified.
Fit view	The plot is shown of the fitted peaks in the fitted region. Once this is shown, the estimated parameters can be modified and the fit repeated.
Integration view	The plot is shown where the user can determine the peak area by integration.
Values of parameters	The values of the estimated and fitted parameters are shown for all the peaks in the region. More on peak shape in the Basics chapter.
Integrate peak	The peak areas in the region are determined by integration. The program switches to the integration view and the user can modify the proposed integration.
Reject integration	The integration performed is discarded and the fit result taken as the final result again.
Spectrum view	The view switches to what can also be selected with the View/Raw spectra option

Insert new peak here.

A new peak is inserted in the list of peaks in the estimate for the region. The peak energy is taken from the mouse click, the shape parameters from the shape calibration, and the area is estimated at 100 counts. Each of the estimated parameters can be modified by hand in the 'Edit peak fit' dialogue box that pops up. It is recommended to perform this action in View Estimate Mode, so the improvement can be seen directly.

Delete peak here.

The peak closest to the clicked-on position is deleted from the estimate. It is recommended to perform this action in View Estimate Mode, so the improvement can be seen directly.

Modify estimate.

The estimate for a region in the spectrum can be modified. After modification, the fit of the peak parameters to the measured spectrum is repeated.

The estimate for a region consists of a set of parameters that apply to the whole region and sets of parameters for the individual peaks.

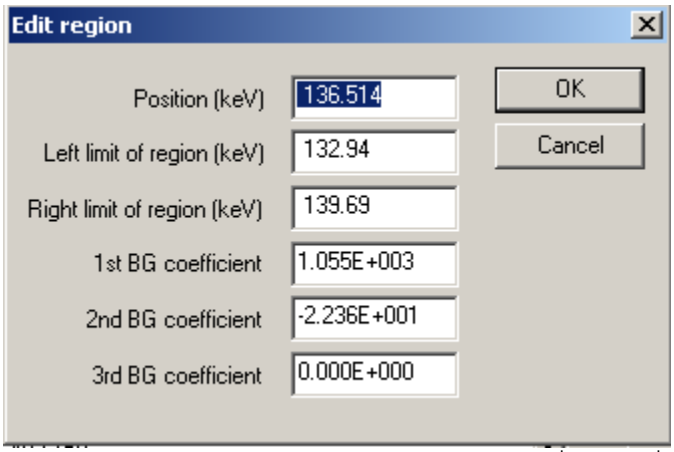
The program shows the complete list of regions with the current region highlighted as the proposed choice, in the *Edit region and peaks* dialogue which is a version of the more general dialogue for editing lists of lists.

When the user chooses to edit the proposed region, the Edit region dialogue pops up. If the user chooses to edit the list of peaks, another dialogue pops up which allows him to edit the list of peaks for the region. This dialogue is a version of the more general dialogue for editing lists.

When editing the list of peaks, the user can choose to insert a new one or modify an existing one, using the Edit peak fit dialogue.

Edit region dialogue.

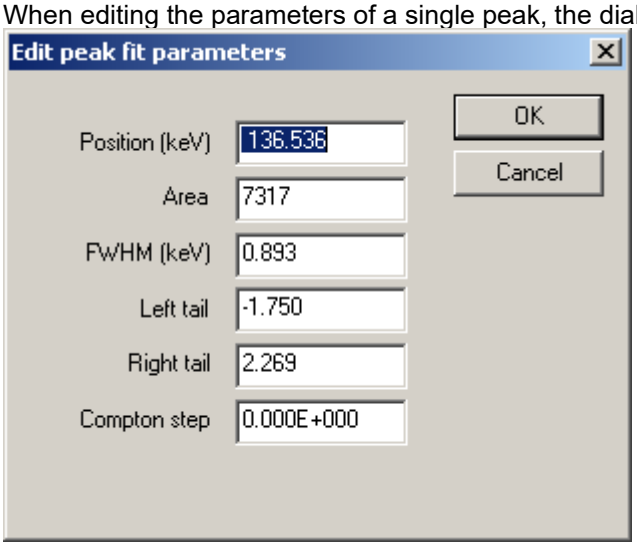
When editing a multiplet, the parameters applying to the whole region are of interest first. These are offered to the user as shown below.



It usually clears up the situation to set the 2nd and 3rd background coefficients to 0, so that the continuum becomes a horizontal line. The left and right limits of the region may need adjustment to stay clear from neighboring peaks, or to extend the region and get better leverage on the continuum under the peak.

Edit peak fit dialogue.

When editing the parameters of a single peak, the dialogue looks like this:



The meaning of these parameters is described in the Basics section.

Curves for the spectra' pop-up menu

The meaning of the peak shape parameters is explained in the Basics section.

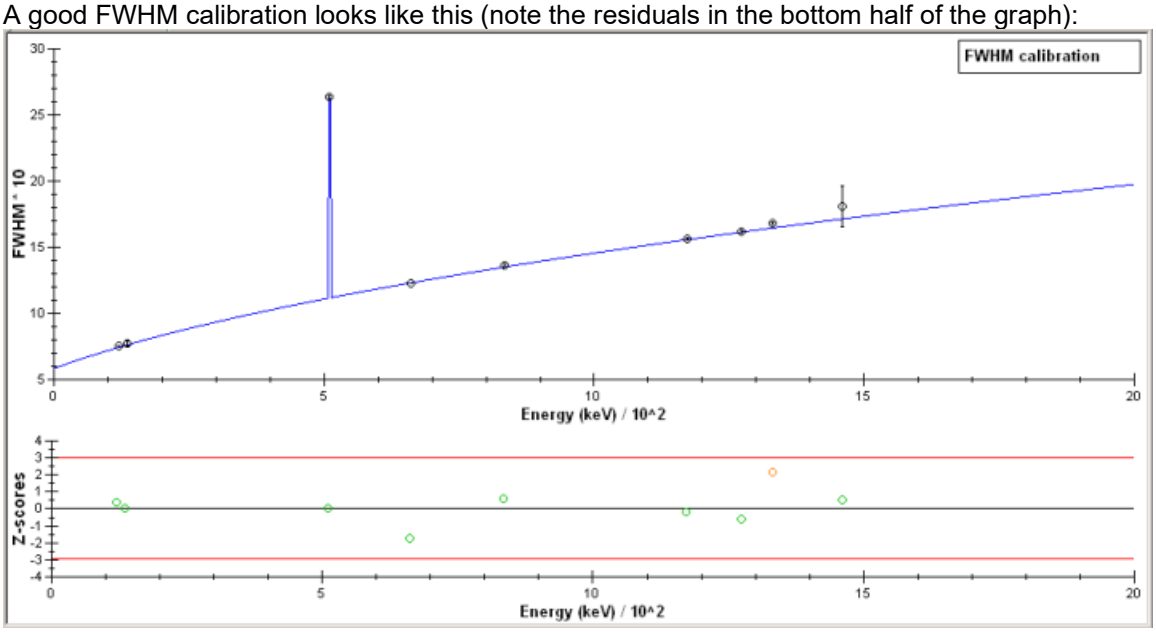
FWHM	Show the history of the sample of interest

Low-energy tail parameter	Show the raw spectra of the sample of interest
High-energy tail parameter	A menu pops up with available curves.
Energy	A menu pops up with available views of fitted regions in the spectrum.

View FWHM curve

More on peak shape in the Basics chapter.

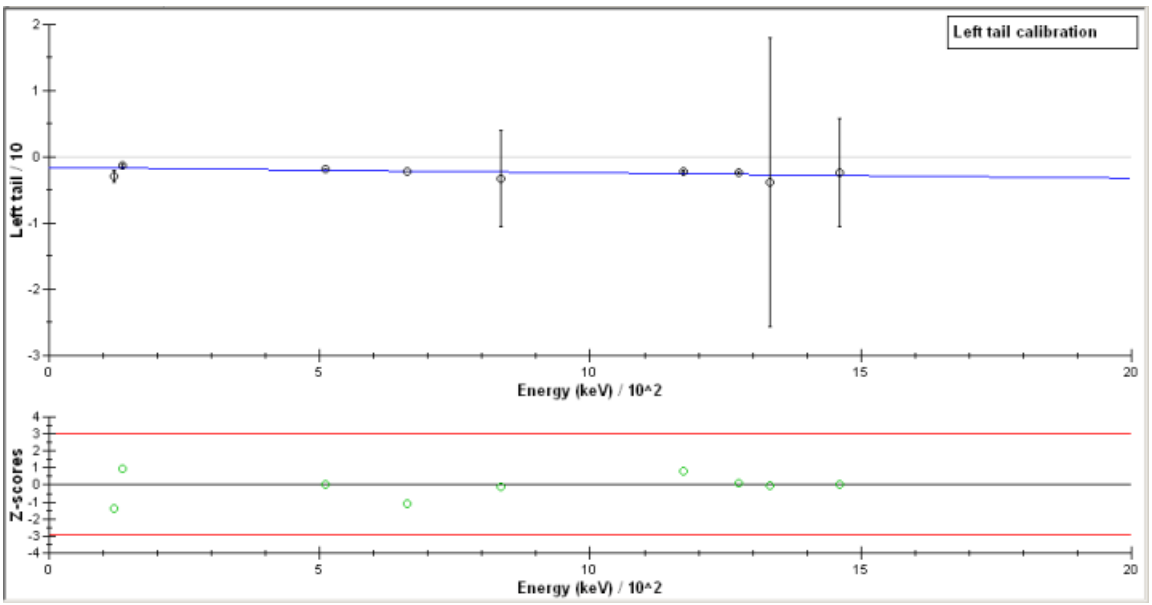
A good FWHM calibration looks like this (note the residuals in the bottom half of the graph):



View low-energy tail parameter.

More on peak shape in the Basics chapter.

A good low-energy (a.k.a. left) tail parameter calibration looks like this (note the residuals in the bottom half of the graph):

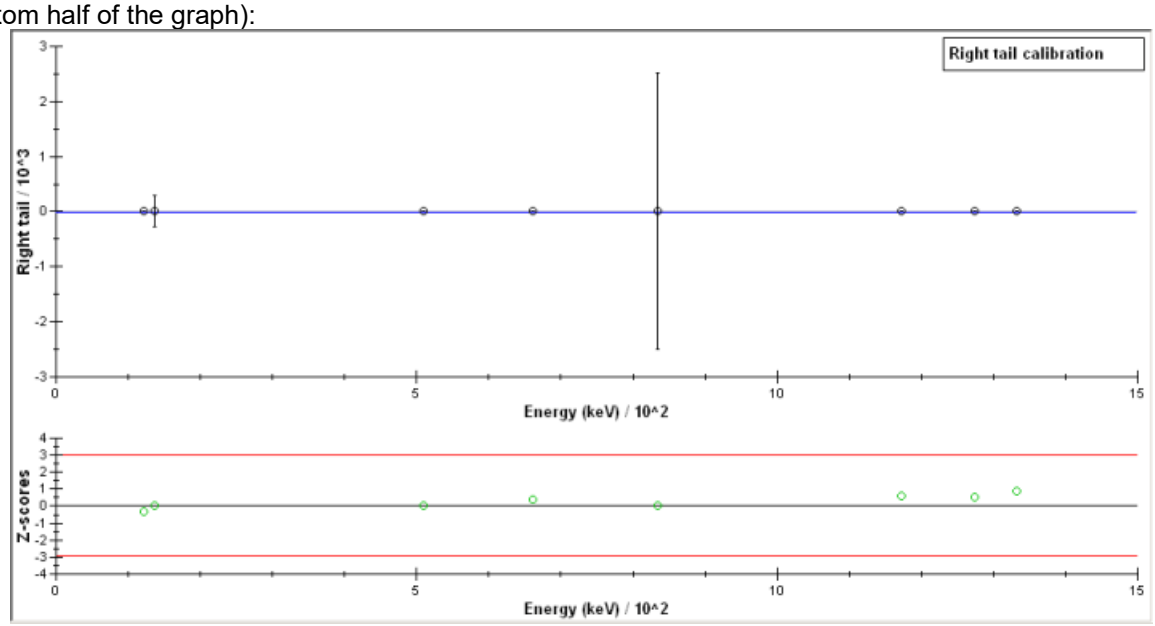


Low-energy tail parameters should normally have values less than -1.6,values closer to 0 suggest overlooked multiplet components or charge collection problems in the detector crystal. More on peak shape in the Basics chapter.

View high-energy tail parameter.

More on peak shape in the Basics chapter.

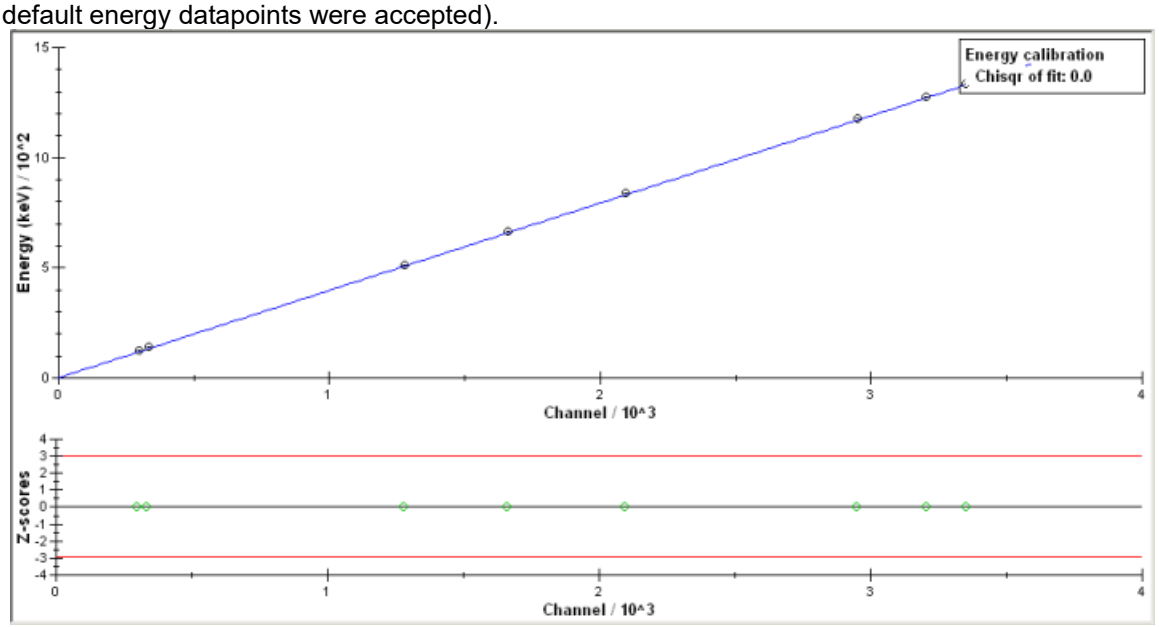
A good high-energy (a.k.a. right) tail parameter calibration looks like this (note the residuals in the bottom half of the graph):



High energy tail parameters should be larger than 1.5. Values closer to 0 suggest overlooked multiplet components or bad pile-up rejection adjustment. More on peak shape in the Basics chapter.

View energy calibration

The energy calibration plot looks like this (the example looks much too good to be true, because the default energy datapoints were accepted).



Peak fit views' pop-up menu

More on peak shape in the Basics chapter.

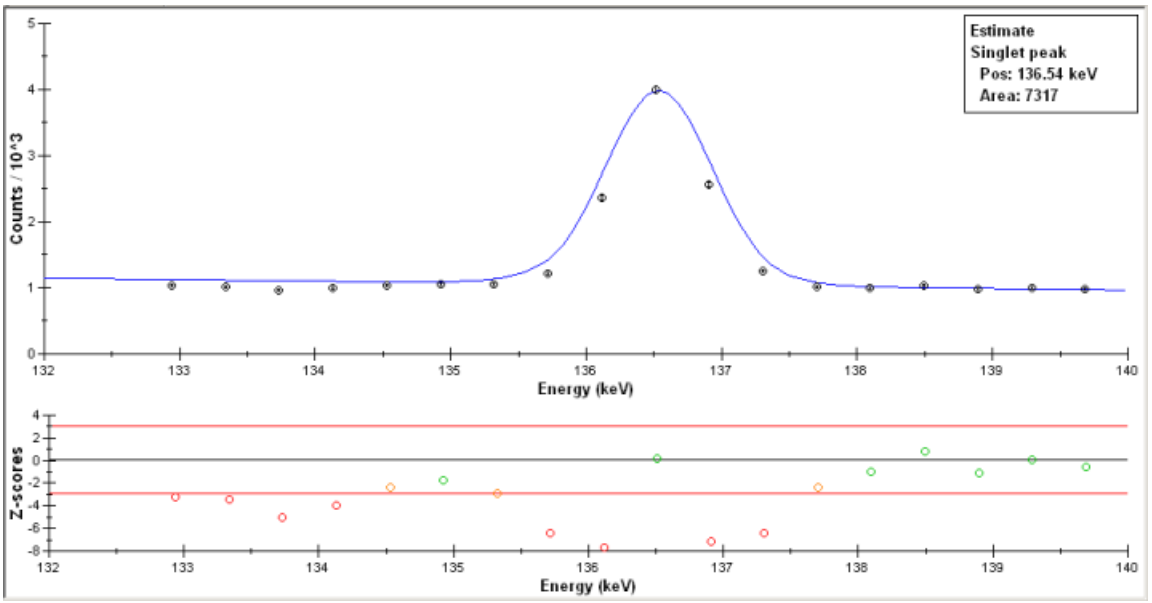
Estimate View	Show the estimate for the region
Fit view	Show the fit for the region
Values of parameters	Show the fitting parameters
Integration view	Integrate the peak area
Next region	The next region is selected.
Previous region	The previous region is selected.

In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes

(estimate, fit, parameter values and integration). The space bar or any other key takes you back to the "View raw spectrum" view mode.

View estimate

An example of a peak estimate is shown below.



Such an estimate can be manipulated by right-clicking and choosing to modify the estimate.

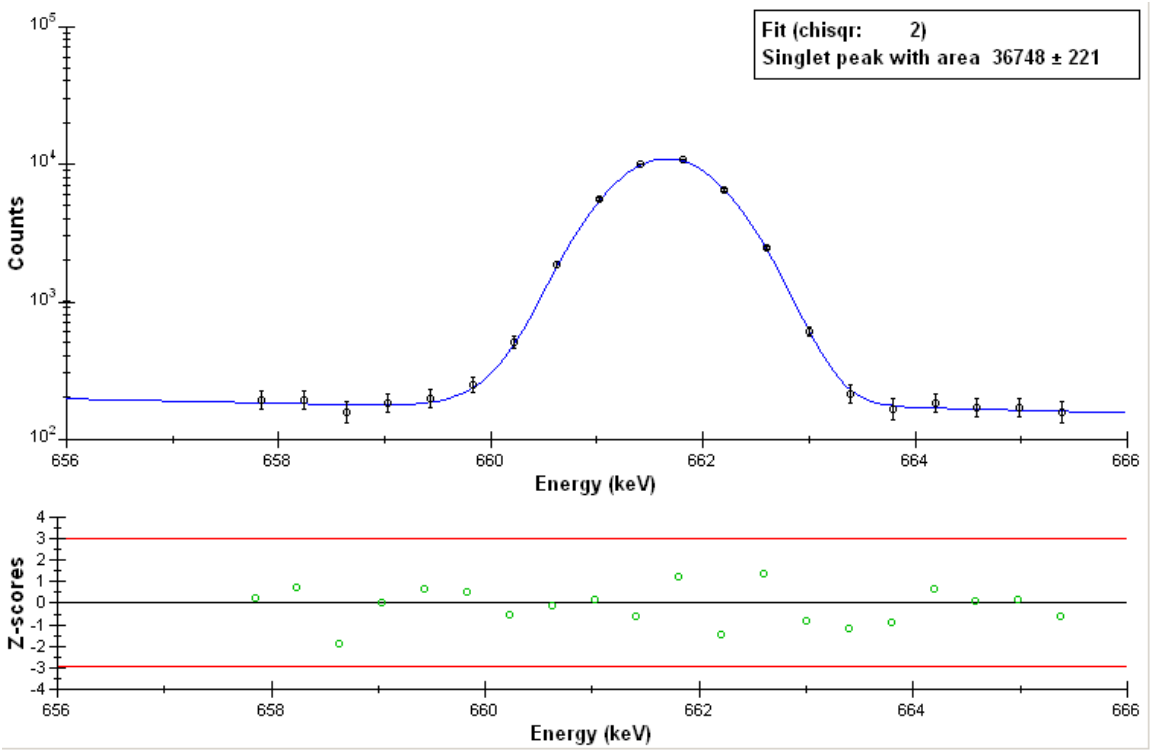
In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes (estimate, fit, parameter values and integration). The space bar or any other key takes you back to the "View raw spectrum" view mode.

View fit

More on peak shape in the Basics chapter.

A good peak fit looks like this (if the y-axis has been set to logarithmic with View/Options for plot):

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In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes (estimate, fit, parameter values and integration). The space bar or any other key takes you back to the "View raw spectrum" view mode.

Values of parameters

All parameters relevant to the fit in the current region are shown:

Singlet near 137 keV
Estimate region from 132.94 to 139.69 keV
Fitted region from 132.94 to 139.69 keV
Chisqr of fit: 2.2

PARAMETER	ESTIMATED VALUE	FITTED VALUE	1 SD.UNCERTAINTY
Sum Gauss area	7317	6283	139
Sum total area	7416	6438	143
Range (keV)	4.0	3.2	
BG coeff. 0	1.055E+003	1.013E+003	2.100E+001
BG coeff. 1	-2.236E+001	-1.544E+001	5.433E+000
BG coeff. 2	0.000E+000	-1.601E+000	4.582E-001
Energy (keV)	136.536	136.532	0.008
Area Gaussian	7317	6283	139
FWHM (keV)	0.90	0.77	0.02
Left tail	-1.75	-1.42	0.19
Right tail	2.00	5.00	291.59
Compton step	0.00E+000	1.05E-002	1.10E-002
Area inc.tails	7317	6438	143
Range (keV)	2.3	1.89	

More on peak shape in the Basics chapter.

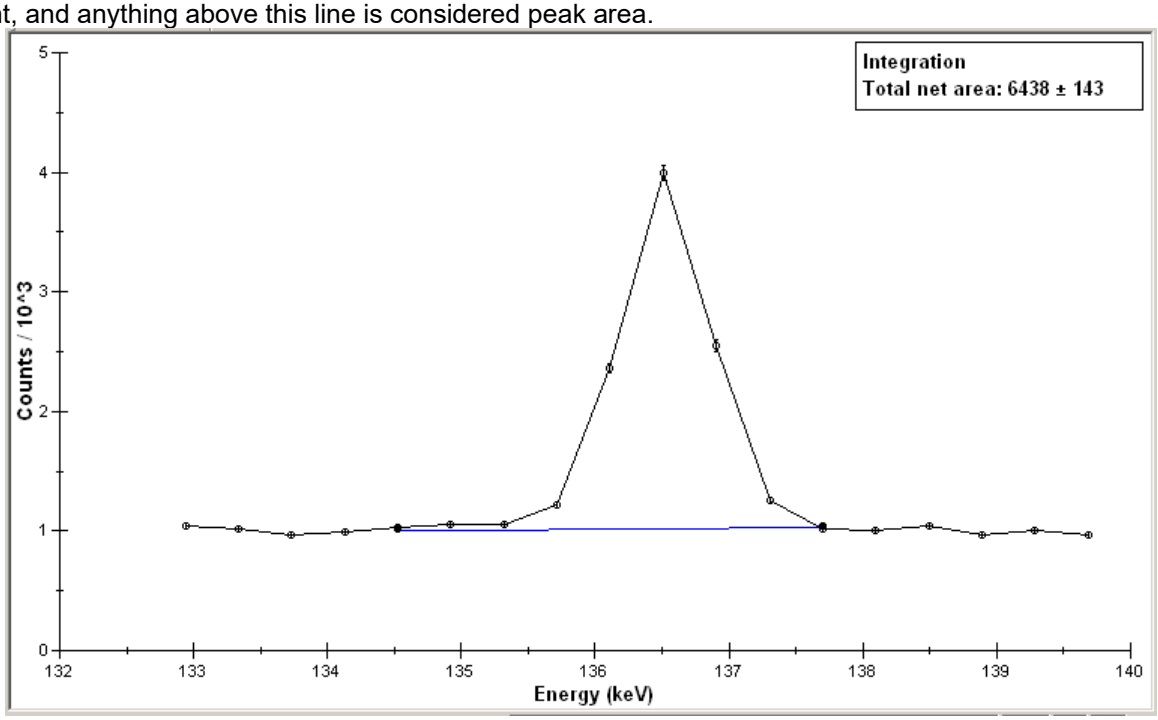
In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes

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(estimate, fit, parameter values and integration). The space bar or any other key takes you back to the “View raw spectrum” view mode.

Integration view

An integrated peak looks like this. The user may select different channels than the program initially suggests to start and stop the integration. The average of 3 channel contents is used to determine the continuum level both left and right of the peak. A straight line is drawn from point to point, and anything above this line is considered peak area.



In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes (estimate, fit, parameter values and integration). The space bar or any other key takes you back to the “View raw spectrum” view mode.

Integrate peak.

The integration view is switched on and the program suggests from where to where the integration might be performed, based on the current fit results. The user can choose to do it differently by left-clicking to the left and right of the peak position.

In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes (estimate, fit, parameter values and integration). The space bar or any other key takes you back to the “View raw spectrum” view mode.

Reject integration.

The selected channels for integration are erased, and the fit again determines what peak area and energy will be written to file in the end.

In any of these views, the right arrow key takes you to the next region, the left arrow to the previous one, and with the up and down arrow keys you can cycle though the four region view modes (estimate, fit, parameter values and integration). The space bar or any other key takes you back to the “View raw spectrum” view mode.

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Efficiency curves for the spectra command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the full-energy peak efficiency and the peak-to-total curves associated with the spectra of the current sample. If the sample was just interpreted, both the curves for the reference geometry and the curve for the actual counting geometry will be shown. The datapoints in the latter curve only serve to indicate what energies were used for the curve conversion.

Flux parameter to view command (View menu)

When this view mode is selected, a dialog box will open that allows for selection of the flux parameter to see in the flux parameter map plot: The thermal flux, the neutron temperature T, the thermal/epithermal ratio f, the alpha parameter or the Fast flux.

Map of flux parameters command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the map of the currently selected flux parameter. The plot only shows the values of the selected parameter in the column of the current sample, along with the polynomial fitted to the measured values as a function of row number. Only row numbers 0 through 255 are available as possible values, but one could use them as position indicators with a mm precision in an irradiation container of ordinary size. The solid plotted point indicates the current sample position, the other point the comparators in the same column.

Graphical results command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the interpretation of the selected spectrum of the current sample in a three-pane representation. The graph is interactive.

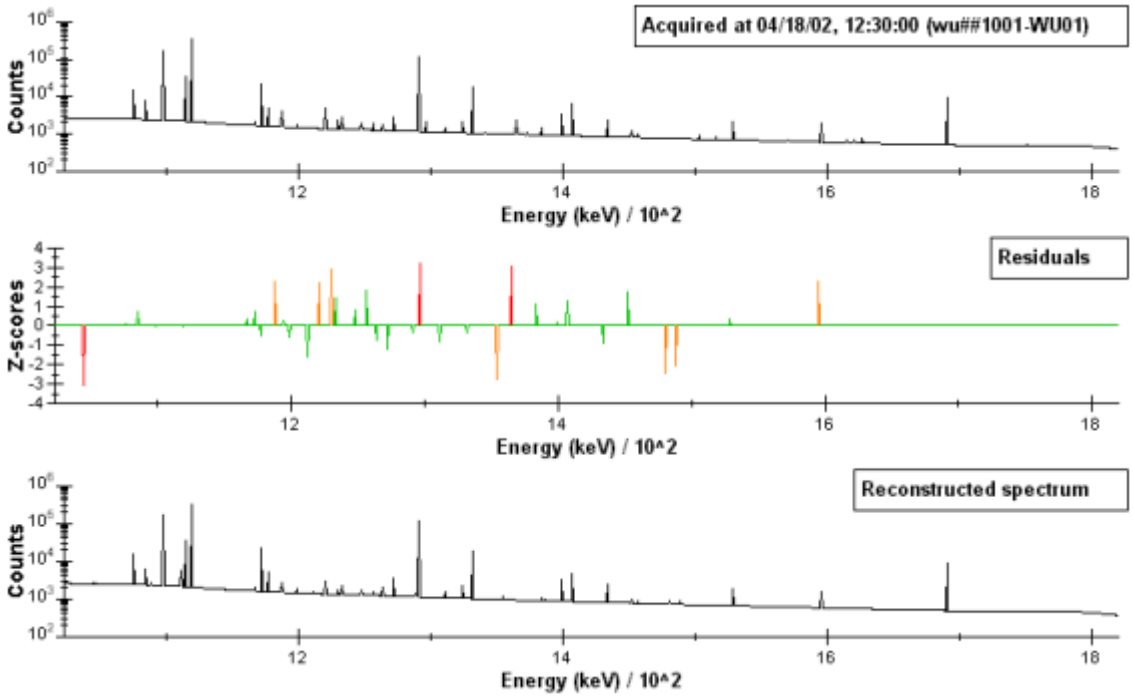
The top pane shows the measured spectrum, but not in the form of raw channel contents. Instead, what is shown is the continuum observed in the raw spectrum, with the peak areas and energies as read from file superposed.

The bottom pane shows the reconstructed spectrum, consisting of the same continuum channel contents, with peak energies and areas superposed that are calculated from the sample history, the efficiency curves and the interpretation results. That is the computed sample composition, for ordinary samples, blanks and reference materials. For comparators, it is the computed set of neutron flux parameters. For calibration sources, it is the efficiency curve that is the interpretation result, the source activities were known from the start.

The middle pane shows the differences between the measure and the reconstructed spectrum, after standardization, that is, the difference divided by its own uncertainty. The resulting values are known as z-scores, and if the interpretation is perfect, they should fall between -2 and 2 in 95% of the cases, and between -3 and 3 in 99% of the cases. Values below 2 are indicated in green, between 2 and 3 are indicated in orange, values exceeding 3 in red.

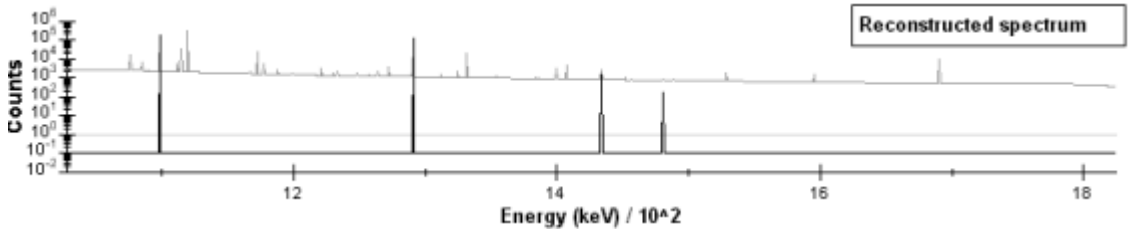
Positive ‘red’ residuals may be the result of unrecognized peaks being present in the spectrum, and in that case have no effect on other results. But negative ‘red’ residuals indicate a real conflict between peaks of one element and require further investigation. Quite often, one will observe positive and negative ‘red’ residuals right next to each other in the high-energy half of the spectrum. This indicates that the energy calibration is off by too much for proper identification of peaks and should be redone.

Escape peaks are usually recognized as such but not used in k0_IAEA, resulting in a peak that is present in the measure spectrum but not in the reconstructed spectrum, and still with a z-score of 0.



A reasonably nice interpretation results, even though there are some red residuals to be seen.

In the View/Plot options dialog, one can choose to see the peaks of an entity of interest highlighted in the lower pane of the three panes. An entity of interest can be an activation reaction (for comparators), a radionuclide (for calibration sources) or an element. It will be plotted as superposed on a zero continuum to make it easier to see. The works best when the y-axis is logarithmic, also as determined in the View/Plot options dialog



The bottom pane of the graph shown above, now with Fe highlighted.

Right-clicking on a peak with the mouse will pop up a window with the interpretation data of the peak, in a format as described for the log file, only this time you are allowed to choose whether the peak is to be deselected in the interpretation process or not. The list of deselected peaks can also be edited with Edit/interpret Options.

Peak information dialog

This dialog shows information about observed and detected peaks near the energy that was pointed at with the mouse. The information is presented in a format as described for the log file, only this time you are allowed to choose whether the peak is to be deselected in the interpretation process or not. (The list of deselected peaks can also be edited with Edit/interpret Options.)

Three buttons are available to this end:

Deselect (some of) these peaks for interpretation.
If only one peak is shown in the dialog window, this peak is added to the list of deselected peaks. If more than one peak is in scope, the general-purpose list edit dialog pops up showing all the peaks in

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scope. Peaks that are to be interpreted should be deleted from this list before exiting with the OK button.

Select (some of) these peaks for interpretation.

If only one peak is shown in the dialog window, this peak is removed from the list of deselected peaks. If more than one peak is in scope, the general-purpose list edit dialog pops up showing all the peaks in scope. Peaks that are not to be interpreted should be deleted from this list before exiting with the OK button.

Deselect all peaks of the Highlighted Entity

All peaks that the current highlighted single entity (to be selected with the View/Options dialog) apparently contributed to are added to the list of deselected peaks. Selecting a single peak of the entity again afterwards is the quickest way to get a concentration from a single peak. Also useful if flux monitor foils were counted separately, to stop the program from expecting Au peaks in a Zr spectrum and vice versa.

Edit list of deselected peaks for interpretation

This button gives the user full access to the list of deselected peaks, no matter which energy was pointed at with the mouse. The exact same access is provided through Edit/interpret Options.

Deselection of peaks

Normally, because of the holistic approach implemented in k0_IAEA, all peaks are considered when interpreting the spectrum or spectra and calculation elemental concentrations. But some peaks are just too hard to handle sometimes. For example, the lead X-rays coming from the detector shielding are not meaningful. The same is usually true for the 511 keV annihilation peak.

These peak energies are deselected by default when a new series is created. Once a sample has been interpreted in the new series, these five peaks can be selected for use after all, and others can be deselected if so desired.

Deselection means that the program sets the uncertainty in the peak area to a very large number in the interpretation process and displays no discrepancies for these peaks afterwards.

The list of deselected peaks applies to the series as a whole. Whenever a peak has been selected or deselected, once you are certain that you did the right thing, all samples should be reinterpreted to ensure that they were all dealt with the same way, and to make the reference material results useful for Quality Assurance.

If the samples in the series have been measured more than once, a list of deselected peaks is maintained for each spectrum.

The deselected peaks are stored in a binary file in the series folder. The default list is stored in the \k0_iaea folder. If a particular set of deselected peaks is found to be useful again and again, one might consider replacing the original default list file with the customized list file. Remember that such custom lists are only applicable if the analysis procedure and the type of material are very similar! The analysis procedure must be the same with respect to the number of measurements per sample, the decay times, and the irradiation time.

Fitted efficiency curve command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the efficiency curve that was just determined by fitting to either a measured spectrum or to imported efficiency data.

Numerical results command (View menu)

When this view mode is selected, the main window of k0_IAEA will show the interpretation results in numerical form. If the sample was just interpreted, some intermediate results will be shown that are not stored in the series database. The information stored in the database is always shown.

Concentrations with precisions and accuracies are shown. Uncertainty propagation is described here.

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Select spectrum of interest command (View menu)

When this view mode is selected, a dialog pops up that allows for the selection of the spectrum of interest. Sometimes it is necessary to select a specific one, that is when efficiency calibrations are being performed, or when the View/Graphical results command is to be used. Sometimes it is nicer to see all spectra or efficiency curves of a single sample at the same time - 'all' can be selected then. When a sample has only one spectrum anyway, the choices are equivalent.

Options for plot/views command (View menu)

When this view mode is selected, a dialog pops up that allows for a number of choices to be made that affect the graphs.

The axis type can be set to linear or logarithmic. This choice will always affect the y-axis, but only the x-axis of efficiency curve plots.

A grid can be plotted.

If an Ortec Zero Dead Time spectrum is being acted on, Poisson statistics do not apply, and each spectrum consists of two parts: The dead-time corrected channel contents and their variances. With the "Variance spectrum" option, the variances can be inspected. For normal spectra with Poisson-distributed channel contents, the two are identical.

An entity of interest can be selected and shown as explained in View/Graphical results.

The 'Nice X-axis' choice determines how smoothly the x-axis will scroll when the user is navigating in spectrum plots.

The 'use energy Calibration' choice determined whether channel numbers or energies are used for the x-axis in the raw spectra plots, the lists of peak positions, the fitted regions, as well as in the dialogues where peak fitting parameters can be adjusted. This even applies to the results plots, to facilitate going back and forth between assignment information from the interpretation and the peak fit.

The "residuals with calculated Uncertainties" option only applies to the Graphical view of the interpretation results, where the middle of the three graphs shows residuals. These residuals are calculated from the difference between the measured peak area and the peak are that the software can account for from the composition and history of the sample, divided by the uncertainty. That uncertainty can be either the uncertainty in the measured area exclusively (when this option is not selected), or the uncertainty in the measured peak areas and the uncertainty in the explained peak area combined (when the option is selected). Discrepancies will be easier to see when the option is not selected.

When the option is not selected, many bad residuals will show up in the graph. This is because it is easy to measure a photopeak with precisions better than 0.1 % - but the theoretical gamma-ray yields and the k0-values have much larger uncertainties that are not accounted for in this view!

Zoom in mode / Zoom out mode command (View menu)

These two options determine how an interactive graph will respond to a left mouse click. Zooming in and out can also be performed with the up and down arrow keys, as well as with the scroll button on the mouse.

Toolbar command (View menu)

Use this command to display and hide the Toolbar, which includes buttons for some of the most common commands in k0_IAEA, such as File Open. A check mark appears next to the menu item when the Toolbar is displayed.

See Toolbar for help on using the toolbar.

Toolbar



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The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to some tools used in k0_IAEA,

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

Click	To
	Open an existing document. k0_IAEA displays the Open dialog box, in which you can locate and open the desired file.
	Go to the previous sample in the current series.
	Go to the next sample in the current series.
	Go to the previous spectrum of the current sample
	Go to the next spectrum of the current sample

Status Bar command (View menu)

Use this command to display and hide the Status Bar, which describes the action to be executed by the selected menu item or depressed toolbar button, and keyboard latch state. A check mark appears next to the menu item when the Status Bar is displayed.

See Status Bar for help on using the status bar.

Status Bar

The status bar is displayed at the bottom of the k0_IAEA window. To display or hide the status bar, use the Status Bar command in the View menu.

The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area similarly shows messages that describe the actions of toolbar buttons as you depress them, before releasing them. If after viewing the description of the toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button.

The middle area of the status bar shows the current sample.

The right-hand areas of the status bar indicate the status of the current sample:

Indicator Description

CMPL All the information needed for interpretation of the current sample is present.

INTThe current sample was just interpreted, and all the intermediate data are still in memory, allowing for interactive checking of the result in the View / Graphical results mode.

RSL Results for the current sample are present in the series database and can be inspected in the View / Numerical results mode.

Interactive graphs

All spectrum plots in k0_IAEA are interactive. When the mouse is mover over a certain area and left-clicked, the plot will zoom in or zoom out depending on the View/Zoom in mode or Zoom out mode settings. The up and down arrow keys will always zoom out and zoom in, independently of these settings. The mouse wheel also allows for zooming in and out. The right and left keys will move the spectrum left and right, the PgUp and PgDn keys also but in larger steps; the Home and End keys will move it all the way to the left and right.

The View/Plot options dialog allows the user to set the 'Nice X axis' option. When this option is selected, the x-axis will not scroll left and right as smoothly, but will contain a nice number of intervals, with ticks at the beginning and end.

When an interpretation result is viewed in the form of a three-pane spectrum plot, information about any specific peak can be retrieved by right-clicking on the peak. The formatting of this information is the same as in the last part of the log file.

The interactive graphs remember what region of the spectrum was last inspected, but in terms of channel numbers.

Irradiation facility menu commands

The irradiation facility menu offers the following commands, which enable you to store the flux parameters determined in the current series in the permanent database for future use in other series.

Irradiation of interest	In case multiple irradiations were performed within this series, choose the irradiation of which the flux parameters are to be stored
Store flux parameters	Store the average of all flux parameters determined for the irradiation of interest in the permanent database.
Plot	Plot the flux parameter of interest as stored in the permanent database as a function of time for the current irradiation facility

Irradiation of interest command (Irradiation facility menu)

This option is necessary if comparators of complex composition have been re-used (as described in the How to... section), to make sure that the right set of flux parameters is saved with the Store flux parameters command.

Store flux parameters command (Irradiation facility menu)

This command will store the average of the flux parameters determined in the current irradiation of interest in the permanent database. They will be tagged with the date and time of irradiation. In the future, when a simple flux comparator has been used and the unknown flux parameters have to be retrieved from the permanent database, the last record preceding the time of irradiation of the simple comparator will be used to fill in the blanks.

Plot (Irradiation facility menu)

Takes the irradiation of interest (in case of reused comparators), otherwise simply the first irradiation of the current sample, retrieves the flux parameters from the permanent database and plots the one of interest (selected with the View/Flux parameter to view menu option) as a function of time.

Detector menu commands

The detector menu offers the following groups of commands, which enable you to store the efficiency curves determined from spectra in the current series in the permanent database for future use in other series. Also, efficiency curves can be exported and imported from here. Finally, raw efficiency datapoints can be exported.

Efficiency curves

Manual efficiency data entry	Enter or edit efficiency datapoints manually one by one.
Import efficiencies from file	Import efficiency data stored in a text file.
Export reference efficiency curves	Store the reference efficiency curves (i.e. **not** adjusted for the current spectrum and sample) in a text file for use in other programs
Export actual efficiency curves	Store the actual efficiency curves (i.e. adjusted for the current spectrum and sample) in a text file for use in other programs
Export efficiency datapoints to file	Store the efficiency datapoints in a text file for use in other programs
Store efficiency curves	Store the fitted efficiency curves in the permanent database.

Energy calibrations

Store current calibration	obvious
List of calibrations	Obvious

Shape calibrations

Store current calibration	Obvious
List of calibrations	Obvious

Background spectra

Store background spectrum	The current spectrum is stored as background. The series that contains the spectrum used for this must remain on the hard disk after this, so it is advisable to always use the same series for background spectrum measurements.
List of background spectra	The list of background spectra is shown and can be modified

List of background spectra

The list of background spectra is one of the lists maintained by the system and it can be edited the standard way. No new background spectra can be entered, and also the contents of the background spectrum cannot be modified.

Import efficiencies from file command (Detector menu)

When this command is given, the program will prompt for a filename for the text file with the efficiencies to import. The format of this text file is described here. The data will be fitted immediately after import, and a message with the resulting chisqr will pop up.

If the chisqr is higher than say, 5, it will be necessary to take a look at the fitted curve and resolve the problem. Perhaps by determining the peak areas better, perhaps by correcting a mistake in the certificate, perhaps some other problem needs to be fixed. The data imported can be edited directly with the manual efficiency data entry command.

It is ok for a datapoint to specify a zero efficiency and a non-zero peak-to-total ratio or vice versa. The 0 values are simply ignored by the program.

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Manual efficiency data entry

Efficiency data can be entered or edited with the Edit list and Edit efficiency dialogs that pop up when this command is given.

Export reference efficiency curves to file command (Detector menu)

The program prompts for a filename. Efficiency data for predefined energies, taken from the curves selected as the best reference curves for the current sample and spectrum, **but not adjusted to the current counting geometry**, are exported to a text file of the same format as used for the import option.

Export actual efficiency curves to file command (Detector menu)

The program prompts for a filename. Efficiency data for predefined energies, taken from the curves selected as the best reference curves for the current sample and spectrum, **and adjusted to the current counting geometry**, are exported to a text file of the same format as used for the import option.

Export efficiency datapoints to file command (Detector menu)

The program prompts for a filename and the datapoints obtained from the current efficiency calibration just performed are exported to a text file of the same format as used for the import option.

Store efficiency curves command (Detector menu)

The newly fitted efficiency curves are stored in the permanent database. If they were fitted to a calibration spectrum by k0_IAEA, the program already knows what the detector and counting geometry are. If the datapoints were imported, the program will prompt for the detector and the sample-detector distance, with the Store efficiencies dialog box.

Store efficiencies dialog

This dialog allows one to choose the detector and set the sample-detector distance (that is the distance between the bottom of the outermost sample container and the end cap of the detector if the cylinder axis of the two are aligned, and the center-of-mass of the sample to the end cap distance in the side-looking geometry.

Edit efficiency dialog.

One datapoint, consisting of the
peak energy,
full-energy peak efficiency,
peak-to-total ratio,
single escape peak to full energy peak area ratio and
double escape peak to full energy peak area ratio

(all with absolute uncertainties) can be entered. Efficiencies are numbers between 0 and 1; peak-to-total ratios are, too. Escape peak ratios could be larger than unity but rarely are.

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Tools menu commands

The Tools menu contains the following commands:

File locations	Choose the permanent_data file location
Export libraries	Export the nuclear library data to text files.

File locations command (Tools menu)

This command allows one to select where in the network the permanent database resides. This will be necessary if one permanent database is to be used by multiple users working on different PCs.

Export libraries command (Tools menu)

Using this command, the user can export the various nuclear library files used by the program to text files. The format is described briefly here:

For k0_ list.txt

```
Na Na-24 1.000
(Element) (Isotope) (additional info for special activation-decay cases)
0
(file type format indicator)
2
( No. of gamma ray)
1368.60 4.680E-002 5.000E-004
(Energy) (k0-value and unc)
2754.00 4.620E-002 5.000E-004
```

For decay_scheme.txt

```
Mg-24
(Isotope)
1
(file type format indicator)
#levels: 5
(No. of Energy Level)
level 1: 1368.60 1.3700E-012 #trns: 1
(Level No.) (Energy) (half life in seconds)  (No. of transitions)
         0 1.0000E+000 1.0000E+000 0.0000E+000
        (to level #)  (probability of trans.) (probability of gamma)(KX-ray over gamma ratio)
level 2: 4122.59 3.8000E-014 #trns: 1
         1 1.0000E+000 1.0000E+000 0.0000E+000
level 3: 4237.90 7.3000E-014 #trns: 2
         1 2.3290E-001 1.0000E+000 0.0000E+000
         0 7.6710E-001 1.0000E+000 0.0000E+000
level 4: 5234.73 7.6000E-014 #trns: 2
         3 2.4952E-002 1.0000E+000 0.0000E+000
         1 9.7505E-001 1.0000E+000 0.0000E+000
#mothers: 1
(# nuclides decaying to this nuclide)
       Na-24 #feeds: 3
                (Isotope)  ( No. of levels feb by this mother)
               4 5.2100E-004 1
               (level #)  (probability)(decay type: 0: EC/Bplus, 1: Bmin, 2: alpha)
                  0.00
                  (max energy of betas (not used))
               2 9.9900E-001 1
                  0.00
               1 4.8948E-004 1
                  0.00
```

For base_cat.txt

```
###KK123#####k######
##KK123#####k######
#KK123#####k######
KK123#####k######
K123#####k######
```

```
Au M: 196.97
(Element) (Atomic Mass)
98.70  0.00   68.80   66.99   77.90   80.20 4.938E-001 2.894E-001 1.704E-001 4.642E-002
(SIGMAa)(SIGMAs)(EKa1)(EKa2)(Ekb1)(Ekb2) (IKa1)(IKa2)(IKb1)(IKb2)
3 produced nuclides
(# radionuclide(s) produced from neutron reaction with exisiting k0-values)
Au-196
Au-198
Au-199
7 isotope(s)
# isotopes of this element in the catalogue
  Z:  79 A: 196 abundance: 0.0000000 0.0000000 Au-196
 (atomic number)(mass number)(abundance and unc) (name)
    2 daughter(s)
   (# daughters of this isotope)
      lambda: 1.200096E-006 1.940961E-009 Pt-196
      (decay constant and unc.)(name of daughter)
      lambda: 9.741925E-008 1.575598E-010 Hg-196
    0 product(s)
    (# products from this isotope)
  Z:  79 A: 196 abundance: 0.0000000 0.0000000 Au-196m1
    1 daughter(s)
      lambda: 8.557373E-002 2.112932E-003 Au-196
    0 product(s)
  Z:  79 A: 196 abundance: 0.0000000 0.0000000 Au-196m2
    1 daughter(s)
      lambda: 1.984958E-005 2.046348E-007 Au-196
    0 product(s)
  Z:  79 A: 197 abundance: 1.0000000 0.0000000 Au-197
    mass: 196.9665500 lambda:    1.0 sigmaP: 1.1746E-027
    (atomic mass of isotope)(always 1.0)(potential scattering cross-section)
    9 E-ssf pars
           7.0000E+006 0.998033
           3.5000E+006 0.996076
           1.0000E+006 0.986464
           3.5000E+005 0.962752
           1.0000E+005 0.885704
           3.5000E+004 0.750440
           1.0000E+004 0.526276
           3.5000E+003 0.355083
           1.0000E+003 0.214071
       (optical size of sample)(epithermal self-shielding factor)
    0 daughter(s)
    2 product(s)
      Au-196
        (name of produced isotope)
       s0: 0.00E+000 0.00E+000 Q0: 4.29E-001 0.00E+000
      (thermal capture cross section and unc.)(Q0 and unc.)
       Er: 1.00E+000 7.10E-002 sF: 2.97E-031 0.00E+000
      (resonance energy and unc.)(fast neutron cross section and unc.)
       0 T-g(T) pairs
      (# Westcot factors in table for this activation reaction)
      Au-198
       s0: 9.88E-027 0.00E+000 Q0: 1.57E+001 2.83E-001
       Er: 5.65E+000 4.01E-001 sF: 0.00E+000 0.00E+000
       21 T-g(T) pairs
            0 1.0056
           (T, g(T))
           20 1.0066
           40 1.0076
           60 1.0086
           80 1.0096
          100 1.0106
          120 1.0116
          140 1.0126
          160 1.0136
          180 1.0146
          200 1.0156
          220 1.0166
          240 1.0176
          260 1.0186
          280 1.0197
          300 1.0207
          320 1.0217
          340 1.0228
          360 1.0238
```

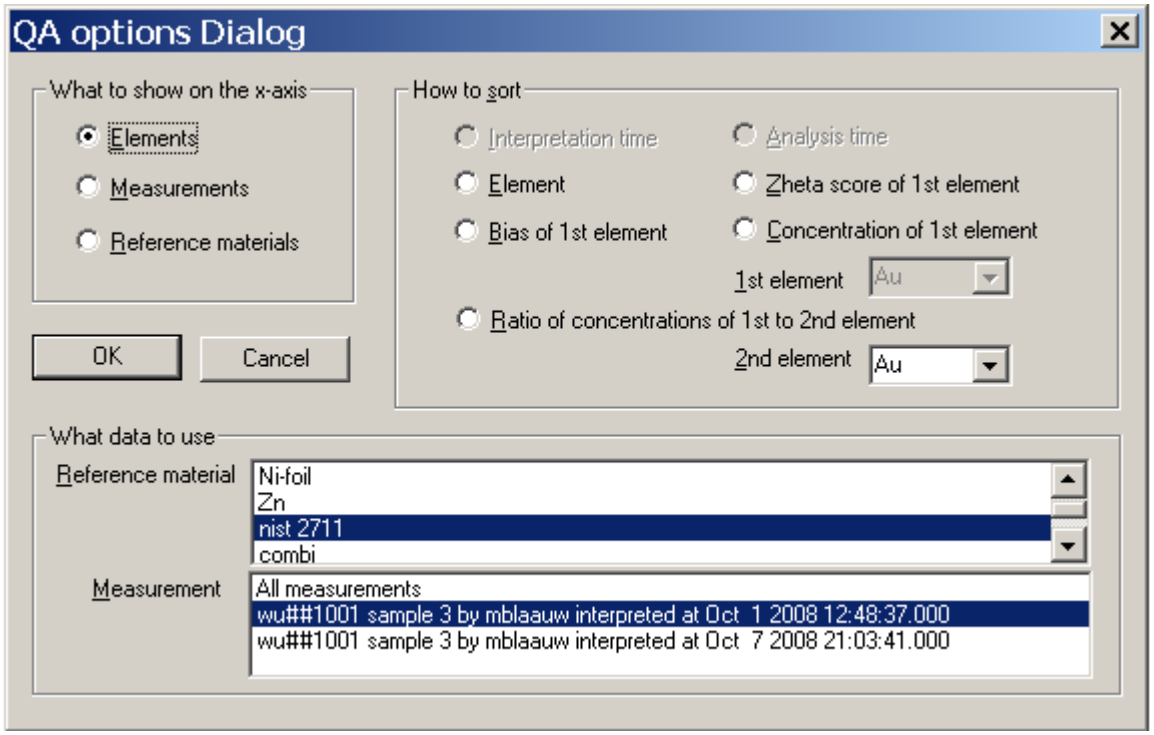
```
         380 1.0248
         400 1.0259
Z:  79 A: 197 abundance: 0.0000000 0.0000000 Au-197m
  1 daughter(s)
    lambda: 8.886502E-002 1.000000E-003 Au-197
  0 product(s)
Z:  79 A: 198 abundance: 0.0000000 0.0000000 Au-198
  1 daughter(s)
    lambda: 2.978480E-006 1.105803E-009 Hg-198
  1 product(s)
    Au-199
      s0: 1.55E-025 1.55E-027 Q0: 1.20E+000 7.71E-003
      Er: 1.00E+001 1.00E-001 sF: 0.00E+000 0.00E+000
      0 T-g(T) pairs
Z:  79 A: 199 abundance: 0.0000000 0.0000000 Au-199
  1 daughter(s)
    lambda: 2.555762E-006 5.699374E-009 Hg-199
  0 product(s)
```

QA/QC menu commands

The QA/QC menu allows you to see how well the analysis of reference materials came out in the past. The interpretation results are stored at the moment of sample interpretation in a database located in: c:\k0-IAEA\QADbase. The location might be elsewhere if you selected a different one with Tools/Select file locations.
The data stored there can be viewed in various ways set with the Options for QA dialogue. The data can be inspected with the Plot QA/QC data command, or with the List of QA/QC results command. The Validation Report Option is special!

Options for QA/QC

This dialogue looks deceptively simple, since it offers a great number of possibilities.
The selectable options depend on what you choose for showing on the X-axis. If you should select "Elements", and the specific reference material chosen was interpreted once or more, the whole dialogue will look like this



where the software will select a sorting method for you if you do not choose one yourself.
What you will get with the Plot QA/QC data or the List of QA/QC results commands depend on these settings.

Showing "elements" on the x-axis means that you will get a plot (or a list) where each chemical element in the certificate of the reference material(s) that was also measured yields a bias factor datapoint. The points are plotted or listed according to your choice, sorted on

- the atomic number of the elements,
- the bias factors of the element,
- the zheta scores of the datapoints,
- the concentrations of the elements, or
- the ratios of the element concentrations to the concentration of a 2nd element.

Showing "Measurements" on the x-axis means that you will be looking at the concentration measured for a specific element in various measurements of on1 reference material. Measurements can be sorted on
Interpretation time (when the result was calculated),
Analysis time (the packaging time of the sample is used for this),

- the bias factors of the measurement,
- the zheta scores of the datapoints, or
- the concentrations of the elements.

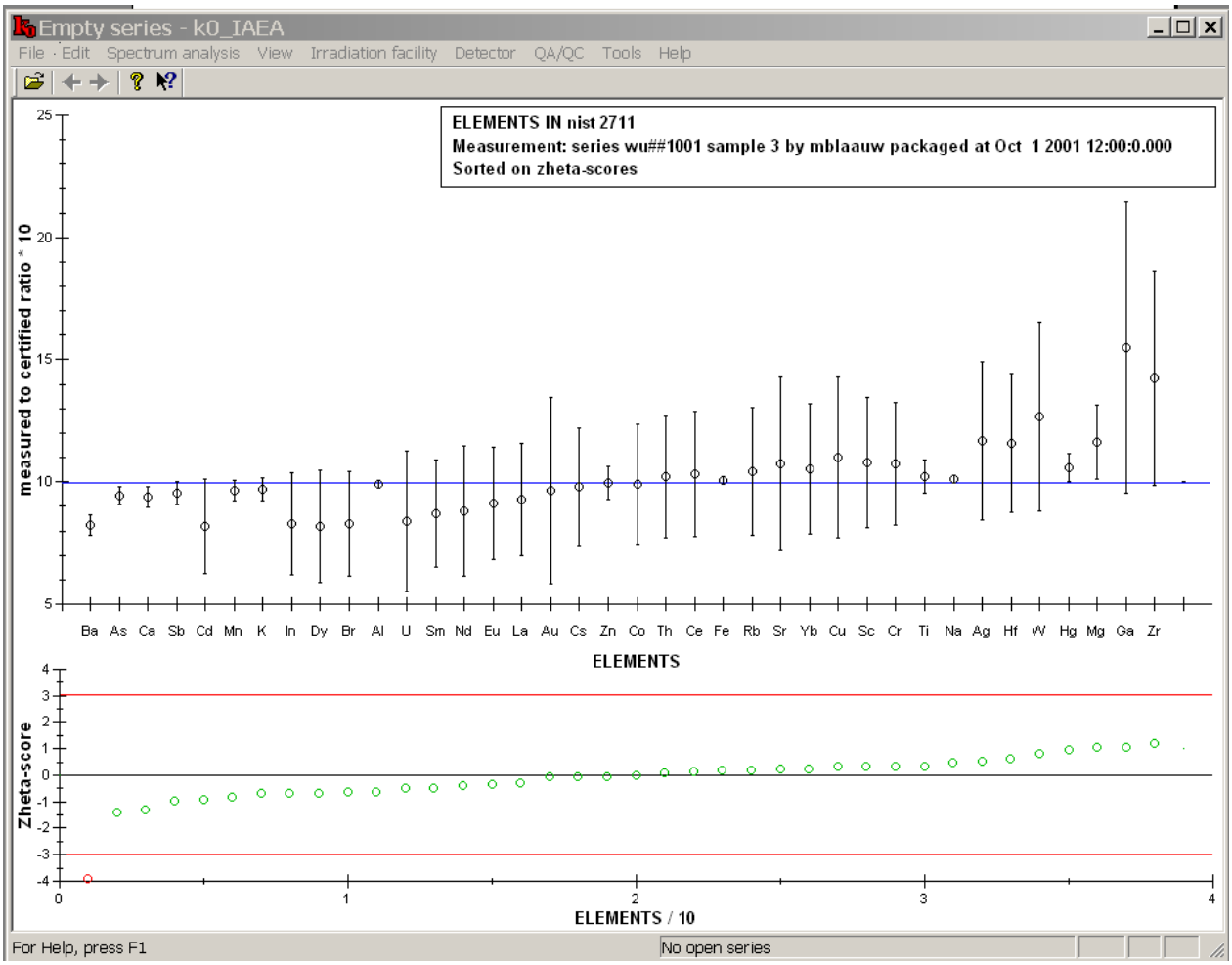
Showing “Reference materials” on the x-axis means that you will be looking at bias factors for one element as it varies from reference material to reference material. The data can be sorted on

- the bias factors for the element,
- the zheta scores of the datapoints,
- the concentrations of the element, or
- the ratios of the element concentrations to the concentration of a 2nd element.

Plot QA/QC data

The main window of the program switches to viewing QA/QC data. One example only is shown here. To discover what all is possible, please go to the Options for QA/QC explanation.

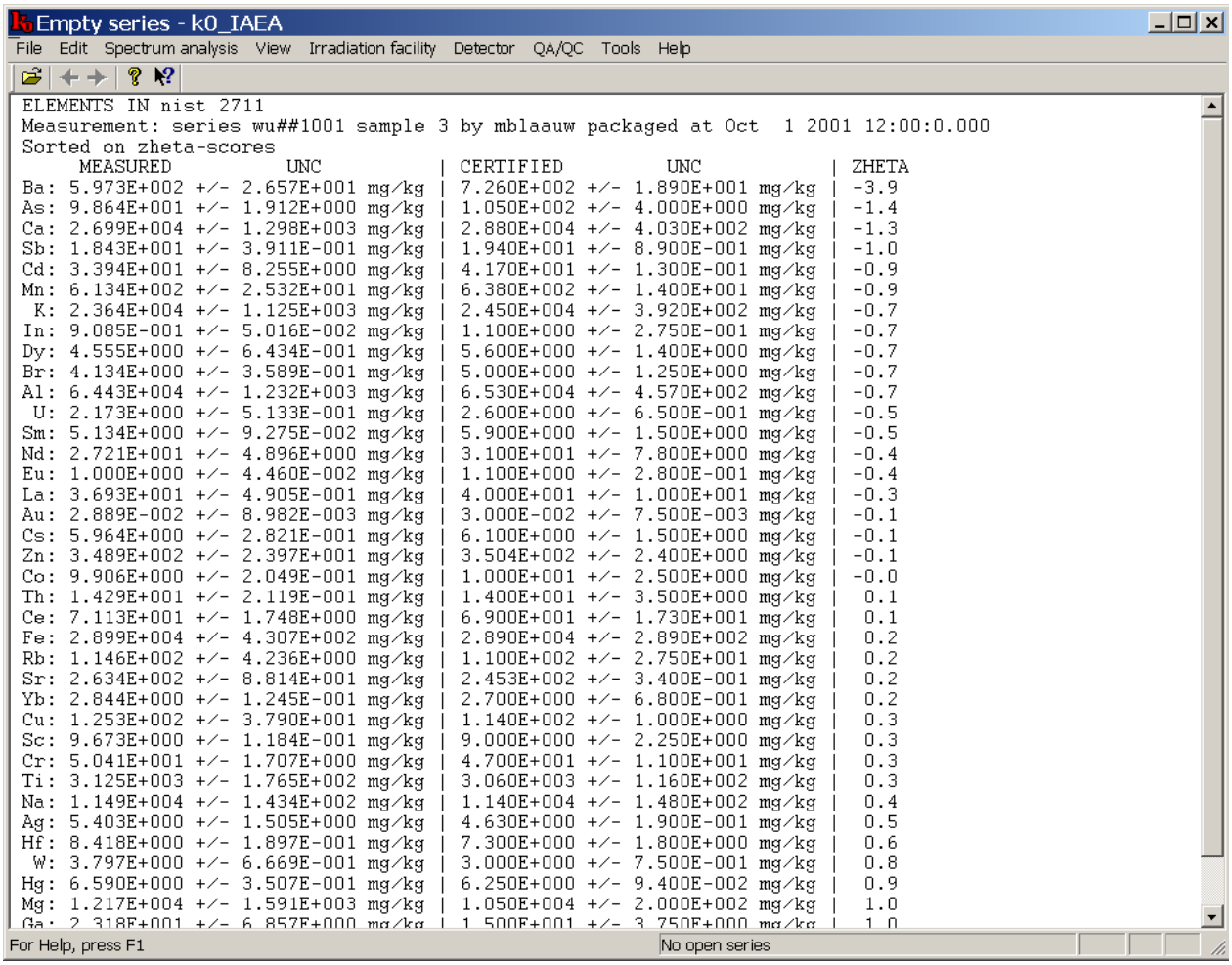
The example shows the results in terms of bias factors, that is the measured to certified concentration ratio. In the upper graph, these ratios are shown with their uncertainties. These 1 s.d. uncertainties are calculated from the reported uncertainties and their accuracies, combined with the uncertainties in the certified concentrations.
In the lower graph, the deviation from unity is shown as a zheta score, that is, the deviation from unity has been divided by the combined measured and certified uncertainties.
The graph can be shown with logarithmic or linear y-axis, and with or without grid. Use the View/Options for plot/views command to this end.



List of QA/QC data

The results stored in the QADbase are presented according to the Options for QA/QC settings. Only one example is shown here.

The example shows the results in measured and certified concentrations. For each result, the difference between the two is shown as a zheta score, that is, the difference has been divided by the combined measured and certified uncertainties.



QA/QC validation report

Validation of a method according to the ISO 17025:2005 standard comprises various aspects of the method. These aspects are discussed in the following paragraphs.

Intended use.
The intended use of the Instrumental Neutron-Activation Analysis (INAA) method as implemented in the k0-IAEA software is to perform multi-element analysis of solids and liquids, where the accuracy and precision of each result are properly estimated. Since INAA as foreseen in the k0-IAEA software is a non-standard method *and* IAEA-designed as well as developed, the software itself provides the tools to validate the method as implemented in a specific location. In this document, we describe the procedures used for the validation, how the results obtained are recorded, and how they should be interpreted.
The validation presented does not cover procedures for sampling, handling or transportation.

Accuracy
In order to avoid confusion, the accuracy of the method is defined for the current purpose as the absence of bias. The requirement for the method is that is that for all elements mentioned in the scope of the laboratory, the bias should be less than 5 %.

The bias of the method is assessed though the analysis over time of a large set of reference materials. For each element in each material, the weighted mean of the measured concentrations and

its external and internal standard errors are calculated. The mean concentration is than divided by the certified concentration to obtain a bias factor with its standard error – the larger of the internal and external standard errors is used to this end. The weighted mean of the bias factors for a given element in all reference materials is than calculated, with its internal standard error. Also, the overall χr^2 is calculated from the zheta-scores of the group averages and the certified concentrations.
This task is performed with the **QA/QC Validation report** option.

An element passes the test when the observed bias factor with its standard error implies a 67 % probability of the true value lying between 0.95 and 1.05 (so that an observed bias factor of 1.00 ± 0.05 just passes the test). It is flagged with “VLD” in the report in that case.

An element fails the accuracy test when the bias factor deviates from unity by more than 5 %, and at the same time deviates from unity by more than 3 standard deviations. It is then flagged with 3 asterisks.

In other cases, the test is inconclusive. If the bias factor deviates from unity by more than 5 %, and at the same time deviates from unity by more than 2 standard deviations, it is flagged with an asterisk in the report. The remaining, meaningless cases are not flagged at all.

Range and linearity

The INAA method is, from first principles, linear in that the induced radioactivity is linearly proportional to the amount of element present, the measured peak area also is, and the algorithm that determines the peak area is as well[1]. Our requirement for the linearity therefore is more stringent than for the accuracy: The contribution of non-linearity to the bias at any concentration level must be smaller than 0.25 %.

Even at very low levels, accurate measurements of elemental concentrations can be obtained by determining peak areas at the energies in the spectrum where the analyte is expected to show up. The precision of such measurements below the detection limits will be very poor, but some users prefer that to no information besides a detection limit. This leads to our requirement for the working range: It should be from 0 to 1 kg/kg.

Still there are a few caveats.

If the element of interest is a major constituent of the material to be analyzed, the neutron self-shielding behavior and/or the gamma-ray self-absorption properties of the sample may become dependent on the analyte concentration, and the induced activity and/or the measured peak area would no longer be linearly proportional to its concentration. Also, if the element to be determined is the major source of radioactivity in the material, the count rates in the measurement will be determined by the analyte concentration and linearity might be at risk due to dead time.
Neutron self-shielding, gamma-ray self-absorption and dead time and the requirements for the accuracy of the corresponding correction methods are discussed separately further down.

The question whether our method as a whole - correction for these effects included - meets the criteria stated above for linearity and range is answered in a similar approach as for the accuracy: The bias factors found in that test are correlated to the certified concentrations by linear regression. An element passes the test when the slope of the regression line with its uncertainty implies a 67 % probability of the true value lying between -0.005 and 0.005 (so that the slope 0.000 ± 0.005 just passes the test). An element fails the linearity test when the slope deviates from zero by more than 0.005, and at the same time deviates from zero by more than 3 standard deviations. In other cases, the test is inconclusive. The results are flagged in the report in a manner that is analogous to the flags in the bias test.

Detection limit

The interference-free detection limits as well as the computation thereof should be specified in the scope of the laboratory. These numbers are derived from the scientific understanding of the method. In practice, the detection limit for a specific element varies due to the noise level in the measurements that is affected by the presence of induced radioactivity from other elements in the sample.

For that reason, the detection limit is calculated for each element in each analysis by the software, from the scientific understanding of the properties of the peak search algorithm. This algorithm and its characteristics have been documented in a scientific publication.

In every analysis run, the detection limits obtained for the elements in the reference material are compared to the certified values. The method fails this test when a certified concentration exceeds

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23#####k######
3#####k######

the calculated reported detection limit and yet the element was not detected. The users of the software can inspect the reports for reference materials analyses for the absence of this flagged occurrence.

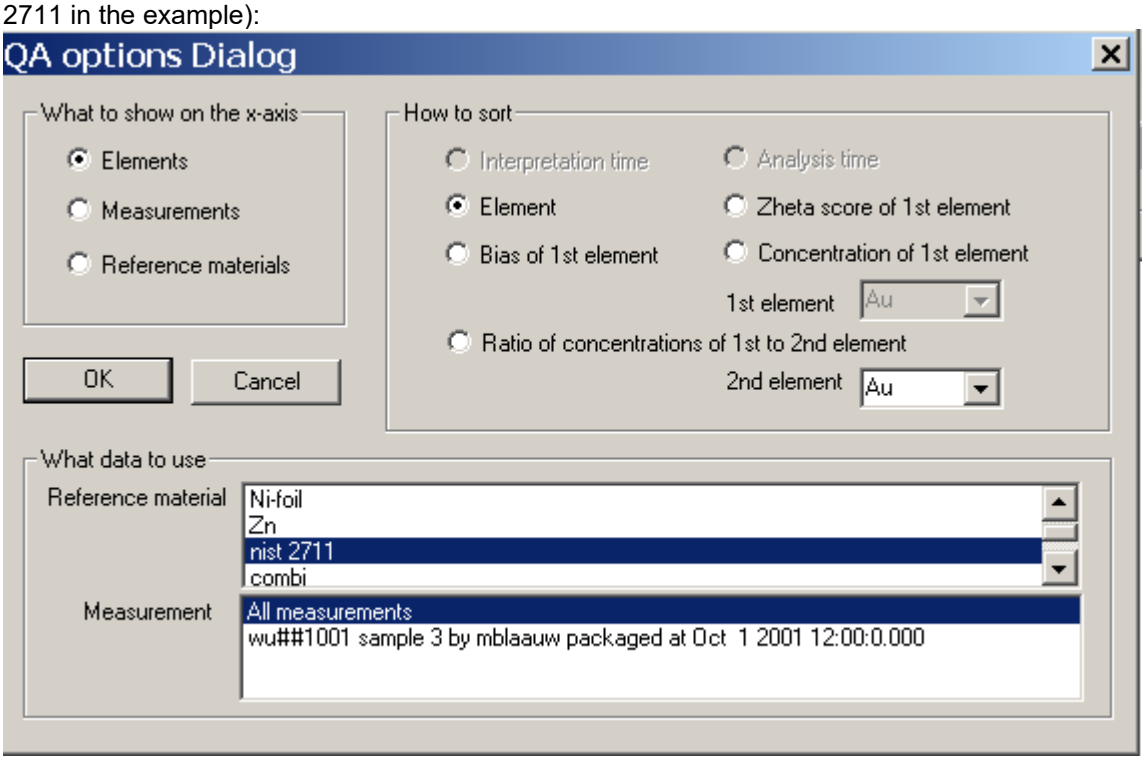
Selectivity
The very high selectivity of the method derives from the high-resolution gamma-ray detectors that are used for the induced radioactivity measurements. Very few radionuclides emit gamma-rays with indistinguishable energies, and if they do, they are not likely to have the same half-life. In selected cases, where only one measurement is done, such ambiguity can still occur (for example Cr-51 and Ti-51). The k0-IAEA software takes this into account and reports the ambiguity as such.

A more common ambiguity results from two elements yielding the same radionuclide (e.g. Al and Na both yield Na-24). Again, the software takes this into account and reports the ambiguity as such.

Repeatability, reproducibility
The k0-IAEA software reports a number for each element in each analysis result that is called the "precision". The number is calculated from the known sources of random uncertainty in the analysis procedure (counting statistics being the main one). If a sample is analyzed repeatedly by the same analysis protocol, this "precision" can be interpreted as the repeatability of the method.
The requirement for the precision is that the SEMext (i.e. observed variation) should not significantly exceed the SEMint (variation expected from calculations) for analysis runs of a homogenous material, performed the same way. If the SEMext should exceed SEMint in the selected case, then the implied unexplained variation should amount to less than 0.5 %. If SEMint should be larger than SEMext, than it should be demonstrated that an additional source of variation of 0.5 % would have increased SEMext significantly in the χ_r^2 –sense, using

$$\chi_r^2 = \left(\frac{\sqrt{V^2/N + SEM_{ext}^2}}{SEM_{ext}} \right)^2 ,$$

where *N* is the number of observations, and *V* is the extra variability.
To perform this test, an element in a homogeneous material with a SEMext as small as possible is selected. This test should be repeated on a regular basis.
To perform the test, set the QA/QC options as follows for the reference material of your choice (NIST 2711 in the example):



And the select the QA/QC List of QA/QC results option.

Reproducibility is tested the same way and at the same time, by selecting a homogeneous material and measurements thereof by different procedures, detectors and technicians. The requirement is that the unexplained variation arrived at from the results should be less than 1 %.

Robustness

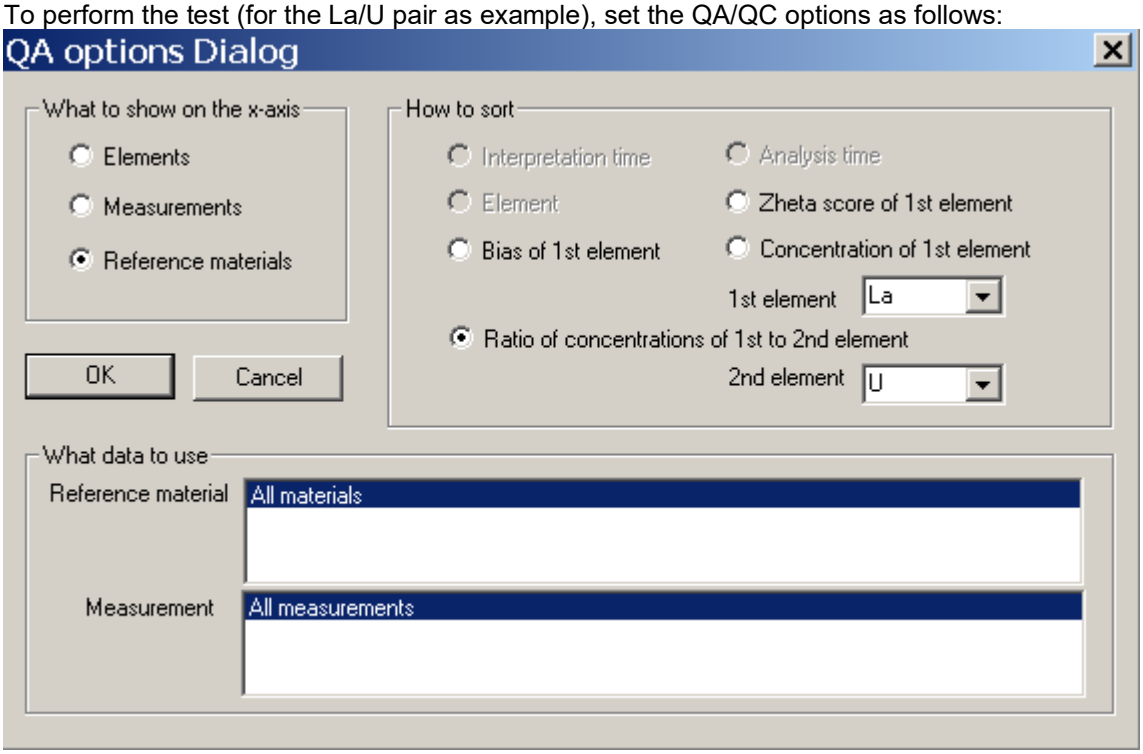
The only external factor potentially affecting the INAA results is the climate in the counting room. Temperature has an effect on the energy calibration of the detectors that might lead to misidentification of radionuclides. Since this is the most serious error that could be made, the requirement is that it should never happen. This requirement is tested along with the accuracy of the method as described above – if robustness should be lacking, the method would fail that test.

Cross-sensitivity

This topic has been addressed in part under “selectivity”. Cross-sensitivity is at stake when a) more than one element contributes to a certain spectral line, or two peaks from different elements are difficult to resolve, b) other elements than the element of interest are present in such large quantities that the linearity of the method is endangered through b1) neutron self-shielding, b2) gamma-ray self-absorption or b3) high count rates.

The requirement for the method with respect to spectral interferences is that the presence of such interferences should not increase the bias. To test for this, the bias factor for a given element is correlated to the concentration of the interfering element in a few selected cases: For example La in the presence of U, Zn in the presence of Sc, and Co in the presence of Br. The test is failed if the slope of the regression line differs from zero significantly in the statistical sense, and at the same time its absolute value exceeds 0.005. Otherwise, the test is passed successfully.

To perform the test (for the La/U pair as example), set the QA/QC options as follows:



and then select the QA/QC Plot QA/QC data. If no trend is observable by eye, the interference is well-corrected.

Neutron self-shielding is kept to a minimum by using small samples. It is corrected for using state-of-the-art equations as specified in the k_0-method, using all available information on the matrix composition of the sample. The equations used were validated by Monte Carlo calculations as described in or referred to in the paper mentioned.

Gamma self-absorption is kept to a minimum by using small samples. It is corrected for using state-of-the-art equations as specified in the k_0-method, using all available information on the matrix composition of the sample.

The validity of the neutron self-shielding and gamma-ray self-absorption correction methods for small samples are not experimentally validated in the development of this software: If failure of the correction

methods contributed noticeably to non-linearity, that would be noticed in the accuracy and linearity tests as described above.

Regular review
All tests described should be performed regularly as an integral part of the periodical evaluation of the reference-material results. This is necessary because the method and its calibration factors are continuously evolving.
This task is performed with the QA/QC options in the k0-IAEA program. The data taken into consideration are the grand total, the data from the last 10 years, the last 5 years, the last 2 years and the data from the last year. Future releases of the software will allow for the setting of the time span of interest. If a test for a more recent dataset is inconclusive, the dataset from the next larger time span can be used to decide on validity.

Conclusion
After performing all the tests described here, a “validity test” report is written, and conclusions drawn. All failures to pass a test are looked into and may require action to be taken.
For some elements, no suitable reference materials exist, so the tests above cannot prove the validity of the method. If determination of such elements is requested by a customer, a traceable standard for that element must be included in the analysis procedure to demonstrate absence of bias.

Help menu commands.

The Help menu offers the following commands, which provide you with assistance for this application:

Help Topics	Offers you an index to topics on which you can get help.
About	Displays the version number of and the credits for this application.

Index command (Help menu)

Use this command to display the opening screen of Help. From the opening screen, you can jump to step-by-step instructions for using k0_IAEA and various types of reference information.

Once you open Help, you can click the Contents button whenever you want to return to the opening screen.

Using Help command (Help menu)

Use this command for instructions about using Help.

About command (Help menu)

Use this command to display the copyright notice and version number of your copy of k0_IAEA.

Context Help command.



Use the Context Help command to obtain help on some portion of k0_IAEA. When you choose the Toolbar's Context Help button, the mouse pointer will change to an arrow and question mark. Then click somewhere in the k0_IAEA window, such as another Toolbar button. The Help topic will be shown for the item you clicked.

Shortcut
Keys: SHIFT+F1

Nuts and bolts.

On these help pages, some detailed information is given that did not seem to belong anywhere else. Unless otherwise stated, all *uncertainties* given and asked by the program are 1 standard deviation uncertainties.

The dead time correction factor entered in Series editor is used only to treat the spectrum continuum for detection limit estimation (by multiplying the channel contents with the dead time correction factor), the peak areas supplied to the program must have been corrected already. If this is not the case, the Edit/Interpret options menu must be used to tell the program to also correct the peak areas for dead time.

Disabled and Irrelevant spectra

The software distinguishes irrelevant and disabled spectra. Irrelevant spectra will occur when a flux monitor is used more than once, in a sequence of alternating irradiations and measurements, and some fluxes have been calculated already. In that case, the spectra that were measured before the irradiation for which the flux still needs to be calculated are irrelevant for the current calculation. They can still be seen on screen but will not be interpreted at all.

Disabled spectra are treated like enabled spectra in all respects, except that the spectrum contents are disregarded in the interpretation step, as if the uncertainty in all the peak areas had been set to infinity. This means that if a sample was measured more than once, one can see what the disregarded spectrum should have looked like to be in agreement with the enabled spectra of the same sample. Problems due to energy calibration shifts or sample mix-ups can be identified rather easily using the 'disable' possibility in the Series database.

The series database and the permanent database

The k0_IAEA program operates on two databases. One is series-specific and is called the 'series database'. The other is of a more general nature and is called the 'permanent database'. The series database contains information like sample histories, sample types and spectrum filenames.

The permanent database contains materials composition definitions, detector geometry data, calibration results and other information that is not likely to change from series to series - or rather, information that one would want to enter in the system only once.

Some information in the database is not actually being used by k0_IAEA. It may be used in the future, or it may be there to help the user in keeping all the information that might be relevant in one place.

The unused information in the permanent database currently is:
Domain and password of users
The uncertainties in the recipient dimensions

The unused information in the Series database is:
Uncertainties in dead time percentage and timing, distance from detector
Uncertainties in sample height.

Information occurring in both databases that is not used:
Uncertainty in neutron temperature.

Blank certificate

The blank certificate is specified in mg/kg, just like a reference material is. But one also needs to enter a mass in the packaging record of a blank in the series. The concentrations entered and this mass must match in order to get good results.

Spectrum files

k0_IAEA can determine peak energies and areas in gamma-ray spectra only starting at version 2.0. It was assumed that most potential users would have a program for that already. This means that in order to calculate anything, the program needs two files related to each single spectrum: One file containing the raw channel contents and one with the peak energies and areas.

Some programs out there allow the user to search for peaks only in a limited region of the spectrum. The k0_IAEA program expects that this region was set to the total number of channels in the spectrum. The interpretation of the spectrum may fail if this condition is not met.

Currently, the program can read IAEA .spe files (that are called .k0s files here), SAMPO .spe files, ORTEC .chn and .spc files, and Canberra .cnf files, for raw channel contents. Some more formats are available through external conversion programs called by k0_IAEA, that can also be used manually by the user in an MS-DOS window. For peak areas and energies, it can read the IAEA .gsr format (like GANAAS produces but called .k0p in the k0_IAEA program), SAMPO .ptf files, GammaVision report files (use the .gvt extension here) and CANBERRA .rpt files. Please note that SAMPO .ptf files can contain no more than 250 peaks, whereas k0_iaea sometimes needs more. For example, if this phenomenon leads to the 2754 keV peak area of Na-24 not being imported, the k0_iaea program will not recognize the 1368 keV peak either, until it has been told to disregard the 2754 keV peak.

The filename extensions named here *must* be used, or else the program will attempt to read a file with the wrong format in mind - and fail as a result.

See also the section on input file formats

The raw channel content files all contain acquisition start and stop times, and usually also dead time information. If the history of a sample has been entered and the main program knows that there must be spectrum files, it will prompt the user for filenames when the sample is selected for the first time and copy these times into the database. So don't go to the trouble of precisely typing that kind of information in the Series database editor.

The k0-program uses the file extensions to recognize the files, so the user is not free to choose his own.

The k0-program reads the raw channel contents first, and the peak area file next. Energy calibration information must be present in one of the two. If it is present in both, the peak area file takes precedence over the raw channel contents file. Peak width calibration information should be given in the peak area file, if not, an estimate is used that is good enough for most practical purposes.

Input file formats

k0_IAEA can read several spectrum file formats for input internally. For channel contents, the ORTEC integer. CHN and .SPC formats can be read. Also, the IAEA .spe format and the Canberra .lis formats are suitable. For some other filetypes, the conversion utilities of the SPEDAC software package are called from k0_IAEA. To read any of these files, the filename extension MUST be set to the extensions listed in the following table:

Description	Read internally by k0_IAEA	
Aptec spectrum files		*.ap0
Aptec v4.3 spectrum files		*.a43
Canberra S100 files		*.mca
Canberra binary spectrum files		*.cnf
Canberra text spectrum files	yes	*.lis
IAEA spectrum files	yes	*.k0s
Nuclear Data Accuspec		*.nda
Nucleus PCA		*.spm
Ortec integer spectrum files	yes	*.chn
Ortec spectrum files	yes	*.spc
Sampo spectrum files	yes	*.spe
Silena EMCAPlus		*.sip
Silena		*.sil

It is also possible to write your own conversion program in order to read your own spectrum files and add it to the set already present in the program folder of the k0_IAEA program. For example, let us assume that your spectrum files have the 'ysf' extension. Then, the conversion program must be named cvt_ysf_k0s.exe, and must be placed in the k0_iaea directory where the main program also resides (this probably is the 'c:\program files\k0_iaea' folder). The conversion program will be called by the main program when a spectrum file is to be read with the 'ysf' extension. It will be called with two

filenames as arguments: The first filename is that of the .ysf spectrum file, the second of the .k0s file that your program needs to create from the data in the .ysf file, in IAEA .spe format. The resulting .k0s file will be deleted after reading by the main program to save disk space.

If your spectrum files have some other extension than .ysf, as they probably do, substitute that extension for .ysf in the text above.

For peak energies and areas, that may have been corrected for dead time and pile-up, the IAEA .gsr format, the Canberra .rpt format and various formats are suitable. To read any of these files, the filename extension MUST be set to the extensions listed in the following table:

Description	Read internally by k0_IAEA	
k0_IAEA	yes	*.k0p
Canberra text spectrum analysis file	yes	*.rpt
SAMPO peak analysis file	yes	*.ptf
GAMMAVISION text peak analysis file	yes	*.gvt
MAESTRO text peak analysis file	yes	*.omt

It is also possible to write your own conversion program in order to read your own peak area files. For example, if your peak area files have the 'ypf' extension, the conversion program must be named cvt_ypf_k0p.exe, and must be placed in the k0_iaea directory where the main program also resides. The conversion program will be called by the main program when a peak area file is to be read with the 'ypf' extension. It will be called with two filenames as arguments: The first filename is that of the .ypf peak area file, the second of the .k0p file, in IAEA .gsr format, that your program needs to create from the data in the .ypf file. The .k0p file will be deleted after reading by the main program to save disk space.

If your peak area files have some other extension than .ypf, substitute that extension for .ypf in the text above. The extension you choose must not be in use already for another spectrum file format. This is also the reason why new extensions were defined for old file formats: too many spectrum acquisition programs used the '.dat' and '.spe' extensions in the past.

If the peak area file does not contain information on the peak width as a function of energy, a reasonably good estimate, typical for a 20 % HPGe detector, is used.

Both the raw spectrum file and the peak area file may contain energy calibration information. If so, the one in the peak area file takes precedence over the one in the raw spectrum file.

For efficiency data, both for import and for export, the .k0e format is used.

IAEA .spe format (also known as .k0s format)

The format is best defined by example:

```
$SPEC_ID:
wu##1001-WU27
$SPEC_REM:
DET# 0
DETDESC# pgt
AP# IAEA_k0 software
$DATE_MEA:
04/19/200204:00:50
$MEAS_TIM:
815 820
$MCA_CAL:
%3
-7.2088893E-017.7965334E-011.0385458E-07
$DATA:
0 4095
0000000000
0000000000
0000000000
0000000000
```

```
... until 4096 channel contents have been printed.
```

Clearly, this is a rather simple file format. k0_IAEA is more forgiving when reading these files than the original GANAAS package: As long as the channel contents are separated by spaces, they will be read correctly. Other numbers also can be specified in any format.

Canberra .lis format

Another rather simple format for spectrum input demonstrated by example. The lines that must be there for k0_IAEA are in red; the others might as well be omitted. The third term in the energy calibration polynomial is disregarded by k0_IAEA - only quadratic polynomials are used internally. This possibly has a slight effect on detection limits exclusively.

```
 ******************************************************
 ***** S P E C T R A L  D A T A  R E P O R T *****
 ******************************************************

 Report Generated On : 16/06/2003 15:46:34
 Data Location : D:\VAX40\SP5734.CNF
 File Description: DET5

 Collector :

 Sample Title:
 Spectrum Description:
 Spectrum Description (cont.):
 Spectrum Description (cont.):
 Spectrum Description (cont.):
 Sample Identification : Steel/sp5734
 Sample Type : U
 Sample Geometry :

 Peak Locate Threshold :5.00
 Peak Locate Range (in channels) : 1 -8192
 Peak Area Range (in channels) : 1 -8192
 Identification Energy Tolerance :0.000 keV

 Sample Size :4.080E+001 mg

 Sample Taken On : 04/03/2003 14:30:00
 Acquisition Started : 12/03/2003 08:10:46

 Live Time :94785.50 seconds
 Real Time :96412.02 seconds

 Decomp Time tilMeasureStart :11140.78 minutes
 Decomp Time til Mid Measurement :11944.21 minutes
 Middle of Measurement at: 12/03/2003 21:34:12

*************ENERGY CALIBRATION COEFFICIENTS*************

Energy Calibrate Performed on:18/11/2002 15:45:19
by:
Energy Calibrate Type:POLY

Energy(keV) =-0.316 + 0.250*ch + -3.82E-009*ch^2 +0.00E+000*ch^3

*************SHAPE CALIBRATION COEFFICIENTS *************

Shape Calibrate Performed on:
by:

FWHM = 0.631+ 0.030*E^1/2

LOW TAIL = 0.0E+000 +0.0E+000*E
```

#####k######

```
 DUAL Efficiency Calibration Equation
 ====================================

No DUAL Equation


Channel| Counts
10
20
30
40
    ....
```

Canberra .rpt format

Another file format for input best defined by example. k0_IAEA looks for the line shown in red and reads everything that follows:

```
Peak Analysis Report 16/06/2003 15:50:14 Page1


*******************************************************************************
***** P E A KA N A L Y S I SR E P O R T*****
*******************************************************************************


 Detector Name:
 Sample Title:
 Peak Analysis Performed on:16/06/2003 15:50:13
 Peak Analysis From Channel:1
 Peak Analysis To Channel: 8192

 PeakROIROIPeakEnergy FWHMNet PeakNet AreaContinuum
No. start endcentroid (keV) (keV)Area Uncert.Counts

1 232-251 246.2561.20 1.262.45E+004 1986.24 9.03E+005
 M2 283-313 292.0372.64 1.217.31E+004713.10 7.24E+005
 m3 283-313 301.2674.95 1.211.27E+005798.40 7.18E+005
 M4 327-360 340.6884.80 1.309.89E+004822.07 7.53E+005
 m5 327-360 351.0587.39 1.313.46E+004691.40 7.08E+005
```

IAEA .gsr format (also known as .k0p format)

This file format was introduced with the IAEA GANAAS package. The only modification made for k0_IAEA was the addition of the peak search threshold lines:

    $THRESHOLD:
    3

```
$MCA_CAL:
%3
 -7.20889E-01 4.23653E-01 1.03855E-07
$RES_CAL:
4.86216E+00 2.66543E-03 0.00000E+00
$PEAKS:
 5
154.52  2.17  65.49 6973 100 1.00
184.11  1.97  78.03 7368 110 1.00
375.84 11.15 159.24 1491  40 1.00
398.62  2.63 168.89 6175  90 1.00
465.65  2.30 197.28 6979  85 1.00
```

####k######
###k######

The MCA_CAL numbers specify a polynomial for the energy calibration. One was also present in the .spe (or .k0s) file specifying the channel contents. In case of conflict between the two, the energy calibration in the .gsr (.k0p) file gets the priority.
What one also needs to know is that the RES_CAL numbers specify a polynomial that yields the squared FWHM (in keV * keV), not the FWHM (in keV) itself. The third coefficient is ignored by k0_IAEA because of being unphysical.
The peaks are specified, each on a line, with position, 1 s.d. uncertainty in position, energy, area, 1 s.d. uncertainty in area, and chisqr of the fit. The k0-IAEA program, when fitting peaks and saving the results, stores the range of the peak as a last, extra column, so that the file looks like this. The range is defined as the width (in keV) of the region where the peak contributes significantly to the spectrum. This is used in the process of identifying peaks: any library energy that matches the peak energy to within the range is considered a possible contribution. Manual and automatic integrations tend to yield large ranges.
The pulser energy is the apparent energy of the pulser peak in the gamma-ray spectrum, the pulser area its area. The pulser information lines are absent if no pulser is present in the spectrum. Alternatively, the pulser energy can be set to -1.0 to indicate its absence.

```
    $THRESHOLD:
    3
$MCA_CAL:
%3
 -7.20889E-01 4.23653E-01 1.03855E-07
$RES_CAL:
4.86216E+00 2.66543E-03 0.00000E+00
$PULSER_ENERGY:
4000.0
$PULSER_AREA:
15000.0
$PEAKS:
 5
154.52  2.17  65.49 6973 100 1.00 3.00
184.11  1.97  78.03 7368 110 1.00 3.00
375.84 11.15 159.24 1491  40 1.00 4.00
398.62  2.63 168.89 6175  90 1.00 4.00
465.65  2.30 197.28 6979  85 1.00 4.00
```

The .k0e format for efficiency import and export

Another very simple format:

```
0
9
50.00 3.710E-3 3.710E-5 1.000E+0 1.000E-2 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 100.00 1.247E-2 1.247E-4 1.000E+0 1.000E-2 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 150.00 1.358E-2 1.358E-4 7.149E-1 7.149E-3 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 200.00 1.092E-2 1.092E-4 5.416E-1 5.416E-3 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 250.00 8.484E-3 8.484E-5 4.366E-1 4.366E-3 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 300.00 6.963E-3 6.963E-5 3.662E-1 3.662E-3 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 350.00 5.916E-3 5.916E-5 3.156E-1 3.156E-3 0.000E+0 1.000E-2 0.000E+0 1.000E-2
 400.00 5.149E-3 5.149E-5 2.774E-1 2.774E-3 0.000E+0 1.000E-2 0.000E+0 1.000E-2
1450.00 4.561E-3 4.561E-5 2.476E-1 2.476E-3 1.000E-4 1.000E-6 1.000E-3 1.000E-6
```

The first 0 is a file format indicator. Then comes the number of data lines in the file. And then the data. First the energy (in keV), then the full-energy peak efficiency, its uncertainty, the peak-to-total ratio and its uncertainty, and the single and double escape peak ratios with their uncertainties. All these must be absolute values. The numbers can be entered in various formats and must be separated with spaces or tabs. It is wise to use the original data for this purpose, rather than data obtained from a curve that was already fitted, because that curve may not match the curve used in k0_IAEA precisely. In case of missing data, simply enter a zero value and the entry will be ignored for that zero efficiency or ratio.

##k######

An alternative format, also understood by the program, is as follows:

```
0
15
50.00 keV: 1.28E-002 (1.0 %), 1.00E+000 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
60.00 keV: 5.07E-002 (1.0 %), 1.00E+000 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
70.00 keV: 1.17E-001 (1.0 %), 1.00E+000 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
80.00 keV: 1.98E-001 (1.0 %), 1.00E+000 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
90.00 keV: 2.79E-001 (1.0 %), 9.20E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
 100.00 keV: 3.49E-001 (1.0 %), 8.50E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
 120.00 keV: 4.38E-001 (1.0 %), 7.42E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
 150.00 keV: 4.59E-001 (1.0 %), 6.29E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
 200.00 keV: 3.60E-001 (1.0 %), 5.07E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
 500.00 keV: 1.22E-001 (1.0 %), 2.56E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
1000.00 keV: 5.74E-002 (1.0 %), 1.53E-001 (1.0 %), 0.00E+000 (0.0 %), 0.00E+000 (0.0 %)
1500.00 keV: 3.78E-002 (1.0 %), 1.13E-001 (1.0 %), 9.16E-003 (1.0 %), 1.26E-002 (1.0 %)
2000.00 keV: 2.83E-002 (1.0 %), 9.13E-002 (1.0 %), 5.55E-002 (1.0 %), 7.08E-002 (1.0 %)
2500.00 keV: 2.25E-002 (1.0 %), 7.73E-002 (1.0 %), 1.53E-001 (1.0 %), 1.82E-001 (1.0 %)
3000.00 keV: 1.84E-002 (1.0 %), 6.75E-002 (1.0 %), 3.11E-001 (1.0 %), 3.46E-001 (1.0 %)
```

Custom report templates

A customized report is produced by creating a new report template or editing an existing one. These templates are plain ASCII files located in the same folder as the permanent_data.k0i file and have .k0t filename extensions. They can be created and edited with a simple word processor like Notepad or WordPad. A few examples are already there to get you started.

The template consists of text to be included in the report, format specifications and location indicators. The format specifications specify how the numbers are to be represented, and the location indicators specify where in the text the numbers are to appear. Finally, there are some general settings to be used.

A template file always must contain four sections: The first is the title page, the second is for ordinary samples, the third is for reference materials and the last is for blanks. Each section begins with a section indicator on its own line: {T}, {S}, {R} and {B}. The title section is used only once, the other sections are repeated as many times as there are samples of that nature present in the series. Section specifications can be empty or absent.

Format specifications in custom report templates

The format specifications are based on those available in the C programming language. A format specification, which consists of optional and required fields, appears by itself on a single line in the report template and has the following form:

%what%[flags] [width][**.**precision] **representation**

Each field of the format specification is a single character or a number signifying a particular format option. The simplest format specification contains only the percent signs, a *what* and a *representation* character (for example, `%c%f`).

Format specification lines determine how numbers are printed starting at the point where the specification appears in the template. It is possible to use different formats in different sections of a report.

The possible choices for the different fields are explained in the following:

what

The *what* character specifies what kinds of numbers or text you are talking about. The possible choices are the same as used in the location indicators.

representation

Required character that determines whether the associated *argument* is interpreted as a character, a string, or a number, and also how to represent it. For reporting purposes, only a few are relevant, as shown in the following table:

Character	Output Format
e	Signed value having the form [–]*d.dddd* **e** [*sign*]*ddd* where *d* is a single decimal digit, *dddd* is one or more decimal digits, *ddd* is exactly three decimal digits, and *sign* is + or –.
E	Identical to the **e** format except that **E** rather than **e** introduces the exponent.
f	Signed value having the form [–]*dddd.dddd*, where *dddd* is one or more decimal digits. The number of digits before the decimal point depends on the magnitude of the number, and the number of digits after the decimal point depends on the requested precision.
g	Signed value printed in **f** or **e** format, whichever is more compact for the given value and precision. The **e** format is used only when the exponent of the value is less than –4 or greater than or equal to the precision argument. Trailing zeros are truncated, and the decimal point appears only if one or more digits follow it.
G	Identical to the **g** format, except that **E**, rather than **e**, introduces the exponent (where appropriate).

#k######
k######
######

s	Text, e.g. for sample descriptions
d	For integer numbers, like the confidence interval number which can only be 1, 2 or 3.

flags
Optional character or characters that control justification of output and printing of signs, blanks, decimal points. More than one flag can appear in a format specification.

Flag	Meaning	Default
–	Left align the result within the given field width.	Right align.
+	Prefix the output value with a sign (+ or –) if the output value is of a signed type.	Sign appears only for negative signed values (–).
0	If *width* is prefixed with **0**, zeros are added until the minimum width is reached. If 0 and – appear, the **0** is ignored. If **0** is specified with an integer format (**i**, **u**, **x**, **X**, **o**, **d**) the **0** is ignored.	No padding.
blank (' ')	Prefix the output value with a blank if the output value is signed and positive; the blank is ignored if both the blank and + flags appear.	No blank appears.
#	When used with the **e**, **E**, or **f** format, the **#** flag forces the output value to contain a decimal point in all cases.	Decimal point appears only if digits follow it.
#	When used with the **g** or **G** format, the **#** flag forces the output value to contain a decimal point in all cases and prevents the truncation of trailing zeros. Ignored when used with **c**, **d**, **i**, **u**, or **s**.	Decimal point appears only if digits follow it. Trailing zeros are truncated.

width
Optional number that specifies the minimum number of characters output.

precision
Optional number that specifies the number of characters printed after the decimal point.

Location indicators in custom report templates

Location indicators can appear in the middle of a line of text and are replaced by characters, numbers or sets of numbers when the report is created. They have the following form

@[what elem]

where the *what* character(s) specifies what to print at this location, and *elem* specifies the element by name. The elem specification is ignored unless specified with the 'c' or 'C' (concentration) or 'e' (element name) *what* charachters. Element names, if needed, are given as e.g. '*W*' or '*As*'.

If the element name is '*X*', results for all elements specified in a list created with the permanent database editor and specified with 'L' general setting will be printed, by repeating the current line in the template for all elements in the list. If the element name is 'x', the current line will be repeated starting at the first 'x' location indicator for those same elements but without line breaks - this is what you need to create a flexible table of results. The 'X' and 'x' element identifiers cannot be mixed with each other or with other element names in one line. Only the first one encountered in one line is used. The available choices for the *what* character are

what	default format	prints
		title page section
i	%1d	1, 2, or 3 depending on how many standard deviations (that is, coverage factors) are used for confidence interval reporting (use the general

#####

		settings to select the value, ‘i’ to print it in the report).
p	%s	name of person who did the analysis
s	%s	name of series
S	%s	series description
l	none	list of deselected peaks
		samples section (also applies to reference materials and blanks)
n	%2d	sample number
t	%s	sample description text
m	%6.2f	sample mass
h	none	sample history (automatically ends with a newline)
e	%2s.....	element name (in case of no interference, the dots represent spaces)
E	%2s (%2d)	element name and interference groups number (in case of interference)
c	%8.3E	measured element concentration
a	%4.1f	uncertainty in measured element concentration including systematic errors (GUM)
u	%4.1f	uncertainty in measured element concentration including only random errors
d	%8.3E	detection limit or uncertainty
		reference materials and blanks sections
N	%s	Certificate name of reference material or blank
C	%8.3E	known element concentration
U	%4.1f	accuracy (GUM uncertainty with coverage factor 1) of known element concentration
z	%4.1f	z-score base on uncertainty in measured element concentration including systematic errors and reference data
		general
@	none	The @ character itself is printed.
T	none	The TAB character is printed.
f	none	The form feed/page break character is printed.

General settings in custom report templates

A general setting, which consists of two characters only, appears by itself on a single line in the report template and has the following form:

$setting argument

Where ‘argument’ provides further information. The following settings are currently available:

Setting character	Effect
D	suppress printing of 100 % detection limits for elements that were not detected. Only affects reports where no list of elements to report was specified in ‘X’ mode (see the *what* character definitions).
A	print elements in alphabetical order (default). Must be specified before the ‘L’ option is used.
Z	print elements sorted on atomic number. Must be specified before the ‘L’ option is used.
R name	name is the name of a list of elements to be reported. Lists of elements named before this one are discarded.
L name	name is the name of an additional list of elements to be reported. This option can be repeated as many times as required
B name mass	name of blank of which the composition is to be used to correct all the

####

	ordinary sample concentrations with. This is where to specify the blank of the series should happen not contain one due to mishaps. The mass is the mass of the blank in mg.
1	print 1 standard deviation uncertainties, i.e. 67 % confidence intervals (default)
2	print 2 standard deviation uncertainties, i.e. 95 % confidence intervals
3	print 3 standard deviation uncertainties, i.e. 99 % confidence intervals
U 1	print concentrations in kg/kg
U 2	print concentrations in mass %
U 3	print concentrations in mass parts-per-thousand
U 4	print concentrations in mg/kg
U 5	print concentrations in ug/kg
U 6	print concentrations in ng/kg
U 7	print concentrations in pg/kg
U 8	print concentrations in fg/kg
r	relative uncertainties in % to be printed (default)
a	absolute uncertainties to be printed
m	sample masses to be printed in mg (default)
g	sample masses to be printed in g
k	sample masses to be printed in kg

Log file format

The log file written at interpretation time for each sample (if the user so commands using the Edit/Interpret options dialog) has a format that depends on the sample type. The peak assignment information is similar for all types and is described at the end of this page, since it appears at the end of the log file.

For **ordinary samples**, **blanks** and **reference materials**, the file starts with information about expected peaks, if the "All Asp in log file of interpretation" box was ticked in the Edit//Interpret options dialog dialogue.

For each element (or only one if View/Options for plot/views was used to select an element of interest), all peaks are listed if the expected area 'A100' is larger than 1 and the peak was considered relevant by the software in view of the maximum concentrations established for each element. For each peak, the following numbers are given:

- Isotope that emits the gamma-ray
- Peak energy in keV
- A100, that is the expected area if the concentration of the element in the sample is 100%.
- R: The activation rate, that is the number of activation reactions per second producing this radionuclide directly or indirectly.
- y: The gamma-ray yield as a fraction of 1.
- e: The detection efficiency as a fraction of 1
- c: the coincidence correction factor
- Asp: The entity known as "specific activity" in the k0-literature. If the gamma-ray yield is non-zero, and the reaction is the simplest (type 1 in the k0 literature), Asp is the product R.y.e.c. In case of sum peaks, Asp is R.P, where P is the probability of detecting a count in the full-energy peak per disintegration of the radionuclide. In case of multiple irradiations, the value shown was calculated from the last irradiation preceding the measurement.

If the peak was detected in a spectrum, a second line follows, and the following information is given:

- Isotope that emits the gamma-ray energy
- Peak energy in keV
- "assigned to": Measured peak energy in keV.
- Peak area and uncertainty
- Max amount calculated from (peak area + 2x uncertainty)/A100.
- One or more codes:
  - ND means not detected.
  - K0 means there is a k0-constant associated with the peak.
  - DR means the peak was deselected / disregarded.

Next come the subsystems of linear equations and their Linear Least Squares solutions, if the "Intermediate results in log file of interpretation" box was ticked in the Edit//Interpret options dialog dialogue. Here one sees Blaauw's holistic interpretation method at work. The method is best explained with a small example:

```
System of equations with 10 observed, 3 expected peaks (so 13 equations) and 2 unknowns
En/ent:  Br          W
  59.7 | 0.00E+000  2.95E+008 |    438 +/- 441 (1) *
 134.2 | 0.00E+000  4.87E+008 |    421 +/- 425 (1) *
 479.5 | 0.00E+000  4.02E+008 |   1633 +/- 145 (1)
 551.5 | 0.00E+000  8.68E+007 |    240 +/- 253 (1) *
 553.9 | 7.65E+008  0.00E+000 |   4114 +/- 570 (1)
 618.9 | 4.21E+008  9.59E+007 |   2748 +/- 140 (1)
 685.7 | 0.00E+000  3.80E+008 |   1517 +/- 133 (1)
 698.3 | 2.41E+008  0.00E+000 |   1113 +/- 129 (1)
 776.5 | 6.62E+008  0.00E+000 |   3278 +/- 195 (1)
 827.9 | 1.81E+008  0.00E+000 |    787 +/- 130 (1)
1044.2 | 1.67E+008  0.00E+000 |    764 +/- 147 (1)
1317.6 | 1.35E+008  0.00E+000 |    708 +/- 98 (1)
1475.2 | 7.40E+007  0.00E+000 |    425 +/- 76 (1)

LLS fit| 5.13E-006  3.79E-006
Chisqr: 1.8

-------------------------------------

###
```

What is shown here is the system of equations for Br and W. These elements must be considered at the same time because both are expected to yield a peak at 618.9 keV. Let's take a look at the line for that energy. If the sample consisted of pure Br, at the given irradiation time, decay time, measurement time et cetera, the peak area at that energy (the "A100") would have been 4.21×10^8 counts (first column). Pure W would have yielded 9.59×10^7 counts (second column). The observed peak area was 2748 ± 140 counts (third and fourth column). But Br also yields peaks that W could not contribute to and vice versa. All the observed peak areas are considered to be the linear sum of the W and Br contributions. There are even some unobserved peaks of which the absence might shed light on the matter, these are shown tagged with a '*'. The area of such peaks is estimated from the continuum at the peak position as described in Blaauw's paper on peak search methods. The (1) indicates that all the peaks in this example belong to the first measured spectrum of the sample.

The resulting system of 13 equations and 2 unknowns is solved by standard LLS methods and the result is shown with its reduced Chisqr. A reduced Chisqr of 1.0 is perfect, lower is ok but less perfect, and above 5 or so something clearly went wrong.

The log file proceeds by listing all the peaks in the spectra that were considered relevant, and the contributions to these peaks. For the 618.9 keV peak from the system of equations above, the example reads

```
Peak at 618.96 keV, 2076 +/- 501 counts
        Significant contributions:
                  619.10 keV, Br, Br-82: (0.694 +/- 0.081) x 5.976E-006,
                         y: 4.324E+001 %, e: 4.954E-003, c: 0.9466, Asp: 2.592E+008
                                        +/- 3.858E+006) (k0)
                  618.34 keV, W, W-187: (0.172 +/- 0.040) x 2.293E-005,
                         y: 6.070E+000 %, e: 4.960E-003, c: 0.9995, Asp: 1.663E+008 +/- 1.298E+006) (k0)
                Total assigned fraction: 0.865 +/- 0.090
        Contributions considered insignificant:
                  620.36 keV, Ag, Ag-110m: (0.004 +/- 0.002) x 1.175E-003,
                         y: 2.825E+000 %, e: 4.945E-003, c: 0.9409, Asp: 9.928E+006 +/- 5.062E+005) (k0)
                  620.04 keV, Ba, Ba-131: (0.025 +/- 0.001) x 2.328E-002,
                         y: 1.570E+000 %, e: 4.947E-003, c:  1.375, Asp: 3.144E+004 +/- 1.833E+003) (k0)
                  620.79 keV, Er, Er-171: (0.000 +/- 0.000) x 1.659E+001,
                         y: 8.896E-002 %, e: 4.942E-003, c: 0.9491, Asp: 1.194E+005 +/- 2.462E+004)
                  617.51 keV, Gd, Gd-159: (-0.000 +/- 0.000) x 3.429E-001,
                         y: 1.400E-002 %, e: 4.966E-003, c: 0.9942, Asp: 1.257E+004 +/- 2.592E+003)
                  618.58 keV, Hf, Hf-181: (0.001 +/- 0.000) x 1.011E-002,
                         y: 4.030E-002 %, e: 4.958E-003, c:  1.097, Asp: 1.445E+006 +/- 2.978E+005)
                  618.33 keV, La, La-140: (0.035 +/- 0.001) x 1.052E-003,
                         y: 5.990E-002 %, e: 4.960E-003, c:  0.955, Asp: 6.717E+005 +/- 1.385E+005)
                  620.02 keV, Mo, Mo-99: (-0.000 +/- 0.000) x 2.339E+000,
                         y: 2.310E-003 %, e: 4.947E-003, c: 0.9711, Asp: 2.092E+002 +/- 4.312E+001)
                  620.37 keV, Nd, Pm-151: (0.000 +/- 0.000) x 2.577E-001,
                         y: 6.900E-002 %, e: 4.945E-003, c:  1.002, Asp: 4.831E+003 +/- 9.960E+002)
                  620.11 keV, Pd, Ag-111: (0.000 +/- 0.000) x 3.016E-001,
                         y: 1.811E-002 %, e: 4.947E-003, c:  1.003, Asp: 1.869E+003 +/- 3.225E+002)
                  616.70 keV, Sb, Sb-122: (0.003 +/- 0.000) x 6.153E-003,
                         y: 1.120E-002 %, e: 4.972E-003, c: 0.9769, Asp: 8.003E+004 +/- 1.650E+004)
                  621.17 keV, U, I-132: (0.001 +/- 0.000) x 1.814E-003,
                         y: 1.580E+000 %, e: 4.939E-003, c: 0.9448, Asp: 2.683E+005 +/- 4.195E+004)
```

The data shown are the measured peak energy, area and uncertainty. Then come the significant contributions to the peak. Shown are the element symbols, the radionuclide yielding the peak, and the peak energy according to the nuclear catalogues, followed by the concentrations of Br and W that the observed peak area corresponds to (5.97×10^{-6} kg/kg Br and 2.293×10^{-5} kg/kg W). This information is followed by the yield of the gamma-ray, the full-energy peak efficiency for that energy in the actual counting geometry, and the coincidence correction factor (if applicable, for artificial peaks like escape peaks or some peaks "N/A" is shown). The k_0 "Specific activity" follows, as defined above. If a peak is associated with a k0-constant, the (k0) tag is printed. If the peak (or rather its position) was used to estimate the detection limit for the element, it is tagged with (dl). All this information is preceded by the fraction of the peak that was assigned to the elements, that is, the final element concentration as reported by the program, divided by the concentration shown here, that is the one corresponding to the complete peak area. The sum of the assigned fractions should be 1 within its uncertainty. In the example, it is a little more than 2 standard deviations off - no reason for alarm, since that is expected to happen in 1 out of 20 cases.

Next come the insignificant contributions. These are just like the significant contributions, only they were disregarded in the system of linear equations, because of being smaller than the uncertainty in the observed peak area, or smaller than the insignificance fraction set by the user. Elements that were not detected at all are shown in this list by denoting the contribution fraction with a '<' sign instead of an uncertainty, meaning that the contribution is smaller than that, as well as that the element

was not detected at all. This approach results in systems of equations that are reasonably sized to solve on a computer, but in the example one can see that the assigned fraction would have been closer to unity if the Ba and La contributions had been taken into account.

Some peaks were not actually observed, but merely expected in the spectrum. The file shows these with the areas that might have been observed at that location in the spectrum.

Some peaks were not observed, but the upper limit for the unobserved peak area determined the upper limit or detection limit for the associated element. These elements are then listed as insignificant contributions with 0 areas and tagged with (dl).

For **comparators**, the output is very similar to the output for ordinary samples. This time, not the elemental concentrations are the unknowns, but the thermal fluxes as observed through the different activation reactions. The file starts with information about expected peaks, if the "All Asp in log file of interpretation" box was ticked in the Edit//Interpret options dialog dialogue.

For each reaction (or only one if View/Options for plot/views was used to select an element of interest), all peaks are listed if the expected area 'A100' is larger than 1 and the peak was considered relevant by the software in view of the maximum concentrations established for each reaction. For each peak, the following numbers are given:

- Isotope that emits the gamma-ray
- Peak energy in keV
- A100, that is the expected area if the neutron flux was $4x10^{16}$ $m^{-2}s^{-1}$.
- R: The activation rate, that is the number of activation reactions per second producing this radionuclide directly or indirectly.
- y: The gamma-ray yield as a fraction of 1.
- e: The detection efficiency as a fraction of 1
- c: the coincidence correction factor
- Asp: The entity known as "specific activity" in the k0-literature. If the gamma-ray yield is non-zero, and the reaction is the simplest (type 1 in the k0 literature), Asp is the product R.y.e.c. In case of sum peaks, Asp is R.P, where P is the probability of detecting a count in the full-energy peak per disintegration of the radionuclide. In case of multiple irradiations, the value shown was calculated from the last irradiation preceding the measurement.

If the peak was detected in a spectrum, a second line follows, and the following information is given:

- Isotope that emits the gamma-ray energy
- Peak energy in keV
- "assigned to": Measured peak energy in keV
- Peak area and uncertainty
- Max amount calculated from (peak area + 2x uncertainty)/A100, if this result is multiplied with $4x10^{16}$ $m^{-2}s^{-1}$, a neutron flux is obtained.
- One or more codes:
  - ND means not detected.
  - K0 means there is a k0-constant associated with the peak.
  - DR means the peak was deselected / disregarded.

Next come the subsystems of linear equations and their Linear Least Squares solutions, if the "Intermediate results in log file of interpretation" box was ticked in the Edit//Interpret options dialog dialogue.

The example is

```
System of equations with 1 observed, 0 expected peaks (so 1 equations) and 1 unknowns
En/ent:  Zn-69m
 438.6 | 4.33E+002 |    737 +/- 31 (1)

LLS fit| 6.80E+016
Chisqr: 0.0
```

Here, the area of $4.33x10^2$ is the expected area for a thermal flux of $4x10^{16}m^{-2}s^{-1}$ - an arbitrary order-of-magnitude estimate for all INAA facilities in the world. The observed peak area is larger, and the flux solved from this system of 1 equation with 1 unknown is $6.8x10^{16}m^{-2}s^{-1}$.

After all the individual activation reaction results, it is shown how all the observed thermal fluxes can be reconciled by also fitting the other flux parameters to the observed activation rates, but only if the comparator composition allows for that and the user did not force only the thermal flux to be determined.

```
RESULT OF FIT OF FLUX PARAMETERS
             Thermal flux: 6.312E+016 +/- 7.235E+014
Chisqr: 3.0

     Target     Product    Rate      err   fitrate    z
 1    Zn-64 ->    Zn-65: 4.660E-012   1.2 4.684E-012 -0.4
 2    Zn-68 ->   Zn-69m: 4.968E-013   4.3 4.609E-013 1.7
```

In the sample, only the thermal flux was determined as the weighted average of the results from two activation reactions. The observed activation rate (captures per second per target atom) is shown, as well as the rate calculated from the flux parameters. The quality of the fit is shown in terms of z-scores and a reduced Chisqr.

In the per-peak information coming next, thermal neutron fluxes corresponding to the peak areas are shown.

For **calibration sources**, the format of the first half of the log file is different. For starters, the file lists the ‘very first estimate’, of which a few lines are shown here. The efficiency values here are calculated directly from the known number of disintegrations of each radionuclide during the measurement, the known gamma-ray yield per disintegration, and the measured peak area. In a coincidence-free counting geometry, these would be correctly calculated efficiencies.

```
E (keV)    effic      err
  24.93 3.238E-004 1.044E-004
  32.19 1.001E-002 4.628E-004
  36.40 2.586E-002 2.006E-003
  88.03 2.264E-001 1.161E-003
 122.06 2.430E-001 8.467E-004
 136.47 2.360E-001 3.188E-003
 165.85 1.910E-001 9.294E-004
 255.07 1.525E-001 7.008E-003
 279.19 1.303E-001 3.170E-002
 391.69 9.688E-002 5.321E-004
 514.00 7.415E-002 3.563E-003
 661.66 6.110E-002 4.041E-004
 898.04 4.022E-002 3.353E-004
1173.24 3.046E-002 1.883E-004
1332.50 2.707E-002 1.617E-004
```

(Note the presence of the Cd-109 and Sn-113 X-rays here!)

The file subsequently lists the observed peak areas and the theoretical peak areas as obtained after the efficiency curve has been fitted to the data, as well as the ratios of these areas, and the standardized differences between them.

```
First estimate after fitting polynomial to very first estimate:
25 Peaks in Measured (v1) and 146 in Recon (v2)
   E    |      v1         e1     |     v2    |    v2/v1  |   v1-v2/e1  |
  24.93 | 2.58E+003 +/- 8.3E+002 | 7.91E+003 |       3.1 |        -6.4 |
  32.19 | 3.05E+004 +/- 1.4E+003 | 2.83E+004 |      0.93 |         1.6 |
  36.40 | 1.79E+004 +/- 1.4E+003 | 1.48E+004 |      0.83 |         2.2 |
  66.47 | 6.18E+002 +/- 2.4E+002 | 1.25E+001 |      0.02 |         2.6 |
  76.50 | 1.50E+003 +/- 3.7E+002 | 1.39E+000 |   0.00093 |           4 |
  88.03 | 9.06E+005 +/- 4.6E+003 | 9.37E+005 |         1 |        -6.7 |
 122.06 | 4.87E+005 +/- 1.7E+003 | 4.80E+005 |      0.98 |         4.5 |
 136.47 | 5.92E+004 +/- 8.0E+002 | 5.72E+004 |      0.97 |         2.5 |
 165.85 | 1.19E+005 +/- 5.8E+002 | 1.23E+005 |         1 |        -6.7 |
 255.07 | 4.90E+003 +/- 2.3E+002 | 4.42E+003 |       0.9 |         2.1 |
 279.19 | 8.88E+002 +/- 2.2E+002 | 8.76E+002 |      0.99 |       0.054 |
 339.65 | 1.09E+003 +/- 2.2E+002 | 8.78E+000 |    0.0081 |           5 |
 352.33 | 2.28E+003 +/- 2.2E+002 | 6.92E+000 |     0.003 |          11 |
 391.69 | 9.99E+004 +/- 5.5E+002 | 1.01E+005 |         1 |        -1.6 |
 461.71 | 9.48E+002 +/- 2.6E+002 | 1.46E-001 |   0.00015 |         3.7 |
 476.12 | 2.11E+003 +/- 5.8E+002 | 1.74E-002 |  8.3E-006 |         3.6 |
```

```
 514.00 | 1.11E+004 +/- 5.3E+002 | 1.13E+004 |         1 |       -0.49 |
 528.96 | 4.97E+002 +/- 2.1E+002 | 5.86E-004 |  1.2E-006 |        2.4 |
 584.33 | 1.95E+003 +/- 1.8E+002 | 3.43E-007 |  1.8E-010 |         11 |
 661.66 | 2.10E+006 +/- 1.4E+004 | 2.03E+006 |      0.97 |        4.8 |
 898.04 | 9.43E+004 +/- 7.9E+002 | 8.80E+004 |      0.93 |          8 |
 912.20 | 1.72E+003 +/- 2.2E+002 | 1.04E-002 |    6E-006 |        7.9 |
1173.24 | 1.19E+006 +/- 7.4E+003 | 1.05E+006 |      0.88 |         20 |
1332.50 | 1.06E+006 +/- 6.3E+003 | 8.89E+005 |      0.84 |         27 |
1764.51 | 6.81E+002 +/- 2.8E+002 | 9.47E-007 |  1.4E-009 |        2.4 |
Unreduced chisqr: 1.743E+003, reduced: 6.976E+001
```

However, in real counting geometries, there is always coincidence summing. So after correction for that, and the fitting of the theoretical peak areas to the observed peak areas by variation of the efficiency curve, the result is nicer as also shown in the log file. In the last step, peaks apparently not due to the radionuclides known to be present in the calibration source have been removed.

```
Final result:
15 Peaks in measured spectrum (v1) and 146 in theoretically reconstructed spectrum (v2)
   E    |      v1         e1     |     v2    |    v2/v1  |   v1-v2/e1  |
  24.93 | 2.58E+003 +/- 8.3E+002 | 7.34E+003 |       2.8 |        -5.7 |
  32.19 | 3.05E+004 +/- 1.4E+003 | 2.49E+004 |      0.82 |           4 |
  36.40 | 1.79E+004 +/- 1.4E+003 | 1.30E+004 |      0.73 |         3.5 |
  88.03 | 9.06E+005 +/- 9.1E+003 | 9.19E+005 |         1 |        -1.5 |
 122.06 | 4.87E+005 +/- 4.9E+003 | 4.81E+005 |      0.99 |         1.2 |
 136.47 | 5.92E+004 +/- 8.0E+002 | 5.74E+004 |      0.97 |         2.3 |
 165.85 | 1.19E+005 +/- 1.2E+003 | 1.22E+005 |         1 |        -2.6 |
 255.07 | 4.90E+003 +/- 2.3E+002 | 4.17E+003 |      0.85 |         3.2 |
 279.19 | 8.88E+002 +/- 2.2E+002 | 8.28E+002 |      0.93 |        0.28 |
 391.69 | 9.99E+004 +/- 1.0E+003 | 9.82E+004 |      0.98 |         1.7 |
 514.00 | 1.11E+004 +/- 5.3E+002 | 1.15E+004 |         1 |        -0.8 |
 661.66 | 2.10E+006 +/- 2.1E+004 | 2.15E+006 |         1 |        -2.5 |
 898.04 | 9.43E+004 +/- 9.4E+002 | 9.49E+004 |         1 |       -0.64 |
1173.24 | 1.19E+006 +/- 1.2E+004 | 1.19E+006 |         1 |       -0.34 |
1332.50 | 1.06E+006 +/- 1.1E+004 | 1.05E+006 |      0.99 |         1.2 |
Unreduced chisqr: 9.856E+001, reduced: 6.637E+000
```

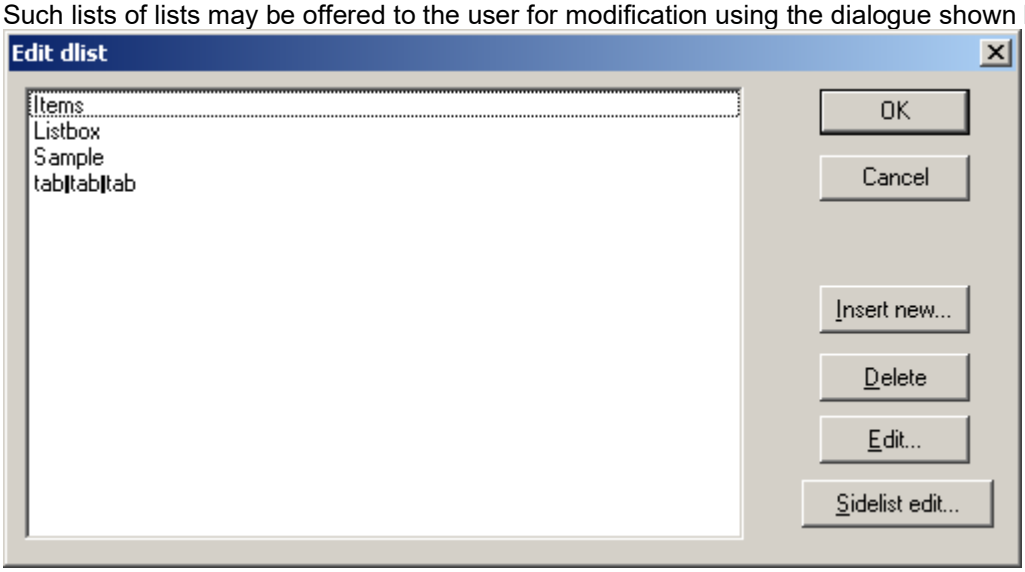
(This final result is not perfect, but not very bad either for a measurement performed right on the end cap of the detector...)

The file proceeds by listing all observed peaks and their interpretation, just as in the case of other kinds of samples. Instead of the concentration or flux corresponding to the peak area, however, the source activity at the start time of packaging is shown. For calibration sources, the start time of the packaging event is taken to be the reference time for the activities. If the timestamps in the permanent database differ from that time, they have been converted in the simplest manner using the radionuclide's half-life. This means that the activity you get, when you multiply the activity corresponding to the total peak area with the assignment factor, is equal to the known activity at the time of sample packaging. To avoid confusion, it is recommended to use the certificate date as the packaging date in case of detector efficiency calibration samples. The packaging time should never precede the certificate reference time. Asp values are meaningless here and shown as 0.0.

Editing list of lists

In a few cases, the k0-IAEA program works with a list of lists. For example, after analyzing a spectrum, there is a list of regions in the spectrum, and for each region there is a list of peaks found in that region.

Such lists of lists may be offered to the user for modification using the dialogue shown here.



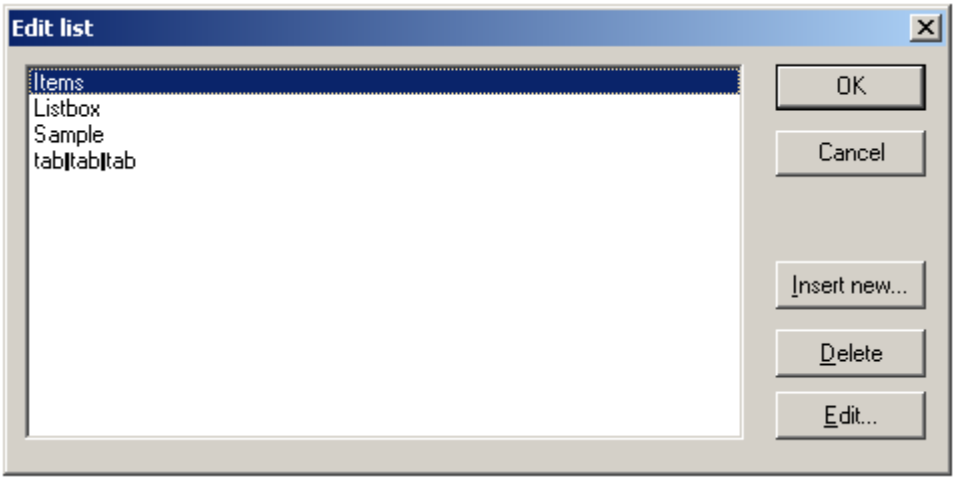
The text in the upper left corner of the window will be different dependent on the list of lists to be modified. Also, the text for the choice on the lower right button will reflect what's to be edited there.

The 'Insert new', 'Delete' and 'Edit' choices may be greyed out or not, depending on the list. The 'Insert new' and 'Edit' choices will result in another dialogue popping up, where the user is allowed to edit the selected or to-be-inserted record.

The 'Sidelist edit' choice will take the user to the 'Edit list' dialogue.

Editing lists

The k0-IAEA program often uses lists of items for various purposes. These lists are sorted on some value (for example, a list of peaks is typically sorted on peak energy) and contain any number of records. All lists that can be edited by the user are first offered up with the 'Edit list' dialogue shown here.



The text at the top left edge of the window is different for the different lists. Also, what is shown in the blank middle area varies from list to list: It should be enough at least to see unambiguously what record is being selected.

##
#

The ‘Insert new’, ‘Delete’ and ‘Edit’ choices may be greyed out or not, depending on the list. The ‘Insert new’ and ‘Edit’ choices will result in another dialogue popping up, where the user is allowed to edit the selected or to-be-inserted record.