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AVERAGE GROUP DATA FOR ^{241}Pu IN THE 0.1 - 21.5 keV ENERGY REGION

N.T. Koyumdzhieva and N.B. Yaneva
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(Translated from a Russian original published in Yadernye Konstanty 4/1990)

Translation editor: Dr. Alex Lorenz

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ABSTRACT

Group neutron data for ^{241}Pu neutron were calculated for the unresolved resonance region (0.1-21.5) keV using multilevel R-matrix formalism.

INTRODUCTION

Neutron data for the heavy isotopes of Pu are essential to improve fuel processing in the U-Pu cycle and also to predict reactor characteristics for a nuclear power plant. Recent efforts have been directed towards obtaining reliable physical models to have a reliable description of available experimental results and also to extrapolate neutron cross-sections in a region for which no (or little) experimental information exists [1].

In recent years several evaluations [2, 3, 4] have been made for ^{241}Pu in the unresolved resonance region. All these evaluations were based on the single-level Breit-Wigner formalism [5] with the addition of elastic scattering from the permanent background to the resonance cross-section to allow for the effect of inter-resonance interference and the contribution of widely spaced resonances. In the present paper the ^{241}Pu neutron data (average neutron cross-sections, resonance self-shielding factors and their Doppler broadening) are calculated. Multilevel R-matrix formalism of the nuclear reactions (Reich-Moore approximation) [6] is used and allowance made for the statistical distributions of average resonance parameters by using the Monte-Carlo statistical method.

Average resonance parameters

Energy averaged resonance parameters are used to parameterize neutron cross-sections in the unresolved resonance region. They are constants for the given energy range (energy group) and their values change when they undergo transition to a different energy group. It is in this sense that we refer to the energy dependence of average resonance parameters.

In this paper we took the average resonance parameter values from the JAERI evaluation [3] and reduced them to the BNAB energy ranges [7] by the linear interpolation method.

The average radiative width $\overline{\Gamma}_\gamma$ and the potential scattering radius R_c are taken as energy independent values. For all spin states $\overline{\Gamma}_\gamma$ = 0.4 eV and R_c = 9.8 fm (Table 1).

The average spacing between the resonances of a compound nucleus with spin J^* is $D_J = \frac{2(2I+1)}{(2J+1)} D_{obs}$, where I is the nuclear target spin, J is the compound nucleus spin, D_{obs} is the average observed spacing between resonances in the low energy region. The energy dependence for D_J starts to develop when E_n > 4 keV, and this dependence is taken into account in D_{obs} (Table 2). Not making allowance for the energy dependence D_{obs} in the energy group (10-21.5) keV leads to a 2.4% drop in the average radiative capture cross-section $\overline{\sigma}_\gamma$ and to a 1.5% drop in the average fission cross-section $\overline{\sigma}_f$.

In our evaluation, we make allowance for the contribution of p-resonance states of the compound nucleus as one state averaged over spin J. We are able to do this because the p-resonance contribution to the neutron cross-sections in the region examined is relatively small (≈10%). Then we obtain the average spacing between the p-resonances from the following equation:

$$\bar{D}_{(p)} = \frac{1}{\sum_J \rho_J} = \frac{1}{\sum_J (1/D_J)} ,$$

where p_j is the resonance density of a compound nucleus with a spin J^*.

The power functions for s-states $\bar{S}_0$ and for p-states $\bar{S}_1$ are heavily energy dependent. We obtain their average group values from the JAERI evaluation by reduction to the corresponding energy groups in the BNAB system by quadratic interpolation.

The average fission widths are also dependent on the energy value. We used the same procedure as for the power functions to obtain the fission widths for each compound nucleus state J^*. In the calculation process we retain the ratio of the fission width in one spin state to the fission width in every other, as it is done in the JAERI evaluation. Since we consider the p-resonance contribution of the compound nucleus as one state averaged over the spin conditions $J^* = 1^-, 2^-, 3^-, 4^-$, then $\overline{\Gamma_{f(p)}}$ is obtained as an average of the fission widths of these states. All the energy dependent average resonance parameters are given in Table 2.

The degrees of freedom for the neutrons (ν_n), the fission (ν_f) and radiative (ν_γ) widths are given in Table 1. For compound nucleus s-resonance states the values ν_n and ν_f are the same as those obtained by other authors [2]. For the generalized p-state we take $\nu_n = 1$ and $\nu_f = 1$. The contribution of each of the two fission channels for the $J^* = 2^+$ state is considered equal as the use of the Porter-Thomas distribution to describe Γ_f fluctuations is only justified in cases of very weakly or very strongly diverging relative contributions of the channels, and when they are equal the integral values of ν can be used rather than ν_{eff} [2]. The average number of prompt fission neutrons $\nu_n = 2.913 + 0.149\ E_n$ agrees with the JAERI evaluation.

Results and discussion

Calculations were carried out using the MNCARL program [8]. Group averages were calculated for the neutron cross-section values. The radiative capture cross-section $\bar{\sigma}_\gamma$ and the fission cross-section $\bar{\sigma}_f$ were calculated using the procedure proposed by Luk'yanov with the aim of optimizing the calculation process. If we write the K-matrix elements in the form: $K_{nn} = A_1 + A_2$, $K_{ff} = B_1 + iB_2$, $K_{nf} = C_1 + iC_2$ then:

$$\bar{\sigma} = 4 \frac{A_2 + 2N + B_2(N-M) + B_1 Q}{|\Delta|^2} \qquad (1)$$

$$\bar{\sigma}_f = 4 \frac{C_1^2 + C_2^2}{|\Delta|^2}, \qquad (2)$$

where:

$$N = A_2 B_2 + C_2^2$$
$$M = A_1 B_1 - C_1^2$$
$$Q = A_1 B_2 + B_1 A_2 - 2C_1 C_2$$
$$|\Delta|^2 = (1 + A_2 + B_2 + N - M)^2 + (A_1 + B_1 + Q)^2.$$

The calculation of the cross-section using formulas (1)-(2) gives identical results to calculations using (1 - iK) matrix elements [9].

The corresponding resonance self-shielding coefficients f_t, f_f, f_γ and f_n and their Doppler broadening $\Delta t^{1,2}$, $\Delta f^{1,2}$, $\Delta \gamma^{1,2}$ and $\Delta n^{1,2}$ were calculated for three temperatures, 300°C, 900°C and 2100°C, and also for the dilution cross-section values σ_0 = 1 b, 10 b, 100 b, 1000 b. Doppler broadening was calculated according to the formulas:

$$\Delta_i^1 = \frac{\sigma_i(900^\circ C) f_i(900^\circ C; \sigma_0) - \sigma_i(300^\circ C) f_i(300^\circ C; \sigma_0)}{\sigma_i(300^\circ C)}$$

$$\Delta_i^2 = \frac{\sigma_i(2100^\circ C) f_i(2100^\circ C; \sigma_0) - \sigma_i(900^\circ C) f_i(900^\circ C; \sigma_0)}{\sigma_i(300^\circ C)},$$

where i ≡ t,f,γ,n. All the calculation results are given in Tables 5-8.

As can be seen from Table 2, the energy dependence $\overline{\Gamma_{f(p)}}$ is very weak. Calculations showed that not making allowance for the energy dependence $\overline{\Gamma_{f(p)}}$ in the energy range (0.1-21.5) keV has no effect on the average radiative capture cross-section values which are very sensitive to the average fission width values. In this case $\overline{\Gamma_{f(p)}}$ was calculated as the average of the initial fission width values of all p-resonance channels; $\overline{\Gamma_{f1}}$ = 960 MeV, $\overline{\Gamma_{f2}}$ = 270 MeV, $\overline{\Gamma_{f3}}$ = 600 MeV, $\overline{\Gamma_{f4}}$ = 230 MeV (see JAERI [3]).

Kon'shin et al. [10] calculated the particle contributions of each spin state J^{π} in average fission cross-sections and of the radiative capture cross-section. From these calculations it can be seen that, owing to p-wave spin states, the fission cross-section is approximately 1% of the total fission cross-section at E_n = 1 keV. The same also applies to the radiative capture cross-section. When E_n = 10 keV, however, these contributions increase respectively by 10% for $\overline{\sigma_\gamma}$ and 20% for $\overline{\sigma_f}$. Then use of one averaged p-resonance state in the 11th energy group results in a 10% reduction in $\overline{\sigma_\gamma}$ and an approximately 18% reduction in $\overline{\sigma_f}$. Therefore we are limited to using one averaged p-resonance state only up to an energy value of E_n = 2 keV. The average fusion widths of the states $J^{\pi} = 1^-$, 2^-, 3^-, 4^- in energy groups 13, 12 and 11 are given in Table 3.

In Table 4 the calculated group cross-sections of the present work are compared with the group cross-sections obtained on the basis of a full system of evaluated data [2]. These are the only average group cross-sections for ^{241}Pu in the BNAB energy ranges known to us. It can be seen that the calculated radiative capture cross-sections $\overline{\sigma_\gamma}$ of the present paper are systematically higher than Kon'shin's group cross-sections. Comparison with the only available experimental data by Weston [11] (Fig. 1) shows good agreement, with the exception of the 17th energy group (100-215) eV. The experimental data are taken from Ref [3].

In Fig. 2 the fission cross-section is compared with experimental results.

Conclusion

The average group data (e.g., average neutron cross-sections, resonance self-shielding coefficients, and their Doppler broadening) were calculated on the basis of a self-consistent approach to the calculation of the resonance structure of neutron cross-sections. The average group data were calculated in the BNAB system energy groups.

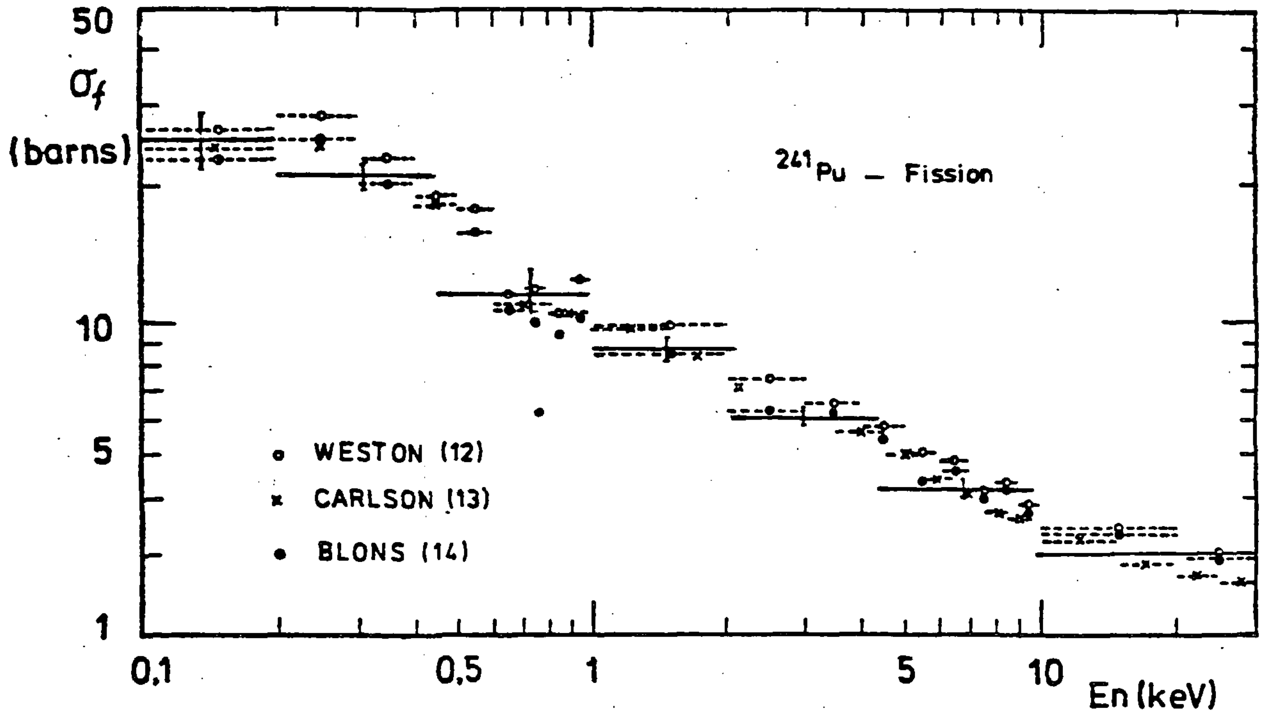

Fig. 1. Comparison of evaluated group radiative capture cross-sections $\overline{\Gamma_\gamma}$ (solid line) with experimental data.

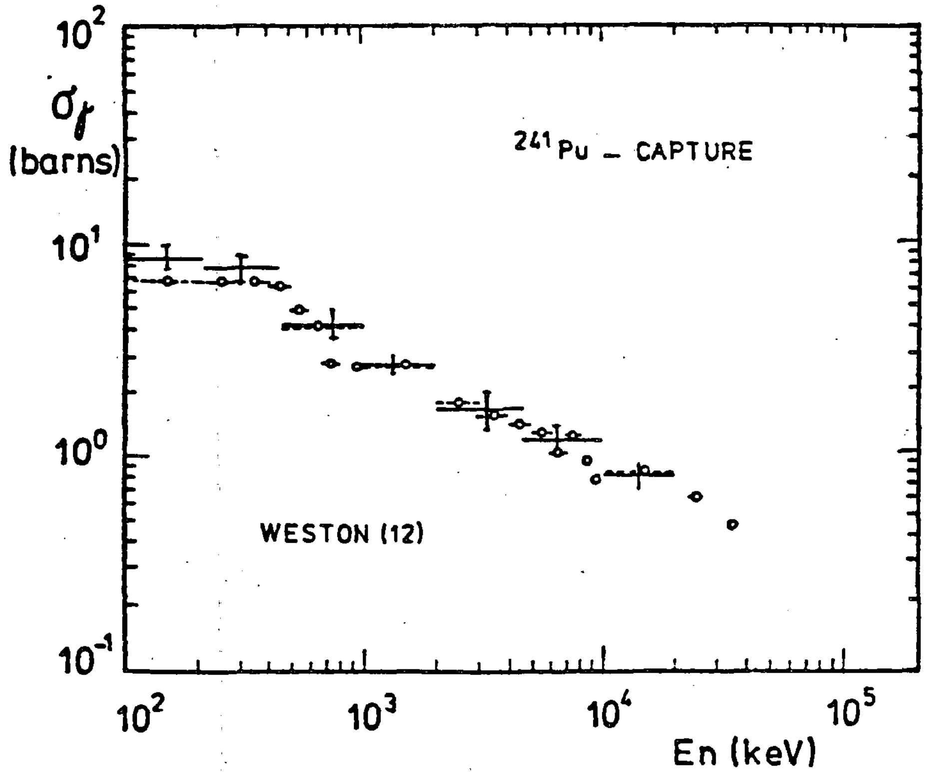

Fig. 2. Comparison of evaluated group fission cross-sections $\overline{\Gamma_f}$ (solid line) with experimental data.

Table 1

Average inter-resonance spacing $\overline{D}_J$ and degrees of freedom for neutrons ν_n, fission ν_f and radiative ν_γ widths for compound nucleus s- and p-resonances

l	J^π	g_J	ν_n	ν_f	ν_γ	R_c fm	$\overline{\Gamma}_\gamma$, eV
0	2^+	0.4167	1	2	∞	9.8	0.04
0	3^+	0.5833	1	1	∞	9.8	0.04
1	1^-	0.2500	1	2	∞	9.8	0.04
1	2^-	0.4167	2	2	∞	9.8	0.04
1	3^-	0.5833	2	2	∞	9.8	0.04
1	4^-	0.7500	1	2	∞	9.8	0.04

1: **orbital moment of s- and p-neutrons,**

J^π: **compound nucleus spin and parity,**

g_J: **statistical factor**

Table 2

Energy dependence of the strength functions $\overline{S}_0$ and $\overline{S}_1$ and of the average fission widths for s- $\overline{\Gamma}_{f(2+)}$ and $\overline{\Gamma}_{f(3+)}$) and p-resonances ($\overline{\Gamma}_{f(p)}$) and D_{obs}

Group	$\overline{S}_0 \cdot 10^{-4}$	$\overline{S}_1 \cdot 10^{-4}$	$\overline{\Gamma}_{f(2^+)}$ eV	$\overline{\Gamma}_{f(3^+)}$ eV	$\overline{\Gamma}_{f(p)}$ eV	D_{obs} eV
17	1.0065	1.4832	1.1420	0.4913	0.6838	0.85
16	1.3376	1.9712	0.7962	0.4770	0.3425	0.85
15	1.0695	1.5761	0.8207	0.3531	0.4914	0.85
14	1.1474	1.6909	0.8356	0.3595	0.5004	0.85
13	1.1728	1.7283	0.9632	0.4144	0.5768	0.8415
12	1.1615	1.7116	1.0141	0.4363	0.6073	0.833
11	1.1446	1.6868	1.0272	0.4419	0.6158	0.8245

Table 3
Average fission widths $\overline{\Gamma f}$ for p-resonance states
above E_n = 1 keV

Group	$J^\pi=1^-$	$J^\pi=2^-$	$J^\pi=3^-$	$J^\pi=4^-$
13	1.0752	0.3024	0.6720	0.2576
12	1.1320	0.3184	0.7075	0.2876
11	1.1467	0.3225	0.7166	0.2748

Table 4
Average group cross-sections $\overline{\sigma_t}$, $\overline{\sigma_f}$, $\overline{\sigma_\gamma}$ and $\overline{\sigma_n}$

Group	$\bar{\sigma}_t$, barn		$\bar{\sigma}_f$, barn		$\bar{\sigma}_\gamma$, barn		$\bar{\sigma}_n$, barn	
	[2]	present work	[2]	Present work	[2]	present work	[2]	present work
17	46.747	48.391	26.006	26.040	6.872	8.651	13.869	13.700
		±5.390		±4.910		±1.648		±0.374
16	43.254	43.450	22.714	21.640	6.773	7.930	13.767	13.880
		±3.678		±1.776		±1.031		±1.143
15	30.234	29.320	12.718	11.440	3.920	4.260	13.596	13.620
		±1.340		+0.920		±0.420		±0.130
14	24.452	24.487	8.460	8.137	2.614	2.890	13.378	13.460
		∓0.338		∓0.120		∓0.146		∓0.153
13	21.145	21.067	6.421	6.003	1.606	1.844	13.102	13.220
		±0.151		±0.010		±0.064		±0.051
12	18.277	18.269	4.460	4.144	1.079	1.225	12.738	12.900
		±0.072		±0.041		±0.018		±0.034
11	16.132	16.169	3.249	2.954	0.697	0.825	12.186	12.390
		±0.067		±0.030		±0.010		±0.012

Table 5
Self-shielding resonance factors f_t and f_f

Group	σ_0 barn	f_t 300°C	f_t 900°C	f_t 2100°C	f_f 300°C	f_f 900°C	f_f 2100°C
17	1	0.4495	0.4804	0.5185	0.5285	0.5752	0.6246
	10	0.5075	0.5422	0.5817	0.5919	0.6368	0.6822
	100	0.7051	0.7455	0.7823	0.7899	0.8234	0.8528
	1000	0.9224	0.9416	0.9550	0.9551	0.9656	0.9733
16	1	0.4731	0.5229	0.5752	0.5551	0.6216	0.6816
	10	0.5318	0.5827	0.6322	0.6209	0.6809	0.7330
	100	0.7320	0.7772	0.8131	0.8196	0.8552	0.8827
	1000	0.9336	0.9506	0.9616	0.9657	0.9742	0.9800
15	1	0.6248	0.6752	0.7150	0.6524	0.7156	0.7622
	10	0.6892	0.7365	0.7717	0.7204	0.7743	0.8129
	100	0.8632	0.8934	0.9129	0.8912	0.9169	0.9338
	1000	0.9766	0.9832	0.9870	0.9832	0.9879	0.9907
14	1	0.7250	0.7683	0.7995	0.7480	0.8016	0.8383
	10	0.7842	0.8216	0.8471	0.8061	0.8491	0.8779
	100	0.9200	0.9383	0.9493	0.9341	0.9509	0.9614
	1000	0.9880	0.9912	0.9930	0.9908	0.9934	0.9949
13	1	0.7943	0.8239	0.8434	0.8158	0.8534	0.8770
	10	0.8470	0.8708	0.8858	0.8645	0.8933	0.9109
	100	0.9520	0.9614	0.9668	0.9595	0.9692	0.9748
	1000	0.9934	0.9948	0.9956	0.9948	0.9961	0.9969
12	1	0.8523	0.8693	0.8791	0.8818	0.9045	0.9174
	10	0.8968	0.9094	0.9165	0.9180	0.9342	0.9433
	100	0.9726	0.9767	0.9788	0.9787	0.9833	0.9858
	1000	0.9966	0.9970	0.9974	0.9974	0.9981	0.9984
11	1	0.8910	0.8988	0.9028	0.9236	0.9340	0.9396
	10	0.9270	0.9323	0.9350	0.9492	0.9562	0.9601
	100	0.9824	0.9838	0.9846	0.9879	0.9897	0.9907
	1000	0.9976	0.9976	0.9976	0.9986	0.9988	0.9989

Table 6
Self-shielding resonance factors f_γ and f_n

Group	σ_0 barn	f_γ 300°C	f_γ 900°C	f_γ 2100°C	f_n 300°C	f_n 900°C	f_n 2100°C
17	1	0.4082	0.4822	0.5546	0.8883	0.8944	0.9004
	10	0.4676	0.5441	0.6142	0.9047	0.9108	0.9165
	100	0.6881	0.7554	0.8078	0.9483	0.9552	0.9607
	1000	0.9250	0.9487	0.9632	0.9874	0.9906	0.9925
16	1	0.4408	0.5261	0.5992	0.8392	0.8533	0.8664
	10	0.5037	0.5870	0.6532	0.8590	0.8723	0.8842
	100	0.7247	0.7876	0.8300	0.9181	0.9304	0.9398
	1000	0.9363	0.9560	0.9672	0.9780	0.9837	0.9872
15	1	0.5961	0.6844	0.7428	0.9032	0.9144	0.9223
	10	0.6684	0.7468	0.7964	0.9233	0.9330	0.9396
	100	0.8641	0.9044	0.9271	0.9697	0.9755	0.9790
	1000	0.9786	0.9859	0.9897	0.9952	0.9964	0.9970
14	1	0.7105	0.7764	0.8192	0.9167	0.9270	0.9335
	10	0.7745	0.8305	0.8628	0.9368	0.9453	0.9503
	100	0.9214	0.9444	0.9564	0.9786	0.9825	0.9846
	1000	0.9869	0.9925	0.9942	0.9970	0.9976	0.9980
13	1	0.7974	0.8426	0.8689	0.9274	0.9350	0.9396
	10	0.8502	0.8853	0.9051	0.9477	0.9535	0.9570
	100	0.9549	0.9669	0.9733	0.9849	0.9871	0.9883
	1000	0.9942	0.9958	0.9967	0.9981	0.9984	0.9986
12	1	0.8725	0.8975	0.9108	0.9385	0.9432	0.9458
	10	0.9111	0.9292	0.9387	0.9579	0.9613	0.9631
	100	0.9767	0.9820	0.9846	0.9894	0.9904	0.9909
	1000	0.9972	0.9978	0.9982	0.9987	0.9989	0.9989
11	1	0.9219	0.9332	0.9389	0.9493	0.9517	0.9528
	10	0.9479	0.9556	0.9596	0.9666	0.9682	0.9690
	100	0.9876	0.9895	0.9905	0.9922	0.9926	0.9928
	1000	0.9985	0.9968	0.9969	0.9991	0.9991	0.9992

Table 7
Doppler broadening of self-shielding factors

Group	σ_0, barn	Δ_t^1	Δ_t^2	Δ_f^1	Δ_f^2
17	1	0.0309	0.0381	0.0467	0.0494
	10	0.0347	0.0395	0.0449	0.0454
	100	0.0404	0.0368	0.0335	0.0294
	1000	0.0192	0.0134	0.0105	0.0077
16	1	0.0503	0.0529	0.0671	0.0607
	10	0.0514	0.0501	0.0606	0.0528
	100	0.0459	0.0367	0.0364	0.0263
	1000	0.0179	0.0119	0.0094	0.0067
15	1	0.0500	0.0403	0.0626	0.0472
	10	0.0468	0.0357	0.0532	0.0393
	100	0.0296	0.0201	0.0249	0.0177
	1000	0.0059	0.0045	0.0038	0.0037
14	1	0.0430	0.0309	0.0534	0.0366
	10	0.0371	0.0251	0.0428	0.0287
	100	0.0179	0.0106	0.0166	0.0107
	1000	0.0026	0.0014	0.0024	0.0018
13	1	0.0296	0.0195	0.0376	0.0236
	10	0.0238	0.0150	0.0288	0.0176
	100	0.0094	0.0054	0.0097	0.0056
	1000	0.0014	0.0008	0.0013	0.0008
12	1	0.0170	0.0098	0.0227	0.0129
	10	0.0126	0.0073	0.0162	0.0091
	100	0.0040	0.0021	0.0046	0.0025
	1000	0.0005	0.0003	0.0006	0.0003
11	1	0.0078	0.0040	0.0104	0.0056
	10	0.0053	0.0032	0.0070	0.0039
	100	0.0014	0.0006	0.0018	0.0010
	1000	0.0000	0.0000	0.0002	0.0001

Table 8
Doppler broadening of self-shielding factors

Group	σ_0,barn	Δ^1_γ	Δ^2_γ	Δ^1_n	Δ^2_n.
	1	0.0740	0.0724	0.0061	0.0060
	10	0.0765	0.0701	0.0061	0.0057
17	100	0.0665	0.0514	0.0069	0.0055
	1000	0.0237	0.0145	0.0032	0.0019
	1	0.0864	0.0728	0.0853	0.0721
	10	0.0845	0.0670	0.0833	0.0662
16	100	0.0646	0.0433	0.0629	0.0424
	1000	0.0217	0.0122	0.0197	0.0112
	1	0.0870	0.0600	0.0112	0.0079
	10	0.0770	0.0514	0.0097	0.0066
15	100	0.0388	0.0248	0.0058	0.0035
	1000	0.0054	0.0061	0.0012	0.0006
	1				
	10	0.0548	0.0316	0.0085	0.0050
14	100	0.0217	0.0113	0.0039	0.0021
	1000	0.0022	0.0010	0.0006	0.0004
	1	0.0452	0.0263	0.0076	0.0046
	10	0.0351	0.0198	0.0058	0.0035
13	100	0.0120	0.0064	0.0022	0.0012
	1000	0.0016	0.0009	0.0003	0.0002
	1	0.0250	0.0133	0.0047	0.0026
	10	0.0181	0.0095	0.0034	0.0018
12	100	0.0053	0.0026	0.0010	0.0005
	1000	0.0007	0.0003	0.0002	0.0000
	1	0.0113	0.0057	0.0024	0.0011
	10	0.0077	0.0040	0.0016	0.0008
11	100	0.0019	0.0010	0.0004	0.0002
	1000	0.0003	0.0001	0.0001	0.0000

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