International Atomic Energy Agency

INDC(CCP)-203/L

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

COMPARATIVE ANALYSIS OF THE NEUTRON CROSS-SECTIONS OF IRON
FROM VARIOUS EVALUATED DATA LIBRARIES

V.M. Bychkov, V.V. Vozyakov, V.N. Manokhin, F. Smoll
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English translation from a paper in

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August 1983

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

Printed by the International Atomic Energy Agency
Vienna, Austria, September 1983
83-05086

INDC(CCP)-203
Distribution: L

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Abstract

COMPERATIVE ANALYSIS OF NEUTRON CROSS-SECTION OF IRON FROM EVALUATED NUCLEAR DATA LIBRARIES. The comperative analysis of neutron cross-sections of iron from evaluated nuclear data libraries SOKRATOR, KEDAK, ENDL is done in energy interval from 0.025 eV to 20 MeV. Some of iron cross-sections from SOKRATOR library are revised and new data, which are obtained by using new experimental data are more comprehensive theoretical methods, are recommended. As a result the new version of the iron neutron cross-section file (BNF-2012) is produced for SOKRATOR library.

L83-20254
Translated from Russian

UDC 539.171: 539.172.4

COMPARATIVE ANALYSIS OF THE NEUTRON CROSS-SECTIONS OF IRON FROM VARIOUS EVALUATED DATA LIBRARIES

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The evaluated neutron data library SOKRATOR was set up in the Institute of Physics and Power Engineering to supply nuclear constants for work in the design and safety of fast reactors and for other practical applications in nuclear physics [1]. In addition to this library, the Nuclear Data Centre of the USSR State Committee on the Utilization of Atomic Energy (GKAE) has a number of foreign evaluated data libraries. Since these libraries are now widely used, it is important to have a qualitative description of them.

This paper contains a comparative analysis of the neutron cross-sections of one of the most important structural elements of a nuclear reactor - iron - from the evaluations of the SOKRATOR library and two foreign libraries - KEDAK [2] and ENDL [3]. The most recent versions of these libraries were used in the analysis; the iron cross-sections for the SOKRATOR library were evaluated by the Nuclear Data Centre in 1975, a description of the file being contained in Refs [4,5].

Apart from comparing microscopic neutron cross-sections and analysing discrepancies between data from the different libraries, the paper revises a number of cross-sections from the SOKRATOR library and recommends new curves plotted on the basis of the latest experimental data or improved methods of theoretical calculation. All changes and additions to the file are recorded in this paper. A new version of the iron file has thus been obtained which replaces the preceding one and is entered in the SOKRATOR library under the old number (BNF-2012).

A comparison of neutron cross-sections was performed for the following energy ranges: the thermal point and the experimentally resolved resonance region of the compound nucleus, the unresolved resonance region and the region of continuum of excited nuclear states. Where necessary, the results of the latest experimental work were used in the analysis of discrepancies between the data from different libraries.

Total cross-section

The total cross-section in the KEDAK and ENDL libraries was evaluated from experimental data on the detailed behaviour of the cross-section, the recommended curve being drawn through the experimental points by hand. The KEDAK library also gives a recommended set of resonance parameters although there is no link between these parameters and the total cross-section curve.

The SOKRATOR library evaluation from the thermal neutron energy region up to 200 keV was carried out using R matrix theory calculations and taking into account inter-resonance interference. The evaluation method and the formalism used for the calculation are described in Refs [5,6]. The evaluation took into account both information on resonance parameters and experimental data on the detailed behaviour of the cross-section. In the region of interference minima, the cross-section was corrected with allowance for the results of transmission measurements made on thick samples. The contribution of the isotopes ^{54}Fe(5.96%), ^{56}Fe(91.78%) and ^{57}Fe(2.28%) was included in the evaluation.

Figures 1a and b show a comparison of the total cross-section curves from the three libraries mentioned above in the experimentally resolved resonance region. Agreement between the data from the various libraries is on the whole satisfactory. The KEDAK and ENDL libraries are in better agreement since they were obtained by the same method. The biggest discrepancy between the evaluations is observed in the 5-8 keV energy range where the KEDAK library curve is significantly higher than the ENDL and SOKRATOR data, which virtually coincide in this region.

In the experimentally resolved resonance region, the SOKRATOR evaluation would seem to be the more reliable since the methodology it employs makes it possible to take into account various ways of presenting the experimental information. In the table, the s-resonance parameters of the isotope ^{56}Fe, which basically determine the total cross-section of natural iron, are compared with the parameters recommended in Ref. [7] (BNL-325) and the preliminary data of Gayther et al. [8].

As the table shows, the SOKRATOR evaluation is in satisfactory agreement with the latest experimental data. The present paper also considers the influence of ^{58}Fe isotope resonances (which were not included in the

SOKRATOR evaluation) on the total cross-section and the radiative capture cross-section of natural iron. The ^{58}Fe resonance parameters were taken from experimental papers [9,10]. The study has shown that the inclusion of the ^{58}Fe isotope resonances has practically no effect on the evaluation results. Its contribution is most appreciable in the region of total cross-section minima, but for that region the SOKRATOR evaluation took into account the results of special transmission measurements made on thick samples of natural iron [11,12].

In the unresolved resonance region, the total cross-section evaluations in each of the three libraries were based on experimental data on the detailed behaviour of the cross-section. In the SOKRATOR data, the resonance structure in the total cross-section is maintained down to an incident neutron energy of 3 MeV, and beyond that a smooth curve is recommended. At present, the resonance parameters for iron are reliably defined up to an energy of about 500 keV. In the energy region up to 3 MeV, the ENDL and SOKRATOR evaluations are in good agreement and show a more pronounced total cross-section resonance structure than the KEDAK evaluation. A comparison of the total cross-section evaluations in the 2-2.5 MeV range is given in Figure 1c. The average cross-sections from these libraries, smoothed over the resonance structures, agree in the region above 3 MeV to within 1.5-2% (Figs 2a,b).

It can be seen that the various total cross-section evaluations in the range of energies above the experimentally resolved resonance region are on the whole also in satisfactory agreement. In this paper, the total cross-section evaluation region in the SOKRATOR file is extended up to an incident neutron energy of 20 MeV; in doing so, we have used the experimental data available for that region and optical model calculations with the potential parameters recommended in Ref. [13].

Neutron radiative capture cross-section

In the SOKRATOR library, the capture cross-section in the range of energies from thermal to 30 keV was evaluated by resonance parameter calculations. The evaluation method is described in Ref. [5]. The KEDAK and ENDL evaluations were obtained on the basis of experimental work in which the detailed behaviour of the cross-section was measured. The data from the different laboratories in this range are compared in Figures 3a, b and c. As the comparison shows, there are considerable discrepancies between the various evaluations in the 0.1-30 keV range. The data from all three libraries tally in the 0.01 eV-100 eV range. The major discrepancy between the recommended curves at energies above 100 eV is that between the data from experimental papers [14,15] and the resonance parameter calculation. The resonances in the KEDAK evaluation at energies below 1 keV correspond to the data in Ref. [14], but are not included in the SOKRATOR or ENDL libraries since they were not confirmed by other measurements. The description of the first two resonances (1.15 and 1.63 keV) in the SOKRATOR and ENDL evaluations were generally in good agreement, while the resonance structure in this region is barely perceptible in the KEDAK file. At energies higher than 5 keV, the KEDAK and ENDL evaluations exceed the recommended curve of the SOKRATOR library by a substantial margin. As has already been noted, the reason for this is that the KEDAK and ENDL evaluations in this region are based on experimental data from Ref. [15], the results of which are much higher than the resonance parameter calculations. So far no explanation has been found for this discrepancy nor for the discrepancy between the data in Refs [14,15] in the energy range above 1 keV.

Figure 4 compares the neutron radiative capture cross-sections in the 30 keV-50 MeV range. All three evaluations virtually coincide in the 0.2-1 MeV energy range, which is a result of the satisfactory agreement of the different experimental data in this region. However, beyond this energy range the SOKRATOR curve diverges sharply from the KEDAK and ENDL data. The experimental data vary widely in the 30-200 keV energy range, and for this reason the SOKRATOR library evaluation was obtained from model calculations based on statistical theory using average resonance parameters: this yields an accuracy of about 30% for the recommended curve. The ENDL and KEDAK evaluations are higher than the SOKRATOR data in the 30-100 keV range, but lower in the 100-200 keV range.

On this account there is need to consider new experimental data on the capture cross-section. Ref. [8] gives preliminary capture cross-section measurement results over a wide range of neutron energies - from a few eV up to 800 keV. The accuracy of the data averaged over the energy ranges is about 20%. These data tally well with the SOKRATOR library evaluation in the 1-10 and 100-800 keV energy ranges. In the 10-20 keV range, where a low minimum is observed between the strong s-resonances of the ^{54}Fe and ^{56}Fe isotopes in the capture cross-section (from the SOKRATOR library), the recommended curve has to be raised by 5 mb in order to fit the data in Ref. [8]. In this energy region, the experiment in Ref. [8] is closer to the KEDAK and ENDL evaluations. In the 30–100 keV region, the data in Ref. [8] lie between the SOKRATOR evaluation (about 20% lower) and the KEDAK and ENDL evaluations (about 30% higher). The discrepancies between the SOKRATOR evaluation and the data in Ref. [8] in this region do not exceed the experimental error and are within the accuracy limits of the evaluated curve (30%).

For energies above 1 MeV, where no experimental capture cross-section data are available, the difference between the curves recommended by the libraries under consideration is due to the difference in the calculation parameters and models used in the evaluations. The method of calculating the capture cross-section recommended by the SOKRATOR library is described in Ref. [4]. That paper takes into account direct and semi-direct neutron capture mechanisms which determine the increase in the cross-section at energies above 10 MeV, and this is also reflected in the curve recommended by the KEDAK library.

Neutron elastic scattering cross-section

The integral cross-section for neutron elastic scattering in all libraries was obtained as the difference between the total cross-section and the cross-section of all non-elastic processes: $\sigma_{el} = \sigma_t - \sigma_{non}$. Accordingly, the elastic scattering cross-section at an incident neutron energy lower than the non-elastic scattering threshold for iron ($E \lesssim 1$ MeV) is virtually identical with the total cross-section (the capture cross-section is small). A comparison of elastic scattering cross-sections from SOKRATOR, ENDL and KEDAK data in the initial neutron energy region of 5-15 MeV is given in Fig. 5. The resonance structure of the cross-section is not indicated in the curve recommended by the SOKRATOR library, while the cross-sections from the other two libraries undergo oscillation up to energies of about 8-10 MeV. The Figure also shows smooth curves from these libraries which were obtained by averaging the cross-section over the 1 MeV range. The biggest discrepancy between the KEDAK and ENDL averaged curves is 7-8% and is due to an uncertainty in the σ_t cross-section (2%) and in the σ_{non} cross-section (about 10%). The recommended curve of the SOKRATOR library lies between the evaluations of the other two libraries. In the new version of the SOKRATOR library, the range in which the elastic scattering cross-section is determined has been increased to 20 MeV. When working out the recommended curve, optical model calculations with the parameters from Ref. [13] were used.

Angular distributions of elastically scattered neutrons

Angular distributions are treated in different ways in the libraries under consideration. The SOKRATOR file gives factors for the expansion of the angular distributions in Legendre polynomials, while the KEDAK and ENDL libraries give a pointwise presentation of the differential cross-sections as a function of the neutron emission angle. In order to compare the data from the different libraries, the angular distributions in the KEDAK and ENDL libraries were expanded in Legendre polynomials $[P_\ell\ (\cos\ )]$. The expansion was carried out in the equation $\sigma(\theta) = \sum_{\ell=0} B_\ell P_\ell(\cos\ \theta)$mb/sr. A comparison of the energy dependence of the first three expansion factors from the libraries under consideration and the evaluation by Bazazyants [16] is given in Figs 6a, b and c.

The best agreement is found between the evaluated data of the SOKRATOR file and Ref. [16]. The largest discrepancies are between the ENDL library data and the other evaluations at energies below 7 MeV. In the energy range above 7 MeV, the results of the various evaluations become closer: this seems to be due to the use in all the evaluations in this energy range of optical model calculations because no experimental data are available in the 7-14 MeV range. A study of these curves carried out by the Technical University in Dresden using optical model calculations and the results of the latest experimental work [17,18] shows that the best agreement is with the curve recommended by the SOKRATOR library.

In the new version of the SOKRATOR library, angular distributions have been evaluated up to an energy of 20 MeV using optical model calculations with parameters taken from Ref. [13]. In addition, at energies above 10 MeV, a pointwise presentation of angular distributions was used since at high energies the polynomial representation requires a much greater number of expansion terms and is unreliable.

Excitation function of levels for neutron non-elastic scattering

The SOKRATOR and KEDAK files give excitation functions for the first few levels of the isotopes ^{54}Fe and ^{56}Fe, while the ENDL file provides only the excitation function of the first level of the ^{56}Fe nucleus. The SOKRATOR evaluation was performed using a statistical prediction and the coupled channel method. Experimental data only were employed in the KEDAK evaluation. The first level excitation functions from the libraries being examined are given in Fig. 7a. The data from the KEDAK and SOKRATOR libraries are on the whole in satisfactory agreement, although the KEDAK evaluation has a more pronounced resonance structure. The ENDL data recommend a smooth curve which lies on average 20% above the data of the other two libraries. Figure 7 also displays the new version of the SOKRATOR library which includes data from the latest experiments [19,20]. A comparison of the excitation functions of the second level E2 = 1.408 MeV (isotope ^{54}Fe) is given in Fig. 7b. Relatively good agreement between the KEDAK and SOKRATOR data is observed only up to an energy of 3 MeV, beyond which the KEDAK evaluation is approximately double that of the SOKRATOR library. The experimental data from Ref. [21] shown in Fig. 7b support the SOKRATOR evaluation.

The excitation functions of the third (2.08 MeV) and fourth (2.655 MeV) levels are shown in Figs 7c and d. Here again a discrepancy is observed between the KEDAK and SOKRATOR data at large energies [E > 4 MeV]. This discrepancy increases at higher levels. Theoretical calculations performed independently at the Institute of Physics and Power Engineering and the Technical University in Dresden confirm the SOKRATOR evaluation.

Non-elastically scattered neutron spectra

In the SOKRATOR and ENDL libraries, neutron emission spectra are presented in the form of points as a function of the energy of the escaping neutron. The KEDAK library gives nuclear temperature values for calculating energy spectra using Maxwell's equation. The new version of the SOKRATOR library recommends calculated spectra obtained on the basis of statistical theory with allowance for pre-equilibrium emission. The emission spectra include the contributions of the (n,pn), (n,np), (n,n') and (n,2n) reactions.

Angular distributions of non-elastically scattered neutrons

The angular distributions of non-elastically scattered neutrons with excitation of the first two levels (0.845 and 1.408 MeV) are given only in the SOKRATOR library, in the form of coefficients for Legendre polynomials.

Total cross-section of neutron non-elastic scattering

A comparison of the evaluations of non-elastic scattering total cross-section is given in Fig. 8. Maximum deviation in the recommended data is about 10%. Changes in the cross-section recommended in the new version of the SOKRATOR library are the result of changes in the excitation functions of the first two levels (see Figs 7a,b) and in the cross-section of the (n,2n) reaction (see Fig. 11). Best agreement is found between the SOKRATOR and ENDL data.

Cross-section of the (n,p) reaction

The excitation functions of the (n,p) reaction from the libraries under consideration are shown in Fig. 9. A major contribution to the cross-section of this reaction for a natural mixture of iron isotopes is made by the isotopes ^{56}Fe and ^{54}Fe for which this reaction has been thoroughly studied in experiments. It is for this reason that the recommended cross-sections from the different libraries virtually coincide. In the new version of the SOKRATOR library, which is shown in Fig. 9, the incident neutron energy range is increased to 20 MeV. In addition, the cross-section near the reaction threshold is re-evaluated and the previous value reduced somewhat as a result.

Cross-section of the (n,α) reaction

Figure 10 gives data from the SOKRATOR libraries (old and new versions) as well as the KEDAK, ENDL and SAND-2 [22] libraries. The considerable deviation among them is explained by the lack of experimental data for the ^{56}Fe (n,α) reaction which makes a major contribution to the cross-section for a natural mixture of isotopes. Consequently, all available evaluations were performed using calculations.

The old SOKRATOR evaluation was obtained on the basis of statistical theory using α-particle penetration factors calculated in a quasi-classical approximation. In this approximation the penetration factors proved to be too high in the energy range below the coulomb barrier of the nucleus with the result that the (n,α) reaction cross-section near the threshold was overestimated. In the new version, the evaluation uses α-particle penetration factors calculated by the optical method; furthermore, measurement results at 14.7 MeV [23] were included.

Thus, the new version of the SOKRATOR library and the KEDAK and SAND-2 evaluations are in satisfactory agreement over the range from the reaction threshold up to an energy of 10 MeV. Above this energy the SAND-2 curve is lower and the KEDAK curve much higher than the SOKRATOR data. The ENDL evaluation is much lower than the data from the other libraries over the whole energy range.

(n,2n) reaction cross-section

The recommended cross-sections from the various libraries and the experimental data [24] are presented in Figure 11. As can be seen from the Figure, the old version of the SOKRATOR library and the KEDAK and ENDL evaluations are in satisfactory agreement in the energy range from threshold to 14 MeV. However, at the time when these evaluations were performed there were no direct measurements of the excitation functions of the (n,2n) reaction. The SOKRATOR evaluation, in particular, was based on indirect data obtained by deducing the calculated spectrum of the first neutron from experimental neutron emission spectra [4]. In the new version of the SOKRATOR library, the (n,2n) reaction excitation function was obtained on the basis of statistical theory and the pre-equilibrium emission model. The experimental results in Refs [24,25] were also taken into account. The evaluation also included the contributions of the isotopes ^{57}Fe and ^{56}Fe.

The new version of the SOKRATOR library generally gives higher values for the (n,2n) reaction cross-section than earlier evaluations.

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Goel B., Krieg B. Report KFK-2234. Karlsruhe, 1975 (KEDAK-3).

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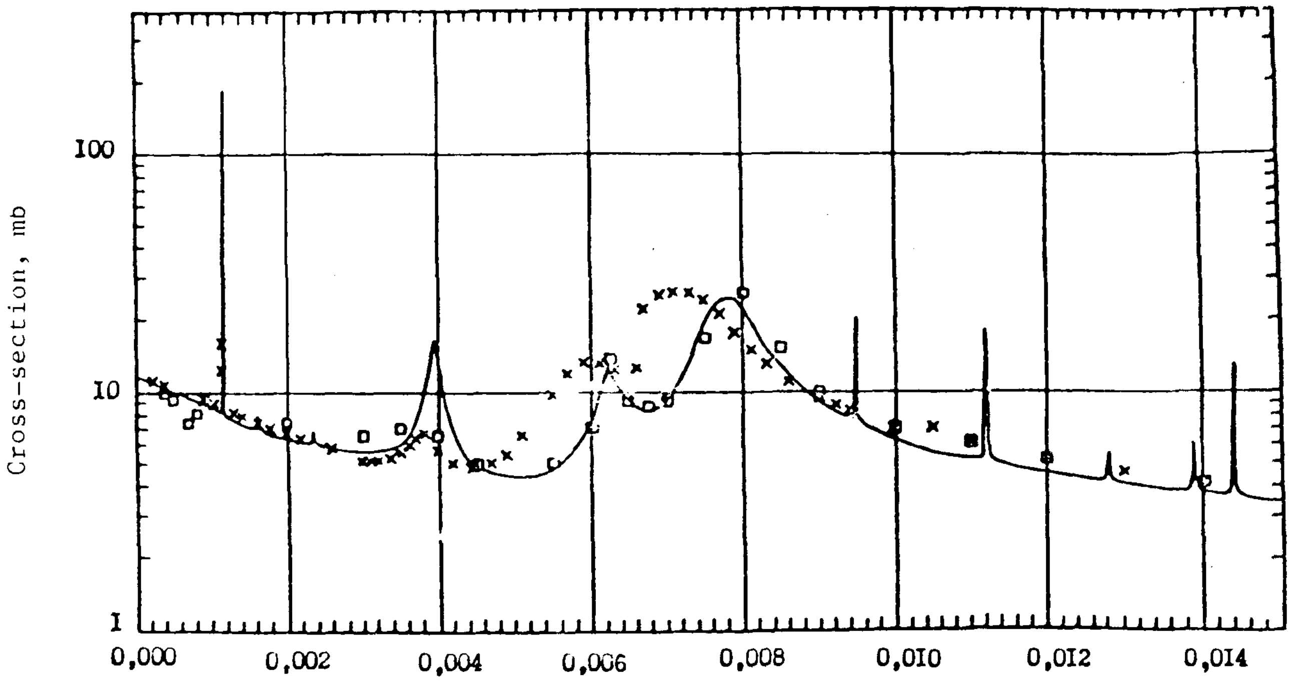
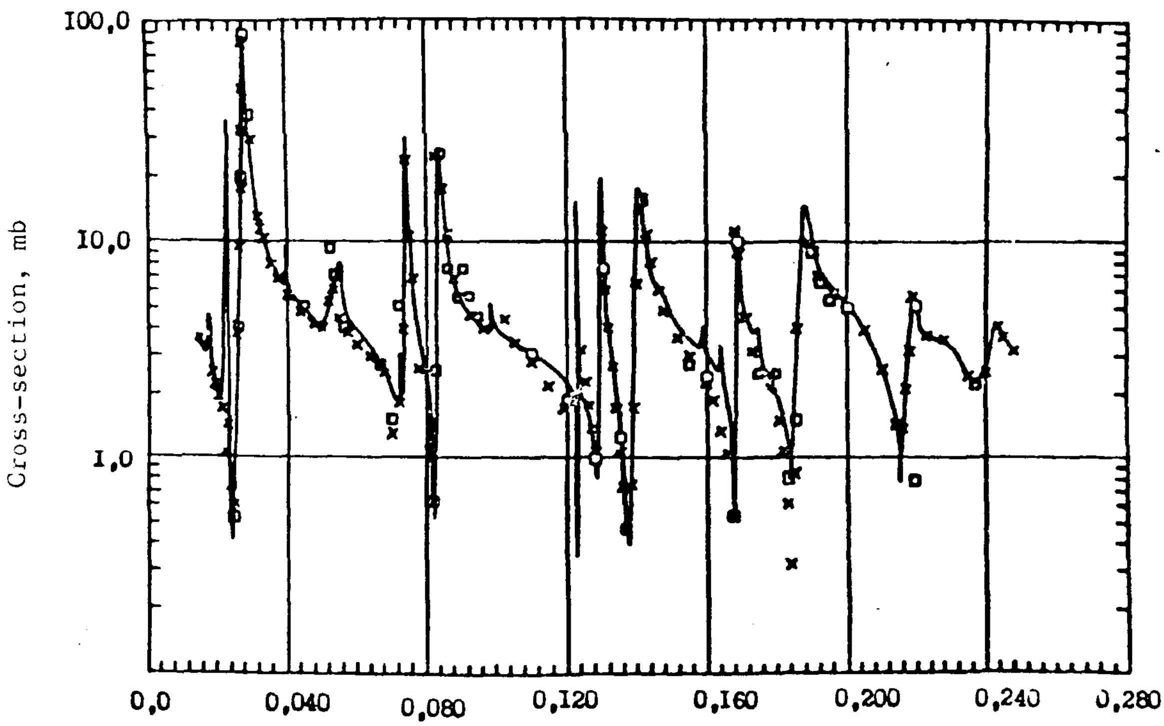


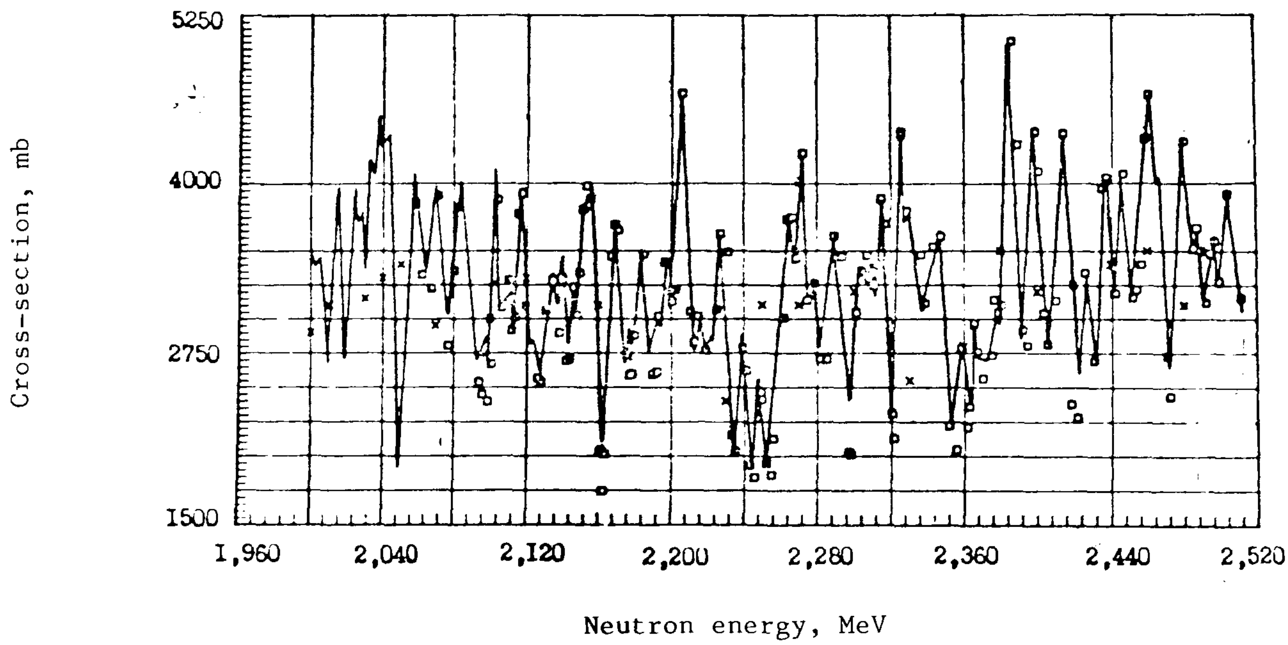
a



b

Fig. 1. Total cross-section in the energy range 1-15 keV (a), 15-250 keV (b), 2-2.5 MeV (c).

X-KEDAK; □ - ENDL; ——— - SOKRATOR

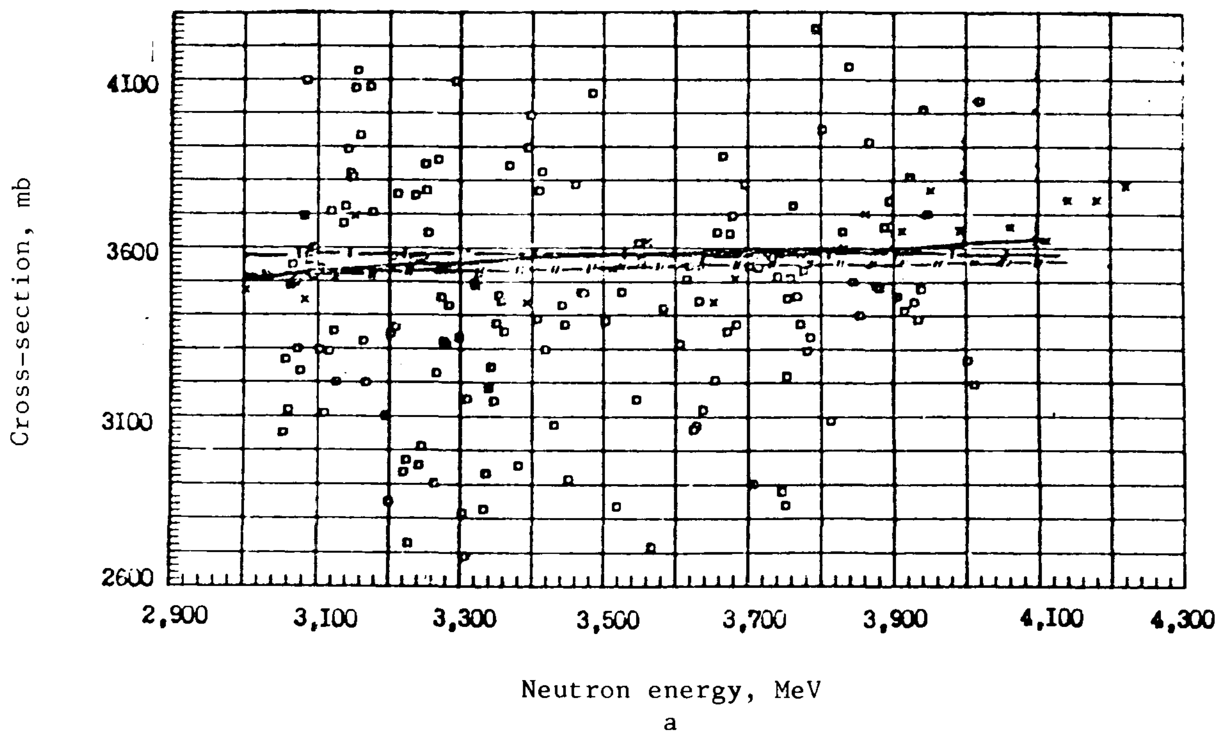


c

Fig. 1

Neutron s-resonance parameters of the ^{56}Fe nucleus

Resonance energy, keV			Neutron width, keV		
BNL-325	SOKRATOR	Ref. [8]	BNL-325	SOKRATOR	Ref. [8]
27,7±0,2	27,66	27,748	1,60±0,05	1,42	1,396
74 ±0,4	73,9	73,933	0,54±0,04	0,54	0,613
83,6±0,4	83,6	83,439	0,96±0,08	1,03	1,182
123,2±0,6	-	-	0,13±0,02	-	-
129,6±0,6	129,6	129,703	0,5 ±0,05	0,66	0,55
139,9±0,7	139,9	140,149	2,37±0,2	2,27	2,608
169,0±0,8	168,7	169,0	0,75±0,065	0,76	0,925
188,0±0,8	187,0	187,266	3,4 ±0,23	3,2	3,246
221 ± 1	222,8	220,268	1,4 ±0,1	1,57	1,211



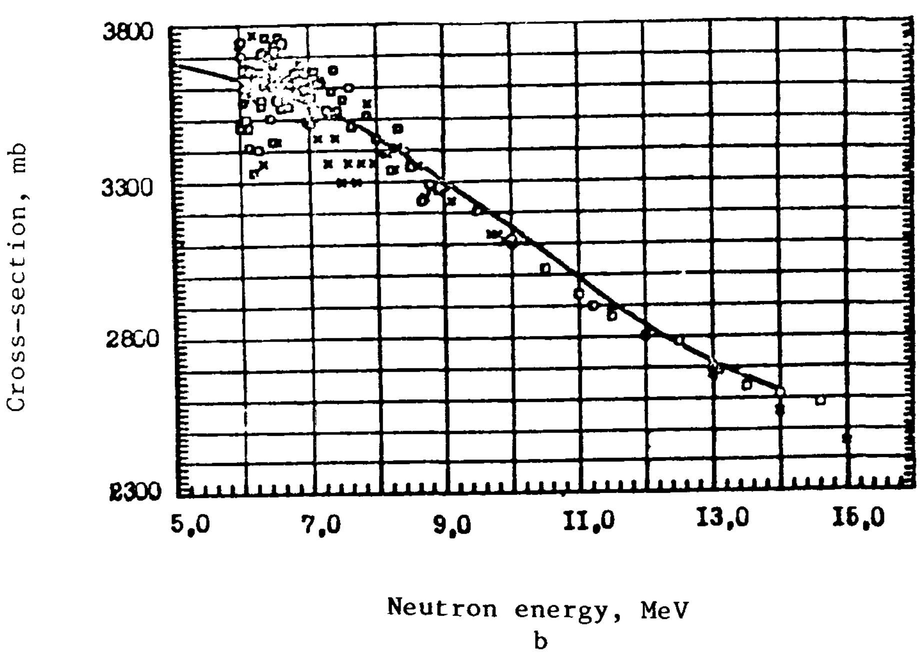
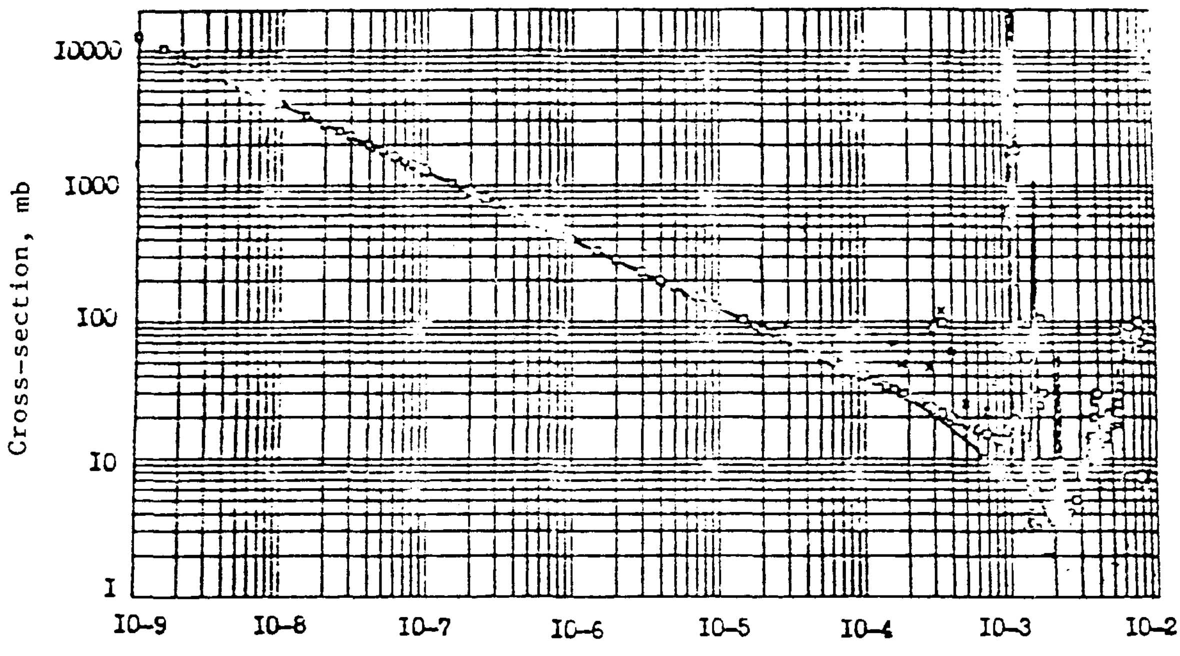
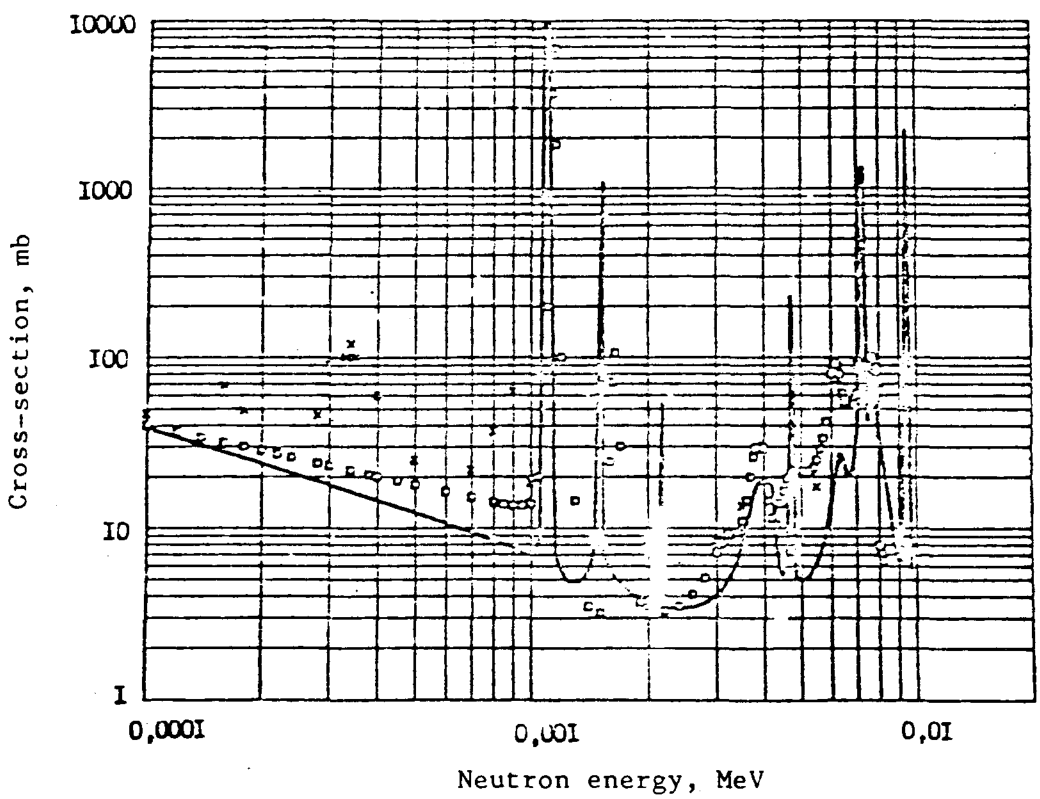


Fig. 2. Total cross-section in the energy range 3-4 MeV (a) and 5-15 MeV (b):
X - KEDAK (——/—— = averaged curve); □ - ENDL (——//—— = averaged curve);
—— = SOKRATOR

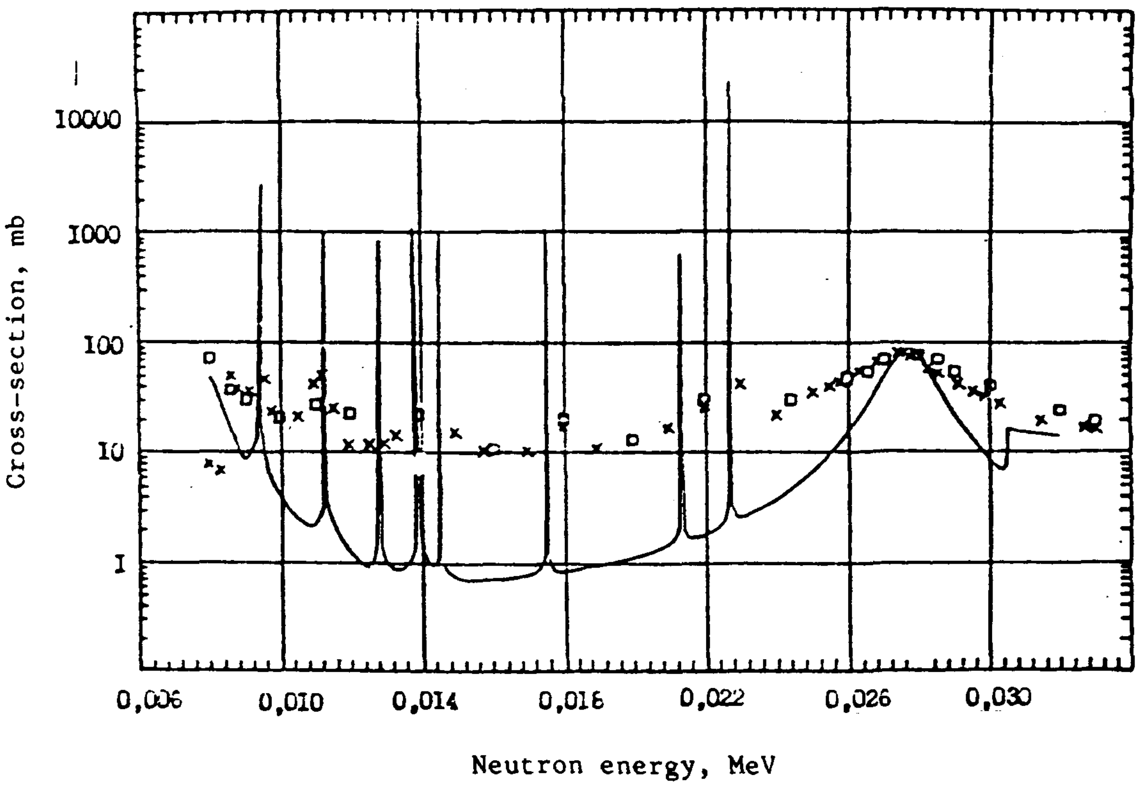


a



b

Fig. 3 Neutron radiative capture cross-section in the energy range 10^{-3}eV - 1 keV (a), 0.1-10 keV (b), 10-30 keV (c): X = KEDAK; □ = ENDL; ——— = SOKRATOR


Cross-section, mb
10000
1000
100
10
1
0,006
0,010
0,014
0,018
0,022
0,026
0,030
Neutron energy, MeV

c

Fig. 3

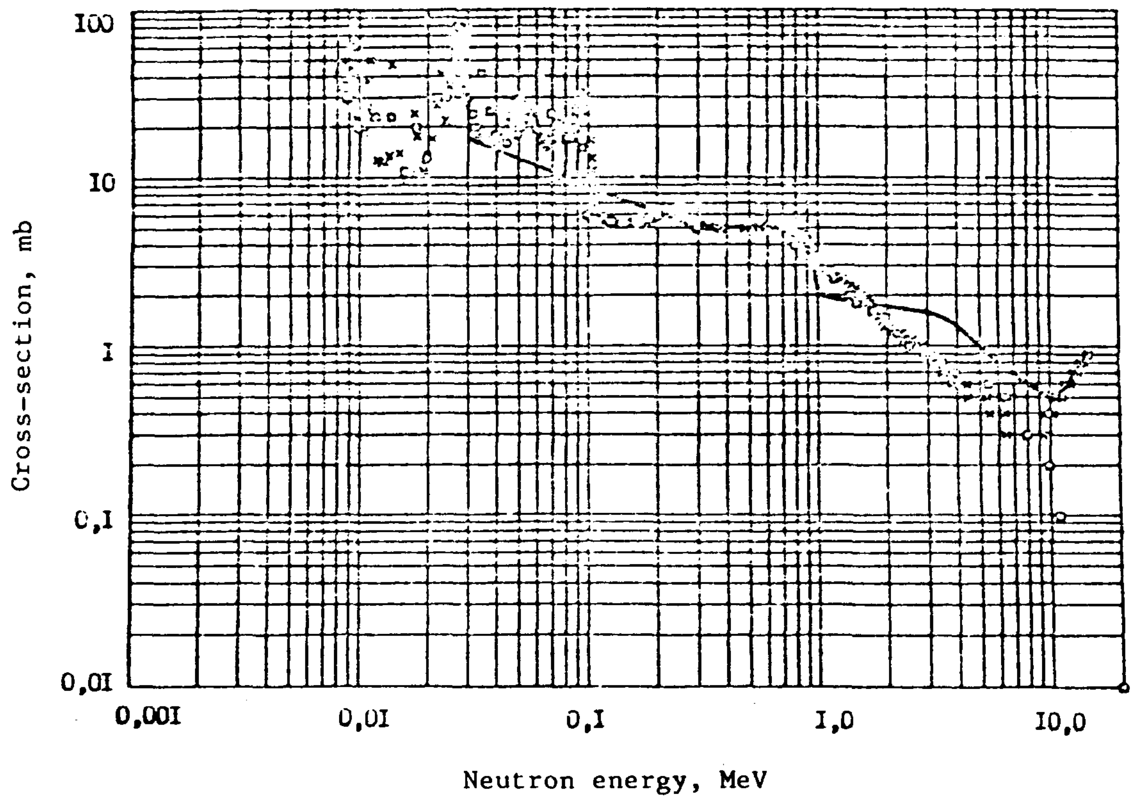


Fig. 4 Neutron radiative capture cross-section in the energy range 30 keV - 15 MeV:
X = KEDAK; ◻ = ENDL; ———— = SOKRATOR

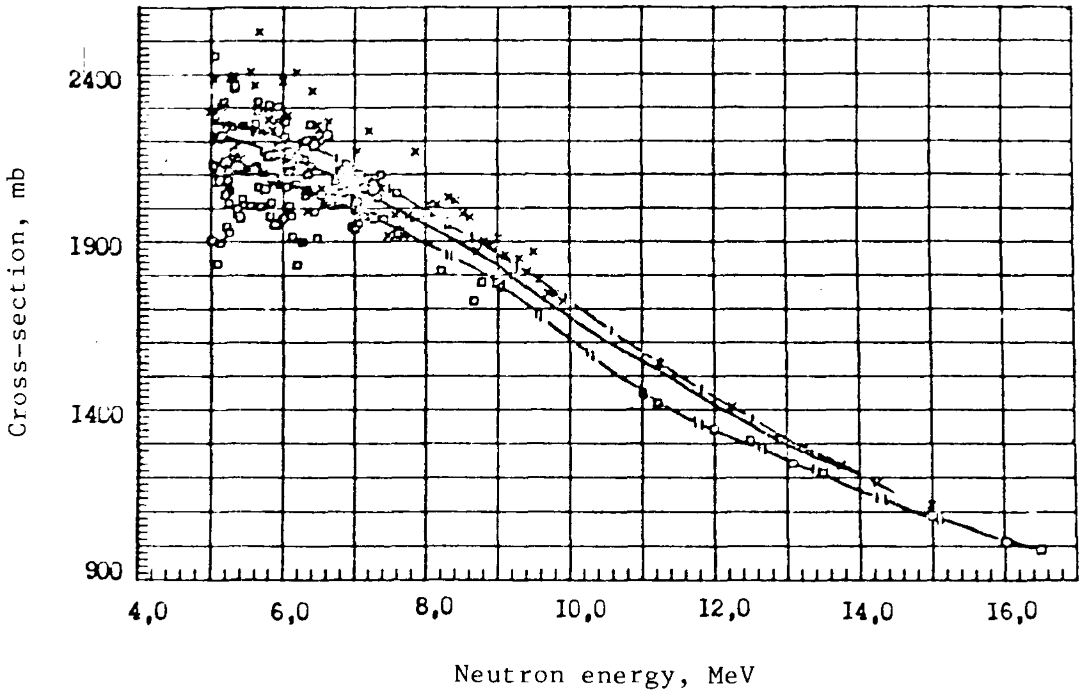
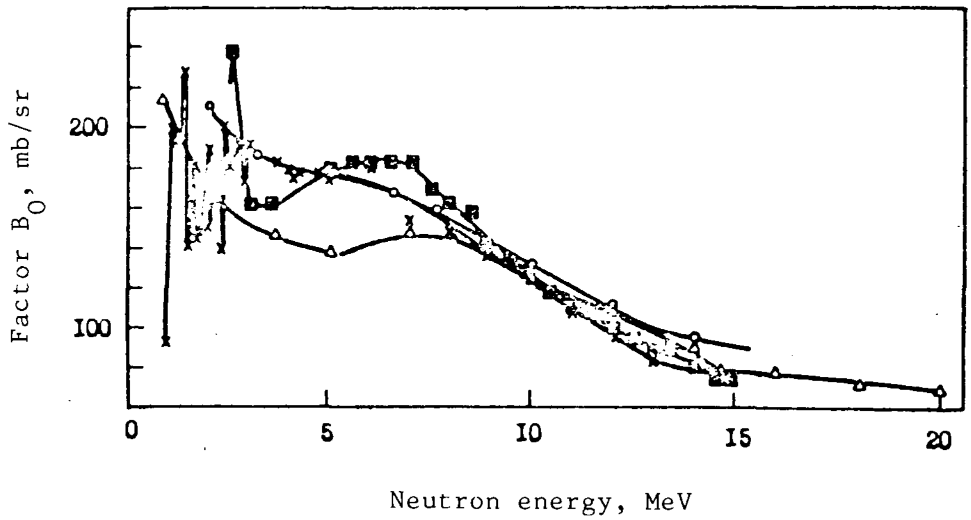
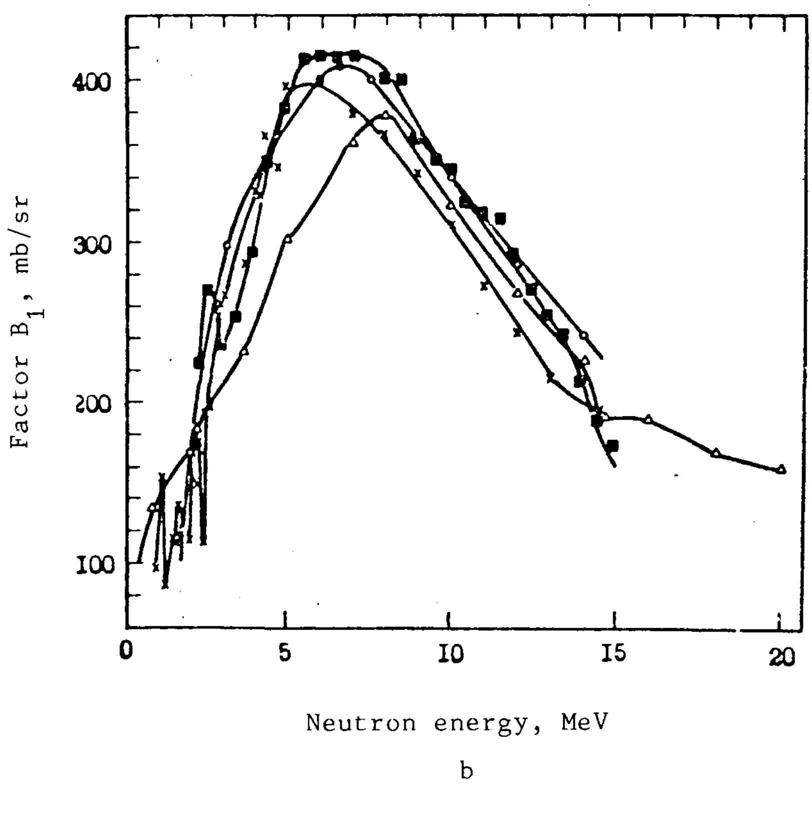


Fig. 5. Neutron elastic scattering cross-section in the 5-15 MeV energy range: x = KEDAK (——/—— = averaged curve); □ = ENDL (——//—— = averaged curve); —— = SOKRATOR

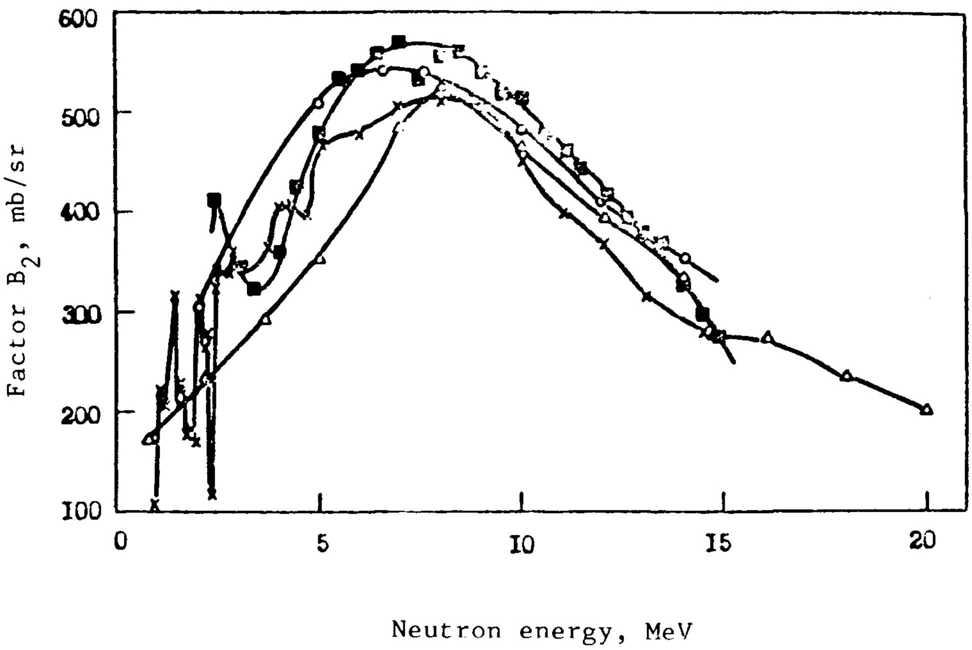


a



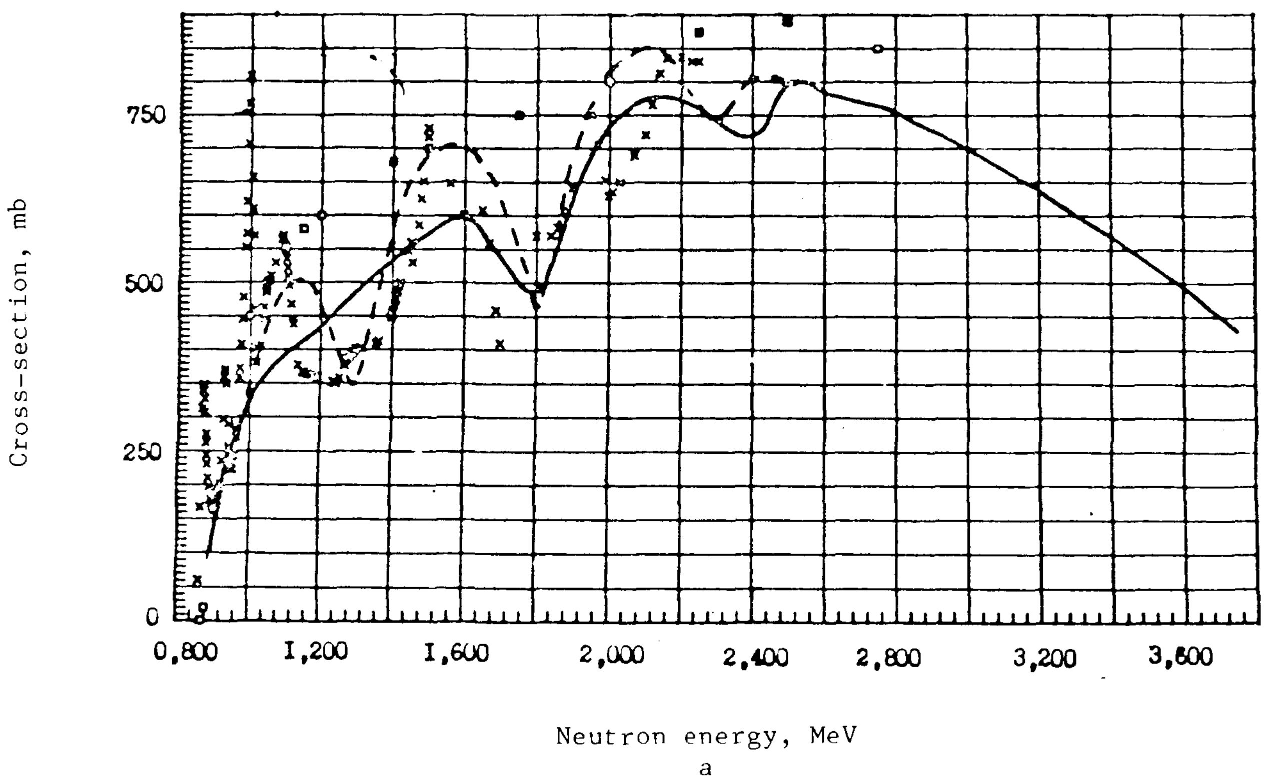
b

Fig. 6. Energy dependence of the factors B_0(a), B_1(b) and B_2(c) in the Legendre polynomial expansion of elastic scattering angular distributions: x = KEDAK; Δ = ENDL; O = SOKRATOR; ■ = Ref.[16]

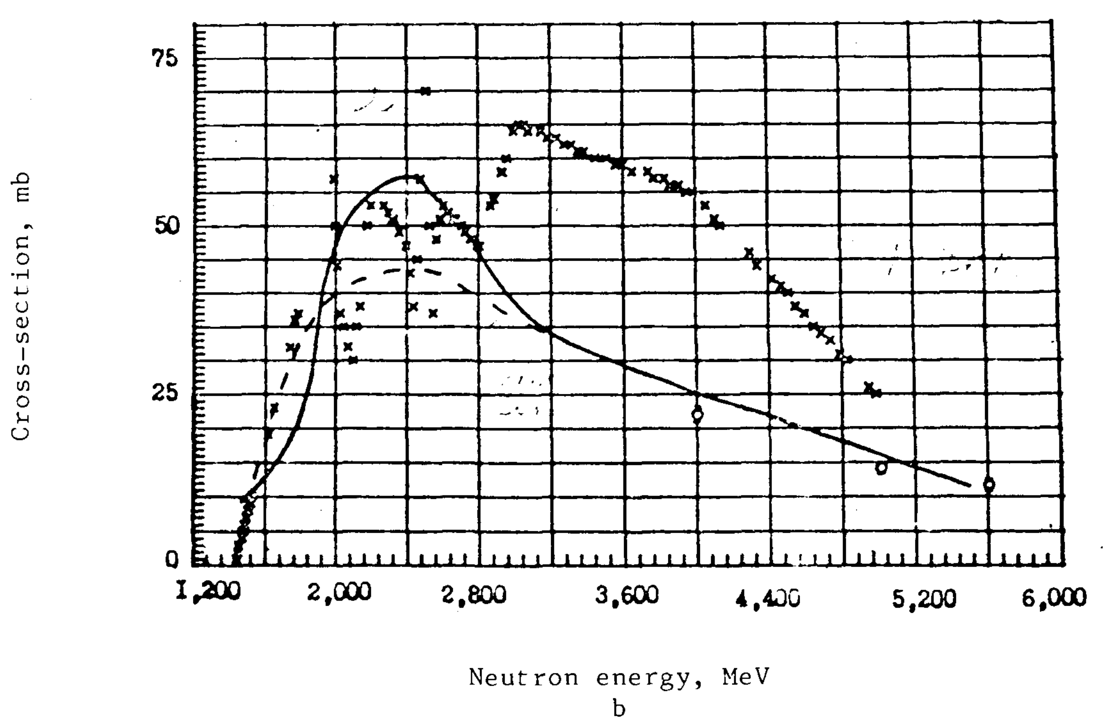

600
500
400
300
200
100
Factor B_2, mb/sr
0
5
10
15
20
Neutron energy, MeV

c

Fig. 6

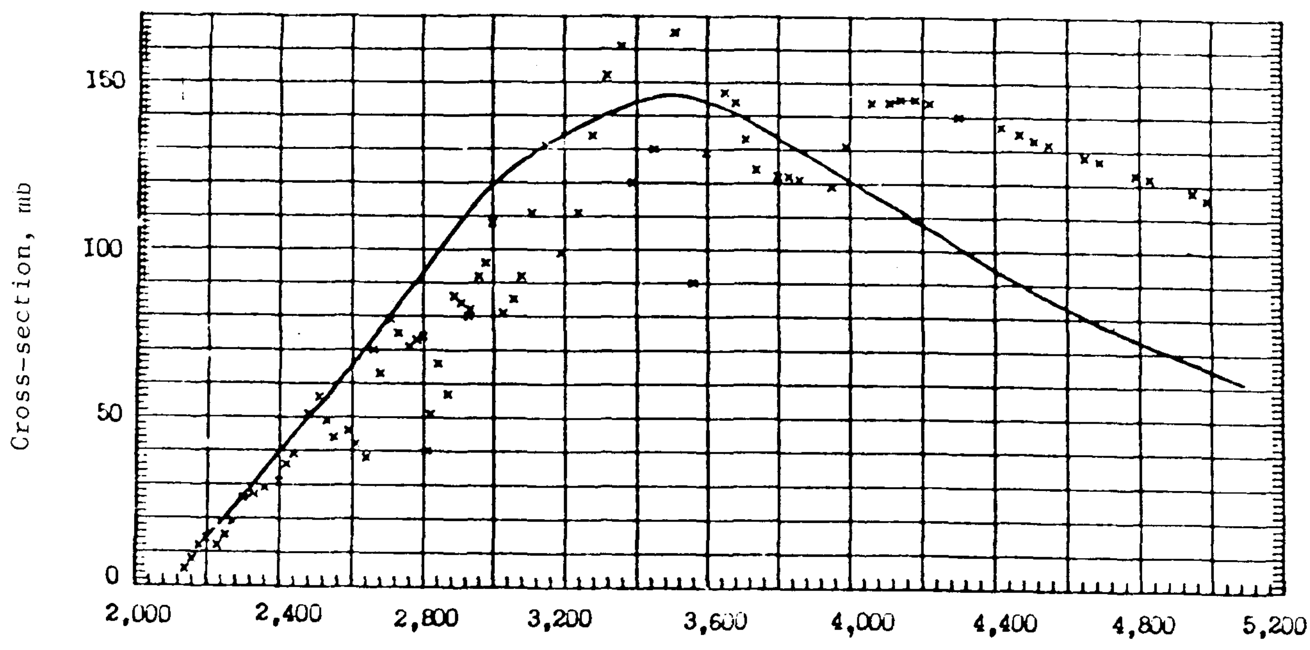


a

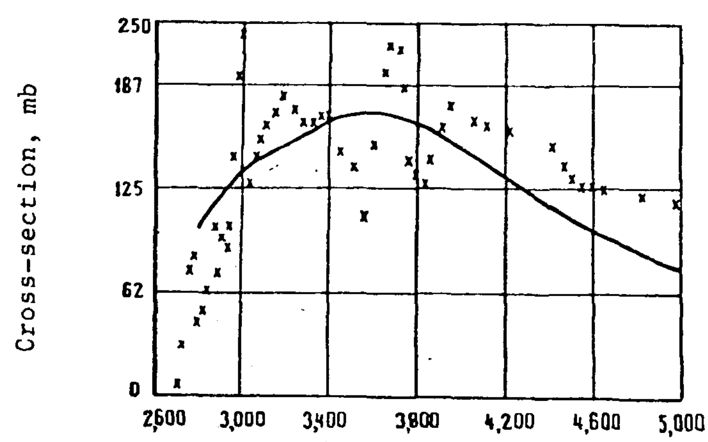


b

Fig. 7. Partial cross-section of neutron non-elastic scattering with excitation of the levels 0.845 MeV (a), 1.408 MeV (b), 2.08 MeV (c), 2.655 MeV (d): X = KEDAK; □ = ENDL; —— = SOKRATOR (old value); --- = SOKRATOR (new version); ♁ = data from Ref. [21].


Cross-section, mb
150
100
50
0
2,000
2,400
2,800
3,200
3,600
4,000
4,400
4,800
5,200
Neutron energy, MeV

c


Cross-section, mb
250
187
125
62
0
2,600
3,000
3,400
3,800
4,200
4,600
5,000
Neutron energy, MeV

d

Fig. 7

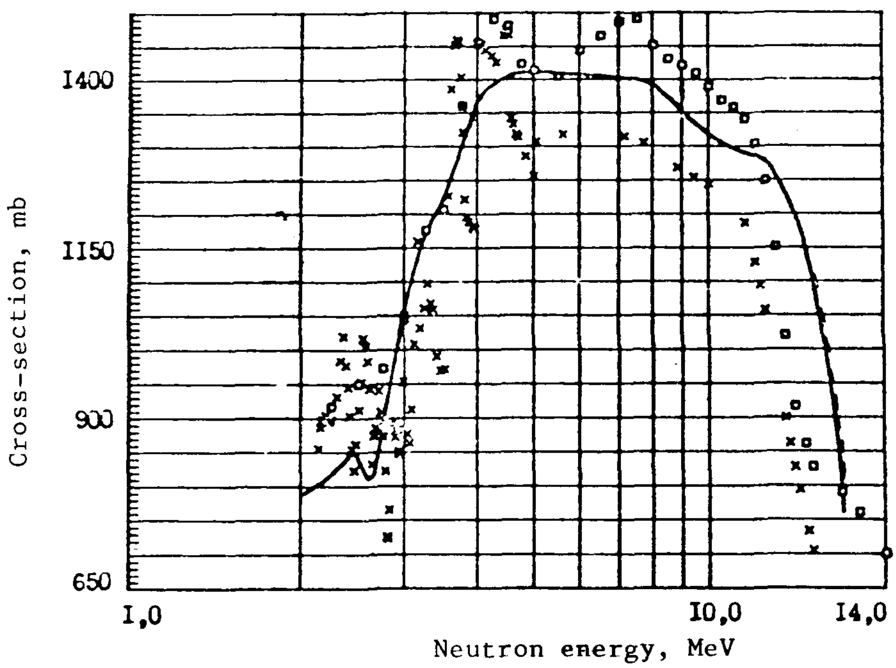


Fig. 8. Total cross-section of neutron non-elastic scattering: X = KEDAK; □ = ENDL; ——— = SOKRATOR (old value); - - - = SOKRATOR (new version).

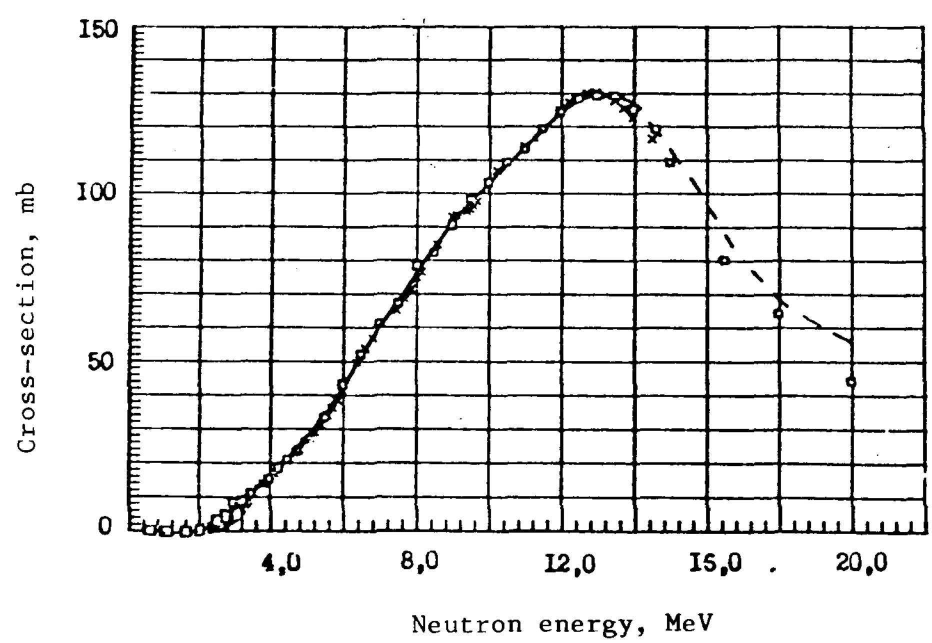


Fig. 9. Cross-section of (n,p) reaction: X = KEDAK; □ = ENDL; ——— = SOKRATOR (old value); --- = SOKRATOR (new version).

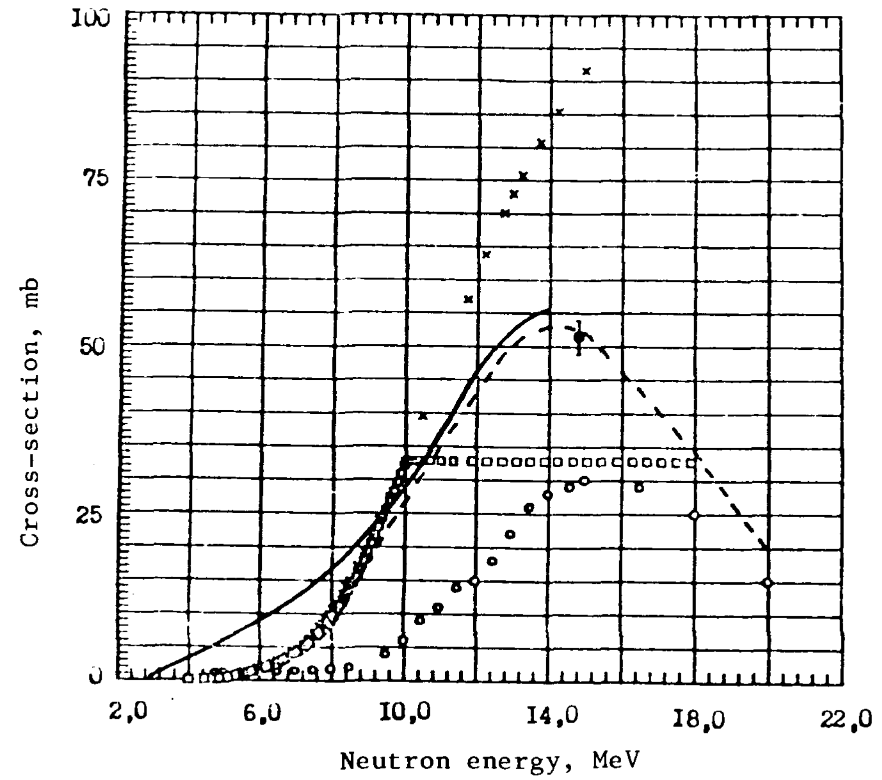


Fig. 10. Cross-section of the (n,α) reaction: X = KEDAK; O = ENDL; ▢ = SAND-2; ——— = SOKRATOR (old value); --- = SOKRATOR (new version); ♀ = experimental value from Ref. [23].

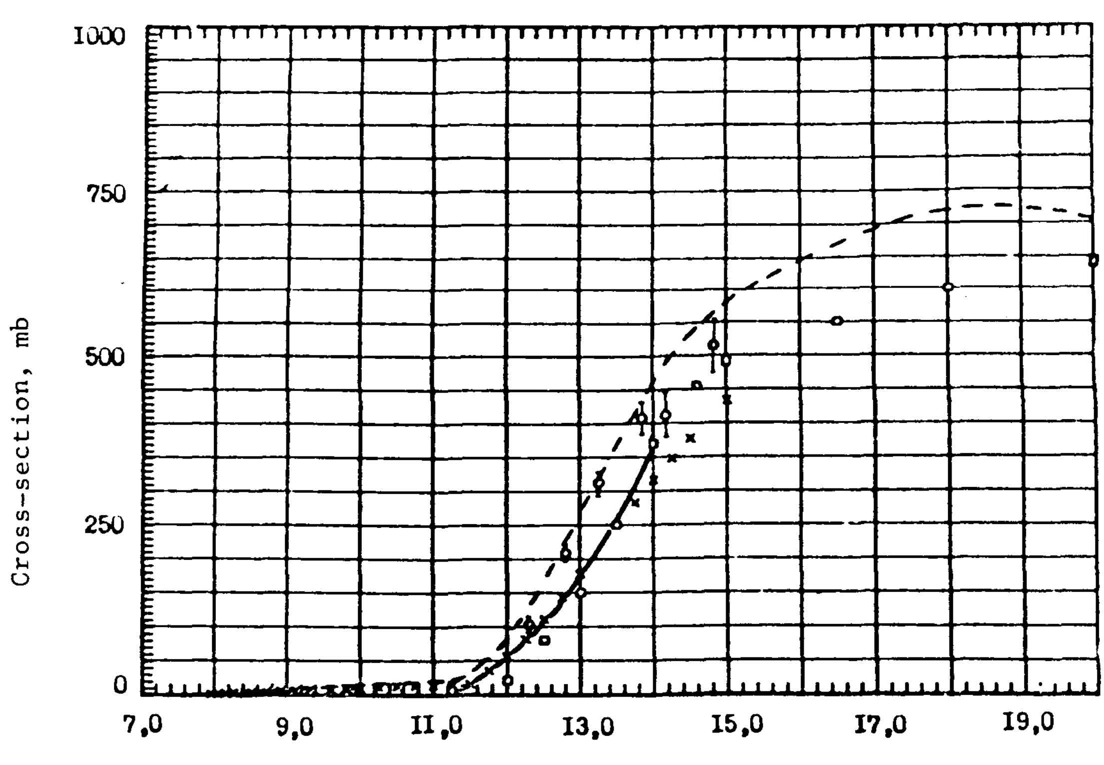


Fig. 11. Cross-section of the (n,2n) reaction: X = KEDAK; ——— = SOKRATOR (old value); --- = SOKRATOR (new version); ♀ = experimental data from Ref. [24].