International Atomic Energy Agency

INDC(CCP)-90/U

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(Extract translation from INDC(CCP)-86/G,
Nuclear Constants, Vol.20 Part 1, 1975)

Translated by the IAEA
June 1976

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

Reproduced by the IAEA in Austria
June 1976
76-4426

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76-2687
Translated from Russian

THE EVALUATION OF NEUTRON CROSS-SECTIONS FOR IRON

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ABSTRACT

This paper gives an evaluation of all the neutron cross-sections for a natural mixture of iron isotopes. The evaluated data are presented in the SOKRATOR format and have been fed into the computer file of evaluated nuclear data at the Nuclear Data Centre (Obninsk).

Introduction

Iron is the most important structural material for reactors and shielding, so that an accurate knowledge of its neutron cross-sections (especially the capture cross-section) is required. The existing iron evaluation at the Nuclear Data Centre, from the KEDAK file [2] and the BNAB*/ 26-group system of constants [1], relies on measurements made before 1965 and does not take into account many new papers which have appeared in recent years. The Nuclear Data Centre accordingly decided to evaluate all the neutron cross-sections for a natural mixture of iron isotopes. All available experimental data were used in the evaluation. In certain areas, where few data were available, or where those that are available proved to be contradictory, the recommended curves were derived from theoretical calculations based on nuclear models. Average group cross-sections were obtained for comparison with the BNAB 26-group system of constants at present used in reactor calculations.

Total cross-section

In the resolved resonance region (up to 200 keV) the recommended cross-section is based on multilevel R-matrix formalism. The collision-

*/ Bazazyants, Nikolaev, Abagyan, Bondarenko.

matrix element is in the following form:

$$U_{nn}^{\nu} = e^{2i\varphi_n^{\nu}} \frac{1+iR^{\nu}}{1-iR^{\nu}};$$
$$R^{\nu} = \frac{1}{2} \sum_{\lambda(\nu)} \frac{\Gamma_{\lambda n}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} + R_0^{\nu}(E); \qquad (1)$$
$$R_0^{\nu} = A^{\nu} + B^{\nu}(E - E_{1/2});$$

where $\Gamma_{\lambda\gamma}$ and $\Gamma_{\lambda n}$ are the radiation and neutron widths of the resonances of the compound nucleus:

E_λ are the resonance energies;

$E_{\frac{1}{2}}$ is the mid-point of the neutron energy interval considered; and

A^{ν} and B^{ν} are parameters introduced to allow for the contribution to the cross-section from resonances to the right and left of the energy interval considered but not included in the $\lambda(\nu)$ summation.

In calculating the resonance cross-sections for natural iron the contributions from the isotopes ^{54}Fe, ^{56}Fe and ^{57}Fe were taken into account with weightings proportional to the isotopic fractions they represent. The s-resonance parameters used in the calculations were selected on the basis of Refs [3-5], which performed multilevel analysis of transmission data. In selecting the p-resonance parameters, account was taken of the results obtained in R-matrix analysis of the radiative capture data in Refs [6, 7]. In cases where only $g\Gamma_n\Gamma_\gamma/\Gamma$ have been measured for p-resonances, the neutron widths Γ_n were obtained on the assumption of constant radiation width ($\Gamma_\gamma = 0.6$ eV). The coefficients A^{ν} and B^{ν} and the negative resonance parameters for ^{56}Fe were found by fitting the calculated curve to the experimental cross-section from Refs [8, 9]. A full set of recommended resonance parameters is given in Tables 4(a) and 4(b). The mean resonance parameters for natural iron are given in Table 5.

In evaluating the total cross-section in the energy range 0.2-14 MeV, use was made of the latest high-resolution measurements [10-12], data from transmission experiments with "poor" resolution [13, 14], the evaluations of Schmidt [2] and Filippov [15], and also the compilation in Ref. [16]. Comparison of the detailed curve of the total cross-sections obtained from high-resolution experiments shows that the positions of the maxima and minima in the cross-section are in good agreement even though the absolute values differ. In Ref. [17] Cerjacks reports that in the processing of the measurements in Ref. [10] the correction for analyser dead time was wrong; this could be the reason why the total cross-section value is too high. The results in later work of Cerjacks [18] in the energy range 0.5-1.3 MeV are lower than the data in Ref. [10].

In the energy range 3-14 MeV the data in Refs [10, 12, 2, 16], averaged with an interval ΔE, which is large enough for smoothing of the resonance structure, and the evaluated results from Ref. [15], agree with an accuracy not worse than $\pm$ 2% in the range 3-5 MeV, 1.5% in the range 5-9 MeV and 1% in the range 9-14 MeV.

In the light of what has been said above, the recommended cross-section values were taken as follows:

In the range 0.2-0.332 MeV - the Schmidt evaluation [2];

In the range 0.332-0.460 MeV - the data from Ref. [11];

In the range 0.46-1.3 MeV - the data from Ref. [12];

and the minima and maxima up to 0.4 MeV were corrected on the basis of the measurements given in Refs [9, 19]. Reference [18] was not taken into account for the correction because, as shown in Ref. [37], this would lead to extremely low values of the self-shielding coefficient. In the energy range above 3 MeV the optical model calculations were taken as recommended cross-sections, fitted to the mean curve of the cross-sections from Ref. [12] in the range 1.3-9.7 MeV and from Ref. [10] in the range 9.7-14 MeV.

Radiative capture cross-section

Since p and d neutrons make an important contribution to the radiative capture cross-section in the resonance range, the calculation from the resonance parameters given in Table 4 is taken as the recommended cross-section only in the range 0.025 eV-30 keV, where the omission of p-resonances is very improbable and the d-wave contribution can be neglected.

In the energy range 30-100 keV there is a marked divergence between two groups of experimental capture cross-section data. The measurements in Refs [20-22] agree satisfactorily with each other but lie considerably lower, by factors of 2 or 3, than the data in Refs [23, 24]. At energies above 100 keV the data of the various authors agree satisfactorily. The reason for the divergence between the different sets of measurements in the range 30–100 keV has not been established and in our evaluation we therefore recommend the statistical theory calculation for this range with the mean resonance parameters given in Table 5. Since the d-wave strength function cannot be found from the experimental data, it is taken to be equal to the s-strength function.

Level excitation functions and neutron inelastic scattering spectra

Level excitation functions with inelastic neutron scattering are evaluated for thirteen ^{56}Fe levels and for the primary level of ^{54}Fe (E_{th} = 1.409 MeV). The level-scheme parameters are shown in Table 3. The theoretical calculations of Ref. [25], based on the generalized optical model and on the Hauser-Feschbach statistical theory, are used in the evaluation.

The excitation function for the first ^{56}Fe level in the range 0.845–3 MeV was evaluated on the basis of the measurements of Gilboy and Towle [26], which are supported by many other experimental data [27]. At energies above 3 MeV the theoretical calculation of Ref. [25] is adopted, in which the contribution of the direct process to the primary-level excitation cross-section is calculated by the coupled-channel*/ method. The excitation functions for the remaining 12 levels of the ^{56}Fe nucleus are also taken from Ref. [25]. The excitation function for the primary level of the ^{54}Fe nucleus is evaluated on the basis of the experimental data of Refs [26, 28] on the assumption that it is similar to the excitation function for the ^{56}Fe nucleus level with E_{th} = 0.845 MeV.

The inelastic scattering spectra at initial neutron energies of 7.9 and 14 MeV were evaluated on the basis of the experimental data in Refs [29–33] and the theoretical calculations in Ref. [25]. In calculating the spectra, account was taken of both the statistical mechanism and the direct excitation mechanism as derived from the disturbed-wave method (DWBA).

*/ N.B. Literal translation.

Cross-sections of the (n,p), (n,α), (n,2n), (non), (inl) and (el) reactions

The (n,p) and (n,α) cross-sections were evaluated for ^{54}Fe and ^{56}Fe on the basis of the experimental data compiled in Ref. [2] and the theoretical calculations in Ref. [25].

The (n,2n) reaction cross-section is recommended on the basis of data obtained by separating the primary neutron spectrum from the measured inelastic scattering spectra [34] and by semi-empirical methods of data systematics [35]. The σ_{non} cross-section was obtained as the sum of the cross-sections of all inelastic processes: $\sigma_{non} = \sigma_{inl} + \sigma_{np} + \sigma_{n\alpha} + \sigma_{n\gamma} + \sigma_{nln}$. The σ_{el} cross-section was found as the difference between the total cross-section and the cross-section of all the inelastic processes: $\sigma_{el} = \sigma_{tot} - \sigma_{non}$.

Comparison of this evaluation with the BNAB data system

The mean group cross-sections $\overline{\sigma_{tot}}$, $\overline{\sigma_c}$, $\overline{\sigma_{in}}$, $\overline{\sigma_{el}}$, and resonance self-shielding coefficients were obtained by point representation of the evaluated results. It should be noted that, in contrast to the BNAB constants, the mean group cross-section $\overline{\sigma_c}$ here does not include the cross-sections of the threshold reactions (n,p), (n,α). This is the reason for the difference in the $\overline{\sigma_c}$ cross-sections in the first two groups. Table 5(a) compares the group constants obtained from our evaluation with the BNAB constants [1]. In addition, the table gives the Fe $\overline{\sigma_c}$ values obtained in the 26-group data system of Ref. [36] from the evaluation of the third version of the American evaluated data file ENDF/B-III. The biggest differences appear in the resonance range (groups 9-14) for the $\overline{\sigma_c}$ cross-section. At energies below 1 keV the group cross-sections from the BNAB system and from our own evaluation coincide almost perfectly.

Table 6(b) gives the resonance self-shielding coefficients f_t and f_c, as calculated from the detailed cross-section curve. The f_c coefficients were derived only for the range 1-30 keV, since at energies above 30 keV the resonance structure of the $\sigma_{n\gamma}$ cross-section was not taken into account in our evaluation. Comparison with the BNAB system self-shielding coefficients also shows a certain discrepancy in the values of f_c and f_t. In the neutron energy range where the resonance structure is significant ($E < 1$ MeV), the values of f_t obtained from our evaluation are systematically lower than the BNAB data (except for groups 9 and 10).

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Table 1

Isotopic composition of natural iron

Isotope	^{54}Fe	^{56}Fe	^{57}Fe	^{58}Fe
Content (%)	5.82	91.66	2.19	0.33

Table 2

The threshold reactions considered and their energies

Isotope	Reaction	Residual nucleus	Q(MeV)
^{54}Fe	(n,n')	^{54}Fe	- 1.409
	(n,p)	^{54}Mn	+ 0.1
	(n,α)	^{51}Cr	+ 0.6
^{56}Fe	(n,n')	^{56}Fe	- 0.845
	(n,p)	^{56}Mn	- 2.9
	(n,α)	^{53}Cr	+ 0.3
	(n,2n)	^{55}Fe	- 11.2

Table 3(a)

Level scheme of residual nuclei

Fe - 56

E, MeV	I^{π}
0	0^+
0,845	2^+
2,08	4^+
2,655	2^+
2,936	0^+
2.956	2^+
3,118	1^+
3.122	4^+
3.367	2^+
3,386	6^+
3,443	3^+
3.450	1^+
3,598	0^+
3,599	2^+

Mn - 56

E, MeV	I^{π}
0	(3^+)
0,026	(2^+)
0,108	(1^+)
0,207	(2^+)

Cr - 53

E, MeV	I^{π}
0	$3/2^-$
0,564	$1/2^-$
1,006	$5/2^-$
1,287	$7/2^-$
1,539	$7/2^-$
1,973	(3/2)

Fe - 54

E, MeV	I^{π}
0	0^+
1,408	2^+
2,534	
2,540	4^+
2,563	
2,960	2^+
3,162	2^+

Table 3(b)

Level density parameters for residual nuclei in the Fermi gas model

Nucleus	a(MeV^{-1})	δ (MeV)
^{56}Fe	6.2	1.0
^{56}Mn	6.1	- 2.0
^{53}Cr	6.05	- 0.5

Table 4(a)

Recommended resonance parameters of iron isotopes

Isotope	l	A^{ν}	$B^{\nu}(eV^{-1})$	R(Fermi)
^{54}Fe	0	0,10	$0,1.10^{-4}$	6
	1	0	0	
^{56}Fe	0	0,11	$0,15.10^{-5}$	6
	1	0	0	
^{57}Fe	0	0,1	$0,1.10^{-5}$	6
	1	0	0	

Table 4(b)

No.	E_0(keV)	Γ_n(eV)	Γ_γ(eV)	ℓ	I^π	Isotope
I	- 2,0I	I77	0,6	0	I/2+	56
2	I,I67±0,0I0	0,056±0,006	0,6±0,I	I	I/2-	56
3	I,62 ±0,0I		0,050±0,0I*	I	0+	57
4	2,35		0,0004*	I	I/2-	56
5	3,96 ±0,05	I77 ±36	I,I4 ±0,06	0	I-	57
6	4,75 ±0,06		0,05I±0,0I*	I	0+	57
7	6,2I ±0,07	396 ±50	I,32 ±0,I5	0	I-	57
8	7,22 ±0,08		0,36 ±0,09*	I	I+	57
9	7,76 ±0,0I	I020 ±20	3,0 ±0,5	0	I/2+	54
I0	7,90 ±0,08		0,I8 ±0,09*	I	I+	57
II	9,48 ±0,02	2,3	0,60*	I	I/2-	54
I2	II,I9 ±0,I	7,0	0,60	I	I/2-	54
I3	I2,8 ±0,I		0,46 ±0,I5*	I	I+	57
I4	I3,9 ± 0,I		0,7 ±0,2*	I	I+	57
I5	I4,4 ±0,I		0,53 ±0,I4*	I	I/2-	54
I6	I7,5 ±0,3		0,7I ±0,35*	I	I+	57
I7	2I,3 ±0,4		I,09 ±0,28*	I	I+	57
I8	22,7 ±0,I		0,I9I±0,022*	I	I/2-	56
I9	27,66±0,2	I420±I00	I,44 ±0,I4	0	I/2+	56
20	29,0 ±0,4	3000±500	4 ± I	0	I-	57
2I	30,7 +0,I	I0	0,6	I	I/2-	54
22	39,I8±0,I2	I5	0,6	I	I/2-	54
23	52,78±0,2	2540±200	I,0	0	I/2+	54
24	7I,86±0,3	I770±200	I,0	0	I/2+	54
25	73,9 ±0,4	540±40	I,0	0	I/2+	56
26	83,6 ±0,4	I030±80	I,0	0	I/2+	56
27	98,5 ±0,4	5I0±I00	I,0	0	I/2+	54
28	I22,5±0,6	I4±5	I,0	0	I/2+	56
29	I29,6±0,6	650±I00	I,0	0	I/2+	56
30	I29,7±0,6	3000±I000	I,0	0	I/2+	54
3I	I39,9±0,7	2270±200	I,0	0	I/2+	56
32	I47,I±0,8	2750±500	I,0	0	I/2+	54
33	I59,0±I,0	I80±90	I,0	0	I/2+	54
34	I68,7±I,0	760±I60	I,0	0	I/2+	56
35	I73,9±I,0	2800 ± I200	I,0	0	I/2+	54
36	I87,0±I,0	3200 ± 230	I,0	0	I/2+	56
37	I9I,2±I,0	42400 ± 500	I,0	0	I/2+	56
38	2I9,5±I,0	I400 ± I00	I,0	0	I/2+	56
39	222,8±I,2	I570 ± I40	I,0	0	I/2+	54

* Value of $\Gamma_n \Gamma_\gamma / \Gamma_0$ is given.

Table 5

Mean resonance parameters of natural iron

ℓ	S	Γ_{γ}(eV)	D(keV)
0	I,6.10^{-4}	I,4	30
I	0,I.10^{-4}	0,6	-
2	I,6.10^{-4}	0,6	-

Table 5(a)

Comparison of mean-group cross-sections with the BNAB data system

Energy range	Group No.	BNAB σ_t (barn)	NDC σ_t (barn)	BNAB σ_c (barn)	NDC σ_c (barn)	BNAB σ_{in} (barn)	NDC σ_{in} (barn)	BNAB σ_e (barn)	NDC σ_e (barn)	ENDF/B σ_e (barn)
6,5 - I0,5 MeV	I	3,40	3,30	0,001	0,001	I,37	I,39	I,39	2,08	I,97
4,0 - 6,5 MeV	2	3,80	3,70	0,005	0,001	I,35	I,4I	2,45	2,24	2,26
2,5 - 4,0 MeV	3	3,50	3,40	0,002	0,002	I,I3	I,I3	2,37	2,30	2,36
I,4 - 2,5 MeV	4	3,30	3,I0	0,003	0,002	0,90	0,68	2,40	2,42	2,37
0,8 - I,4 MeV	5	2,90	2,70	0,004	0,002	0,37	0,3I	2,33	2,39	2,2
0,4 - 0,8 MeV	6	3,30	3,I	0,005	0,005	0,0I	0,004	3,78	3,09	3,06
0,2 - 0,4 MeV	7	3,00	2,9	0,006	0,005	-	-	2,99	2,9	2,9
0,I - 0,2 MeV	8	3,70	4,2	0,006	0,007	-	-	3,69	4,I9	3,7
46,5- I00 keV	9	5,30	5,I	0,007	0,0II	-	-	5,29	5,I	5,3
2I,5-46,5 keV	I0	I4,5	I2,8	0,0I7	0,0I9	-	-	I4,5	I2,8	I3,5
I0,0-2I,5 keV	II	4,0	3,6	0,005	0,009	-	-	3,99	3,6	2,8
4,65-I0,0 keV	I2	8,40	9,9	0,004	0,022	-	-	8,40	9,9	I0,0
2,I5-4,65 keV	I3	5,90	6,8	0,0II	0,009	-	-	5,89	6,6	6,8
I,0 -2,I5 keV	I4	7,50	7,2	0,I06	0,202	-	-	7,39	7,0	8,6
465 -I000 eV	I5	I0,0	9,9	0,0I5	0,0I0	-	-	I0,0	9,9	9,9
2I5 - 465 eV	I6	II,0	II,0	0,026	0,0I8	-	-	II,0	II,0	II,0
I00 - 2I5 eV	I7	II,4	II,3	0,037	0,030	-	-	II,4	II,3	II,3
46,5- I00 eV	I8	II,5	II,5	0,053	0,047	-	-	II,4	II,4	II,4
2I,5- 46,5 eV	I9	II,5	II,5	0,072	0,07I	-	-	II,4	II,4	II,4
I0,0- 2I,5 eV	20	II,5	II,5	0,I05	0,I05	-	-	II,4	II,4	II,4
4,65- I0,0 eV	2I	II,5	II,6	0,I54	0,I55	-	-	II,4	II,4	II,4
2,I5 - 4,65 eV	22	II,6	II,6	0,220	0,220	-	-	II,4	II,4	II,4
I,0 - 2,I5 eV	23	II,7	II,7	0,330	0,337	-	-	II,4	II,4	II,4
0,465- I,0 eV	24	II,9	II,9	0,490	0,484	-	-	II,4	II,4	II,4
0,2I5- 0,465 eV	25	I2,I	I2,I	0,720	0,726	-	-	II,4	II,4	II,4
0,0252 eV	26	I3,9	I3,9	2,53	2,55	-	-	II,4	II,4	II,4

Table 5(b)

Comparison of resonance self-shielding coefficients for $\sigma_0 = 0$

Energy range	Group No.	f_t^{BNAB}	f_t^{NDC}	f_c^{BNAB}	f_c^{NDC}
6,5 - I0,5 MeV	I	-	-	-	-
4,0 - 6,5 MeV	2	0,96	I,0	0,97	-
2,5 - 4,0 MeV	3	0,94	0,93	0,95	-
I,4 - 2,5 MeV	4	0,74	0,83	0,90	-
0,8 - I,4 MeV	5	0,6I	0,65	0,79	-
0,4 - 0,8 MeV	6	0,45	0,46	0,63	-
0,2 - 0,4 MeV	7	0,55	0,42	0,62	-
0,I - 0,2 MeV	8	0,39	0,35	0,50	-
46,5- I00 keV	9	0,34	0,45	0,53	-
2I,5- 46,5 keV	I0	0,03	0,06	0,39	0,40
I0,0- 2I,5 keV	II	I,0	0,77	0,75	0,65
4,65- I0,0 keV	I2	0,86	0,63	0,60	0,68
2,I5- 4,65 keV	I3	I,0	0,90	0,77	0,79
I,0 - 2,I5 keV	I4	I,0	0,96	0,37	0,2I