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JEF-DOC - 336

NATURAL Cr AND Fe ISOTOPES EVALUATED FILES FOR JEF-2

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JEF/EFF Meeting, Saclay 3-6 Dec.1990.

In addition to the papers, presented as JEF-DOC reports at the previous JEF Meetings, on natural Cr and Fe isotope evaluated files and the corresponding preparation of processed libraries in the frame of a preliminary validation and testing, the present document is intented to briefly outline the last actions fulfilled according to the indications from the last Meeting.

i) Preliminary testing of the Fe files through NJOY code processing showed a number of negative values for kerma factors in ultra-fine group descriptions. As pointed out in NJOY feature description report kerma factors sometimes depend on relatively small differencies between large numbers when they are computed by the "energy-balance method", by wich "the energy allocated to neutrons and photons is simply subtracted from the available energy to obtain the energy carried away by the charged particles".

In this context it is very important to ensure the consistency of neutron and photon yields and average energies. By a carefull investigation inconsistencies were found coming from numerical errors in threshold energies and mainly from statistical fluctuation correction factors in yields and cross section data calculations respectively.

These inconsistencies were properly removed in the model and file processing (ULIXES code) chain and the resulting iron files gave rise to kerma factor as shown in figures 1 to 4.

The corrected files in ENDF/B-6 format were sent to NEA-Data Bank for JEF-2 purposes at the end of June 1990.

ii) For the puposes of benchmark testing of Fe data files, at the last JEF meeting, it was suggested to investigate the influence of extending the fine structure in the energy range above .862 MeV for elastic cross section as observed by experiments, but not taken into account by model code calculations. To this aim an "ad hoc" working file for Fe-56 was prepared by adopting elastic fluctuating (broad resolution) cross section from ENDF/B-6 in the energy range 0.862-5.15 MeV, even if in absence of the requested mean resonance parameters, and changing total

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cross section accordingly. The working File was made available to the NEA-DB for distribution to the mentioned purposes.

iii) Concerning Cr isotope evaluations in resolved resonance region, the selected parameters for bound levels as presented and discussed at previous JEF Meeting (within the comparison of calculated thermal cross sections and resonance integrals with experimental data) were finally adopted in the last Cr file release.

iv) As requested for completing the documentation already produced on Cr and Fe evaluation criteria and results, the presentation is made (figures 5 to 9 in the following) of additional typical cross section data of reaction leading to nuclides relevant for material activation estimate, according to the suggestion from previous JEF Meeting. In two significant cases comparison is also made with respect to JEF-1 data.

v) additional testing of the validity of evaluation models and methods concerned the comparison with experimental data of discrete gamma-ray emission data for Cr-52 and -53 and Fe-56 calculated upon request for gamma ray spectroscopy applications in activation analysis.
Significant examples are shown in annected figure 10 and tables I and II.

vi) In order to avoid errors by the checking programmes procedures the following rules were adopted by ULIXES code for file preparation:
- angular distribution (MF=4) are described by an even number of Legendre polynomial coefficients when necessary adding 0. value as the last coefficient; at lower energies, when a smaller number of coefficients was evaluated, a number of 0. values were added as many as needed to allow interpolation with higher energy values;
- in elastic scattering angular distibution (MF=4,MT=2) description at energies below the continuum region (where model anisotropic distribution were calculated) isotopic behaviour is assigned (including to lowest energy limit of the file);
- for emitted particle energy distributions description (MF=5 and MF=6) at threshold energies a conventional approach was assigned allowing for consistent calculations avoinding errors in checking programmes;
- emitted gamma yields (MF=12) as obtained at the lowest energy value considered in model calculations (KeV region) were assumed valid also at the lower file energies; the same rule was adopted for emitted gamma energy distribution (MF=15).

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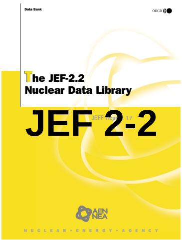

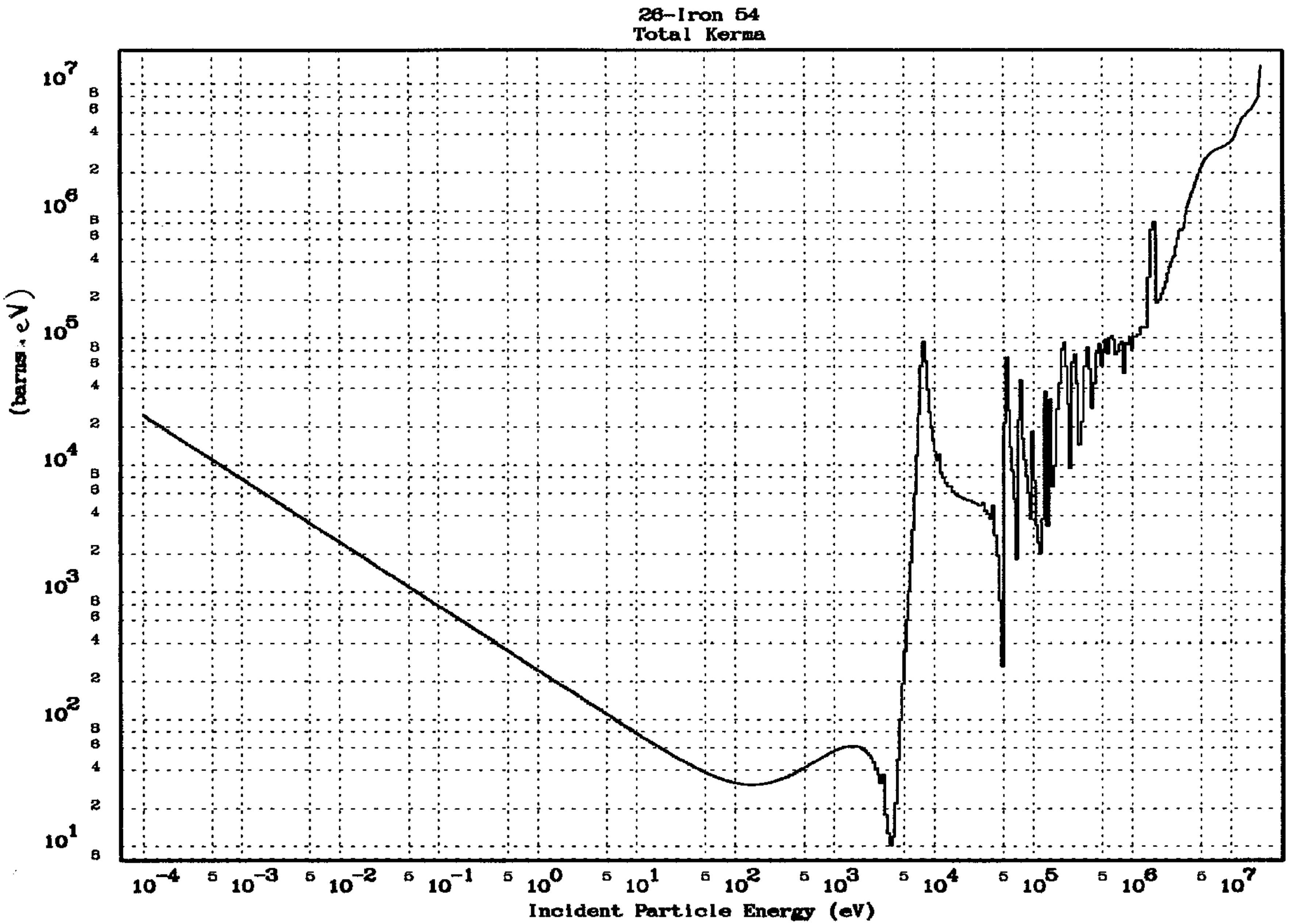

Fig. 1

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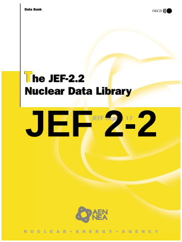

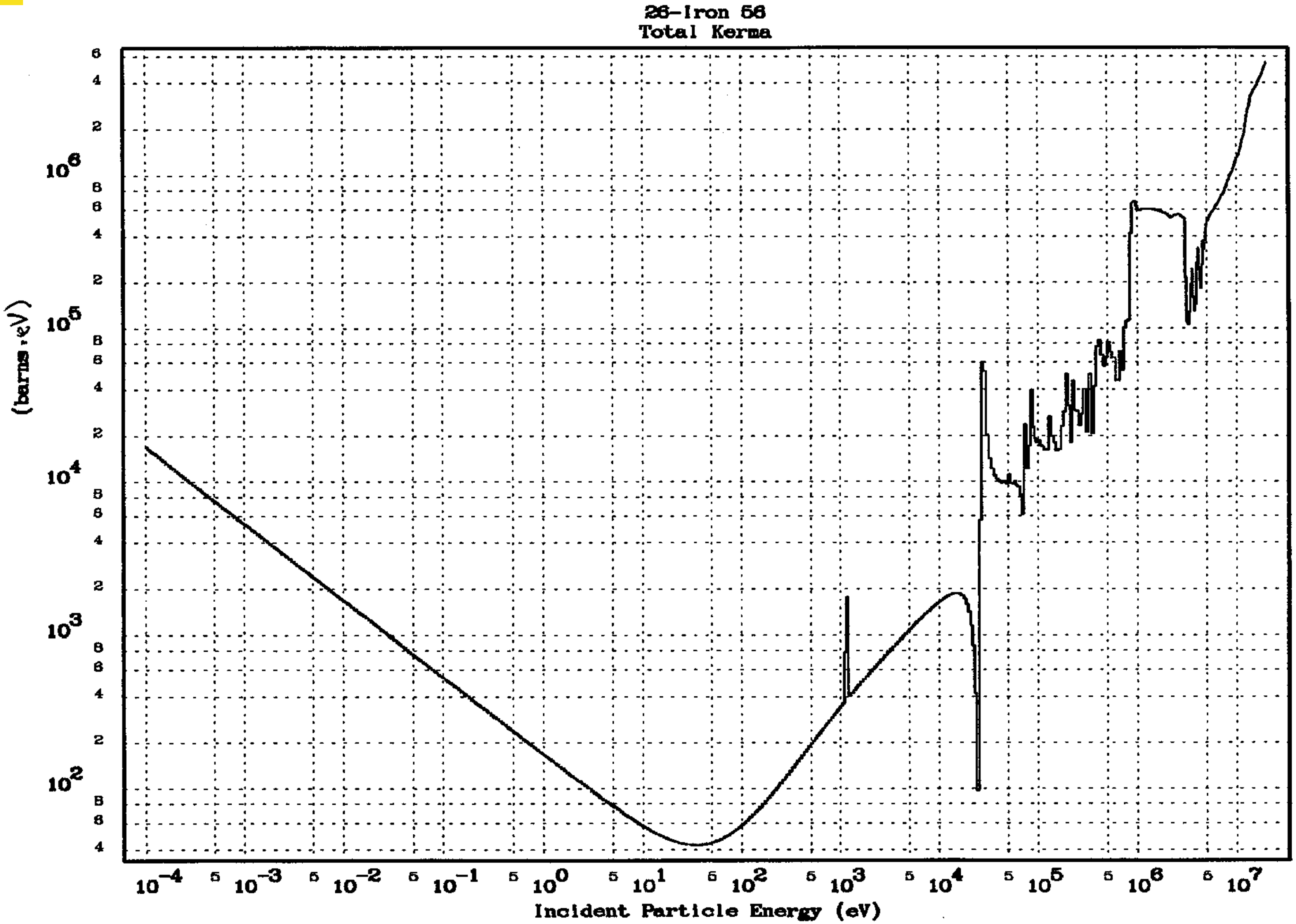

Fig. 2

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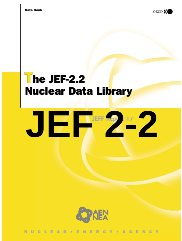

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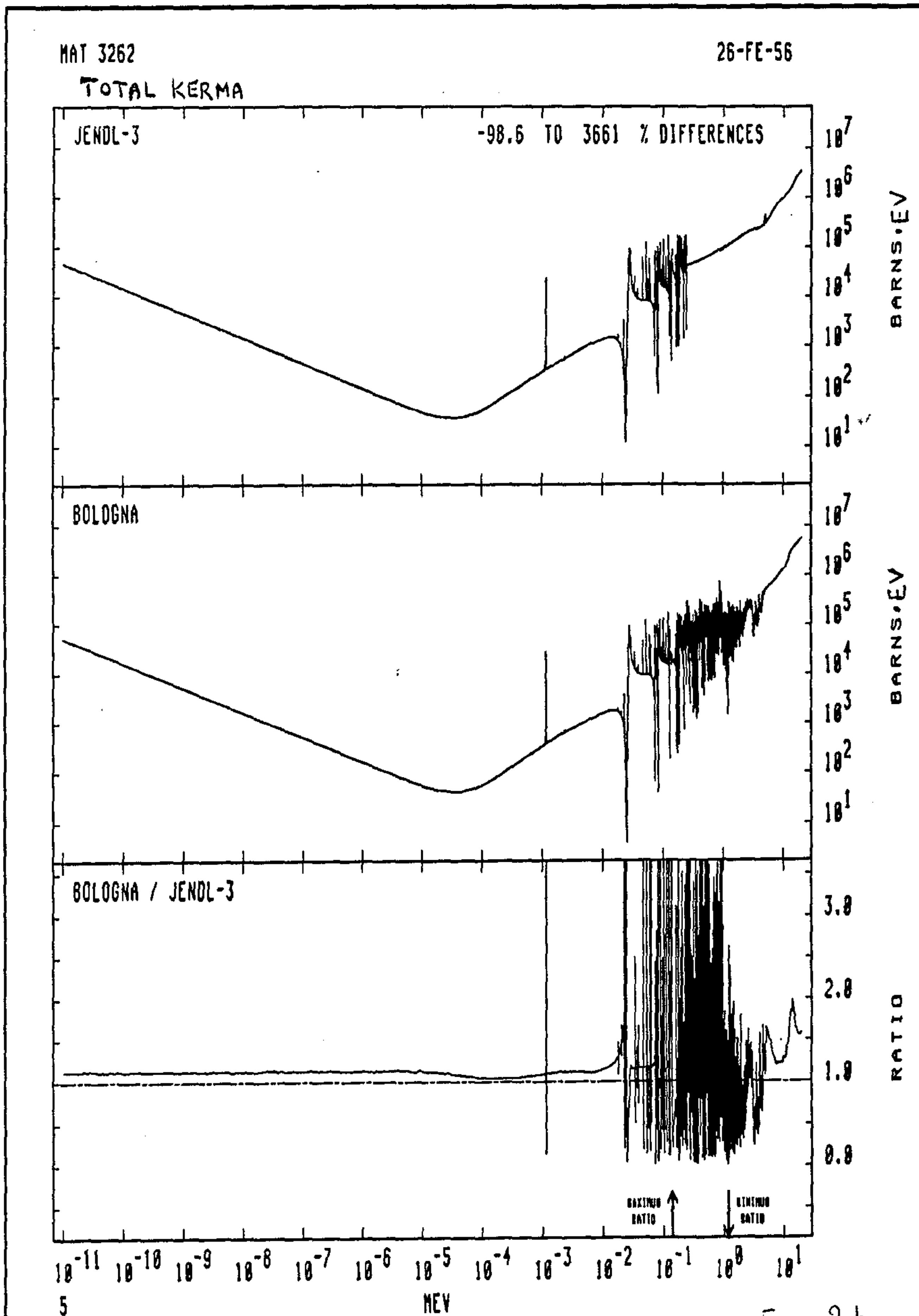
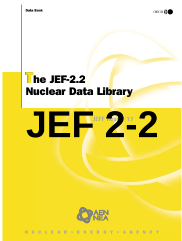


MAT 3262
26-FE-56
TOTAL KERMA
JENDL-3
-98.6 TO 3661 % DIFFERENCES
BOLOGNA
BOLOGNA / JENDL-3
BARNS.EV
BARNS.EV
RATIO
MAXIMUM RATIO
MINIMUM RATIO
MEV
5

Fig. 2b



MAT 3263 26-FE-57

TOTAL KERMA

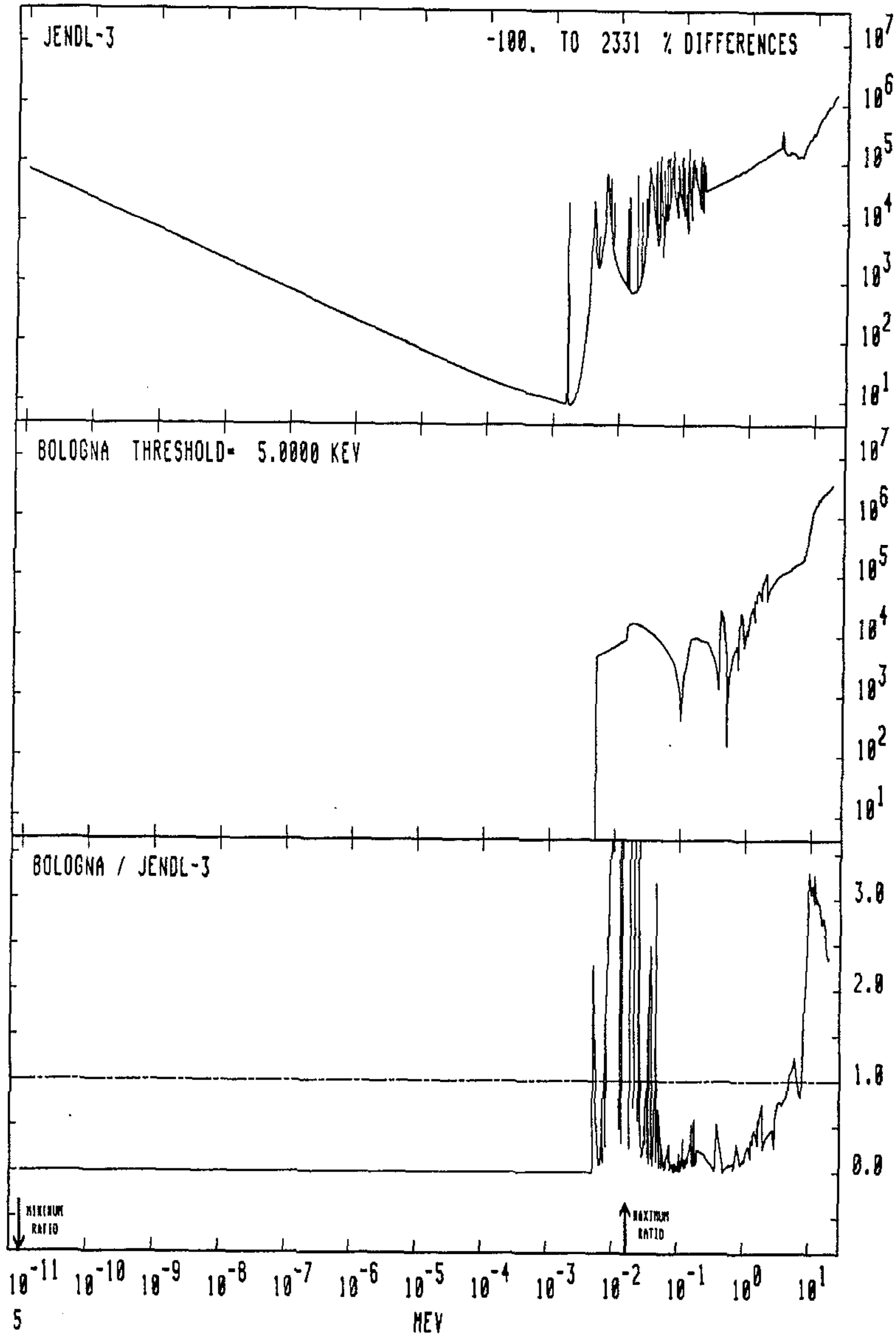
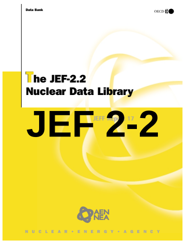


Fig. 3



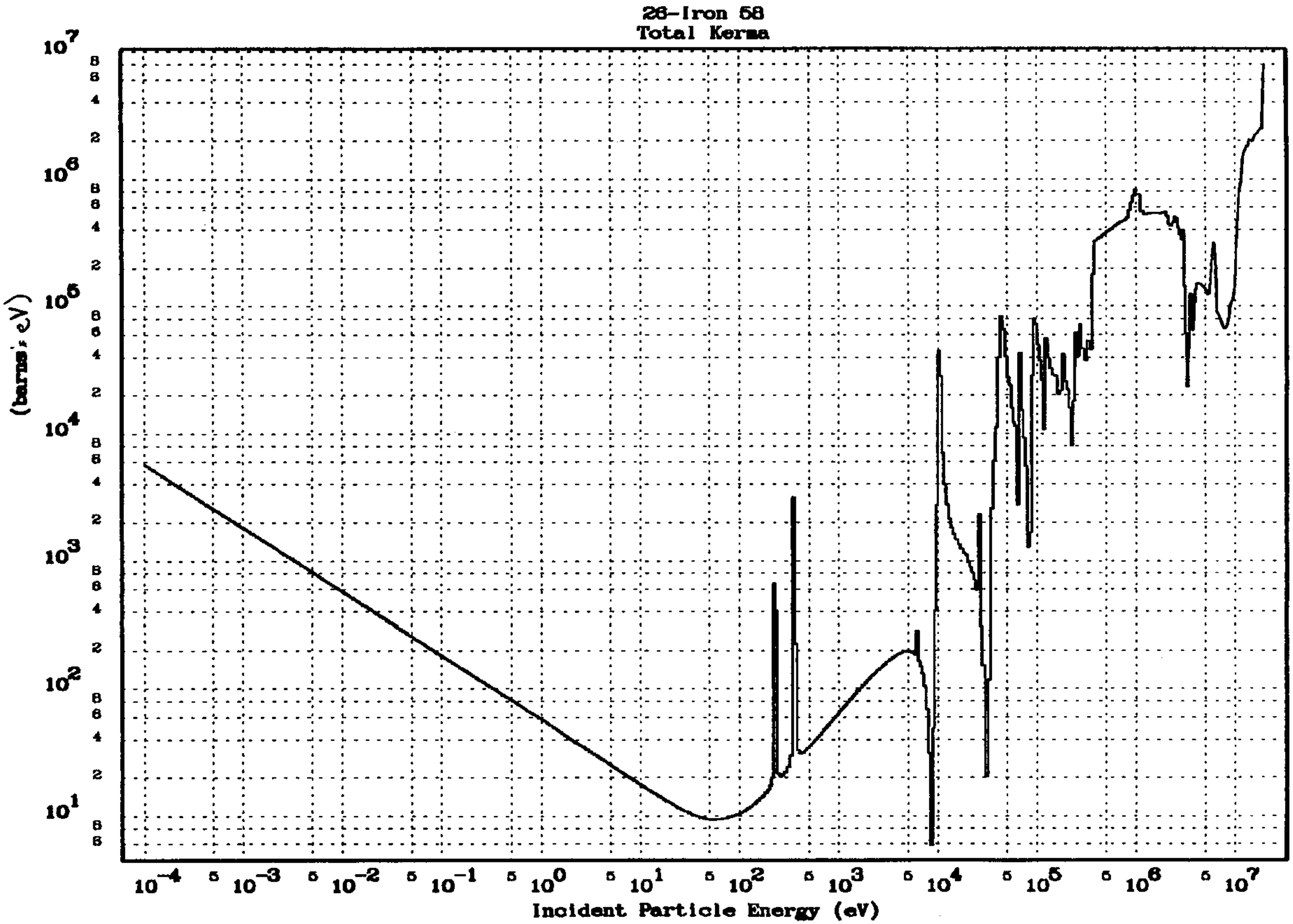


Fig. 4

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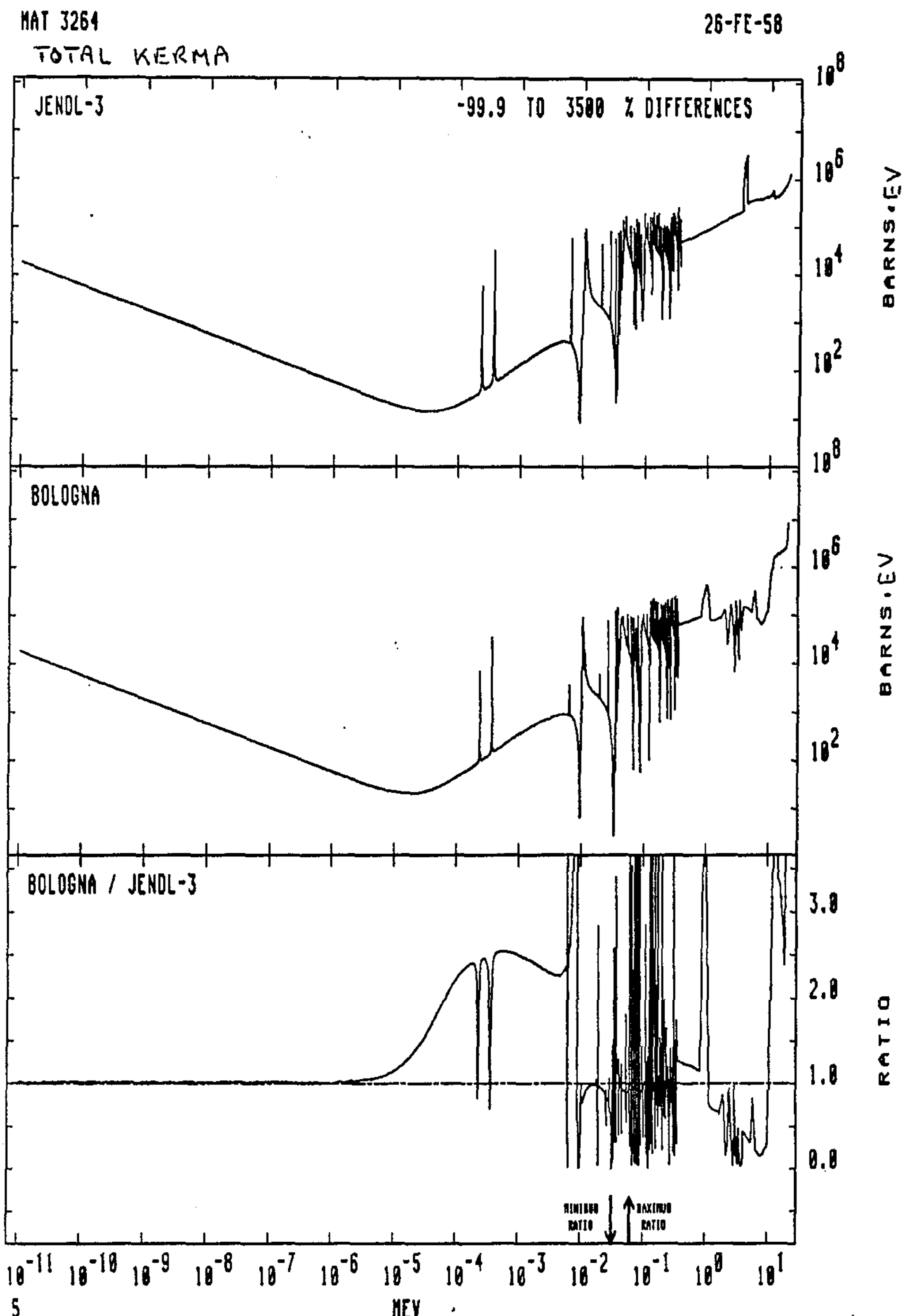

Fig. 4b

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SELECTED EXPERIMENTAL DATA FROM EXFOR

CHROMIUM-53 (N,P),,SIG

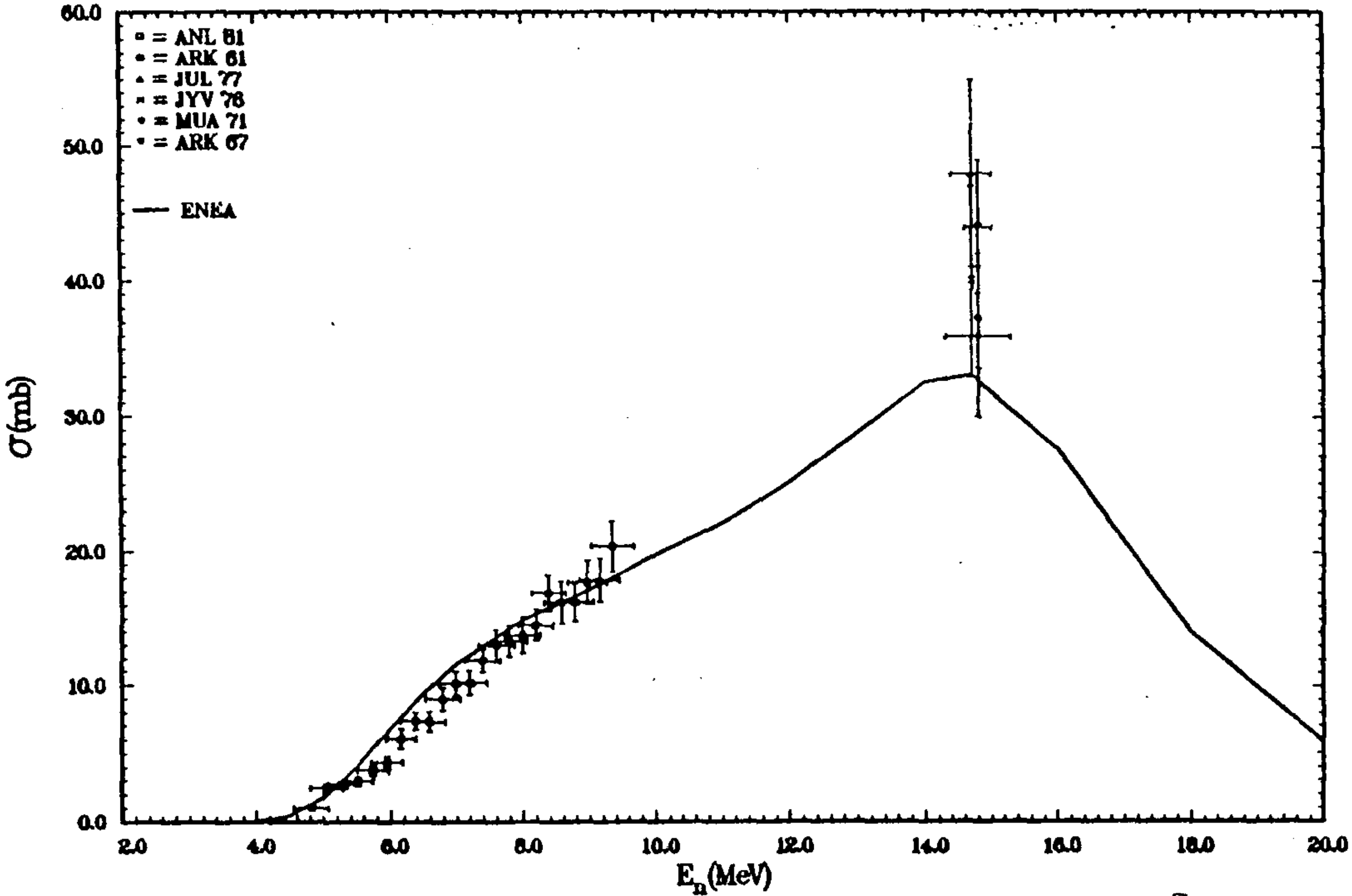

fig. 5

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SELECTED EXPERIMENTAL DATA FROM EXFOR

CHROMIUM-52 (N,2N),,SIG

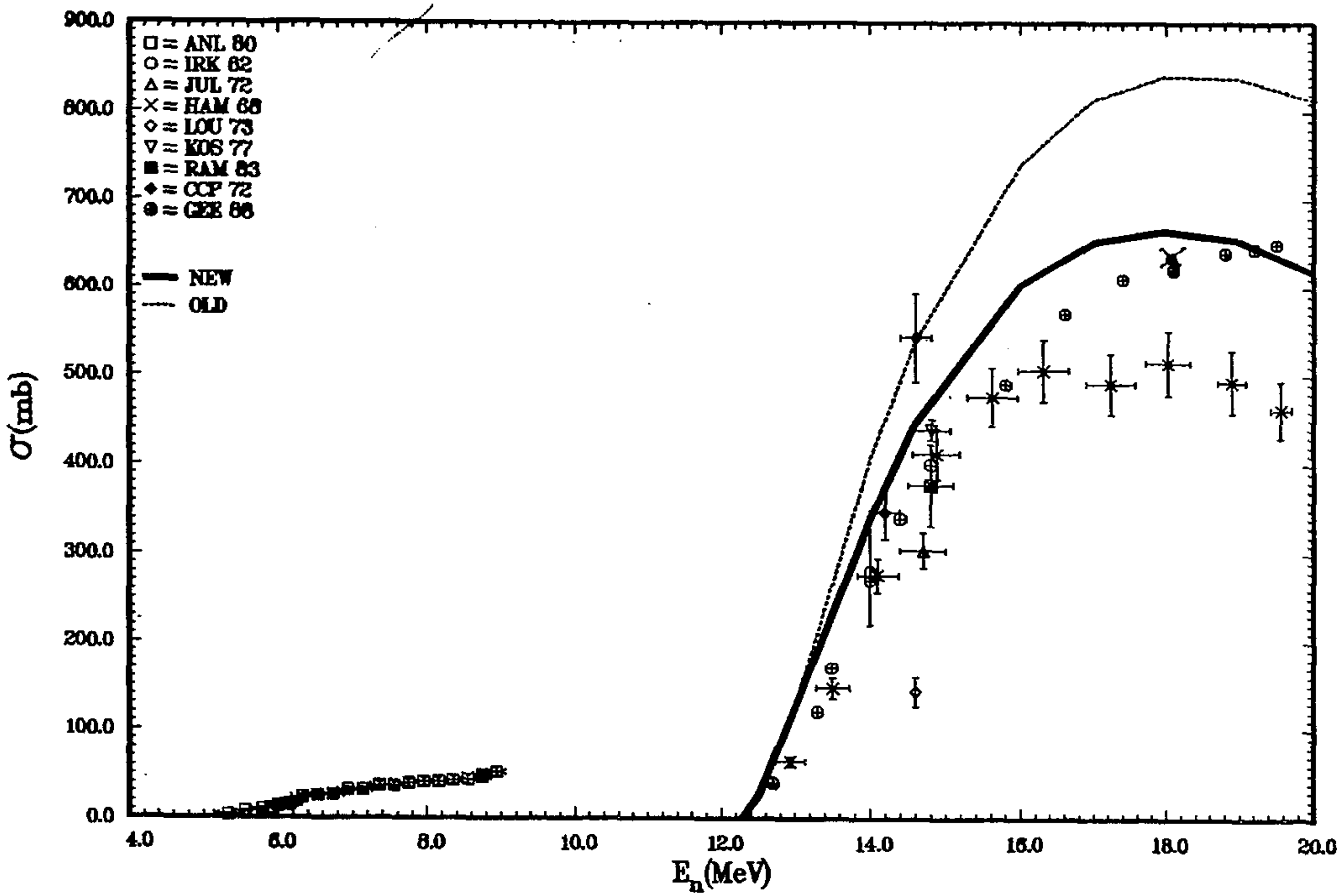

Fig. 6

✗ Recent (July '89) datum from

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SELECTED EXPERIMENTAL DATA FROM EXFOR

IRON-56 (N,P),,SIG

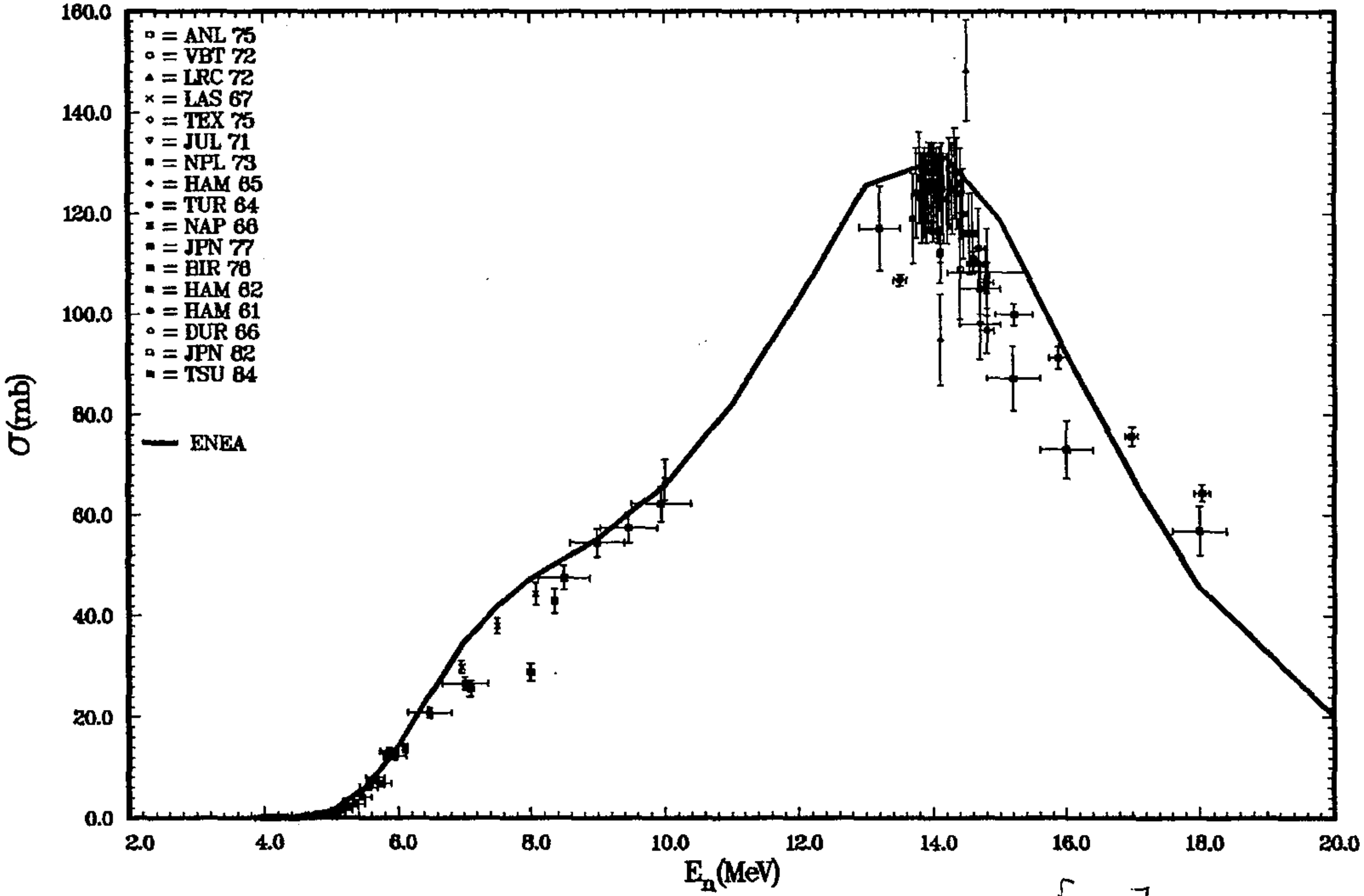

Fig. 7

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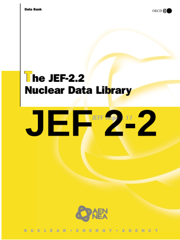

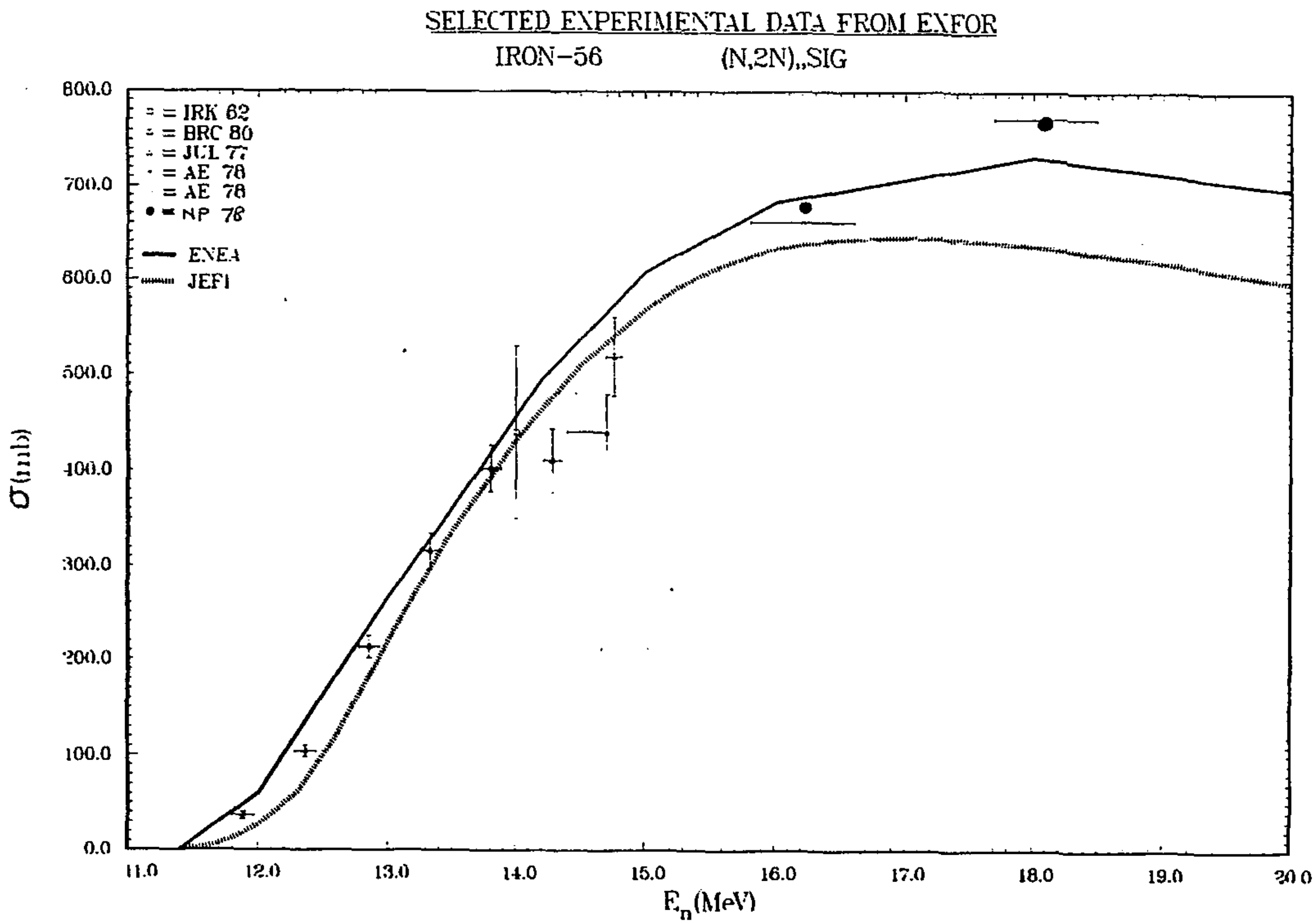

Fig. 8

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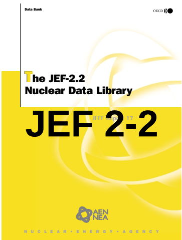

SELECTED EXPERIMENTAL DATA FROM EXFOR

NATURAL IRON (N,A),,SIG

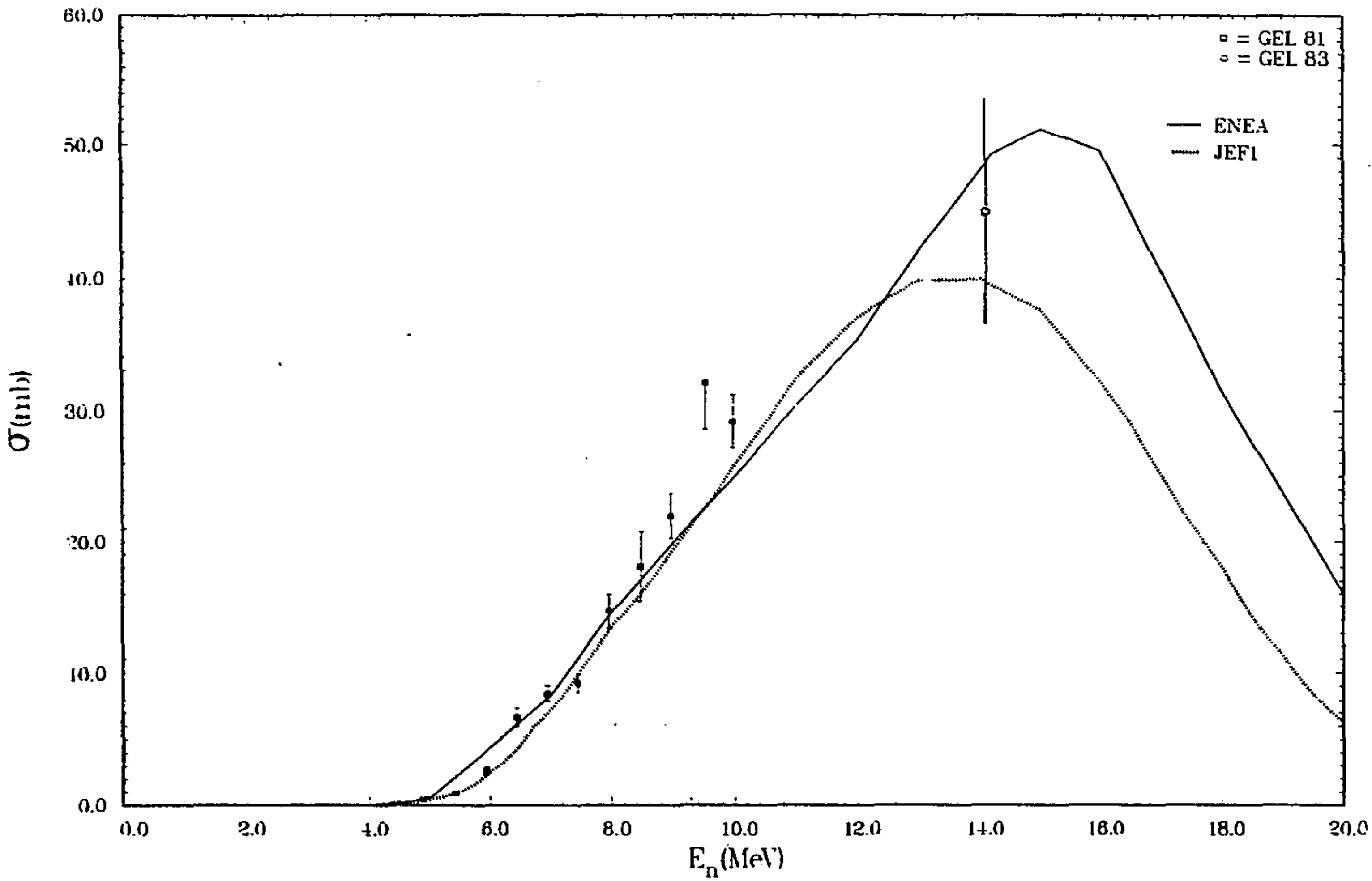

Fig. 9

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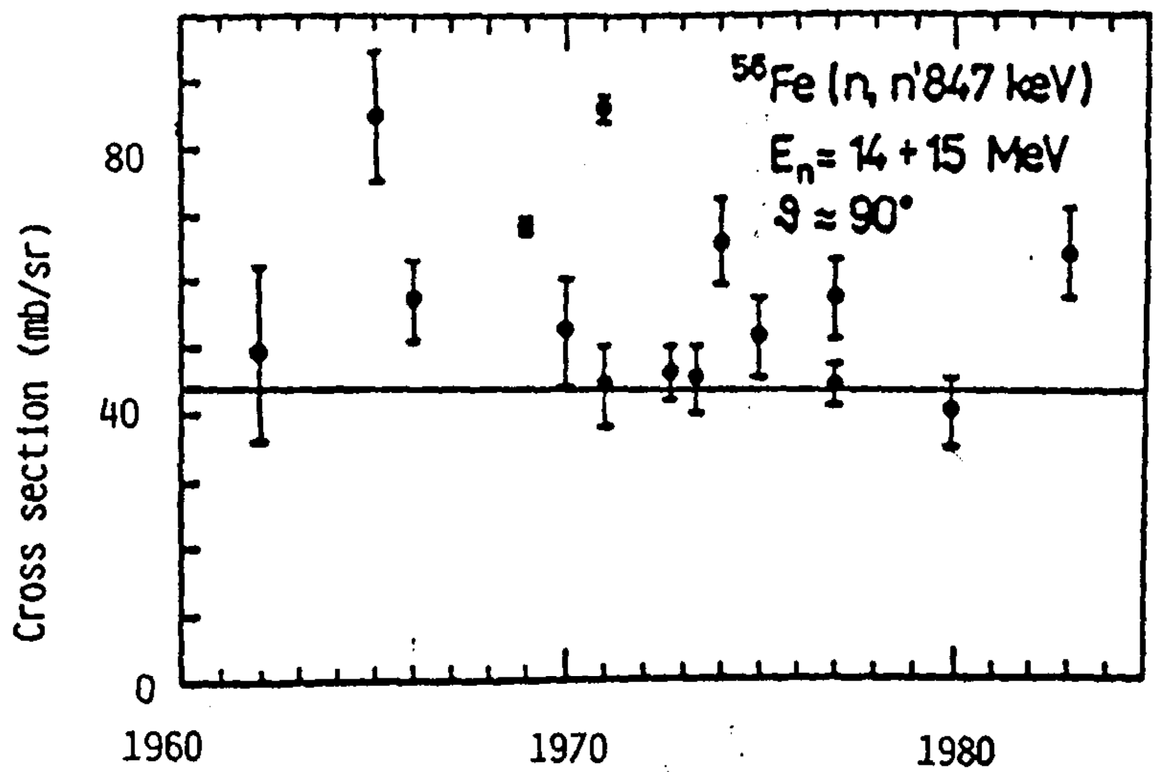
Fig.10



Production cross section for the 847 keV gamma line at 90° from ^{56}Fe(n,n' gamma) reaction measured in several laboratories. Solid line: present calculations.

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TABLE I

GAMMA-RAY PRODUCTION RATES FOR ^{52}CR(N,N'γ) REACTION AT E_n = 14.2 MeV

TRANSITION $J^{\pi}_{i} - J^{\pi}_{f}$	E_{γ} (MeV)	$\sigma_{n,n'\gamma_i} / \sigma^{TOT}_{n,n'\gamma}$ (%) EXP.	CALC.
2^+_3 2^+_1	1.728	3.3 ± 0.6 (2)	3.5
2^+_2 2^+_1	1.531	5.1 ± 0.6 (2)	4.7
2^+_1 0^+_1	1.434	---	91.8
4^+_2 2^+_1	1.334	24.3 ± 1.8 (2), 30.0 ± 6.7 (4)	25.3
5^+_1 4^+_1	1.246	4.3 ± 0.5 (2)	3.8
4^+_1 2^+_1	0.936	26.5 ± 1.8 (2), 26.8 ± 5.7 (4)	34.7
5^+_1 4^+_2	0.848	4.1 ± 0.5 (2)	2.7
6^+_1 4^+_1	0.744	7.9 ± 0.7 (2)	14.2
3^+_1 4^+_2	0.704	4.7 ± 0.5 (2)	5.8
4^+_3 4^+_2	0.647	7.8 ± 0.9 (2)	6.2

TABLE II

Gamma-ray production rates for $^{56}Fe(n,n'\gamma)$ reaction at E_n = 14.2 MeV and $\theta = 125°$

transition $J_i^\pi \rightarrow J_f^\pi$	E_γ (kev)	$d\sigma/d\Omega$ $(n,n'\gamma)$ (mb/sr) calc.	expt.		
$2_1^+ \rightarrow 0_1^+$	847	42.3	45.6 ± 5.0[a]	86.3 ± 7.5[b]	48.6 ± 4.0[d] 65.6 ± 7.0[c] 65.4 ± 4.6[e]
$4_2^+ \rightarrow 4_1^+$	1038	3.78		4.8 ± 0.8[b]	4.0 ± 0.8[d] 5.9 ± 0.6[e]
$4_1^+ \rightarrow 2_1^+$	1238	20.4	25.2 ± 3.0[a]	40.0 ± 3.5[b]	26.2 ± 1.9[d] 29.7 ± 2.1[e]
$6_1^+ \rightarrow 4_1^+$	1303	3.77		9.0 ± 1.0[b]	8.8 ± 1.0[d] 5.7 ± 0.6[e]
$3_1^+ \rightarrow 4_1^+$	1360	0.29			0.72 ± 0.24[e]
$2_2^+ \rightarrow 2_1^+$	1811	1.85		7.3 ± 0.8[b]	2.4 ± 0.6[d] 5.4 ± 0.6[e]
$0_2^+ \rightarrow 2_1^+$	2095	0.20			0.53 ± 0.37[e]*
$2_3^+ \rightarrow 2_1^+$	2112	0.84		2.1 ± 1.1[b]	1.9 ± 0.5[e]
$1_1^+ \rightarrow 2_1^+$	2273	0.47			0.64 ± 0.45[e]
$2_4^+ \rightarrow 2_1^+$	2521	0.43		3.6 ± 1.0[b]	1.7 ± 0.5[e]
$3_1^+ \rightarrow 2_1^+$	2596	1.14		4.7 ± 1.1[b]	2.8 ± 0.7[d] 3.0 ± 0.6[e]
$3_1^- \rightarrow 0_1^+$	3070	4.74			

(a) ref. (18) ; E_n = 14.2 Mev; $\theta = 90°$
(b) ref. (7) ; E_n = 14.8 Mev; $\theta = 125°$
(c) ref. (19) ; E_n = 14.2 Mev; $\theta = 122°$
(d) ref. (20) ; E_n = 14.1 Mev; $\theta = 90°$
(e) ref. (21) ; E_n = 14.9 Mev; $\theta = 90°$

(*) Without identification in ref.(20) ; transition proposed in this work.

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