

The 2012 recommended k_0 database

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Abstract Many overview papers have been published with recommended nuclear data for use in the k_0 method of NAA and made available in scientific journals or in the form of a downloadable database. In September 2009, the k_0 -International Scientific Committee formed the k_0 -Nuclear Data Committee (k_0 -NDC) whose first task was to collect all these data at a single place to facilitate updating and to correct any evident errors. This task of the k_0 -NDC was successfully completed in March 2012 when the 2012 recommended k_0 database was published in the form of an Excel file.

Keywords k_0 method of NAA · k_0 database · Nuclear data · The IUPAC k_0 database

Introduction

As is well-known, the k_0 standardisation method of neutron activation analysis (k_0 -NAA) was introduced by Simonits et al.

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[1], whereby absolute nuclear data were replaced by k_0 factors, which were experimentally determined. Compared to the relative method, the k_0 method greatly reduces the need for the preparation of standards. It uses gold as the standard and composite nuclear constants for analytically interesting nuclides are normalised to gold nuclear data. During the last 30 years the k_0 method has been introduced in many laboratories around the world for multi-element NAA and the method is continuously improving, along with its nuclear data [2–7]. In 2003, these data were made available by the International Union of Pure and Applied Chemistry (IUPAC) in the form of the Access database (http://www.iupac.org/home/projects/project-db/project-details.html?tx_wfqbe_pi1%5Bproject_nr%5D=2001-075-1-500) created by Kolotov and De Corte [8, 9]. In the process of validation of the consistency of the nuclear data inside the k_0 _IAEA software with the IUPAC k_0 database, several inconsistencies were investigated by Blaauw and De Corte [10] in 2009 and published in 2010.

During the 5th International k_0 Users' Workshop in September 2009, Belo Horizonte, Brazil, the k_0 -Nuclear Data Committee (k_0 -NDC) was formed by the k_0 -International Scientific Committee (k_0 -ISC). The k_0 -NDC is responsible for reviewing all new developments in the nuclear data used with the k_0 method of NAA, which includes ensuring the consistency in the k_0 database. The latter task was successfully fulfilled in March 2012 when the 2012 recommended k_0 database was published in the form of an Excel file (see weblink: <http://www.kayzero.com/k0naa/k0naa/News/News.html>) dated 2012-03-14.

Results and discussion

The 2012 recommended k_0 database is based on the data published in Refs. [2–10]. The values, references and

Table 1 Changes in the “ k_0 ” sheet of the 2012 recommended k_0 database

El	A	S	E_γ (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 in Ref. [7]
Cu	64	1	1,345.8	4.98E–04	0.9	2002-08-28	Removed Ref. [3], old $k_0 = 4.91\text{E}–4$. Published in Ref [7]
Ga	72	1	2,507.9	7.29E–03	1.3	2021-08-28*	Published in Ref. [7] * Typo error, should be 2002-08-28. Not corrected by the k_0 -Nuclear Data Committee during the revision in year 2012.
Se	75	1	264.7	7.11E–03	0.7	2002-08-28	Removed Ref. [3], old $k_0 = 7.25\text{E}–3$. Published in Ref. [7]
Se	75	1	279.5	3.00E–03	1.2	2002-08-28	Removed Ref. [3], old $k_0 = 3.06\text{E}–3$. Published in Ref. [7]
Se	75	1	400.7	1.43E–03	0.8	2002-08-28	Removed Ref. [3], old $k_0 = 1.45\text{E}–3$. Published in Ref. [7]
Zr	95	1	756.7	1.10E–04	1.3	2011-12-07	Typo error in Ref. [7] for k_0 , E-5 instead of E-4. Published in Ref. [10]
Rh	104	1	555.8	6.92E–02	1.5	2011-12-07*	Typo error in Ref. [7] for $\gamma_{555.8}(\text{m/F2 g})$, 0.0691 instead of 0.0651. * The last publication Ref. [10] is also incorrect, with typo error 0.651 instead of 0.0651. The correct value of 0.0651 is given in original Ref. [5]. An inappropriate correction was made by the k_0 -Nuclear Data Committee in the Excel file during the revision in year 2012.
Pd	111	2	172.2	1.07E–05	1.4	2002-08-28	Removed Ref. [3], old $k_0 = 9.04\text{E}–6$. Published in Ref. [7]
Sn	117	2	158.6	1.33E–05	1	2002-08-28	Removed Ref. [3], old $k_0 = 1.35\text{E}–5$. Published in Ref. [7]
Tm	170	1	84.3	3.26E–02	1.7	2000-12-31	Removed Ref. [3], old $k_0 = 4.30\text{E}–2$. Published in Ref. [7]
Ta	182	1	152.4	1.62E–02	0.7	2011-12-07	Removed Ref. [3], old $k_0 = 1.61\text{E}–2$. Published in Ref. [7]

For definition and explanation of symbols and notations, see Ref. [7] and the Excel file <http://www.kayzero.com/k0naa/k0naa/News/News.html>

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 above mentioned Excel-sheet.

In this work, the Access version of the IUPAC database [9] has been converted into an Excel file. 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 k_0 database can be opened in the 2003 version of Excel, and it contains the following worksheets:

k_0

This sheet summarizes the 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 1).

Capture

This sheet lists the neutron capture cross-sections, the resonance integrals (RI) and the ratios of the two (Q_0), as

well as the effective resonance energies (E_r) for the nuclides appearing in the k_0 table (see Table 2).

Decay

Here, the 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 this sheet (see “Decay” sheet in the Excel file).

Nuclides

The properties of the target and product nuclides can be seen in this sheet. 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 3).

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 here (see “decay code (ng)” and “decay code (nf)” in the Excel file).

There are two sheets, which contain the most important k_0 and decay code data for nuclides produced by the neutron-induced fission of uranium (see Table 4).

Table 2 Changes in the “Capture” sheet of the 2012 recommended k_0 database

El	A	S	Q_0	dQ_0 (%)	E_r , eV	dE_r (%)	El ₁	A ₁	S ₁	Revised	Comments to revision
Na	23	10	0.59		3,380	11	Na	24	1	2011-12-14	$dQ_0 = 4.7$ is removed
Si	30	10	1.11	6.0	2,280	0.4	Si	31	1	2011-12-14	Add dQ_0 from Ref. [7]
Cl	37	10	0.69		13,700	14	Cl	38	1	2011-12-14	$dQ_0 = 4.1$ is removed
K	41	10	0.87	3.0	2,960	7.1	K	42	1	2011-12-14	New Q_0 and dQ_0 from Ref. [7]. Removed Ref. [3], old $Q_0 = 0.97$ and no data for dQ_0
Sc	45	10	0.43		5,130	17	Sc	46	1	2011-12-14	Add dE_r from Ref. [2]
Cr	50	10	0.53		7,530	11	Cr	51	1	2011-12-14	$dQ_0 = 2.4$ is removed
Mn	55	10	1.053	3.0	468	11	Mn	56	1	2011-12-14	New dQ_0 from Ref. [7]. Removed Ref. [3], old $dQ_0 = 2.6$
Co	59	10	2		136	5.1	Co	60	2	2011-12-14	Add dE_r from Ref. [2]
Co	59	10	1.993	3.0	136	5.1	Co	60	1	2011-12-14	New dQ_0 from Ref. [7]. Removed Ref. [3], old $dQ_0 = 2.7$
Cu	65	10	1.06		766	17	Cu	66	1	2011-12-14	$dQ_0 = 4.9$ is removed
Zn	64	10	1.908	5.0	2,560	10	Zn	65	1	2011-12-14	New dQ_0 from Ref. [7]. Removed Ref. [3], old $dQ_0 = 4.9$
Se	76	10	0.77		577	8	Se	77	2	2011-12-14	Add dE_r from Ref. [2]
Br	81	10	19.3	3.0	152	9.2	Br	82	1	2011-12-14	New dQ_0 from Ref. [7]. Removed Ref. [3], old $dQ_0 = 3.1$
Rb	87	11	23.3	3.0	364	3	Rb	88	1	2011-12-14	New dQ_0 from Ref. [7]. Removed Ref. [3], old $dQ_0 = 2.9$
Sr	84	10	13.2		469	7	Sr	85	1	2011-12-14	Add E_r and dE_r from Ref. [2]
Mo	100	10	18.8	4.0	672	14	Mo	101	1	2011-12-14	New Q_0 and dQ_0 from Ref. [7]. Removed Ref. [3], old $Q_0 = 18.84$ and $dQ_0 = 4.3$
Rh	103	10	6.81	3.5	1.45	0.7	Rh	104	2	2011-12-14	Add dQ_0 from Ref. [7]
Pd	108	10	25.0		39.7	5	Pd	109	2	2011-12-14	X_{sec} , dX_s , RI and Q_0 from IUPAC Data base Q_0 is the same in Ref. [7]
Ag	107	10	2.9		38.5	4.9	Ag	108	1	2011-12-14	$dQ_0 = 4.0$ is removed
Ag	109	10	18.4		6.08	1	Ag	110	1	2011-12-14	Add dE_r from Ref. [2]
Sn	124	10	17.2	12	74.2	7	Sn	125	1	2011-12-14	Keep $dQ_0 = 12$ from Ref. [4] instead of 11 $dQ_0 = 11$ in Ref. [7] is typo error!
Sb	123	10	19.9		28.2	6.4	Sb	124	2	2011-12-14	Add dE_r from Ref. [2]
Au	197	10	15.7	1.8	5.65	7.1	Au	198	1	2011-12-14	Kept dQ_0 from Ref. [3]

For definition and explanation of symbols and notations, see Ref. [7] and the Excel file <http://www.kayzero.com/k0naa/k0naa/News/News.html>

Table 3 Changes in the “Nuclides” sheet of the 2012 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	1E+09	1993-03-15	No info in Ref. [7]
Nb	94	1	0	20,300	Y	1,600	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]
Lu	176	11	2.59	3.6E+10	Y	2E+09	1993-03-15	No info in Ref. [7]
Re	187	11	62.6	5E+10	Y	2E+09	1993-03-15	No info in Ref. [7]
Th	232	11	100	1.4E+10	Y	6E+07	1993-03-15	No info in Ref. [7]
U	238	11	99.28	4.5E+09	Y	3E+06	1993-03-15	No info in Ref. [7]

Recommended to use
1 y = 365.2422 d; for definition and explanation of symbols and notations, see Ref. [7] and the Excel file <http://www.kayzero.com/k0naa/k0naa/News/News.html>

The last three sheets resolve abbreviations and codes used in the database (see “S”, “RA Decay” and “Reac” sheets in the Excel file).

In this work, changes were made to the “ k_0 ” (Table 1), “Capture” (Table 2), “Nuclides” (Table 3) and “ k_0 (nf)”

(Table 4) sheets. All changes are relative to the IUPAC k_0 database dated 2002-10-01, version 4 [9]. The changes were approved by the k_0 -NDC on 2012-03-14 and the resulting Excel file was published (see weblink: <http://www.kayzero.com/k0naa/k0naa/News/News.html>). It should

Table 4 Changes in the “ k_0 (nf)” sheet of the 2012 recommended k_0 database

El.	A	S	E_γ , keV	k_0	dk_0 (%)	Revised	Revision information
Ru	103	1	610.3	6.05E-05		2011-12-07	Removed Ref. [7], old $k_0 = 9.87E-5$. Published in Ref. [10]
Rh	105	2	129.6	1.85E-05		2011-12-07	Removed Ref. [7], old $k_0 = 2.29E-5$. Published in Ref. [10]
Nd	147	1	91.1	2.41E-04		2011-12-07	k_0 -Nuclear data committee, typo error in Ref. [6]: E-3 instead of E-4

For definition and explanation of symbols and notations, see Ref. [7] and the Excel file <http://www.kayzero.com/k0naa/k0naa/News/News.html>

be noted that in many cases the only change in the Excel file relative to the previous the IUPAC k_0 database is that the revision information is now said to be found in Ref. [7] rather than in the original publication of the data. If this was the only change for a given case, the change is not explicitly mentioned in Tables 1–4.

The k_0 -NDC recommends the use of this Excel file of 2012-03-14 as the official k_0 database. Users that modify data in this Excel file for their own use break the link to this recommended k_0 -NAA database and therefore lose traceability to the k_0 factors therein. This database is a compilation of the best data available up to 2003. Since then, many papers have been published containing new measurements of k_0 and Q_0 values and even new E_r values and half-lives. Undoubtedly, some of the new values will one day be accepted as being more accurate than the corresponding values in the recommended database. It is now the priority of the k_0 -NDC to evaluate these new values, as well as others which will be published soon, and to update the recommended database.

Conclusion

The different versions of the k_0 database Refs. [2–10] have been carefully checked for consistency and correctness. The different types of mistakes and typos were identified and corrected. The database is established in the form of an easily accessible Excel file freely downloadable at <http://www.kayzero.com/k0naa/k0naa/News/News.html>. The k_0 -Nuclear Data Committee is now working to review all the recently measured nuclear data in order to update this database.

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