Title
Comparison of IUPAC k0 Values and Neutron Cross Sections to Determine a Self-consistent Set of Data for Neutron Activation Analysis

Permalink
https://escholarship.org/uc/item/4p90c5kk

Author
Firestone, Richard B

Publication Date
2010-09-15

Peer reviewed
Comparison of IUPAC k0 Values and Neutron Cross Sections to Determine a Self-consistent Set of Data for Neutron Activation Analysis

Richard B. Firestone1,* and Zsolt Revay2

1 Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
2 Institute of Isotope and Surface Chemistry, H-1525, Budapest, Hungary

*Author for correspondence (E-mail: rbfirestone@lbl.gov).

Received; accepted

Abstract. Independent databases of nuclear constants for Neutron Activation Analysis (NAA) have been independently maintained by the physics and chemistry communities for many year. They contain thermal neutron cross sections \( \sigma_0 \), standardization values \( k_0 \), and transition probabilities \( P_\gamma \). Chemistry databases tend to rely upon direct measurements of the nuclear constants \( k_0 \) and \( P_\gamma \) which are often published in chemistry journals while the physics databases typically include evaluated \( \sigma_0 \) and \( P_\gamma \) data from a variety of experiments published mainly in physics journals. The IAEA/LBNL Evaluated Gamma-ray Activation File (EGAF) also contains prompt and delayed \( \gamma \)-ray cross sections \( \sigma_\gamma \) from Prompt Gamma-ray Activation Analysis (PGAA) measurements that can also be used to determine \( k_0 \) and \( \sigma_0 \) values. As a result several independent databases of fundamental constants for NAA have evolved containing slightly different and sometimes discrepant results. An IAEA CRP for a Reference Database for Neutron Activation Analysis was established to compare these databases and investigate the possibility of producing a self-consistent set of \( \sigma_0 \), \( k_0 \), \( \sigma_\gamma \), and \( P_\gamma \) values for NAA and other applications. Preliminary results of this IAEA CRP comparison are given in this paper.

Introduction

Several sources of nuclear data are available for Neutron Activation Analysis (NAA). The chemistry community has largely adopted the \( k_0 \) standardization method for NAA. A comprehensive database of \( k_0 \) values has been adopted by the International Union of Pure and Applied Chemistry [1] that is based primarily on the measurements of F. De Corte and A. Simonits [2]. These \( k_0 \) values can also be derived from total radiative thermal neutron cross sections \( \sigma_0 \) that were evaluated by S. Mughabghab [3] and the \( P_\gamma \) transition probabilities that are available from two main sources, ENDF [4] and the Table of Radionuclides [5]. In addition, prompt and delayed \( \gamma \)-ray cross sections \( \sigma_\gamma \) were measured with guided neutron beams at the Budapest Reactor [6], evaluated as part of an IAEA Coordinated Research Project [7], and published in the Evaluated Gamma-ray Activation File (EGAF) [8].

The varying sources of \( k_0 \), \( \sigma_0 \), \( \sigma_\gamma \), and \( P_\gamma \) data contain inconsistent and sometimes discrepant values. This problem was recognized by the IAEA which organized a Coordinated Research Project (CRP) on a Reference Database for Neutron Activation Analysis [9,10]. A preliminary comparison of the NAA data for all activation products has been completed and some typical examples of discrepant data are discussed in this paper. The complete and self-consistent database of \( k_0 \), \( \sigma_0 \), \( \sigma_\gamma \), and \( P_\gamma \) data is being developed by these authors for inclusion in the next version of the EGAF database and dissemination to the user community.

The \( k_0 \) standardization method

Neutron Activation Analysis (NAA) for the determination of elemental concentrations was traditionally standardized by either absolute or comparator modes [11,12]. The absolute method suffers from the inaccuracy of nuclear data for activation and decay and the single-comparator method is dependent on local irradiation and counting conditions. The \( k_0 \) standardization method was developed by Simonits and De Corte [13] to determine elemental concentration using \( k_0 \) factors that are experimentally determined composite nuclear constants.

The concentration \( Q_x \) of an analyte \( x \) is measured by the \( k_0 \) standardization method as shown in the following equation.

\[
Q_x = \frac{(N_p/W_t mSDC)_x}{(N_p/W_t mSDC)_{Au}} \times \frac{1}{k_{0,\text{Au}}(x)} \times \frac{f + Q_{0,\text{Au}}(\alpha)}{f + Q_{0,x}(\alpha)} \times \varepsilon_{p,\text{Au}} \times \varepsilon_{p,x}
\]  

(1)
Here Au is the co-irradiated gold monitor ($E_\gamma=411.8$ keV), $N_p$ is the number of counts in the $\gamma$-ray peak, $W$ is the weight of the sample, $w$ is the weight of the gold monitor, and $t_m$ is the counting time. $S=1 - \exp(-\lambda t_m)$ where $\lambda$ is the decay constant and $t_m$ is the irradiation time. $D=\exp(-\lambda t_d)$ where $t_d$ is the decay time, $C=[1 - \exp(-\lambda t_0)]/\lambda t_0$, $f$ is the thermal to epithermal neutron flux ratio, and $Q_0=I_0/\sigma_0$ where $I_0$ is the count rate and $\sigma_0$ is the 2200 ms$^{-1}$ neutron cross section. The epithermal neutron flux distribution is approximated by $1/E^{1+\alpha}$, assuming the cross section varies as $1/E$, and $\epsilon_p$ is the full-energy peak detection efficiency.

The $k_{0,Au}(x)$ factor is defined in the following equation.

$$k_{0,Au}(x) = \frac{M_{Au} \theta_{x} \sigma_{0,x} P_{\gamma,x}}{M_x \theta_{Au} \sigma_{0,Au} P_{\gamma,Au}}$$

Here $M$ is the atomic weight, $\theta$ is the isotopic abundance, and $P_{\gamma}$ is the emission probability. The gold monitor can be replaced by another monitor $m$ in which case

$$k_{0,m}(x) = \frac{k_{0,Au}(x)}{k_{0,Au}(m)}$$

If the cross section in the thermal neutron energy region deviates from $1/E$, then $f+Q_{0,Au}(\alpha)\epsilon_p f+Q_{0,0}(\alpha)\epsilon_p s_0$, then $Q_{0,0}$ should be replaced by

$$g_{Au}(T_n) + r(\alpha) \sqrt{t_n / T_0} \times s_{0,Au}(\alpha)$$

$$g_{x}(T_n) + r(\alpha) \sqrt{t_n / T_0} \times s_{0,x}(\alpha)$$

where $g(T_n)$ is the Westcott g-factor which depends on Maxwellian neutron temperature $T_n$ and measures the deviation from $1/E$ cross section dependence. The spectral index is $r(\alpha) \sqrt{T_n / T_0}$ where $T_0=293.6^o$K and $s_0(\alpha)$ modifies the $1/E^{1+\alpha}$ epithermal neutron cross section distribution. If the cross section follows a $1/E$ dependence then

$$s_0 = \frac{2}{\sqrt{\pi}} Q_0 - 0.484$$

The conversion of $Q_0(\alpha)$ to $Q_0(0)$ and $s_0$ to $s_0(\alpha)$ is given by

$$Q_0(\alpha) = \left[ \frac{Q_0 - 0.429}{(E_{\gamma})^{\alpha}} + \frac{0.429}{(2\alpha+1)(E_{Cd}^{\alpha})} \right] (1 \text{ eV})^{\alpha}$$

and

$$s_0(\alpha) = s(E_{Cd})^{-\alpha}(1 \text{ eV})^{\alpha}$$

where $E_{Cd}=0.55$ eV is the cadmium cut-off energy and $E_{\gamma}$ is the effective resonance energy defined by

Ryves [14]. The (1 eV)$^\alpha=1.0$ term is from the definition of the epithermal neutron flux distribution [15,16].

**Data Sources**

The relationship between the nuclear constants $k_0$, $\sigma_0$, and $P_{\gamma}$ is shown in Eq. (2). The quantity $\sigma_p$ is defined simply as $\sigma_p = P_{\gamma} \sigma_0$. Values for these constants can be obtained from various, partially independent nuclear databases. The goal of this project is to evaluate a unified, self-consistent set of nuclear constants from all sources.

**Total radiative thermal neutron cross sections $\sigma_0$ and $k_0$ values**

The IUPAC $k_0$ database [1] is derived primarily from the direct experimental measurements of De Corte and Simonits [2] without consideration of other relevant nuclear decay data. These values were precisely measured although their uncertainties appear to reflect mainly statistical error. The De Corte and Simonits measurements are sometimes used in Mughabghab’s evaluation of total radiative neutron cross sections, published in the *Atlas of Neutron Resonances* [3] which is largely based on measurements compiled in the CSISRS library [17]. Many of those measurements are from unpublished private communications or difficult to obtain reports. The CSISRS coverage of cross sections published in physics and engineering journals in is very good although cross sections published in chemistry journals or measured by the $k_0$ method are often missed. Significant improvement in the $\sigma_0$ data can be expected from an intercomparison of data from the Atlas, the IUPAC $k_0$ database, and other sources of data.

**Gamma-ray transition probabilities $P_{\gamma}$**

$P_{\gamma}$ data are available for all isotopes in ENSDF [4]. This file is generally organized to display data representative of each experiment for the purpose of adopting nuclear level properties. The decay data in ENSDF does not necessarily represent the best decay information that could be obtained from all available sources. ENSDF transition probabilities $P_{\gamma}$ are not given explicitly but must instead be calculated through a series of intensity normalizations, each with their own explicit uncertainty. There are no guidelines for calculating the $\Delta P_{\gamma}$ uncertainty for individual $\gamma$-rays in ENSDF. Cut-off dates for the ENSDF evaluations are commonly more than 10 years old so the data may be out of date. Conversion coefficients, necessary for determining decay scheme normalizations, are calculated with older, less reliable methods in most ENSDF decay datasets.
Pγ data are also available for a limited number of isotopes of applied interest from the Table of Radionuclides [5] which is evaluated by the Decay Data Evaluation Project. These data are available in ENSDF format but they are still not widely adopted by ENSDF evaluators. The Table of Radionuclides is evaluated with stricter standards than ENSDF and is aimed at providing the best Eγ, Pγ and t1/2 data from all sources without requiring ENSDF type normalizations for Pγ. The coverage of the Table of Radionuclides is limited to selected isotopes and does not include the full range of isotopes of interest for NAA.

**Budapest Reactor guided neutron beam measurements**

Neutron capture -ray cross sections for elemental targets with Z = 1 – 83, 90, 92, except for He and Pm, have been measured at the 10 MW Budapest Reactor with a guided thermal neutron beam [18]. These data have been published in the Handbook of Prompt Gamma Activation Analysis [6]. The target station is located ≈30 m from the Reactor where both primary and secondary γ-rays can be measured in low background conditions. Neutrons enter the evacuated target holder and continue to the beam stop at the rear wall of the guide hall. The thermal-equivalent neutron flux was 2×109 n cm⁻² s⁻¹.

Prompt gamma-rays from the target were measured with an n-type high-purity, 25% efficient, germanium (HPGe) detector with closed-end coaxial geometry located 23.5 cm from the target. The detector is Compton-suppressed by a BGO-scintillator guard detector annulus surrounded by 10-cm thick lead shielding. Counting efficiency was calibrated from 50 keV to 10 MeV with radioactive sources and (n,γ) reaction gamma rays to a precision of better that 1% from 500 keV to 6 MeV and better than 3% at all energies [19].

Thermal neutron γ-ray cross sections were determined using either stoichiometric compounds or accurately prepared mixtures containing the standard elements H, N, or Cl whose γ-ray cross sections are precisely known [20]. The γ-ray cross sections for isotopes of interest were then accurately determined from their intensity ratios to the standard γ-ray transition intensities of the comparators. These measurements are independent of target composition or neutron flux. The neutron beam used in these measurements is a pure thermal beam so the measured -ray cross sections do not need to be corrected for epithermal contributions.

**Budapest Reactor σ0 measurements**

Numerous σ0 measurements discussed in this paper were measured at the Budapest Reactor. Gamma-ray cross sections σγ for the decay of short-lived activation products were observed together with the prompt γ-rays in the Budapest Reactor experiments. These σγ measurements, corrected for saturation when half-lives are long with respect to the measurement time, can be used with either Pγ data from ENSDF or the Table of Radionuclides to determine σγ or with σ0 data from the Atlas to determine Pγ.

Prompt σγ data for low-Z isotopes can also be used to determine σ0 when the decay scheme is complete. In these cases σγ=Σσγ(Ground State)=Σσγ(Primary γ-rays). The Budapest Reactor guided neutron beam measurements are the only comprehensive source of experimental σγ data. Many other precise measurements of the relative neutron capture Iγ intensities, sometimes normalized to per 100 neutron captures, have also been measured. In many cases the Budapest isotopic data, measured on natural elemental targets, is incomplete because of either low isotopic abundance or low cross section. The Budapest σγ data can be used to renormalize the Iγ data from the other experiments to get a more complete set of σγ data.

For heavy isotopes (Z≥20) the prompt neutron capture γ-ray decay spectra generally are too complex to resolve a large continuum of weak transitions. In these cases only strong transitions deexciting lower lying levels and intense primary γ-rays are resolved. In order to measure σ0 it is necessary to determine the statistical contribution to the level scheme. This has been done with the statistical mode code DICEBOX [21] which calculates simulated level schemes for the higher levels above a cut-off energy Ecut and uses experimental level/gamma properties for levels below Ecut and measured primary γ-ray cross sections feeding levels below Ecut. A variety of level density functions and γ-ray strengths are supported by DICEBOX to produce the simulated level schemes which can be regenerated many times to determine the statistical fluctuations in the theory. The DICEBOX calculations are normalized to experiment by comparing the calculated feeding to levels below Ecut with the experimental cross section depopulating those levels. A discussion of the use of DICEBOX calculation to determine σ0 has been given by Krticka et al [22].

**Selected discrepant σγ/k0/Pγ values**

The majority of data from the different data sources have only minor variations, however in some cases the data are discrepant and must be reconciled by evaluation and/or further measurements. Several interesting examples follow.
$^{12}\text{C}(n,\gamma)^{13}\text{C}$ and $^2\text{H}(n,\gamma)^3\text{H}$

The simple $^{12}\text{C}(n,\gamma)^{13}\text{C}$ decay scheme, measured at the Budapest Reactor, is shown in Fig. 1. The cross section $\sigma_0(^{12}\text{C})=3.90\pm0.06$ mb determined from these complete decay scheme data is compared with previous measurements in Table 1. The new value is inconsistent with the Atlas [3] adopted value, which was based on the measurement by Jurney et al [23], but consistent with five other values. The average of comparable the cross section measurements in Table 2 is $\sigma_0(^{13}\text{C})=3.84\pm0.06$ mb.

Jurney et al [23] also used their $\sigma_0(^{13}\text{C})$ value in the same paper to determine the $^2\text{H}(n,\gamma)$ cross section. The new $^{13}\text{C}$ cross section suggests that Jurney et al’s value should be increased to $552\pm16$ mb which is consistent with four other previous measurements. We propose an adopted cross section $\sigma_0(^{2}\text{H})=549\pm10$ mb, based on the average of comparable values. This new value needs to be confirmed by future experiments.

$^{23}\text{Na}(n,\gamma)^{24}\text{Na}$

The $^{23}\text{Na}(n,\gamma)^{24}\text{Na}$ decay scheme is shown in Fig. 2 where the activation $\sigma_0$ cross sections measured at the Budapest Reactor for the production of the 1368.6- and 2754.0-keV $\gamma$-rays ($P_\gamma=1.0$) are shown. The average activation cross section from these measurements $\sigma_0(^{23}\text{Na})=542\pm3$ mb is compared with previous measurements in Table 2. This new value is higher than the adopted value $\sigma_0(^{23}\text{Na})=517\pm4$ mb from the Atlas [3] but it is comparable to several other measurements.

$^{30}\text{Si}(n,\gamma)^{31}\text{Si}$

The cross section $\sigma_0(^{31}\text{Si})=107\pm2$ mb adopted in the Atlas [3] is consistent with the Budapest Reactor value of $112\pm6$ mb. For $k_0(1266.2\gamma)=1.45\pm0.01\times10^{-7}$ from De Corte and Simonits [2], $\sigma_0=0.0630\pm0.0004$ mb. The transition probability $P_\gamma(1266.2)=\sigma_\gamma/\sigma_0=5.89\pm0.12\times10^{-4}$ which is more precise that $P_\gamma=5.0\pm0.4\times10^{-4}$ measured by McGuire and Hossain [24].
Table 2. Comparison of $^{23}$Na(n,γ) cross section measurements. The new EGAF [8] value is higher than the Atlas [8] value but consistent with other high values.

| $^{23}$Na | Author (Year) | $\sigma_0 \pm \Delta \sigma$ (mb) |
|----------|---------------|---------------------------------|
|          | Coltman (1946) | 470±40                          |
|          | Pomerance (1951) | 470±24                          |
|          | Meadows (1961) | 470±60                          |
|          | Brooksbook (1955) | 500±50                         |
|          | Koehler (1963) | 500±20                          |
|          | Yamamuro (1970) | 500±30                          |
|          | Harris (1953) | 503±5                           |
|          | Grimeland (1955) | 510±30                         |
|          | De Corte (2003) | 513±6                           |
|          | Kennedy (2003) | 515±21                          |
|          | Heft (1978) | 523±5                           |
|          | Ryves (1970) | 527±5                           |
|          | Szentmiklosi (2006) | 527±8                        |
|          | Bartholomew (1953) | 530±32                       |
|          | Wolf (1960) | 531±8                           |
|          | Cocking (1958) | 536±6                           |
|          | Jowitt (1959) | 536±8                           |
|          | Rose (1959) | 539±8                           |
|          | Budapest-PGAA | 540±4                           |
|          | Budapest-NAA | 542±3                           |
|          | Gleason (1975) | 540±20                          |
|          | Kaminishi (1963) | 577±8                         |
|          | Seren (1947) | 630±130                         |
|          | Atlas         | 517±4                           |
|          | Adopted       | 541±4                           |

$^{36}$S(n,γ)$^{37}$S

The Atlas [3] cross section $\sigma_0(36S)=236±6$ mb is inconsistent with $\sigma_0(36S)=160±3$ mb derived from $k_0(3103.1\gamma)=1.96(4)\times10^{-6}$ measured by De Corte. These $\sigma_0/k_0$ values are the only information available for neutron activation analysis of sulfur. The Atlas value is based on two consistent measurements, $\sigma_0(36S)=233±2$ mb by Raman et al [25] and $\sigma_0(36S)=249±14$ mb by Beer et al [26]. Both measurements were with isotopically enriched targets. The problem with $k_0(37S)$ is that the abundance of $^{36}$S is 0.02±0.01% and varies widely in the environment. We recommend $k_0=3.05(10)\times10^{-6}$ which is based upon the adopted $\sigma_0$ value assuming an isotopic abundance =0.02%. This value cannot be used for analytical purposes unless the isotopic abundance has first been measured.

$^{37}$Cl(n,γ)$^{38}$Cl

The Atlas [3] cross section $\sigma_0(37Cl)=433±6$ mb is consistent with the $\sigma_0(37Cl)=436±8$ mb derived from the De Corte and Simonits [2] $k_0$ values. From ENSDF [4] for $^{37}$Cl ($t_1/2=37.230±0.014$ m) decay, $P_1(1643.4)=0.333±0.005$ and $P_1(2167.5)=0.444±0.009$ based on the well-known γ-ray branching ratios and assuming a ground state $\beta^+$ feeding of 55.6±0.9%.

From the De Corte and Simonits $k_0$ values we determine that $P_1(1643.4)=0.319±0.006$ and $P_1(2167.5)=0.430±0.008$ which are consistent with the γ-ray branching ratios and a ground state $\beta^+$ feeding of 57.2±0.8%. This new ground state feeding is consistent with 57.6±1.3% measured by van Klinken et al [27] but discrepant with 55.2±0.6% from Miyahara et al [28].

$^{39,40,41}$K(n,γ)$^{40,41,42}$K

Table 3. Comparison of cross section measurements for the potassium isotopes.

| Author (Year) | $\sigma_0 \pm \Delta \sigma$ (b) |
|---------------|--------------------------------|
| **$^{39}$K**  |                                |
| Pomerance (1952) | 1.87±0.15                      |
| Gillette (1966) | 1.4                            |
| Hansen (1949)  | 2.9±0.7                        |
| von Egidy (1984)* | 2.206±0.025                    |
| **Atlas**      | 2.1±0.2                        |
| **Adopted**    | 2.21±0.03                      |
| **$^{40}$K**   |                                |
| Asghar (1978)  | 30                             |
| Beckstrand (1971) | 30±8                          |
| Pomerance (1952) | 66±20                           |
| Gillette (1966) | 70                            |
| Krusche (1984)* | 90±3                           |
| **Atlas**      | 30±8                           |
| **Adopted**    | 90±3                           |
| **$^{41}$K**   |                                |
| Seren (1947)   | 1.0±0.2                        |
| Pomerance (1952) | 1.19±0.10                       |
| Koehler (1967) | 1.2±0.1                        |
| Gryntakis (1976) | 1.28±0.06                      |
| De Corte (2003) | 1.42±0.02                      |
| Gleason (1975) | 1.43±0.03                      |
| Heft (1978)    | 1.43±0.03                      |
| Lyon (1960)    | 1.45                           |
| Ryves (1970)   | 1.46±0.03                      |
| Kappe (1966)   | 1.49±0.03                      |
| Kaminishi (1982) | 1.57±0.17                     |
| Krusche (1985)* | 1.523±0.022                    |
| **Atlas**      | 1.46±0.03                      |
| **Adopted**    | 1.522±0.022                    |

* Data were normalized to the Budapest cross section measurements.

Gamma-ray cross sections $\sigma_0$ for the three potassium isotopes were measured at the Budapest Reactor. These data can be used to renormalize the nearly complete neutron capture γ-ray intensities of Krusche et al [29,30,31] to obtain $\sigma_0$ for $^{39,40,41}$K(n,γ). These results are summarized in Table 3 where they are compared with previous measurements. For $^{40}$K(n,γ) the Budapest renormalized von Egidy [29] cross section $\sigma_0(40K)=2.206±0.025$ b is more precise and consistent with the Atlas [3] value.
A new $\sigma_d^{(50)K}$=90±3 b value, based on the Budapest Reactor $\sigma_d$(1293.6)=35.3±1.8 b which was used to renormalize the data of Krusche et al [30] is 3x the Atlas [3] value and consistent with the measurement of Pomerance [32].

The new $\sigma_d^{(41)K}$=1.523±0.022 b is based on the renormalization of Kappe [33] data and is consistent with measurements by Ryves [34] and Kaminishi [35] but higher than the value derived from the De Corte and Simonits [2] $42^{\text{K}} k_0$ values. This value is based on the measurement of prompt $\gamma$-rays while most lower values are based activation experiments suggesting that the difference may be due to a problem with the decay scheme $\gamma$-ray normalization.

The cross section $\sigma_d^{(70)Zn}$=93.5±3.7 b is also given 4.28±0.04% IT and 95.72±0.04% EC decay branching intensities for $^{114}In^{m+g}$ which disagree with the ENSDF [8] branchings reported as 3.25±0.24% IT and 96.75±0.24% EC.

$^{99}Tc(n,\gamma)^{100}Tc$

The cross section $\sigma_d^{(99)Tc}$=22.8±1.3 b was adopted in the Atlas [3]. A new value $\sigma_d^{(99)Tc}$=24.2±0.2 b can be derived from $\sigma_d$(539.5)=1.604±0.014 b and $\sigma_d$(590.8)=1.296±0.011 b from Budapest Reactor data, published by Molnar et al [45], and an improved $^{100}Tc$ (15.46±0.19 s) decay scheme normalization by Furutaka et al [46]. No $k_0$ values are given for $^{100}Tc$ in the IUPAC compilation [1] and we adopt $k_0$(539.5γ)=0.033±0.0003 and $k_0$(590.8γ)=0.0272±0.0007 here.

$^{103}Rh(n,\gamma)^{104}Rh^{m+g}$

The decay scheme for $^{104}Rh^{m+g}$ is shown in Fig. 3. From ENSDF [8] $P_\gamma$(555.8)=0.020±0.005 is poorly known because of a large uncertainty in the excited state feeding intensity. De Corte and Simonits [2] have measured $k_0$(555.8γ)=0.0692±0.0010 for the combined isomer and ground state feeding which corresponds to $\sigma_d$(555.8γ)=3.41±0.05 b. Assuming the adopted cross section $\sigma_d^{(103)Rh^{m+g}}$=143.5±1.5 b from the Atlas [3] we get a more precise value $P_g$(555.8)=0.0238±0.0004.

---

$^{74}Ge(n,\gamma)^{75}Ge^{m}$

The cross section $\sigma_d^{(74)Ge^{m}}$=163±5 mb in the Atlas [3] was adopted from EGAF data [8] but is inconsistent with $\sigma_d^{(74)Ge^{m}}$=138±1 mb that has been derived from $k_0$(139.7γ)=5.73±0.06×10^{-4} measured by De Corte and Simonits [2]. The EGAF values is consistent with $k_0=6.76±0.03×10^{-4}$. A new neutron activation measurement is necessary to confirm this new value.

---

$^{45}Sc(n,\gamma)^{46}Sc^{m}$

The ratio of the isomer $^{46}Sc^{m}$ to ground state cross sections $\sigma_d(^{45}Sc^{m})/\sigma_d(^{45}Sc^{g})=0.56±0.04$ was measured by Simons [36] in the thermal column of their reactor. The Atlas [3] has adopted $\sigma_d^{(45)Sc^{m}}=9.9±1.1$ b assuming $\sigma_d^{(45)Sc^{g}}=17.4±1.1$ b. A new, more precise measurement of $\sigma_d^{(45)Sc^{m}}=7.77±0.21$ b at the Budapest Reactor has been published by Szentmiklosi et al [37]. No $k_0$ value exists for the 142.5 keV $\gamma$-ray from $^{46}Sc^{m}$ decay in the IUPAC database [1] although this short-lived activity can give more rapid analytical results for Sc than $\gamma$-rays from $^{46}Sc^{g}$ decay ($t_{1/2}=83.788±0.022$ d). We recommend the value $k_0$(142.5γ)=0.226±0.005.

$^{70}Zn(n,\gamma)^{71}Zn^{g}$

The cross section $\sigma_d^{(70)Zn^{g}}=83±5$ mb was adopted in the Atlas [3] based mainly on the measurement of Mannhart and Vonach [38]. This value is supported by four other less precise measurements [39,40,41,42]. De Corte and Simonits [2] report $k_0$(511.6γ)=1.55±0.3×10^{-6} which gives $\sigma_d^{(70)Zn^{g}}=22$ mb assuming $P_\gamma$(511.6)=0.32 from Zoller et al [43] as adopted in ENSDF. An alternate decay scheme normalization by Thwaites and Pratt [44] is $P_\gamma$(511.6)=0.13 gives $\sigma_d^{(70)Zn^{g}}=63$ mb which is in better agreement with the Atlas value. Assuming the Atlas cross section is correct and adopting the De Corte and Simonits $k_0$ value we get $P_\gamma$(511.6)=0.085±0.005.
105Pd(n,γ)106Pd

The prompt γ-ray decay scheme form 105Pd(n,γ)106Pd is incomplete because of the contribution of unresolved continuum γ-rays. Statistical model calculations have been performed with the DICEBOX code to determine the missing statistical feeding to the ground state. The population/depopulation plot for 105Pd(n,γ) is shown in Fig. 4. The agreement between experiment and calculation is excellent. Krčíka et al [22] determined the total radiative neutron capture cross sections σ₀ in this way for all of the palladium isotopes using DICEBOX and the Budapest data and these results are summarized in Table 4.

113In(n,γ)114In

The decay scheme for 114In m1 is shown in Fig 5. The 114In m1 decay scheme consists of three γ-rays whose k₀ values have been measured by De Corte and Simonits [2]. From these data, after correction for internal conversion, we get σ_{γ+e}(190.3)=8.28±0.09 b, σ_{γ+e}(558.4)=0.368±0.003 b, and σ_{γ+e}(725.2)=0.372±0.002 b. These data give σ₀(114In m1)=8.65±0.09 b which is more precise and in good agreement with σ₀(114In m1)=8.1±0.8 b from the Atlas [3].

127I(n,γ)128I

The cross section σ₀(127I)=6.15±6 b adopted in the Atlas [3] is consistent with many precise measurements that don’t involve neutron activation. P(442.9)=0.1261±0.0008 was measured by Miyahara et al [47], and σ₀(127I)=5.39±0.06 b assuming the k₀ data of De Corte and Simonits [2] or σ₀(127I)=5.63±0.08 b assuming the σ₉ data of Szentmiklosi et al [37]. For an average value σ₀(127I)=5.48±0.12 b from the two activation measurements, P(442.9)=0.112±0.003 which is in substantial disagreement with the Miyahara et al measurement.

Fig. 4. Population/Depopulation plot for 105Pd(n,γ)106Pd. The spin distribution of the neutron capture state was determined by a least-squares minimization of the DICEBOX fit to the data.

Fig. 5. Main features of the 114In m1 decay scheme. The decay branchings are from ENSDF [8].

Table 4. Palladium total radiative thermal neutron cross sections.

| Isotope | σ₀ (literature) (barns) | σ₀ (this work) (barns) |
|---------|-------------------------|------------------------|
| 104Pd   | 1.6±0.2                 | 1.1±0.4                |
| 106Pd   | 0.65±0.30               | 0.75±0.26              |
| 108Pd   | 21.0±1.5                | 21.7±0.5               |
| 109Pd   | 0.30±0.03               | 0.36±0.10              |
| 110Pd   | 7.6±0.5                 | 8.6±0.6*               |
| 112Pd   | 0.70±0.17               | 0.34±0.10              |

*Value from Ref. [22] has been revised here.
**151Eu(n,γ)152Eu**

The cross section \(\sigma_0(151\text{Eu})=5900\pm200\) b was adopted in the Atlas [3] based largely on the data of Gryntakis [48]. De Corte and Simonits data [2] \(k_0\) data give \(\sigma_0(151\text{Eu})=6885\pm15\) b which is consistent with Budapest Reactor data that give \(\sigma_0(151\text{Eu})=6750\pm170\) b. We recommend a new adopted value of \(\sigma_0(151\text{Eu})=6880\pm100\) b.

**181Ta(n,γ)182Ta**

The cross section \(\sigma_0(181\text{Ta})=20.5\pm0.5\) b was adopted in the Atlas [3] based on many consistent measurements. This cross section is also consistent with the \(k_0\) measurements from De Corte and Simonits [2] for \(E_γ\geq152.4\) keV but inconsistent with two lower energy \(\gamma\)-rays from \(^{181}\text{Ta}\) (\(\text{t}_{1/2}=114.43\pm0.03\) d). The transition probabilities for these two \(\gamma\)-ray are well established in the Table of Radionuclides and we adopt \(k_0(67.8\gamma)=0.0975\pm0.0028\) and \(k_0(100.1\gamma)=0.0334\pm0.0008\) based on the adopted \(P_γ\) and \(\sigma_0\) values.

| \(^{186}\text{W}\) | Author (Year) | \(\sigma_0\pm\Delta\sigma\) (b) |
|----------------|--------------|-----------------|
| Gillette (1966) | 33           |                 |
| Pomerance (1952) | 34.1.0±2.7   |                 |
| Seren (1947)     | 34.2±7       |                 |
| Beitins (1992)   | 42.3±0.4     |                 |
| De Corte (2003)  | 42.2±0.22    |                 |
| Szentmiklosi (2006) | 42.8±0.4 |                 |
| Damle (1967)     | 35.4±0.8     |                 |
| Bondarenko (2008) | 35.9±1.1   |                 |
| Heft (1978)      | 36.6±0.8     |                 |
| Gleason (1977)   | 37.0±1.5     |                 |
| Anufriev (1981)  | 37±3         |                 |
| Nguyen (2008)    | 37.2±2.1     |                 |
| Friesenhahn (1966) | 37.8±1.2 |                 |
| Knopf (1987)     | 38.5±0.8     |                 |
| Uddin (2008)     | 38.7±2.3     |                 |
| Karadag (2004)   | 39.5±2.3     |                 |
| Hogg (1970)      | 40.0±1.5     |                 |
| Lyon (1960)      | 41.3         |                 |
| Lyon (1960)      | 51.0         |                 |
| **Atlas**        | 38.1±0.5     |                 |
| **Beitins (1992)** | 34.8±0.3    |                 |
| **De Corte (2003)** | 34.72±0.18  |                 |
| **Szentmiklosi (2006)** | 35.2±0.3 |                 |

* Value based on new decay scheme normalization [51].

**185W(n,γ)186W**

The cross section \(\sigma_0(185\text{W})=38.1\pm0.5\) b was adopted in the Atlas [3] based on the measurements reported in Table 5. Significant variation exists in these measurements. The precise \(\sigma_0\) values in Table 4 measured by Beitins et al. [49], De Corte and Simonits [2], and Szentmiklosi et al. [37] are all much higher than those measured by other methods. Previous activation data were all based on an older decay scheme normalization [50]. A new decay scheme normalization measured by Marnada et al. [51] leads to a new, more precise adopted value \(\sigma_0(185\text{W})=34.8±0.2\) b that is in better agreement with other measurements.

**Conclusions**

Significant progress has been made on the intercomparison of \(k_0\), \(\sigma_0\) and \(P_γ\) data from various sources. Several discrepancies discussed here have been tentatively resolved. Still a large body of slightly different nuclear constants needs to be resolved into a single self-consistent data base. Recently a \(k_0\) nuclear data committee, headed by Zsolt Revay, has been formed by the \(k_0\) users group to look into this problem and develop the next generation \(k_0\) database for nuclear applications. A parallel effort is underway to incorporate a new set of \(k_0\) and \(\sigma_0\) values into the next version of the EGAF database for the eventual adoption by ENSDF, ENDF, and DDEP evaluators.

**Acknowledgements.** We thank Andrej Trkov, Institute Jožef Stefan, and Mark Kellett, IAEA, for organizing and running the IAEA CRP on a Reference Database for Neutron Activation Analysis that got this project started. Valuable discussions at the CRP meetings with Maria Arribére, Centro Atómico Bariloche, Argentina; Frans De Corte, Ghent University, Belgium; Sunday Jonah, Ahmadu Bello University, Zaria; Radojko Jaćimović, Institute Jožef Stefan, Slovenia; Peter Schillebeeckx, IRMM, Belgium; Menno Blaauw, Reactor Institute Delft, Netherlands; and Maria Angela Menezes, CDTN/CNEN, Brazil are especially appreciated. This work was performed under the auspices of the U.S. Department of Energy by the University of California, supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy at Lawrence Berkeley National Laboratory under Contract No. DE-AC02-05CH11231.

**References**

1. Kolotov, V.P., De Corte, F.: Compilation of \(k_0\) and related data for Neutron Activation Analysis (NAA) in the form of an electronic database. Pure Appl. Chem. 76, 1921-1925 (2004).
2. De Corte, F., Simonits A.: Recommended nuclear data for use in the \(k_0\) standardization of neutron activation analysis. Atomic Data and Nuclear Data Tables 85, 47–67 (2003).
3. Mughabghab, S.: Atlas of Neutron Resonances, Elsevier (2006).
4. Evaluated Nuclear Structure Data File – a computer file of experimental nuclear structure and decay data maintained by the National Nuclear Data Center, Brookhaven National Laboratory.
5. Table of Radionuclides, decay data for radionuclides important for applied research and detector calibration evaluated by the Decay Data Evaluation Project and maintained by the Bureau International des Poids et Mesures, France.
6. Handbook of Prompt Gamma Activation Analysis, edited by G.L. Molnar, Kluwer Academic Publishers (2004).
7. Choi, H.D., Firestone, R.B., Lindstrom, R.M., Molnar, G.L., Reddy, A.V.R., Tan, V.H., Zhou, C.M., Poviotto-Coercuera, R., Trkov, A.: Development of a Database for Prompt Neutron Activation Analysis. J. Nucl. Sci. Tech. Supplement 2, 1372-1375 (2002).
8. Firestone, R.B., Choi, H.D., Lindstrom, R.M., Molnar, G.L., Mughabghab, S.F., Poviotto-Coercuera, R., Revay, Zs., Zerkin, V., Zhou, C.M.: Database of Prompt Gamma Rays from Slow Neutron Capture for Elementary Analysis, IAEA STI/PUB/1263, 251 pp (2007).
9. Firestone, R.B., Trkov, A.: Summary Report: First Research Coordination Meeting on Reference Database for Neutron Activation Analysis. INDC(NDS)-0477 (2005).
10. Kellett, M.A., Firestone, R.B.: Second Research Coordination Meeting on Reference Database for Neutron Activation Analysis. INDC(NDS)-0514 (2008).
11. Girardi, F., Guzzi G., Pauli J.: Activation analysis by absolute gamma-Ray counting and direct calculation of weights by nuclear constants. Anal. Chem. 36, 1588-1594 (1964).
12. Girardi, F., Guzzi G., Pauli J.: Reactor neutron activation analysis by the single comparator method. Anal. Chem. 37, 1085-1092 (1965).
13. Simonits, A., De Corte, F., Hoste, J.: Single-comparator methods in reactor neutron activation analysis. J. Radioanal. Nucl. Chem. 24, 31-46 (1975).
14. Ryves, T.B.: A new thermal neutron flux convention. Metrologia 5, 119-124 (1969).
15. De Corte, F., Moens, L., Jovanovic, S., Simonits, A., De Wispelaere, A.: Applicability of the 1/E1st epithermal spectrum representation and the effective resonance energy E∞ in NAA. J. Radioanal. Nucl. Chem. 102, 37-57 (1986).
16. De Corte, F., Bellemans, F., De Neve, P., Simonits, A.: The use of a modified Westcott-formalism in the k∞-standardization of NAA: The state of affairs. J. Radioanal. Nucl. Chem. 179, 93-103 (1994).
17. The CSISRS library contains an extensive compilation of experimental nuclear reaction data up to 1 GeV. Neutron reactions have been compiled systematically since the discovery of the neutron, while charged particle (up to carbon) and photon reactions have been covered less extensively. CSISRS is maintained by the National Nuclear Data Center, Brookhaven National Laboratory.
18. Belgya, T., Révay, Zs., Fazekas, B., Héjja, I., Dabolczi, L., Mohnár, G.L., Kis, Z., Östör, J., Kaszás Gy.: The new Budapest capture gamma-ray facility. in Proc. 9th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics, Budapest, Hungary, Oct. 8-12, Eds. G. Molnár, T. Belgya, Zs. Révay, Springer Verlag Budapest, Berlin, Heidelberg 1997 p. 826.
19. Firestone, R.B., Shirley, V.S., Table of Isotopes, 8th edition (Wiley, New York, 1996).
20. Handbook for Calculations of Nuclear Reactions Data, IAEA, Vienna, Report No. IAEA-TECDOC-1024, 1998.
21. Béčvár, F.: Simulation of γ cascades in complex nuclei with emphasis on assessment of uncertainties of cascade-related quantities. Nucl. Phys. A417, 434-449 (1998).
22. Krtiška, M., Firestone, R.B., McNab, D.P., Sleveland, B., Agvaanluvsan, U., Belgya, T., Révay, Zs.: Thermal neutron capture cross sections of the palladium isotopes. Phys. Rev. C 77, 054615 (2008).
23. Jurney, E.T., Bendt, P.J., Browne J.C.: Thermal neutron capture cross section of deuterium. Phys. Rev. C25, 2810 (1982).
24. McGuire, S.C., Hossain, T.Z.: 1266-keV gamma branch in 31Si decay. Phys. Rev. C 48, 1434-1437 (1993).
25. Raman, S., Ratynski, W., Jurney, E.T., Bunker, M.E., Starner, J.W.: 26S(n,γ)28Si reaction with thermal neutrons and decay of 27Si to levels in 37Cl. Phys. Rev. C30, 26-30 (1984).
26. Beer, H., Coceva, C., Hofinger, R., Mohr, P., Oberhumer, H., Sedgeshev, P.V., Popov, Yu.P.: Measurement of direct neutron capture by neutron-rich sulfur isotopes. Nucl. Phys. A621, 235c-238c (1997).
27. van Klinken, J., Pleiter, F., Dijksra, H.T.: Beta- and Gamma-ray measurements on the decay of 35Cl. Nucl. Phys. A112, 372-384 (1968).
28. Miyahara, H., Yoshida, A., Wurdnyanto, G., Hara, K., Yanagida, K., Mori, C.: Precise measurement of the gamma-ray emission probabilities of 37Cl. Nucl. Instrum. Methods Phys. Res. A369, 494-497 (1996).
29. von Egidy, T., Daniel, H., Hungerford, P., Schmidt, H.H., Lieb, K.P., Krusche, B., Kerr, S.A., Bunker, G., Borner, H.G., Brissot, R., Hofmeyr, C., Rascher, R.: Levels and gamma transitions of 40K studied by neutron capture. J. Phys. G. Nucl. Phys. 10, 221-239 (1984).
30. Krusche, B., Lieb, K.P., Ziegeler, L., Daniel, H., von Egidy, T., Rascher, R.: Spectroscopy of 40K by thermal neutron capture in 40K. Nucl. Phys. A417, 231-255 (1984).
31. Krusche, B., Winter, Ch., Lieb, K.P., Hungerford, P., Schmidt, H.H., von Egidy, T., Scheere, H.J., Kerr, S.A., Borner, H.G.: Level structure of 42K from the 41K(n,γ) and 41K(d,p) reactions. Nucl. Phys. A439, 219-252 (1985).
32. Pomerance, H.: Thermal neutron capture cross sections. Phys. Rev. 88, 412-413 (1952).
33. Kappe, D.W.: A self-consistent set of thermal neutron activation cross sections. Diss. Abstr. B27, 919 (1966).
34. Ryves, T.B.: Activation measurements of thermal neutron capture cross-sections and resonance integrals. J. Nucl. Energy 24, 35 (1970).
35. Kaminishi, K., Shuin, T.: Thermal neutron cross-sections of Na-23 and K-41. Japanese J. Appl. Phys. 21, 636 (1982).
36. Simons, G.G.: Isomeric cross section ratios for the Sc-46, Cs-134, and Re-188 isomers. Lawrence Radiation Laboratory Report TID-22165 (1962).
37. Szentmiklósi, L., Revay, S., Belgya, T.: Measurement of partial $\gamma$-ray production cross-sections and $k_0$ factors for radionuclides with chopped-beam PGAA. Nucl. Instr. Meth. Phys. Res. A 564, 655-661 (2006).
38. Mannhart W., Vonach, H.: Isomeric cross section ratios for the 2-P-1/2 and 1-G-9/2 shell model states formed by thermal neutron capture. Zeit. Phys. 210, 13-31 (1968).
39. Hughes, D.: private communication published in the SCISRS database (1951).
40. Thwaites, T.T., Pratt, W.W.: Decay of Zn71 isomers. Phys. Rev. 124, 1526-1531 (1961).
41. Arino, H., Kramer, H.H., Molinski, V.J., Tlisbury, R.S., Wahl, W.H., Stier, P.M.: Research in activation analysis. USAEC Report NYO-10175 (1964).
42. Mangal, S.K., Gill, P.S.: Thermal neutron activation cross-section for isomer production. Nucl. Phys. 36, 542-548 (1962).
43. Zoller, W.H., Walters, W.B., Gordon, G.E.: Decay of 2.4 min $^{71}$Zn and 3.9 h $^{71}$Zn to levels of $^{71}$Ga. Nucl. Phys. A142, 177-203 (1970).
44. Thwaites, T.T., Pratt, W.W.: Decay of the Zn$^{71}$ isomers. Phys.Rev. 124, 1526-1531 (1961).
45. Molnár, G. L., Belgya, T., Révay, Zs, Qaim, S. M.: Partial and total thermal neutron capture cross sections for non-destructive assay and transmutation monitoring of $^{99}$Tc. Radiochim. Acta 90, 479–482 (2002).
46. Furutaka, K., Harada, H., Nakamura, S., Katoh, T., Fujii, T., Yamana, H., Raman, S.: Cross Section of Thermal-Neutron Capture Reaction by $^{99}$Tc. J. Nucl. Radiochem. Sci. 6, 283-286 (2005).
47. Miyahara, H., Matamoto, H., Wurdiyanto, G., Takenaka, T., Yoshida, A., Mori, C.: Gamma-ray emission probability measurement by a two-dimensional $4\pi\beta-\gamma$ Coincidence System. Nucl.Instrum.Methods Phys.Res. A353, 229-233 (1994).
48. Gryntakis, T.: Evaluation of the G(Tn)-function and determination of cross sections for Eu-isotopes. Thesis DM-6909, Technical University of Munich (1976)
49. Beitins, M.R., Boneva, S.T., Khitrov, V.A., Malov, L.A., P.Popov, Yu., Prokofjev, P.T., Rezvaya, G.L., Simonova, L.L., Sukhovoj, A.M., Vasilieva, E.V.: Study of the $^{187}$W states excited in the (n,\(^\gamma\)) reaction. Z. Phys. A341, 155-170 (1992).
50. Firestone, R.B.: A=187. Nucl. Data Sheets 62, 159-269 (1991).
51. Marnada, N., Nagata, H., Ueda, N., Ikeda, K., Hayashi, N., Mori, C., Miyahara, H.: Precise measurement of gamma-ray emission probabilities for $^{187}$W by using a two-dimensional $4\pi\beta-\gamma$ coincidence system. J. Nucl. Sci. Technol. (Tokyo) 36, 1119-1124 (1999).
DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.