JAERI-Research
95-068

UNCERTAINTIES IN EVALUATED TOTAL CROSS-SECTION DATA FOR 14 NUCLIDES CONTAINED IN JENDL-3.2

October 1995

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編集兼発行　日本原子力研究所
印　　　刷　いばらき印刷㈱

JAERI-Research 95-068

Uncertainties in Evaluated Total Cross-Section Data for 14 Nuclides Contained in JENDL-3.2

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(Received October 2, 1995)

Variances and covariances of total cross sections have been estimated for 14 nuclides contained in JENDL-3.2. Least-squares analyses using the GMA code were performed to obtain them. Information on the uncertainties of those measurements, which the JENDL-3.2 evaluation was based on, was derived from the associated references and fed into the GMA code system. The results obtained from the present analysis are illustrated.

Keywords: JENDL-3.2, Variance, Covariance, Total Cross Section, Least-squares Analysis

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ＪＥＮＤＬ－3.2に収納されている14核種の全断面積の誤差

日本原子力研究所東海研究所原子炉工学部
中村　雅弘*・柴田　恵一

（1995年10月2日受理）

評価済核データライブラリーＪＥＮＤＬ－3.2に収納されている14核種について、その全断面積の分散及び共分散の推定を行った。推定には、最小自乗法に基づく計算コードＧＭＡを用いた。ＪＥＮＤＬ－3.2の評価の際に用いられた個々の実験値の誤差情報は関連する文献より求められ、ＧＭＡコードに入力された。今回の計算結果は図で示される。

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1. Introduction

Variances and covariances of evaluated data are required to estimate uncertainties in reactor calculations from the viewpoint of reliability, safety and economics. The recent evaluated data libraries such as ENDF/B-VI[1)] and JEF-2[2)] contain error files to meet the requirement. However, the second version of JENDL-3 (referred to as JENDL-3.2[3)]), which was made available in 1994, did not contain error files although some users strongly requested them. Moreover, the first version of JENDL Dosimetry File[4)] which was based on JENDL-3 took variance and covariance data from IRDF-85[5)]. Therefore, it is an urgent task to make our own error files.

One of the difficulties in making error files is due to the fact that there is no established procedure to derive variance-covariance data. In general, data evaluation is performed on the basis of experimental data, more or less, but few experimenters give detailed error information to evaluators. Thus, it is needed to carry out error analyses with limited experimental information.

A least-squares program GMA[6)] was developed at ANL to derive variance and covariance data from a set of experiments with minimal information. With this code, the percentage of the systematic error to the cross-section value is required as input. The correlation matrix for data points in each experiment is calculated from this percentage. The procedure is very simple and appropriate for producing error files without knowing the detailed error information for each experiment. The present work was undertaken to study the applicability of the GMA code to the production of variances and covariances of evaluated data in JENDL-3.2. Estimated were the uncertainties in the total cross sections of fourteen nuclides ^{6}Li, ^{7}Li, ^{9}Be, ^{12}C, ^{16}O, ^{23}Na, Ti, Cr, Fe, Ni, ^{235}U, ^{238}U, ^{239}Pu and ^{240}Pu, where the nuclide without a mass number stands for a natural element.

Chapter 2 describes the mathematical method used in the GMA code. Chapter 3 deals with information on errors of measurements for each nuclide. The results are graphically given in chapter 4.

2. Method

Variances and covariances of total cross sections for fourteen nuclides were estimated by using the GMA code system. A flow chart of the calculation procedure is shown in Fig. 1. Experimental data are retrieved from a database NESTOR-2[7], and the data format is converted using a utility program EXPTOGMA. Energy grids are determined by prior data. Experimental values from one data set are extrapolated to neighboring energy grids by using the shape of prior cross sections as shown in Fig. 2, and then the weighted average value is calculated at the energy grid. The cross-section error at this grid consists of a systematic error given by input and a reduced statistical error calculated from contributing data. This processing is performed by another utility DATGMA. The cross sections in JENDL-3.2 were used for the prior cross sections. A set of experimental data, Y, is defined as

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \cdot \\ \cdot \\ Y_n \end{pmatrix} \tag{1}$$

,where Y_i stands for each experiment involving one or multiple data points after being averaged at the grids. In GMA, a correlation coefficient $C_{i,jk}$ of the experiment i is calculated by the formula

$$C_{i,jk} = \begin{cases} \dfrac{\Delta\sigma^{sys}_{i,j} \cdot \Delta\sigma^{sys}_{i,k}}{\Delta\sigma^{total}_{i,j} \cdot \Delta\sigma^{total}_{i,k}} & (j \neq k) \\ 1.0 & (j = k) \end{cases} \tag{2}$$

, where $\Delta\sigma^{total}_{i,j}$ and $\Delta\sigma^{sys}_{i,j}$ are total and systematic errors at the j-th grid. The total error is given by combining systematic and statistical errors, i.e.,

$$\Delta\sigma^{total}_{i,j} = \sqrt{\left(\Delta\sigma^{sys}_{i,j}\right)^2 + \left(\Delta\sigma^{sta}_{i,j}\right)^2} \tag{3}$$

, where $\Delta\sigma^{sta}_{i,j}$ stands for a statistical error. A covariance matrix element $V_{i,jk}$ is given by

$$V_{i,jk} = \Delta\sigma^{total}_{i,j} \bullet \Delta\sigma^{total}_{i,k} \bullet C_{i,jk} \ . \tag{4}$$

The total covariance matrix V should have the form

$$V = \begin{pmatrix} V_1 & & & 0 \\ & V_2 & & \\ & & \cdot & \\ & & & \cdot \\ 0 & & & V_n \end{pmatrix} \ . \tag{5}$$

A design matrix Φ is introduced as

$$\Phi_{ij} = \begin{cases} 1 \ \text{if } i\text{-th datum lies in } j\text{-th grid} \\ 0 \ \text{if otherwise} \ . \end{cases} \tag{6}$$

The best estimate X is obtained from the following equation:

$$X = (\Phi^T V^{-1} \Phi)^{-1} \Phi^T V^{-1} Y \tag{7}$$

, where T denotes the transpose. The covariance matrix M associated with the best estimate is obtained from

$$M = \chi^2 (\Phi^T V^{-1} \Phi)^{-1} \tag{8}$$

,where χ^2 is a measure of fitting, and is expressed by

$$\chi^2 = \frac{(Y-X)^T V^{-1} (Y-X)}{d-g} \ . \tag{9}$$

In eq. (9), the symbols d and g stand for the dimension of V and the number of energy grids, respectively. The χ^2 value is applied to eq. (8) when it is larger than unity.

3. Determination of Systematic Errors for Each Experiment

With the GMA calculation, it is required to identify systematic errors for each

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3. Determination of Systematic Errors for Each Experiment

With the GMA calculation, it is required to identify systematic errors for each measurement in order to produce a covariance matrix V_i. The systematic errors were taken from the references associated with the experiment as much as possible. In some cases where no error information is available, guess-values are assigned. Error information for each experiment is given as follows:

1) ^{6}Li for $E_n \geq 1$ MeV

Knitter et al.[8] (1977) E_n = 80 keV - 3 MeV

Total error is given in the data.

Systematic error:	no. of ^{7}Li atoms	0.5 %
	sample size	0.25 %
	dead time	0.34 %
	sum	0.65 %

Lamaze et al.[9] (1979) E_n = 3 - 50 MeV

Statistical error is given in the data.
No information is available on systematic error.
A systematic error of 1 % is assumed.

Smith et al.[10] (1982) E_n = 500 keV - 4.7 MeV

Statistical error is given in the data.
A systematic error of 2 % due to the sample.

2) ^{7}Li for $E_n \geq 100$ keV

Meadows and Whalen[11] (1970) E_n = 100 keV - 1.5 MeV

Statistical error is given in the data.
A systematic error of 0.82 % due to the sample.

Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 15 MeV

Total error is given in the data.
A systematic error of 0.5 % due to the sample.

Goulding et al.[13] (1972) E_n = 700 keV - 30 MeV

Statistical error is given in the data.
No information is available on systematic error.
A systematic error of 1 % is assumed.

Lamaze et al.[9] (1979) E_n = 3 - 50 MeV

Statistical error is given in the data.
No information is available on systematic error.
A systematic error of 1 % is assumed.

3) ^{9}Be for $E_n \geq 830$ keV

Schwartz et al.[14] (1971) E_n = 500 keV - 20 MeV

Statistical error is given in the data.
No information is available on systematic error.
A systematic error of 1 % is assumed.

Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 15 MeV

Total error is given in the data.
A systematic error of 0.4 % due to the sample.

Auchampaugh et al.15) (1979) $E_n = 1 - 14$ MeV
Statistical error is given in the data.

Systematic error:	sample thickness	0.7 %
	background	1.0 %
	normalization	1.0 %
	dead time	0.5 %
	sum	1.7 %

Finlay et al.16) (1993) $E_n = 5 - 600$ MeV
Statistical error is given in the data.
A systematic error of 0.5 % due to normalization.

Sugimoto et al.17) (1989) $E_n = 1 - 10$ MeV
Statistical error is given in the data.
A systematic error of 1.5 % is assumed.

4) ^{12}C for $E_n \geq 4.8$ MeV

Lamaze et al.9) (1979) $E_n = 2.5$ MeV - 40 MeV
Statistical error is given in the data.
No information is available on systematic error.
A systematic error of 1 % is assumed.

Auchampaugh et al.15) (1979) $E_n = 1.2 - 13.9$ MeV
Statistical error is given in the data.

Systematic error:	sample thickness	0.7 %
	background	1.0 %
	normalization	1.0 %
	dead time	0.5 %
	sum	1.7 %

Cierjacks et al.18) (1980) $E_n = 3 - 32$ MeV
Total error is given in the data.
A systematic error of 1 % is assumed.

Finlay et al.16) (1993) $E_n = 5 - 600$ MeV
Statistical error is given in the data.
A systematic error of 0.5 % is given by the authors.

5) ^{16}O for $E_n \geq 3$ MeV

Cierjacks et al.18) (1980) $E_n = 3 - 32$ MeV
Total error is given in the data.
A systematic error of 0.5 % is assumed.

Larson19) (1980) $E_n = 2 - 71$ MeV
Statistical error is given in the data.
A systematic error of 3 % is deduced.

6) ^{23}Na for $E_n \geq 350$ keV

Cierjacks et al.[20] (1969) E_n = 290 keV - 32 MeV

Total error is given in the data.

A systematic error of 2 % is deduced.

Langsford et al.[21] (1965) E_n = 180 keV - 120 MeV

Total error is given in the data.

A systematic error of 3 % is assumed.

Stoler et al.[22] (1971) E_n = 650 keV - 45 MeV

Statistical error is given in the data.

A systematic error of 1.5 % due to background.

Larson et al.[23] (1976) E_n = 32 keV - 37 MeV

Statistical error is given in the data.

A systematic error of 3 % is deduced.

7) Ti for $E_n \geq 100$ keV

Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 15 MeV

Total error is given in the data.

A systematic error of 0.5 % due to sample thickness.

Cabe and Cance[24] (1973) E_n = 150 keV - 4 MeV

Total error is given in the data.

A systematic error of 3.5 % is deduced.

Schwartz et al.[25] (1974) E_n = 500 keV - 4 MeV

Statistical error is given in the data.

A systematic error of 3 % due to normalization.

Barnard et al.[26] (1974) E_n = 100 keV - 1.5 MeV

Statistical error is given in the data.

A systematic error of 3 % is deduced.

8) Cr for $E_n \geq 300$ keV

Cierjacks et al.[27] (1968) E_n = 500 keV - 32 MeV

Total error of 3 % is given the data.

A systematic error of 2.8 % is deduced.

Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 1.5 MeV

Total error is given in the data.

A systematic error of 0.5 % is deduced.

Perey et al.[28] (1973) E_n = 180 keV - 30 MeV

Statistical error is given in the data.

A systematic error of 4 % is assumed.

Larson[19] (1980) E_n = 2 - 81 MeV

No error information is available.

The error given is assumed to be statistical.

A systematic error of 4 % is assumed.

9) Fe for $E_n \geq 250$ keV

Carlson and Cerbone[29] (1970) E_n = 460 keV - 9 MeV

Statistical error is given in the data.

A systematic error of 4 % is assumed.

Cierjacks et al.[30] (1968) E_n = 500 keV - 32 MeV

Total error of 3 % is given in the data.

A systematic error of 2.8 % is assumed.

Perey et al.[31] (1972) E_n = 190 keV - 49 MeV

Statistical error is given in the data.

Systematic error:	impurities in sample	0.14 %
	sample thickness	0.5 %
	dead time	2.0 %
	flux normalization	1.0 %
	background	0.1 %
	sum	2.3 %

Pattenden et al.[32] (1973) E_n = 200 eV - 1.1 MeV

Statistical error is given in the data.

A systematic error of 3 % is assumed.

Schwartz et al.[25] (1974) E_n = 500 keV - 15 MeV

Total error is given in the data.

A systematic error of 1 % is assumed.

10) Ni for $E_n \geq 557$ keV

Larson et al.[33] (1983) E_n = 2.2 keV - 20 MeV

Total error is given in the data.

A systematic error of 0.61 % is deduced.

Larson[19] (1980) E_n = 2 - 80 MeV

Statistical error is given in the data.

A systematic error of 5 % is assumed.

11) ^{235}U for $E_n \geq 30$ keV

Uttley et al.[34] (1966) E_n = 150 eV - 950 keV

Total error is given in the data.

A systematic error of 0.5 % is assumed.

Böckhoff et al.[35] (1972) E_n = 5.8 - 270 keV

No error is given in the data.

A systematic error of 3 % and a statistical error of 3 % are assumed.

Schwartz et al.[36] (1974) E_n = 500 keV - 15 MeV

Statistical error is given in the data.

A systematic error of 1.1 % is deduced.

Green and Mitchell[37] (1973) E_n = 500 keV - 10 MeV

Statistical error is given in the data.

A systematic error of 3 % is assumed.

Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 15 MeV
Total error is given in the data.
A systematic error of 0.5 % is deduced.
Poenitz et al.[38] (1981) E_n = 48 keV - 4.8 MeV
Total and statistical errors are given in the data.
A systematic error of 0.6 % is deduced.
Poenitz and Whalen[39] (1983) E_n = 1.8 - 20 MeV
Total error is given in the data.

Systematic error:	sample thickness	0.3 %
	background	0.3 %
	dead time	0.5 %
	sum	0.66 %

12) ^{238}U for $E_n \geq$ 150 keV
Whalen and Smith[40] (1971) E_n = 100 keV - 1.5 MeV
Statistical error is given in the data.
A systematic error of 3 % is assumed.
Poenitz et al.[38] (1981) E_n = 48 keV - 4.8 MeV
Total and statistical errors are given in the data.
A systematic error of 0.4 % is deduced.
Tsubone et al.[41] (1984) E_n = 23 - 930 keV
Total error is given in the data.
A systematic error of 2.2 % is deduced.
Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 15 MeV
Total error is given in the data.
A systematic error of 0.5 % due to sample thickness.
Bratenahl et al.[42] (1958) E_n = 7 - 14 MeV
Total error is given in the data.
A systematic error of 0.5 % is given by the authors.
Peterson et al.[43] (1960) E_n = 17 - 29 MeV
Total error is given in the data.
A systematic error of 0.5 % is given by the authors.

13) ^{239}Pu for $E_n \geq$ 7 MeV
Schwartz et al.[36] (1974) E_n = 500 keV - 15 MeV
Statistical error is given in the data.
A systematic error of 1.1 % is deduced.
Foster, Jr. and Glasgow[12] (1971) E_n = 2.3 - 15 MeV
Total error is given in the data.
A systematic error of 0.5 % due to sample thickness.
Nadolny et al.[44] (1973) E_n = 500 keV - 31 MeV
Statistical error is given in the data.
A systematic error of 1 % is deduced.

Poenitz et al.[39] (1983) E_n = 1.8 - 21 MeV

Total error is given in the data.

Systematic error:	sample thickness	0.75 %
	background	0.3 %
	dead time	0.3 %
	sum	0.93 %

14) ^{240}Pu for En ≥ 40 keV

Smith et al.[45] (1972) E_n = 120 keV - 1.5 MeV

Total and systematic errors are given in the data.

A systematic error of 3 % is deduced.

Poenitz et al.[38] (1981) E_n = 48 keV - 4.8 MeV

Total error is given in the data.

A systematic error of 1.2 % is deduced.

Poenitz and Whalen[39] (1983) E_n = 1.8 - 21 MeV

Total error is given in the data.

Systematic error:	sample thickness	0.75 %
	background	0.3 %
	dead time	0.45 %
	sum	0.93 %

4. Results and Discussion

The calculated results are shown in Figs. 3-23, where the best-fit curves (solid lines) are given together with standard deviations (dashed lines). It was easy to give a fit to smooth cross sections of the nuclides such as ^{6,7}Li, ^{9}Be, ^{235,238}U and ^{239,240}Pu in the energy region considered. As seen in Fig. 2, original experimental data are moved to a grid in parallel with a prior cross-section curve, and then an average value is calculated at the grid. Thus, fine grids should be set when resonance-shaped cross sections are involved.

Enhancement factors which are defined by the square root of eq. (9) are given in Table 1. The values for Ti, Cr and Fe are fairly large, since the measurements for each nuclide are discrepant with one another in the resonance energy region below several MeV. It seems unreasonable to apply these large values to obtain standard deviations in the high energy region where no resonance structure is seen. In these cases, the enhancement factors were recalculated in the resonance and non-resonance energy regions separately, and they were used to obtain the standard deviations in each region.

Figures 24-37 show the correlation matrices normalized to 1000. A strong correlation

Poenitz et al.[39] (1983) E_n = 1.8 - 21 MeV

Total error is given in the data.

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	dead time	0.3 %
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is seen in the figures except for heavy nuclides, since one or two measurements with a huge number of data points are emphasized in the calculations.

5. Conclusion

Error analyses were performed for the total cross section of fourteen nuclides contained in JENDL-3.2. Variances and covariances were determined using the GMA code system, and the results were illustrated. The method used in the present work is very simple, and can be applied to produce the error files of JENDL-3.2.

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Table 1 Enhancement factor F*)

Nuclide	F	Nuclide	F	Nuclide	F
^{6}Li	2.33	^{23}Na	2.83	^{235}U	2.39
^{7}Li	3.39	Ti	13.29, 13.29¹⁾, 0.66²⁾	^{238}U	1.51
^{9}Be	5.20	Cr	17.82, 20.80³⁾, 4.72⁴⁾	^{239}Pu	1.29
^{12}C	4.76	Fe	16.97, 18.94⁵⁾, 3.64⁶⁾	^{240}Pu	1.34
^{16}O	6.53	Ni	0.21		

*) Defined by the square root of eq. (9).
1) Calculated below 5 MeV.
2) Calculated above 5 MeV.
3) Calculated below 4.5 MeV.
4) Calculated above 4.5 MeV.
5) Calculated below 3 MeV.
6) Calculated above 3 MeV.

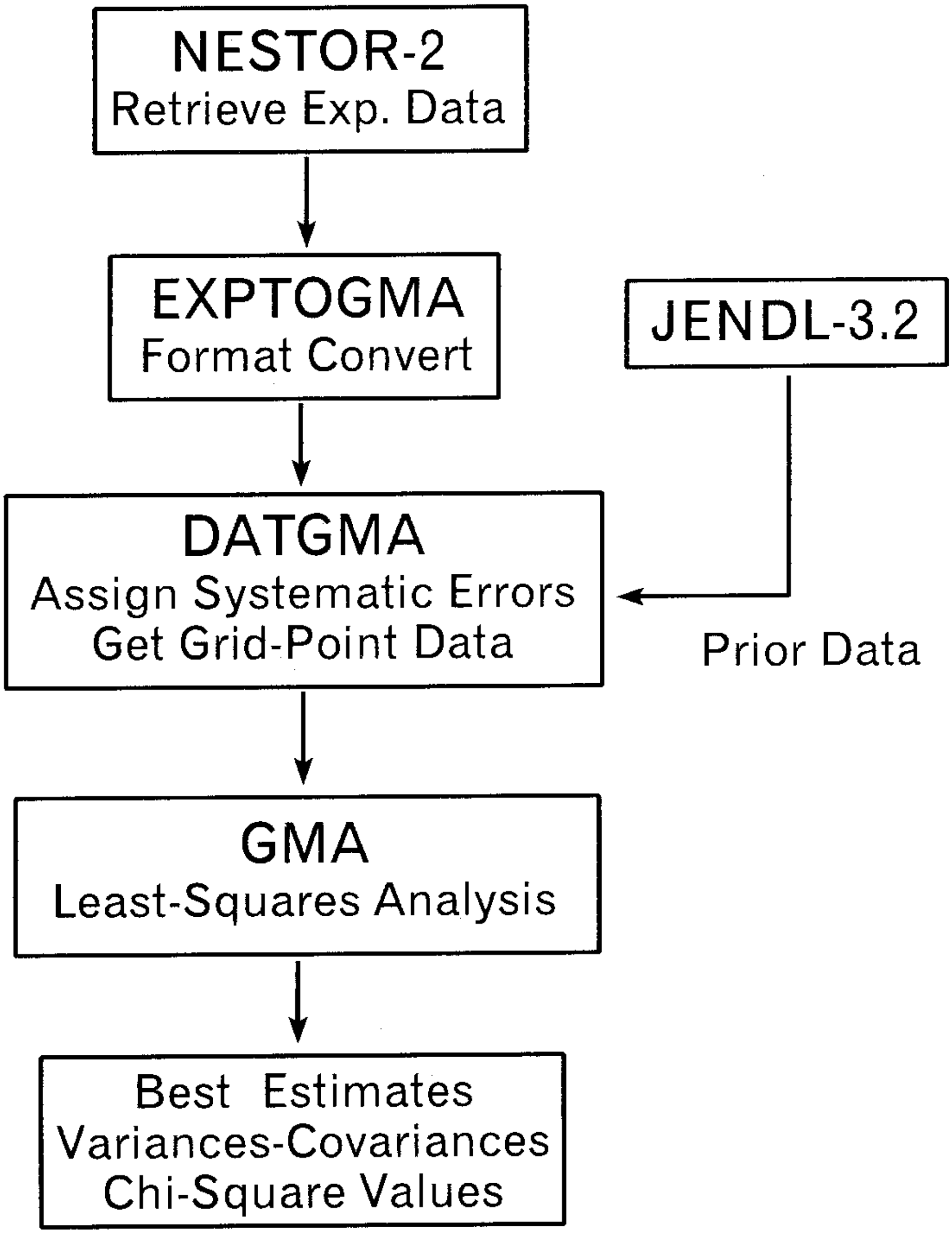

Fig. 1 Flow chart of the GMA code system.

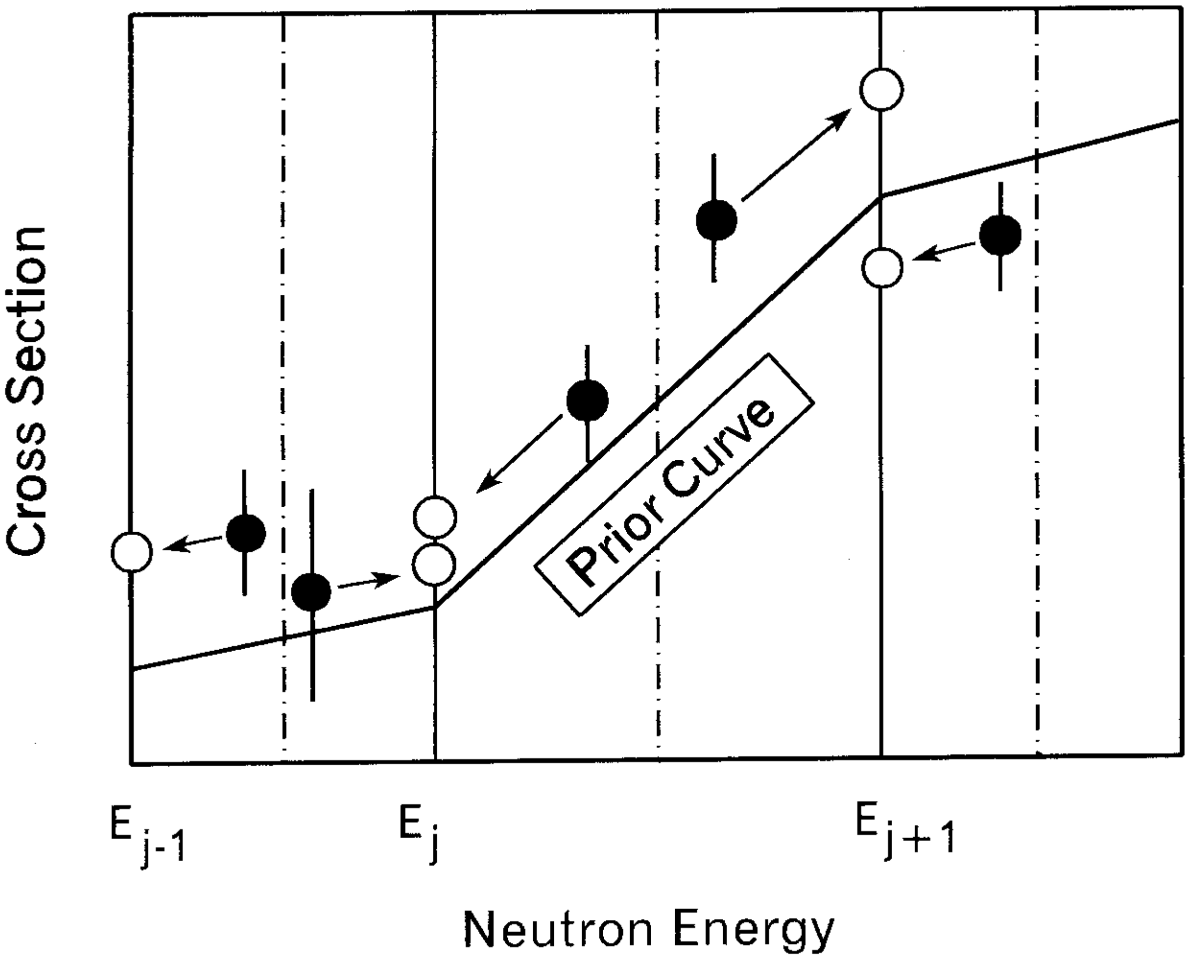

Fig. 2 Procedure to obtain experimental values at a grid energy.
Original data are moved to a grid energy in parallel with a prior curve.

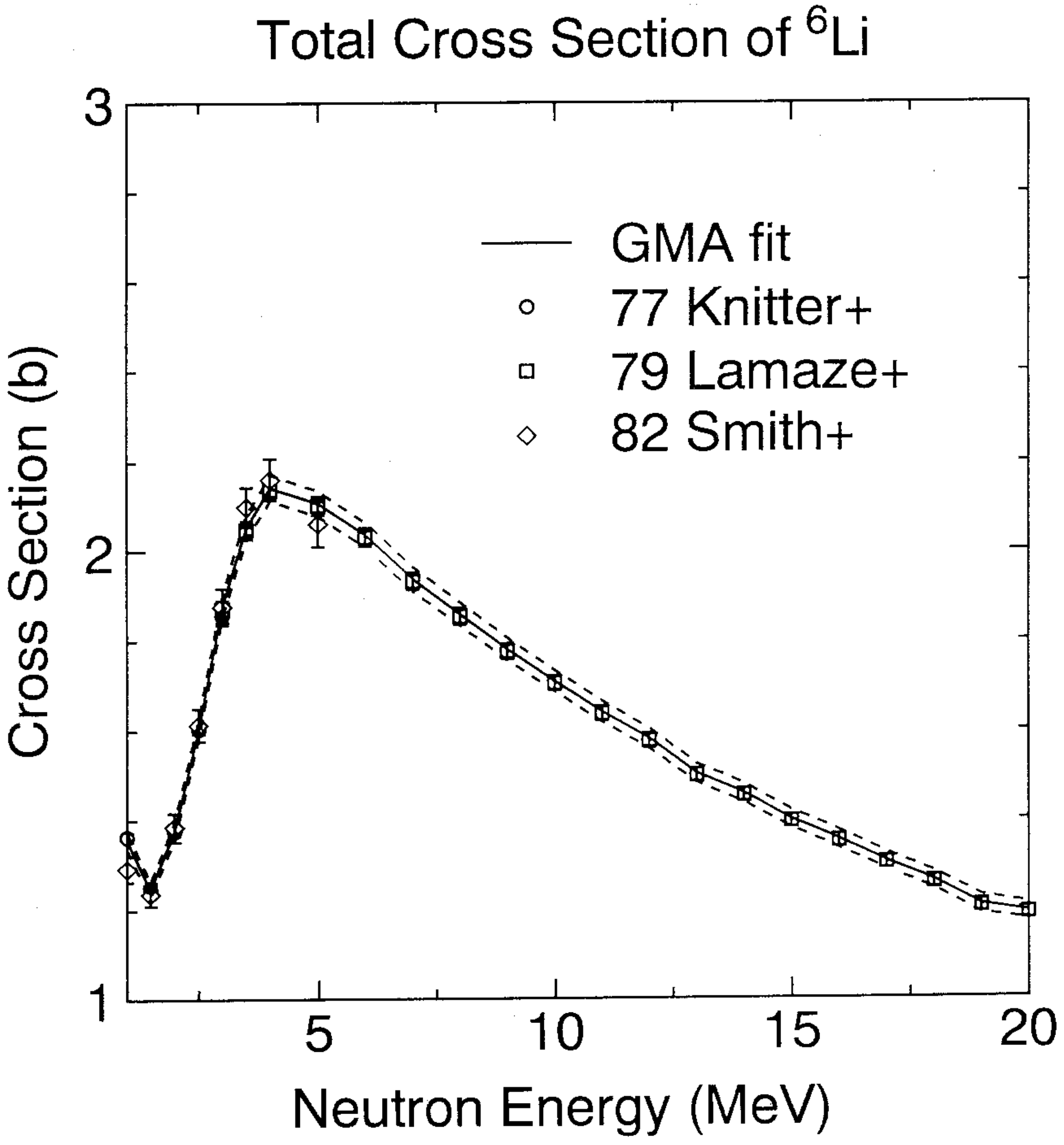

Fig. 3 Total cross section of ^{6}Li.
The solid line is the best estimate, and the dashed lines standard deviations.

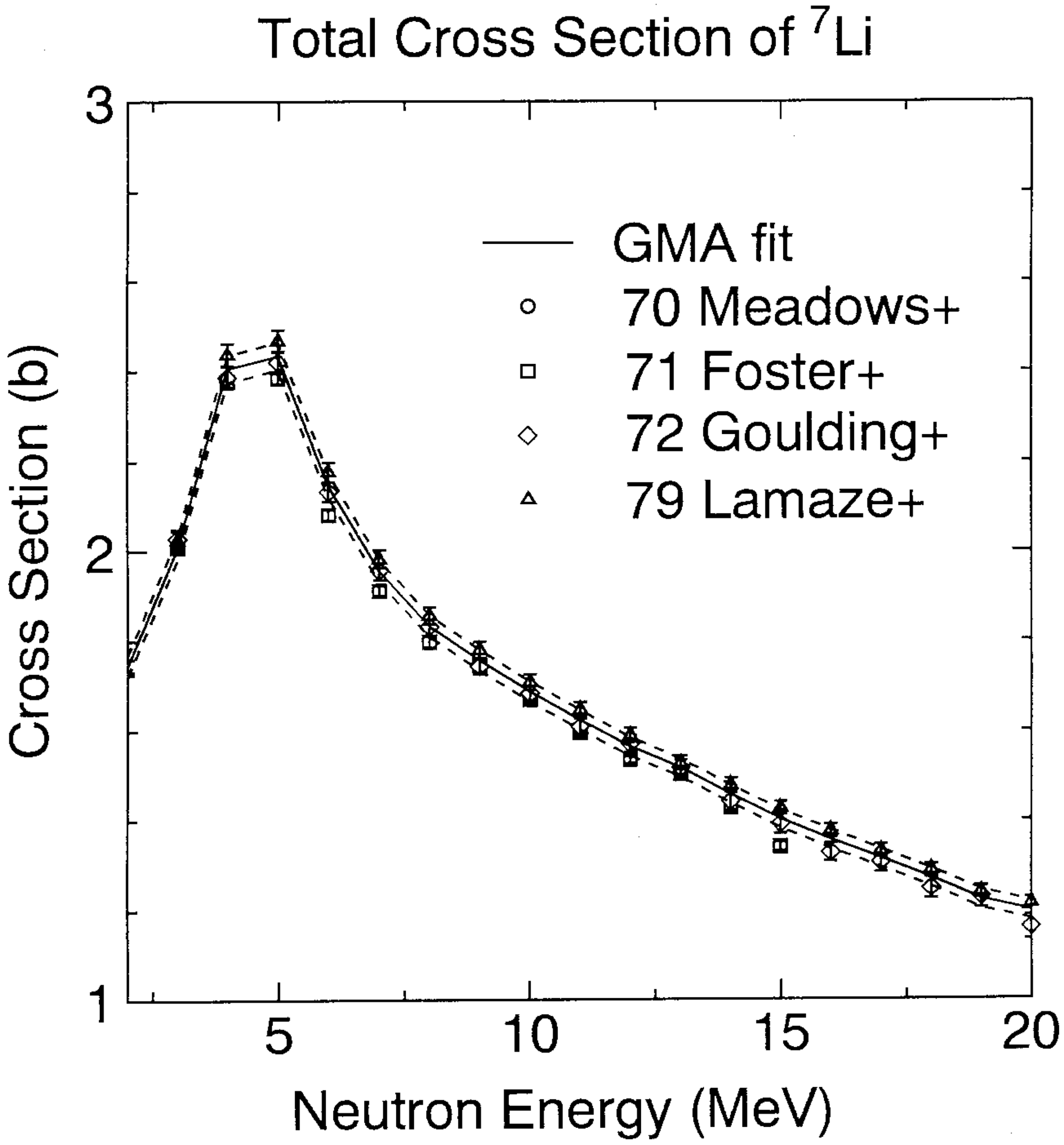

Fig. 4 Total cross section of ^{7}Li.

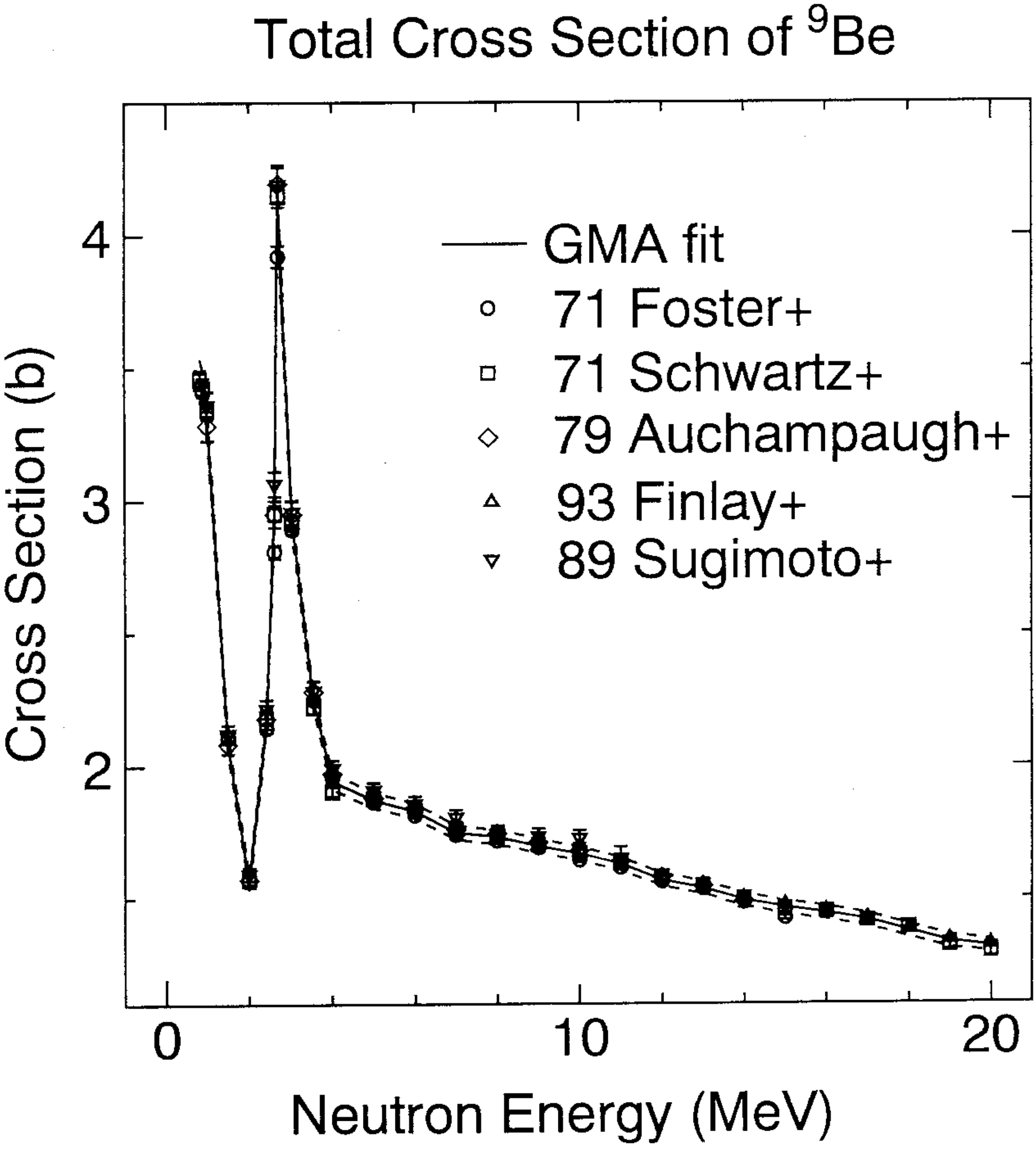

Fig. 5 Total cross section of ^{9}Be.

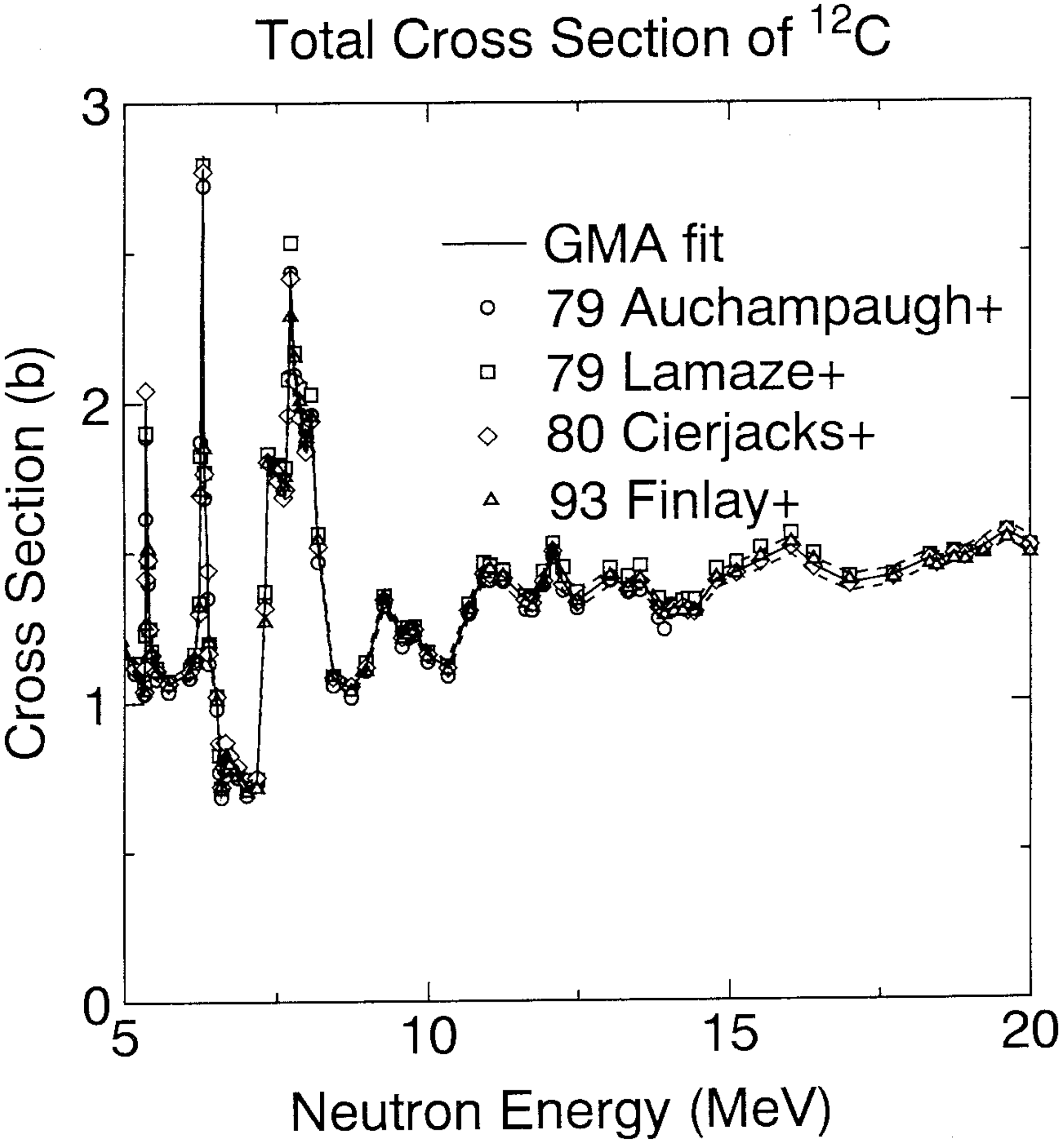

Fig. 6 Total cross section of ^{12}C.

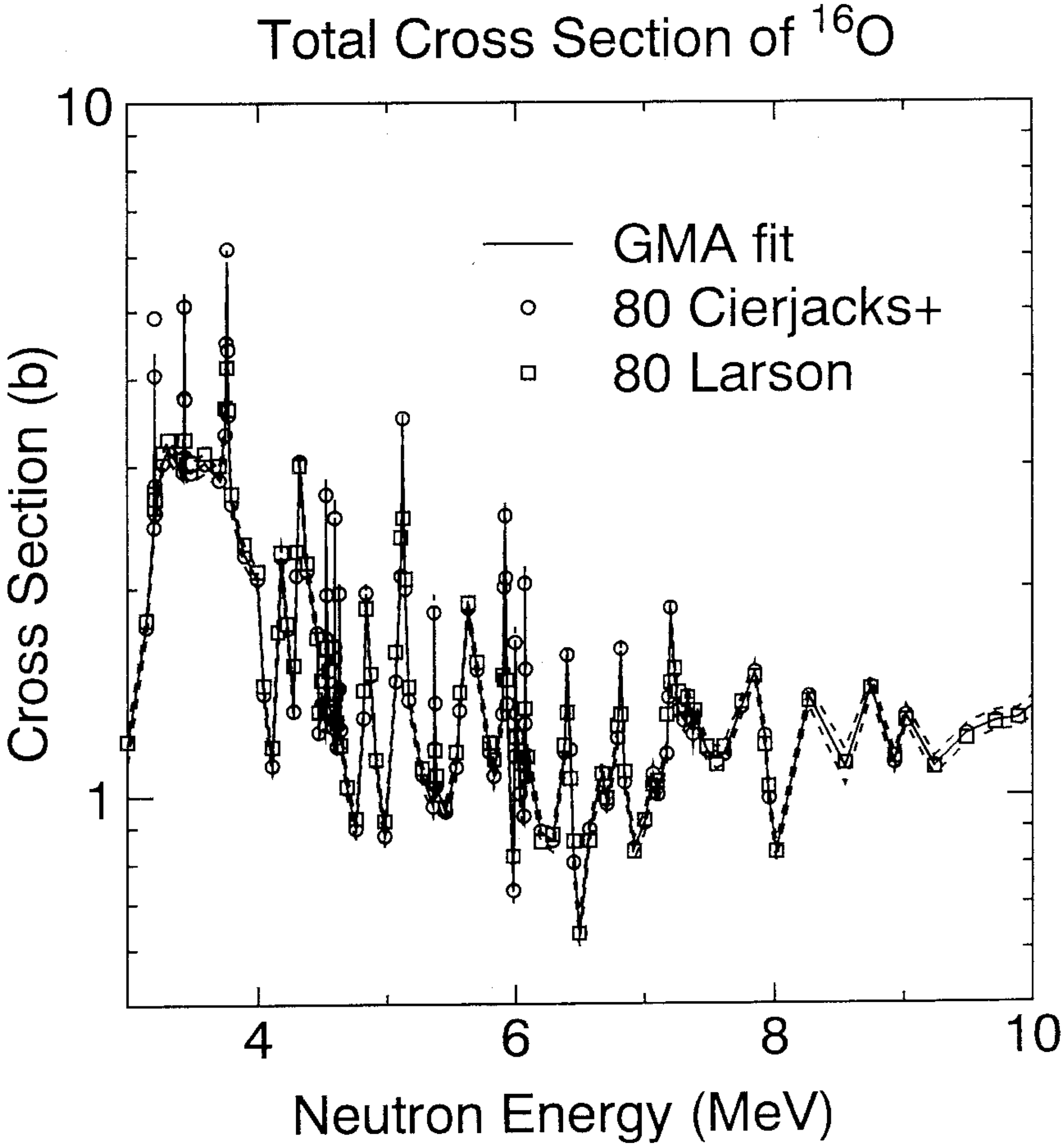

Fig. 7 Total cross section of ^{16}O below 10 MeV.

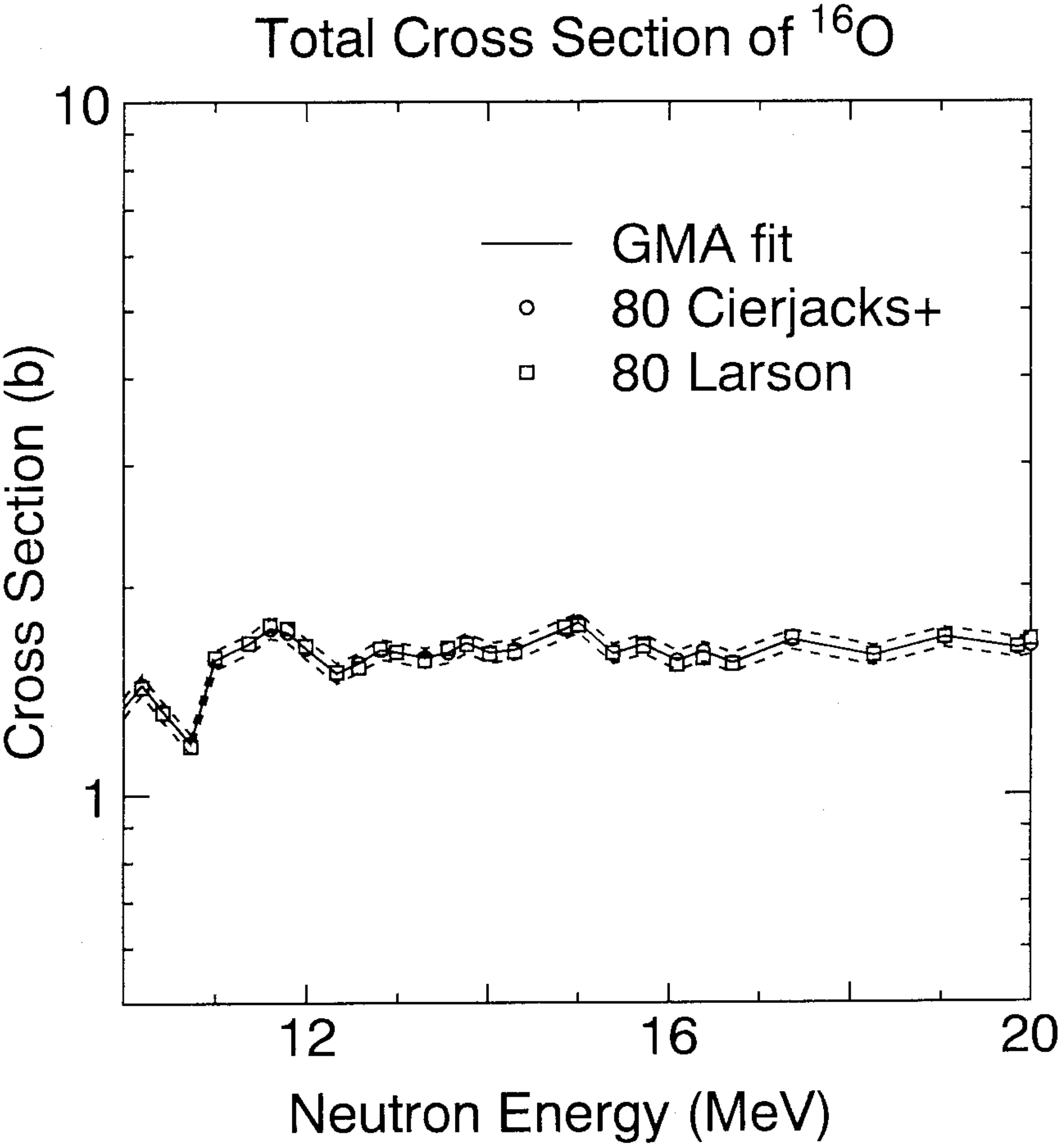

Fig. 8 Total cross section of ^{16}O above 10 MeV.

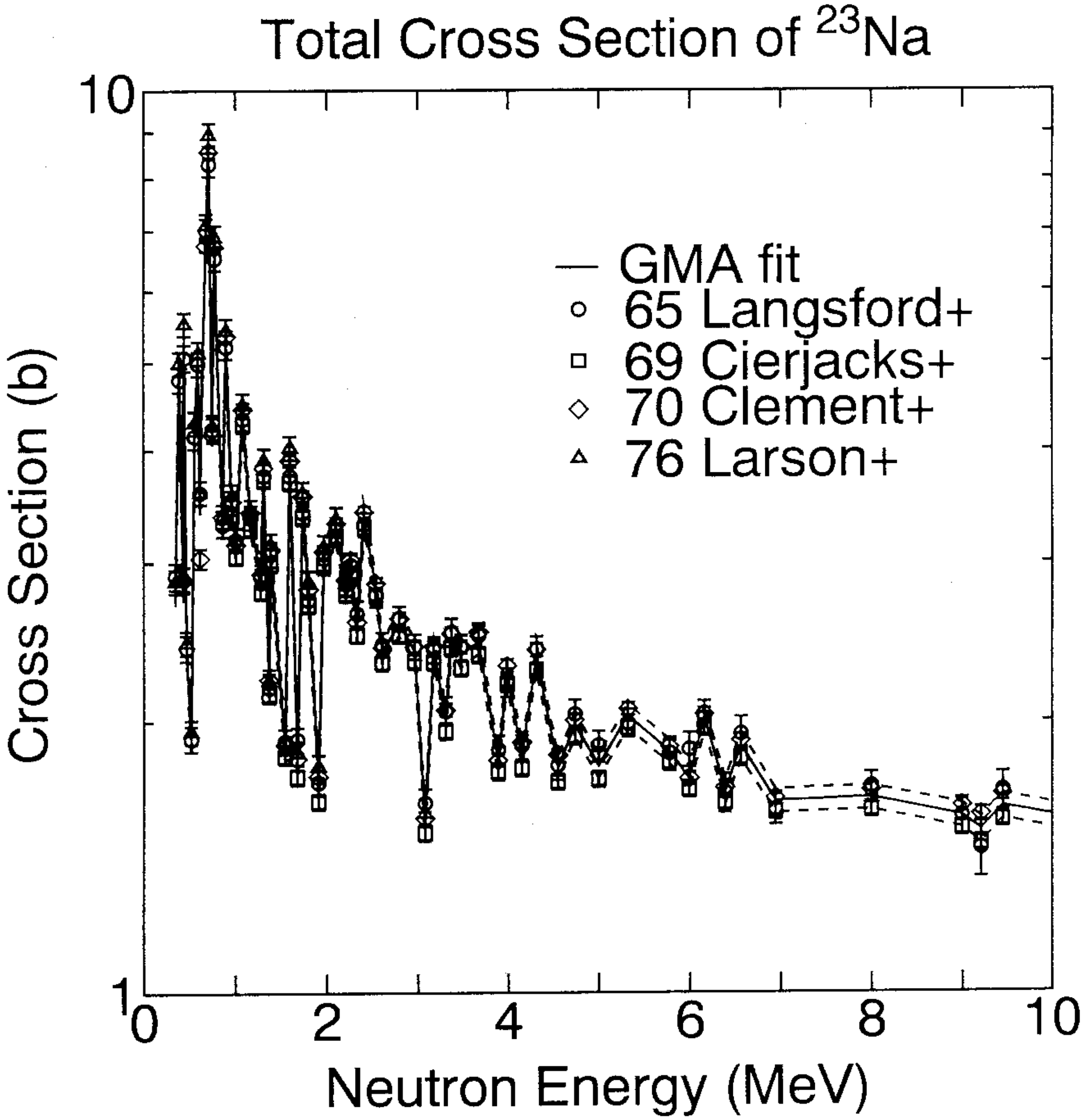

Fig. 9 Total cross section of ^{23}Na below 10 MeV.

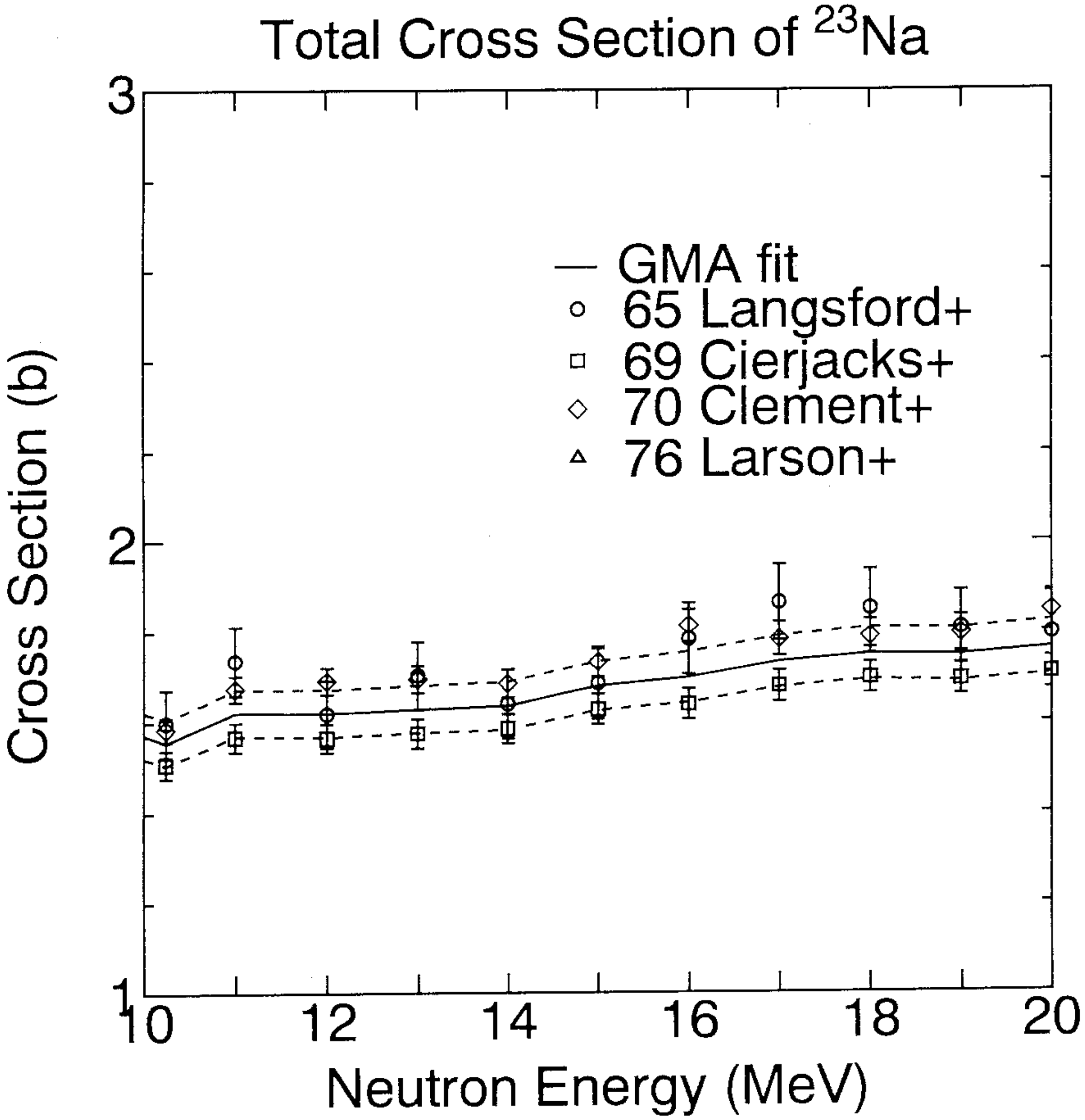

Fig. 10 Total cross section of ^{23}Na above 10 MeV.

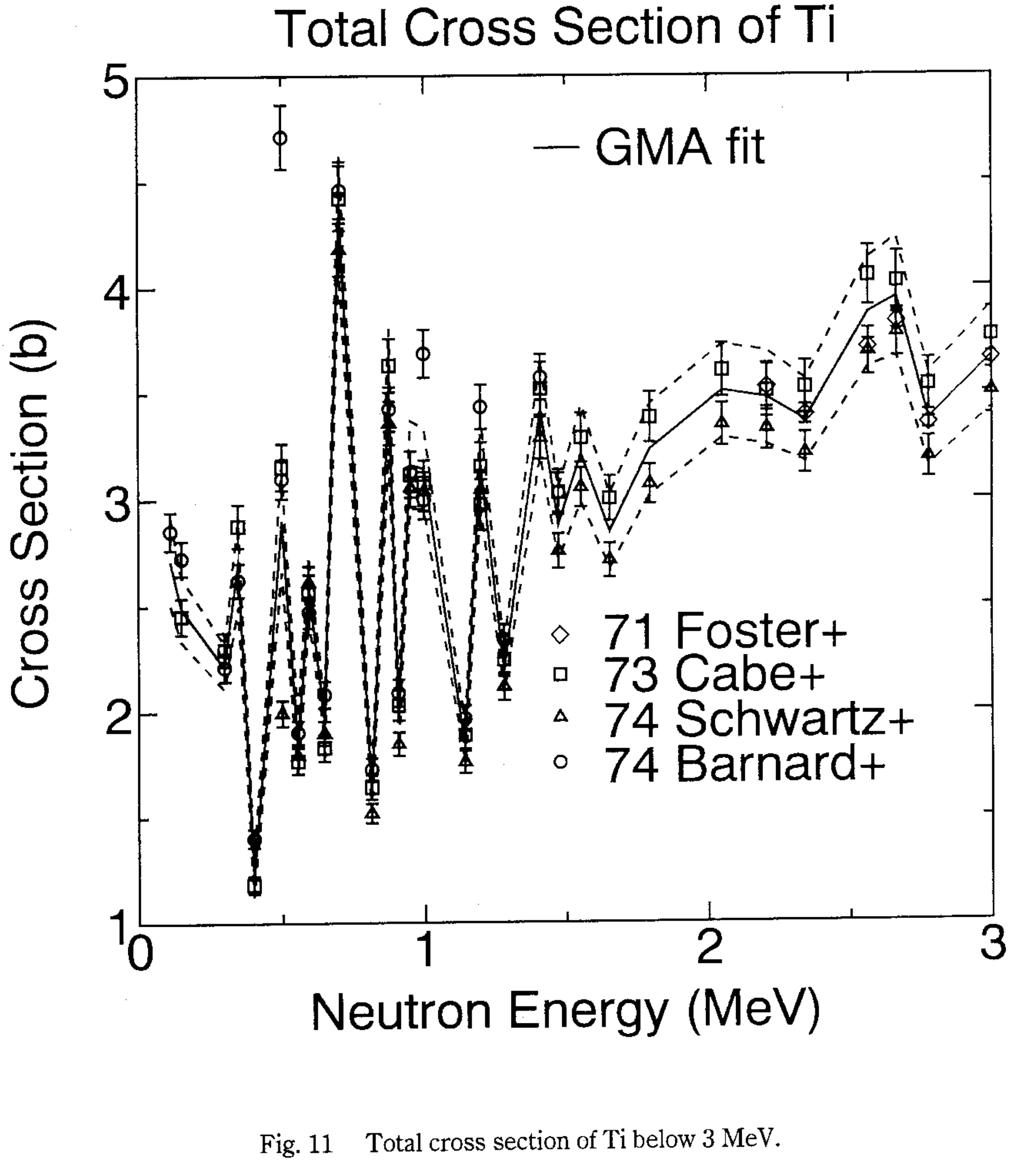

Fig. 11 Total cross section of Ti below 3 MeV.

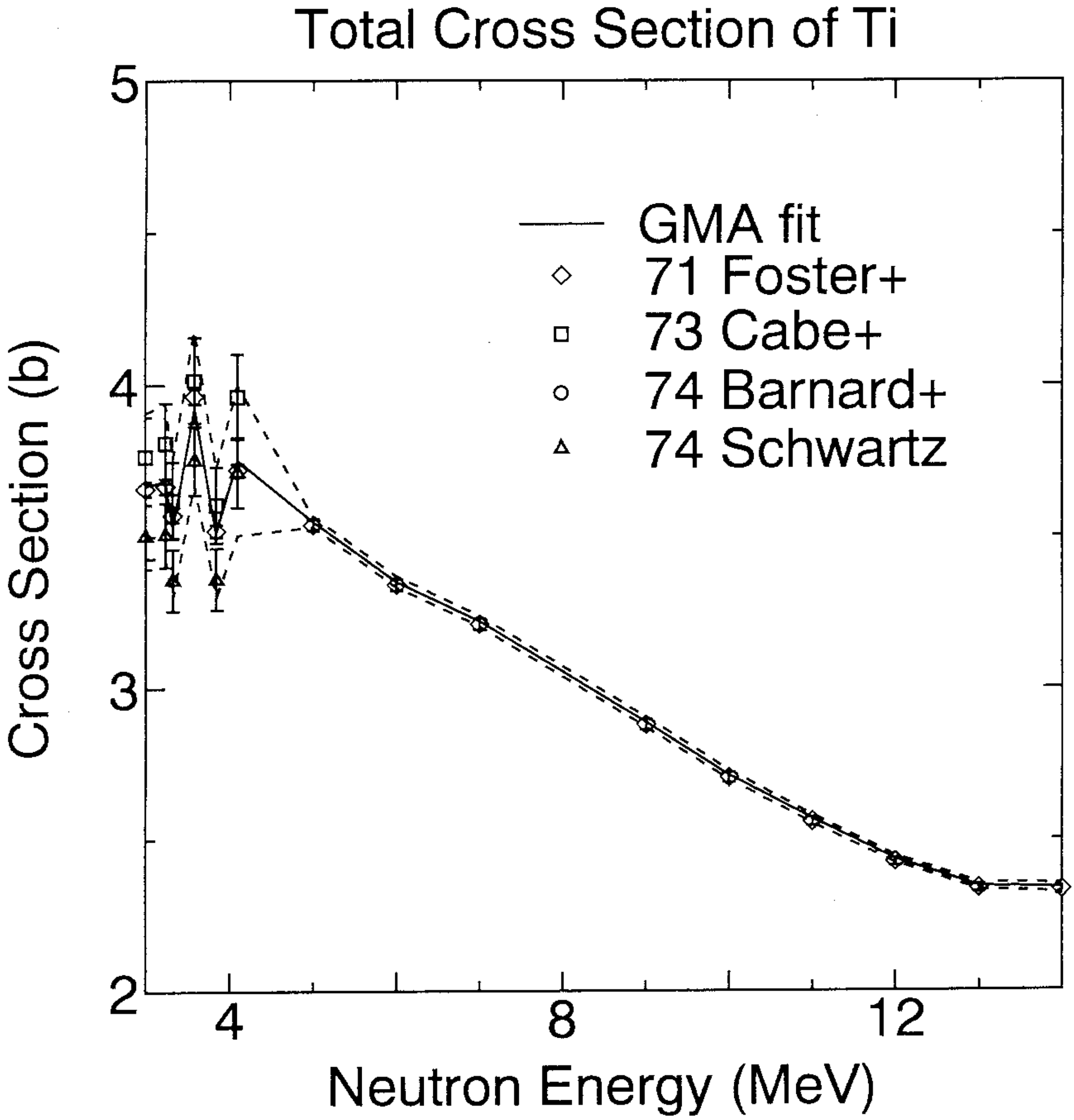

Fig. 12 Total cross section of Ti above 3 MeV.

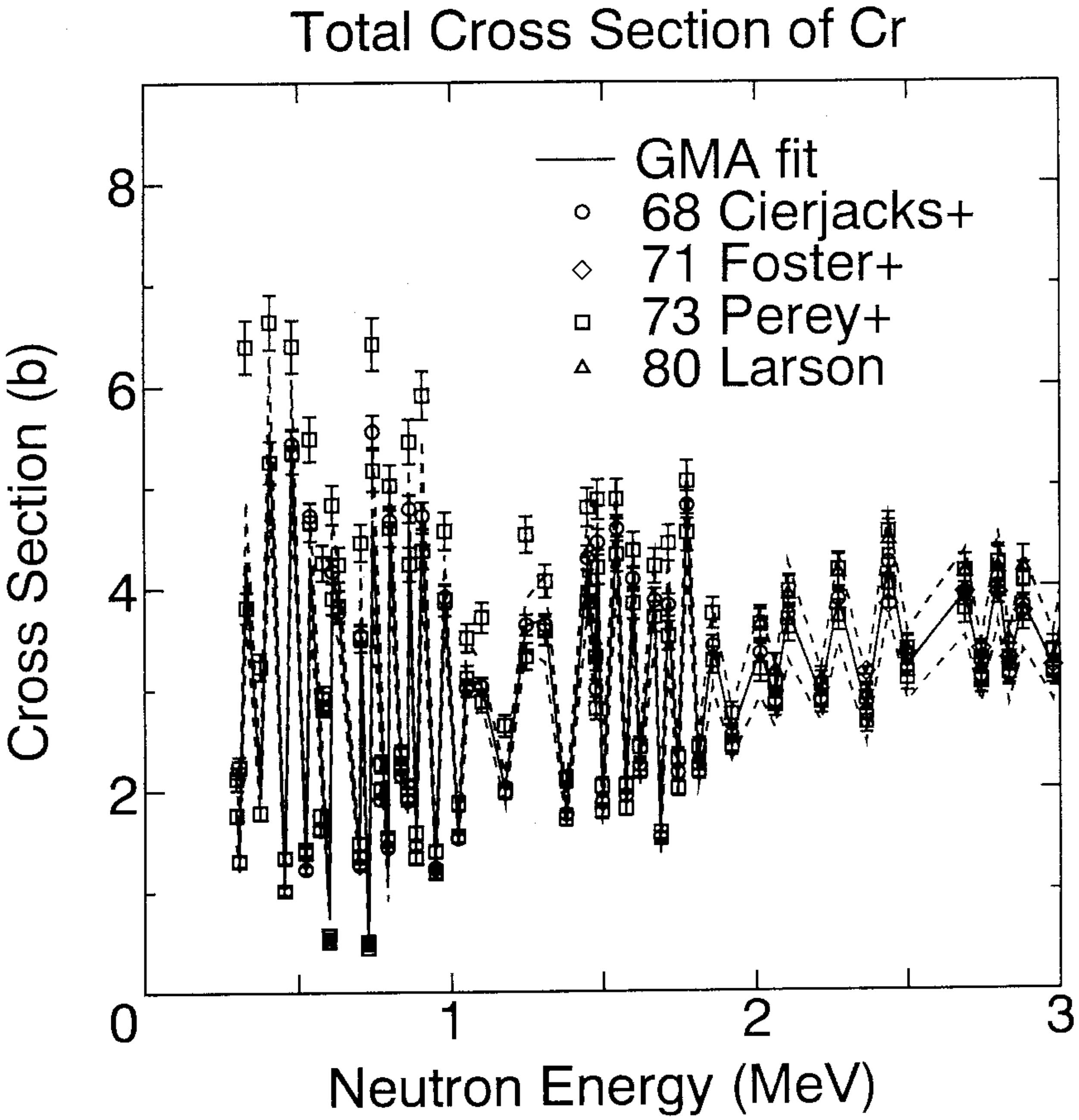

Fig. 13 Total cross section of Cr below 3 MeV.

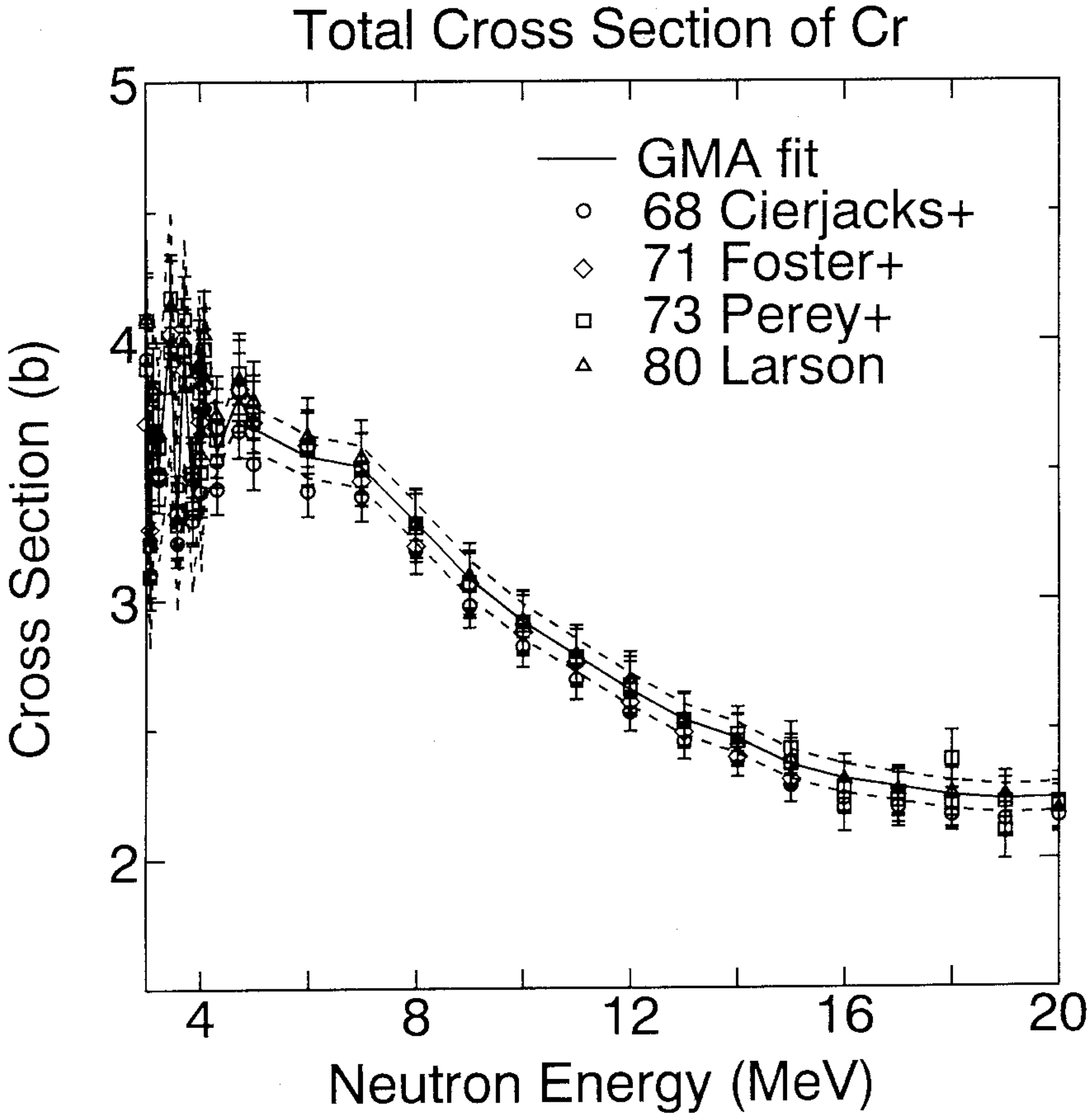

Fig. 14 Total cross section of Cr above 3 MeV.

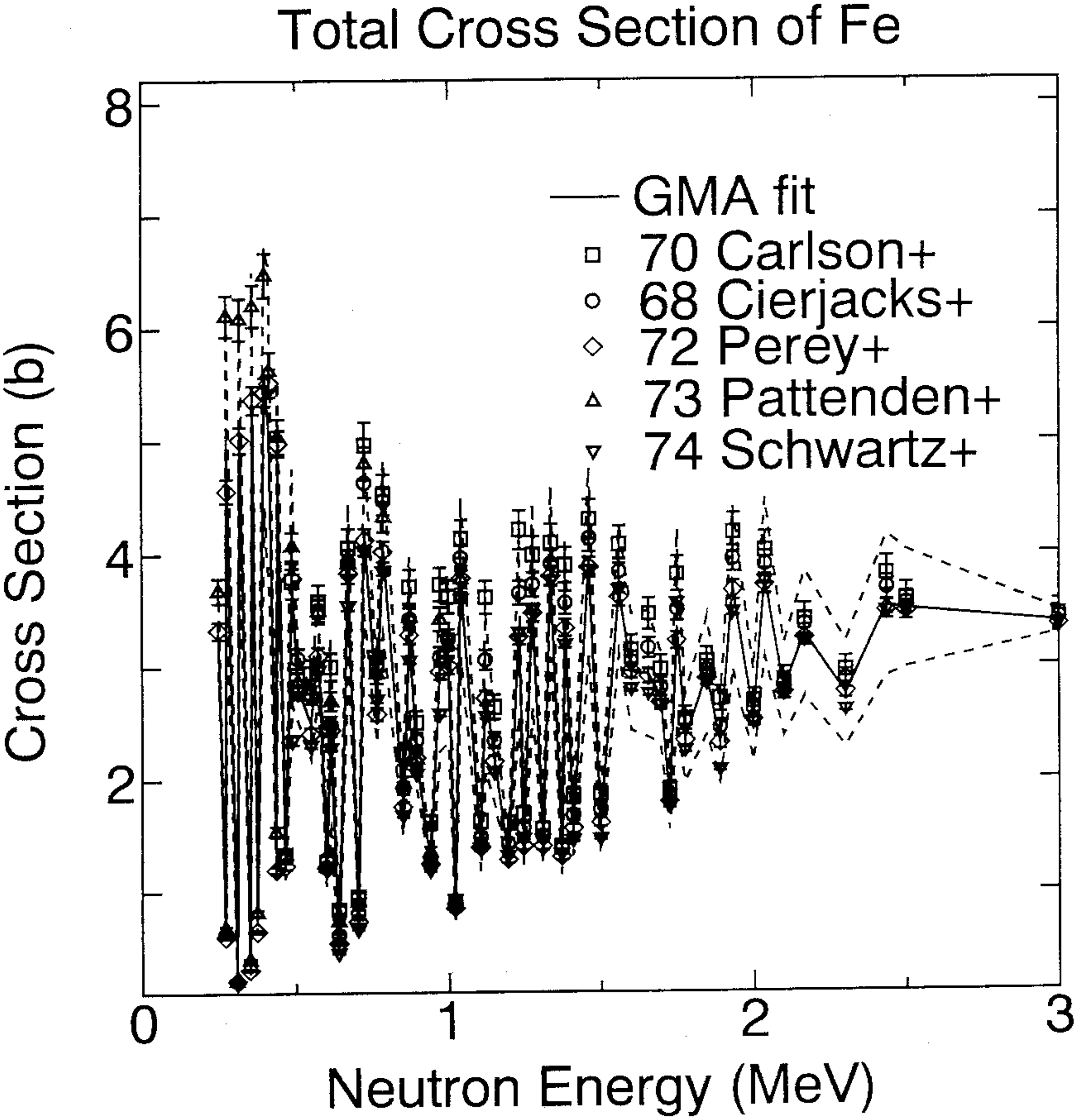

Fig. 15 Total cross section of Fe below 3 MeV.

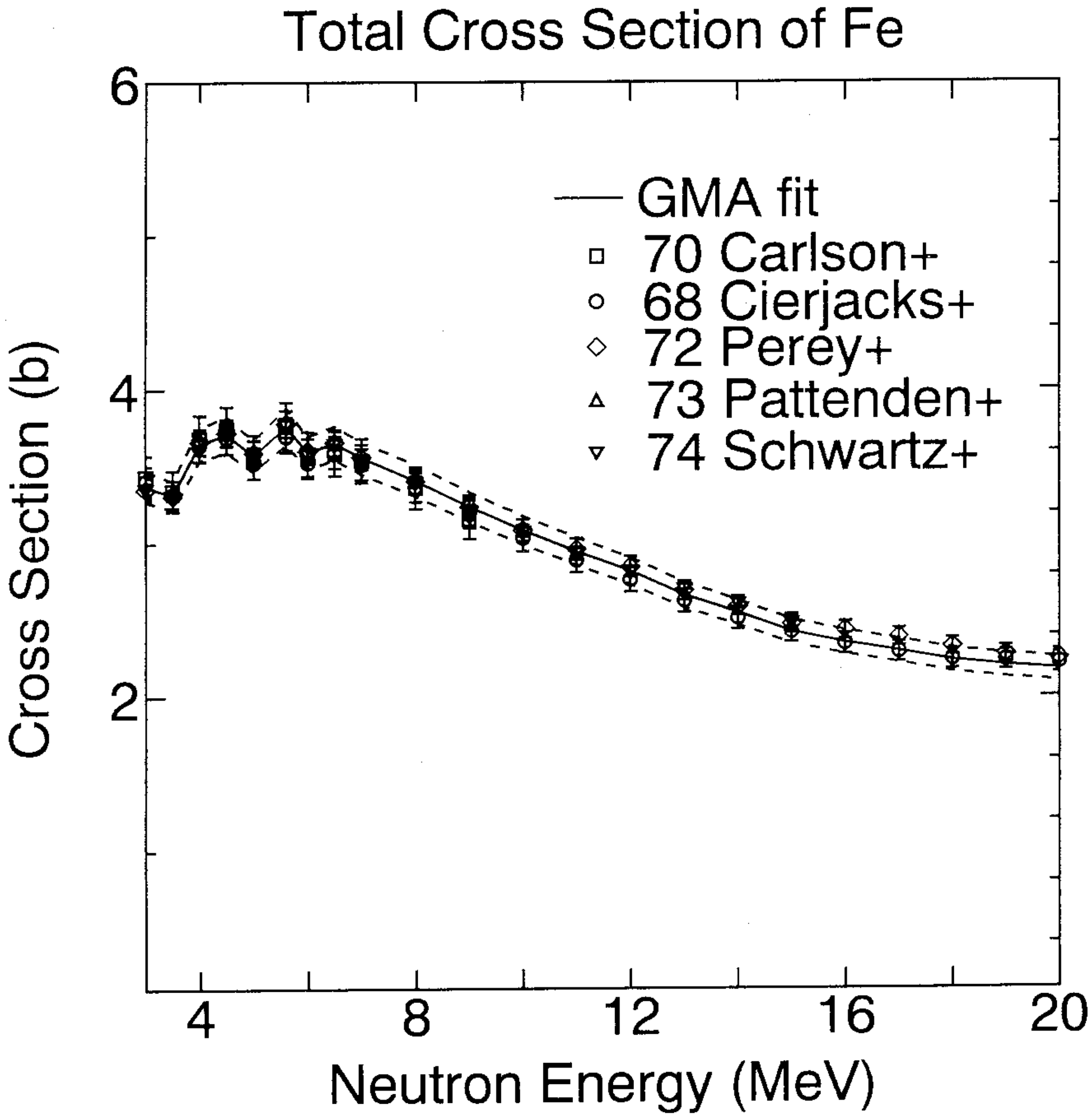

Fig. 16 Total cross section of Fe above 3 MeV.

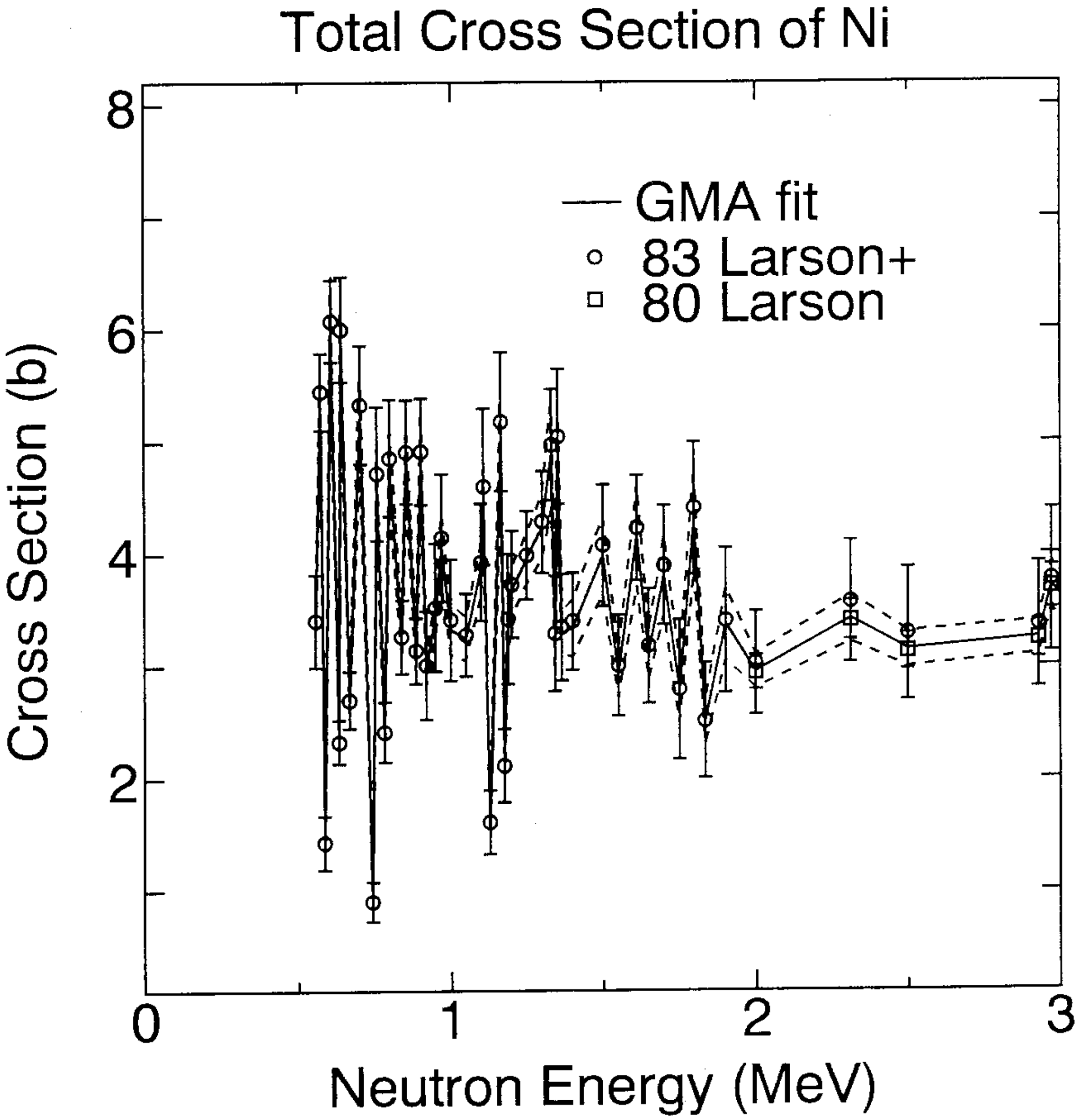

Fig. 17 Total cross section of Ni below 3 MeV.

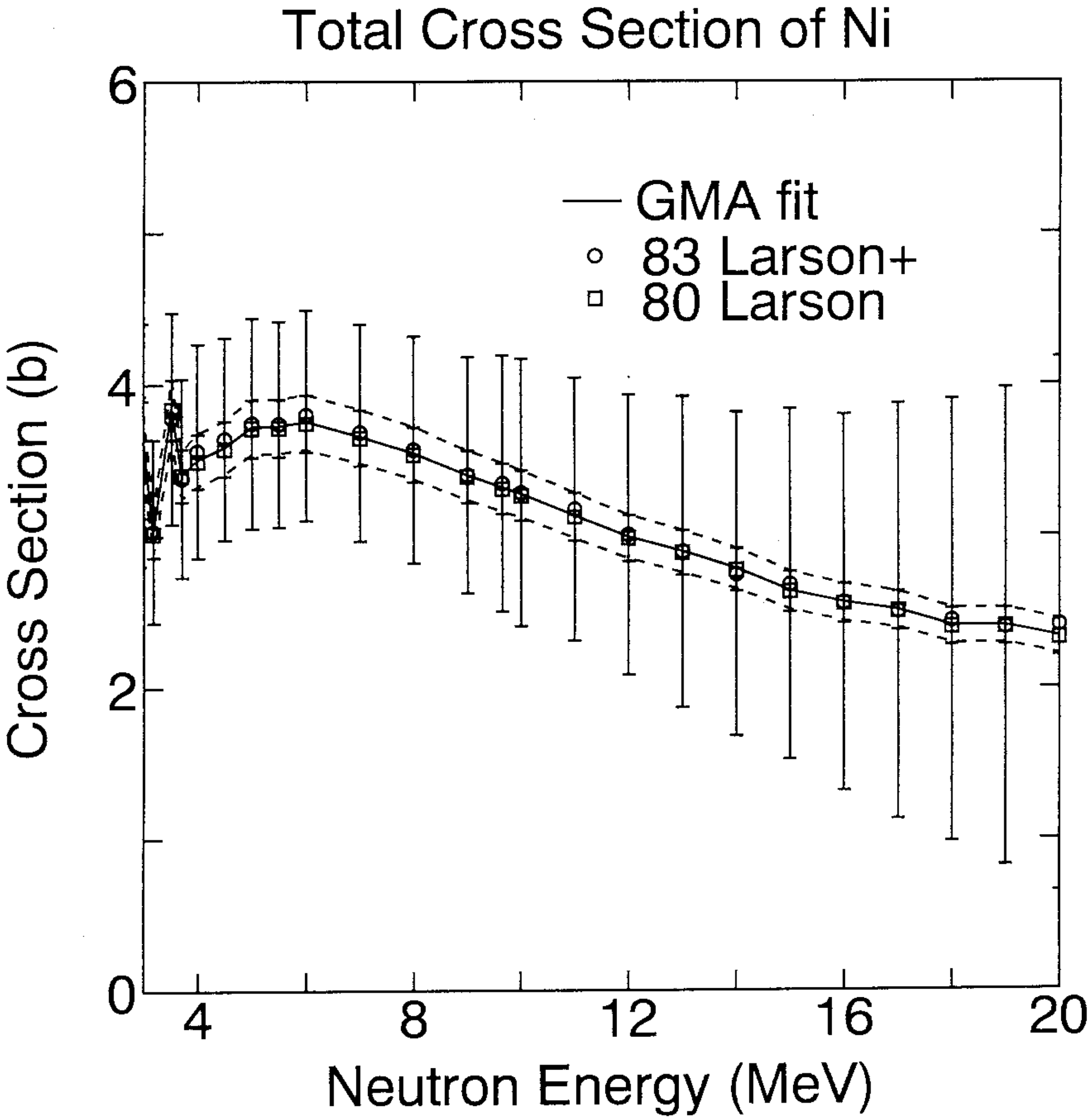

Fig. 18 Total cross section of Ni above 3 MeV.

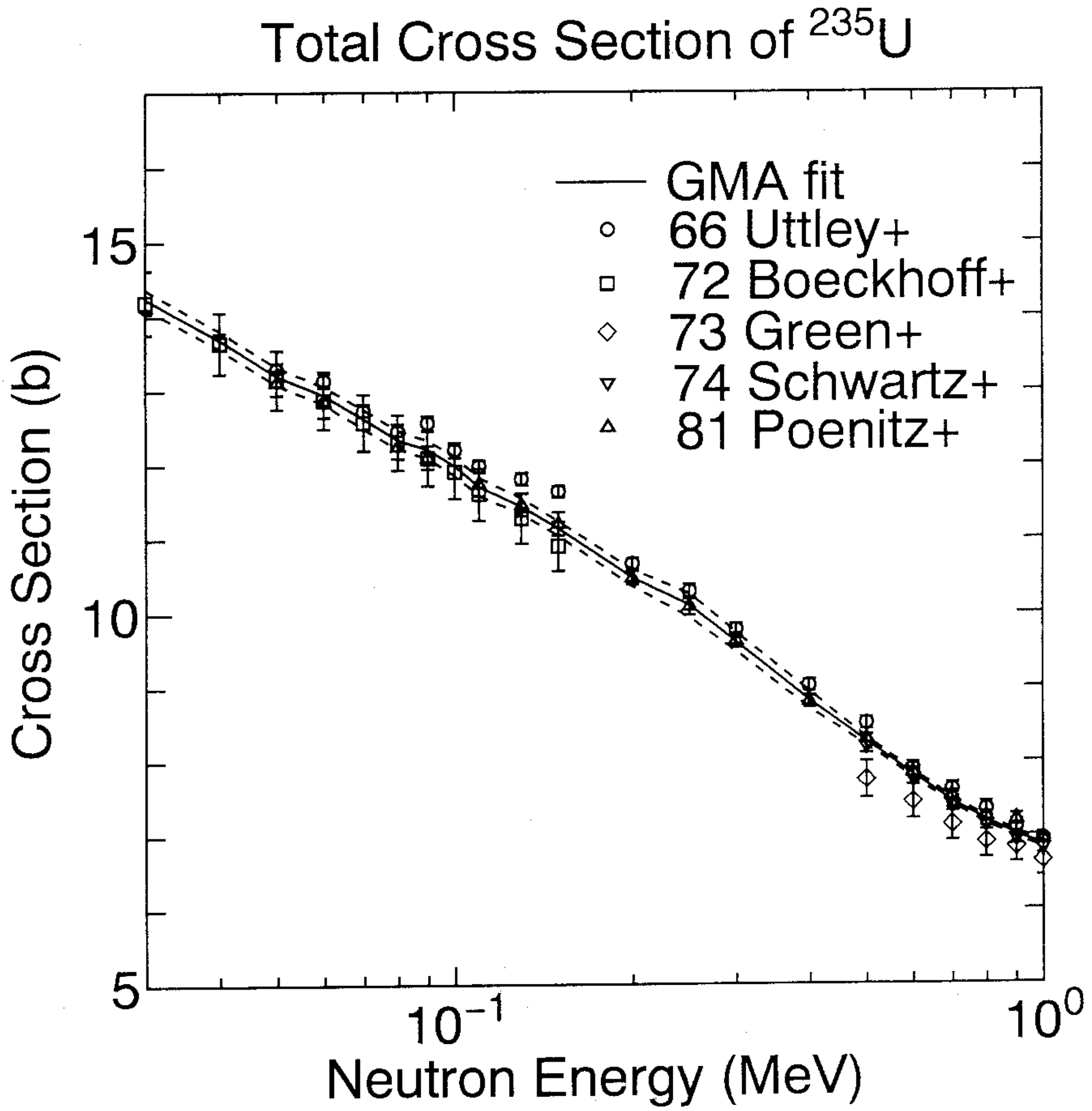

Fig. 19 Total cross section of ^{235}U below 1 MeV.

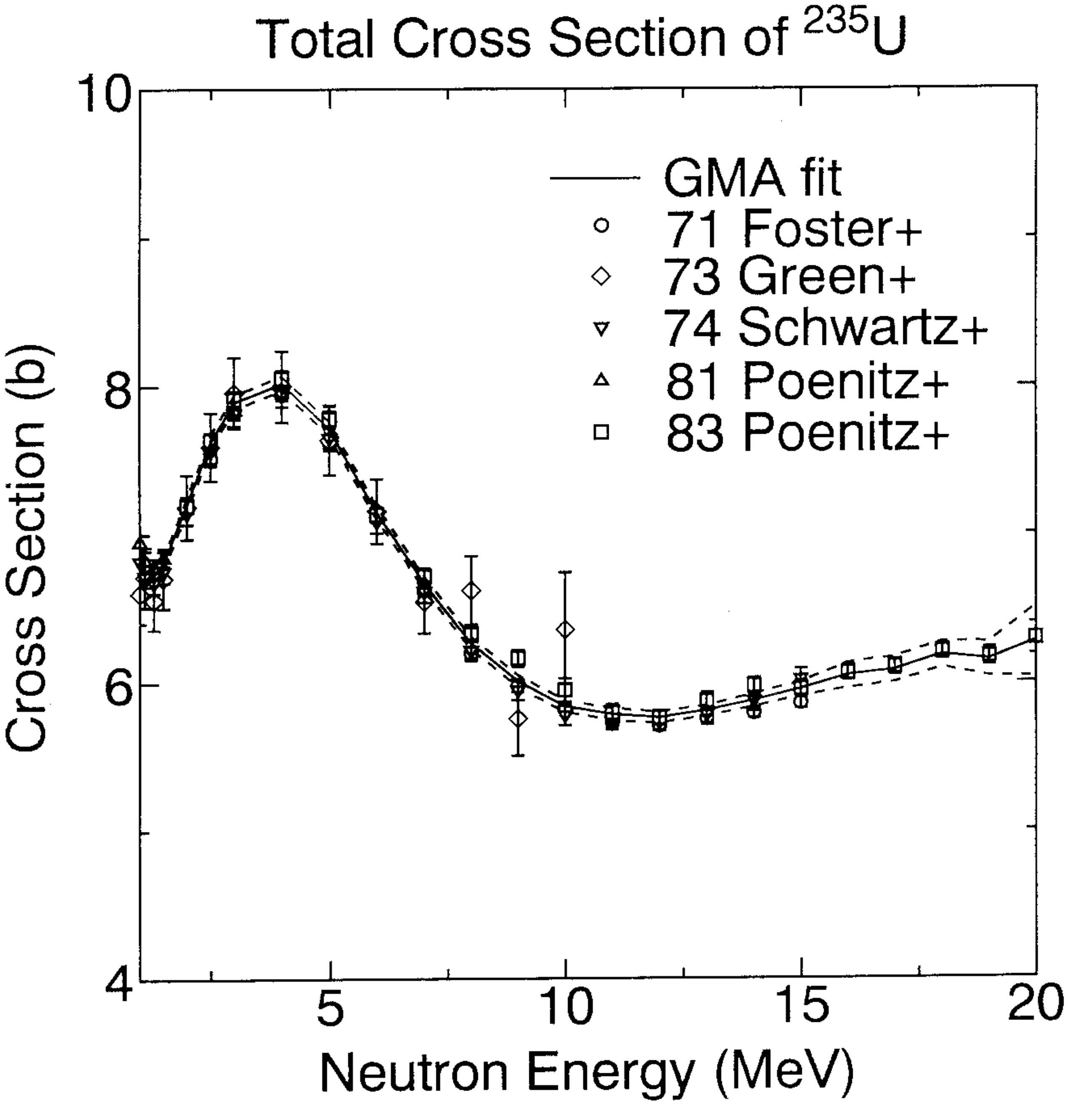

Fig. 20 Total cross section of ^{235}U above 1 MeV.

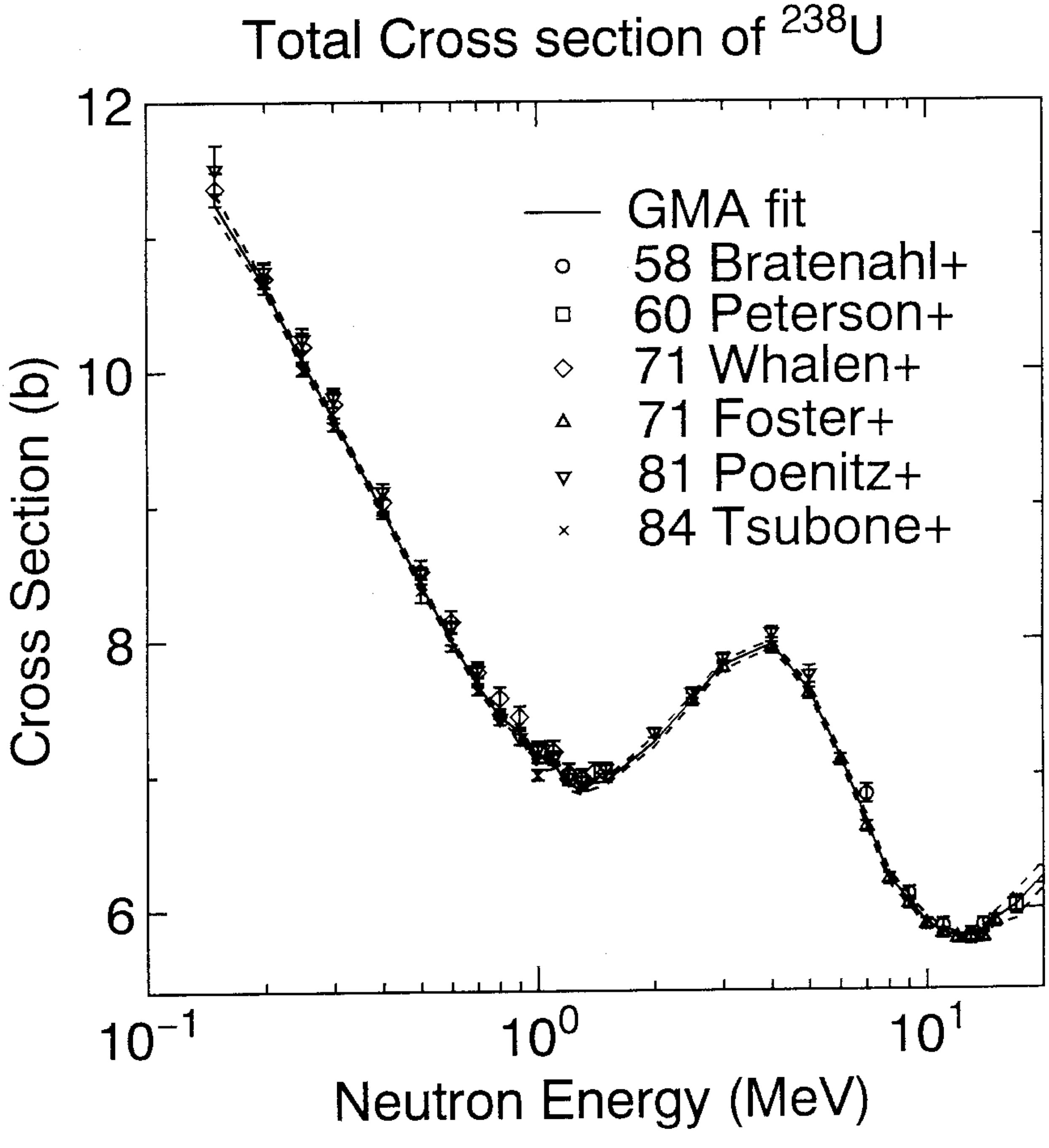

Fig. 21 Total cross section of ^{238}U.

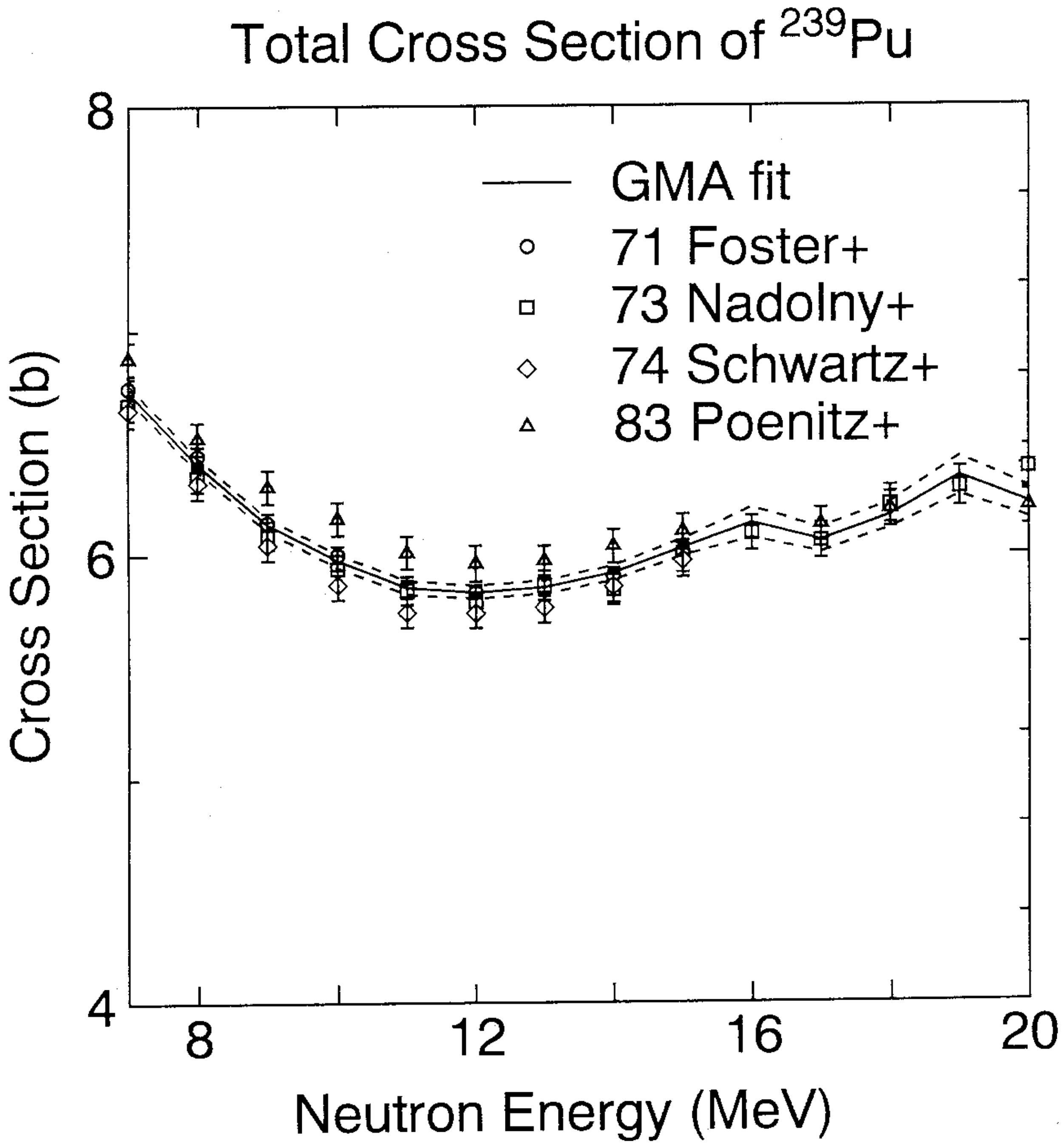

Fig. 22 Total cross section of ^{239}Pu.

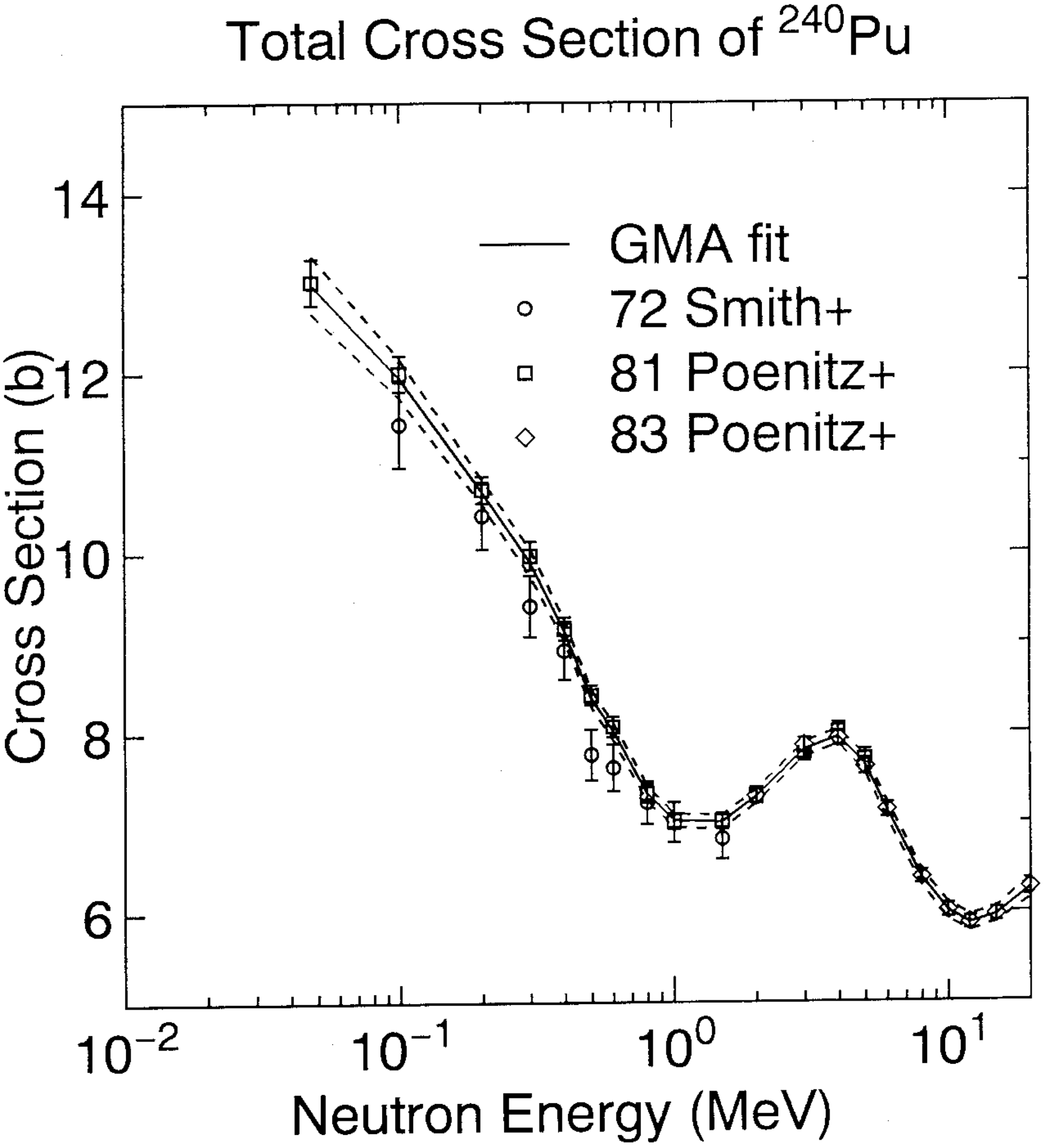

Fig. 23 Total cross section of ^{240}Pu.

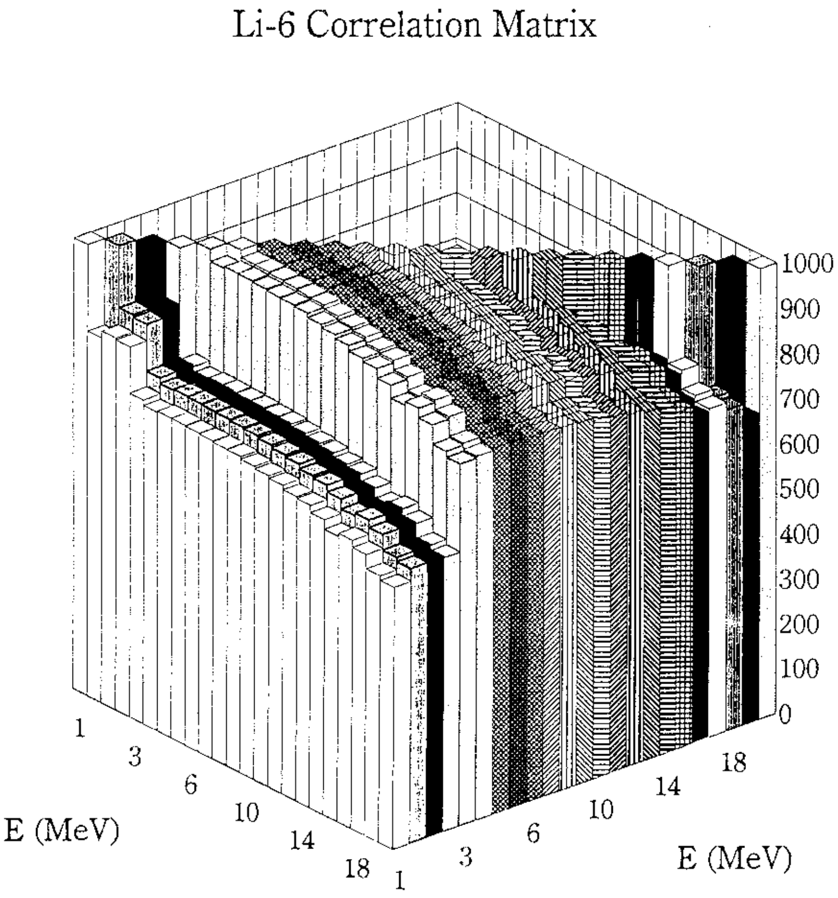

Fig. 24 Correlation matrix for ^{6}Li.

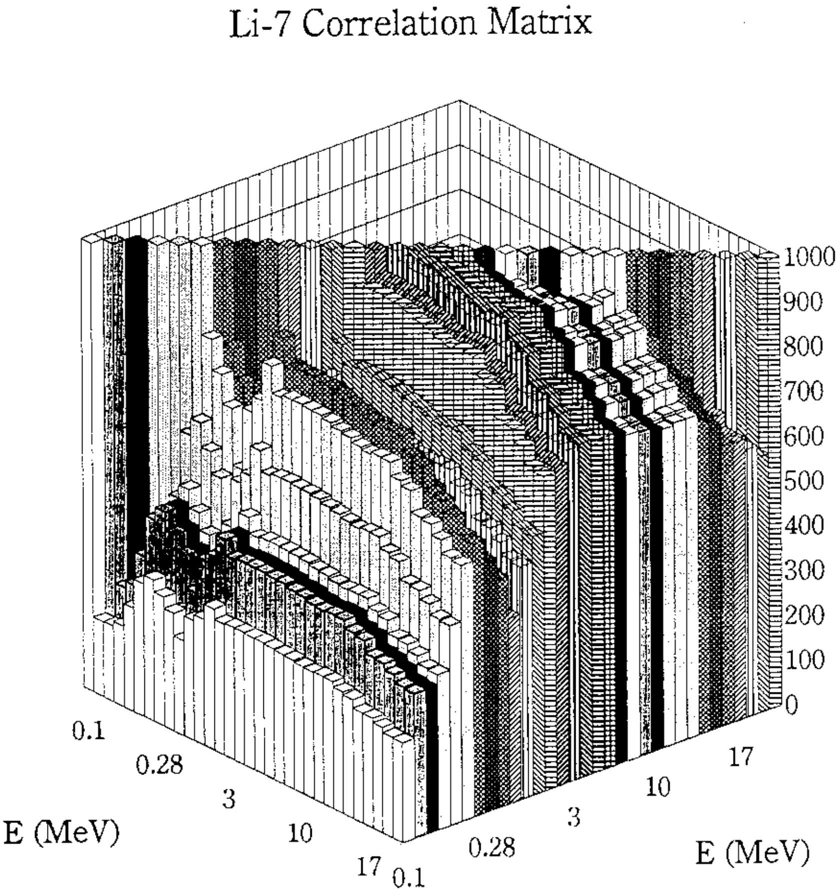

Fig. 25 Correlation matrix for ^{7}Li.

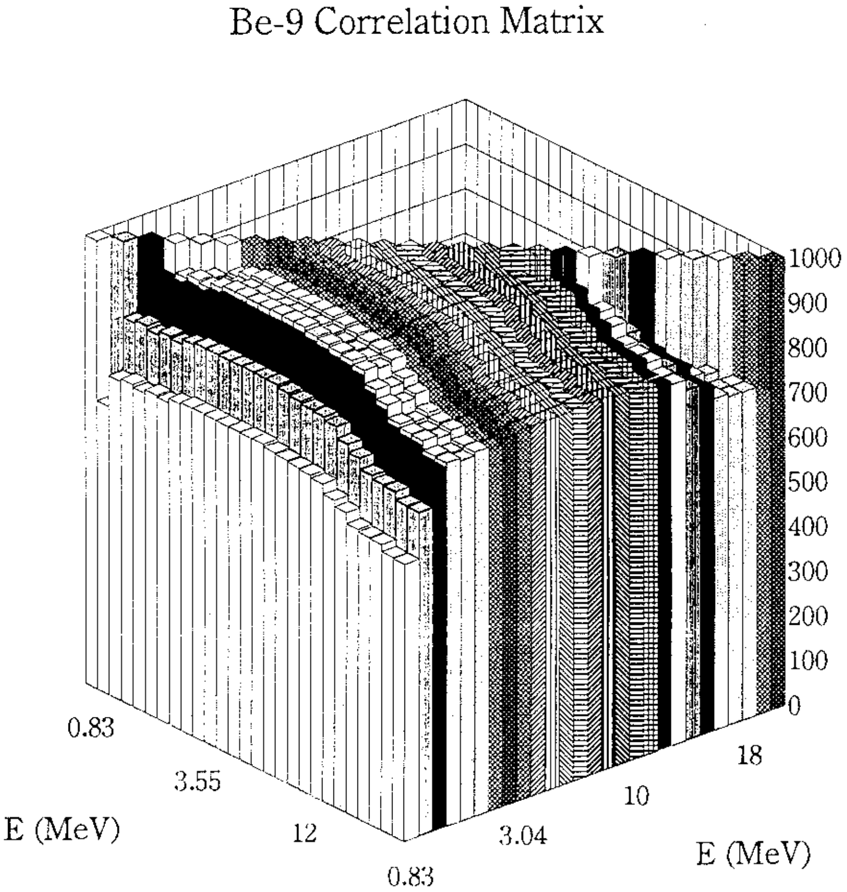

Fig. 26 Correlation matrix for ^{9}Be.

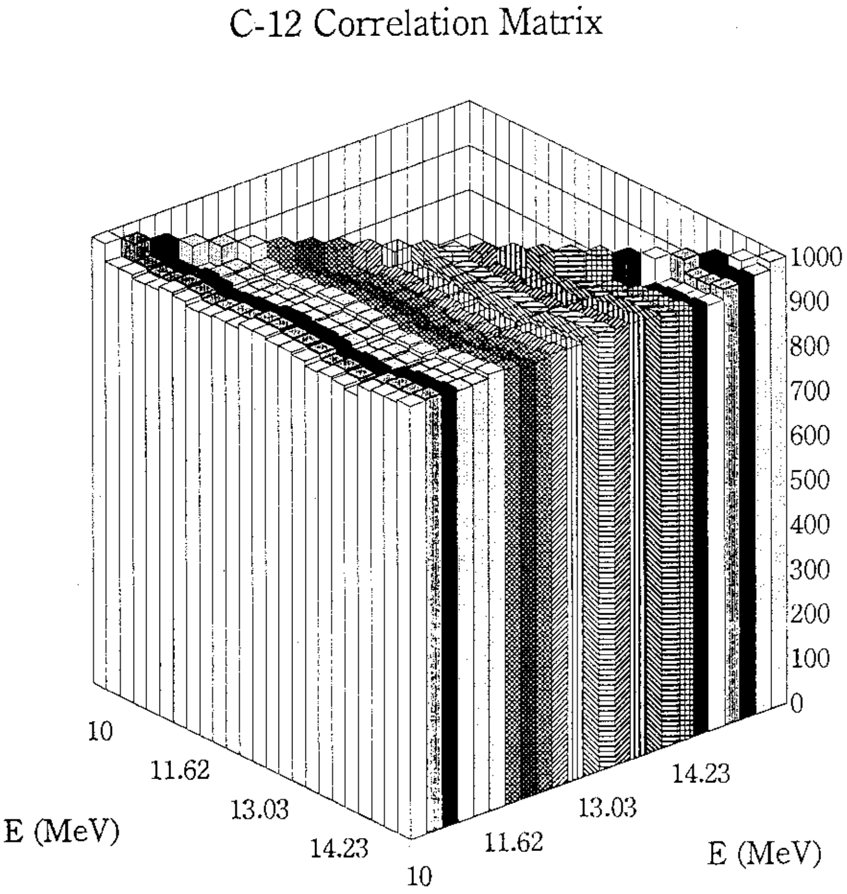

Fig. 27 Partial correlation matrix for ^{12}C above 10 MeV.

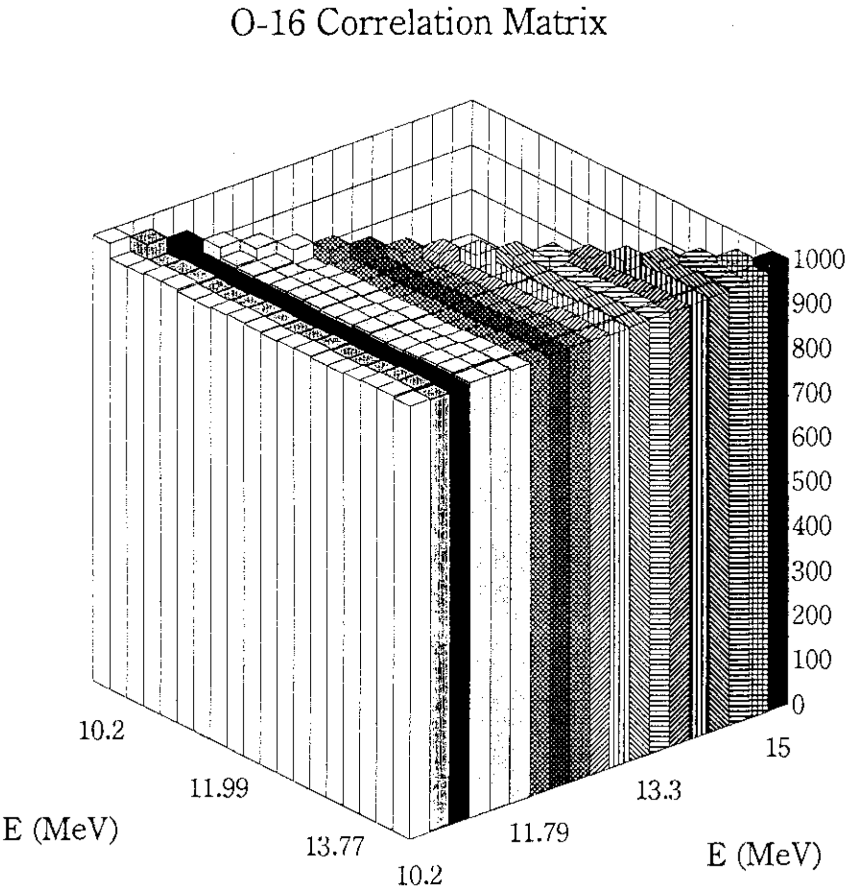

Fig. 28 Partial correlation matrix for ^{16}O above 10 MeV.

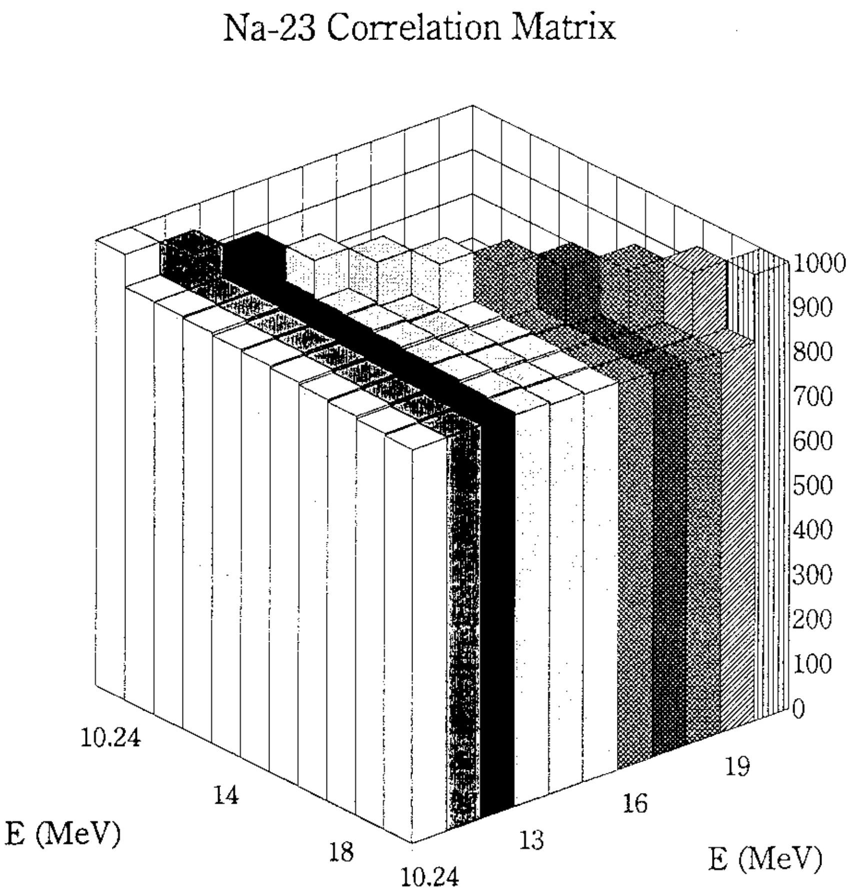

Fig. 29 Partial correlation matrix for ^{23}Na above 10 MeV.

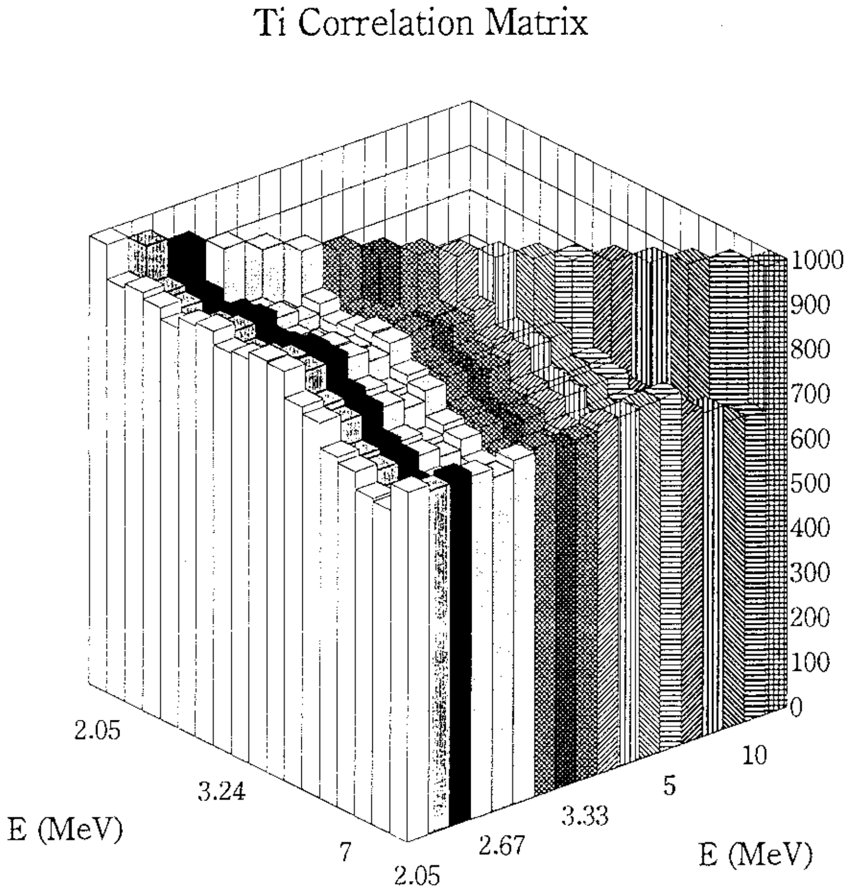

Fig. 30 Partial correlation matrix for Ti between 2 and 10 MeV.

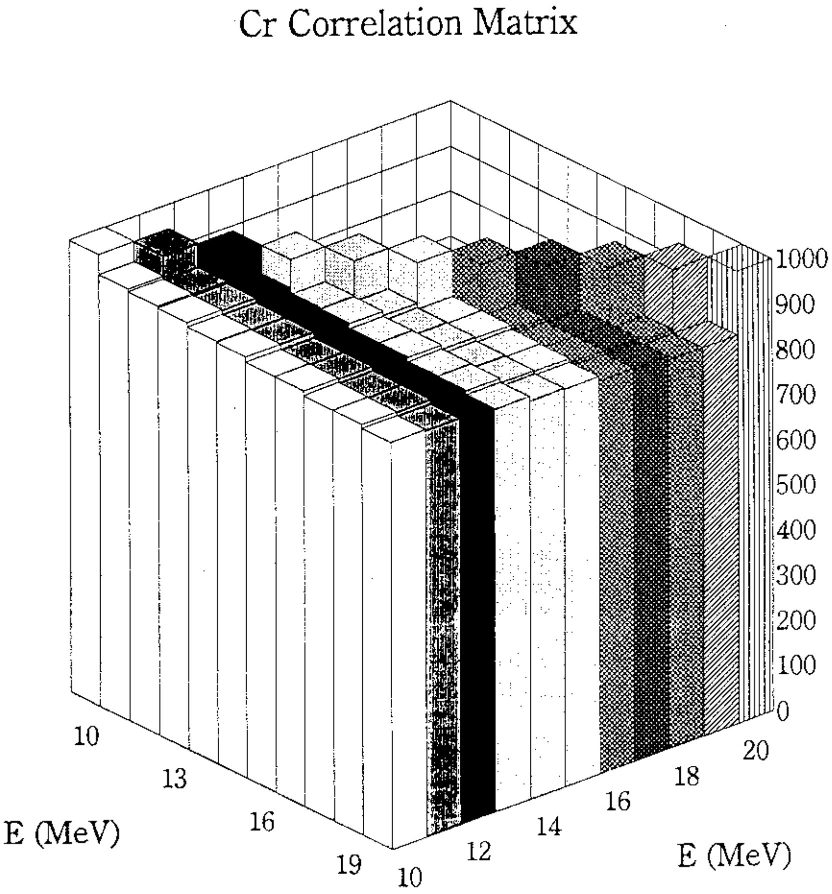

Fig. 31 Partial correlation matrix for Cr above 10 MeV.

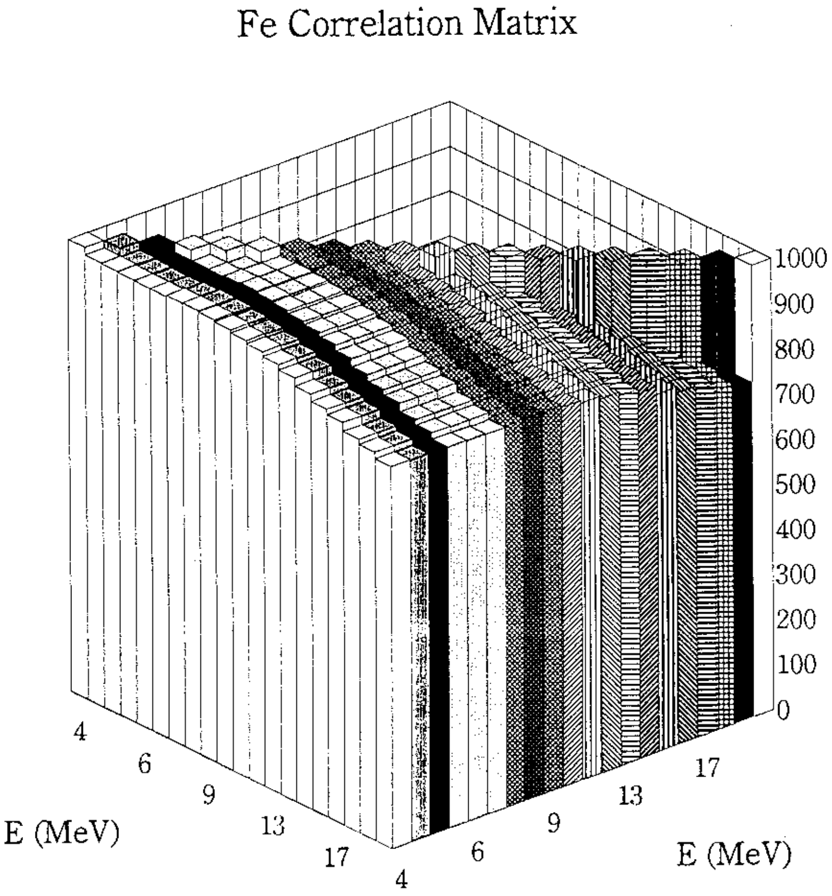

Fig. 32 Partial correlation matrix for Fe above 4 MeV.

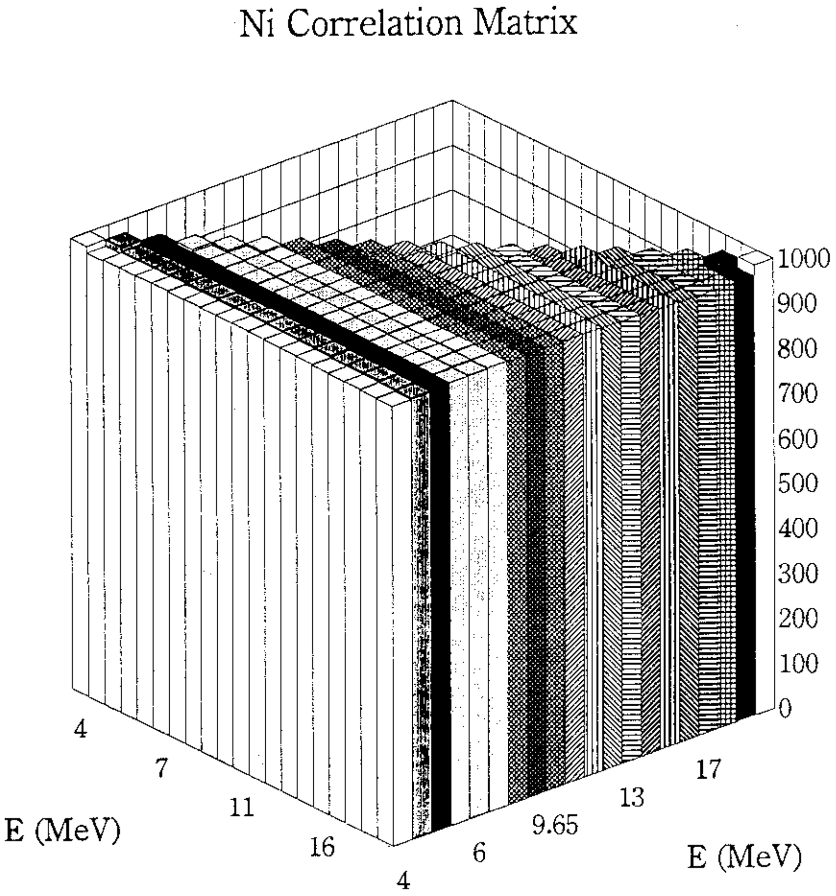

Fig. 33 Partial correlation matrix for Ni above 4 MeV.

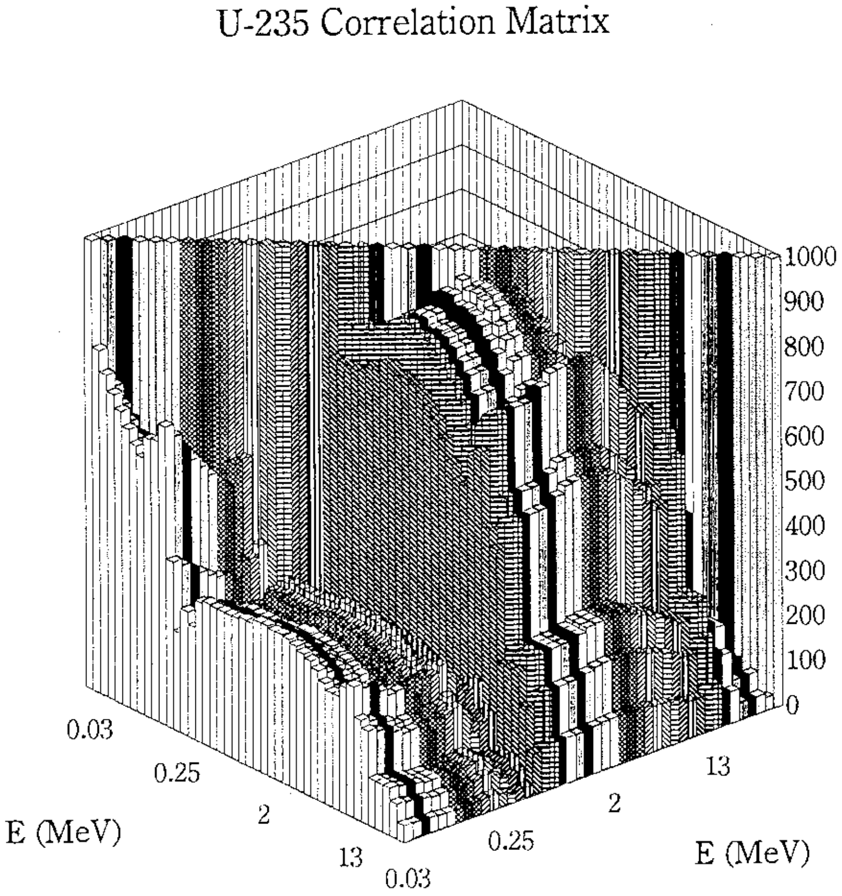

Fig. 34 Correlation matrix for ^{235}U.

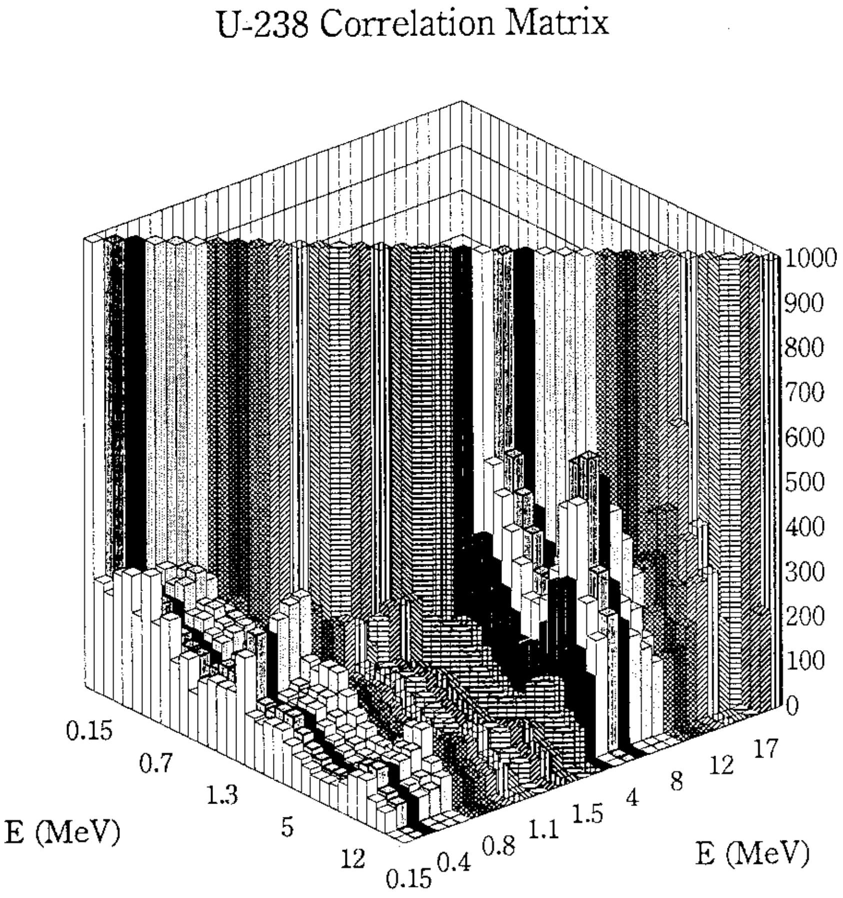

Fig. 35 Correlation matrix for ^{238}U.

Pu-239 Correlation Matrix

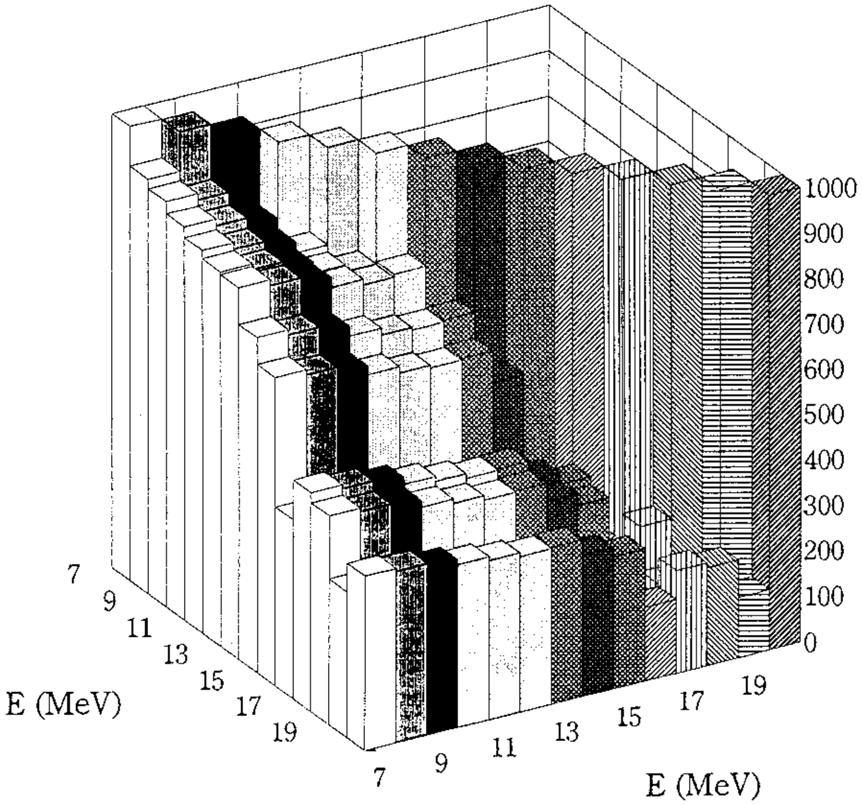

Fig. 36 Correlation matrix for ^{239}Pu.

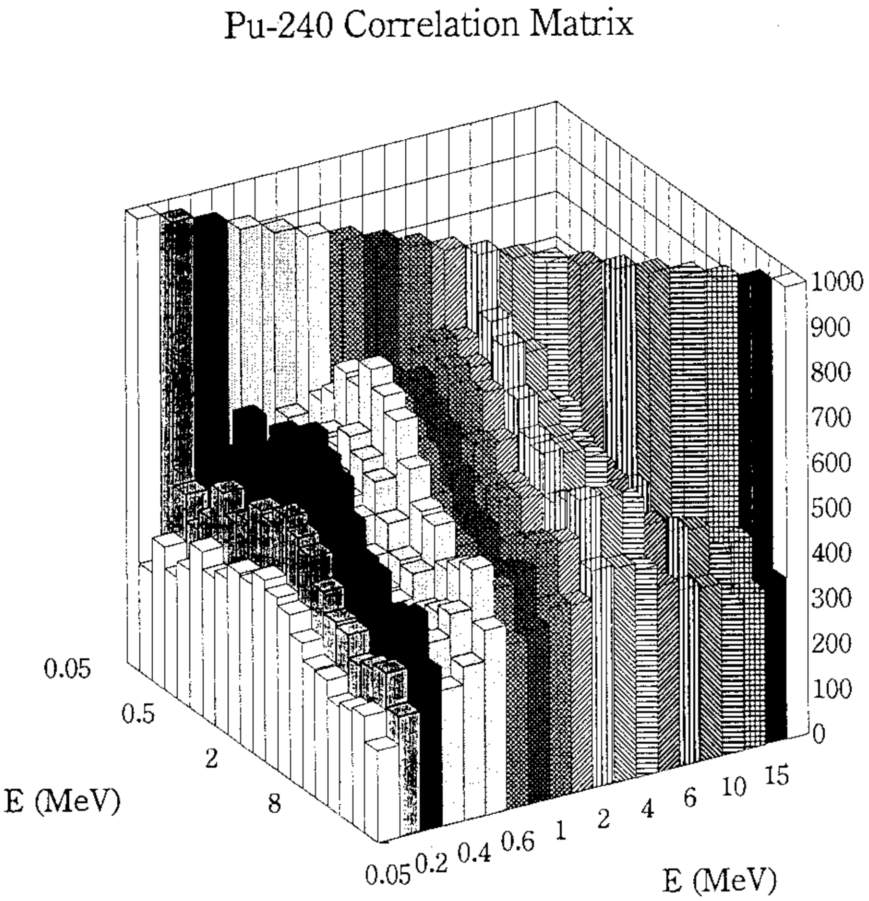

Fig. 37 Correlation matrix for ^{240}Pu.