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TEMPERATURE DEPENDENCE OF THE WESTCOTT *g*-FACTOR FOR NEUTRON REACTIONS IN ACTIVATION ANALYSIS

(Technical Report)

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Temperature dependence of the Westcott g -factor for neutron reactions in activation analysis (Technical Report)[†]

Abstract: The Westcott g -factors, which allow the user to determine reaction rates for nuclear reactions taking place at various temperatures, have been calculated using data from the Evaluated Neutron Nuclear Data Library, ENDF/B-VI. Nuclides chosen have g -factors which are significantly different from unity and result in different reaction rates compared to nuclides whose neutron capture cross-section varies as the reciprocal of the neutron velocity. Values are presented as a function of temperature up to 673.16 K (400 °C).

INTRODUCTION

In performing activation measurements using a nuclear reactor, neutron capture reaction rates are determined as the product of the neutron flux at the sample location and the neutron capture cross-section of the material. For a given nuclide, the neutron capture cross-section at a particular neutron energy is the probability that a neutron at that energy will be captured by the nuclide. The standard energy for tabulation of thermal neutron cross-sections is that of room temperature of 293.59 K or 20.43 °C, corresponding to a neutron energy of 4.05×10^{-21} J, i.e. 0.0253 eV or a neutron velocity of 2200 m/s. This standard energy is chosen because sample irradiation locations in many reactors are at approximately ambient temperatures. (See Beckurts & Wirtz [1] for a general discussion of neutrons and neutron reaction rates in reactors.)

As most reactors do not operate at a temperature of exactly 20 °C, there must be some mechanism for converting the cross-section, σ_0 , at the tabulated energy to the effective cross-section, σ , at the actual temperature of the reactor. Westcott [2] developed a method for converting σ_0 to σ by describing the neutron spectrum as a combination of a Maxwellian–Boltzmann velocity distribution function which is characterized by a temperature, T , and a component of epithermal energy neutrons, whose neutron flux distribution is proportional to the reciprocal of the neutron energy, i.e. dE/E . For a nuclide whose neutron capture cross-section does not vary inversely with the neutron velocity, $\sigma = \sigma_0(g + rs)$, where g is the Westcott g -factor, the epithermal index, r , is approximately the fraction of the total neutron density in the epithermal component, and s is a temperature-dependent quantity related to the reduced resonance integral.

In the absence of an epithermal component, $r=0$. In this case, the g -factor is the ratio of the Maxwellian averaged cross-section, σ_r , to the 2200 m/s cross-section, σ_0 , given by the following expression

$$g = \sigma_r/\sigma_0 = (1/v_0\sigma_0) \int (4/\sqrt{\pi})(v/v_0)^3 \sigma(v) \exp(-v/v_0)^2 dv$$

If $\sigma(v)$ varies as $1/v$, the Maxwellian cross-section is equivalent to the 2200 m/s value and $g = 1$ and $s = 0$.

For many nuclides, there are particular energies for which the probability of capturing a neutron becomes very large. These large probabilities are referred to as resonances in the capture cross-section for the nuclide at that neutron energy. For nuclides which have resonances in the cross-section in the thermal neutron energy range, their corresponding g -factors are different from unity. The values of the g -factors for these nuclides are also temperature dependent.

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CALCULATIONAL RESULTS

In this work, a number of nuclides in the evaluated neutron data library, ENDF/B-VI [3], whose neutron capture cross-sections have resonances in the thermal neutron energy region, have been analyzed to determine their Westcott *g*-factors as a function of various Maxwellian temperatures from 273.16 K (0 °C) to 673.16 K (400 °C). This temperature range would cover the operating conditions for most reactor sample irradiation facilities that would be available for neutron activation analysis.

The resulting *g*-factor temperature dependence is listed in Tables 1–4 for the neutron capture reaction of 25 nuclides from ^{103}Rh to ^{238}U at 21 different reactor temperatures. The *g*-factor for the ^{197}Au neutron capture standard reaction is also given. The *g*-factors for some of the nuclides listed are greater than unity and the values increase with increasing temperature. Other nuclides have *g*-factors which are less than unity and the values decrease with increasing temperature. A few nuclides have *g*-factors whose values go through a maximum or a minimum as the temperature changes.

Table 1 Westcott *g*-factors for neutron capture reactions

<i>T</i> (°C)	<i>E_n</i> (eV)	^{103}Rh	^{113}Cd	^{115}In	^{135}Xe	^{148}Pm	^{149}Sm	^{151}Sm
0	0.0236	1.0219	1.2682	1.0167	1.1381	1.3806	1.6124	0.9499
20	0.0253	1.0246	1.3324	1.0205	1.1613	1.4758	1.7090	0.9291
40	0.0270	1.0292	1.3999	1.0243	1.1814	1.5771	1.7997	0.9093
60	0.0287	1.0339	1.4700	1.0282	1.1985	1.6836	1.8841	0.8904
80	0.0305	1.0386	1.5421	1.0321	1.2127	1.7940	1.9615	0.8723
100	0.0322	1.0435	1.6155	1.0360	1.2243	1.9072	2.0320	0.8550
120	0.0339	1.0484	1.6897	1.0400	1.2335	2.0219	2.0956	0.8384
140	0.0356	1.0533	1.7642	1.0440	1.2404	2.1374	2.1524	0.8225
160	0.0374	1.0583	1.8383	1.0481	1.2453	2.2523	2.2028	0.8072
180	0.0391	1.0634	1.9117	1.0522	1.2484	2.3662	2.2469	0.7925
200	0.0408	1.0685	1.9838	1.0564	1.2497	2.4781	2.2853	0.7784
220	0.0425	1.0737	2.0544	1.0606	1.2496	2.5874	2.3182	0.7648
240	0.0443	1.0790	2.1233	1.0648	1.2481	2.6837	2.3461	0.7518
260	0.0460	1.0844	2.1900	1.0691	1.2453	2.7965	2.3694	0.7392
280	0.0477	1.0898	2.2544	1.0735	1.2416	2.8956	2.3883	0.7270
300	0.0494	1.0953	2.3165	1.0779	1.2368	2.9906	2.4033	0.7153
320	0.0512	1.1009	2.3760	1.0823	1.2312	3.0815	2.4148	0.7040
340	0.0529	1.1065	2.4328	1.0868	1.2249	3.1679	2.4229	0.6931
360	0.0546	1.1123	2.4870	1.0913	1.2179	3.2501	2.4281	0.6825
380	0.0563	1.1181	2.5385	1.0958	1.2103	3.3278	2.4305	0.6723
400	0.0580	1.1240	2.5873	1.1006	1.2022	3.4011	2.4305	0.6624

In Table 5, the *g*-factors at 293.16 K (20 °C) for each of the nuclides calculated here are compared with earlier determinations from Westcott's 1960 report [4], from a 1973 version of the ENDF/B file [5] and from a 1975 calculation by Gryntakis & Kim [6]. Some of the nuclides have similar *g*-factors over the past 40 years, but there are significant differences for other nuclides.

DISCUSSION

The values of the *g*-factor, and whether these values increase or decrease with temperature, depend upon the energy and the width at half-maximum of the resonance in the neutron cross-section for the nuclides. The parameters for these cross-section resonances, such as the energy, the neutron scattering width and the neutron capture width, have been tabulated. The contribution from each of these resonances to the cross-section at a given energy can be calculated, using the tabulated resonance parameters [7].

As the energy increases above the resonance value, the cross-section decreases rapidly from its peak value at the center of the resonance. At higher energies beyond the width at the half-maximum, the decrease in the cross-section becomes less rapid and the energy dependence of the cross-section becomes

Table 2 Westcott g -factors for neutron capture reactions

$T(^{\circ}\text{C})$	E_n (eV)	^{151}Eu	^{152}Eu	^{153}Eu	^{154}Eu	^{155}Eu	^{155}Gd	^{157}Gd
0	0.0236	0.9225	0.9469	0.9799	1.1839	1.0462	0.8586	0.8642
20	0.0253	0.9014	0.9272	0.9741	1.2278	1.0573	0.8443	0.8521
40	0.0270	0.8817	0.9083	0.9685	1.2736	1.0688	0.8296	0.8393
60	0.0287	0.8634	0.8902	0.9630	1.3212	1.0807	0.8147	0.8259
80	0.0305	0.8464	0.8729	0.9576	1.3701	1.0929	0.7996	0.8122
100	0.0322	0.8307	0.8562	0.9523	1.4201	1.1057	0.7845	0.7983
120	0.0339	0.8164	0.8402	0.9471	1.4707	1.1189	0.7695	0.7843
140	0.0356	0.8033	0.8248	0.9421	1.5218	1.1326	0.7547	0.7703
160	0.0374	0.7915	0.8099	0.9372	1.5730	1.1470	0.7400	0.7563
180	0.0391	0.7810	0.7956	0.9323	1.6239	1.1620	0.7256	0.7425
200	0.0408	0.7717	0.7819	0.9276	1.6744	1.1778	0.7115	0.7288
220	0.0425	0.7637	0.7686	0.9230	1.7243	1.1945	0.6976	0.7154
240	0.0443	0.7569	0.7557	0.9185	1.7732	1.2122	0.6841	0.7022
260	0.0460	0.7514	0.7434	0.9141	1.8211	1.2310	0.6708	0.6892
280	0.0477	0.7471	0.7314	0.9097	1.8678	1.2511	0.6579	0.6765
300	0.0494	0.7440	0.7198	0.9055	1.9131	1.2726	0.6453	0.6640
320	0.0512	0.7421	0.7086	0.9014	1.9570	1.2957	0.6331	0.6519
340	0.0529	0.7414	0.6977	0.8973	1.9994	1.3206	0.6211	0.6400
360	0.0546	0.7419	0.6872	0.8933	2.0402	1.3474	0.6095	0.6284
380	0.0563	0.7435	0.6770	0.8894	2.0793	1.3764	0.5982	0.6170
400	0.0580	0.7463	0.6671	0.8856	2.1169	1.4078	0.5872	0.6060

Table 3 Westcott g -factors for neutron capture reactions

$T(^{\circ}\text{C})$	E_n (eV)	^{164}Dy	^{175}Lu	^{176}Lu	^{177}Hf	^{182}Ta	^{185}Re
0	0.0236	0.9906	0.9825	1.6051	1.0177	1.5178	1.0056
20	0.0253	0.9880	0.9771	1.7458	1.0217	1.6385	1.0066
40	0.0270	0.9854	0.9719	1.8922	1.0257	1.7641	1.0076
60	0.0287	0.9829	0.9669	2.0421	1.0298	1.8932	1.0085
80	0.0305	0.9804	0.9620	2.1932	1.0340	2.0238	1.0095
100	0.0322	0.9779	0.9572	2.3441	1.0382	2.1545	1.0105
120	0.0339	0.9754	0.9525	2.4928	1.0424	2.2840	1.0115
140	0.0356	0.9729	0.9480	2.6383	1.0468	2.4112	1.0125
160	0.0374	0.9705	0.9436	2.7793	1.0511	2.5350	1.0136
180	0.0391	0.9681	0.9393	2.9151	1.0556	2.6548	1.0146
200	0.0408	0.9656	0.9351	3.0451	1.0601	2.7700	1.0156
220	0.0425	0.9632	0.9310	3.1687	1.0646	2.8800	1.0167
240	0.0443	0.9608	0.9270	3.2857	1.0693	2.9847	1.0177
260	0.0460	0.9585	0.9231	3.3960	1.0740	3.0838	1.0188
280	0.0477	0.9561	0.9193	3.4994	1.0788	3.1772	1.0199
300	0.0494	0.9537	0.9156	3.5959	1.0836	3.2648	1.0209
320	0.0512	0.9514	0.9120	3.6857	1.0885	3.3468	1.0220
340	0.0529	0.9491	0.9084	3.7689	1.0935	3.4231	1.0232
360	0.0546	0.9468	0.9050	3.8456	1.0986	3.4939	1.0243
380	0.0563	0.9445	0.9016	3.9161	1.1038	3.5593	1.0254
400	0.0580	0.9422	0.8983	3.9807	1.1091	3.6196	1.0265

Table 4 Westcott *g*-factors for neutron capture reactions

<i>T</i> (°C)	<i>E_n</i> (eV)	¹⁸⁷ Re	¹⁹⁷ Au	²³¹ Pa	²³³ Pa	²³⁵ U	²³⁸ U
0	0.0236	0.9973	1.0056	0.9981	0.9868	0.9875	1.0036
20	0.0253	0.9962	1.0066	0.9960	0.9812	0.9832	1.0040
40	0.0270	0.9950	1.0076	0.9947	0.9758	0.9792	1.0045
60	0.0287	0.9938	1.0086	0.9942	0.9708	0.9755	1.0049
80	0.0305	0.9927	1.0096	0.9946	0.9660	0.9722	1.0053
100	0.0322	0.9915	1.0106	0.9963	0.9614	0.9692	1.0057
120	0.0339	0.9904	1.0116	0.9993	0.9571	0.9665	1.0062
140	0.0356	0.9892	1.0126	1.0041	0.9530	0.9641	1.0066
160	0.0374	0.9881	1.0136	1.0107	0.9491	0.9621	1.0070
180	0.0391	0.9869	1.0146	1.0195	0.9454	0.9603	1.0074
200	0.0408	0.9858	1.0156	1.0307	0.9419	0.9588	1.0079
220	0.0425	0.9847	1.0166	1.0447	0.9385	0.9576	1.0083
240	0.0443	0.9835	1.0176	1.0617	0.9354	0.9567	1.0087
260	0.0460	0.9824	1.0186	1.0818	0.9324	0.9560	1.0092
280	0.0477	0.9813	1.0197	1.1054	0.9295	0.9554	1.0096
300	0.0494	0.9802	1.0207	1.1325	0.9269	0.9551	1.0100
320	0.0512	0.9791	1.0217	1.1632	0.9243	0.9550	1.0105
340	0.0529	0.9780	1.0228	1.1977	0.9219	0.9550	1.0109
360	0.0546	0.9769	1.0238	1.2360	0.9197	0.9552	1.0113
380	0.0563	0.9758	1.0248	1.2781	0.9176	0.9554	1.0118
400	0.0580	0.9474	1.0259	1.3240	0.9156	0.9558	1.0122

$(1/E)^{1/2}$ or $1/\nu$. In the absence of any positive energy resonance in the thermal neutron region, a resonance at large negative energy is usually postulated with parameters to fit the cross-section value at the thermal energy of 0.0253 eV. The neutron capture cross-section would vary as $1/\nu$ and the *g*-factor would be unity as mentioned above.

If there are resonances in the cross-section but the energy of the strongest resonance (the resonance whose parameters give the largest calculated contribution to the cross-section) is not very close to the thermal energy of 0.0253 eV, the *g*-factor would still be close to unity. This is the case for ¹⁹⁷Au, ²³⁸U, ¹⁸⁵Re and ¹⁸⁷Re, where the strongest resonance for each nuclide is at an energy of from about 2 eV to 5 eV, compared to the thermal energy range of from 0.025 eV (20 °C) to 0.058 eV (400 °C). The *g*-factors for these nuclides differ from unity by less than 0.7% at 20 °C.

Whether the *g*-factor is larger than unity or smaller than unity and whether the value increases or decreases with temperature will depend upon whether the strongest resonance (the major contributor to the cross-section value) is at a positive neutron energy or at a negative neutron energy (a bound neutron level). When the strongest resonance corresponds to a bound neutron energy level (a resonance at a negative energy), the cross-section in the vicinity of the resonance decreases more rapidly than $1/\nu$. As a $1/\nu$ energy dependence corresponds to a unit *g*-factor, averaging a Maxwellian distribution of neutron energies over a cross-section, which decreases faster than $1/\nu$, would lead to a *g*-factor less than unity. As the temperature increases, the peak of the Maxwellian distribution moves to a higher neutron energy and the cross-section falls even lower than $1/\nu$. The *g*-factor is less than unity and it decreases with increasing temperature. This is the case for ¹⁵¹Sm, ^{151,152,153}Eu, ^{155,157}Gd, ¹⁶⁴Dy, ¹⁷⁵Lu, ¹⁸⁷Re, ^{231,233}Pa and ²³⁵U, where the *g*-factor is less than unity and decreases as the temperature increases.

When the strongest resonance is at a positive neutron energy, the cross-section will be increasing as the energy approaches the resonance peak energy. The *g*-factor will be larger than the $1/\nu$ dependent *g*-factor value of unity. As the temperature increases, the Maxwellian distribution of neutron energies will further approach the peak cross-section value and the *g*-factor will increase with increasing temperature. This is the case for ¹⁰³Rh, ¹¹³Cd, ¹¹⁵In, ¹³⁵Xe, ¹⁴⁸Pm, ¹⁴⁹Sm, ^{154,155}Eu, ¹⁷⁶Lu, ¹⁷⁷Hf, ¹⁸²Ta, ¹⁸⁵Re, ¹⁹⁷Au, ²³⁸U, where the *g*-factor is greater than unity and increases as the temperature increases.

Table 5 Comparison of *g*-factor calculations at 20 °C

Nuclide	This work	Westcott (1960)	ENDF/B (1973)	Gryntakis (1975)
¹⁰³ Rh	1.0246	1.0230	1.0225	—
¹¹³ Cd	1.3324	1.3203	1.3349	1.3266
¹¹⁵ In	1.0205	1.0192	—	1.0175
¹³⁵ Xe	1.1613	—	1.1616	—
¹⁴⁸ Pm	1.4758	—	—	—
¹⁴⁹ Sm	1.7090	1.6170	1.6381	1.5860
¹⁵¹ Sm	0.9291	0.9130	0.90498	—
¹⁵¹ Eu	0.9014	—	0.89201	0.8992
¹⁵² Eu	0.9272	—	—	—
¹⁵³ Eu	0.9741	1.0264	0.98159	1.0290
¹⁵⁴ Eu	1.2278	—	1.07407	—
¹⁵⁵ Eu	1.0573	—	1.0001	—
¹⁵⁵ Gd	0.8443	—	0.84278	0.8387
¹⁵⁷ Gd	0.8521	—	0.85068	0.8561
¹⁶⁴ Dy	0.9880	—	0.98763	—
¹⁷⁵ Lu	0.9771	—	0.97662	—
¹⁷⁶ Lu	1.7458	1.7011	1.74827	1.6914
¹⁷⁷ Hf	1.0217	—	—	—
¹⁸² Ta	1.6385	—	1.63932	1.6880
¹⁸⁵ Re	1.0066	—	1.00548	—
¹⁸⁷ Re	0.9962	—	0.98162	—
¹⁹⁷ Au	1.0066	1.0053	1.00506	1.0038
²³¹ Pa	0.9960	—	—	1.0378
²³³ Pa	0.9812	—	0.99413	1.0759
²³⁵ U	0.9832	0.9900	0.99073	1.0052
²³⁸ U	1.0040	1.0017	1.00230	1.0009

For some nuclides, the half-width of the strongest resonance exceeds the resonance energy or the width occurs in the energy region of the Maxwellian distribution, where the cross-section shape changes. As a result, the *g*-factor can go through a maximum or a minimum depending upon whether it is increasing or decreasing at that point, respectively. This is the case for ¹³⁵Xe, ¹⁴⁹Sm, ¹⁵¹Eu, ²³¹Pa and ²³⁵U.

Most of the *g*-factors in Table 5 have been consistent over the past 40 years. In a few cases, resonance parameters have been measured during the past 25 years. If there were no previously measured resonance parameters, a *g*-factor = 1 was assumed. This would account for the variation from previously presumed *g* ≈ 1 values, such as ¹⁴⁸Pm, ¹⁵²Eu and ¹⁷⁷Hf. In other cases, negative energy resonances have now been postulated to better fit the neutron cross-section value at 0.025 eV. For these nuclides, *g*-factors greater than unity have become *g*-factors less than unity, such as ¹⁵³Eu and ^{231,233}Pa.

UNCERTAINTIES IN *g*-FACTORS

James [8] has estimated the uncertainty in the *g*(*T*) of a nuclide according to the expression $\Delta g = (1/A) \{T \cdot (1/g) \cdot (dg/dT)\}$, where *A* is the ratio of the mass of the nuclide to the neutron mass. James found the uncertainties to be on the order of 0.7% or less.

The uncertainties of *dg/dT* have also been analyzed by Westcott [9] from evaluated cross-section curves for the fissile nuclides ²³³U, ²³⁵U, ²³⁹Pu and ²⁴¹Pu at room temperatures. The uncertainties varied by 0.3% or less. As the *g*-factors for the fissile nuclides have been extensively studied over the years, there are more data available on these values than for any other nuclides. As a result of the extensive database, the uncertainty for these nuclides would be expected to be lower, which they are.

As mentioned earlier, in the absence of resonances, the *g*-factor is unity. In this work, the uncertainty in the difference between the *g*-factors and a unit value has been estimated by using the uncertainties in

the values of the resonance energy and the neutron scattering and the neutron capture half-widths. These estimated uncertainties are 1.5% or less. The largest uncertainties are found in the g-factors which have the largest differences in value from unity.

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