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International Atomic Energy Agency

INDC(CPR)-037
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A SIMULTANEOUS EVALUATION OF NEUTRON INDUCED REACTION CROSS SECTIONS FOR ^{56}Fe at E_n = 14.1 MeV

by

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IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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A Simultaneous Evaluation of Neutron Induced Reaction Cross Sections for ^{56}Fe at E_n = 14.1 MeV

Zhou Delin

(China Nuclear Data Center, CIAE)

Abstract

A simultaneous evaluation of neutron induced reaction (i. e., (n,total), (n,n), (n,non), (n,n′), (n,2n), (n,nα), (n,np), (n,γ), (n,p), (n,d), (n,α), (n,n−em), (n,p−em), (n,d−em) and (n,α−em) reaction) cross sections on ^{56}Fe at E_n = 14.1 MeV is carried out. The evaluated cross sections are compared with the corresponding measured values and the evaluations for CENDL−2, ENDF / B−6, JEF−2.2, JENDL−3 and BROND−2.

Introduction

We have provided comprehensive evaluations for particle (n, p, d, α) emission and related partial reaction cross sections of all isotopes of Fe, Cr and Ni respectively as 'benchmarks' for the 'Intercomparisons of Evaluations (Calculations) of 14.1 MeV Particle Emission Data of Cr, Fe, Ni for Various Libraries' for IAEA / FENDL advisory group meeting[1]. There, by 'comprehensive evaluation' we meant that it was carried out based on the evaluations of the particle emission and related reaction cross sections performed individually, and considering the constraint relations :

$$\sigma(\text{total}) = \sigma(\text{n}) + \sigma(\text{n}') + \sigma(2\text{n}) + \sigma(\text{n}\alpha) + \sigma(\text{np}) + \sigma(\text{p}) + \sigma(\text{d}) + \cdots$$
$$\sigma(\text{non}) = \sigma(\text{n}') + \sigma(2\text{n}) + \sigma(\text{n}\alpha) + \sigma(\text{np}) + \sigma(\text{p}) + \sigma(\text{d}) + \cdots$$
$$\sigma(\text{n}-\text{em}) = \sigma(\text{n}') + 2 \times \sigma(2\text{n}) + \sigma(\text{n}\alpha) + \sigma(\text{np})$$
$$\sigma(\text{p}-\text{em}) = \sigma(\text{np}) + \sigma(\text{p})$$
$$\sigma(\alpha-\text{em}) = \sigma(\text{n}\alpha) + \sigma(\alpha)$$
$$\sigma(\text{d}-\text{em}) = \sigma(\text{nd}) + \sigma(\text{d})$$

Actually, in Ref. [1], for getting evaluated values, the measured data for (n,n′), (n,2n) reactions and for n−em, p−em, and α−em cross sections have been reviewed and analysed carefully, and for some reasons, some other cross sections (σ(non), σ(p), $\sigma(\gamma)$, for example) and the ratios of some cross sections (σ(np) / σ(p), $\sigma(n\alpha)$ / $\sigma(\alpha)$ for example) were quoted from available evaluations. And we have pointed out that 'the nonelastic scattering cross sections as well as the total inelastic scattering cross sections for the main isotopes remain to be improved'. And also pointed out that 'a simultaneous evaluation of total cross section, nonelastic scattering cross section, elastic scattering cross section, etc., on an experimental data base might be a way for further improving the evaluation of these data'[1].

So, at first, it is important to have reliable evaluation(s) for total, nonelastic and / or elastic scattering cross sections. Since the large component of the direct inelastic scattering to the first excited state (846 keV) of ^{56}Fe, more difficulties exist in the elastic and nonelastic scattering cross section measurements, then more difficulties exist in the evaluation work.

1 Individual Evaluations of Various Reaction Cross Sections

1.1 Total Cross Section

Five measurements of total cross section are available by using white neutron source or 'spot' thick target Li(d,n) neutron source by Cierjacks et el. (68), Perey et al. (72), Schwartz et al. (74), Larson et al. (80) and Foster et al. (71) respectively. Total cross sections at 14.1 MeV are obtained via smoothing the measured points around 14 MeV from EXFOR data base. Four measurements performed by Perey et al., Cierjacks et el., Larson et al. and Foster et al. are adopted for this work.

1.2 Elastic Scattering Cross Section

Except Tak92, all those measurements in which the cross sections of elastic and inelastic scattering to 1st excited state are analysed and provided simultaneously are in good agreement with each other[2]. Although the elastic scattering cross section of Tak92 is also in agreement with others within its large quoted error, it is too low to compare with the differences of the measured total and nonelastic scattering cross sections. Anyway, five measurements including Tak92 (i. e., Sch94, Tak92, Elk82, Hya75, Coo52)[2] are adopted in this work.

1.3 Nonelastic Scattering Cross Section

The measurements of nonelastic scattering cross section at 14 MeV were often carried out by using spherical transmission method in 1950's and early 1960's. It seems that in almost all these nonelastic scattering measurements the large inelastic scattering cross section (totaled up to 74.0 ± 5 mb, mainly from direct interaction) to 1st excited state was not corrected properly. Three such measurements for which the detector bias have been mentioned explicitly are adopted in this evaluation after correcting them to 'real' nonelastic scattering cross section :

(i) Mac57[3]. The measured values of nonelastic scattering cross section depend on the thresholds of the detector as shown in Table 1 :

Table 1 Nonelastic scattering cross section measured by MacGregor et al.[3] at 14.2 MeV energy spread 300 keV

E(thr) (MeV)	13.1	12.75	12.6	12.35	12.0	11.4	11.0	10.5	9.4	7.7
σ(non) (b)	1.39	1.37	1.35	1.36	1.36	1.36	1.33	1.34	1.30	1.21

In this case, 1.36 ± 0.03 b is reported by the authors. Obviously the component of inelastic scattering to 1st excited state was not included. So a value of 74.0 mb should be add to 1.360 and then 1.434 b obtained.

(ii) Fle56[4]. In this measurement the neutrons from inelastic scattering to 1st excited state were detected as neutrons of elastic scattering considering that its detector were biased at 9~ 12 MeV. 74.0 mb should be added to its results of 1.380 ± 0.020 mb then 1.454 ± 0.02 b is obtained.

(iii) Gra53[5]. The detector biased at 2 / 3 of the primary neutron energy. To add the contribution of the inelastic scattering to 1st excited state to its measured value then result in 1.344 ± 0.04 b.

1.4 Total Inelastic Scattering

Fortunately the most important isotopes of Fe, Cr and Ni are even–even nuclides. So the total inelastic scattering cross sections of these nuclides can be obtained from γ–production cross sections to 2^+ to ground state. Actually about 90% (95 % for ^{56}Fe) of the inelastic scattering processes are de–excited through 2^+ to ground state[6].

For ^{56}Fe, eight measurements of γ–production data[6~13] are available as shown in Table 2. After correcting the incident neutron energy to 14.1 MeV and gamma detection angle to 125 degree, the measurements (i. e., Abb73, Suk70, Lar85, and Xin88) which are in agreement with each other are adopted.

Table 2 Measured total inelastic scattering cross section of ^{56}Fe

	Orp75 [7]	Lac74 [8]	Eng67 [9]	Abb73 [10]	Suk70 [11]	Lar85 [6]	Xin88 [12]	Yan88 [13]
E_n (MeV)	14.1	14.1	14.7	14.2	14.1	14.1	14.2	14.7
Angle (deg.)	125	125	90	125	90	–	55	90
Sig (mb / sr)	36.5	70 ± 7	57.6 ± 6	57.4 ± 6	52 ± 8			67.14 ± 3.4
Sig (125)	36.5	70	66.2	57.4	59.8		58.9	71.5
Sig (14.1)	36.5	70	77	59.0 ± 6	59.8 ± 9	60.0 ± 6	60.5 ± 6	83.4
Sig (total)	482	924	1016	778 ± 78	789 ± 118	792 ± 79	798 ± 79	1100
Adopted				778 ± 78	789 ± 118	792 ± 79	798 ± 79	

1.5 (n,2n) Reaction Cross Section

The experimental data of (n,2n) reaction cross section for Fe around 14 MeV by using various methods have been collected as far as possible[14~19]. The measurements of Refs. [16~ 18] are in agreement with each other. (see Table 3). As pointed out by Pavlik and Vonach [20], Frehaut et al.'s measurements are underestimated systematically by about 10%. Considering this point, and

Table 3 Measured Fe(n,2n) reaction cross section

	Fre80 [14]	Qai77 [15]	Ach77 [16]	Koz78 [17]	Sal72 [18]	Ash58 [19]
	Fe	^{56}Fe	Fe	Fe	Fe	Fe
E_n (MeV)	14.1	14.7	14.7	14.6	14.36	14.1
Sig (E_n)	385 ± 30	440 ± 40	485 ± 39	480 ± 50	460 ± 40	480 ± 40
Sig (14.1)	385	374	412	416	423	480
Adopted	423	374	412	416	423	407
^{56}Fe#	434 ± 30	374 ± 40	422 ± 40	426 ± 45	434 ± 37	417 ± 40

All values measured on Fe are corrected to ^{56}Fe supposing the (n,2n) cross sections for ^{54}Fe, ^{57}Fe and ^{58}Fe are 5., 1000., 1000. mb respectively.

through the comparisons of the measurements of Ashby et al. with other measured or evaluated ones as shown in Table 4, we may conclude that Ashby et al.'s measurements are overestimated by about 20% systematically.

Table 4 Comparisons of Ashby's measurements with others at 14.1 MeV

Ashby	Frehaut	Ryves	Zhou	Ashby / other
Mn 900			755	1.19
Co 870			720	1.21
Cu 740			609	1.21
Au 2520		2073		1.22
Pb 2650			2252	1.18
Ti 520	340			1.39
V 640	460			1.26
Fe 480	380			1.26
Cu 740	560			1.32
Zr 1250	910			1.37
Mo 1590	1100			1.31
Ta 2560	1910			1.34
W 2800	1920			1.33
Bi 2520	2014			1.25

After correcting the values to neutron energy of 14.1 MeV and 10% and 20% corrections to Frehaut et al.'s and Ashby et al.'s measurements respectively, all measurements are in agreement except Qaim's measurement (by activation method) which by about 10% lower than others. One may notice that around 14 MeV an overestimation of 2% of the neutron energy could cause 8% underestimation of the (n,2n) reaction cross section. Anyway, it is difficult to make sure that what caused this discrepancy, the data set shown in last row of Table 3 are all adopted in this evaluation.

1.6 Neutron Emission Cross Section

An evaluation of angle–energy–integrated neutron emission cross section for Fe at 14.1 MeV has been performed[1]. The evaluated value of 1610 mb for Fe is adopted for this evaluation. After correcting it, a value of 1653 mb for ^{56}Fe is obtained.

1.7 Charged Particle (p, α, d) Emission Data

A series of total (angle–energy–integrated) p–emission and α–emission cross sections have been reported by[21~24] from the measurements of emission spectra. And a series of total α–emission cross section measurements have been performed by Kneff et al. by using isotope–dilution gas mass spectrometer[25].

Intercomparison of these measurements, and comparisons of these measurements with those measured by activation method demonstrate that almost all Grimes′ measurements on p–emission cross sections are higher by about 10% systematically than others, as shown in Table 5. So in present evaluation for p–emission cross section, the Grimes′ measurement for ^{56}Fe is adopted after 10% reduction.

As shown in Table 6, Grimes′ results of α–emission cross section measurements coincide with comparable ones measured by activation method; and most of the Kneff′s measurements are about 10 percent higher than Grimes′ and Fisher′s measurements as well as other comparable ones measured by activation method. In the present evaluation for α–emission cross section, Grimes′, Fisher′s and Kneff′s (after 10% reduction) are adopted.

A more recent measurement from threshold to over 30 MeV on α–emission including spectrum and angular distribution is carried out using the spallation source at WNR / LAMPF and detector telescopes consisting of a low–pressure gas proportional counter and a large area silicon detector[26]. The result of this measurement at 14.1 MeV (42 ± 2 mb) also adopted in present work is in good agreement with Grimes et el.′s measurement and the evaluated value obtained in[1].

Only one measured value of (d–em) cross section is available[21]. This measurement is adopted in this evaluation as (n,d–em), also as (n,d) reaction cross section.

Table 5 Comparisons of measured results of measured and evaluated p–emission cross section and evaluated at 14.8 MeV

	Grimes et al.	Zhou et al. or others				Grimes / others
	(p–em)	(n,p)	(n,np)	(n,2p)	(p–em)	
^{48}Ti	85	62	16.8		78.8	1.16
^{50}Cr	830	294	291	5	590	1.40
^{54}Fe	900	280	362	17	659	1.36
^{58}Ni	1002	937	937	20	957	1.05
^{60}Ni	325	142	79		221	1.47
^{63}Cu	320	125	150		275	1.16
^{65}Cu	44	20	22		44	1.00
^{92}Mo	967	37	744		781	1.24
^{96}Mo	64	24	6		30	1.78

Table 6 Comparisons of measured results of α–emission cross section

	Kneff et al.	Grimes et al.	Fishers et al.	Eval. or meas. by other meth.	
				(n,α)	(n,nα)
^{51}V	18.5 ± 1.1 #	17 ± 0.2 #		17.0 ± 0.2	0.07 ± 0.01 #
^{27}Al	143 ± 7 #	121 ± 25 #		115.5 ± 1.2	– #
^{59}Co	40 ± 3 #		33 ± 1.7 *	31 ± 1 #	
Mg	28 ± 2 #		24.4 ± 1.3 *		
			(23.4 ± 1.5 #)		
^{56}Fe	46 ± 3 #	41 ± 7 #	44 ± 3 *		
	(45.3 ± 3 *)	(40.4 ± 2 *)			

E_n = 14.8 MeV, * E_n = 14.1 MeV

1.7 Partial Cross Sections Relevant to Charged Particle Emission

As a standard, $^{56}Fe(n,p)$ cross section has been well measured and evaluated and an evaluated value of 114.5 mb at 14.1 MeV is adopted for this work. Incorporating with evaluated p–em and α–em cross sections and the shapes of the excitation function of (n,p), (n,np), (n,α) and (n,nα) reactions, the rest of the partial cross sections relevant to charged particle emission are determined for this evaluation.

1.8 (n,γ) Reaction Cross Section

For the minor reaction cross section $\sigma(\gamma)$, a select evaluation (calculation) of 0.74 mb at 14.1 MeV is used in the present evaluation.

1.9 Uncertainties of the Adopted Data

Generally, the uncertainties reported by the authors are quoted. For some measured cross sections, such as (n,2n) cross sections by Frehaut et al. and Ashby et al., p–emission cross section by Grimes et al., α–emission cross section by Kneff et al., which have been modified to more reliable values in the present evaluation, so their uncertainties have been reduced properly.

2 Simultaneous Evaluation of All Measurable Cross Sections

Based on the analyses and evaluations on the measured cross section for all (totalled 15) reactions, i. e., (n,n), (n,n′), (n,2n), (n,nα), (n,np), (n,γ), (n,p), (n,d)

((n,d−em) in the present case), (n,α), as well as (n,total), (n,non), (n,n−em), (n,p−em), (n,α−em) and (n,d−em) individually (i. e., independently as far as possible), a simultaneous evaluation is carried out by using a least squares code LSCC with the constraints :

$$\sigma(\mathrm{total}) = \sigma(\mathrm{n}) + \sigma(\mathrm{n}') + \sigma(2\mathrm{n}) + \sigma(\mathrm{n}\alpha) + \sigma(\mathrm{np}) + \sigma(\gamma) + \sigma(\mathrm{p}) + \sigma(\mathrm{d}) + \sigma(\alpha) + \cdots$$

$$\sigma(\mathrm{non}) = \sigma(\mathrm{n}') + \sigma(2\mathrm{n}) + \sigma(\mathrm{n}\alpha) + \sigma(\mathrm{np}) + \sigma(\gamma) + \sigma(\mathrm{p}) + \sigma(\mathrm{d}) + \sigma(\alpha) + \cdots$$

$$\sigma(\mathrm{n{-}em}) = \sigma(\mathrm{n}') + 2 \times \sigma(2\mathrm{n}) + \sigma(\mathrm{n}\alpha) + \sigma(\mathrm{np})$$

$$\sigma(\mathrm{p{-}em}) = \sigma(\mathrm{p}) + \sigma(\mathrm{np})$$

$$\sigma(\alpha\mathrm{{-}em}) = \sigma(\alpha) + \sigma(\mathrm{n}\alpha)$$

$$\sigma(\mathrm{d{-}em}) = \sigma(\mathrm{d})$$

All measured cross sections and their uncertainties of 15 (for ^{56}Fe, actually 14) reactions adopted for this evaluation are used as input data set : measurement vector Y^* and its covariance V_y^*. It is supposed that all measured cross sections are independently (uncorrelated), except p−emission and α−emission relevant cross sections σ(p), σ(np) and $\sigma(\alpha)$, $\sigma(\mathrm{n}\alpha)$, they are deduced from the measured emission cross sections so the σ(p) and $\sigma(\alpha)$ are correlated with σ(np) and $\sigma(\mathrm{n}\alpha)$ respectively, and four total inelastic scattering measurements are correlated via the common correction factor 1.05[6].

The output of LSCC consists of the evaluated values of all reaction cross sections mentioned above and their covariances, as showing in Table 7. The comparisons of the evaluated values with the corresponding measurements as well as the evaluations for various libraries are shown in Fig. 1 and Table 8. From Fig. 1 we can see that all evaluated values are consistent with all measured data in quoted error.

Table 7 Results of simultaneous evaluation

total and partial cross sections (mb)

total	elast.	incl.	n,2n	n,nα	n,np	n,γ	n,p	n,d	n,α
2561	1158	779.7	418.6	1.448	40.34	0.740	114.5	7.965	40.04

Covariance

1.7E+02	8.7E+01	7.0E+01	6.3E+00	7.3E−03	1.1E+00	1.1E−03	1.5E−01	4.0E−01	5.5E−02
8.7E+01	2.7E+02	−1.7E+02	−1.5E+01	−1.8E−02	−2.7E+00	−2.7E−03	−3.7E−01	−9.5E−01	−1.3E−01
7.0E+01	−1.7E+02	4.5E+02	−1.8E+02	−2.4E−01	−2.3E+01	−1.6E−02	−1.8E+00	−5.8E+00	−7.3E−01
6.3E+00	−1.5E+01	−1.8E+02	2.1E+02	−4.4E−02	−3.1E+00	−1.5E−03	−7.4E−02	−5.3E−01	−5.4E−02
7.3E−03	−1.8E−02	−2.4E−01	−4.4E−02	6.9E−01	−4.1E−03	−1.7E−06	−4.9E−05	−6.1E−04	−3.8E−01
1.1E+00	−2.7E+00	−2.3E+01	−3.1E+00	−4.1E−03	3.2E+01	−2.6E−04	−5.7E+00	−9.4E−02	−1.2E−02
1.1E−03	−2.7E−03	−1.6E−02	−1.5E−03	−1.7E−06	−2.6E−04	2.2E−02	−3.6E−05	−9.3E−05	−1.3E−05
1.5E−01	−3.7E−01	−1.8E+00	−7.4E−02	−4.9E−05	−5.7E+00	−3.6E−05	5.0E+00	−1.3E−02	−1.9E−03
4.0E−01	−9.5E−01	−5.8E+00	−5.3E−01	−6.1E−04	−9.4E−02	−9.3E−05	−1.3E−02	7.8E+00	−4.6E−03
5.5E−02	−1.3E−01	−7.3E−01	−5.4E−02	−3.8E−01	−1.2E−02	−1.3E−05	−1.9E−03	−4.6E−03	1.4E+00

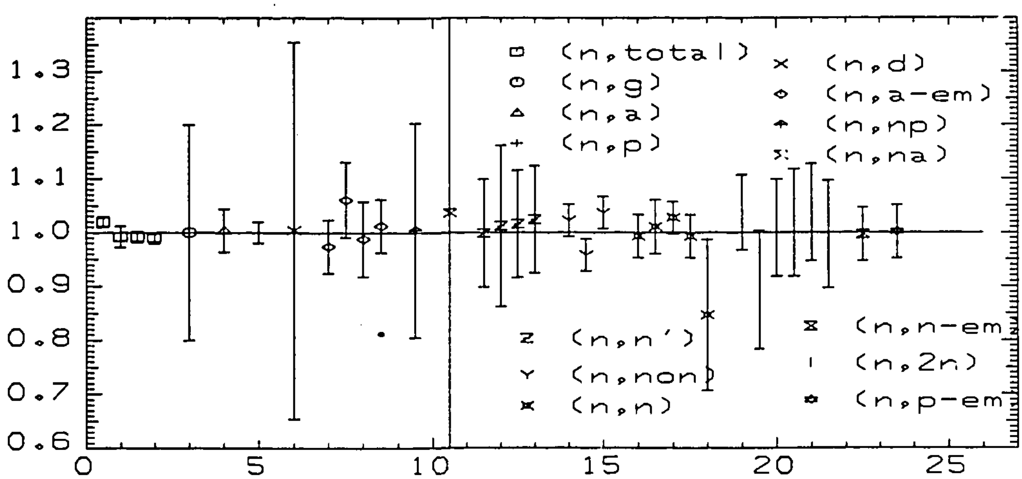

Fig 1. Comparisons of evaluated values with measureed data

Fig. 1 Comparisons of evaluated values with measured data

Table 8 Comparisons of this evaluations with the evaluations for various libraries[27]

MT	This work		CENDL-2	JEF-2.2	ENDF/B-6	JENDL-3.2	BROND-2
	14.1	14.0	14.0	14.0	14.0	14.0	14.0
3 1	2561.	2573.	2550.	2570.	2596.	2574.	2590.
3 2	1158.	1167.	1157.	1192.	1205.	1137.	1266.
3 3	1403.	1405.	1400.		1391.	1427.	
3 4	779.7	798.9	773.8	688.0	774.4	769.3	692.1
3 16	418.6	405.3	416.2	414.4	402.0	439.1	419.0
3 22	1.448	1.324	.8186		1.297	0.840	
3 28	40.34	37.53	38.49		46.71	70.94	
3102	.7399	.7279	.7300	.2138	.7300	.0995	.8100
3103	114.5	116.8	115.2	118.8	115.1	114.0	114.0
3104	7.965	7.694	7.436	.9235	6.300	–	
3107	40.04	40.09	40.18	45.00	44.30	40.90	38.00
3201		1648.	1646.		1626.	1719.	
3203		154.3	153.7		161.8	184.9	
3207		41.41	41.00		45.60	41.74	

3 Discussion and Conclusion

One may notice that Perey et al.'s total cross section measurement at 14.1 MeV is higher by 2.8 ~ 3.0% (about 70 mb) than other three measurements which are in very good agreement with each other and consistent with Qaim's measurement of (n,2n) reaction cross section by activation method. One may also notice that all individual evaluations mentioned above favour Perey et al.'s measurement at least the results near 14.1 MeV. Before the solving an / or explaining of the discrepancies existed in total and other reaction cross section measurements, a simultaneous evaluation just like this work should be the most reasonable way to compromise and optimize the evaluated data set based on wide–spread available experimental information.

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