

INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION



INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONES: 224281/2/3/4/5/6
CABLE: CENTRATOM - TELEX 460392-1

SMR/108-5

WORKSHOP ON NUCLEAR MODEL COMPUTER CODES

16 January – 3 February 1984

REPORT ON THE INTERNATIONAL NUCLEAR MODEL CODE INTERCOMPARISON
SPHERICAL OPTICAL AND STATISTICAL MODEL STUDY

Enrico SARTORI

NEA Data Bank
91191 Gif-sur-Yvette Cedex
France

These are preliminary lecture notes, intended only for distribution to participants.
Missing or extra copies are available from Room 231.



Report on the
International Nuclear Model Code Intercomparison
Spherical Optical and Statistical Model Study

A. Prince, BNL, Brookhaven, USA

G. Reffo, ENEA-Bologna, Italy

F. Sartori, CECOD/NEA Data Bank

Work carried out at NEA Data Bank, 91191 Gif-sur-Yvette CEDEX; France

"The will is infinite and the
execution confined, the desire
is boundless and the act a
slave to limit"

E. Cesàro

I. INTRODUCTION

International Code Intercomparisons have been carried out during the last decade on different topics: Radiation Shielding, Reactor Safety, Reactor Dynamics, Reactor Noise and also Nuclear Models. They follow a rather regular pattern.

After a first comparison, which normally shows rather discrepant results, the exercise is repeated with some additional specifications, which are intended to limit the use of personal judgement in the choice of some parameters. The new results agree better, but to obtain good agreement, some codes have to be modified. It is interesting to observe that this happens also when everybody is using the "same" program.

To use computer codes, i.e. to translate a physical or mathematical problem into a program input, requires a certain craftsmanship that can only be acquired with experience. The "turn the handle" approach often leads to erroneous results.

It is also with this in mind that such benchmark exercises are carried out. The different iterations needed to obtain "convergence" of the results given by the different participants provide much insight for both participants and later users about how to use the different codes, their fine qualities and deficiencies as well as the limitations in the way a physical process in the code is modelled.

After the first intercomparison on the 59-Co cross sections, an improved version of the spherical optical model code was submitted by the French Code Intercomparison Working Group (CIWG) under the chairmanship of A. Prince (BNL). This study resulted in a significant improvement in agreement for calculations of total, elastic, inelastic, capture and threshold reaction cross sections for the six codes of US origin considered.

Prince then suggested an extension of this comparative study to include codes of European and Japanese origin, with the collaboration of the Nuclear Energy Agency Nuclear Data Committee and the Nuclear Energy Agency Data Bank. He suggested using the same cross section calculation for 59-Co as already carried out in the frame of CSFWG NMCS.

Thus the present study is an intercomparison of cross section calculations made with various nuclear model codes. We do not aim to achieve agreement with experimental data, but to pin-point errors and deficiencies in codes and to create confidence in code calculations where experimental data is non-existent.

The parameter specification of the exercise is given in Appendix I.

Each participant was asked to use the same:

- set of parameters (e.g. optical model parameters, level density parameters, level schemes, mass excesses);
- giant resonance parameters;
- normalization for the radiative width;
- level density formulation;
- spin and parity distribution laws;
- optical model and statistical model formalisms.

Due to the special features and limitations of some of the codes used, input and model differences were introduced by some participants with respect to the original formulation of the exercise. These cases are pointed out in the tables and discussed in the section dealing with the analysis of the results.

At energies above about 14 MeV, pre-equilibrium processes contribute appreciably to the cross sections. These may be calculated in several different ways, and a detailed comparison of these will be made in a later report.

The results are presented in comparative tables and graphs. The computed quantities are shown for each incident energy and each code and for each reaction separately.

In this exercise the participants went through two iterations. Better convergence of the results have been achieved in this way because some of the participants have tried, in the second iteration, to comply as strictly as possible with the parameter specifications.

This exercise will be useful to those who are just starting on neutron cross section calculations. It will also help the user to verify the validity of different computer codes by comparing the results obtained from different computer codes and trying to implement the "standard" codes against the results provided by "experimental" codes used in this exercise.

This study should also prove useful to those who are just starting on neutron cross section calculations.

The results included in this report also show the present state of the art in the statistical model calculations and indicate the degree of confidence one can place in the cross sections derived from them. It is hoped that authors of codes used in this study will be willing to make them available, preferably with reasonably full documentation, for distribution through NEA Data Bank.

Codes are normally requested from authors and tested for inclusion in our master files when a specific user request is received. However, some of these are already available: SCAT-2, ELIESE-3, HAUSER-5, CERBERO, ERINNI, SASSI and the latest version of ABACUS called A-THREE (from the CPC library in Belfast, U.K.).

2. PARTICIPANTS AND COMPUTER CODES USED IN THIS EXERCISE

Program	User and Author	Establishment	Country
1. SCAT-2 (Ref. 1)	O. Bersillon	CEA Bruyères-le-Chatel	France
2. ABACUS-2 (Ref. 2)	E. Correa de Oliveria	IEACTA Sao José dos Campos	Brazil
3. OPTICAL (Ref. 3)	T.W. Phillips	LLNL, Livermore	USA
4. ABACUS-NEARPEX (Ref. 4)	E. Ramstrom	SSRL, Nykoeping	Sweden
5. NGROGI (Ref. 5)	Y. Harima M. Kawai	RLNR-TIT, Tokyo NAIG-NRL, Tokyo	Japan
6. EMPIRE (Ref. 6)	M. Herman	IBJ, Warsaw	Poland
7. ELIESE-3 (Ref. 7)	G. Vasiliu, S. Mateescu S.B. Garg, V.K. Shukla Amar Sinha	INPR, Bucharest BARC, Bombay	Rumania India
8. HAUSER-5 (Ref. 8)	S.B. Garg, V.K. Shukla Amar Sinha	BARC, Bombay	India
9. CERBERO (Ref. 9)	H.A.J. Van der Kamp H. Gruppelaar G. Reffo	ECN, Petten ENEA, Bologna	Netherlands Italy

10. FRINNI (Ref. 10)	H.A.J. Van der Kamp H. Gruppelaar G. Reffo	ECN, Petten ENEA, Bologna	Netherlands
11. SASSE-ECN (Ref. 11)	H.A.J. Van der Kamp H. Gruppelaar	ECN, Petten	Netherlands
12. IDA (Ref. 12)	G. Reffo, F. Fabbri	ENEA, Bologna	Italy
13. ABAREX (Ref. 13)	P.A. Moldauer	ANL, Argonne	USA

The description of these codes, their special features when compared to others and their limitations with respect to this exercise are given in Appendix II.

3. PRESENTATION OF THE RESULTS

The results received have been arranged in such a way as to make a fast comparison possible, that is:

- i) optical model cross sections (Tables 1 to 17);
- ii) integrated cross sections below the threshold of second-particle emission (Tables 1 to 9);
- iii) integrated cross sections for multiple particle emissions (Tables 9 to 17);
- iv) graphical presentation of each reaction cross section (Graphs 1-32).

4. COMPARISON OF RESULTS

4.1 Optical Model Cross Sections

Only the codes OPTICAL, POLIFEMO, NAUSIKAA and ABACUS-2 used the optional energy dependence of the nucleon radii in the neutron optical potential real and imaginary well depths; we can therefore divide the code responses into two code groups. Within each group an agreement within a few per cent at all energies among all the codes was found.

The use of the energy dependent radii produced higher cross sections with differences that increase with incident energy up to 6% at $E_n = 14$ MeV. This effect is shown clearly by T. Phillips who gave results for both parametrizations. However, on the whole good agreement (within a few per mil) was observed among the codes using each option, and these are shown in the graphs by different curves (Figs. 1-12).

The calculations with HAUSER-5 do not include the spin-orbit potential; this accounts for the somewhat higher values of the compound nucleus cross section (Figs. 11, 12). The program EMPIRE sets the spin-orbit radius $r_{so} = r_1$, and interpolates the incoming neutron transmission coefficients from a precomputed table, and this may account for the somewhat different values obtained for the compound nucleus cross section.

As far as the matching region is concerned, some participants have used the built-in value of their program instead of the one proposed in the exercise. However, no significant discrepancies could be found which were attributable to such differences.

4.2 Results for the Hauser-Feshbach Theory Calculations (continued)

The following differences were found which may influence the present comparison in all or in part of the energy range:

- i) Mr. Vasiliu used an older Moldauer theory with inclusion of an interference term in the elastic channel which is not any longer in use.
- ii) No indication was given in the exercise as to how the spin distribution between Γ_{exp} and Γ_0 should be taken. This was linearly interpolated between $\sigma^2(U)$ at $E = E_{\text{cut}}$ and $\sigma^2(\Gamma_{\text{exp}})$ at $E = E_{\text{cut}}$ by Roffo, Van der Kamp and Herman. ($\sigma^2(\Gamma_{\text{exp}})$ being the spin cut off derived from fitting the proposed spin distribution law to the discrete level spin distribution with the maximum likelihood method.) The other participants did not specify their assumptions. Some code users are accustomed to extrapolate $\sigma^2(U)$ down to $E = E_{\text{cut}}$; this procedure is probably wrong and makes this comparison less exact.
- iii) The width fluctuation correction used by Herman is that of Hoffman, Richert, Tepel and Weidermüller (Ref. 14). His approach is different from all the other participants who used the usual width fluctuation integral formulae. In addition Moldauer, Roffo and Van der Kamp used an effective number of degrees of freedom greater than one for the χ^2 width distribution law, according to the latest Moldauer theory (Ref. 13), whereas the remaining participants used a Porter-Thomas distribution law. In SASSI-ECN the width fluctuation correction method of Hoffman et al. was used above $E = 1.09$ MeV (first excited state of Co-59). Below that energy the usual width fluctuation integral was used with Porter-Thomas distribution law.

4.2.1 Neutron Radiative Capture (Figs. 15, 16)

For neutron radiative capture, we observed good agreement (see Tables 1 to 17) between the results of CERBERO-ERINNI on the one hand and IDA system on the other. Discrepancies start increasing at neutron energies above ~ 14 MeV. This may be due to numerical differences in the integration procedures which influence very low capture values. The capture cross sections given by SASSI-ECN appear to be some 40% higher; this being interpreted by the author as due to a different normalization in total radiative widths. In fact in SASSI-ECN the gamma-decay width of the neutron resonances is taken (as requested) $\Gamma_Y = 500$ for any λ whereas in CERBERO, ERINNI, PENELOPE, NAUSIKAA it is spin and parity dependent; the normalization adopted is indicated in the table below:

J	$\pi = +$	$\pi = -$
3	507. MeV	262 MeV
4	497. MeV	224 MeV

The results given by EMPIRE and HAUSER-5 differ from each other up to 25% in the region below 6 MeV. Above 6 MeV no (n,γ) values were available from the EMPIRE code.

The values about 40% lower given by the EMPIRE and HAUSER-5 codes, with respect to the ENCA codes, cannot be due to different width fluctuation corrections because discrepancies are observed in the whole considered energy range; the effect is most probably due to a different or no normalization of Γ_Y . This assumption can be verified by examining the Γ_Y normalization for all J^π . At higher energies other types of discrepancies appear between the above mentioned codes, these are probably attributable to numerical integration differences with respect to both neutron and gamma-ray channels. Differences in the weighted spin distributions of continuum levels may also be responsible in part for these discrepancies.

In ABARD-X only one giant resonance can be specified; the one at 19.12 MeV was chosen in this exercise; however, the relative neutron-gamma widths over spacings have been correctly normalized according to the exercise specifications.

Also in SASSI-ECN only one giant dipole resonance was assumed at $E = 19.5$ MeV with a width of 6 MeV. The reason for the high values of the radiative capture cross section above 14 MeV of SASSI-ECN is due to the inclusion of a direct and collective component.

4.2.2 Neutron Inelastic Scattering (Figs. 13, 14)

The inelastic cross sections given by some participants could not be compared because they provided the compound elastic and inelastic neutron scattering cross sections added together. The (n,n') results agree within approximately 10% in the region of the maximum. Again Vasiliu's values appear to be higher because he used an earlier Moldauer theory for the width fluctuation correction with the inclusion of the resonance interference contribution.

The cross sections obtained with HAUSER-5 are appreciably higher; this can be attributed to the use of a potential without a spin-orbit term as mentioned previously. The results provided by the ENEA set of codes are consistent with each other over the whole energy range.

4.2.3 Results for $(n,2n)$ (Figs. 25, 26)

Good agreement (within 5%) is observed at all energies between the NGROGI code and the ENCA codes. Exception is made for 12 MeV where the NGROGI results are 20% lower.

4.2.4 Results for (n,p) (n,α) (Figs. 17-20)

While the set of ENEA codes agree well with each other up to 8 MeV, the energy around which the (n,pn) reaction has its threshold, NGROGI and EMPIRE disagree with them. The neglection of the discrete inelastic scattering in NGROGI might enhance the proton emission. Above 8 MeV there is reasonable agreement in the trend and in the values between ERINNI, PENELOPE and NGROGI. Note that above 12 MeV the proton volume potential changes from $W_p = 0.22E - 2.7$ to $W_p = 0$.

In the case of the (n,α) reaction there is a reasonable agreement between the different codes at energies above 12 MeV. The results of NGROGI are discrepant with those provided by the other codes for energies above 12 MeV.

4.2.5 Results for Two Particle Emission Processes

Comparison of the following reactions show substantial discrepancies:

$$\sigma(n,\alpha n), \sigma(n,\alpha\alpha), \sigma(n,pn), \sigma(n,np)$$

However, the values for $\sigma(n,\alpha x) = \sigma(n,\alpha) + \sigma(n,\alpha n)$ are in quite good agreement apart from the results of NGROGI at lower energies.

5. CONCLUSIONS

From the short comparative analysis outlined above for the results from the different codes one may conclude that the optical model cross sections are in reasonable agreement. The statistical model cross sections are more or less discrepant.

In particular:

- i) The optical model quantities σ_1 , and σ_R for neutrons are in good agreement. We are unable to compare the proton and alpha optical model calculations involved as only a few users have provided results for it. We therefore cannot say to what extent the observed discrepancies in particle emissions are due to differences in the calculated transmission coefficients.
- ii) Large discrepancies in $\sigma(n,2n)$ and in $\sigma(n,2n) + \sigma(n,n')$ which represent the dominant competition, give even larger discrepancies for weak and very weak competitions which share what is left over of the compound nucleus cross section. In some cases one observes differences of one order of magnitude between the results of different codes for the single and multiple particle emissions involving charged particles. Also these differences tend to increase with energy. Discrepancies seem to explode above 12 MeV where the $(n,2n)$, (n,pn) , $(n,\alpha n)$, (n,np) , $(n,\alpha\alpha)$ competitions start rising fast.
- iii) According to the conclusions in (i) such discrepancies can hardly be attributed to the optical model calculations for the neutron, so one has to look for other possible explanations such as:
 - a) Differences in accuracy of the numerical integration techniques (e.g. integration method, number of steps, etc.).
 - b) Differences in the level density formulae used which result in different weights for channel reactions involved.
 - c) Discrepancies in the charged particle optical model transmission coefficients.
 - d) As far as discrepancies in $\sigma(n,\gamma)$ are concerned these might be due to different F_ν normalization for different J and π and differences in the treatment of gamma-ray competition.

- vi) It is highly desirable that authors examine their codes to identify the sources of the discrepancies noted under paragraph (iii). Until this is done, it is not possible to make reliable statistical model calculations of many of the reaction channels studied in this exercise.

6. FUTURE PROGRAMME

This series of program intercomparisons is being extended by exercises on:

- i) coupled channel calculations;
- ii) pre-equilibrium reactions;
- iii) charged particle optical model calculations.

The specifications for these intercomparisons are available on request.

7. ACKNOWLEDGEMENTS

NEA Data Bank wishes to thank all the participants who have made the present program comparison possible and who have contributed their comments to this report. Several of them have, in addition, made comparison runs of their programs with modified input parameters that conform better with the exercise specifications. The work of Dr. P. Hodgson in checking and suggesting modifications to this report has been particularly valuable.

Data Bank staff who have joined in this project and in the preparation of the report are Ms. S. Greenstreet, P. Johnston, P. Nagel, Ms. R. Posca and N. Tubbs.

8. REFERENCES

- /1/ a. O. Bersillon, "SCAT-2: Un Programme de Modèle Optique Sphérique", CEA-N-2227 (October, 1981).
- b. M.A. Melkanoff et al., Methods in Computational Physics, Vol. 6 (1966).
- /2/ a. E.H. Auerbach, "ABACUS-2", BNL-6592 (1964).
- b. E. Correa de Oliveira, "International Nuclear Model Code Comparison Exercise 2: Spherical Optical Model Calculations", 1981, Private Communication.
- /3/ M.E. Smith and H.S. Camarda, "Optical Model Calculation of Neutron-Nucleus Scattering Cross Sections", UCID-18737 (1980).
- /4/ a. E.H. Auerbach, "ABACUS-2", BNL-6592 (1964).
- b. P.A. Moldauer, C.A. Engelbrecht and G.J. Duffy, "NEARREX, A Computer Code for Nuclear Reaction Calculations", ANL-6970, December, 1964.

- c. G. Ramphuwa, "Contribution to the Interpretation and Calculation of Neutron-induced Reaction Cross Sections in Co-60 Using the Spherical Optical Model and the Statistical Model", 1981, Private Communication.
- /5/ a. H. Takahashi, Proc. of EANDC Topical Discussion on Critique of Nuclear Models and Their Validity in the Evaluation of Nuclear Data, Tokyo, JAERI-M-5984, p. 257 (1975).
- b. S. Igarasi, "Program ELIESE-2, A FORTRAN-IV Program for Calculation of the Nuclear Cross Sections by Use of the Optical Model and Hauser-Feshbach's Method", JAERI-1169 (1968).
 - c. Y. Harima, M. Kawai, "Contribution to International Nuclear Model Comparison, Spherical Optical and Statistical Model Study", 1981, Private Communication.
- /6/ a. M. Herman, "EMPIRE", unpublished.
- b. M. Herman, "International Nuclear Model Code Comparison Spherical Optical and Statistical Model Study", 1981, Private Communication.
 - c. W.R. Smith, "SCAT", Computer Phys. Commun. 1, 106 (1969).
- /7/ a. S. Igarasi, "Program ELIESE-3, Program for Calculation of the Nuclear Cross Sections by Using Local and Non-Local Optical Models and Statistical Model", JAERI-1224 (1972).
- b. S. Mateescu and G. Vasiliu, "International Nuclear Model Code Comparison, Spherical Optical and Statistical Model Study, 59-Co Reaction Calculation", 1981, Private Communication.
- /8/ a. F.M. Mann, "HAUSER-5, A Computer Code to Calculate Nuclear Cross Sections", HEDL-TME 78-83, July 1979.
- b. C. Kalbach, "PRECO-B, Program for Calculating Pre-Equilibrium Energy Spectra", Triangle Universities Nuclear Laboratory and North California State Chemistry Department, Informal Report, 1977.
 - c. D.L. Hill and J.A. Wheeler, "Nuclear Constitution and the Interpretation of Fission Phenomena", Physical Review, Vol. 89, No. 5, pp. 1102-1145, 1 March, 1953.
 - d. M. Blann, "Pre-equilibrium Decay", Annual Review of Nuclear Science, Vol. 25, pp. 123-166, 1975.
 - e. S.B. Garg, V.K. Shukla and Amar Sinha, "Neutron-induced Reaction Cross Sections of 59-Co", 1981, Private Communication.
- /9/ a. Fabbri and G. Reffo, "CERBERO-Version 1979: Improved Version of the CERBERO Computer Code for Calculation of Nuclear Reaction Cross Sections", 1979, Private Communication; see also CNLN Reports RT/FI(74) 36 (1974) and RT/FI(77) 6 (1977).
- b. H.A.J. van der Kamp and H. Gruppelaar, "Optical Model and Statistical Model Calculations for 59-Co + n Cross Sections", ECN FYS-STEK-Memo-96, Petten, June 1981.
 - c. G. Reffo, "Theory and Application of Moment Methods in Many Fermion Systems", p. 167, edited by B.J. Dalton, S.M. Grimes, J.P. Vary and S.A. Williams, Plenum 1980.
- /10/ a. F. Fabbri and G. Reffo, "ERJNNI: An Optical Model FORTRAN-IV Code for the Calculation of Multiple Cascading Particle Emissions", CNEN, RT/FI(77) 4 (1977) and Private Communications (1979).
- b. H. Gruppelaar and G. Reffo, "Some Properties of the Width Fluctuation Factor", Nucl. Science and Eng. 62, 756 (1977).
 - c. H.A.J. van der Kamp and H. Gruppelaar, "Optical Model and Statistical Model Calculations for 59-Co + n Cross Sections", ECN FYS-STEK-Memo-96, Petten, June 1981.
- /11/ a. V. Benzi et al., "SASSI: A FORTRAN Programme for the Calculation of Neutron Scattering from a Spherical Optical Model", CNEN, RT/FI(71) 6 (1971).
- b. R. Vennink, unpublished ECN Report and H. Gruppelaar, revisions.
 - c. H.A.J. van der Kamp and H. Gruppelaar, "Optical Model and Statistical Model Calculations for 59-Co + n Cross Sections", ECN FYS-STEK-Memo-96, Petten, June 1981.
- /12/ G. Reffo and F. Fabbri, "The IDA Modular System for Neutron Reaction Cross Section Calculation", unpublished.
- /13/ a. P.A. Moldauer, "Statistics and the Average Cross Section", Nucl. Phys. A344, 185 (1980).
- b. Private Communication.
- /14/ H.M. Hoffman, M. Richert, J.W. Tepel and H.A. Weidenmüller, Z.Phys. A297, 153 (1980).
- /15/ C. Kalbach-Cline, Nucl. Phys. A210, 590 (1973).

CODE(S) USER SIGN.	SCAT2 E	ABACUS2 OPTICAL	ABACUS-NEARREX NCRGCI	EMPIRE	ELIESE3* HAUSER S	CERBEROS L	SASSI ECN L	IDA EL	AGAREX
TOTAL	4657	4856	4859 4811E	4657	4858*	4858	4859	4877	4859
COMP. NUCL.	2500	2497	2502	2459	2543	2699*	2496	2699	2503
ELASTIC: HF	2557S	2563S	2557S 2573SC	4854 4824	2357S	4858H*	4849 4849H	4847	4860 4869
n n HF									
n n HF+NFC									
n d HF									
n g HF+NFC									
n g HF									
n n g HF+NFC									
n p HF									
n D HF+NFC									
n d HF									

S = shape elastic

H = modified transmission coefficients ($t_{ij} = \Theta_{1,j} - 250\Theta_{1,j}^3$)^{1/2} are used according to Holdauer's theory

L = linear interpolation of spin cut-off in the intermediate continuum region

E = energy dependence of the nucleon radii in the neutron optical potential

Table 1

Table 2

CODE(S) USER SIGN.	SCAT2 E	ABACUS2 OPTICAL	ABACUS-NEARREX NCRGCI	EMPIRE	ELIESE3* HAUSER S	CERBEROS L	SASSI ECN L	IDA EL	AGAREX
TOTAL	3825	3825	3819 3856	3829	3825	3826*	3828	3843	3826
COMP. NUCL.	2361	2361	2377 2364C	2303	2380	2404 2399	2380	2380	2384
ELASTIC: HF	14445	14465	14435 14515E	14445 14515E	3824 3796	3826* 38184	3819 3826	3835 3836	14445 3820
n n HF									
n n HF+NFC									
n d HF									
n d HF+NFC									
n p HF									
n d HF									

S = shape elastic

H = modified transmission coefficients ($t_{ij} = \Theta_{1,j} - 250\Theta_{1,j}^3$)^{1/2} are used according to Holdauer's theory

L = linear interpolation of spin cut-off in the intermediate continuum region

E = energy dependence of the nucleon radii in the neutron optical potential

Table 2

En = 1.0

MeV

1.0

Table 2

MeV

Table 3

 $E_n = 1.5$ MeV

	CODE (S)	SERIAL	ABACUS2	OPTICAL	ARACUS-NEARTEX	NENCI	EMPIRE	ELIESET*	ELIESET*	SASSI	ELIESET*	ELIESET*	GRUPPELAAR	REFCO	REFCO	GRUPPELAAR	REFCO	HOLDAER
SP	USER																	
SIGMA	BERILLON DE OLIVEIRA	PHILLIPS	RANSTROM		HARTIG-KNAUT		HERMAN	GARG	VASILIU									
TOTAL	3503	3498	3498	3506	3502	3502*	3502*	3502	3502*	3502	3502	3502*	3502	3502	3502	3502	3502	
CHEP-NUL.	2259	2256	2256	2241	2258	2258	2258	2258	2258	2257	2257	2258	2258	2245	2245	2245	2245	
CLASTIC:																		
Hf	12645	12605	12625	2163	12645	2763*	2763*	2759	2759	2755	2755	2754	2754	2736	2736	2735	2735	
Hf+HFC			12555F	2976														
n n				739				738	738									
n n					497			504	504	560	560	552	552	545	545	545	545	
Hf+HFC								504	504	560	560	552	552	545	545	545	545	
n X								4.17	3.09	4.21	4.21	4.12	4.12	4.06	4.06	4.06	4.06	
Hf																		
n X																		
Hf+HFC																		
n p																		
Hf																		
n D																		
Hf+HFC																		
n S																		
Hf																		

S = shape elastic

M = modified transmission coefficients ($t_{ij} = \Theta_{ij} - 250_{ij}\Theta_{jj}^t$) λ^2 are used according to Holdauer's theory

L = linear interpolation of spin cut-off in the intermediate continuum region

E = energy dependence of the nucleon radii in the neutron optical potential

Table 3

 $E_n = 1.5$ MeV

Table 4

 $E_n = 2.0$ MeV

	CODE (S)	SERIAL	ABACUS2	OPTICAL	ABACUS-NEARTEX	NENCI	EMPIRE	ELIESET*	ELIESET*	SASSI	ELIESET*	ELIESET*	GRUPPELAAR	REFCO	REFCO	GRUPPELAAR	REFCO	HOLDAER
SP	USER																	
SIGMA	BÉZIUTON DE OLIVEIRA	PHILLIPS	RANSTROM		HARTIG-KNAUT		HERMAN	GARG	VASILIU									
TOTAL	3500	3328	3367	3371	3369	3369*	3369*	3369	3369	3366	3366	3366	3366	3362	3362	3362	3362	
CHEP-NUL.	2.54*	2047	2049	2049	2070	2047*	2047*	2047	2047	2045	2045	2045	2045	2049	2049	2049	2049	
CLASTIC:																		
Hf	12225	12765	13265	2191	13225	2091*	2091*	2089	2089	2293	2293	2293	2293	2259	2259	2259	2259	
Hf+HFC			12955F	2365														
n n					1277			1278	1278					1280	1280			
Hf																		
n X																		
Hf																		
n D																		
Hf+HFC																		
n S																		
Hf																		

S = shape elastic

M = modified transmission coefficients ($t_{ij} = \Theta_{ij} - 250_{ij}\Theta_{jj}^t$) λ^2 are used according to Holdauer's theory

L = linear interpolation of spin cut-off in the intermediate continuum region

E = energy dependence of the nucleon radii in the neutron optical potential

Table 4

135

En = 2.5										En = 4.0			
CODE (S)	SCA12	ABACUS2	OPTICAL	ABACUS-NEARREX	NIGROJ	EMPIRE	ELIESE*	CERBERO3	SASSI ECN	IDA	ABAREX	EL	
USER	BERILLON	DE OLIVEIRA	PHILLIPS	RAMSTRÖM	HARITH-KAWAI	HERMAN	GARG	VASILIU	GRUPPELAAR	REFDO	MOLDAUER		
TOTAL	3343	3300	3342	3341	3342	3341*	3341	3337	3340	3318	3342		
CFTRP-NCL,	1868		1890	1888	1890	1890*	1888	1887	1888	1800	1808		
ELASTIC:	14545	13995	14535 14215E	1865 2080	14545	1978*	1865 1999H	1862 2020	2005	1834 2001	14545 2010		
n f			1473		1314	1473	1472			1481			
n n				1231	1342	1339H	13307	1330		1314	1329		
n f + HF C						1.69		2.49			2.55		
n X								2.50	4.44		2.56		
n G								2.10			2.38		

S = Shore elastic

$S = \text{shear elastic}$
 $\tau_{ij} = \text{realized transmission coefficients } (\tau_{11} = \Theta_{11} - 2\Theta_{12}, \Theta_{1j})^T$ are used according to Holdauer's theory

— linear interpolation of spin cut-off in the intermediate continuum region

The dependence of the nucleon radius on the neutron optical potential

ପ୍ରକାଶକ ପରିଷଦ୍ୟ ମହିନେ ପରିବର୍ତ୍ତନ କରିଛନ୍ତି

Tables

ϵ_s = Shore elastic

Ergonomics in Design 30(2) 11–16 © 2018 Taylor & Francis Ltd

$L =$ linear interpolation of spin cut-off in the intermediate continuum region

200

Table 2

En = 4.0 MeV

CODE (S) USER	SCAT2	ABACUS2 OPTICAL E	ABACUS-NEARREY	NCRGCI	EMPIRE	ELIESE3* HAUSER S	ELIESE3 L	SASSI ECN	CERBEROS	GRUPPELAAR	IDR EL	REFD	MOLDAUER?
BERILLON DE OLIVEIRA PHILLIPS		3576	3562 3595C	3556	3556*	3549	3547	3560	3560	3560	3560	3560	3560
CCMP+MCL.	1683	1686 1729C	1683	1671	1683*	1683	1682	1680	1724	1724	1724	1724	1662
ELASTIC: HF HF+HF/C	18735	19565	18755 18665C	18725	2043*	1992 2127N	1990 2055	2040	1854 2024	1854 2024	1854 2024	1854 2024	1854 2024
n n HF HF+HF/C					1675	1559	1547				1552	1545	
n n HF HF+HF/C					1512	14634	1479	1499			1511		
n n HF HF+HF/C					1.35		2.02				2.13		
n n HF HF+HF/C					1.48		2.02	3.351			2.14	2.15	
n n HF HF+HF/C											.66	.65	
n p HF HF+HF/C					.67	5.36	4.35	3.05	5.43		5.32		
n p HF HF+HF/C						4.054	5.38						
n p HF HF					0.13	.005							

S = shape elastic

H = modified transmission coefficients ($t_{1,j} = \Theta_{1,j} - .25\Theta_{1,j}\Theta_{1,j}^2$)^{1/2} are used according to Moldauer's theory

L = linear interpolation of spin cut-off in the intermediate continuum region

C = energy dependence of the nucleon radii in the neutron optical potential

Table 3

En = 4.0 MeV

CODE (S) USER	SCAT2	ABACUS2 OPTICAL E	ABACUS-NEARREY	NCRGCI	EMPIRE	ELIESE3* HAUSER S	ELIESE3 L	SASSI ECN	CERBEROS	GRUPPELAAR	IDR EL	REFD	MOLDAUER?
BERILLON DE OLIVEIRA PHILLIPS		3758	3639 3740E	3635	3635*	3635	3637	3724	3724	3724	3724	3724	3724
CCMP+MCL.	1594	1594 1640E	1594	1594	1594*	1583	1577	1595	1593	1593	1593	1593	1593
ELASTIC: HF HF+HF/C	20425	21065	2055 2105E	20625	2063*			2068	2092	2092	2123	2123	2055
n n HF HF+HF/C					1500	1643	1541				1585	1573	
n n HF HF+HF/C											1514		
n p HF HF+HF/C					0.83	0.76					1.35	.7	
n p HF HF+HF/C											1.23	2.0	
n p HF HF+HF/C											1.24		
n p HF HF+HF/C											7.4	17.9	17.55
n p HF HF+HF/C											22.55		
n p HF HF+HF/C											.21	1.29	0.91

CODE (S) USER	SCAT2	ABACUS2 OPTICAL E	ABACUS-NEARREY	NCRGCI	EMPIRE	ELIESE3* HAUSER S	ELIESE3 L	SASSI ECN	CERBEROS	GRUPPELAAR	IDR EL	REFD	MOLDAUER?
BERILLON DE OLIVEIRA PHILLIPS		3758	3639 3740E	3635	3635*	3635	3637	3724	3724	3724	3724	3724	3724
CCMP+MCL.	1594	1594 1640E	1594	1594	1594*	1583	1577	1595	1593	1593	1593	1593	1593
ELASTIC: HF HF+HF/C	20425	21065	2055 2105E	20625	2063*			2068	2092	2092	2123	2123	2055
n n HF HF+HF/C					1500	1643	1541				1585	1573	
n n HF HF+HF/C											1514		
n p HF HF+HF/C					0.83	0.76					1.35	.7	
n p HF HF+HF/C											1.23	2.0	
n p HF HF+HF/C											1.24		
n p HF HF+HF/C											7.4	17.9	17.55
n p HF HF+HF/C											22.55		
n p HF HF+HF/C											.21	1.29	0.91

S = shape elastic

H = modified transmission coefficients ($t_{1,j} = \Theta_{1,j} - .25\Theta_{1,j}\Theta_{1,j}^2$)^{1/2} are used according to Moldauer's theory

L = linear interpolation of spin cut-off in the intermediate continuum region

C = energy dependence of the nucleon radii in the neutron optical potential

Table 4

En = 6.0 MeV

Table 9

May 1984

S = shade elastic

S_1 = modified transmission coefficients ($S_1 = -a$) - 250-600 JJC are used according to Malsauer's theory

\perp linear interpolation of spin cut-off in the intermediate continuum region

11

Δ = shape elastic

= linear interpolation of spin cut-off in the intermediate continuum region

= energy dependence of the nuclear radii in the neutron optical potential

$$G(n,s) \geq G(n,s) + G(n,s)$$

Table 10

Table 11

En = 0 MeV

CODE(S) CSER	SCAT2	ABACUS2 E	OPTICAL	NDRG1	EMPIRE *	HANSENS	FRINNI L	SASSI ECN L	IDA EL	ABREX
SIGMA	PERSILLON	DE OLIVEIRA	PHILLIPS	HARIMA-KAWAI	HERMAN	DARG	GROFFELAAR	GROFFELAAR	REFTO	MULDER
TOTAL	3377	3509	3379	3377			3381	3355	3522	3357
COMP.MUL.	1514		1533	1534	1529	1667	1535	1539	1577	1535
ELASTIC:										
HF	15435		19175	18465	18435		1051	1026	1050	1074
n										
n p										
n np										
n nn										
n nnp										
n npn										
n npn										
n np										
n pn										
n pp										
n pY										
n d										
n t										
n 3										
n 4										
n 5										
n 6										
n 7										
n 8										
n 9										
n 10										
n 11										
n 12										
n 13										
n 14										
n 15										
n 16										
n 17										
n 18										
n 19										
n 20										
n 21										
n 22										
n 23										
n 24										
n 25										
n 26										
n 27										
n 28										
n 29										
n 30										
n 31										
n 32										
n 33										
n 34										
n 35										
n 36										
n 37										
n 38										
n 39										
n 40										
n 41										
n 42										
n 43										
n 44										
n 45										
n 46										
n 47										
n 48										
n 49										
n 50										
n 51										
n 52										
n 53										
n 54										
n 55										
n 56										
n 57										
n 58										
n 59										
n 60										
n 61										
n 62										
n 63										
n 64										
n 65										
n 66										
n 67										
n 68										
n 69										
n 70										
n 71										
n 72										
n 73										
n 74										
n 75										
n 76										
n 77										
n 78										
n 79										
n 80										
n 81										
n 82										
n 83										
n 84										
n 85										
n 86										
n 87										
n 88										
n 89										
n 90										
n 91										
n 92										
n 93										
n 94										
n 95										
n 96										
n 97										
n 98										
n 99										
n 100										
n 101										
n 102										
n 103										
n 104										
n 105										
n 106										
n 107										
n 108										
n 109										
n 110										
n 111										
n 112										
n 113										
n 114										
n 115										
n 116										
n 117										
n 118										
n 119										
n 120										
n 121										
n 122										
n 123										
n 124										
n 125										
n 126										
n 127										
n 128										
n 129										
n 130										
n 131										
n 132										
n 133										
n 134										
n 135										
n 136										
n 137										
n 138										
n 139										
n 140										
n 141										
n 142										
n 143										
n 144										
n 145										
n 146										
n 147										
n 148										
n 149										
n 150										
n 151										
n 152										
n 153										
n 154										
n 155										
n 156										
n 157										
n 158										
n 159										
n 160										
n 161										
n 162										
n 163										
n 164										
n 165										
n 166										
n 167										
n 168										
n 169										
n 170										
n 171										
n 172										
n 173										
n 174										
n 175										
n 176										
n 177										
n 178										
n 179										
n 180										
n 181										
n 182										
n 183										
n 184										
n 185										

Table 15

 $E_n = 16$

MeV

CODE(S)	SLATE2	AGACUS2	OPTICAL	NRCG1	EMPIRE	HAUSERS	ERINNI	SASSI ECN	IDR	ABAREX
USER	Σ	Σ	Σ	HARINA-KAWAI	*	HERMAN	L	L	EL	MOLDAUER
BERSILLON	2406	2580	2407	2406		2405	2404	2404	2553	2411
DE OLIVEIRA	1405	1405	1405	1405		1405	1406	1405	1465	1411
PHILLIPS	1465C	1465C								
ELASTIC:	1001S	1106S	1000S	1001S			1007	999	1000	1000
HF			1008SE							
r o										
n m										
n np										
n nn										
n nnn										
n nnnp										
n p										
n pn										
n pp										
n p&										
n &										
n &n										
n &pn										
n &pp										
n d										
n t										

S = Shape elastic

L = Linear interpolation of spin cut-off in the intermediate continuum region

E = Energy dependence of the nucleon radii in the neutron optical potential

$$\star \quad G(n,\omega) \equiv G'(n,\omega) + G(n,\Delta\omega)$$

Table 15

MeV

Table 16

MeV

CODE(S)	SLATE2	AGACUS2	OPTICAL	NRCG1	EMPIRE	HAUSERS	ERINNI	SASSI ECN	IDR	ABAREX
USER	Σ	Σ	Σ	HARINA-KAWAI	*	HERMAN	L	L	EL	MOLDAUER
BERSILLON	1375	1375	1375	1375		1375	1441	1376	1375	1374
DE OLIVEIRA	1436C	1436C	1436C	1436C						
PHILLIPS										
ELASTIC:	993S	1005S	993S	993S			997	998	1002	991
HF			997SE							
r o										
n m										
n np										
n nn										
n nnn										
n nnnp										
n p										
n pn										
n pp										
n p&										
n &										
n &n										
n &pn										
n &pp										
n d										
n t										

S = Shape elastic

L = Linear interpolation of spin cut-off in the intermediate continuum region

E = Energy dependence of the nucleon radii in the neutron optical potential

$$\star \quad G(n,\omega) \equiv G'(n,\omega) + G(n,\Delta\omega)$$

Table 16

MeV

S = Shape elastic

L = Linear interpolation of spin cut-off in the intermediate continuum region

E = Energy dependence of the nucleon radii in the neutron optical potential

$$\star \quad G(n,\omega) \equiv G'(n,\omega) + G(n,\Delta\omega)$$

Table 16

MeV

Table 17

En = 20 MeV

CODE(S) USER mb SIGMA	SCAT2	ABACUS2	OPTICAL E	NGROGI HARTHA- KNAIJ	EMPIRE *	HAUSERS	ERINNI L	SASSI ECN L	IDA EL	ABAREX
TOTAL	2360	2389	2299	2300			2301	2307	2372	2303
CIMP. NUCL.	1345	2570E	1345	1345	1347	1349	1346	1344	1409	1357
ELASTIC:	954S	974S	954S	954S			955	963	963	946
H.F.							14.8	10.0	13.0	
n n				1692			1107	1110	1126	
n nn				101			94		103	
n np				12.9			9.9		26.4	
n nx									.6	
n nnx									16.6	
n nnx									3.2	
n nnx									.21	
n npn										
n npn										
n pnp										
n pnp										
n pp										
n pp										
n pδ										
n d										
n t										

S = shape elastic

L = linear interpolation of spin cut-off in the intermediate continuum region

E = energy dependence of the nucleon radii in the neutron optical potential

• $\sigma_{n,\alpha} \equiv \sigma(n,\alpha) + \sigma'(n,\alpha)$

Table 17

En = 20 MeV

12

GRAPHS

Abbreviations used:

AX	(n,n) + (n,αn) cross section
TOT	total cross section
COM	compound nucleus cross section
SHE	shape elastic cross section
ELA	elastic cross section
N	total inelastic cross section
G	(n,γ) cross section
P	(n,p) cross section
A	(n,α) cross section
NN	(n,2n) cross section
NP	(n,np) cross section
NA	(n,na) cross section
PN	(n,npn) cross section
PP	(n,2p) cross section
AN	(n,αn) cross section
HF or H	Hauser-Feshbach
WF or W	Hauser-Feshbach + width fluctuation correction
E	energy dependence option

Abbreviations for the computer codes:

ABA	ABACUS-2
ABN	ABACUS-NEARREX
ABX	ABAREX
CER	CERBERO-3
ELI	ELIESE-3, ELV=ELI run by Vasiliu
EMP	EMPIRE
ERI	ERINNI
HAU	HAUSER*5
IDA	IDA
NGR	NGROGI
OPT	OPTICAL
SAS	SASSI-ECN
SCA	SCAT-2

.....

line drawn through cross section values for which an energy independent nucleon radius was used in the neutron optical potential

line drawn through cross section values for which an energy dependent nucleon radius was used in the neutron optical potential

Cross Section (Barn)

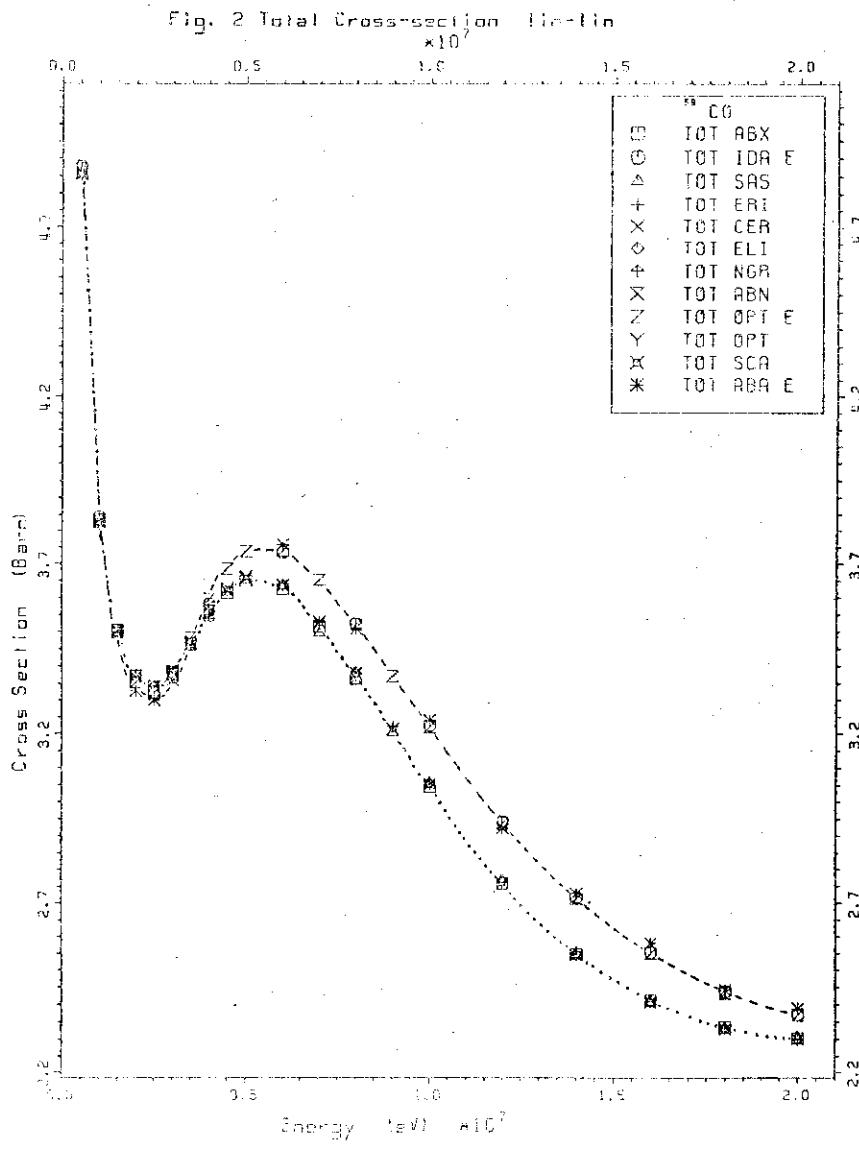
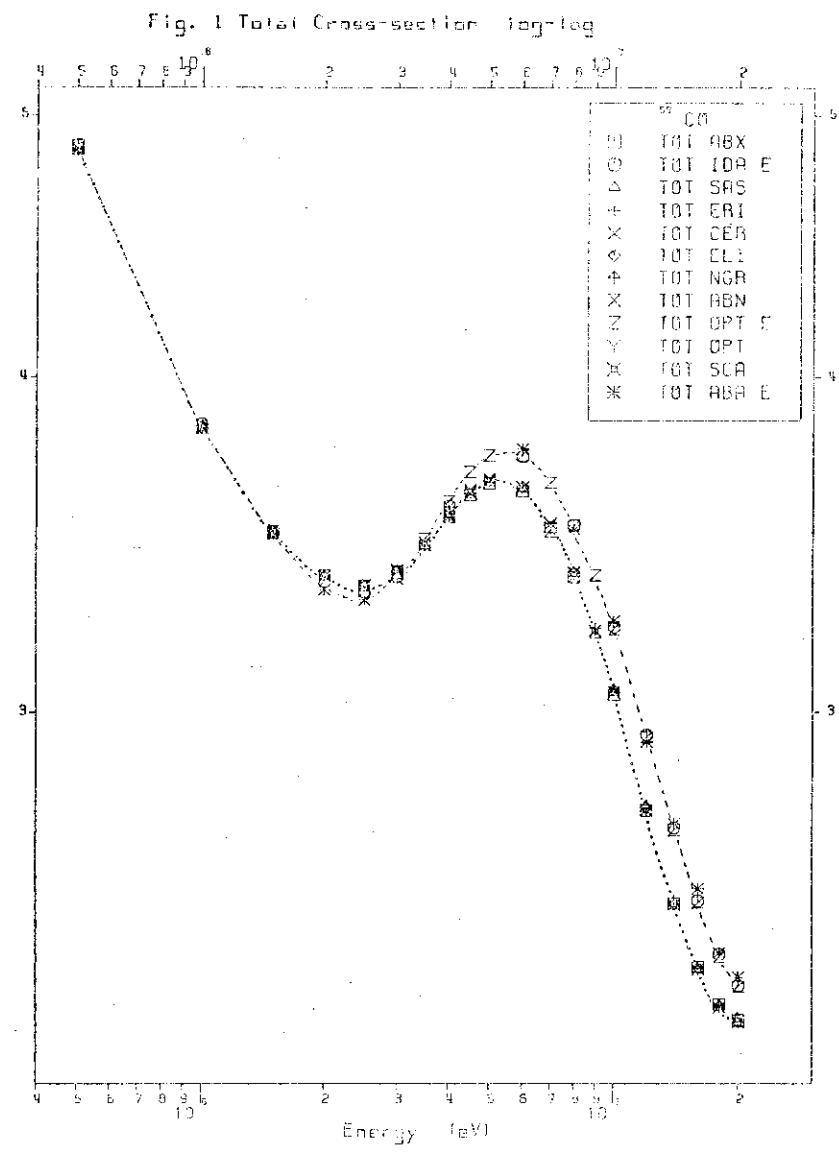


Fig. 3 Shape-elastic Cross-section log-log

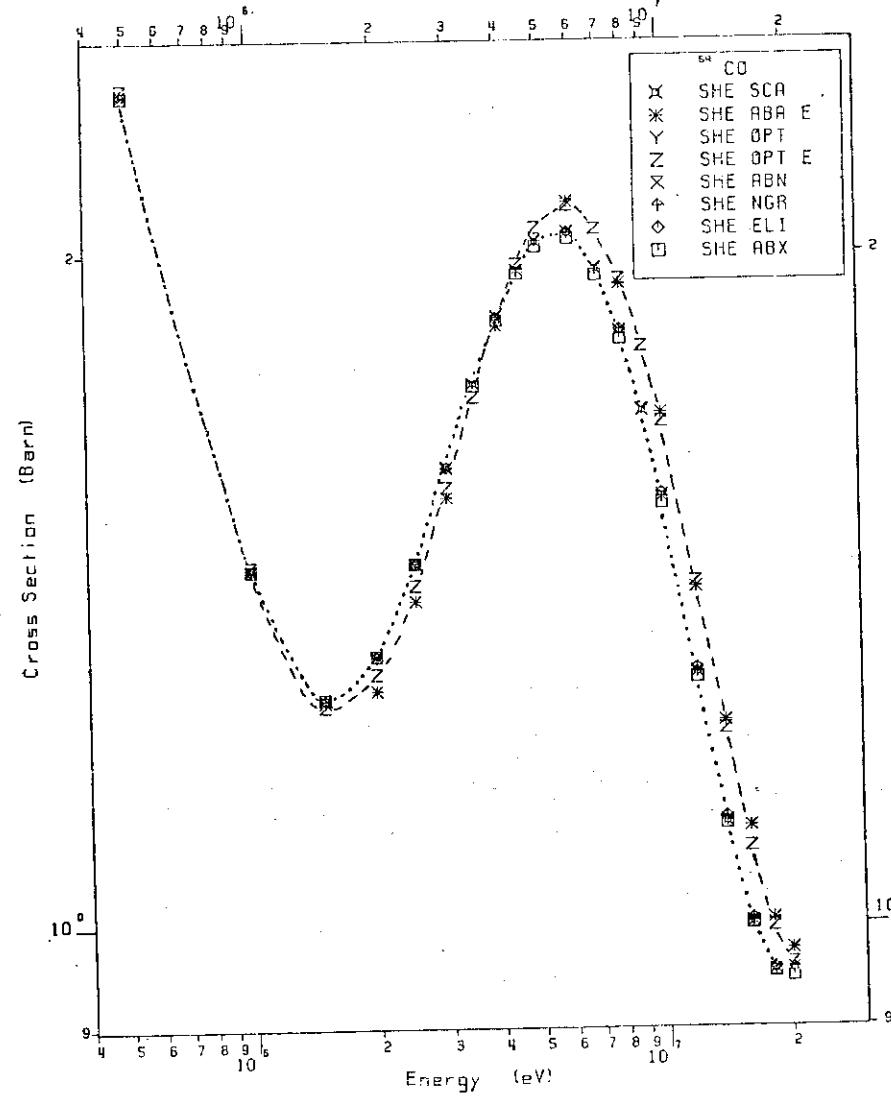


Fig. 4 Shape-elastic Cross-section lin-lin
 $\times 10^7$

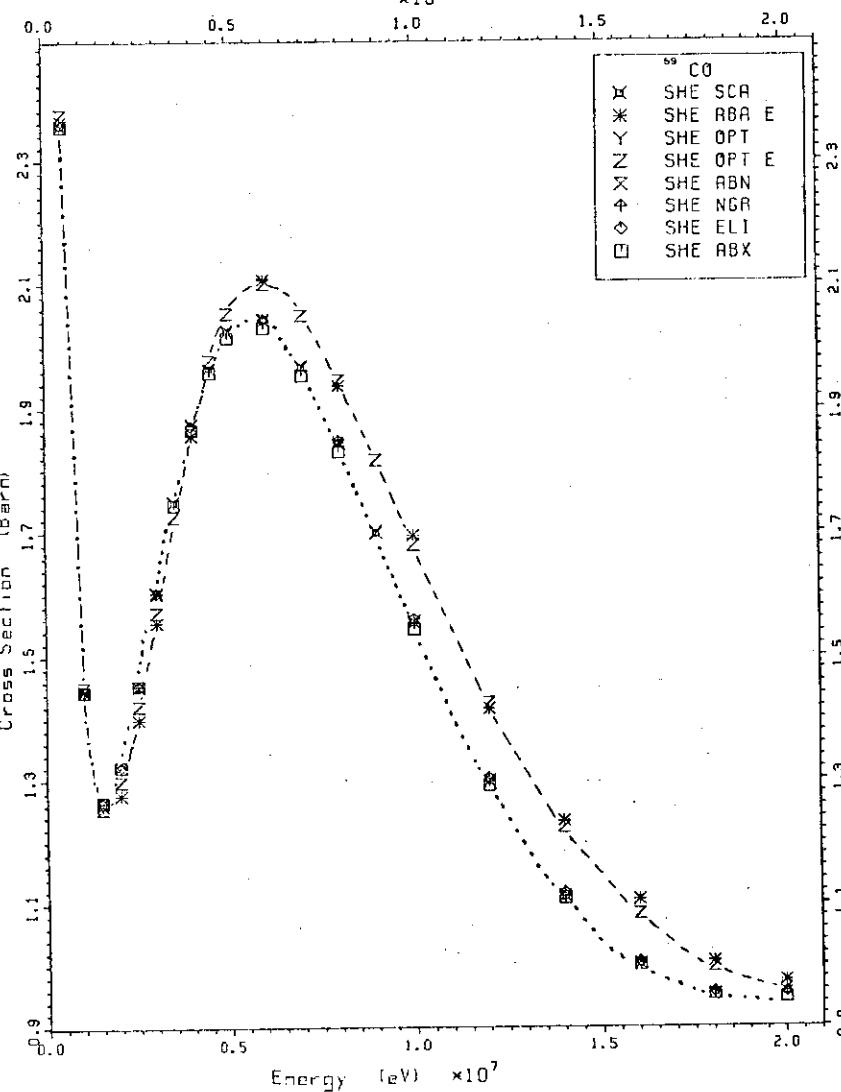


Fig. 5. Elastic Cross-section (HF) log-log

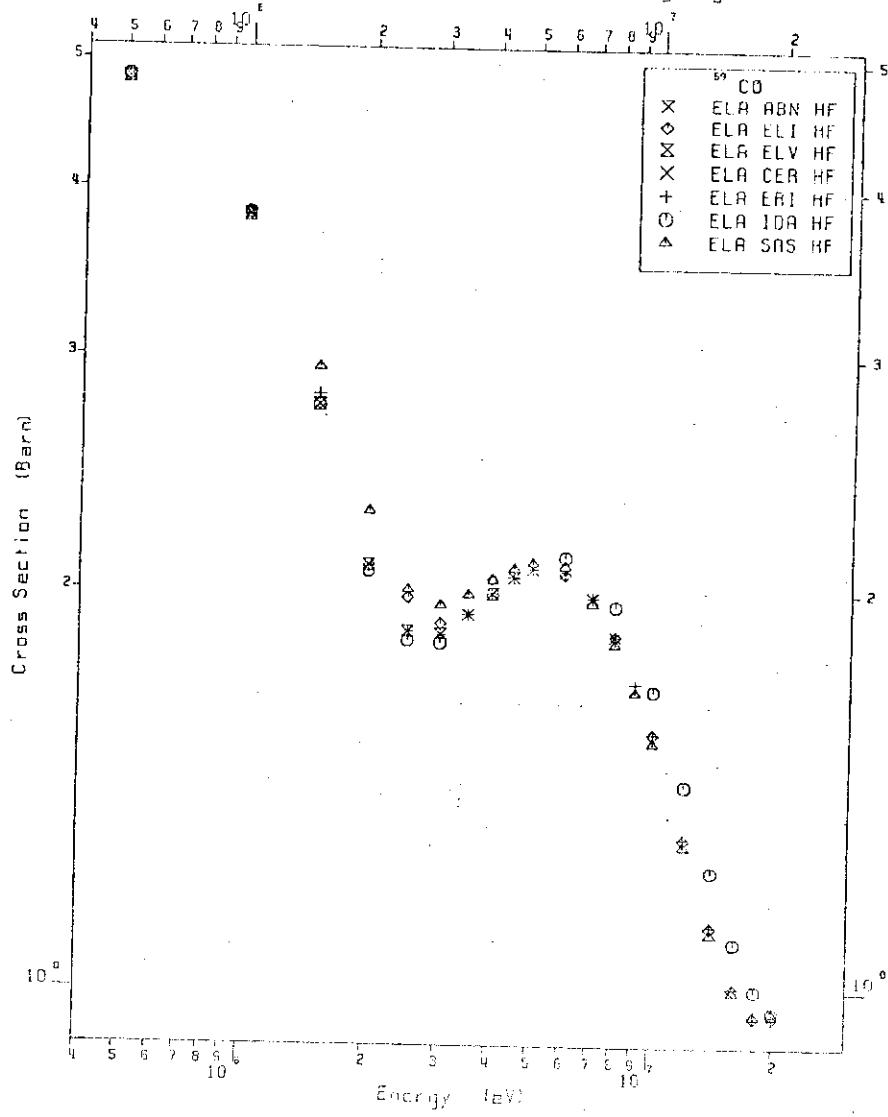
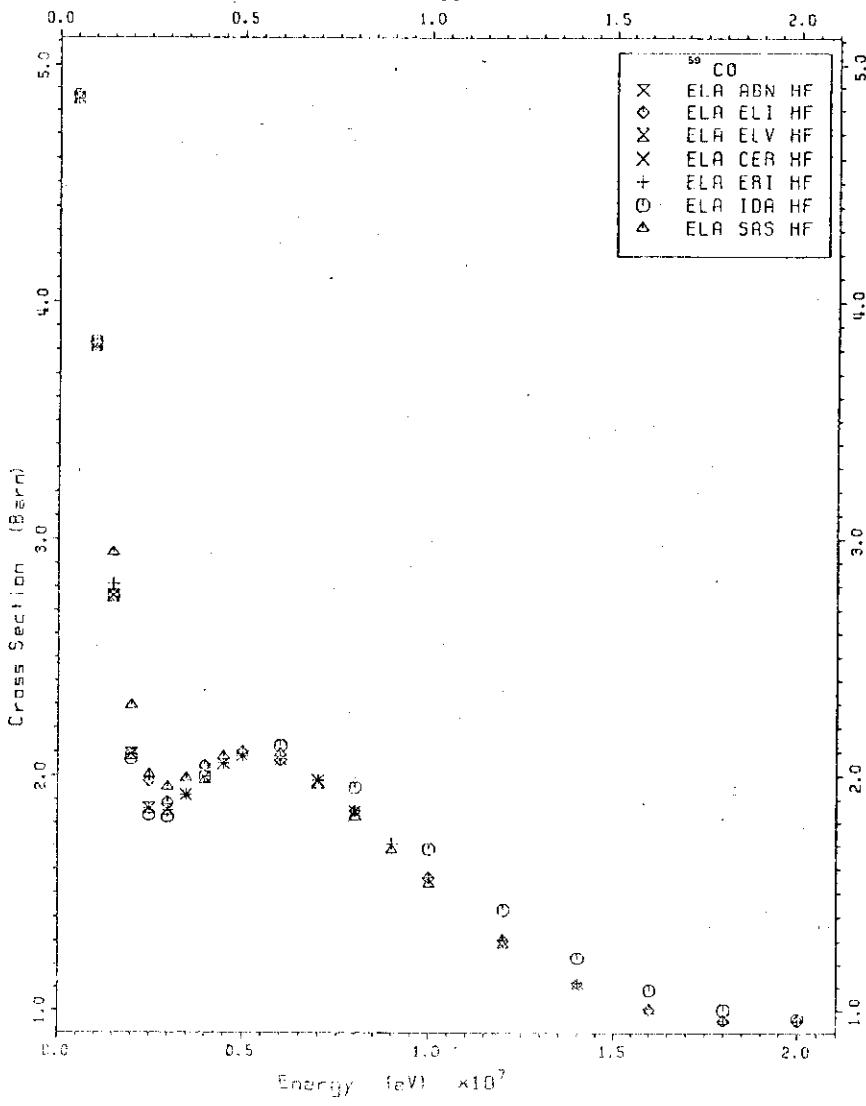


Fig. 6 Elastic Cross-section (EF) Line-
 ×10⁷



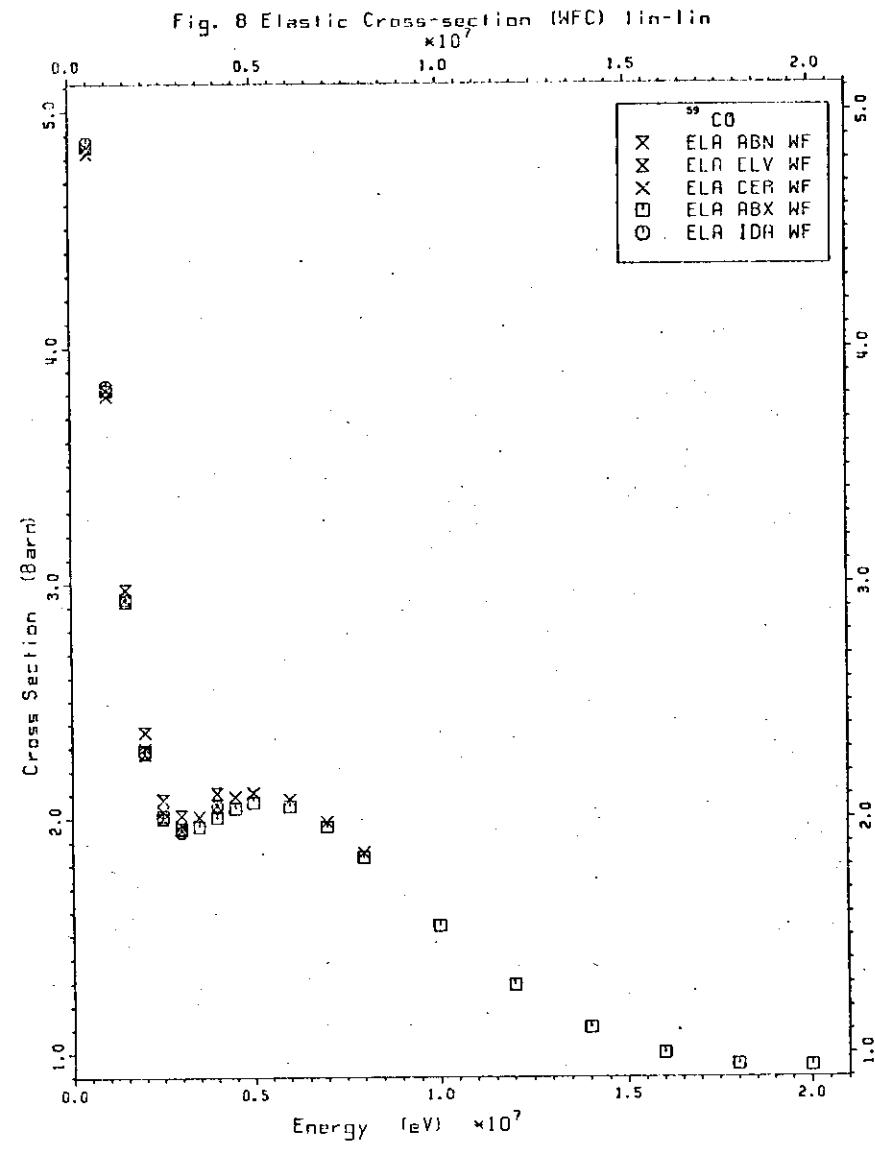
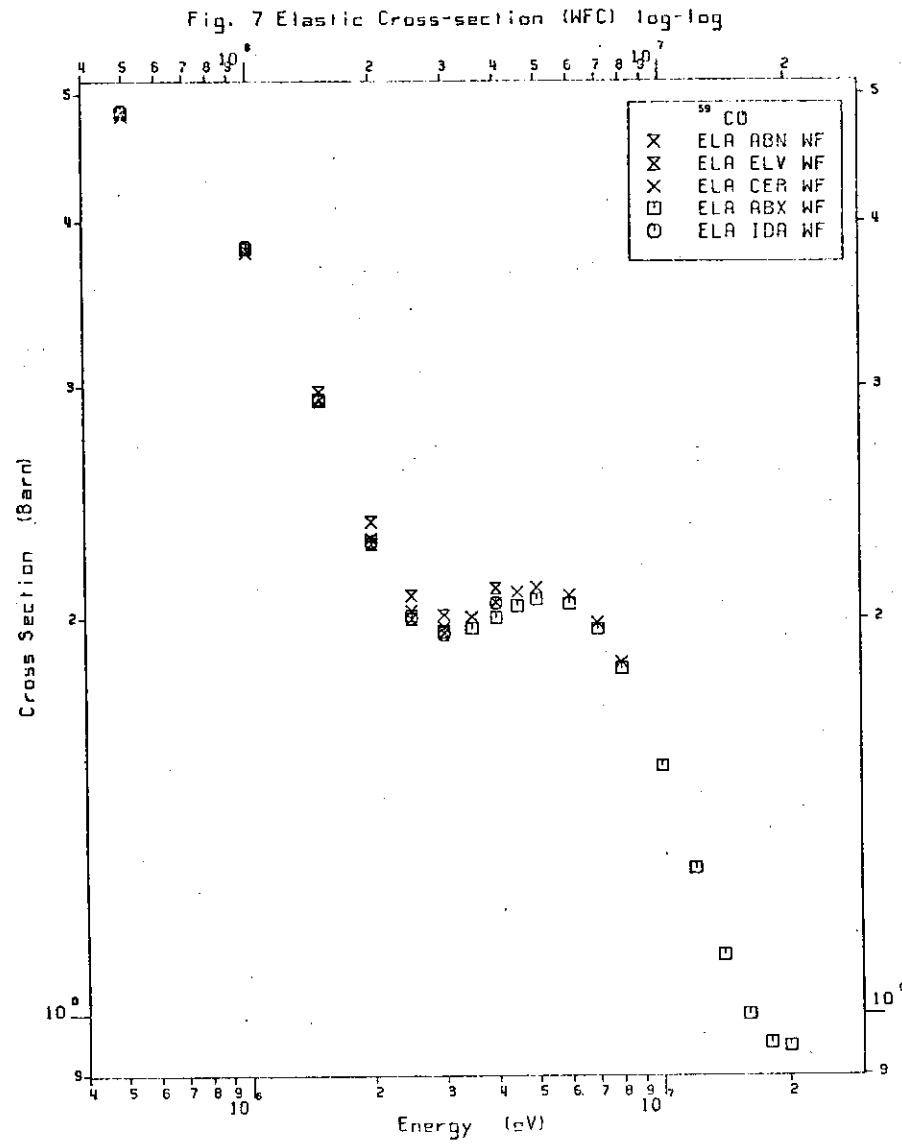


Fig. 9 Elastin Cross-section from BM&RFOI - overlay

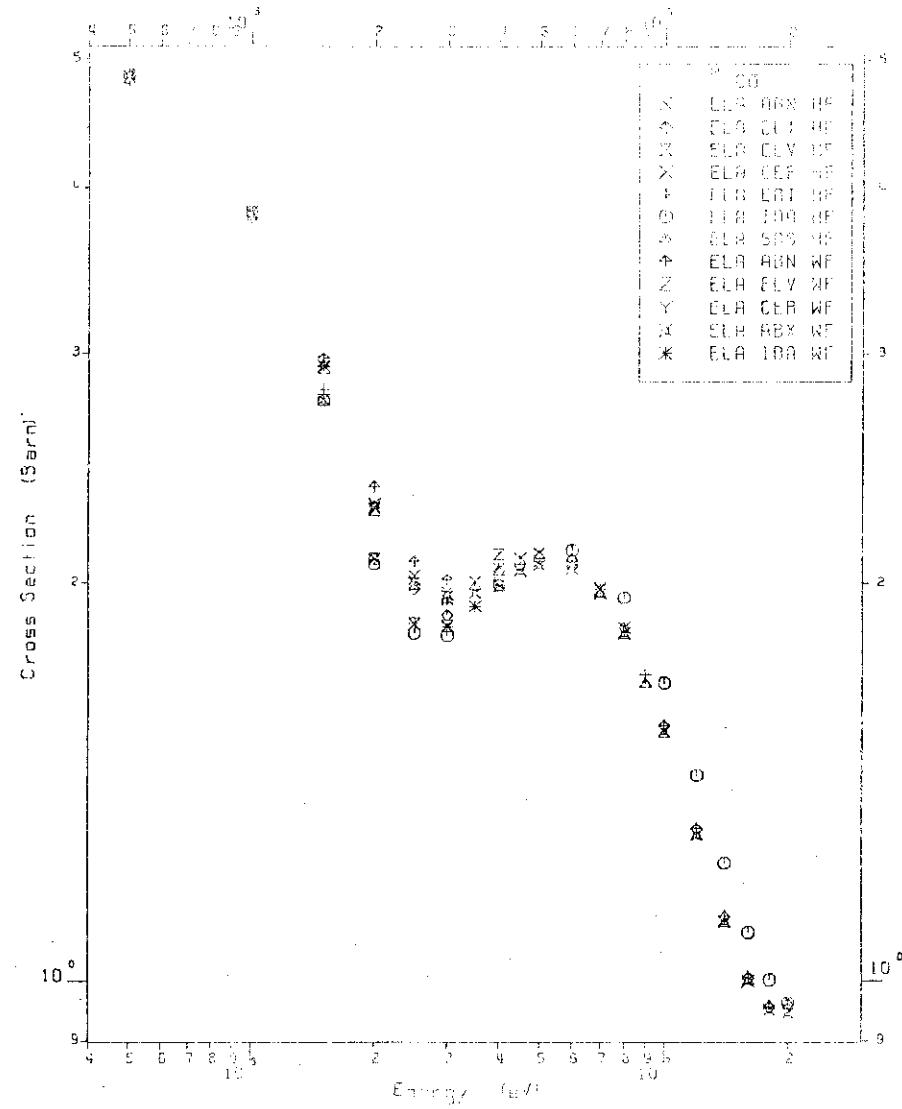


Fig. 10. Elastic-Plastic Interaction (HEA&RFO) Element

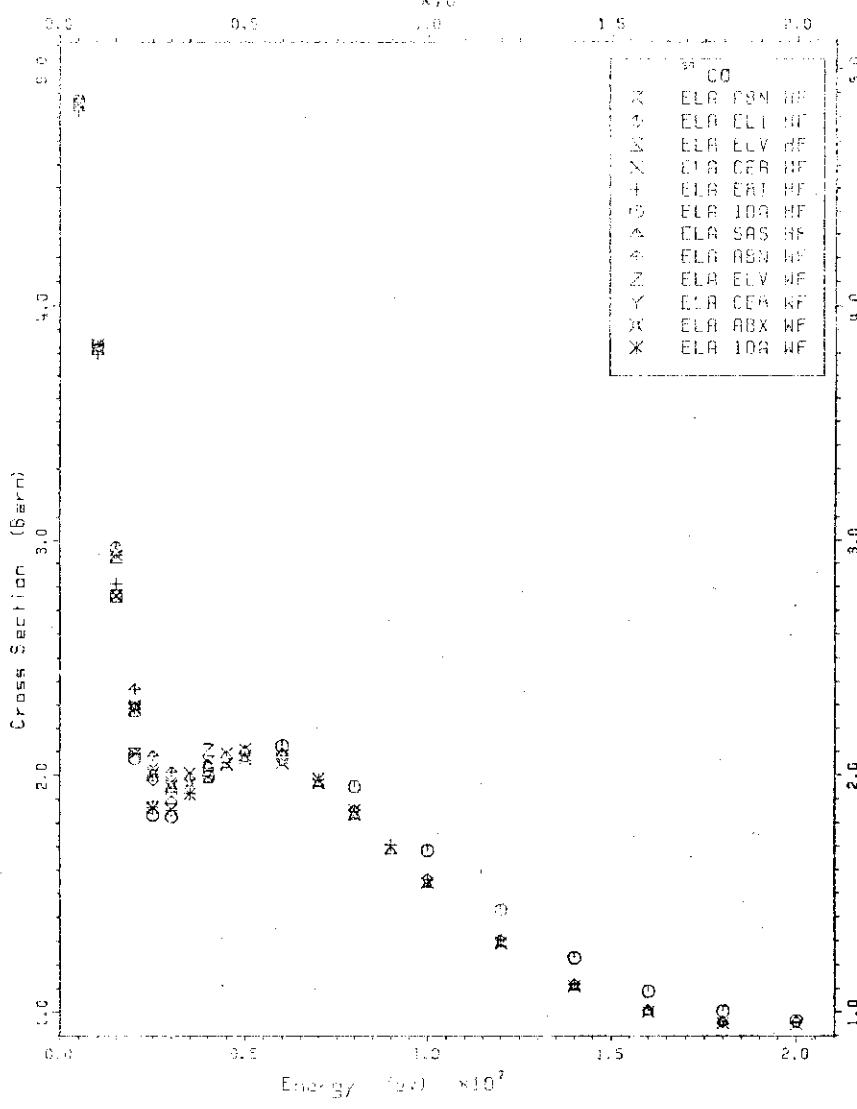


Fig. 11 Compound-nucleus Cross-section log-log

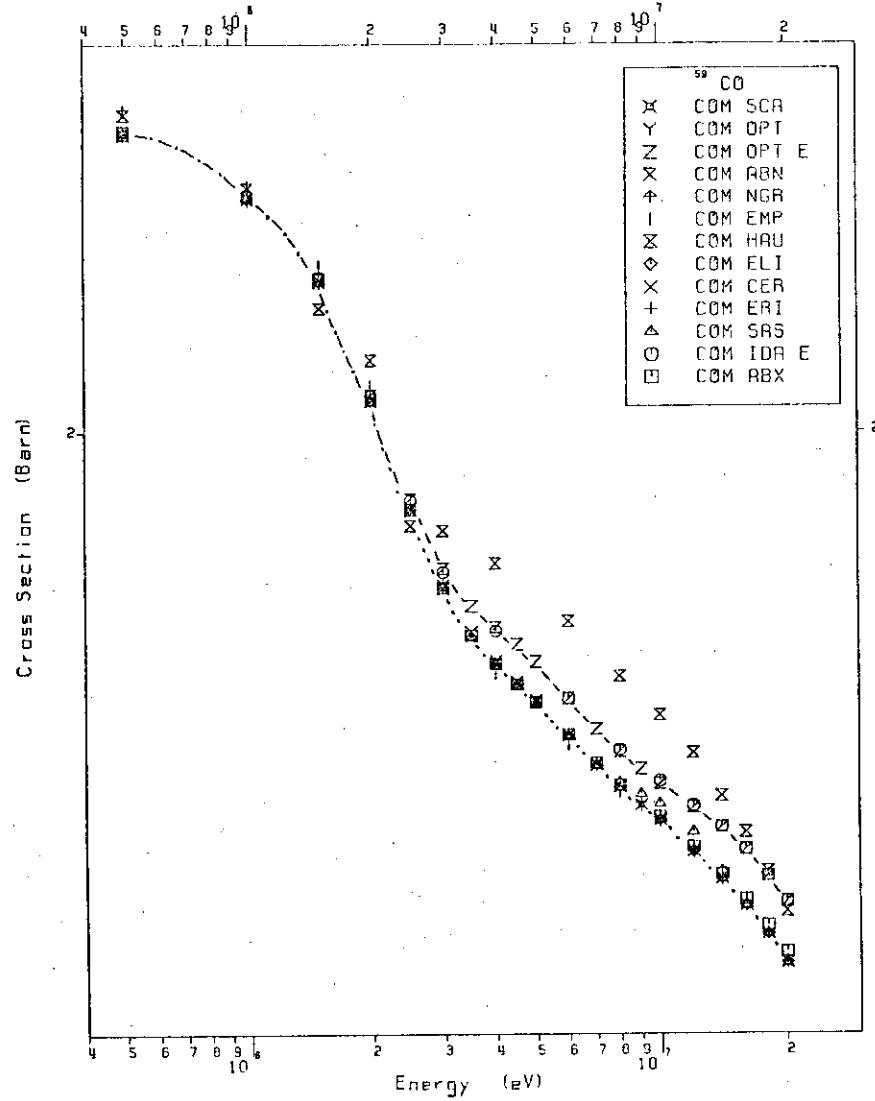


Fig. 12 Compound-nucleus Cross-section lin-lin
 $\times 10^7$

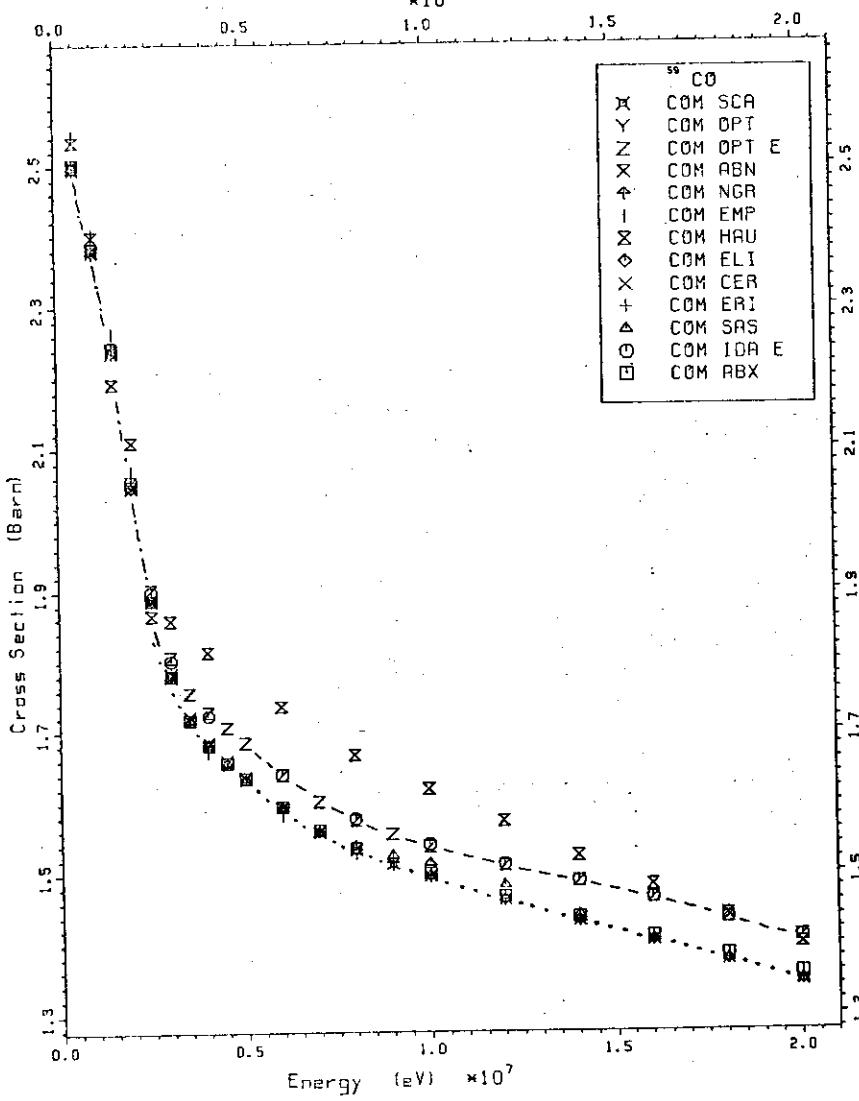


Fig. 13 Inelastic (n,n') Cross-section log-log

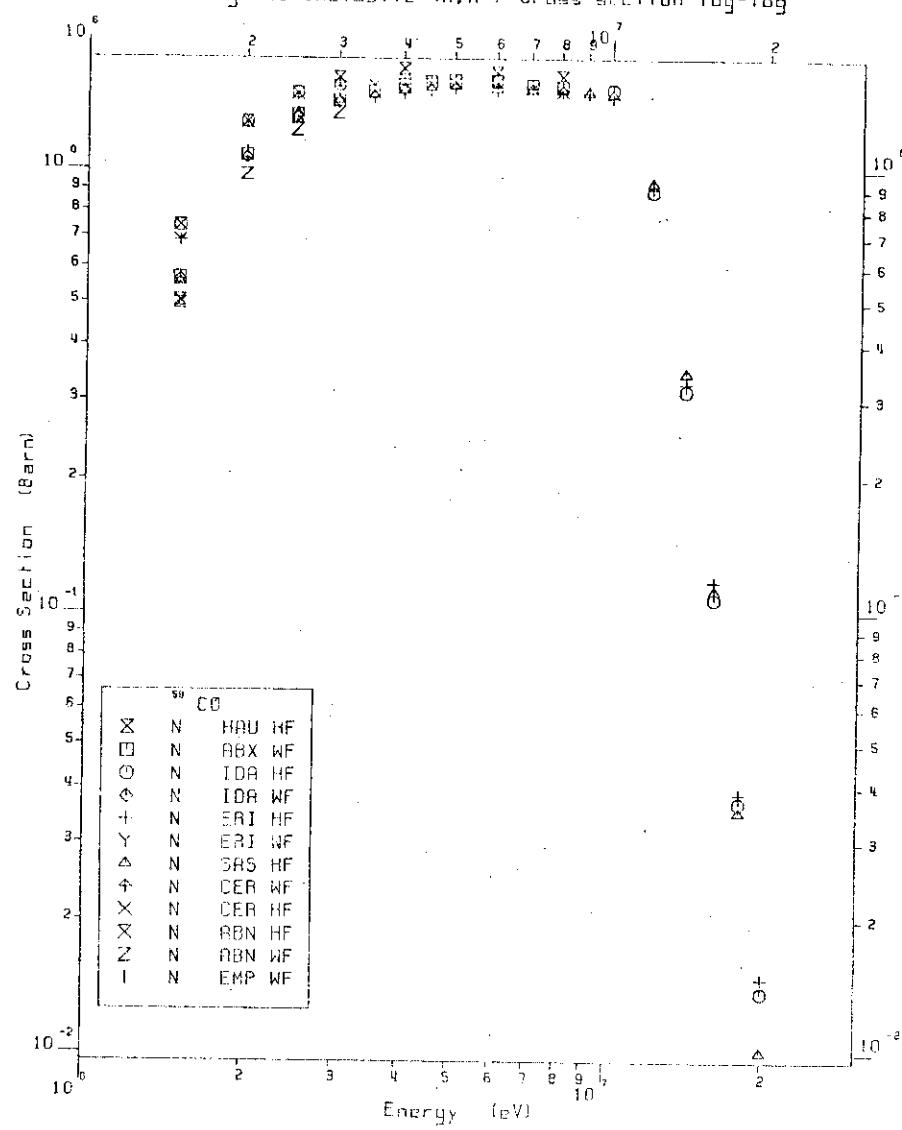
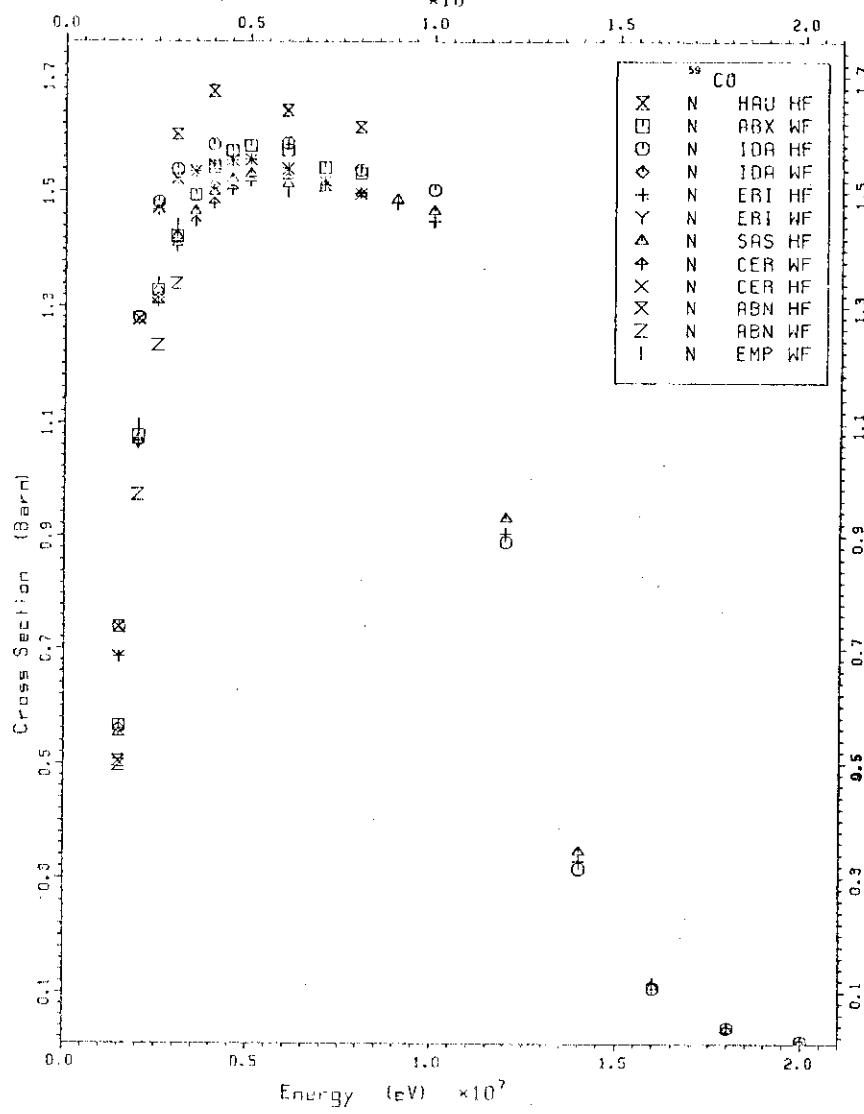
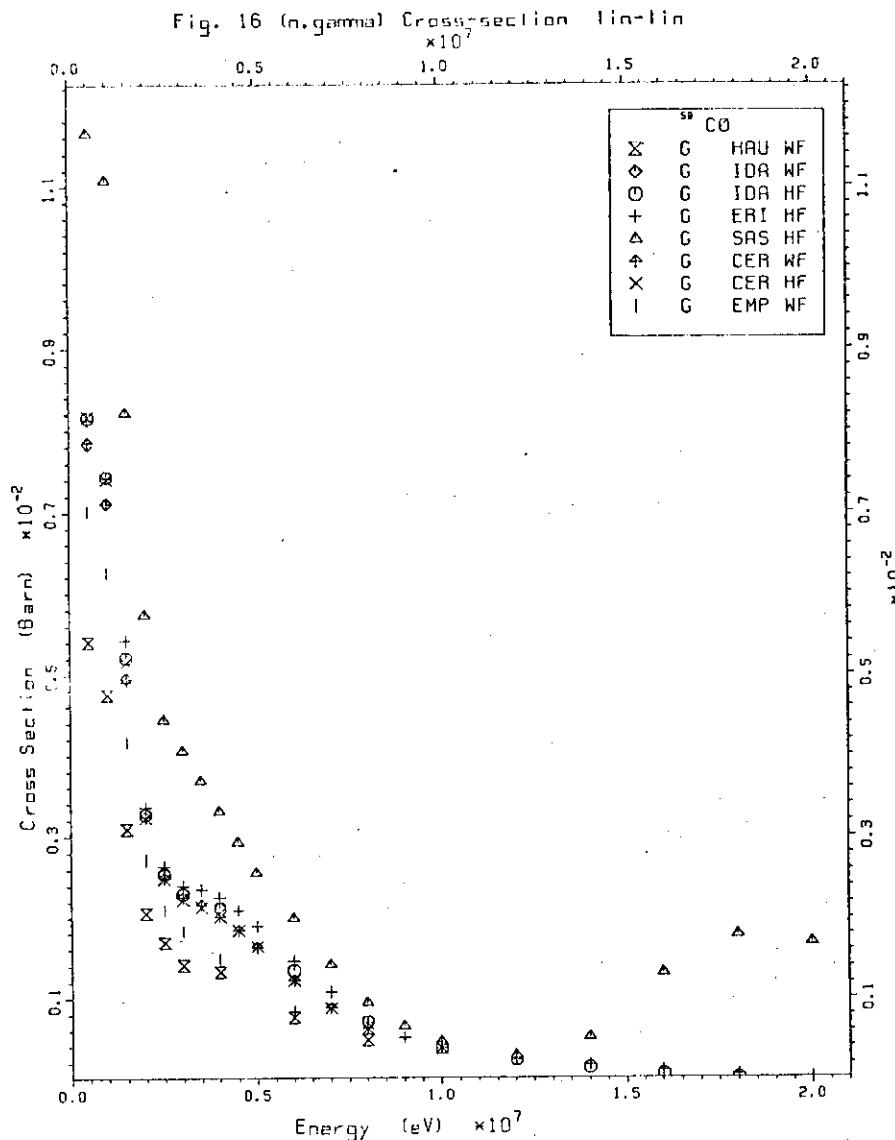
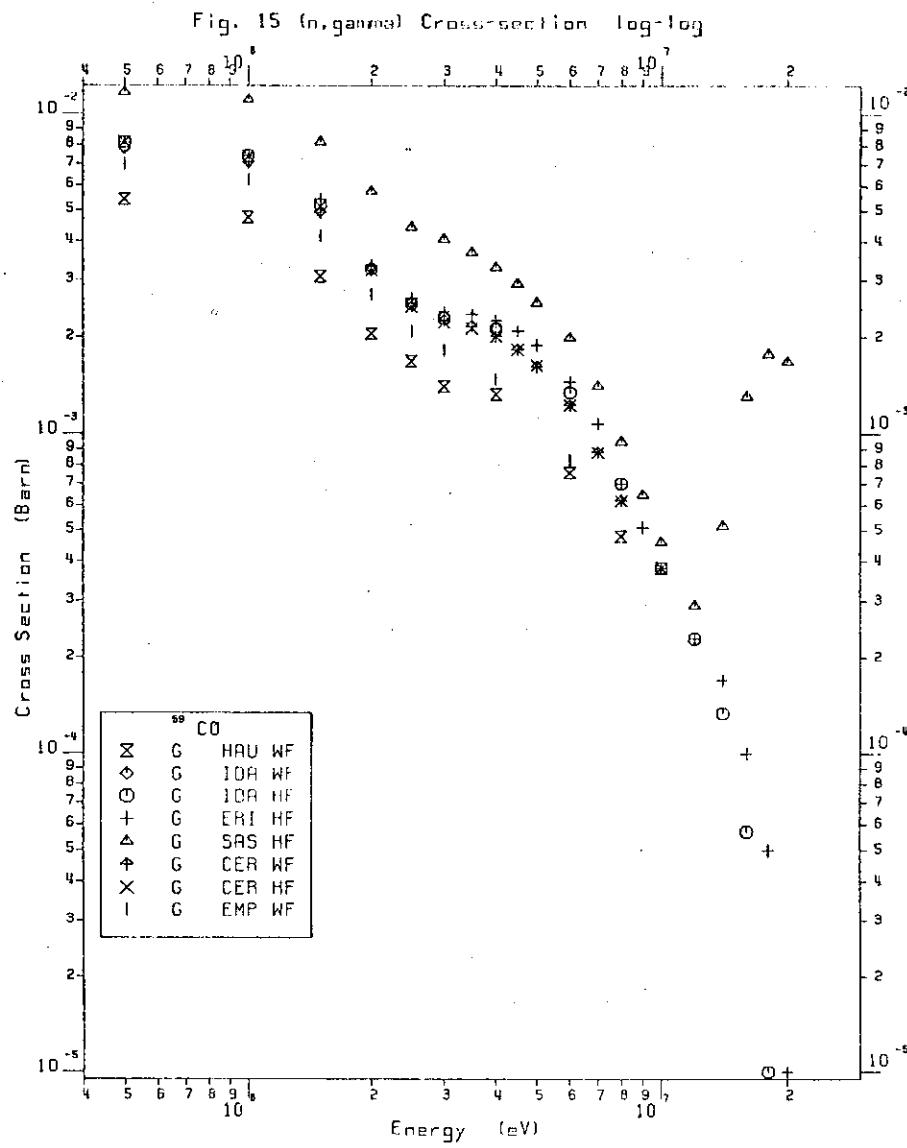
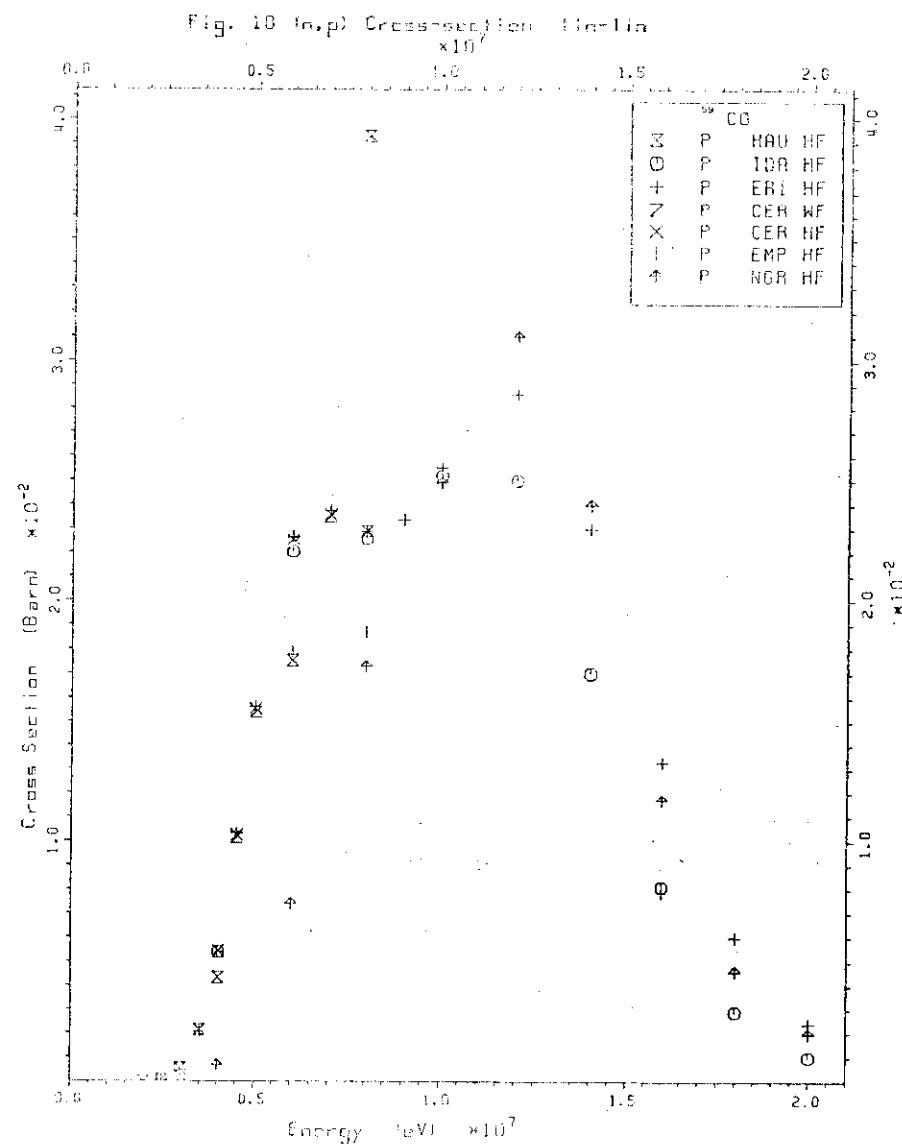
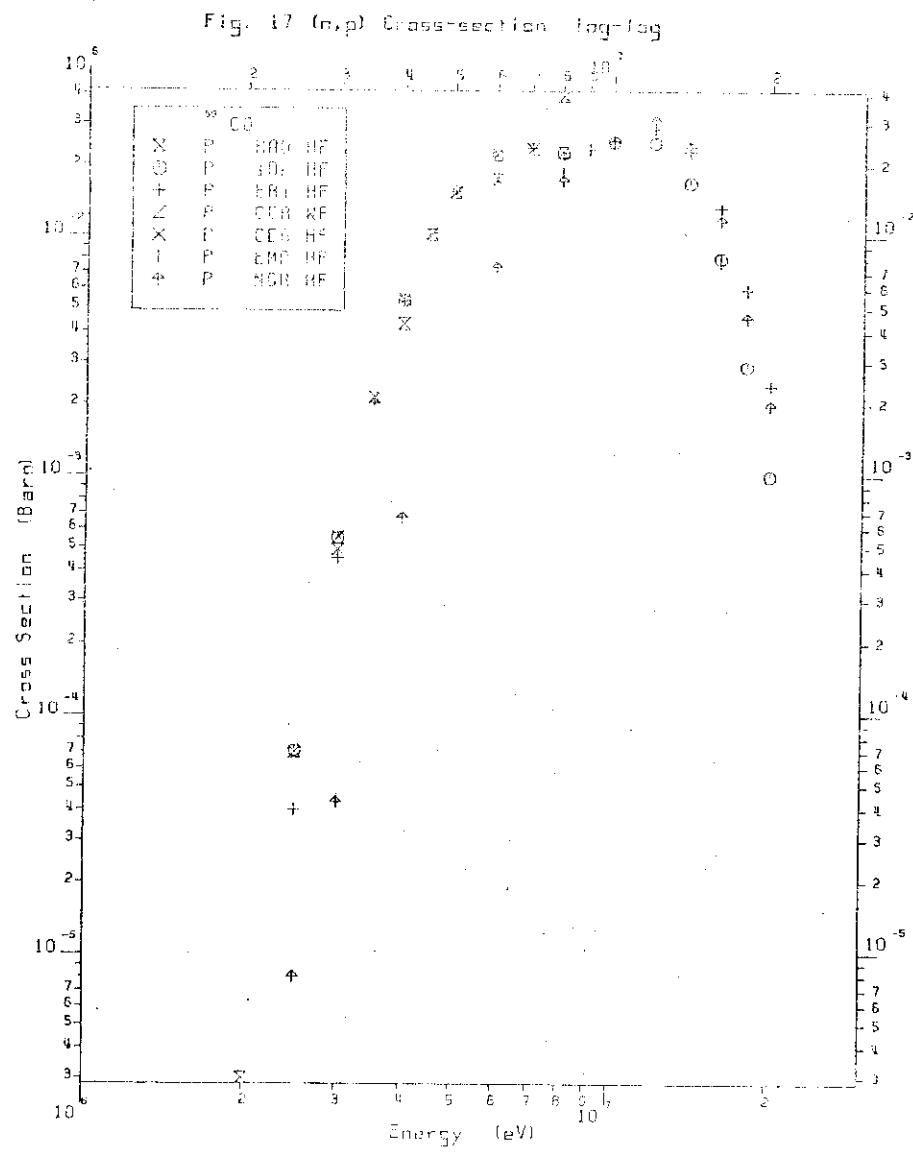


Fig. 14 Inelastic (n,n') Cross-section lin-lin







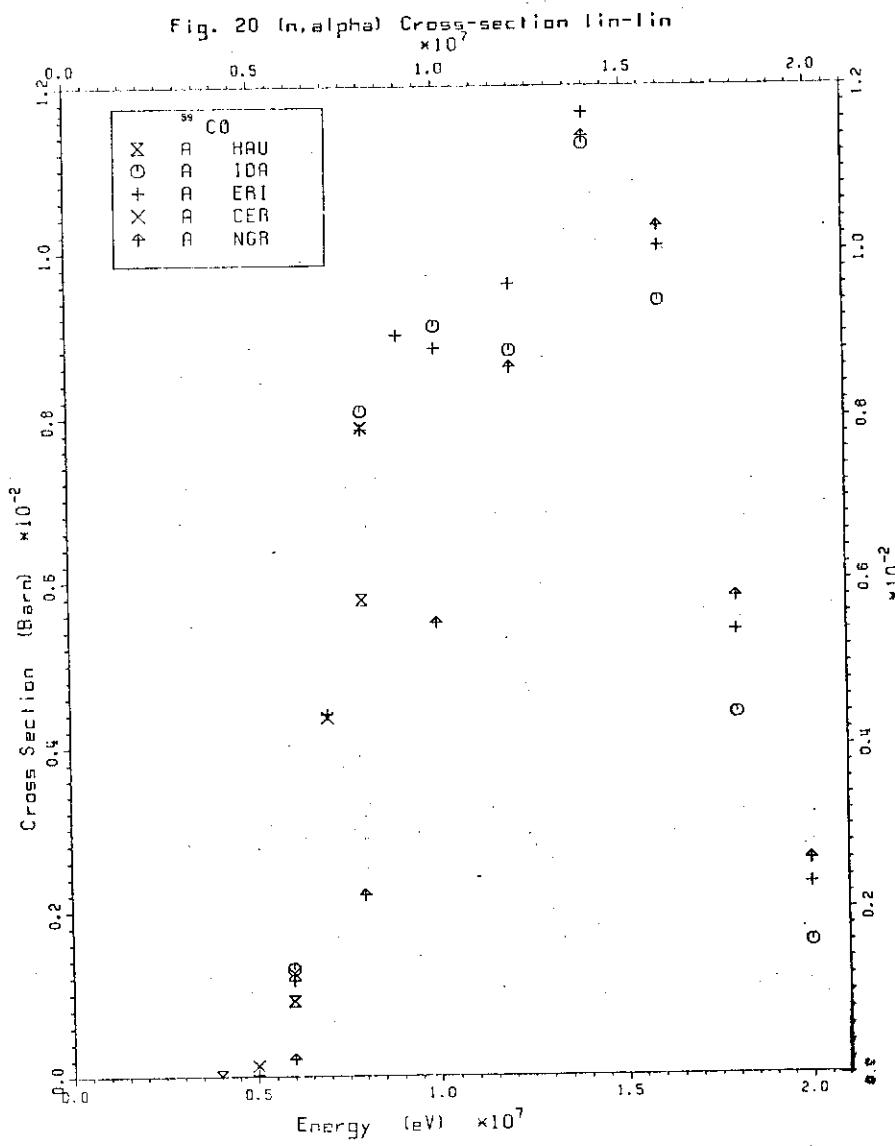
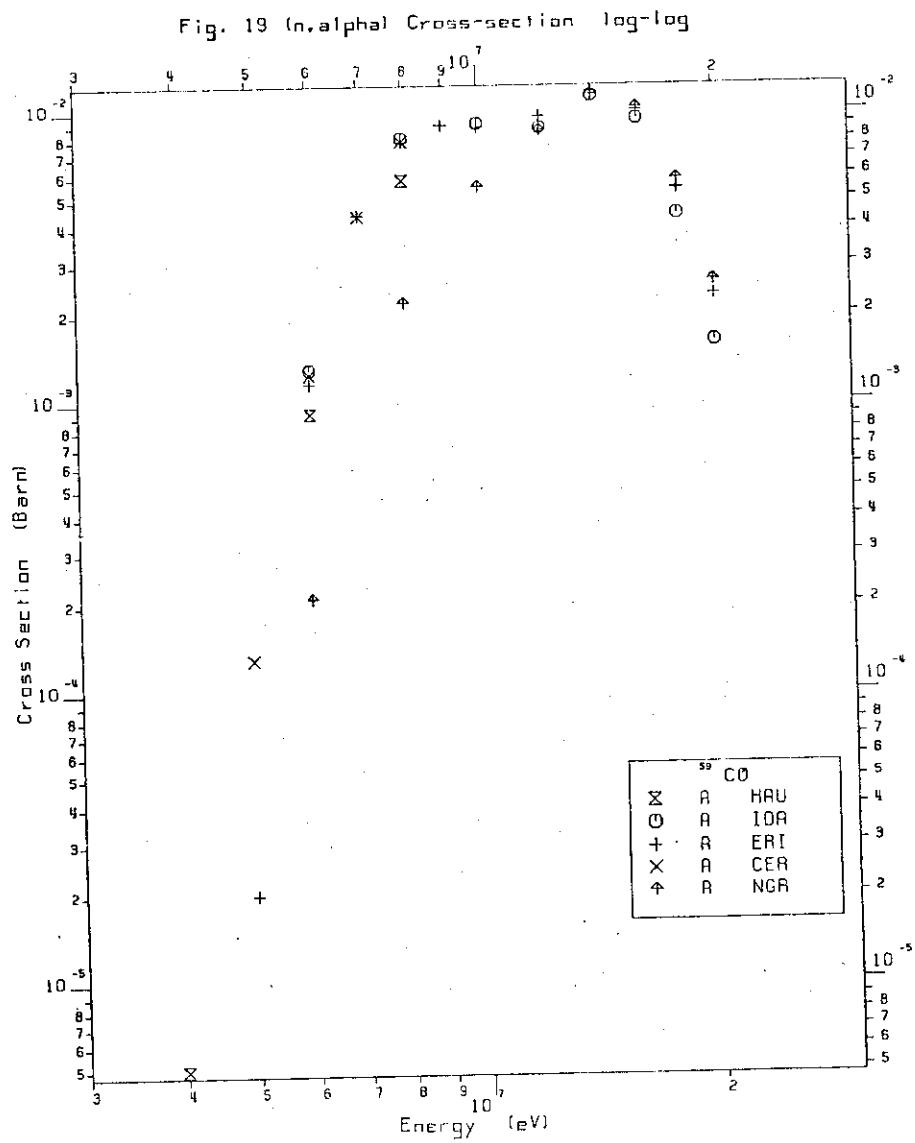


Fig. 21 (α , α) Cross-section log-log

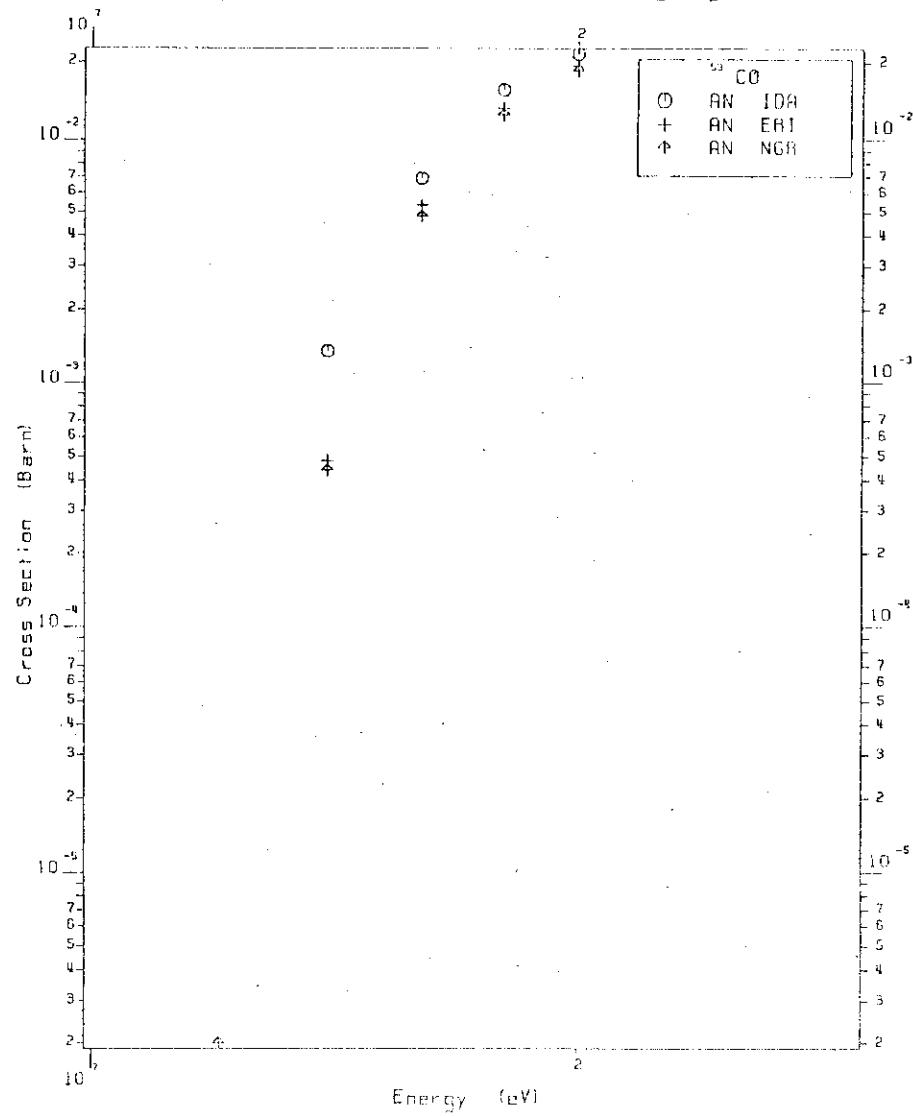


Fig. 22 (α , α) Cross-section lin-lin
 $\times 10^7$

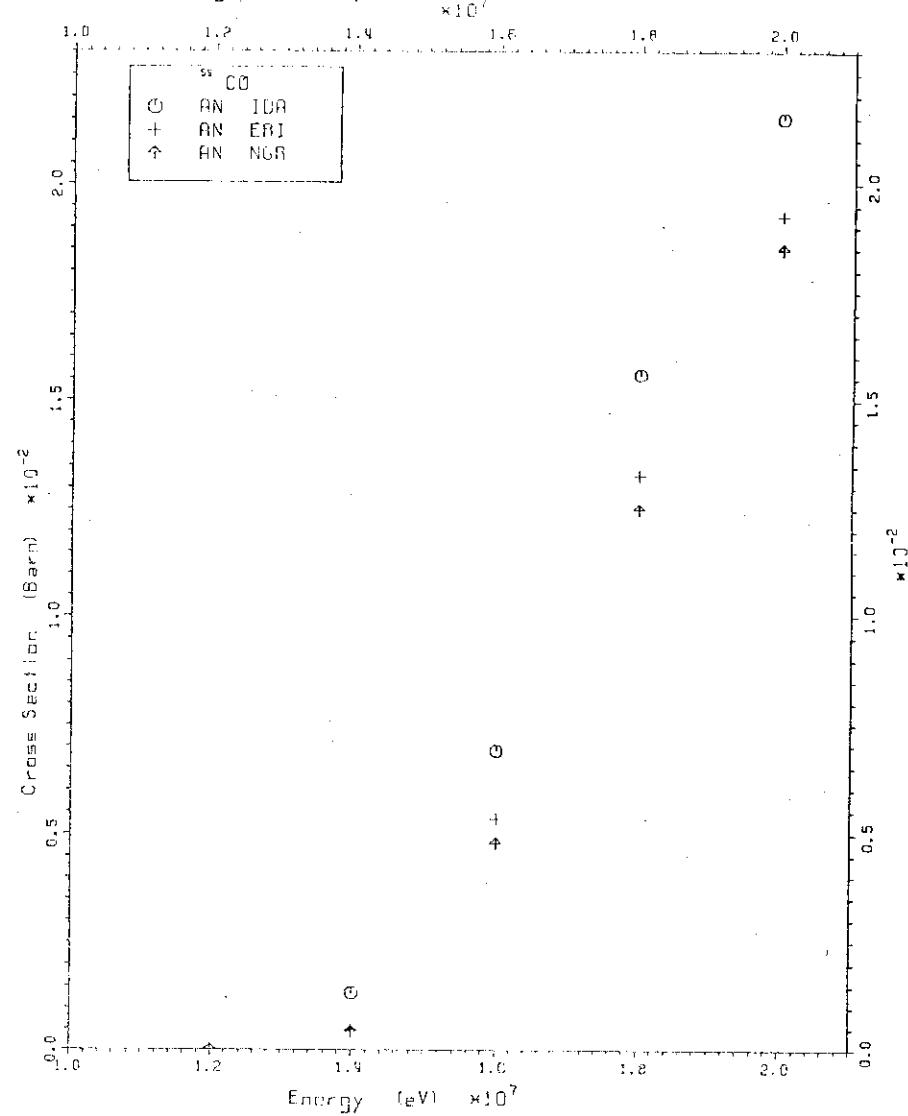


Fig. 23 $(n,\alpha)_\gamma + (n,\alpha)_\gamma n$ Cross-section log-log

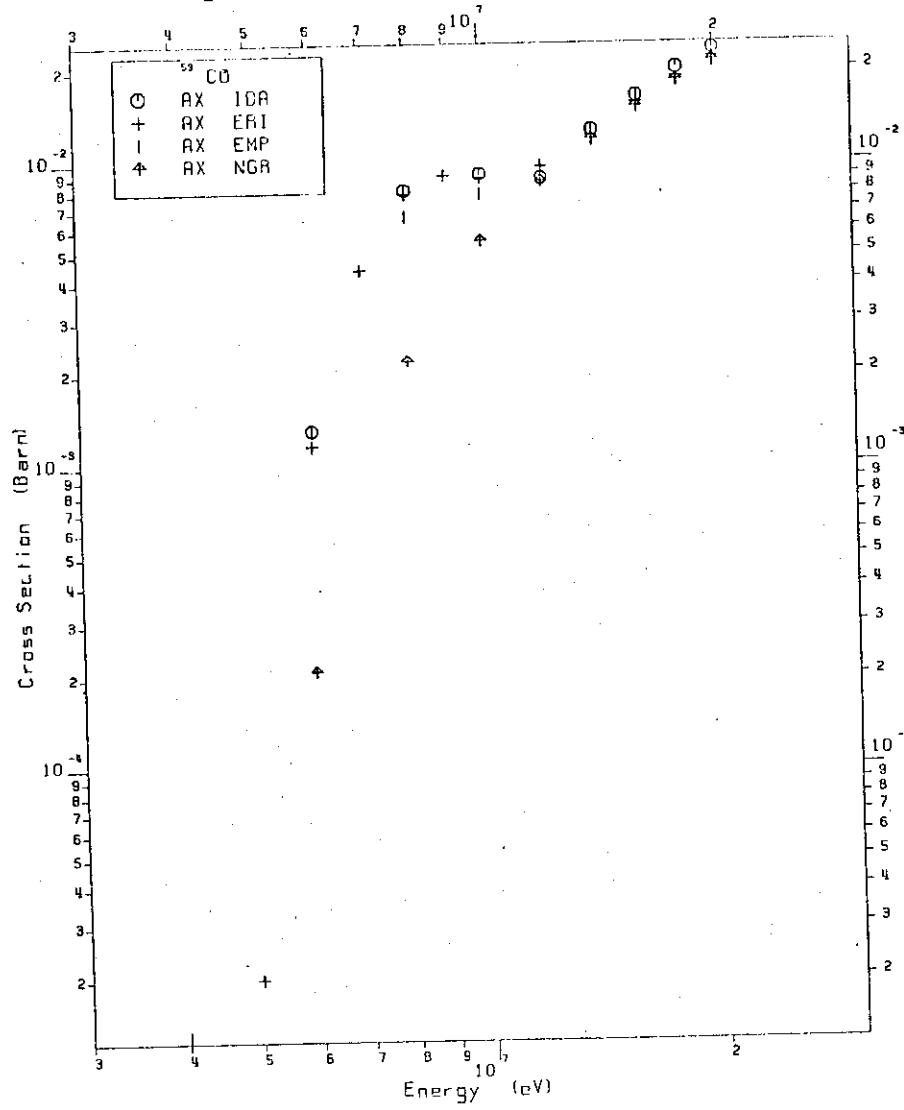


Fig. 24 $(n,\alpha)_\gamma + (n,\alpha)_\gamma n$ Cross-section lin-lin

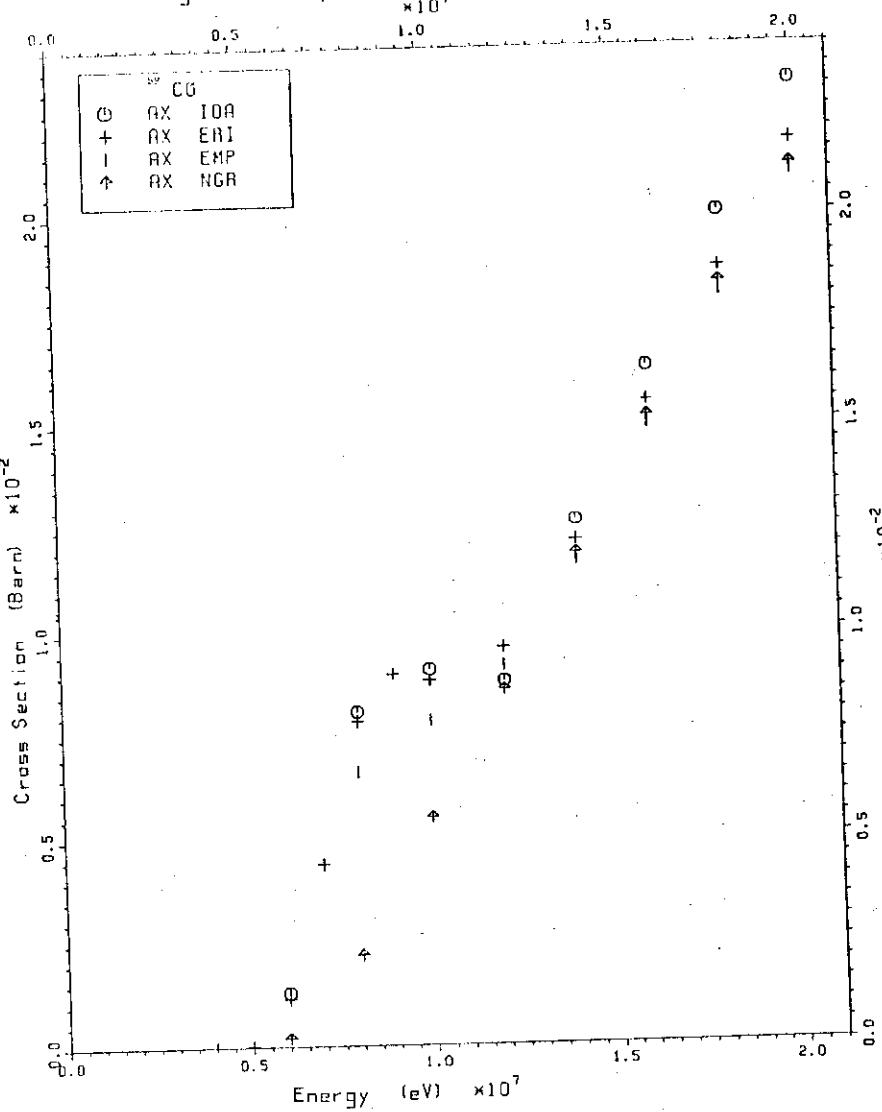


Fig. 25 (cont.) Cross-section log-log

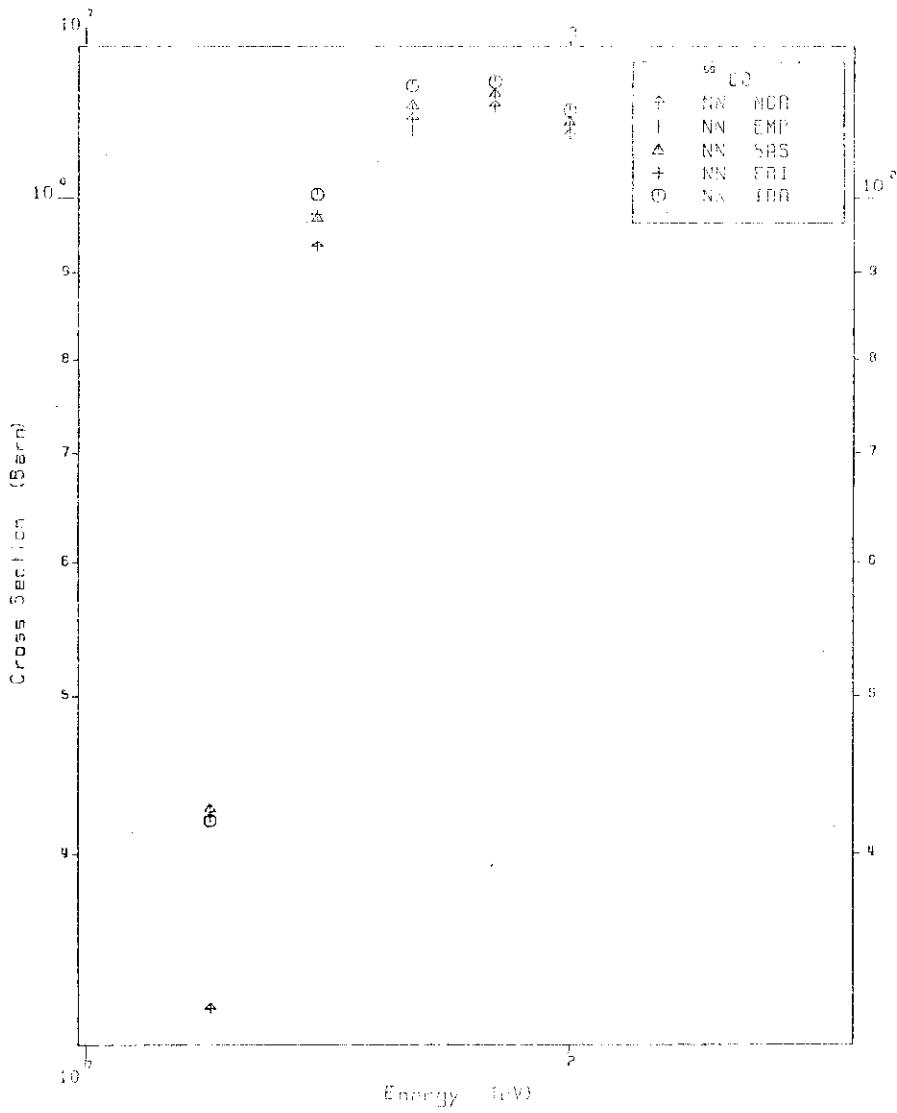


Fig. 26 (cont.) Cross-section line-1

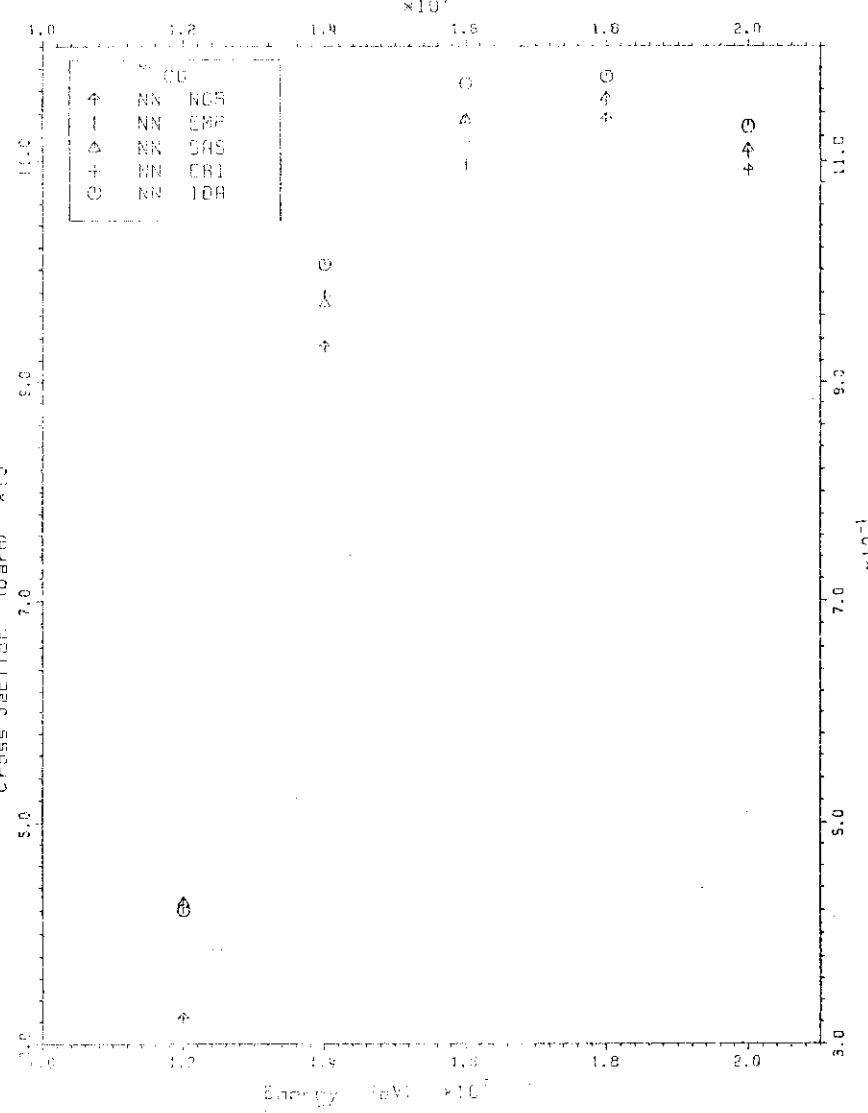


Fig. 27 (n, np) Cross-section log-log

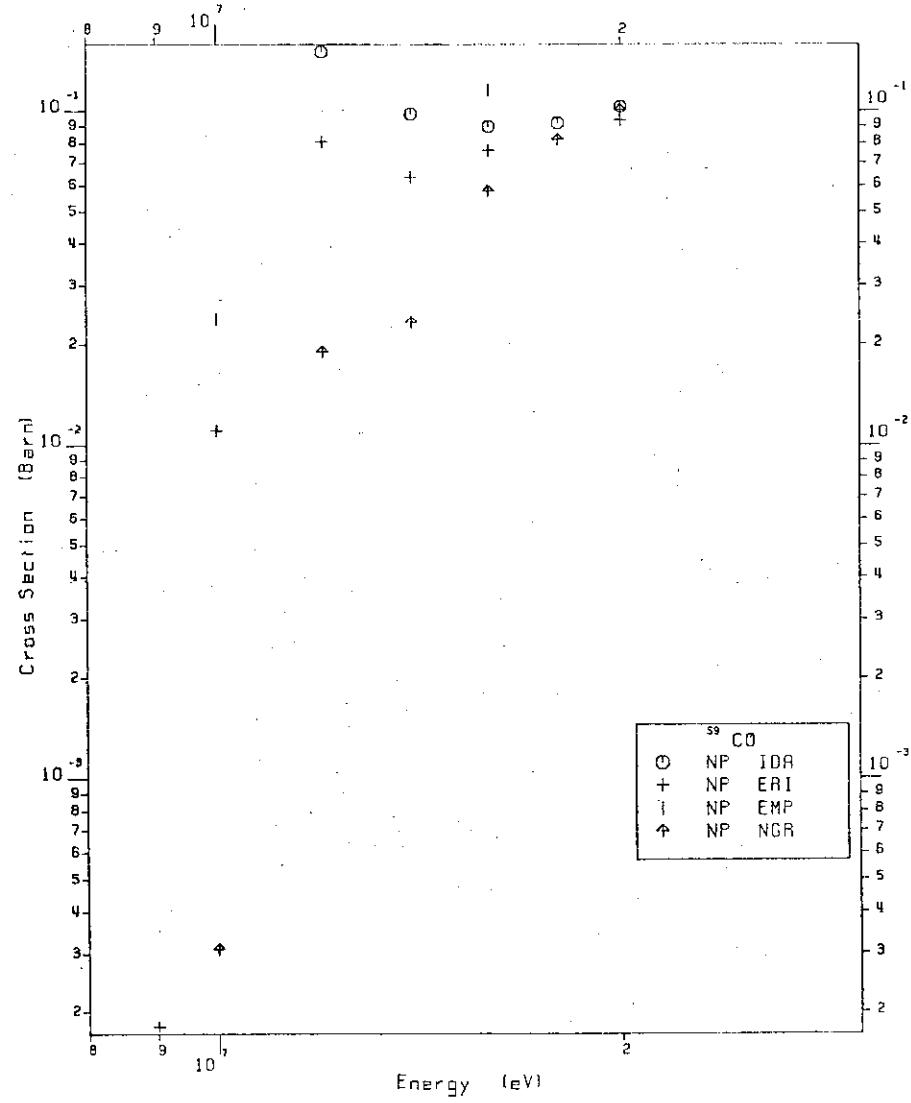


Fig. 28 (n, np) Cross-section lin-lin

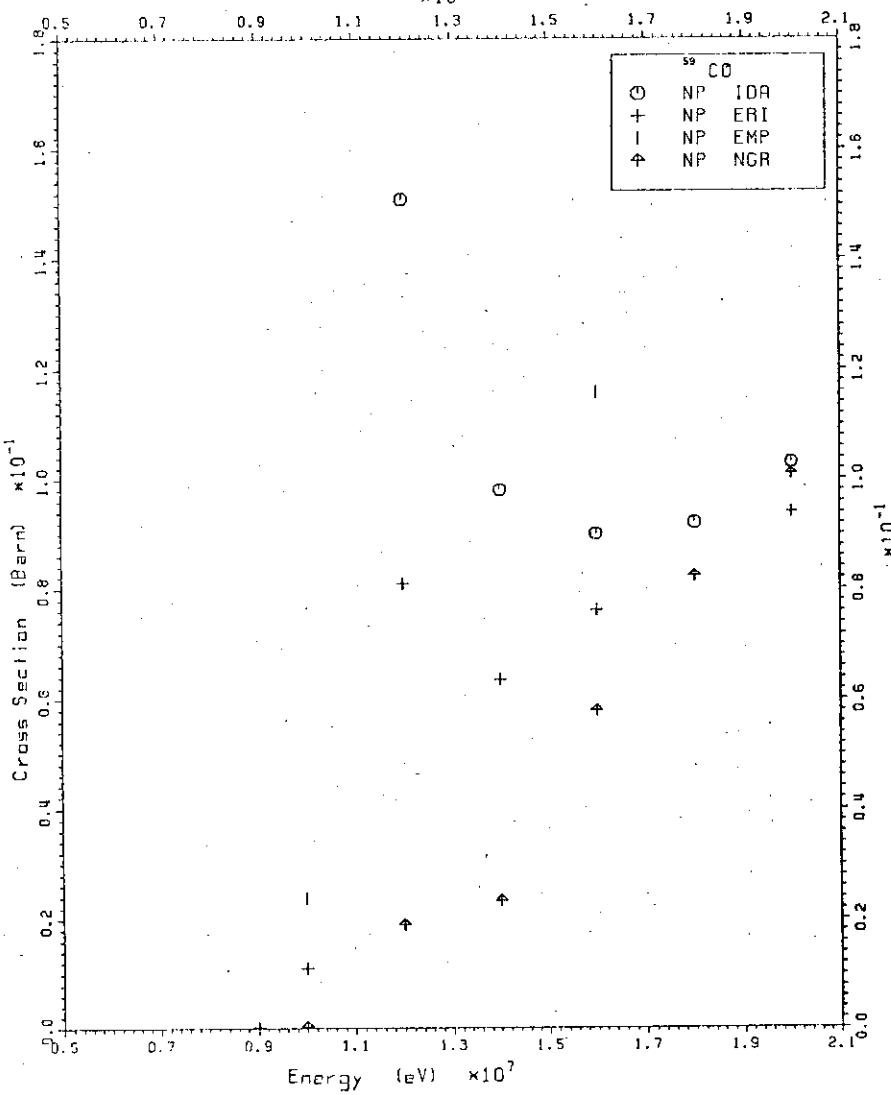


Fig. 29 (n,n) alpha Cross-section log-log

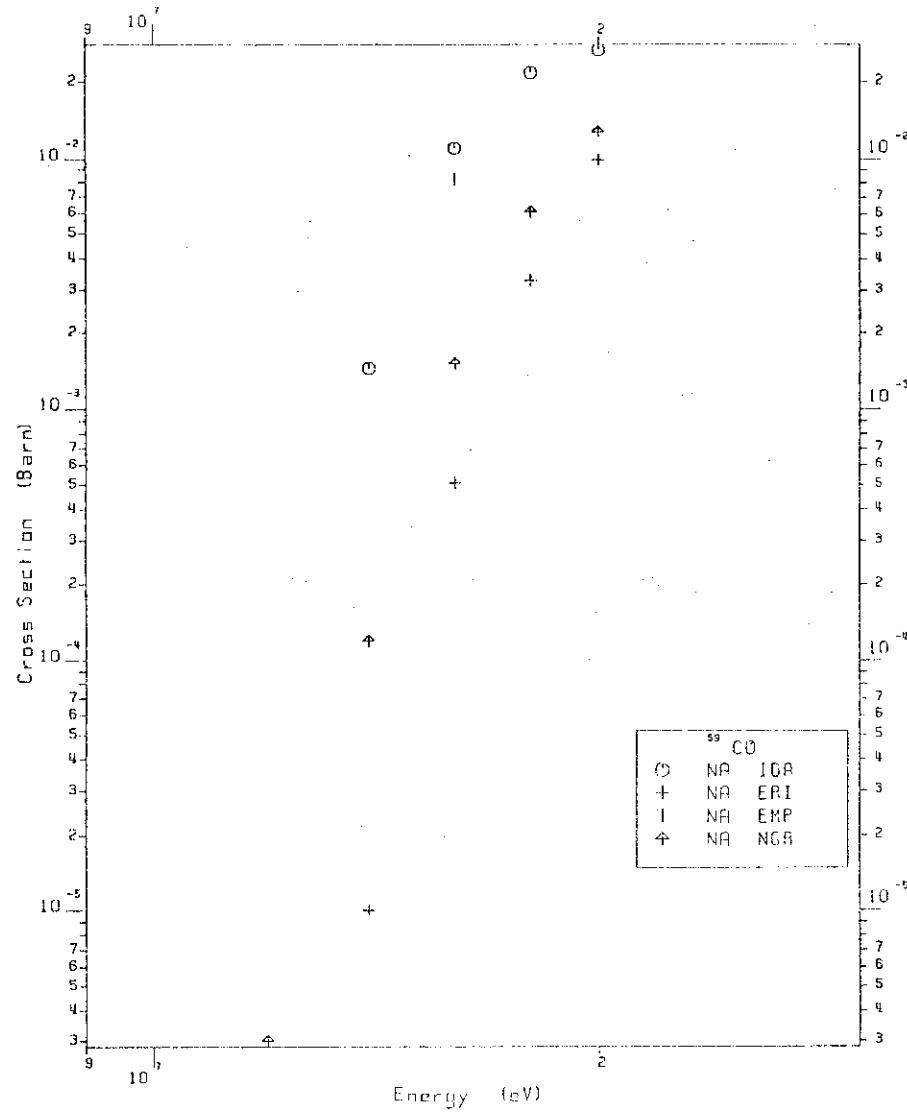
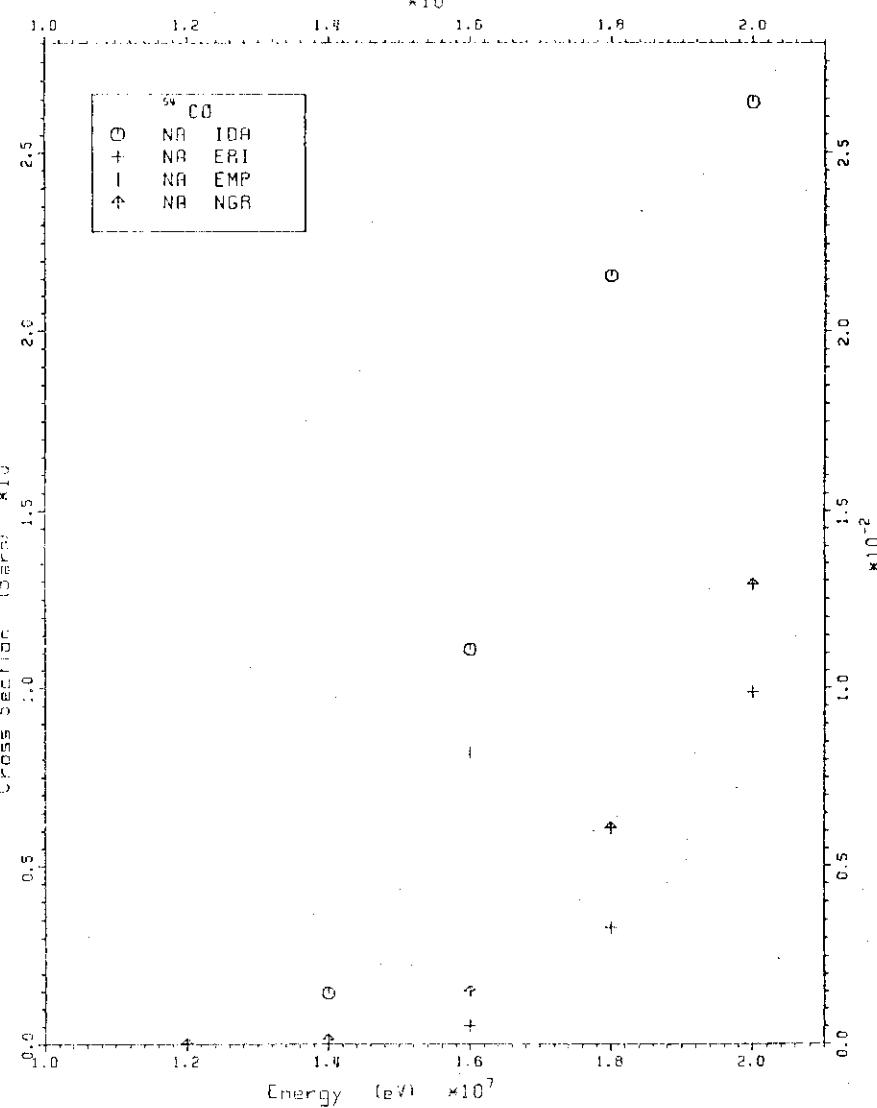
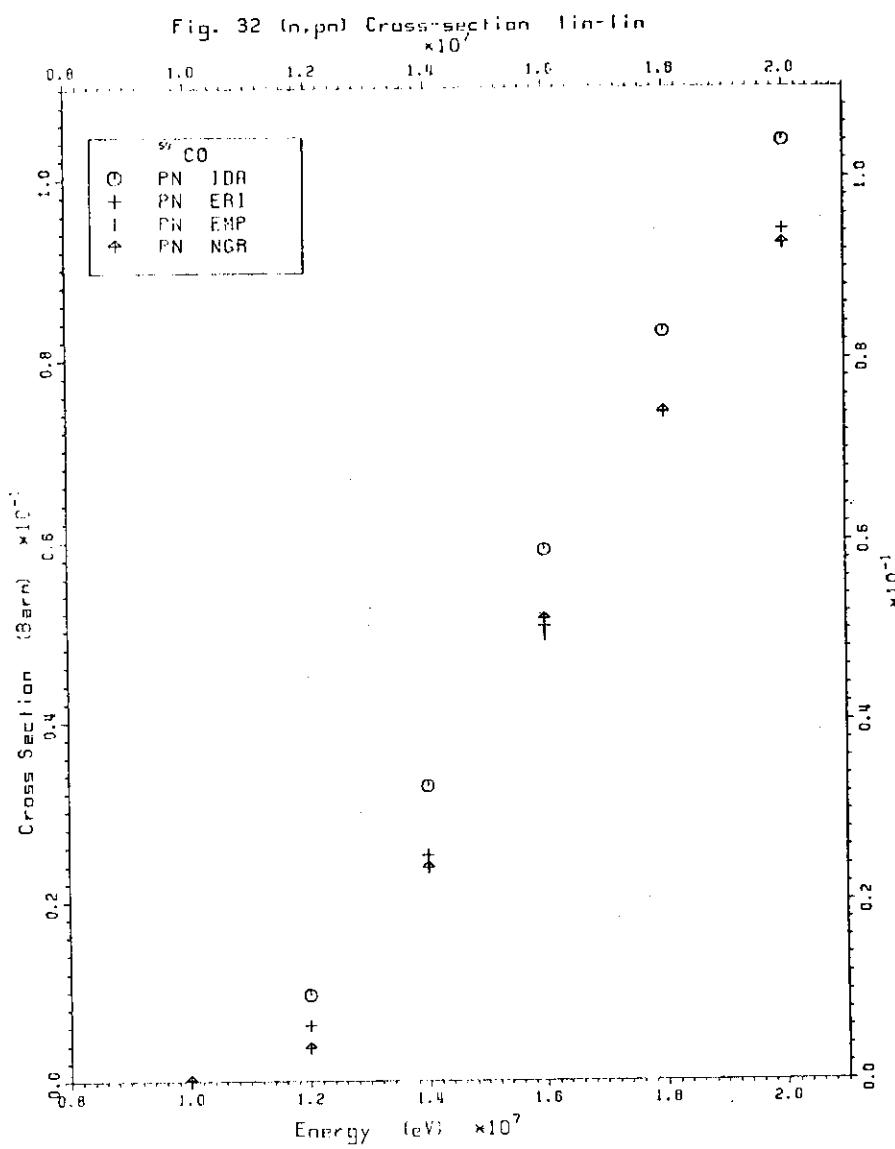
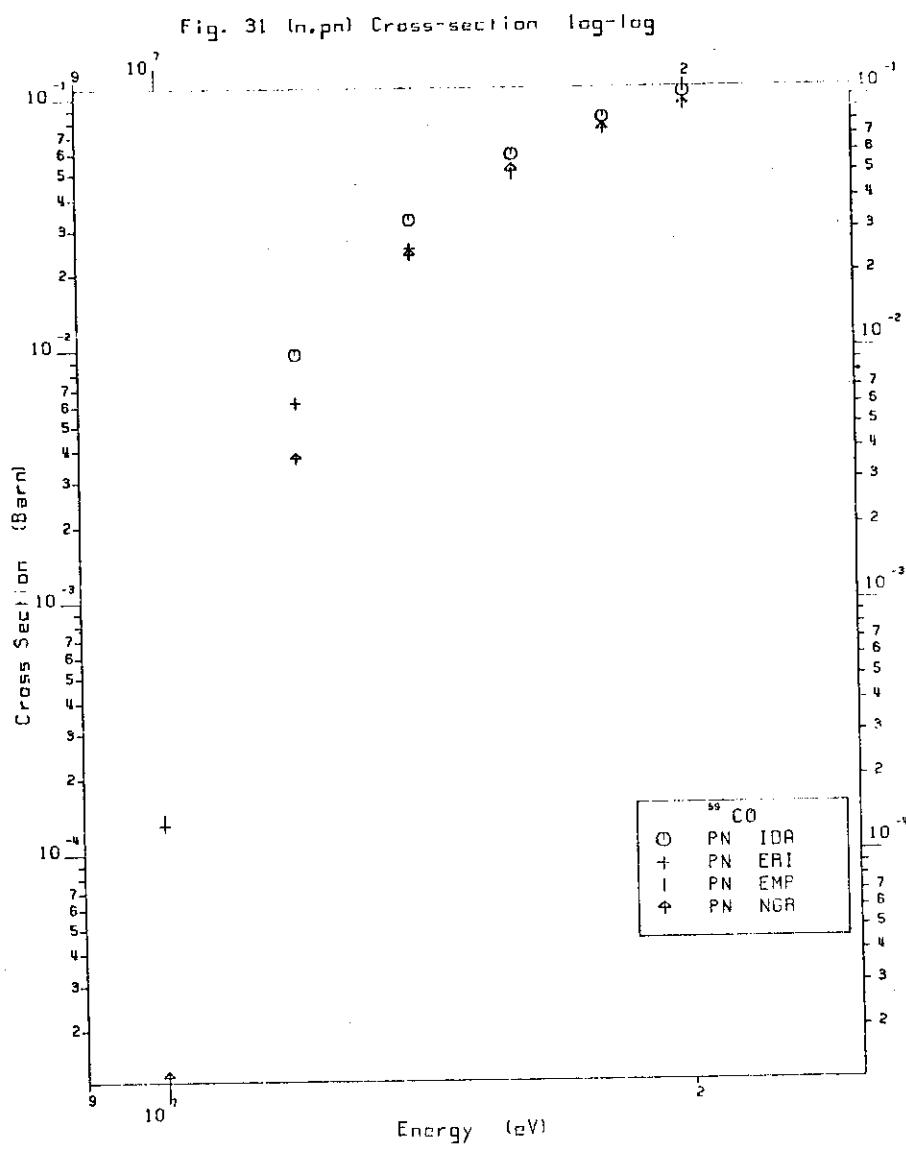


Fig. 30 (n,n) alpha Cross-section lin-lin
 $\times 10^7$





Problem Description1. The calculation and results

Participants should calculate the cross sections of as many of the possible neutron induced reactions on Mo-99 as their codes allow. Parameters are given for calculation of all the following reactions:

Total, Elastic, inelastic, (n, γ) , (n, p) , (n, α) , (n, d) , $(n, ^3\text{He})$, $(n, 2n)$, (n, np) and (n, pn) , $(n, n\gamma)$, $(n, 2p)$, $(n, 3n)$, $(n, 2n(p))$, $(n, 2n+\alpha)$.

For those who wish to carry out only a subset of these reactions, it is suggested that they omit those involving d and ^3He .

a) The calculated quantities to be compared

Calculated cross sections should be given at incident neutron energies between 0.5 and 20 MeV. An adequate choice of energy intervals that will permit to analyse competition between different reaction channels is the following:

- ½ MeV intervals between 0.5 and 5 MeV.
- 1 MeV intervals between 5 and 10 MeV.
- 2 MeV intervals between 10 and 20 MeV.

Another acceptable set of energies would be the following:

- ½ MeV intervals up to 3 MeV.
- 2 MeV intervals up to 20 MeV.

i.e. 0.5, 1, 1.5, 2, 2.5, 3, 4, 6, 8, 10, 12, 14, 16, 18, 20 MeV.

The choice between these two sets is left to the participant.

The calculation falls into two distinct phases, and in order to identify more easily the origin of any discrepancies that may arise, participants should also give the transmission coefficients generated by the spherical optical model part of the calculation, and used as input in the statistical model calculations.

b) Options

Both energy independent and energy dependent optical model parameters are given. The set appropriate to the code normally used by the participant should be chosen. The energy dependent parameters give a slightly better fit to experimental data for the total cross section.

In the energy range up to 5 MeV the calculation can be done either with or without width flip, and with or without W_{SF} , and, in theory, that must mean the total cross section can be fitted in three ways.

International Nuclear Model Codes Comparison

A. Prince - BNL (USA)

Definition of Optical Potential

(according to Bechetti & Greenlees, Phys. Rev. 162, 1190 (1967))

	<u>expression</u>	<u>validity range</u>	<u>explanation</u>
$U_{\text{opt}}(r) = -V_R f_R$			central real
$+ (\frac{\hbar}{m_e c})^2 \frac{V_{SC}}{r} (\frac{d}{dr} f_{SC}) - \vec{p}^* \cdot \vec{f}$			spin orbit
$+ \begin{cases} \frac{(Zze)^2}{2R_c} (3 - (\frac{r}{R_c})^2) & \text{for } r < R_c \\ \frac{(Zze)^2}{r} & \text{for } r > R_c \end{cases}$			Coulomb
$- iW f_I$			imaginary volume
$+ i4a_I W_{SF} (\frac{d}{dr} f_I)$			imaginary surface
where $f_X = f(r, R_X, a_X) = [1 + \exp(r - R_X)/a_X]^{-1}$			
$R_X = r_X^{1/3}$			
$r_c = \text{Coulomb radius}$			

Note: Whenever a parameter is omitted, it is assumed that the corresponding potential is not considered.

Optical Model ParametersNeutron Parameters

$$v_R = 47.4 - 0.463 E + 0.0022 E^2 \quad (E \text{ in MeV-Lab})$$

$$r_R = 1.26 \text{ fm} \quad a_R = 0.7835 \text{ fm}$$

$$r_R = 1.26 + 0.00286 E \quad (E \text{ in MeV-Lab}) \text{ fm} \quad \text{Energy dependent option}$$

$$W_{SF} = 17.5 + 0.358 E - 0.007 E^2$$

$$r_I = 1.3136 \text{ fm} \quad a_I = 0.6319 \text{ fm}$$

$$r_I = 1.3136 - 0.0007 E \quad (E \text{ in MeV-Lab}) \text{ fm} \quad \text{Energy dependent option}$$

$$v_{SO} = 6.44$$

$$r_{SO} = r_R \quad a_{SO} = a_R$$

$$\text{Matching Radius } R_m = 15.585 \text{ fm or } R_m = R + 10.7 \text{ fm.}$$

The real potential is of the Woods-Saxon form; the imaginary potential is surface type with a gaussian form and the spin orbit potential of the Thomas form.

Proton Parameters: Becchetti & Greenlees Phys. Rev. 182, 1190 (1969)

$$v_R = 54.0 - 0.32 E + 0.4Z/A^{1/3} + 24.0(N-Z)/A \quad \text{MeV}$$

$$r_R = 1.17 \quad a_R = 0.75$$

$$W_V = 0.22E - 2.7 \text{ or zero, whichever is greater}$$

$$W_{SF} = 11.8 - 0.25E + 12.0(N-Z)/A, \quad \text{MeV}$$

or zero, whichever is greater

$$r_I = 1.32 \text{ fm} \quad a_I = 0.51 + 0.7(N-Z)/A \quad \text{fm}$$

$$v_{SO} = 6.2 \text{ MeV}$$

$$r_{SO} = 1.01 \text{ fm} \quad a_{SO} = 0.75 \text{ fm}$$

$$r_c \text{ (coulomb radius)} = 1.25 \text{ fm}$$

Deuteron Parameters: Perey & Perey, Phys. Rev. 132, 755 (1963)

$$v_R = 81.0 - 0.22E + 2.0(Z/A)^{1/3}$$

$$r_R = 1.15 \text{ fm}, \quad a_R = 0.81 \text{ fm}$$

$$W_{SF} = 14.4 + 0.24E$$

$$r_I = 1.34 \text{ fm}, \quad a_I = 0.68 \text{ fm}$$

$$r_c = 1.25 \text{ fm}$$

Helion Parameters

Becchetti-Greenlees - Proc. Third Int'l Symposium, Madison, Wisc. (1970)

682.

$$v_R = 151.9 - 0.17 E + 50 (N-Z)/A \quad \text{MeV}$$

$$W_V = 41.7 - 0.33 E + 44 (N-Z)/A \quad \text{MeV}$$

$$r_R = 1.20 \text{ fm.}, \quad a_R = 0.72 \text{ fm}$$

$$r_I = 1.40 \text{ fm.}, \quad a_I = 0.88 \text{ fm}$$

$$v_{SO} = 2.5 \text{ MeV}$$

$$r_{SO} = r_R + a_{SO} \cdot a_R$$

$$r_c = 1.30 \text{ fm.}$$

Tritons

Becchetti - Greenlees - ibid

$$V_R = 165.0 - 0.17 E - 6.4 (N-Z)/A \text{ MeV}$$

$$W_V = 46.0 - 0.33 E - 110 (N-Z)/A \text{ MeV}$$

$$r_R = 1.20 \text{ fm}, \quad a_R = 0.72 \text{ fm}$$

$$r_I = 1.40 \text{ fm}, \quad a_I = 0.84 \text{ fm}$$

$$V_{SO} = 2.5 \text{ MeV}$$

$$r_{SO} = r_R, \quad a_{SO} = a_R$$

$$r_c = 1.30 \text{ fm.}$$

Alpha Parameters

McFadden & Satchler, Nucl. Phys. 84, 177 (1966)

$$V_R = 164.7 \text{ MeV}$$

$$r_R = 1.442 \text{ fm} \quad a_R = 0.520 \text{ fm.}$$

$$W_V = 22.4 \text{ MeV}$$

$$r_I = r_R, \quad a_I = a_R$$

$$r_c = 1.25 \text{ fm.}$$

Energy Level Schemes for $^{59}\text{Co}(n,xn)$ Reactions

$^{60}\text{Co}(n,\gamma)$

E(MeV)	J ^π
0.0000	5.0 ⁺
0.0590	2.0 ⁺
0.2780	4.0 ⁺
0.2880	3.0 ⁺
0.4360	5.0 ⁺
0.5062	3.0 ⁺
0.5427	3.0 ⁺
0.6144	3.0 ⁺
0.7388	1.0 ⁺
0.7836	4.0 ⁺
1.0056	4.0 ⁺
1.2157	1.0 ⁺
1.5159	4.0 ⁺

$^{59}\text{Co}(n,n)_x(n,n')$ (cont.)

E(MeV)	J ^π
2.1830	3.5 ⁻
2.2060	2.5 ⁻
2.3950	4.5 ⁻
2.4790	2.5 ⁻
2.5420	2.5 ⁻
2.5850	4.5 ⁻
2.7810	1.5 ⁻
2.8240	4.5 ⁻
2.9620	2.5 ⁻

$^{59}\text{Fe}(n,p)$

E(MeV)	J ^π
0.0000	1.5 ⁻
0.2870	0.5 ⁻
0.4750	2.5 ⁻
0.5700	1.5 ⁻
0.7280	1.5 ⁻
1.0300	3.5 ⁻
1.1620	1.5 ⁻
1.2100	0.5 ⁻
1.5200	4.5 ⁺
1.5700	2.5 ⁻
1.9620	0.5 ⁻

$^{59}\text{Co}(n,n)_x(n,n')$

E(MeV)	J ^π
0.0000	3.5 ⁻
1.0993	1.5 ⁻
1.190	4.5 ⁻
1.2915	1.5 ⁻
1.4340	0.5 ⁻
1.4600	5.5 ⁻
1.4810	2.5 ⁻
1.7440	3.5 ⁻
2.0620	3.5 ⁻
2.0870	2.5 ⁻
2.1530	6.5 ⁻

Table I

Energy Level Schemes for $\text{Co}^{59}(\text{n},\text{xn})$ Reactions (cont.)

$^{56}\text{Mn}(\text{n},\alpha)$
also
 (n,nHe^3)

E(MeV)	J ^π
0.0	3.0 ⁺
0.0266	2.0 ⁺
0.1105	1.0 ⁺
0.2120	4.0 ⁺
0.2151	2.0 ⁺
0.3355	5.0 ⁺
0.3410	3.0 ⁺
0.4543	4.0 ⁺
0.4863	3.0 ⁺
0.7162	3.0 ⁺
0.7540	3.0 ⁺
0.8404	3.0 ⁺
1.1664	1.0 ⁺
1.5094	2.0 ⁺
1.7429	2.0 ⁺
1.8333	1.0 ⁺

 $^{58}\text{Co}(\text{n},2\text{n})$

E(MeV)	J ^π
0.0000	2.0 ⁺
0.0249	5.0 ⁺
0.0530	4.0 ⁺
0.1114	3.0 ⁺
0.3656	3.0 ⁺

 $^{58}\text{Co}(\text{n},2\text{n})$ (cont.)

E(MeV)	J ^π
0.3740	5.0 ⁺
0.4575	4.0 ⁺
0.8859	4.0 ⁺
1.0400	3.0 ⁺
1.0760	6.0 ⁺
1.1845	5.0 ⁺
1.2366	2.0 ⁺
1.3690	1.0 ⁺
1.4243	1.0 ⁺

$^{58}\text{Fe}(\text{n},\text{np})$
 (n,pn) also (n,d)

E(MeV)	J ^π
0.0000	0.0 ⁺
0.8106	2.0 ⁺
1.6747	2.0 ⁺
2.0763	4.0 ⁺
2.1338	3.0 ⁺
2.2570	0.0 ⁺
2.6000	4.0 ⁺
2.7818	1.0 ⁺
2.8761	2.0 ⁺
2.9700	5.0 ⁻
3.0380	2.0 ⁺
3.2300	2.0 ⁺
3.2442	0.0 ⁺
3.5372	1.0 ⁺
3.6300	2.0 ⁺

Table I

Energy Level Schemes for $\text{Co}^{59}(\text{n},\text{xn})$ Reactions (cont.) $^{57}\text{Co}(\text{n},3\text{n})$

E(MeV)	J ^π
0.0000	3.5 ⁻
1.2237	4.5 ⁻
1.3775	1.5 ⁻
1.5047	0.5 ⁻
1.6894	5.5 ⁻
1.7572	1.5 ⁻
1.8969	3.5 ⁻
1.9196	2.5 ⁻
2.1331	2.5 ⁻
2.3113	3.5 ⁻
2.6111	3.5 ⁻

$^{57}\text{Fe}(\text{n},\text{p},2\text{n})$ also
 (n,t)
 $(\text{n},\text{n},\text{d})$

E(MeV)	J ^π
0.0000	0.5 ⁻
0.0144	1.5 ⁻
0.1366	2.5 ⁻
0.3667	1.5 ⁻
0.7067	2.5 ⁻
1.0080	3.5 ⁻
1.1980	4.5 ⁻
1.2651	0.5 ⁻
1.3568	3.5 ⁻
1.6277	1.5 ⁻
1.7257	1.5 ⁻
1.9750	0.5 ⁻
1.9894	4.5 ⁻
2.1170	2.5 ⁻

 $^{54}\text{Mn}(\text{n},2\text{n},\alpha)$

E(MeV)	J ^π
0.0000	3.0 ⁺
0.0545	2.0 ⁺
0.1562	4.0 ⁺
0.3678	5.0 ⁺
0.4078	3.0 ⁺
0.8389	4.0 ⁺
1.0097	3.0 ⁺
1.0732	6.0 ⁺
1.1366	5.0 ⁺

 $^{57}\text{Mn}(\text{n},\text{He}^3)$

E(MeV)	J ^π
0.0000	2.5 ⁻
0.0840	3.5 ⁻
0.8510	1.5 ⁻
1.0590	0.5 ⁻
1.0740	4.5 ⁻
1.2270	5.5 ⁻

 $^{58}\text{Mn}(\text{n},2\text{p})$

E(MeV)	J ^π
0.0000	3.0 ⁺

Table I

Table I
Energy Level Schemes for $\text{Co}^{59}(\text{n},\text{n}\alpha)$ Reactions (cont.)

$\text{Mn}^{55}(\text{n},\text{n}\alpha)$

E(MeV)	J ^π
0.0000	2.5 ⁻
0.1260	3.5 ⁻
0.9843	4.5 ⁻
1.2920	5.5 ⁻
1.5280	1.5 ⁻
1.8850	3.5 ⁻
2.1990	3.5 ⁻
2.3660	2.5 ⁻
2.4286	0.5 ⁻
2.5647	1.5 ⁻

$\text{Fe}^{56}(\text{n},\text{n}\alpha)$

Levels Taken from J. Lachlear, et al., NSE 55, 168 (1974)

Excitation Energy (keV)	J ^π	Excitation Energy (keV)	J ^π
0.0	0 ⁺	4458.4	3 ⁺
846.8	2 ⁺	4510.0	3 ⁻
2025.1	4 ⁺	4539.5	1 ⁺
2657.6	2 ⁺	4554.0	3 ⁺
2941.7	3 ⁺	4612.3	2 ⁺
2960.0	2 ⁺	4660.0	3 ⁺
3120.0	1 ⁺	4684.7	3 ⁺
3123.0	4 ⁺	4729.9	0 ⁺
3370.2	2 ⁺	4739.6	2 ⁺
3388.1	6 ⁺	4878.0	2 ⁺
3445.4	3 ⁺		
3449.3	1 ⁺		
3601.9	2 ⁺		
3607.0	0 ⁺		
3755.0	6 ⁺		
3832.0	2 ⁺		
3856.5	2 ⁺		
4049.0	3 ⁺		
4100.3	3 ⁺		
4120.0	4 ⁺		
4298.2	4 ⁺		
4302.0	0 ⁺		
4395.0	3 ⁺		
4401	2 ⁺		

Statistical Model Parameters

The level density formalism is based on the analytical methods of Gilbert and Cameron, (Can. J. Phys. 43 (1965) 1446), and some of the parameters are given in Table II.

The normalization constants may be determined from the gamma ray strength functions (s wave) given as $\frac{\Gamma_\gamma}{2\pi} \frac{<\Gamma_\gamma>}{<D>}$

$$\text{For } {}^{59}\text{Co} \quad <\Gamma_\gamma> = 0.5 \text{ eV}$$

$$<D> = 1400 \text{ eV}$$

The Brink-Axel giant dipole resonance form is to be used for determining the gamma-ray transmission coefficients where

$$\Gamma_1 = 2.86 \text{ MeV} \quad E_1 = 16.50 \text{ MeV} \quad \sigma_1 = 0.059 \text{ b}$$

$$\Gamma_2 = 5.50 \text{ MeV} \quad E_2 = 19.12 \text{ MeV} \quad \sigma_2 = 0.061 \text{ b}$$

The gamma ray strength functions for the residual nuclei are not specified here. The participant may either use the same as for ${}^{59}\text{Co}$ or specify his own. In the latter case, the values used should be specified.

Table II

Statistical Model Parameters

Reaction	n,γ	n,n	n,p	n,α	n,2n	n,np	n,na
Residual Nucleus	${}^{60}\text{Co}_{27}$	${}^{59}\text{Co}_{27}$	${}^{59}\text{Fe}_{26}$	${}^{56}\text{Mn}_{25}$	${}^{58}\text{Co}_{27}$	${}^{58}\text{Fe}_{26}$	${}^{55}\text{Mn}_{25}$
P(N)	0	1.29	0	0	0	1.29	1.27
P(Z)	0	0	1.54	0	0	1.54	0
S(N) *	15.60	14.92	15.60	14.13	14.13	14.92	13.26
S(Z) *	-17.36	-17.36	-16.37	-15.53	-17.36	-16.37	-15.53
a ⁽¹⁾	8.372	7.900	8.370	7.233	6.518	7.465	6.665
U _x (MeV)	5.0	5.04	5.04	5.18	5.086	5.086	5.227
E _x (MeV)	5.0	6.33	6.58	5.18	5.086	7.916	6.497
E _{cut} ⁽²⁾ (MeV)	1.6	3.0	2.0	1.9	1.5	3.7	2.6

1) It might be necessary to renormalize the level parameter for ${}^{60}\text{Co}$ to obtain agreement with the recommended level spacing $< D >$

2) E_{cut} = Continuum cut-off energy

* This information is redundant and has been included for completeness only.

Explanations of symbols used in Table I

$P(N)$, $P(Z)$ pairing energies

$S(N)$, $S(Z)$ shell corrections

E_x excitation energy of the tangency point

U_x energy at the tangency point (minus pairing energy)

a level parameter

Level density formulae (Gilbert & Cameron)

Fermi gas Formula

$$\rho_2 = \exp(2\sqrt{aU}) / [12\sqrt{2} a^{1/4} U^{5/4} \sigma]$$

ρ_2 is the density of levels of all angular momenta J

where $U = E - P(Z) - P(N)$

$$\sigma^2 = 0.146 \sqrt{aU} \cdot A^{2/3} \quad \text{the spin cut-off factor}$$

This formula is valid for all energies greater than E_x' , where

$$U_x' = 2.5 + 150/A$$

$$E_x' = U_x' + P(Z) + P(N)$$

Below this energy the constant temperature formula is adopted

$$\rho_1 = (1/T) \exp[(E - E_o)/T]$$

which smoothly joins ρ_2 : i.e. $\rho_1(E_x') = \rho_2(U_x')$

This gives for E_o and T the following relations:

$$1/T = (\frac{a}{U_x'})^{1/2} - \frac{3}{2U_x'} \quad ; \quad E_o = E_x' - T \log[T\rho_2(U_x')]$$

Table III

Mass Excesses

Isotope	$-\Delta$ (MeV)
^{57}Co	59.3470
^{58}Co	59.8472
^{59}Co	62.2357
^{60}Co	61.6556
^{54}Mn	55.5570
^{55}Mn	57.7100
^{56}Mn	56.9087
^{57}Mn	57.6200
^{58}Mn	56.6060
^{56}Fe	60.6094
^{57}Fe	60.1838
^{58}Fe	62.1551
^{59}Fe	60.6700

Appendix II

Description of the Computer Codes Used

SCAT-2 (D. Bersillon)

Spherical optical model code employing recent numerical methods in particular for the Coulomb function calculations.

ABACUS-2 (A.E. Auerbach)

This code is a combination of the Optical Model and the Hauser-Feshbach formalism. It has a 4 class capability:

- Class 1 - scattering by an optical potential: gives σ_T , σ_{SE} , and σ_R only.
- Class 2 - computes the bound state radial wave function for a specific ℓ and j .
- Class 3 - uses method of Class 1 to generate transmission coefficients for use in Hauser-Feshbach Theory. Computes σ_T , σ_{SE} , σ_{CE} , and σ_{nn} .
- Class 4 - calculates radial integrals from partial waves generated by Class 1 and 2. A multidimensional search procedure is included for obtaining best optical model parameters.

OPTICAL (M.E. Smith, S. Camarda, with modifications by T.W. Phillips)

Spherical optical model code for calculation of σ_I , σ_{el} , σ_R , $d\sigma_{el}/d\theta$. An option for INMC potential has been included by Phillips.

ABACUS-NEARREX (P.A. Moldauer, S. Zawadski)

It is a combination of ABACUS (optical model code) and NEARREX (Hauser-Feshbach + Moldauer theories code) which computes neutron-induced, average fluctuation (or compound nucleus) cross sections. Provision is made for the computation of compound elastic and inelastic neutron cross section, radiative capture and fission cross sections, as well as other processes, such as proton emission. It can also be used to compute proton-induced average cross sections.

ABAREX (P.A. Moldauer)

A revised and improved version of ABACUS-NEARREX. The neutron channel fluctuation degrees of freedom are calculated according to the formula given in Ref. 13.

- The width fluctuation correction can be computed for all compound nucleus sections, including capture.
- In addition to the n-gamma cross section ABAREX can compute the capture cross section which is obtained from n-gamma by subtracting the effect of neutron re-emission. This can be significant above 1 MeV.
- ABAREX is capable of fitting neutron s and p wave strength functions and R' and total cross sections and differential cross sections for elastic and inelastic neutron scattering to individual or lumped levels, simultaneously for several incident neutron energies.

ABAREX permits only one giant resonance to be specified.

NGROGI (Y. Harima, M. Kawai)

Improved version of GROGI III by Takahashi. Uses the ELIESE-2 module for spherical optical model calculations. Wapstra-Bos's mass table is incorporated. The Gilbert-Cameron type composite formula for level density calculation is built into the code. As another option, Lang's formula can be used. Several kinds of gamma-ray strength functions are available: Brink-Axel type profile function, Berman type strength function, Weisskopf's single particle model (optionally), E1 sum-rule for dipole transition, E2 sum-rule for quadrupole transition (optionally); Yраст energies which are not given by the user are calculated in the code by $E_J = J(J+1)/aR$, $aR = 2\sigma_0^2/T$, where a is the level density parameter, σ_0 is the spin cut-off factor and T is the nuclear temperature.

NGROGI is capable of calculating the pre-equilibrium process based on the Kalbach-Cline procedure (Ref. 15).

EMPIRE (M. Herman, A. Marcinkowski)

Pre-equilibrium and equilibrium decay, both angular momentum dependent, are included. Populations of discrete levels are calculated due to the angular momentum conservation and full gamma cascade are accounted for. The code is designed for calculations of capture and multistep reactions. The precompound mechanism is included in the first step of the decay, according to the geometry dependent HYBRID model of M. Blann. The method of Hofmann, Richert, Tepel and Weidenmüller with an improved formula for the elastic enhancement factor (Ref. 14) is used to account for width fluctuations. The code is capable of treating reactions with neutrons, protons, alphas and gammas. Deuterons are treated in the incoming channel only.

ELIESE-3 (S. Igarasi)

Calculates elastic and inelastic scattering cross sections and any kind of reaction cross sections involving absorption and emission of neutrons, protons, deuterons and alpha particles. Polarization is also calculated. Local and non-local spherical optical models and Hauser-Feshbach theory with and without the width fluctuation corrections are allowed.

ENSIERAS (J.M. Monr)

Calculated angle-integrated reaction cross sections can now include capture and pickup channels. To simplify, the differential cross sections may be requested. Cross sections for discrete levels or compound states can be calculated, as well as the total for each reaction type. Fission rates can be calculated in two variants of energy release. There is no restriction on the spins of the particles. The code uses the model of nuclear fission: the statistical firebreak model, the pre-equilibrium model (excited-particle), and a statistical model for direct reactions. Transition probabilities are incorporated from a table of previously-calculated transmission coefficients which can be supplied as input data or calculated by solving the Schrödinger equation with a spherical potential using Fermi's method using the value as read from CECDB. The real spherical potential is taken to be the Woods-Saxon shape and the derivatives can be three-times or Gaussian shapes. The fission transmission coefficients are based on the Hill-Wheeler equation. ENSIERAS is designed to predict nuclear cross sections over and beyond 10 MeV from threshold up to 60 MeV. Finally, the only statistical direct model is included in the (n, alpha) pickup reaction. The Coulomb function is used to be replaced if energy lies far below the Coulomb barrier threshold. A number of other reaction processes can be calculated. Incident nuclei can be described by IBM discrete levels and/or the constant temperature level, or alpha and/or the Fermi-gas level descriptions; the angular transfer of nuclear spin between incoming and outgoing fragments is T₀. The angular distribution expressed in equally spaced angles from 0 to 90 degrees can be calculated for up to 20 discrete states. The program does not follow gamma-ray cascades from fission.

CERNPRO-3 (C. Reffo, L. Ferri)

Local and non-local spherical optical model calculations are allowed. Hauser-Feshbach and Brink-Axel theories are included. Multi-asculations can be calculated for scattering to an effective number of degrees of freedom as described in the first works by Haldenius. It calculates σ_{tot} , σ_{dis} , σ_{cap} (angle-integrated or angle-differential as well as any type of binary reaction (x, a) where x can be *indifferently* n, p, α , γ). Particle and primary gamma-ray spectra are given as well as the cross section for discrete level excitations of all residual nuclei involved. The cross section is also given for those processes (e.g. $n + \gamma, n$) initiated by gamma-ray emission and followed by subsequent particle emission. As a calculation test on integration techniques involved at the end of such run the percentage difference is given between optical model compound nucleus formalism cross section and the sum of all compound elastic and inelastic contributions. Only El transitions are considered in gamma decay which is treated according to the Brink-Axel model. The code is designed for the use below threshold for the second emission.

ERINNI (F. Fabbri, G. Reffo)

Computes multiple particle emissions like $(x:y:b)$ x,y,b being n,p, γ , *independently*, and c α,β,γ in and γ . The code is designed for calculations between 5-20 MeV. There is a problem on particle statistics, i.e., one cannot only the final state of a multi-emission process, one has to calculate the intermediate states too.

SACCHETTA (M. Benzi, F. Fabbri, L. Ferri, improved by R. Scopelaine)

Initially the code calculated σ_{tot} , σ_{pp} , total and differential σ_{el} and also carried out linear-potential calculations for neutrinos only. Scopelaine has added the calculation of $(n, 2n)$ in which neutron radiative capture with width fluctuation corrections. There is an option to use the method of Fermi, i.e., for the calculation of the width, instead of using above a given energy. Fission cross sections are used to reduce the compound-nucleus cross sections. In this way a possibility of charged-particle cross-sections is supported here.

IDA Radiation System (G. Ferro, F. Fabbri)

It consists of a code-system; the most important codes are: POLIFEMO, NAUGIKAA, ILEMACO.

POLIFEMO is designed for binary reactions.

Direct and compound reaction contributions to the excitation of discrete levels are calculated as well as angle-differential cross sections for elastic and inelastic contributions. Particles and gamma-ray spectra are calculated. Valence capture is calculated according to Lyman or Landau-Feshbach models. The fission contribution is included, as a consistency test the percentage difference between the optical model reaction cross section and the sum of all direct and compound reactions cross section contributions, are printed. The model involved can optimally select a part or all the data in a shared data library containing mass excesses, evaluated level schemes, giant resonance parameters, optical model data sets, local systematics for level density parameters, etc.

NAUGIKAA is designed for multiple-particle and gamma-ray cascading emitters. (Eleven subcascades emitters are possible, of which each of the first four can be *independently* a, p, α , γ while last seven can only be γ). In addition to complete channel correlations the pre-equilibrium component of the first emission is computed within the framework of a unified model accounting for any projectile and emitted p, α, γ (Ref. 12); consider momentum and parity conservation are considered. When partial cross sections are summed over all the excited numbers, the unified model option is used for pre-equilibrium and equilibrium emitters. The fission competitor is included.

ILEMACO receives the output of NAUGIKAA to produce the requested spectra for any particle in the cascade. Separate spectra for all particles and gamma-rays emitted in any cascading emission may be requested as well as the total spectrum for a particular emission type at any given energy. Isomeric ratios can also be calculated. ILEMACO can display partial and/or total spectra together with evaluated experimental data sets taken from a data base.

RELATIONS BETWEEN THE CODES

- The codes SCAT-2, ABACUS-2, OPTICAL only compute the optical model cross sections like σ_T , σ_R , $a_{\text{sh},\text{el}}$. They have been independently developed and therefore no particular relation exists among them.
- ABACUS-NEARREX consists of the fusion of the two codes: ABACUS-2 for calculating the optical model quantities and NEARREX for the Hauser-Feshbach theory calculations with width fluctuation corrections. ABAREX is an improved version of ABACUS-NEARREX and contains the latest developments in width fluctuation correction factors.
- EMPIRE is a general code which accounts for equilibrium and pre-equilibrium emissions with inclusion of spin and parity conservation, giving integrated and energy differential cross sections. Where necessary the width fluctuation correction is also used. It has been developed recently and independently from other codes used in this exercise.
- ELIESE-3. The set of ELIESE codes are very well known and widely used for optical model and Hauser-Feshbach calculations with width fluctuation cross sections for binary reactions.
- NGROGI is an extended version of ELIESE-2 and includes multiple cascading emissions and pre-equilibrium effects.
- CERBERO, POLIFEMO, SASSI, ERINNI, NAUSIKAA belong to a complex and integrated chain of codes. They all share the same modules: SMOG (spherical) and CIRCE (deformed) for the optical model and CERBERO for the statistical model. The first two are designed for binary reactions and the second is a more general and versatile version of the first. The last three are designed for multiple particle emissions and can be used each up to incident energies of ~ 15 MeV, ~ 20 MeV, ~ 50 MeV, respectively.