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COMPILATION OF k_0 AND RELATED DATA FOR NEUTRON-ACTIVATION ANALYSIS (NAA) IN THE FORM OF AN ELECTRONIC DATABASE**

(IUPAC Technical Report)

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Compilation of k_0 and related data for neutron-activation analysis (NAA) in the form of an electronic database

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Abstract: This report describes the principles underlying a comprehensive electronic database that contains data essential for calculation of analytical results from neutron-activation analysis (NAA) and that is available through IUPAC. The method used is a comparator method called the k_0 method, where k_0 is a dimensionless factor which is experimentally measured with high accuracy for more than 130 isotopes and which makes use of the gamma spectroscopic line for an analyte isotope relative to a gold comparator. The database contains recommended values for k_0 and other relevant nuclear data.

INTRODUCTION

The conventional method of quantitative reactor neutron-activation analysis (NAA) is based on the relative method of standardization with the use of suitable reference materials. By optimal selection of reference materials, various interference effects (nuclear, measurement, etc.) may be neglected due to compensation. At the same time, the relative method of NAA has a number of restrictions: limited number of suitable reference samples, often nonoptimal for NAA with respect to concentration of the certified elements, difficulties in performing panoramic analysis, unavailability for determination of "unexpected" elements, etc.

To expand the versatility of NAA, standardless approaches based on mathematical modeling of all steps of analysis have been suggested and developed since the end of the 1960s. The "absolute" (parametric) method did not achieve broad popularity because of its inherent limitations, which led to lower accuracy. That is why attention was paid to the development of alternative comparator methods which combine the flexibility of "absolute" with the accuracy of relative standardization. The essence of a comparator method consists in co-irradiation of the analyzed samples with a suitable element of known mass (comparator), and combining this with the results of gamma-ray spectrometry. Various precalibrations and nuclear data enable one to compute the concentration of any element via the comparator.

The nuclear data for the comparator must be known with high accuracy. Usually gold, zirconium, or other suitable elements can be chosen. The k_0 factor of an analyte isotope/gamma-line relative to the gold comparator is defined by the ratio:

$$(k_{0,\mathrm{Au}})_{\mathrm{a}} = \frac{M_{\mathrm{Au}}\Theta_{\mathrm{a}}\sigma_{0,\mathrm{a}}\gamma_{\mathrm{a}}}{M_{\mathrm{a}}\Theta_{\mathrm{Au}}\sigma_{0,\mathrm{Au}}\gamma_{\mathrm{Au}}} \quad (1)$$

where M_x, Θ_x, σ_x, γ_x are the atomic mass, the isotopic abundance, the thermal (n, γ) cross-section, and the yield of the analytical gamma-line. The k_0 factors for the majority of the elements that can be determined via NAA were experimentally measured with high accuracy and are tabulated in the literature.

The formula for computing the analyte mass fraction c_a is:

$$c_a = \frac{\left(\frac{N_p / t_m}{SDCW}\right)_a}{\left(\frac{N_p / t_m}{SDCW}\right)_{Au}} \times \frac{1}{(k_{0,Au})_a} \times \frac{\varepsilon_{p,Au}}{\varepsilon_{p,a}} \times \frac{f_i + Q_{0,Au}(\alpha)}{f_i + Q_{0,a}(\alpha)} \quad (2)$$

where the first term describes the results of the gamma-ray spectrometry measurements of the analytical radionuclide and the comparator, the second term is the corresponding k_0 factor, the third term is related to the full energy peak efficiency calibration of the detector, and the last term accounts for the contribution of the epithermal activation.

The list of the symbols used is as follows:

N_p net peak area of the measured gamma-line (corrected for pulse losses)
t_m measuring time
S $1 - \exp(-\lambda t_{irr})$, with t_{irr}: irradiation time
D $\exp(-\lambda t_d)$, with t_d: decay time
C $[1 - \exp(-\lambda t_m)]/\lambda t_m$, with t_m: measurement time
W mass of irradiated sample/comparator
λ decay constant
$\varepsilon_{p,x}$ full energy peak detection efficiency for measuring E_γ
Q_0 I_0/σ_0 with σ_0 (n, γ) cross-section for thermal neutrons (velocity 2200 m s^{-1}) and I_0: resonance integral;
α measure of the nonideal epithermal neutron flux distribution, approximated by a $1/E^{1+\alpha}$ behavior.

The subscripts "a" and "Au" refer to analyte and gold comparator.

The theory of the k_0 method is described in numerous publications, for example, see [1].

ESSENCE OF THE PROJECT

Comparator standardization based on the k_0 method has been launched into the practice of NAA at the end of the 1970s [2]. From that time, due to intensive investigations by an international group of scientists, the method has been developed significantly with respect to both the methodology and the nuclear data used for computations. Nowadays, the method is in active use in numerous laboratories all over the world. The usefulness and high efficiency of the method for radioanalytical practice is confirmed by a series of dedicated International Workshops held in Ghent, 1992 [3], and Ljubljana, 1996 [4], followed by a recent 3rd Workshop in Bruges, 2001 [5], and special sessions of other radiochemical/radioanalytical conferences, for example, the most recent conferences of the series "Modern Trends in Activation Analysis", MTAA10 [6] and recently passed MTAA11 [7].

As it is a single comparator method, the k_0 standardization is based on the application of special computer programs for performing the quite cumbersome computations. For running these computer programs, various nuclear datasets are required. Usually these data exist as "home-made" libraries (text, binary, or other types of files), compiled on the basis of recommended published data or obtained and evaluated in the laboratory. As a rule, the libraries have no unified format and their comparison or interchange between different laboratories may need additional efforts for developing the corresponding programs (converters). The manual data input also is not free from possible random errors. The possible data discrepancy may result in problems in comparing results of analyses made in different laboratories.

The goal of the project was to make a compilation of recommended k_0 and related nuclear data in the form of an electronic database (MS Access database management system). The developed database is available on a CD-ROM and is distributed by IUPAC (<http://www.iupac.org>) freely on request of the interested organizations/persons.

A few compilations of the k_0 data can be found in the literature [1,17]. Some data were published stepwise in a number of consecutive compilations, with several extensions and updates over the course of several years [8–16]. These partial and fragmentary datasets were assembled [17] and inserted into the tables of the present database. The electronic database consists of few main tables covering activation, k_0 and decay data, and a few auxiliary tables. All tables are relationally linked with each other to support database integrity. The detailed structure of the database and its capabilities and user interface are described in a separate paper [18].

The selection of a database of MS Access type is explained by its wide distribution as a component of MS Office and the possibility to use internal programming for data handling (viewing forms, exporting, multiple SQL queries, etc.). Advantages of using MS Access are its extended capabilities for exporting data in various formats, its support of SQL queries for extraction of the needed data for those who use Excel as a media for computations or use stand-alone special programs written in higher-level programming languages. Additionally, such a solution permits easy migration to the MS SQL server, which may be interesting for those who use distributed computations (including those accessible via the Internet).

The architecture of the database supports traceability of future data updating or appending, which implies easy recomputation of analytical data using any set of data, either the latest or previous ones.

DATABASE DISTRIBUTION

The database is available in three different forms: files IUPAC_k0NAA_v.4_Access97p.mdb, IUPAC_k0NAA_v.4_Access2000p.mdb (for Access97 and Access2000, respectively) and a special set of installation files for those who do not have MS Access installed. In the latter case, the installation routine will install a runtime version of MS Access2000 and the corresponding version of the database file.

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