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A review of nuclear data for the k_0-based neutron activation analysis

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Abstract: Nuclear data for the k_0-based neutron activation analysis (k_0-NAA) including: k_0-factors – combination of nuclear constants (atomic mass, isotopic abundance, gamma-ray yield and thermal neutron capture cross section); Q_0 – the ratio of the resonance integral to thermal neutron capture cross section; and $\bar{E}_r$ – effective resonance energy, along with the related nuclear data are presented and evaluated in the presentation. Accuracy and capability of k_0-NAA depends considerably on the reliability of the above mentioned nuclear data. In general, the evaluation of nuclear data is essential and necessary in the field of nuclear science and technology, and this work is conducted by the nuclear data centers on the world as well as the research institutions where the nuclear data are used for R&D. Therefore, the evaluation of the nuclear data used in k_0-NAA should also be performed so that some of data may no longer be appropriate should be redetermined. The evaluation of nuclear data in k_0-NAA would contribute to the improvement of accuracy and reliability of the method, moreover, it would also contribute to the establishment a nuclear database in Vietnam in the future.

Keywords: *Nuclear data, neutron activation analysis, k_0-standardized method.*

I. INTRODUCTION

The k_0-based neutron activation analysis (k_0-NAA) is based on the k_0 factors – the combined constant of nuclear data, determined by experiment. Therefore, the accuracy of the method depends on reliability of the k_0 factors. In addition, there are other related nuclear data such as thermal neutron capture cross section (σ_0), integral resonance (I_0) (or $Q_0 = I_0/\sigma_0$) and the effective resonance energy ($\bar{E}_r$). Currently, the first version of database and the updated version [1,2] has widely used. However, recent references show that some data have only been determined just once 30 years ago but they have never been verified or updated. Some k_0 factors are considered as "not yet approved". Moreover, some of data of first version have not yet been verified [3,4]. A number of laboratories around the world have reviewed the nuclear data of interest, but their findings have not been included in the library of new database, and so on. Therefore, this presentation reviews all of the nuclear data (k_0, Q_0 and $\bar{E}_r$) for the elements of interest in k_0-NAA. After reviewing, some data will be chosen for re-determining and then the experimental determination of selected data should be carried out.

The nuclear data (k_0, Q_0 and $\bar{E}_r$) has been determined by experiment mainly in the laboratories of Europe: Belgium, Hungary and the Netherlands. Then, some other laboratories in the US, Canada and Japan have been involved in the implementation.

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Recently, the international scientific committee of k_0-NAA has recommended for re-determining of a number of k_0 factors and related nuclear data. It should be immplemented a review the k_0 factors and related nuclear data in k_0-NAA, aiming to evaluate and re-determine some nuclear data of interest. Nuclear data including 300 gamma energy levels, 55 radionuclides, with 17 types of reactions and decays of nuclear states in k_0-NAA should be reviewed. Choose the necessary data to re-determine by experiment based on the updated criteria. The establishment of the nuclear database includes, i.e. k_0, Q_0 and $\overline{E}_r$ for the elements with relevance radionuclides of interest in k_0-NAA, so is essential and necessary.

The re-determination some of nuclear data in k_0-NAA will contribute to the world's nuclear database. Experimental methods used in the nuclear research reactor are characterized such as neutron flux, energy spectrum deviation, coefficient of cadmium, and so on measured by the spectrometers based on HPGe detectors and the data processing by specialized software. To evaluate the new nuclear data and apply to real samples using k_0-NAA. Compare the results using the new data and the old data to prove the improvement of the new data.

II. METHODOLOGY

Review of reference documents related to nuclear data in k0-NAA problem, from which the nuclear data are summarized for reviewing and choosing the appropriate cases to re-determine by experiment in consideration of ability of the laboratories the nuclear research reactor as a neutron source causing nuclear reactions for research and measurement systems as well as computer software for data processing.

Experimental nuclear physics methods used by bombarding the targets using pure standards of the elements of interest in the neutron field of the nuclear research reactor, then use the HPGe detector based-spectrometer to measure the gamma-ray spectrum. Finally, using computer software to process the data and calculate the results.

Isotopes under investigation and chosen convention

For all the determinations use was made of the standards to which these materials, mostly foils and wires, are especially suited because of the minimum preparation required, negligible chances of mass losses, homogeneity, stability and low uncertainty in the certified content. Furthermore, several of the diluted Al alloys or spiked paper filters can be regarded as free from strong neutron self-shielding effects during irradiations. The use of the much simpler Høgdahl convention [5] over the Westcott formalism [6] was chosen since from Holden [7] it can be seen that only the rhenium isotopes deviate slightly from the 1/v expected behavior. Their deviations are 0.8 % at 60 ^{0}C, while the temperature of our channels is estimated to be 30 ^{0}C. Table 1 displays the $k_{0,Au}$ factors and related nuclear data for use in k_0-NAA.

Experimentally measured $k_{0,Au}$ factors and related nuclear data for use in k_0-standardized neutron activation analysis (k_0-NAA) are given. Data for which the percent uncertainty (relative standard error, s, in %) is denoted as (–) bear an uncertainty estimated to be about 5% (for k_0) or about 10% (for Q_0). The symbols in Table 1 are explained as followings:

El - Chemical symbol of the element; Target isotope - Isotope of the target element; Q_0=$I0/\sigma_0$ - resonance integral to 2200-m/s cross-section ratio; The relative standard error, S, in %; $\overline{E}_r$ - Effective resonance energy, in keV; Formed isotope Isotope formed in the reaction, together with the activation/decay code; $T_{1=2}$ - Half-life; $E\gamma$- Gamma-ray energy, in keV, adopted from Isotope Explorer (1999); $k_{0,Au}$ - Measured $k_{0,Au}$ ratio, with the relative standard error, S, in %; In our notation, 9.98E-4 = 9.98×10^{-4} , etc.

III. RESULTS AND DISCUSSION

The recommended nuclear data are based on the data published in Refs. [8–10]. The values, references and comments have been verified carefully and corrected where typographical errors, data-handling (e.g. rounding) errors, inconsistencies, or other mistakes were found. All questionable data were discussed one by one, and were modified after a common agreement. All modifications to the data and the rationale behind the modification are traceable in the tables.

In this work, the access version of the IUPAC database [9] has been used in a table. The obvious rounding errors (smaller than 0.1 %) were corrected and the all k_0 factors are written in the scientific format. Thus the values listed in the tables contain the proper number of significant digits. The present data contains the followings:

k_0 – values, it lists the elements, their isotopes and the gamma-ray energies together with the k_0 values and their uncertainties. In further columns it is also indicated if the value is affected by true coincidence summing or is derived from summing a multiplet. The revision dates and the relevant references are also shown (see Table I). Neutron capture cross-sections, resonance integrals and the ratios of the two (Q_0), as well as the effective resonance energies ($\bar{E}_r$) for the nuclides appearing in the table (see Table II).

Decay modes of the radioactive nuclides formed during the activation can be found: either β decays or isomeric transitions. The branching ratios between β decays and isomeric transitions also appear in the table. Nuclides, the properties of the target and product nuclides can be seen in the table. The target nuclides are stable and their isotopic abundances are given, while the products are radioactive and their half-lives are shown in the traditional units (see Table III).

Decay codes, most decays are type I, where the radioactive state decays directly to the very-short-lived gamma-emitting state. Decays through several steps have the codes from II to VII, which can be seen as “decay code (n, γ)” and “decay code (n, f)” in Ref [10]. There are data, which contain the most important k_0 and decay code for nuclides produced by the neutron-induced fission of uranium (see Table IV).

Table I. Changes in the “k_0” values of the recommended data.

El	A	S	Eγ (keV)	k_0	dk_0 (%)	Revised	Revision information
F	20	1	1,633.6	9.98E−04	1.2	2002-08-28	Old revision on 2001-06-14. Published [7]
Cu	64	1	1,345.8	4.98E−04	0.9	2002-08-28	Removed Ref. [3], old k_0 = 4.91E−4. Published [7]
Ga	72	1	2,507.9	7.29E−03	1.3	2021-08-28*	Published in Ref. [7] *Type error, should be 2002-08-28.
Se	75	1	264.7	7.11E−03	0.7	2002-08-28	Removed Ref. [3], old k_0 = 7.25E−3. Published [7]
Se	75	1	279.5	3.00E−03	1.2	2002-08-28	Removed Ref. [3], old k_0 = 3.06E−3. Published [7]
Se	75	1	400.7	1.43E−03	0.8	2002-08-28	Removed Ref. [3], old k_0 = 1.45E−3. Published [7]
Zr	95	1	756.7	1.10E−04	1.3	2011-12-07	Eror in Ref. [7] for k_0, E-5 instead of E-4. Published [8].
Rh	104	1	555.8	6.92E−02	1.5	2011-12-07*	Type error in Ref. [7] for $c_{555.8}$(m/F2g), 0.0691 instead of
*The last publication Ref. [10] is also incorrect, with type error 0.651 instead of 0.0651. The correct value of 0.0651							
Pd	111	2	172.2	1.07E−05	1.4	2002-08-28	Removed Ref. [3], old k_0 = 9.04E−6. Published in Ref. [7]
Sn	117	2	158.6	1.33E−05	1	2002-08-28	Removed Ref. [3], old k_0 = 1.35E−5. Published in Ref. [7]
Tm	170	1	84.3	3.26E−02	1.7	2000-12-31	Removed Ref. [3], old k_0 = 4.30E−2. Published in Ref. [7]
Ta	182	1	152.4	1.62E−02	0.7	2011-12-07	Removed Ref. [3], old k_0 = 1.61E−2. Published in Ref. [7]

Table II. Changes in the "Capture" data of the recommended k_0 database.

El	A	S	Q0	dQ0 (%)	Er, eV	dEr (%)	El 1	A1	S1	Revised	Comments to revision
Na	23	10	0.59		3,380	11	Na	24	1	2011-12-14	dQ0 = 4.7 is removed
Cl	37	10	0.69		13,700	14	Cl	38	1	2011-12-14	dQ0 = 4.1 is removed
K	41	10	0.87	3.0	2,960	7.1	K	42	1	2011-12-14	New Q0 and dQ0 from Ref. [7]. Removed Ref. [3], old. Q0 = 0.97 and no data for dQ0
Sc	45	10	0.43		5,130	17	Sc	46	1	2011-12-14	Add dEr from Ref. [2]
Cr	50	10	0.53		7,530	11	Cr	51	1	2011-12-14	dQ0 = 2.4 is removed
Mn	55	10	1.053	3.0	468	11	Mn	56	1	2011-12-14	New dQ0 from Ref. [7]. Removed Ref. [3], old dQ0 = 2.6
Co	59	10	2		136	5.1	Co	60	2	2011-12-14	Add dEr from Ref. [2]
Cu	65	10	1.06		766	17	Cu	66	1	2011-12-14	dQ0 = 4.9 is removed
Zn	64	10	1.908	5.0	2,560	10	Zn	65	1	2011-12-14	New dQ0 from Ref. [7]. Removed Ref. [3], old dQ0 = 4.9
Sb	123	10	19.9		28.2	6.4	Sb	124	2	2011-12-14	Add dEr from Ref. [2]
Au	197	10	15.7	1.8	5.65	7.1	Au	198	1	2011-12-14	Kept dQ0 from Ref. [3]

Table III. Changes in the "Nuclides" data of the recommended k_0 database.

El	A	S	Abu (%)	$T_{1/2}$	Unit	$dT_{1/2}$	Revised	Comment
Co	60	1	0	1,925.3	D	0.3	2002-09-01	$T_{1/2}$ = 5.271 Y in Ref. [7]
Rb	86	2	0	1.017	M	0.003	1993-03-15	$T_{1/2}$ = 1.02 M in Ref. [7]
Rb	87	11	27.835	4.8E+10	Y	1E09	1993-03-15	No info in Ref. [7]
Sb	125	1	0	2.73	Y	0.03	1993-03-15	No info in Ref. [7]
Ba	140	1	0	12.746	D	0.01	1993-03-15	No info in Ref. [7]
Th	232	11	100	1.4E+10	Y	6E07	1993-03-15	No info in Ref. [7]
U	238	11	99.28	4.5E+09	Y	3E06	1993-03-15	No info in Ref. [7]

Table IV. Changes in the "k_0 (n,f)" data of the recommended k_0 database

El.	A	S	Eγ,	k0	dk0	Revised	Revision information
Ru	103	1	610.3	6.05E−05		2011-12-07	Removed Ref. [7], old k0 = 9.87E−5.
Rh	105	2	129.6	1.85E−05		2011-12-07	Removed Ref. [7], old k0 = 2.29E−5. Ref. [10]
Nd	147	1	91.1	2.41E−04		2011-12-07	k0-data, type error in Ref. [6]: E3 instead of E−4

IV. CONCLUSIONS

An attempt has been made here to present the state of the art concerning nuclear data for k_0-NAA. In order to be on the safe side, the experimentalist may follow a few practical guidelines, which are given below. Traceability of the experimental procedure is guaranteed only if data from well-documented sources are used. Recommended data libraries or at least data sets evaluated are the best choice. Such are the neutron cross sections and resonance parameters, half-lives and gamma-ray data from the Evaluated Nuclear Structure and Decay Data File (ENSDF), as well as the recommended set of gamma-ray standards for detector calibration. Quality assurance mandates that only data with clearly specified uncertainties are used. The data sources that are recommended here all satisfy this requirement. On the other hand, some frequently used books, tables of decay gamma-rays, do not.

Old handbooks and compilations should be used with precaution, or rather avoided entirely, in that many of the data they contain may have been superseded. (This does not imply, however, that old data are wrong!) Sometimes even widely used handbooks quote data which should be disregarded as, for instance, the Handbook of Radioanalytical Chemistry reproducing the outdated tables.

The most up-to-date resources are usually those available on the Internet home pages of professional data evaluation and distribution centres, such as the IAEA Nuclear Data Section, the NEA Data Bank, and the US National Nuclear Data Center. A caution is required, however, concerning uncontrolled Internet sites providing various kinds of nuclear data.

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