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Covariances between gamma-ray energies

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Abstract

Covariances between experimental data are as significant as variances both in the evaluation of uncertainties and to perform statistical tests. If standard data are used in calibrations, covariances must be taken into account. Covariances are also necessary in order to update values every time when new data are obtained. In this paper we determined covariances between the most important gamma-ray energies for use in Ge-semiconductor detectors calibration recently published by Helmer and van der Leun (Nucl. Instr. Meth. A 450 (2000) 35).

1. Introduction

A consistent set of gamma-ray energies recommended for use in energy calibration was recently published by Helmer and van der Leun [1]. Those data are, however, correlated and these correlations must be taken into account both in calibrations and in statistical tests, as the chi-squared test, especially in the cases where the correlation coefficients are near ± 1.

In this paper the correlation coefficients of those data were estimated by using the matrix formalism of the Least-Squares Method (LSM) with level energy relations included as constraints in the fitting.

2. Energy calibration: input data and least-squares procedure

Helmer and van der Leun [1] used four types of input data in order to update gamma-ray energies. Those data were taken into account in this analysis in order to determine the correlation coefficients. The four types of data set are described below.

(a) Measured wavelengths of 22 gamma-ray transition energies using double-flat Si crystal. The Si lattice parameter adopted in Ref. [1] is $d = 0.192015540(40)$ nm. Since gamma-ray wavelengths depend on the common factor d, they are correlated. In order to determine the covariance matrix of the data, data from Table 3 of Ref. [1] were transformed back to the ratio between d and gamma-ray wavelengths, and the uncertainties were "unpropagated". The data considered in this analysis are $R_i = \lambda_i/d$, and the gamma-ray energies in eV are related to R_i by $R_i = f/E_i$, where $f = hc/ed$. The fundamental constant hc/e was taken as $1.23984244(37)10^{-6}$ eV m. The data R_i were supposed to be statistically independent.

(b) Another group of data are gamma-ray energies relative to the 412 keV transition of ^{198}Au determined from relative wavelength measurements. (Data with the superscript h in Table 4 of Ref. [1] were not taken into account.) Those data

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are identified below as F_i ($F_i = E_i/E_{\mathrm{Au}}$). At this stage, only the measured uncertainties of F_i were taken into account; uncertainty of the 412 keV transition was not propagated to F_i.

(c) Gamma-ray energy differences were taken into account without transformation. They are identified as $D_{ij} = E_i - E_j$.

(d) The last set of data are gamma-ray energies measured with Ge-detectors and are identified in this paper by $G_i = E_i$.

$$\begin{pmatrix} R_i - f_c/E_{ic} \\ F_i - E_{ic}/E_{\mathrm{Auc}} \\ D_{ij} - (E_{ic} - E_{jc}) \\ G_i - E_{ic} \\ f - f_c \end{pmatrix} = \begin{pmatrix} 0 & \frac{-f_c}{E_{ic}^2} & 0 & 0 & \cdots & \cdots & \frac{1}{E_{ic}} \\ \vdots & & & & & & \vdots \\ \frac{-E_{ic}}{E_{\mathrm{Auc}}^2} & 0 & \cdots & \frac{1}{E_{\mathrm{Auc}}} & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 1 & 0 & \cdots & -1 & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} \Delta E_{\mathrm{Au}} \\ \Delta E_1 \\ \vdots \\ \Delta E_n \\ \Delta f \end{pmatrix} + \mathbf{e}' \tag{4}$$

where E_i is the ith gamma-ray energy and E_{Au} is the energy of the 412 keV transition from ^{198}Au decay. In this equation the subscript c indicates the current value of the parameter in the iterative procedure.

Since some data were taken in the same measurement at the same laboratory, they are affected by common errors and, as a consequence, are correlated. However, these correlations were neglected in this paper; in Section 4, we discuss the consequence of this hypothesis.

The constant f was considered both as experimental data and as a parameter to be fitted. The other parameters to be fitted are the gamma-ray energies.

The Least-Squares Method equations were used as below. If $\boldsymbol{Y}$ is a set of experimental data with covariance matrix $\boldsymbol{V}$, $\boldsymbol{A}_0$ a set of parameters and $\boldsymbol{X}$ a design matrix, the linear model equation is

$$\boldsymbol{Y} = \boldsymbol{X}\cdot\boldsymbol{A}_{\mathbf{o}} + \boldsymbol{e} \tag{1}$$

where $\boldsymbol{e}$ is the column vector formed by the errors. The solution given by the LSM is (see for example Ref. [2] or Appendix E of Ref. [3])

$$\tilde{\boldsymbol{A}} = \boldsymbol{V}_{\tilde{A}}\cdot\boldsymbol{X}^t\cdot\boldsymbol{V}^{-1}\cdot\boldsymbol{Y} \tag{2}$$

where

$$\boldsymbol{V}_{\tilde{A}} = (\boldsymbol{X}^t\cdot\boldsymbol{V}^{-1}\cdot\boldsymbol{X})^{-1} \tag{3}$$

is the covariance matrix of $\tilde{\boldsymbol{A}}$, and $\boldsymbol{V}$ is the covariance matrix of $\boldsymbol{Y}$ defined by $V_{ij} = \langle e_i\cdot e_j\rangle$, where $\langle\,\rangle$ stands for expected values.

Since some relations between gamma-ray energies and the experimental data are not linear, an iterative procedure of the LSM was adopted. The explicit form of Eq. (1) is

Data of types (a) and (b) above were supposed to be statistically independent. However, gamma-ray energies and the fundamental constant f are correlated,

$$\mathrm{cov}(E_i, f) = E_i\sigma_f^2/f. \tag{5}$$

As a consequence, data of types (c) and (d) are correlated both between them and to f.

As expected, the fundamental constant f remains unchanged in the fit since no new experimental data on f were included. Covariances between f and the gamma-ray energies were changed but the correlation coefficients (related to covariance by $\rho_{ij} = \mathrm{cov}_{ij}/\sigma_i\sigma_j$) remain unchanged.

Added to the experimental data, some decay scheme relations were imposed in Ref. [1]. In this paper those relations have also been considered, too.

3. Results

Apart from some details, the procedure developed in this paper gives the same results quoted by Helmer and van der Leun in Ref. [1]. The only relevant difference is the covariance matrix, not given in Ref. [1]. The Tables given below show the most important correlation coefficients ($\rho \geq 0.7$ and $\rho \leq -0.5$) between gamma-ray energies.

The origin of correlation between gamma-ray energies can be seen by inspecting the experimental data and the fitting procedures. Some examples are given below:

(i) *Experimental origin of correlation*: Some correlations come from experiments, as is the case of the 1275 keV from ^{22}Na decay and the 1292 keV from the ^{59}Fe decay. In this case, the correlation is due to the fact that the 1275 keV transition was determined from energy difference with relation to the 1292 keV. The experimental result is 17.053(3) keV (see Table 7 of Ref. [1]). Since the uncertainty of the 1292 keV is 6 eV, the uncertainty of the 1275 keV is $\sqrt{36}9$ eV ≈ 7 eV. From the covariance matrix propagation formula (see Appendix B), the correlation between both gamma-ray energies is

$$\rho_{1275,1292} = \frac{(6\,\mathrm{eV})^2}{7\,\mathrm{eV}\cdot 6\,\mathrm{eV}} \approx 0.86.$$

This example also shows how a new measurement of a quantity can affect both the adopted value of other quantities and their standard deviation. For instance, a new and better measurement of the 1292 keV will change both the adopted value of the 1275 keV energy and its uncertainty. Also, a new measurement of the 1275 keV transition will change both the adopted value and the uncertainty of the 1292 keV transition. These changes can be accomplished if and only if, one knows the entire correlation matrix of all involved quantities [4,5].

(ii) *Cascade-crossover relation*: Some gamma-ray energies were determined mainly by cascade-crossover relations. For instance, 1157, 1189, 1221, 1231, 1257, 1274, 1289, 1374 and 1387 keV from ^{182}Ta decay were determined from cascade-crossover relations involving 1121 keV (standard deviation of 3 eV) and some low-energy transitions measured with curved crystal in relation to the ^{198}Au 412 keV. Since these low-energy transitions have uncertainties less than 1 eV, the uncertainties of the above energies are almost equal to the uncertainty of 1121 keV and they are strongly correlated both to this energy and between themselves. For example, 1189 keV was determined from the sum of 1121 keV and 68 keV (uncertainty of 0.1 eV); from covariance matrix propagation the correlation coefficient between 1189 and the 1121 keV is

$$\rho_{1189,1121} = \frac{(3\,\mathrm{eV})^2}{\sqrt{((3\,\mathrm{eV})^2 + (0.1\,\mathrm{eV})^2)}\cdot 3\,\mathrm{eV}} \approx 1.$$

(iii) *Negative correlation*: Some cascade-crossover relations give rise to negative correlation between gamma-ray energies. For example, the 199 keV transition from ^{75}Se decay was determined from a least-squares fit including some other gamma-rays and its energy was mainly determined from the difference between 264 keV (standard deviation 0.9 eV) and 66 keV (standard deviation 0.8 eV). So, using covariance matrix propagation formula, the correlation between 199 and 66 keV is

$$\rho_{199,66} = \frac{-0.8^2}{\sqrt{0.8^2 + 0.9^2}\cdot 0.8} = -0.66.$$

Small differences between correlation coefficients calculated in these examples and values quoted in Tables 1 and 2 are due to rounding both in our calculation and in Ref. [1], and also due to the fact that in our calculations standard deviations were not multiplied by the square root of the reduced χ^2.

4. Conclusion

When a correlation coefficient is positive, then if a datum is overestimated (underestimated) the other datum is *probably* overestimated (underestimated), too. When the correlation is negative, then if a datum is overestimated (underestimated) the other datum is *probably* underestimated (overestimated). These probabilities are greater if the correlation coefficient is great, and they turn a certainty if the correlation coefficient is ± 1. So, if the correlation of two gamma-ray energies is near ± 1, it must be taken into account in every calibration and statistical test.

Table 1
Positive correlation coefficients between some gamma-ray energies (second and fourth columns, in keV) recommended for use in energy calibrations

^{22}Na	1274.5	^{59}Fe	1291.6	0.78
^{46}Sc	889.3	^{84}Rb	881.6	0.82
^{46}Sc	889.3	^{94}Nb	871.1	0.74
^{46}Sc	889.3	^{110}Ag	884.7	0.74
^{56}Co	977.4	^{56}Co	2015.2	0.84
^{56}Co	977.4	^{56}Co	3253.4	0.76
^{56}Co	1037.8	^{56}Co	2212.9	0.72
^{56}Co	1175.1	^{56}Co	2212.9	0.73
^{56}Co	1175.1	^{56}Co	3451.1	0.77
^{56}Co	1175.1	^{182}Ta	1121.3	0.71
^{56}Co	1175.1	^{182}Ta	1189.0	0.71
^{56}Co	1175.1	^{182}Ta	1221.4	0.71
^{56}Co	1175.1	^{182}Ta	1273.7	0.70
^{56}Co	1175.1	^{182}Ta	1289.1	0.71
^{56}Co	1175.1	^{182}Ta	1373.8	0.70
^{56}Co	1175.1	^{182}Ta	1387.4	0.70
^{56}Co	1238.3	^{56}Co	3451.1	0.78
^{56}Co	1238.3	^{182}Ta	1121.3	0.81
^{56}Co	1238.3	^{182}Ta	1189.0	0.81
^{56}Co	1238.3	^{182}Ta	1221.4	0.81
^{56}Co	1238.3	^{182}Ta	1231.0	0.80
^{56}Co	1238.3	^{182}Ta	1257.4	0.79
^{56}Co	1238.3	^{182}Ta	1273.7	0.80
^{56}Co	1238.3	^{182}Ta	1289.1	0.81
^{56}Co	1238.3	^{182}Ta	1373.8	0.80
^{56}Co	1238.3	^{182}Ta	1387.4	0.80
^{56}Co	1360.2	^{56}Co	2598.4	0.84
^{56}Co	1771.3	^{56}Co	3009.6	0.87
^{56}Co	1810.7	^{56}Co	2598.4	0.80
^{56}Co	1963.7	^{66}Ga	1918.3	0.75
^{56}Co	1963.7	^{66}Ga	2751.8	0.73
^{56}Co	2015.2	^{56}Co	3253.4	0.91
^{56}Co	2034.8	^{56}Co	3273.0	0.92
^{56}Co	2212.9	^{56}Co	3451.1	0.92
^{56}Co	3009.6	^{56}Co	3451.1	0.76
^{56}Co	3202.0	^{66}Ga	2189.6	0.88
^{56}Co	3202.0	^{66}Ga	3228.8	0.94
^{56}Co	3451.1	^{182}Ta	1121.3	0.76
^{56}Co	3451.1	^{182}Ta	1189.0	0.76
^{56}Co	3451.1	^{182}Ta	1221.4	0.76
^{56}Co	3451.1	^{182}Ta	1231.0	0.76
^{56}Co	3451.1	^{182}Ta	1257.4	0.74
^{56}Co	3451.1	^{182}Ta	1273.7	0.76
^{56}Co	3451.1	^{182}Ta	1289.1	0.76
^{56}Co	3451.1	^{182}Ta	1373.8	0.76
^{56}Co	3451.1	^{182}Ta	1387.4	0.76
^{59}Fe	1291.6	^{160}Tb	1271.9	0.75
^{66}Ga	1508.2	^{66}Ga	3380.9	0.87
^{66}Ga	1918.3	^{66}Ga	2751.8	0.94
^{66}Ga	2189.6	^{66}Ga	3228.8	0.94
^{66}Ga	3422.0	^{66}Ga	4461.2	0.95
^{75}Se	198.6	^{75}Se	264.7	0.73
^{75}Se	264.7	^{75}Se	400.7	0.77
^{84}Rb	881.6	^{94}Nb	871.1	0.82
^{94}Nb	702.6	^{124}Sb	722.8	0.75
^{94}Nb	702.6	^{144}Ce	696.5	0.76
^{95}Tc	582.1	^{124}Sb	602.7	0.86
^{95}Tc	582.1	^{124}Sb	1325.5	0.71
^{95}Tc	820.6	^{95}Tc	835.1	0.70
^{95}Tc	835.1	^{95}Tc	1039.3	0.76
^{108}Ag	433.9	^{125}Sb	427.9	0.95
^{108}Ag	433.9	^{125}Sb	463.4	0.96
^{108}Ag	614.3	^{125}Sb	600.6	0.78
^{108}Ag	614.3	^{125}Sb	636.0	0.74
^{110}Ag	657.8	^{110}Ag	1475.8	0.72
^{110}Ag	677.6	^{110}Ag	1384.3	0.77
^{110}Ag	677.6	^{110}Ag	1562.3	0.72
^{110}Ag	706.7	^{110}Ag	1384.3	0.79
^{110}Ag	818.0	^{110}Ag	1475.8	0.87
^{110}Ag	884.7	^{110}Ag	1505.0	0.71
^{110}Ag	884.7	^{110}Ag	1562.3	0.83
^{110}Ag	1475.8	^{110}Ag	1505.0	0.72
^{110}Ag	1475.8	^{110}Ag	1562.3	0.78
^{110}Ag	1505.0	^{110}Ag	1562.3	0.79
^{124}Sb	602.7	^{124}Sb	1325.5	0.81
^{124}Sb	645.8	^{137}Cs	661.7	0.72
^{124}Sb	713.8	^{124}Sb	790.7	0.91
^{124}Sb	713.8	^{124}Sb	1436.6	0.94
^{124}Sb	722.8	^{124}Sb	790.7	0.71
^{124}Sb	722.8	^{124}Sb	1436.6	0.82
^{124}Sb	790.7	^{124}Sb	1436.6	0.93
^{124}Sb	968.2	^{124}Sb	1045.1	0.82
^{124}Sb	968.2	^{124}Sb	1691.0	0.85
^{124}Sb	1045.1	^{124}Sb	1691.0	0.88
^{124}Sb	1368.2	^{124}Sb	2090.9	0.96
^{125}Sb	427.9	^{125}Sb	463.4	0.92
^{125}Sb	600.6	^{207}Bi	569.7	0.78
^{125}Sb	636.0	^{137}Cs	661.7	0.71
^{133}Ba	223.2	^{133}Ba	276.4	0.88
^{137}Cs	661.7	^{144}Ce	696.5	0.74
^{144}Ce	1489.1	^{144}Ce	2185.6	0.93
^{152}Eu	367.8	^{152}Eu	778.9	0.86
^{152}Eu	678.6	^{152}Eu	1089.7	0.96
^{152}Eu	688.7	^{152}Eu	810.5	1.00
^{152}Eu	867.4	^{152}Eu	1112.1	0.99
^{152}Eu	919.3	^{152}Eu	1408.0	0.89
^{152}Eu	1212.9	^{152}Eu	1457.6	1.00
^{153}Gd	103.2	^{153}Gd	172.9	0.75
^{154}Eu	444.5	^{154}Eu	692.4	0.91
^{154}Eu	1246.1	^{154}Eu	1494.0	0.99
^{160}Tb	879.4	^{160}Tb	966.2	0.97
^{160}Tb	962.3	^{160}Tb	1178.0	0.86
^{161}Tb	25.7	^{161}Tb	48.9	0.92
^{161}Tb	25.7	^{161}Tb	74.6	0.97
^{161}Tb	25.7	^{182}Ta	67.8	0.86
^{161}Tb	48.9	^{161}Tb	74.6	0.99
^{161}Tb	48.9	^{182}Ta	67.8	0.94
^{161}Tb	74.6	^{182}Ta	67.8	0.93
^{169}Yb	63.1	^{169}Yb	261.1	0.79

(cont.).

conti.
Table 1

^{169}Yb	109.8	^{169}Yb	130.5	0.79
^{169}Yb	109.8	^{169}Yb	177.2	0.82
^{169}Yb	109.8	^{169}Yb	307.7	0.86
^{169}Yb	109.8	^{192}Ir	205.8	0.74
^{169}Yb	109.8	^{192}Ir	612.5	0.70
^{169}Yb	109.8	^{198}Au	411.8	0.80
^{169}Yb	130.5	^{169}Yb	177.2	0.77
^{169}Yb	130.5	^{169}Yb	198.0	0.87
^{169}Yb	130.5	^{169}Yb	261.1	0.86
^{169}Yb	130.5	^{169}Yb	307.7	0.92
^{169}Yb	130.5	^{192}Ir	205.8	0.83
^{169}Yb	130.5	^{192}Ir	296.0	0.70
^{169}Yb	130.5	^{192}Ir	604.4	0.78
^{169}Yb	130.5	^{192}Ir	612.5	0.78
^{169}Yb	130.5	^{198}Au	411.8	0.86
^{169}Yb	177.2	^{169}Yb	198.0	0.91
^{169}Yb	177.2	^{169}Yb	261.1	0.89
^{169}Yb	177.2	^{169}Yb	307.7	0.96
^{169}Yb	177.2	^{192}Ir	205.8	0.82
^{169}Yb	177.2	^{192}Ir	604.4	0.78
^{169}Yb	177.2	^{192}Ir	612.5	0.78
^{169}Yb	177.2	^{198}Au	411.8	0.88
^{169}Yb	198.0	^{169}Yb	261.1	0.96
^{169}Yb	198.0	^{169}Yb	307.7	0.95
^{169}Yb	198.0	^{192}Ir	205.8	0.83
^{169}Yb	198.0	^{192}Ir	296.0	0.71
^{169}Yb	198.0	^{192}Ir	604.4	0.78
^{169}Yb	198.0	^{192}Ir	612.5	0.79
^{169}Yb	198.0	^{198}Au	411.8	0.88
^{169}Yb	261.1	^{169}Yb	307.7	0.93
^{169}Yb	261.1	^{192}Ir	205.8	0.83
^{169}Yb	261.1	^{192}Ir	296.0	0.71
^{169}Yb	261.1	^{192}Ir	604.4	0.78
^{169}Yb	261.1	^{192}Ir	612.5	0.79
^{169}Yb	261.1	^{198}Au	411.8	0.90
^{169}Yb	307.7	^{192}Ir	205.8	0.87
^{169}Yb	307.7	^{192}Ir	296.0	0.74
^{169}Yb	307.7	^{192}Ir	316.5	0.72
^{169}Yb	307.7	^{192}Ir	604.4	0.82
^{169}Yb	307.7	^{192}Ir	612.5	0.83
^{169}Yb	307.7	^{198}Au	411.8	0.93
^{172}Hf	78.7	^{172}Hf	81.8	0.70
^{182}Ta	84.7	^{182}Ta	152.4	0.96
^{182}Ta	113.7	^{182}Ta	179.4	0.81
^{182}Ta	156.4	^{182}Ta	222.1	0.89
^{182}Ta	198.4	^{182}Ta	264.1	0.88
^{182}Ta	1121.3	^{182}Ta	1189.0	1.00
^{182}Ta	1121.3	^{182}Ta	1221.4	1.00
^{182}Ta	1121.3	^{182}Ta	1231.0	0.98
^{182}Ta	1121.3	^{182}Ta	1257.4	0.97
^{182}Ta	1121.3	^{182}Ta	1273.7	0.99
^{182}Ta	1121.3	^{182}Ta	1289.1	1.00
^{182}Ta	1121.3	^{182}Ta	1373.8	0.99
^{182}Ta	1121.3	^{182}Ta	1387.4	0.99
^{182}Ta	1189.0	^{182}Ta	1221.4	1.00
^{182}Ta	1189.0	^{182}Ta	1231.0	0.98
^{182}Ta	1189.0	^{182}Ta	1257.4	0.97
^{182}Ta	1189.0	^{182}Ta	1273.7	0.99
^{182}Ta	1189.0	^{182}Ta	1289.1	1.00
^{182}Ta	1189.0	^{182}Ta	1373.8	0.99
^{182}Ta	1189.0	^{182}Ta	1387.4	0.99
^{182}Ta	1221.4	^{182}Ta	1231.0	0.98
^{182}Ta	1221.4	^{182}Ta	1257.4	0.97
^{182}Ta	1221.4	^{182}Ta	1273.7	0.99
^{182}Ta	1221.4	^{182}Ta	1289.1	1.00
^{182}Ta	1221.4	^{182}Ta	1373.8	0.99
^{182}Ta	1221.4	^{182}Ta	1387.4	0.99
^{182}Ta	1231.0	^{182}Ta	1257.4	0.95
^{182}Ta	1231.0	^{182}Ta	1273.7	0.99
^{182}Ta	1231.0	^{182}Ta	1289.1	0.98
^{182}Ta	1231.0	^{182}Ta	1373.8	0.99
^{182}Ta	1231.0	^{182}Ta	1387.4	0.99
^{182}Ta	1257.4	^{182}Ta	1273.7	0.96
^{182}Ta	1257.4	^{182}Ta	1289.1	0.97
^{182}Ta	1257.4	^{182}Ta	1373.8	0.96
^{182}Ta	1257.4	^{182}Ta	1387.4	0.96
^{182}Ta	1273.7	^{182}Ta	1289.1	0.99
^{182}Ta	1273.7	^{182}Ta	1373.8	1.00
^{182}Ta	1273.7	^{182}Ta	1387.4	0.99
^{182}Ta	1289.1	^{182}Ta	1373.8	0.99
^{182}Ta	1289.1	^{182}Ta	1387.4	0.99
^{182}Ta	1373.8	^{182}Ta	1387.4	0.99
^{192}Ir	205.8	^{192}Ir	296.0	0.71
^{192}Ir	205.8	^{192}Ir	604.4	0.78
^{192}Ir	205.8	^{192}Ir	612.5	0.78
^{192}Ir	205.8	^{198}Au	411.8	0.84
^{192}Ir	296.0	^{192}Ir	604.4	0.86
^{192}Ir	296.0	^{192}Ir	612.5	0.87
^{192}Ir	296.0	^{198}Au	411.8	0.72
^{192}Ir	308.5	^{192}Ir	604.4	0.89
^{192}Ir	316.5	^{192}Ir	612.5	0.90
^{192}Ir	316.5	^{198}Au	411.8	0.71
^{192}Ir	416.5	^{192}Ir	588.6	0.91
^{192}Ir	416.5	^{192}Ir	884.5	0.89
^{192}Ir	588.6	^{192}Ir	884.5	0.97
^{192}Ir	604.4	^{192}Ir	612.5	0.84
^{192}Ir	604.4	^{198}Au	411.8	0.80
^{192}Ir	612.5	^{198}Au	411.8	0.81
^{198}Au	675.9	^{198}Au	1087.7	0.98
^{203}Pb	401.3	^{203}Pb	680.5	0.94

Table 2
Negative correlation coefficients between some gamma-ray energies

^{75}Se	66.1	^{75}Se	198.6	−0.66
^{75}Se	96.7	^{75}Se	303.9	−0.68
^{75}Se	121.1	^{75}Se	279.5	−0.75
^{75}Se	136.0	^{75}Se	264.7	−0.51
^{110}Ag	446.8	^{110}Ag	937.5	−0.65
^{133}Ba	160.6	^{133}Ba	223.2	−0.76
^{133}Ba	160.6	^{133}Ba	276.4	−0.69

This paper gives the most intense (negative and positive) correlation coefficients between gamma-ray energies adopted as reference in detector calibration. These correlation coefficients must be taken into account in every calibration, as explained in Appendix A. If one does not intend to use the correlation coefficients, he/she must avoid the use of highly correlated data in the same calibration.

Finally, we must consider that the experimental data used as input of the LSM in this paper can be correlated. Data from types (a) and (b) can be correlated due to common errors affecting all results from the same laboratory. Data of type (c) can be correlated if some energy differences were measured in the same experiment and using the same channel × energy calibration curve. This effect also occurs with data of type (d) determined using the same calibrated detector. In order to test the consequence of these initial correlation coefficients, we considered the hypothesis of correlation coefficients 0.4, typical of wavelength measurement with Si crystals [6], between all data of type (a). Only 25 (over about 200) correlation coefficients greater than 0.7 were changed more than 10%. This fact accords with the result obtained in Ref. [6]. where a relatively large range of the initial correlation coefficients would give practically the same final results. Correlation coefficients between data of types (b) and (c) are expected to be less important, since part of the uncertainties come from the channels and they are, as usual, non-correlated. For instance, from the 456 correlation coefficients between gamma-ray energies from ^{152}Eu and ^{192}Ir given in Ref. [7], only about 20 are greater than 0.4. Since we have not taken into account possible correlation between input data, we can estimate that the correlation coefficients given in Tables 1 and 2 are precise within about 10%.

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Appendix A

This appendix shows how to include covariance between gamma-ray energies in a calibration procedure.

Consider a calibration function given by

$$E = a_1 + a_2 \cdot C + a_3 \cdot C^2 ... + a_m \cdot C^{m-1} \tag{A.1}$$

where E is the energy and C is the channel where the correspondent energy peak was observed. In this case the fitted parameters are given by Eq. (2), where $\boldsymbol{Y}$ is the vector given by the calibration energies,

$$\boldsymbol{Y} = \begin{pmatrix} E_1 \\ E_2 \\ \vdots \\ E_n \end{pmatrix} \tag{A.2}$$

and $\boldsymbol{X}$ is the design matrix given by

$$\boldsymbol{X} = \begin{pmatrix} 1 & C_1 & \cdots & C_1^{m-1} \\ 1 & C_2 & & C_2^{m-1} \\ \vdots & & & \vdots \\ 1 & C_n & \cdots & C_n^{m-1} \end{pmatrix} \tag{A.3}$$

where n is the number of experimental points used in the fitting.

The covariance matrix of $\boldsymbol{Y}$, $\boldsymbol{V}$, is given by

$$\mathbf{V} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \cdots & \rho_{1n}\sigma_1\sigma_n \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & & \rho_{2n}\sigma_2\sigma_n \\ \vdots & & & \vdots \\ \rho_{1n}\sigma_1\sigma_n & \rho_{2n}\sigma_2\sigma_n & \cdots & \sigma_n^2 \end{pmatrix} + \boldsymbol{V}_{\mathrm{C}} \tag{A.4}$$

where σ_i is the standard deviation of the gamma-ray energy E_i given in ref. [1], ρ_{ij} is the correlation coefficient between E_i and E_j given in this paper, and $\boldsymbol{V}_C$ is the covariance matrix of the peak positions. Usually, the peak positions are not correlated (since doublets are not used in energy calibrations) and, as a consequence, $\boldsymbol{V}_C$ is a diagonal matrix. Terms with exponents greater than 1 in the calibration function (Eq. (A.1)) are usually negligible when errors are to be propagated from the "independent" variable C to the "dependent" variable E. In this case $\boldsymbol{V}_C$ is given by

$$\mathbf{V}_C = g^2 \begin{pmatrix} \sigma_{C1}^2 & 0 & \cdots & 0 \\ 0 & \sigma_{C2}^2 & & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & \sigma_{Cn}^2 \end{pmatrix} \tag{A.5}$$

where g is the gain (energy/channel) parameter and σ_{Ci} is the standard deviation of the ith peak position.

The chi-square test can be performed by

$$\chi^2 = (\boldsymbol{Y} - \boldsymbol{X}\cdot\tilde{\boldsymbol{A}})^t \cdot \boldsymbol{V}^{-1} \cdot (\boldsymbol{Y} - \boldsymbol{X}\cdot\tilde{\boldsymbol{A}}). \tag{A.6}$$

The variable χ^2 obeys a chi-squared distribution with $n - m$ degrees of freedom.

In order to show how large the effect of including covariance terms is, we simulated a calibration with 11 data between 1010 and 3510 keV in steps of 250 keV. The uncertainties of those data were 5 ev and the correlation coefficients between them were all equal to 0.8. These data simulate approximately a calibration using the ^{56}Co gamma-ray energies. The calibration used in the simulation was $E = a + b\cdot C = 10 + C$, where C is the channel number. The calibration was supposed to have an uncertainty due to the channels equivalent to 3 eV and null covariances. The simulated data are shown in Table 3.

This simulated experience was first analyzed considering the total covariance matrix of the data and, after that, neglecting the correlation coefficients. Since this simulation corresponds to a calibration procedure, energies of channels 1400 and 1500 were interpolated. The results are shown in Table 4. The fitted parameters of the calibration curve, a and b, do not change if one neglects the covariance terms in this case of equal correlation coefficients. The most important changes are the chi-squared values and the uncertainties and correlation of interpolated energies. Neglecting covariances, the chi-squared values was reduced and its confidence level was increased from 47 to 94%. As a consequence, the test is no more a good quality of fit test and some systematic errors could be disguised. The uncertainties of the interpolated values were reduced by about a factor of 2 when covariances are neglected and, as a consequence, the experiment seems better than it really is.

Table 3
Data of the simulated experiment: the energy uncertainties are equal to 5 eV with correlation coefficient equal to 0.8; the uncertainties of the channels are equivalent to 3 eV and not correlated

Energy (keV)	Channel
1010.0051	1000.0019
1259.9968	1249.9969
1510.0013	1499.9924
1760.0009	1749.9982
2010.0023	2000.0017
2260.0036	2249.9994
2510.0011	2500.0043
2760.0057	2749.9988
3010.0019	2999.9971
3260.0017	3250.0023
3510.0003	3500.0004

Table 4
Results of the analysis of the simulated experiment: taking into account the total covariance matrix (A), and neglecting the covariance terms (B)

Results of the fitting	A	B
$a(\sigma_a)$	10.0046(56)	10.0046(53)
$b(\sigma_b)$	0.9999991(14)	0.9999991(22)
$\rho_{a,b}$	− 0.57	− 0.94
$\chi^2_{exp}(P(\chi^2 \geqslant \chi^2_{exp}))$	8.7 (47%)	3.6 (94%)
Interpolated uncertainty at channel 1400, σ_{E1}	4.8 eV	2.6 eV
Interpolated uncertainty at channel 1500, σ_{E2}	4.7 eV	2.4 eV
$\rho_{E1,E2}$	0.9996	0.998

Appendix B

Consider a set of experimental data $(y_1, y_2, \ldots y_n)$ and a set of functions $z_1(y_1, \ldots y_n), \ldots z_m(y_1, \ldots y_n)$. If the covariance matrix of $\boldsymbol{Y}$ is $\boldsymbol{V}_{\mathbf{Y}}$, then the covariance matrix of $\boldsymbol{Z}$ is given by

$$\boldsymbol{V}_{\mathbf{Z}} \approx \boldsymbol{D} \cdot \boldsymbol{V}_{\mathbf{Y}} \cdot \boldsymbol{D}^{t} \tag{B.1}$$

where

$$D_{ij} = \frac{\partial z_i}{\partial y_j}. \tag{B.2}$$

The derivatives are calculated in the experimental values of the independent variables. Eq. (B.1) is exact if z_j are linear functions of y_i.

If $m \leq n$ then $\boldsymbol{V}_{\mathbf{Z}}$ is a true covariance matrix. Otherwise, $\boldsymbol{V}_{\mathbf{Z}}$ is a singular matrix meaning that there are constraints between some elements of $\boldsymbol{Z}$ and that the probability density function of $\boldsymbol{Z}$ is concentrated on a lower-dimensional subspace [4].

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