The Abdus Salam International Centre for Theoretical Physics

International Atomic Energy Agency

Modelling with EMPIRE nuclear reaction code and nuclear data evaluation

Joint ICTP-IAEA Workshop on *Nuclear Reaction Data for nuclear power applications*, 22-26 Sept. 2014, Trieste

Roberto Capote, r.capotenoy@iaea.org
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OUTLOOK

- Background: ND for energy applications
- New U-238 evaluation
  - Nuclear reaction modelling in EMPIRE
  - Differential data
  - Integral and quasi-differential data
- Nuclear data validation using SPA cross sections and dosimetry libraries
- Challenges

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Do we need another ^{238}U evaluation?

OECD/NEA WPEC Subgroup 26 Final Report:
" Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations",
M. Salvatores (coordinator), R. Jacqmin (monitor), Technical report NEA No. 6410, OECD 2008.

The request for improved cross sections and emission spectra and their accuracies for neutron induced reactions on ^{238}U is an important issue that emerges in several of cases studied. High accuracy requirements were placed on inelastic cross-sections **^{238}U(n,inl)** in the whole energy range up to 20 MeV …

A. Santamarina, ND-2013, target uncertainty 5% (current ~ 15%)

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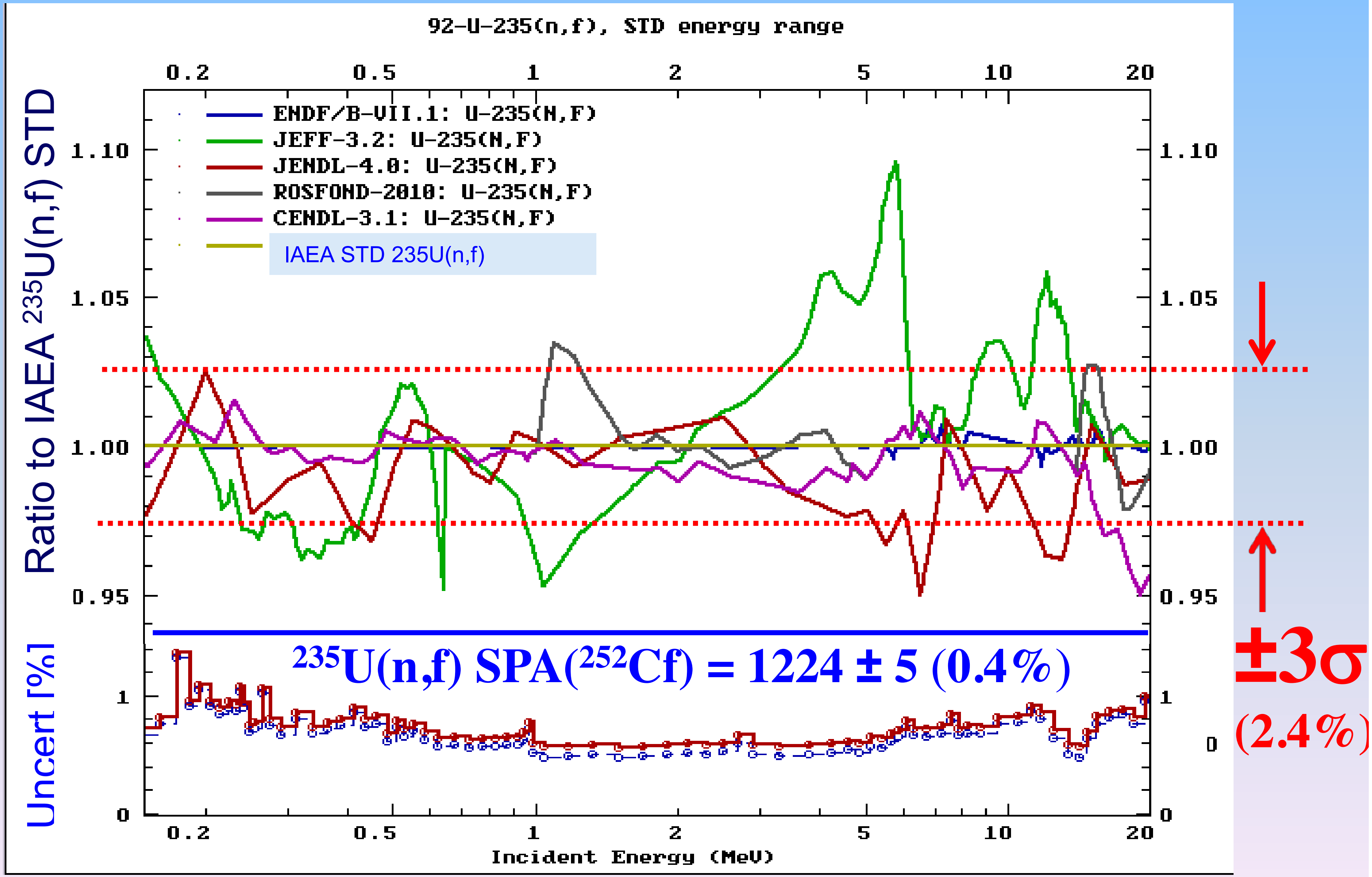
Evaluated ^{235}U(n,f) vs. STD cross section



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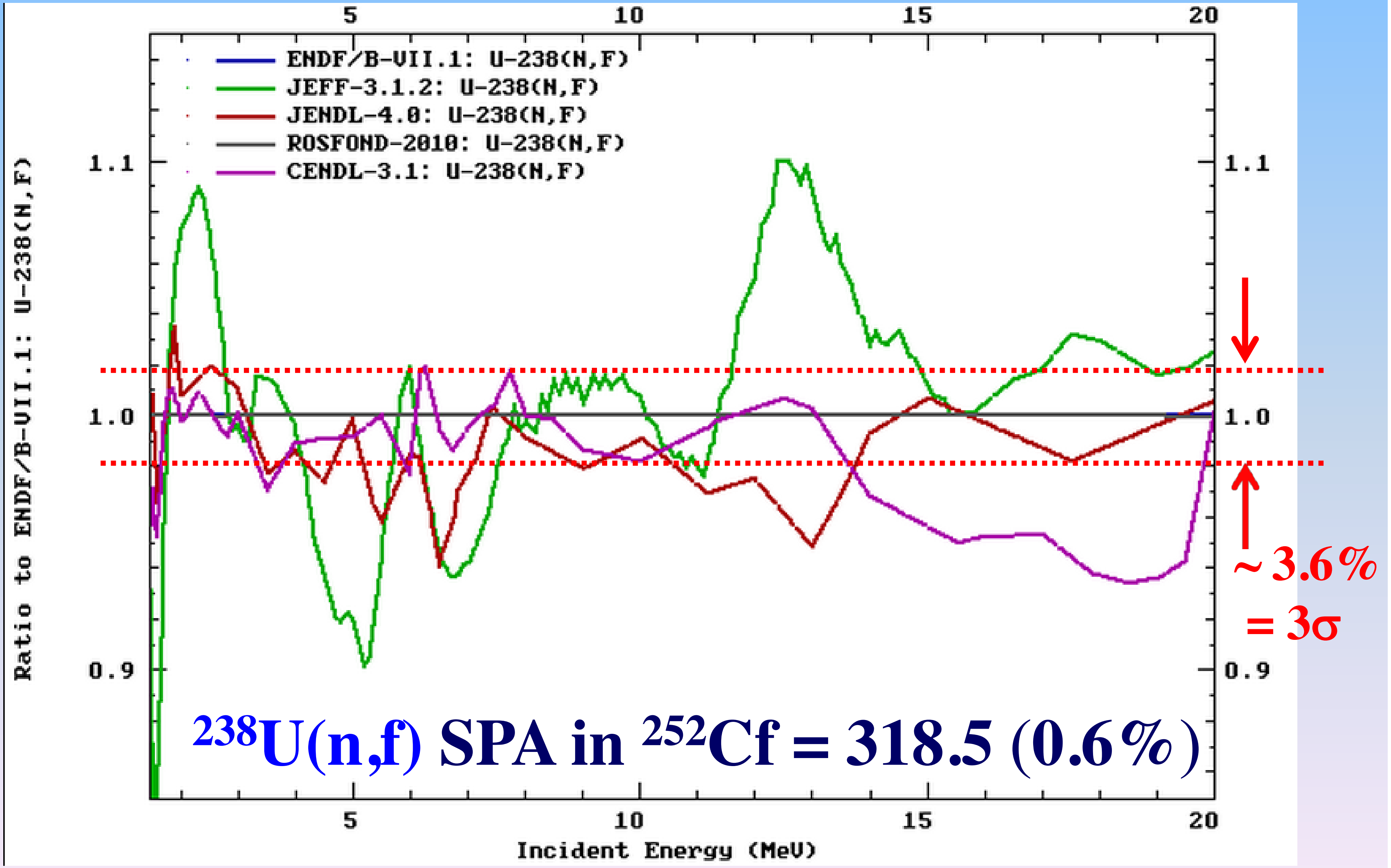
DOES EVAL.FISSION AGREES with STDs?



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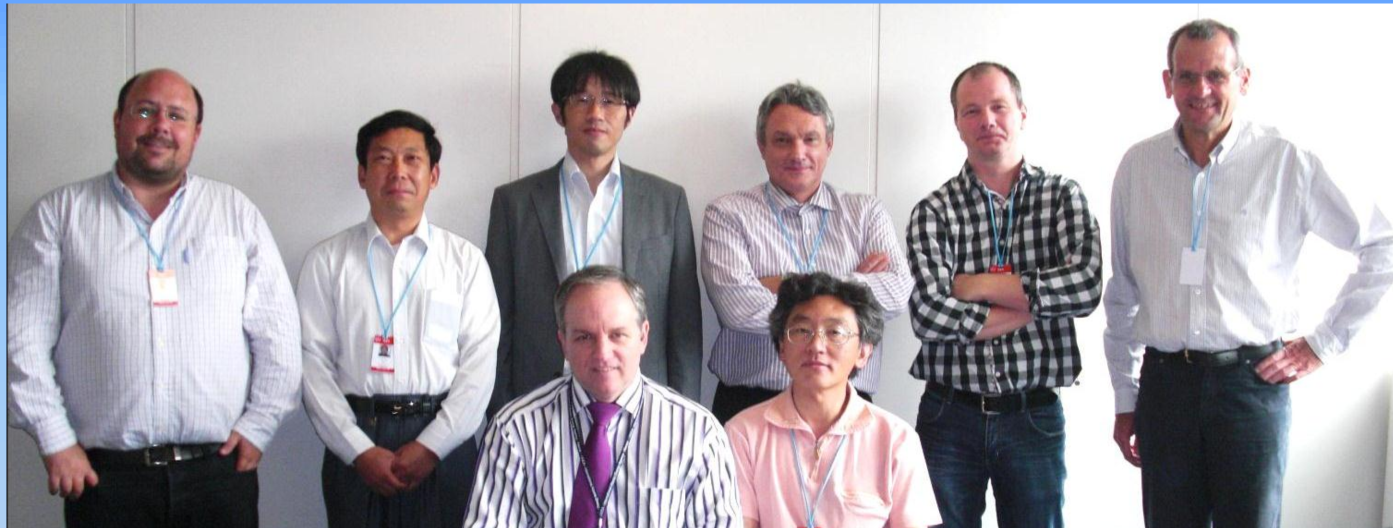
IAEA TM 2011



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INDC(NDS)-0597
Distr. J+NM

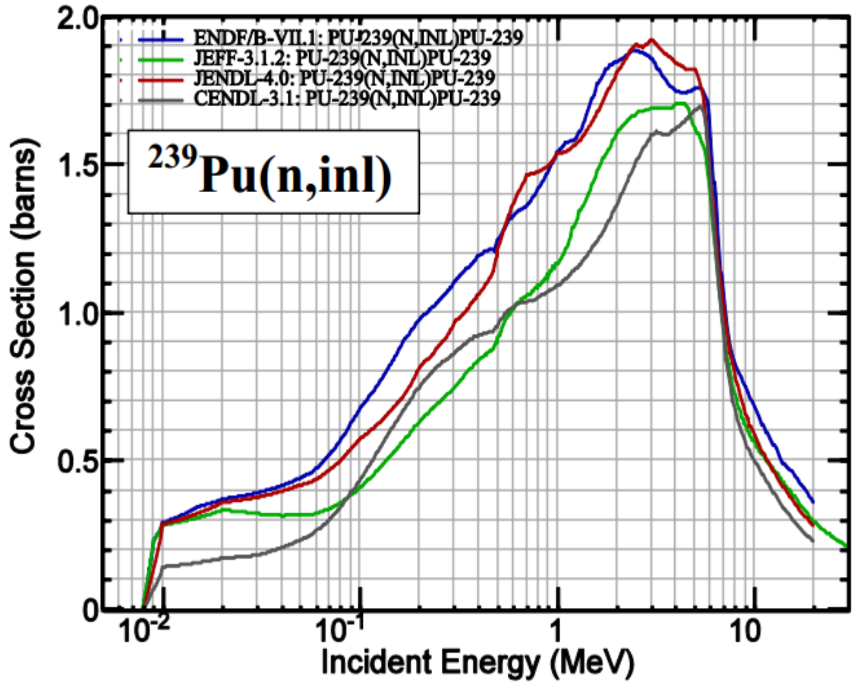
INDC International Nuclear Data Committee

Summary Report

Technical Meeting on

Inelastic Scattering and Capture Cross-section Data of Major Actinides in the Fast Neutron Region

IAEA Headquarters
Vienna, Austria
6 – 9 September 2011



A.J. Plompen, T. Kawano and RC, Technical report INDC(NDS)-0597 (IAEA,Vienna,2012)
http://www-nds.iaea.org/publications/indc/indc-nds-0597.pdf

IAEA TM recommendations ^{238}U(n,inl)

7. For the low energy range (<3 MeV) the compound decay introduces additional degrees of freedom (level densities, strength functions, fission, width fluctuations). For better understanding the compound nuclear reaction mechanism on actinides a simple system must be studied. Predictions for neutron induced reactions on ^{238}U below 1 MeV should be compared.

^{238}U(n,f) and ^{238}U(n,γ) – fitted in STD

^{238}U(n,γ) SPA in ^{252}Cf: 67.5 ± 0.7 mb (1.0%)

^{238}U(n,f) SPA in ^{252}Cf: 318.5 ± 2.1 mb (0.6%)

➡ **^{238}U is the ideal test nucleus for elastic/inelastic studies**

A.J. Plompen, T. Kawano and RC, Technical report INDC(NDS)-0597 (IAEA,Vienna,2012)
http://www-nds.iaea.org/publications/indc/indc-nds-0597.pdf

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First problem:
Elastic and inelastic cross sections

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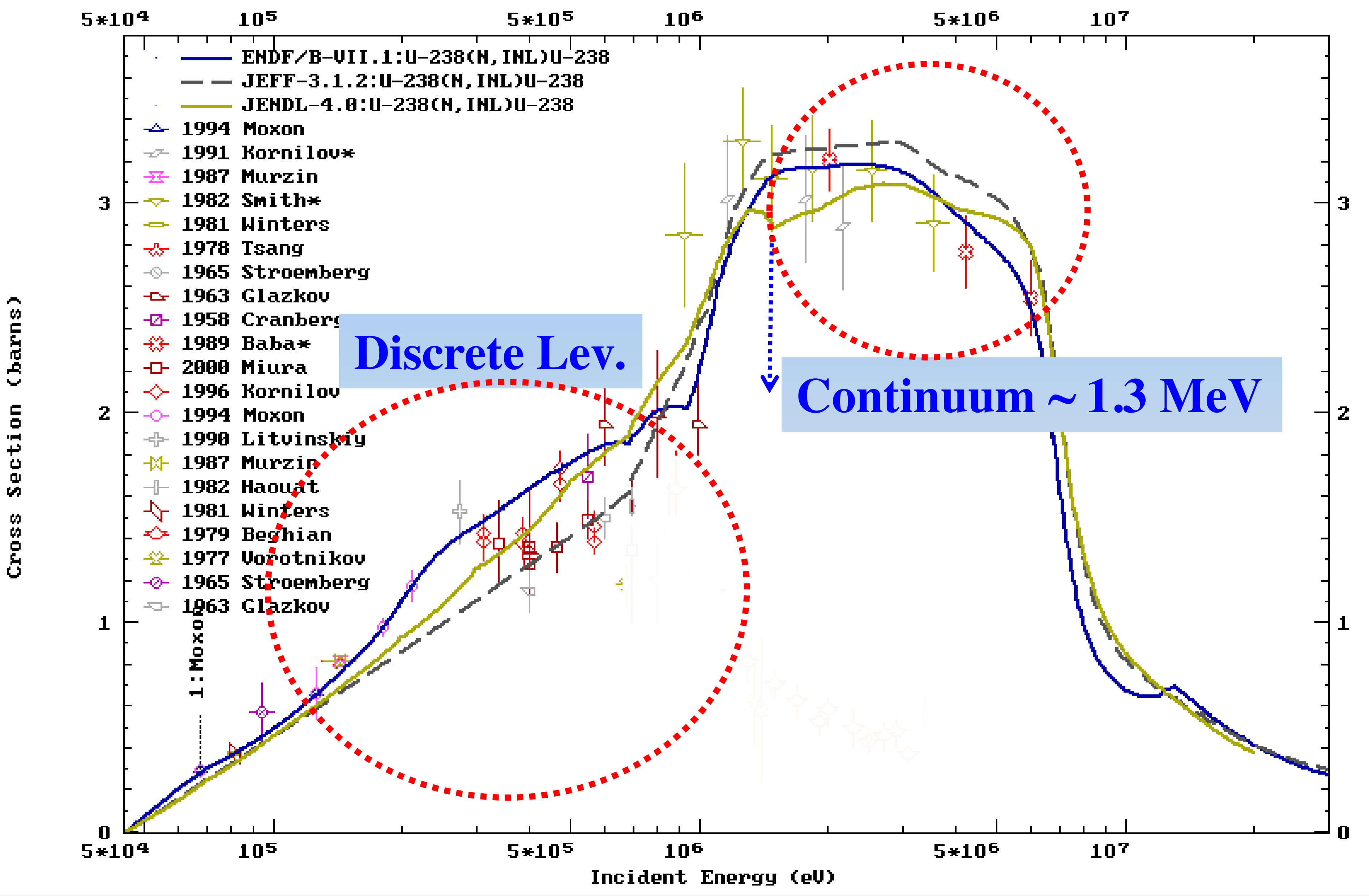
DISCREPANCIES in $^{238}U(n,inl)$



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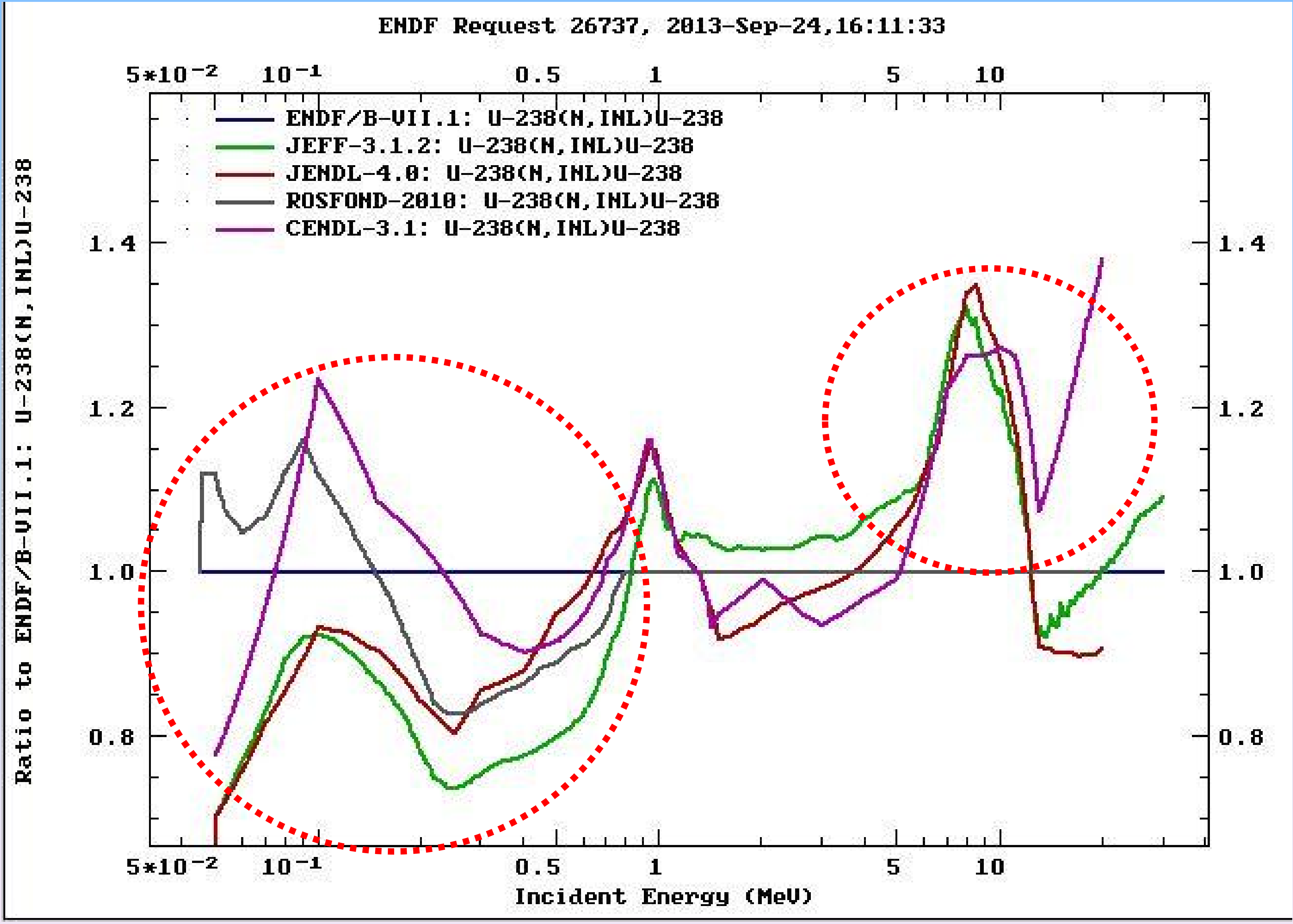

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Nuclear Data Sheets **108** (2007) 2655

EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

M. Herman[1,*], R. Capote[2], B.V. Carlson[3], P. Obložinský[1], M. Sin[4], A. Trkov[5], H. Wienke[6], and V. Zerkin[2]
[1] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
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[5] *Jozef Stefan Institute, Reactor Physics Division R-1, Jamova 39, 1000 Ljubljana, Slovenia and*
[6] *Belgonucleaire, Dessel, B2480, Belgium*

+ recent relevant modelling advances

- ***Dispersive Lane consistent coupled-channel OMPs**:***
  neutron inelastic scattering to discrete levels;
- ***DIR-CN interference effects (as predicted by Moldauer);***
- ***neutron inelastic scattering treatment;***
- ***improved fission formalism (descriptive capability)***

*J.M. Quesada *et al*., EPJ Web of Conferences **42** 02005 (2013)
J.M. Quesada *et al*., ND2013 conference

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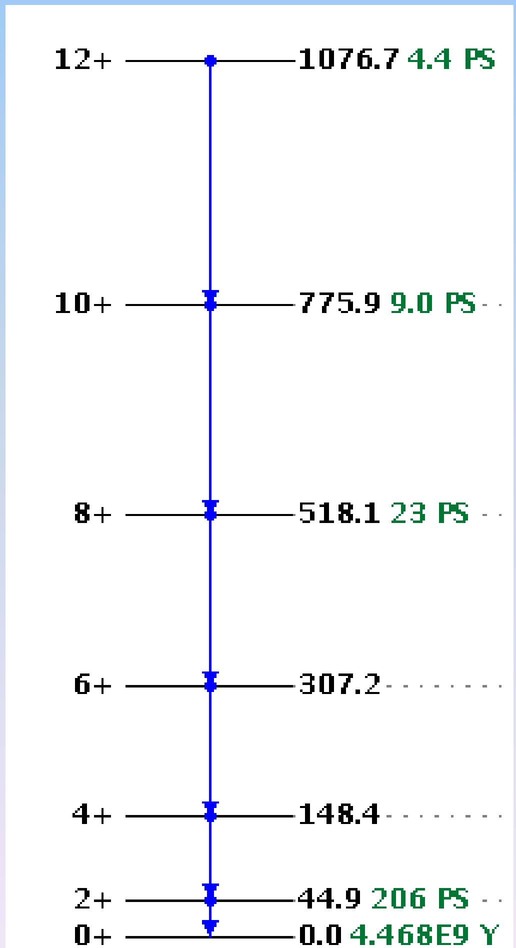
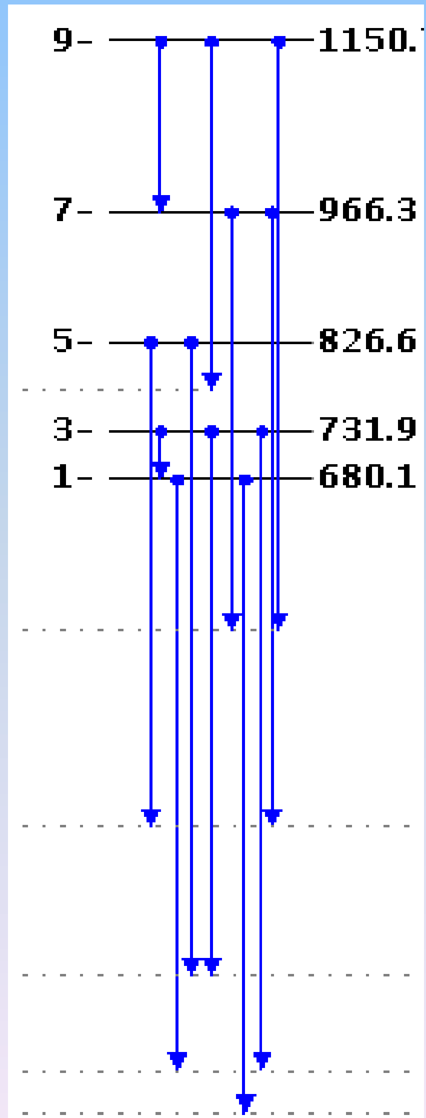
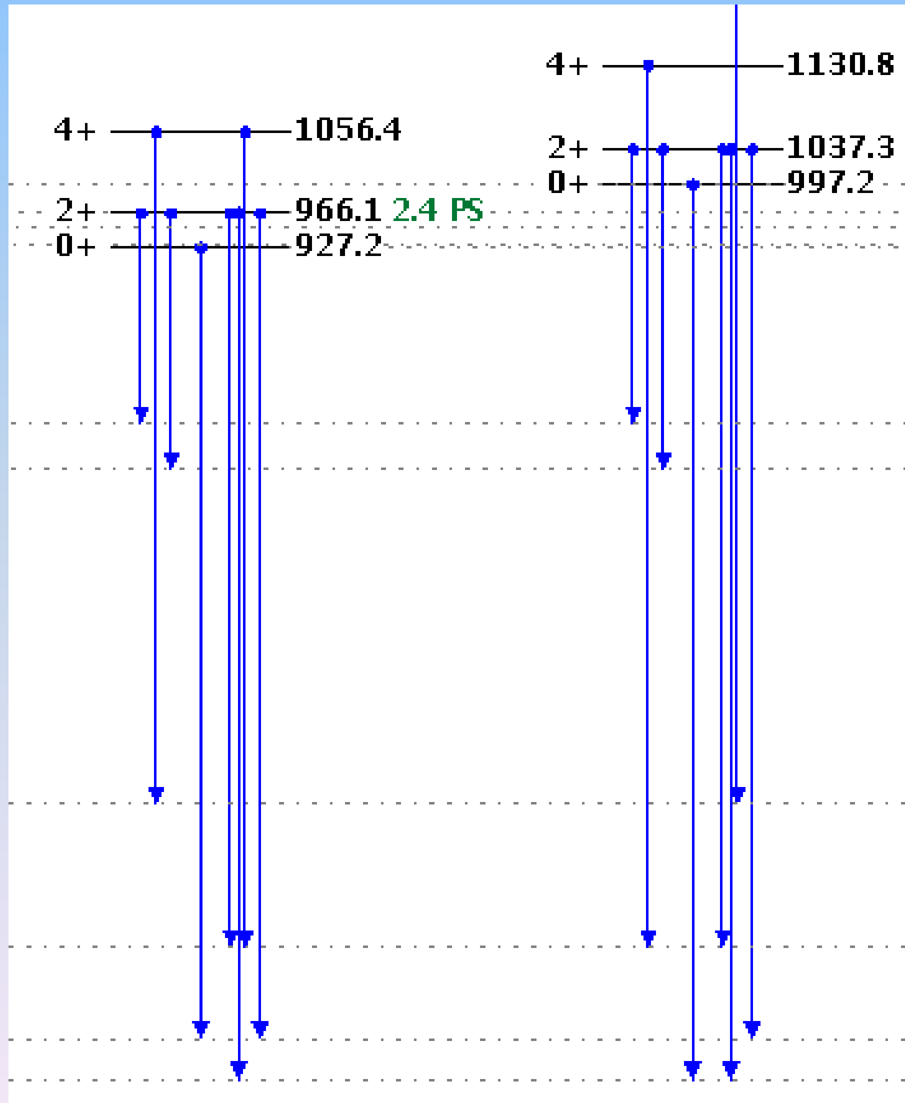
DCCOMP: rigid rotor with soft-rotor corrections

^{238}U







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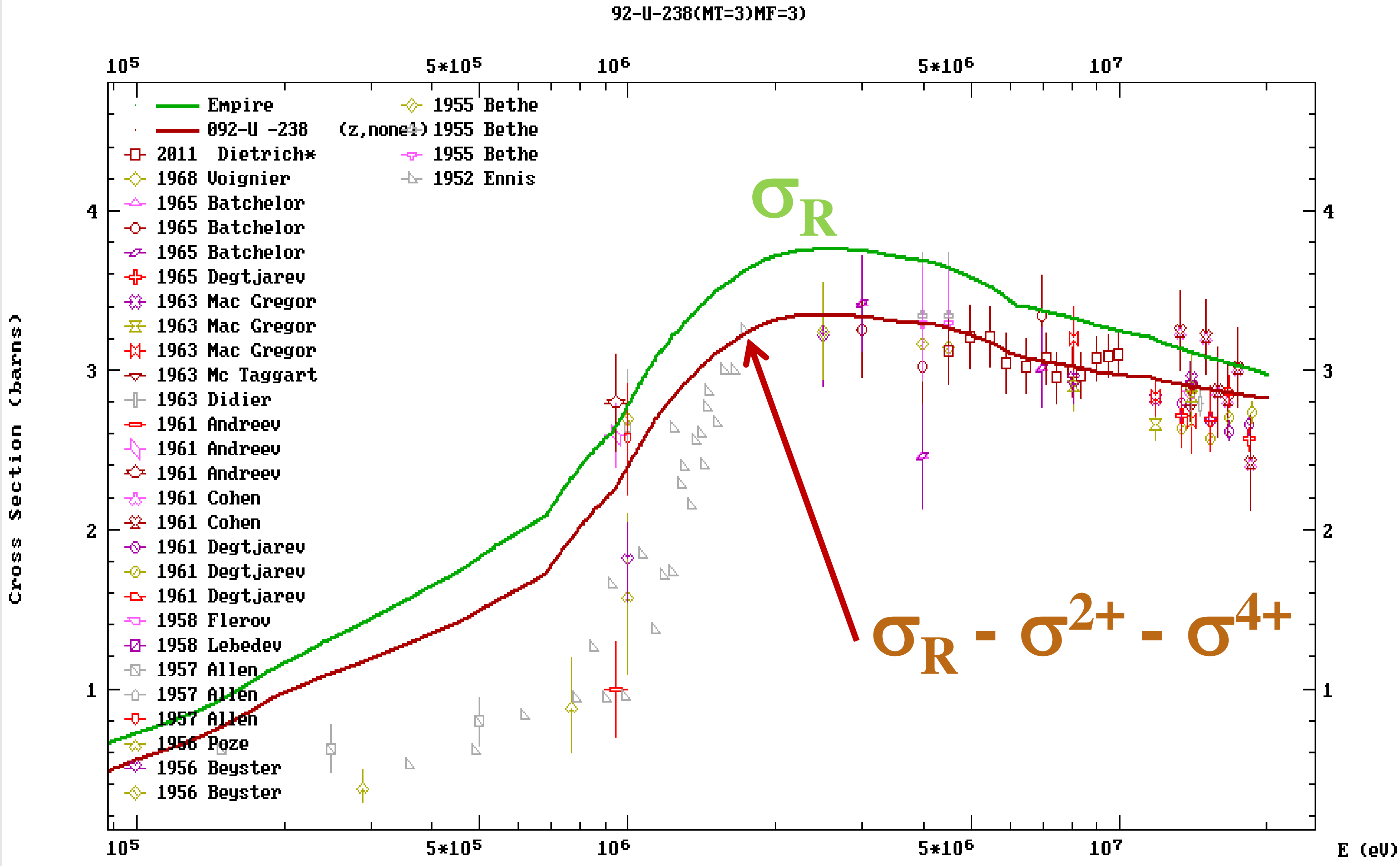
nonelastic cross sections



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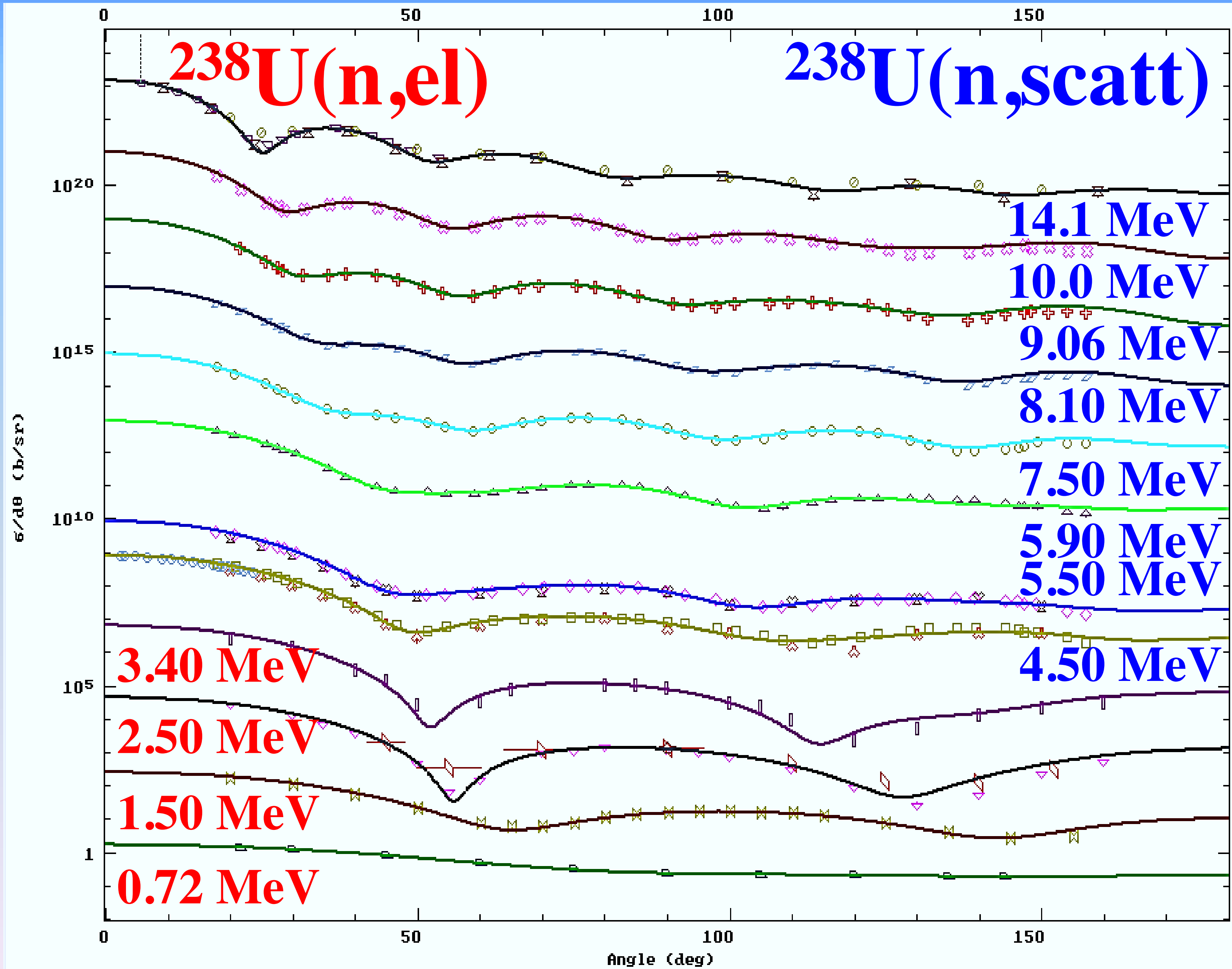

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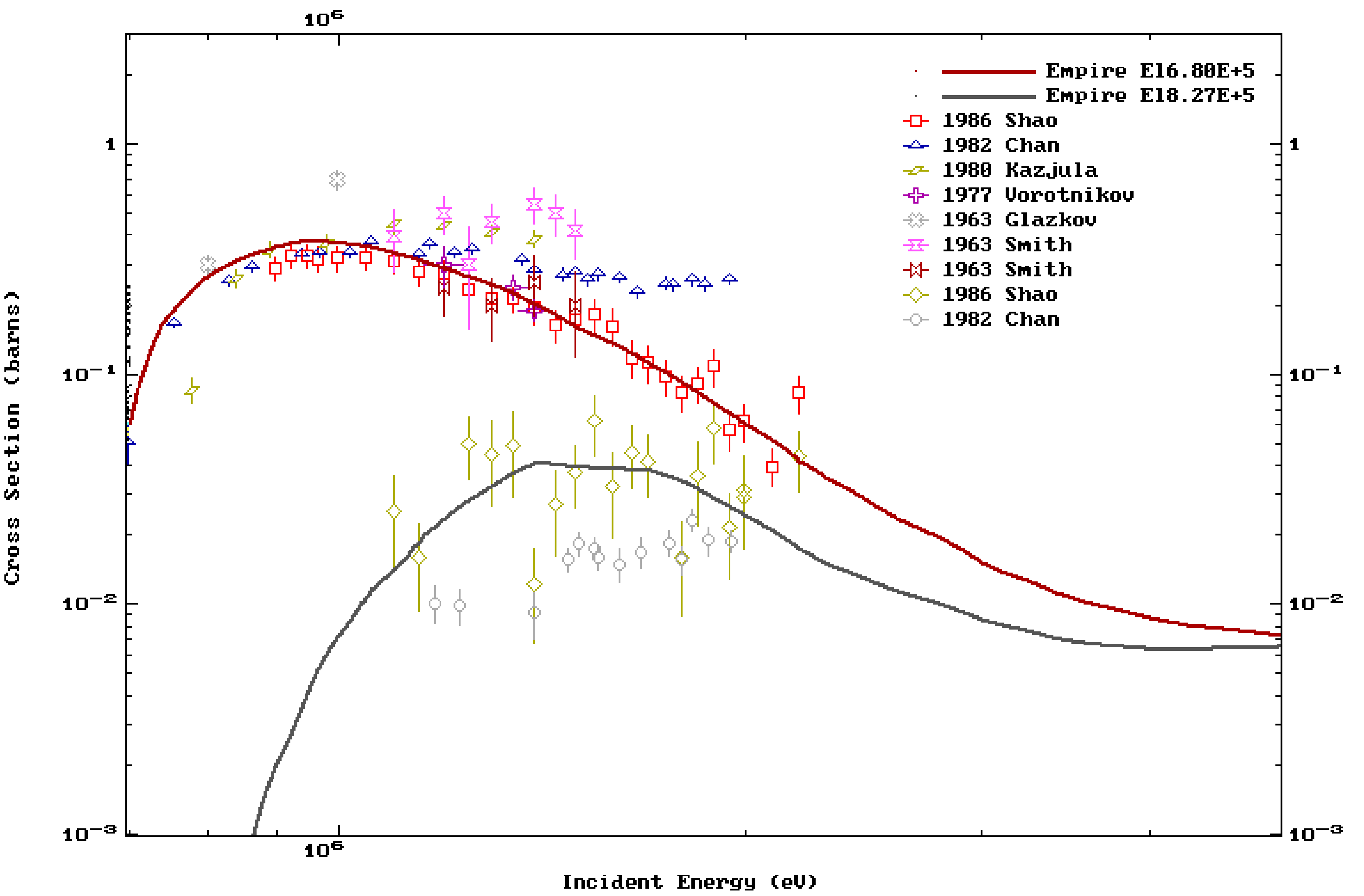
Impact of octupolar band



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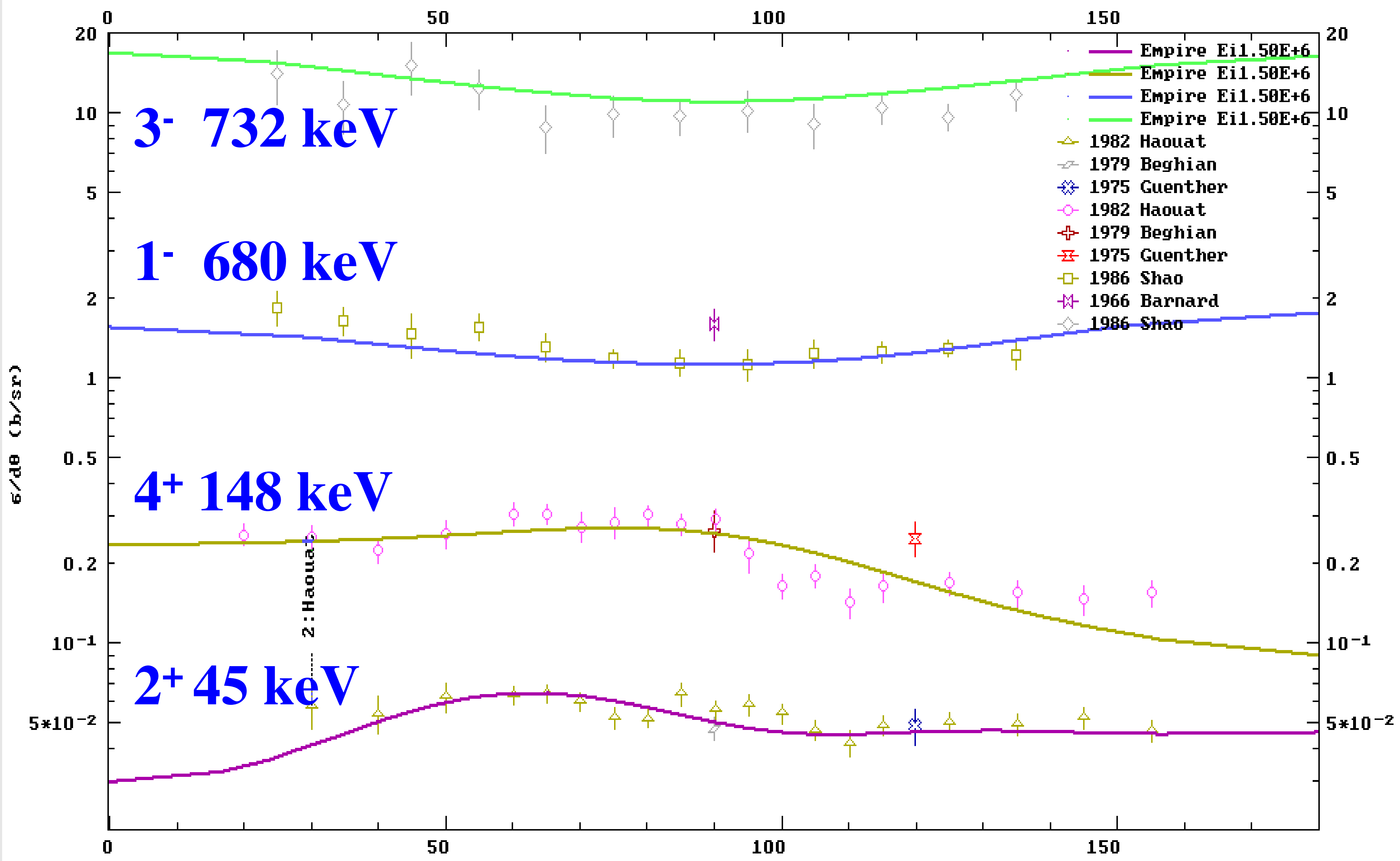
Inelastic angular distributions E_n=1.5 MeV



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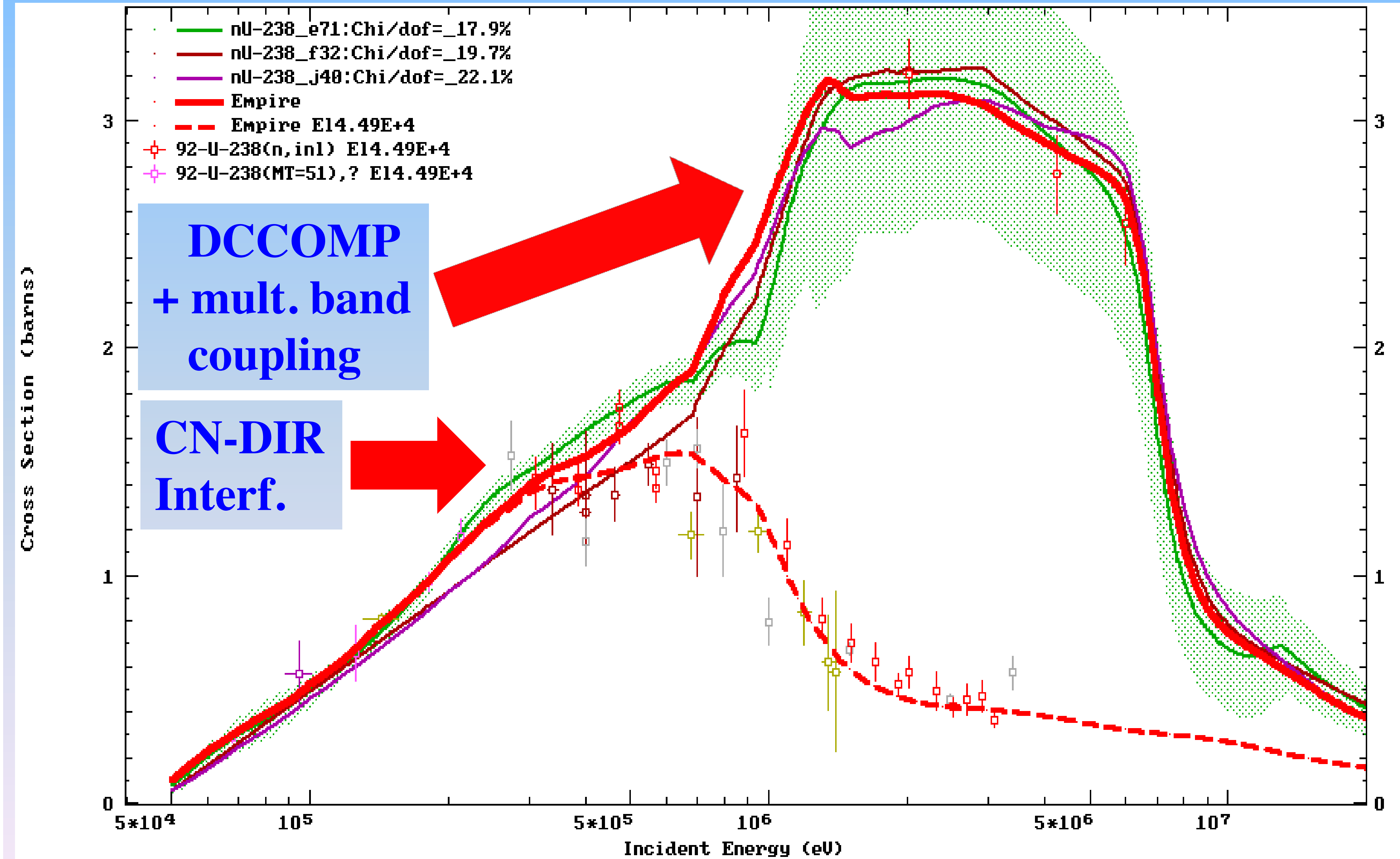
total (and 1st lev) inelastic cross sections



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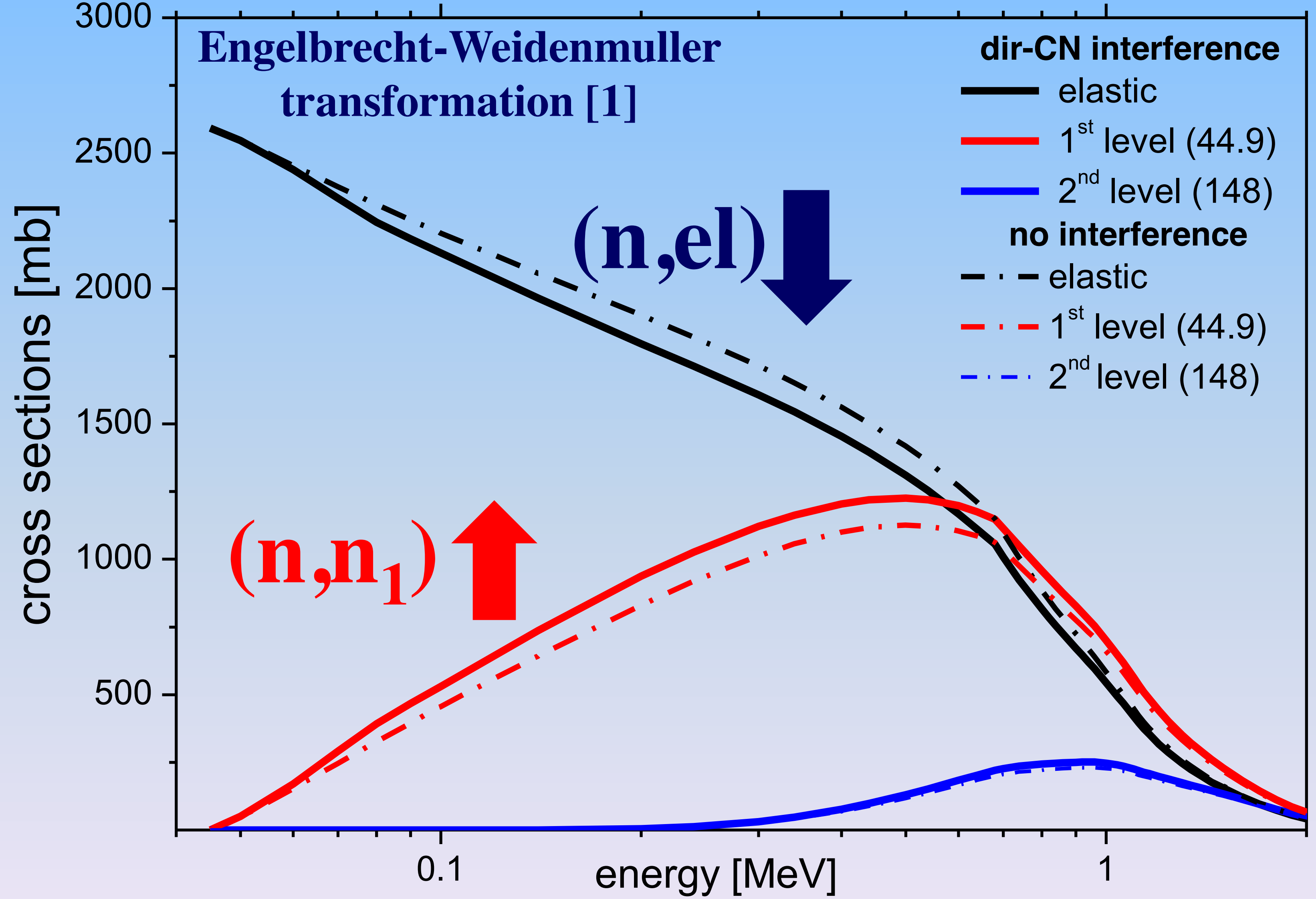
new physics: DIR-CN interference



[1] C.A. Engelbrecht, H.A. Weidenmuller, "Hauser--Feshbach theory and Ericson fluctuations in the presence of direct reactions", Phys.Rev. **C8** (1974) 859-862

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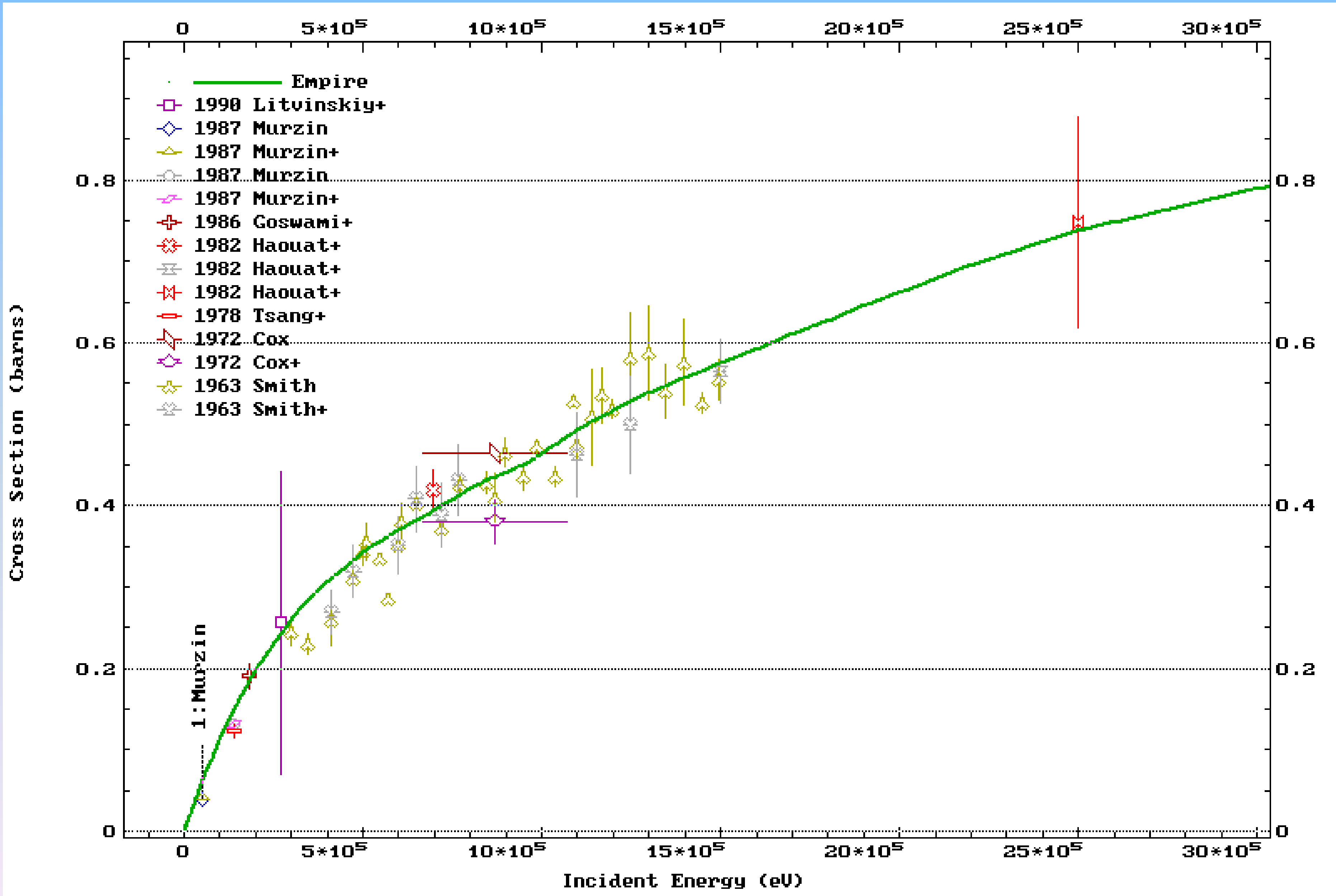
elastic μ-bar (P1 component)



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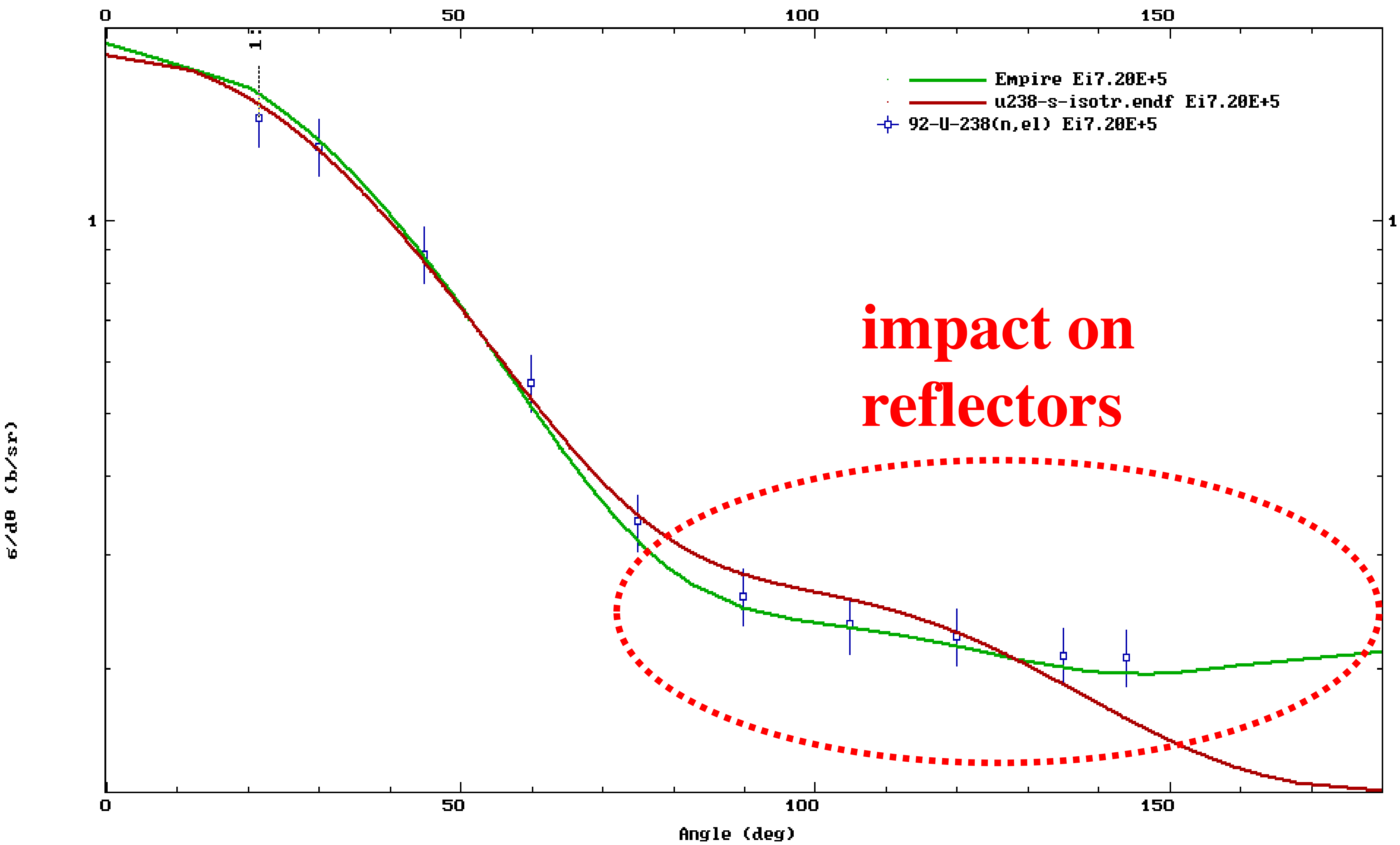
Elastic angular distribution 720 keV



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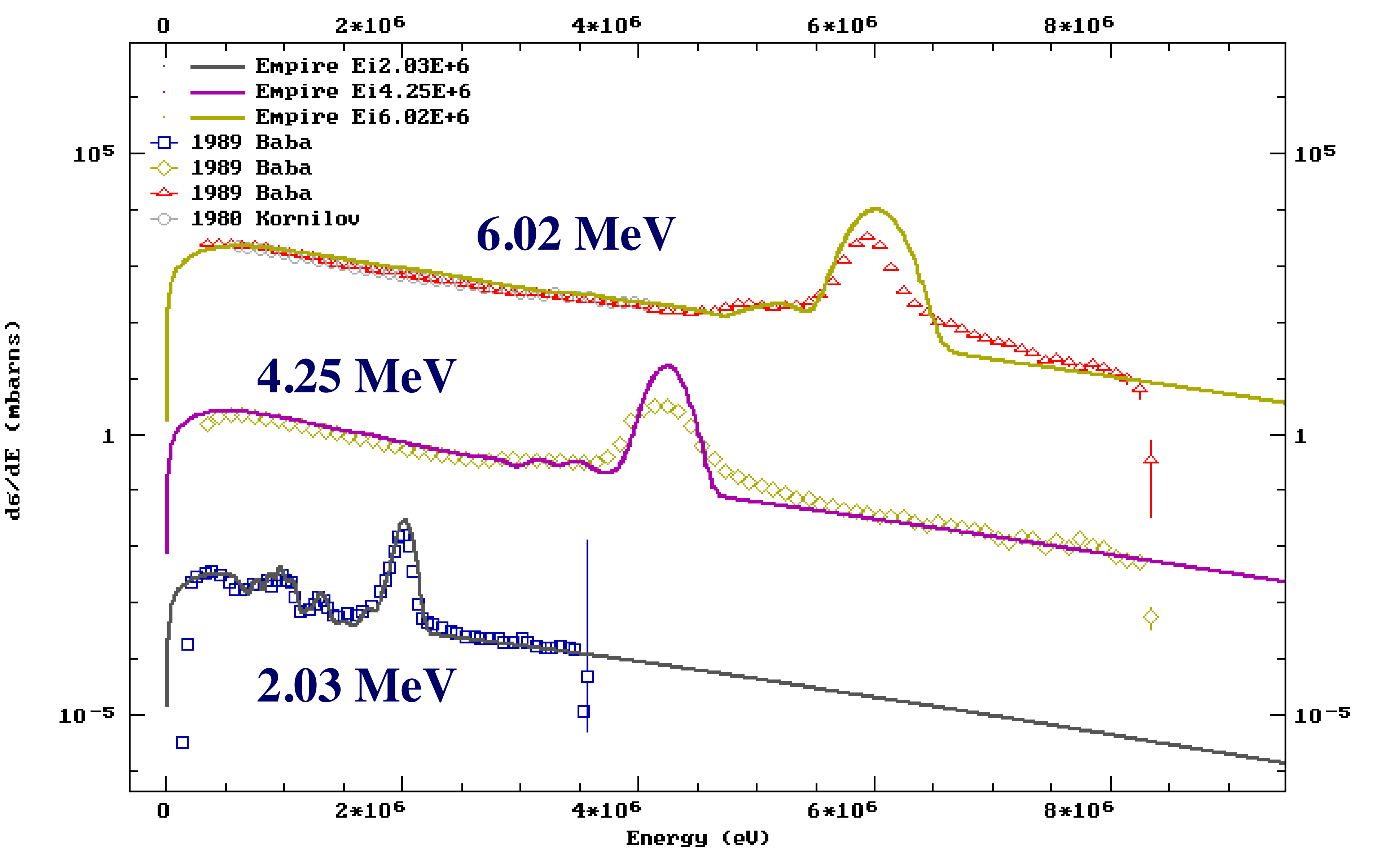
Neutron emission spectra (2-6 MeV)



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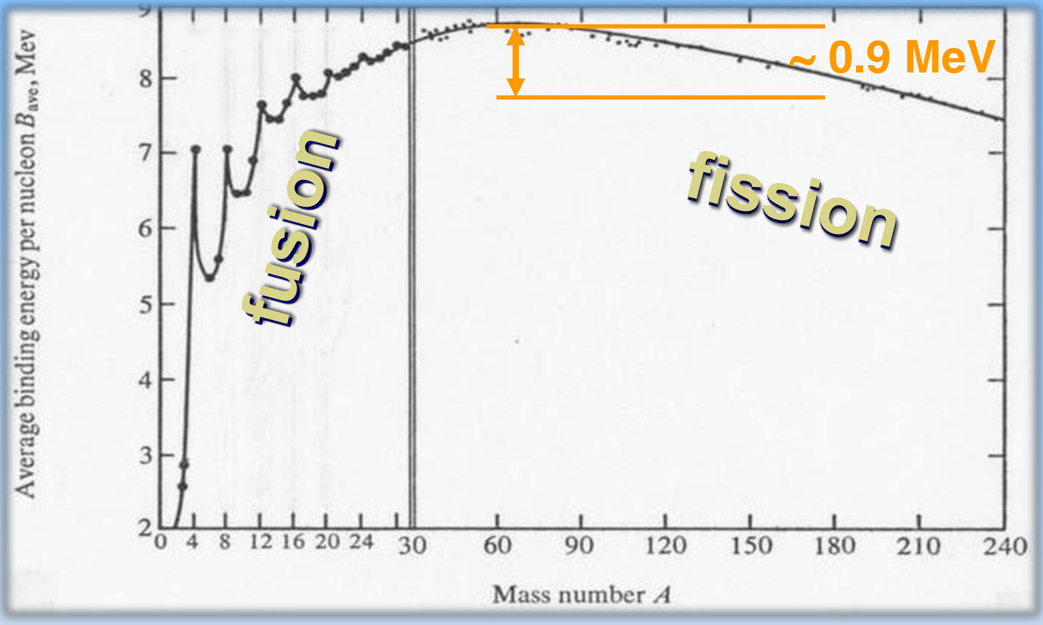
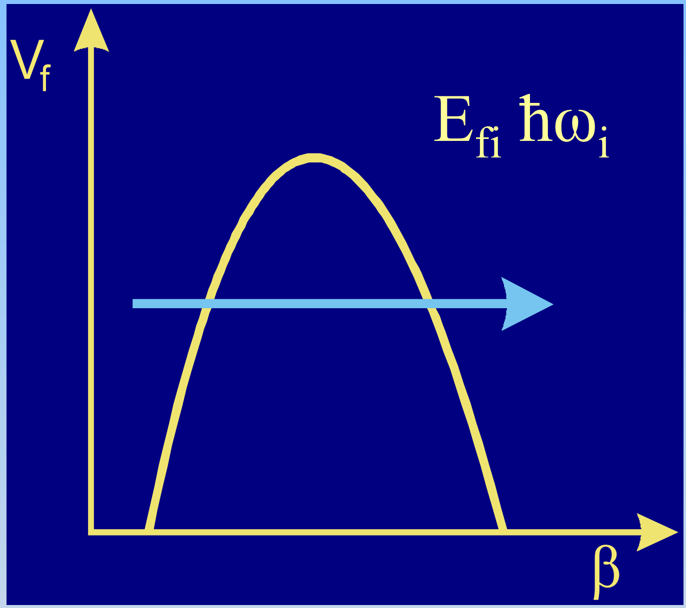
FISSION PROCESS



Parabolic barrier



Transmission coefficients

The origin of the nuclear energy is the difference of binding energy

Hill-Wheeler formula for the Transmission coefficient through a parabolic barrier:

$$T_i = \frac{1}{1 + \exp\left(\frac{2\pi}{\hbar\omega_i} (E_{fi} - E^*) \right)}$$

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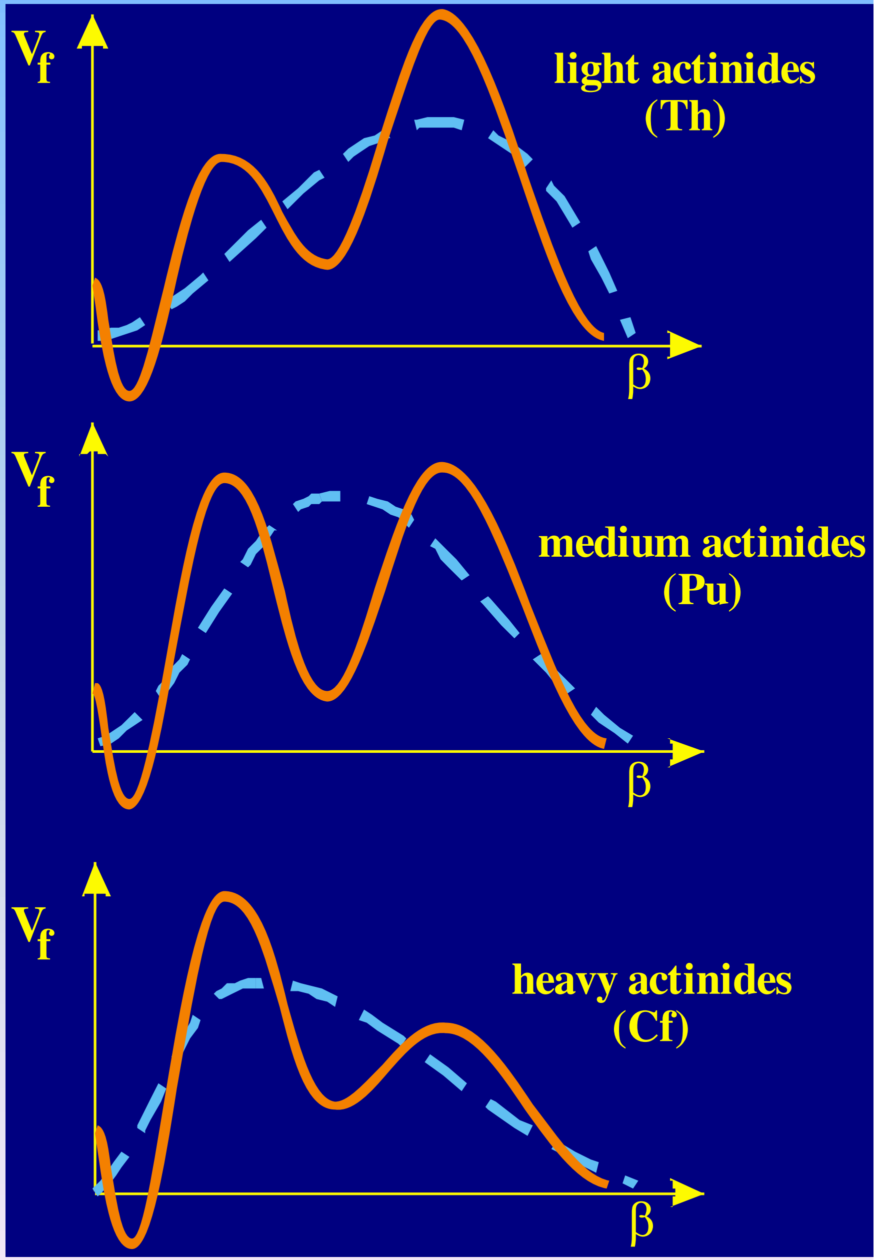
FISSION BARRIERS

Shell correction dependence on Z,N and the dependence of the LD potential on the fissility parameter ($E_C/2E_S$) make fission barrier specific to each nucleus;

- inner barriers almost constant 5-6 MeV for the main range of actinides; fall rapidly in Th region;

- secondary well's depth around 2 MeV;

- outer barriers fall quite strongly from the lighter actinides (6-7 MeV for Th) to the heavier actinides (2-3 MeV for Fm).



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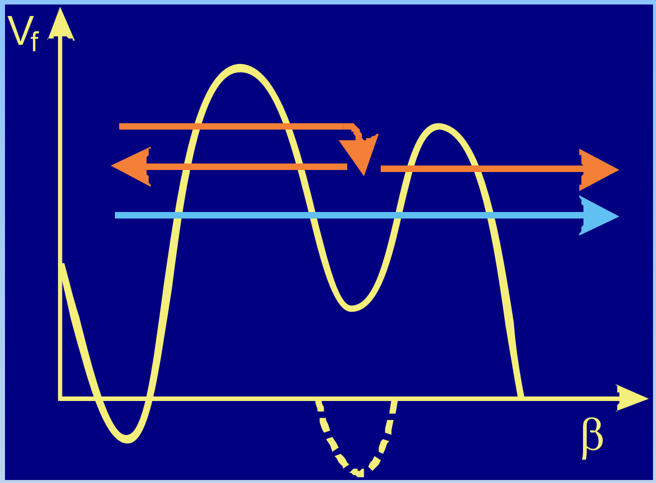

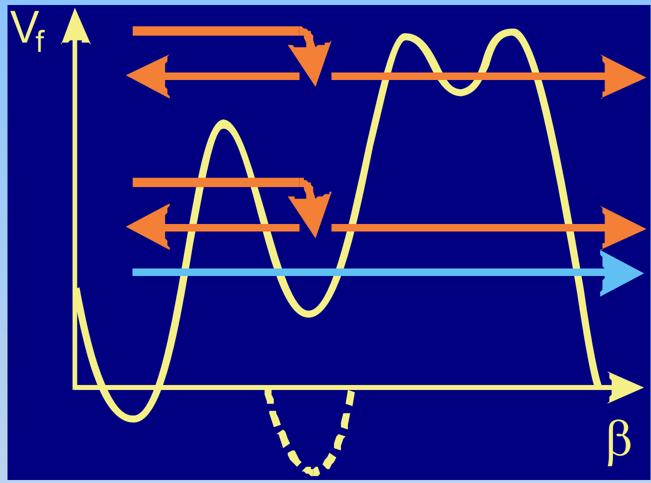

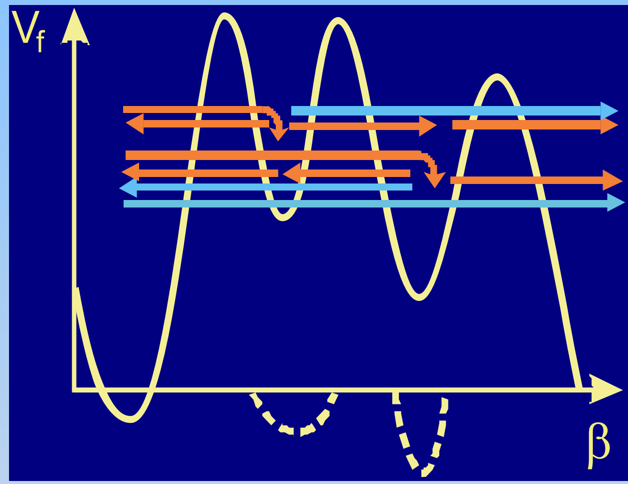

$$T_f = T_{dir} + T_{ind} = T_{dir} + T_{abs}\frac{T_B}{T_A + T_B}$$

$$T_f = T_{dir} + T_{ind} = T_{dir} + T_{abs}\frac{T_{BC}}{T_A + T_{BC}}$$

$$T_f = T_{dir} + T_{ind\,1} + T_{ind\,2}$$

imaginary part:

$$W = -\alpha[E^* - V_f]$$

$$T_{abs} = T_{dir}\frac{e^{2\delta} - (1 - T_2)e^{-2\delta} - T_2}{T_2}$$

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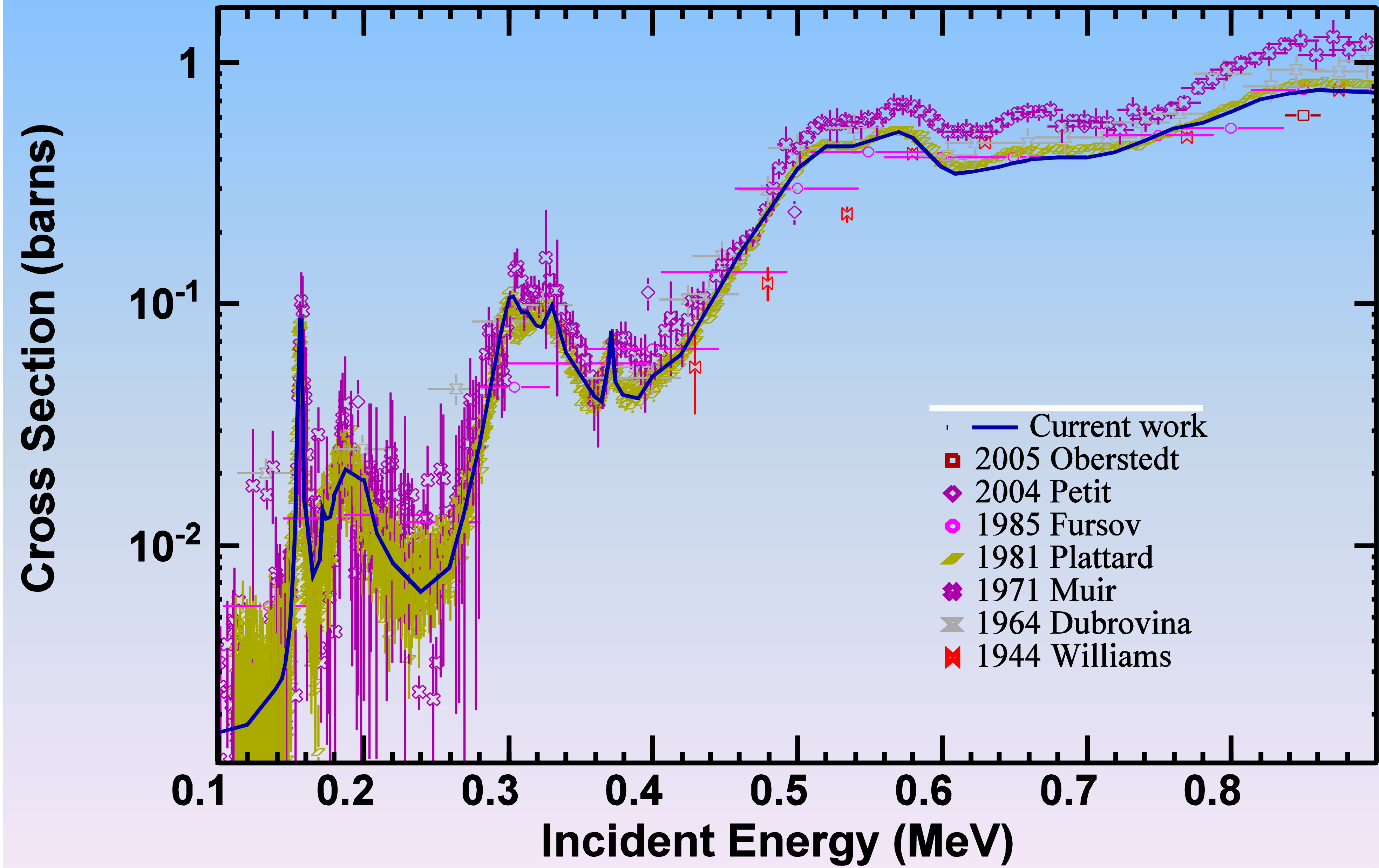

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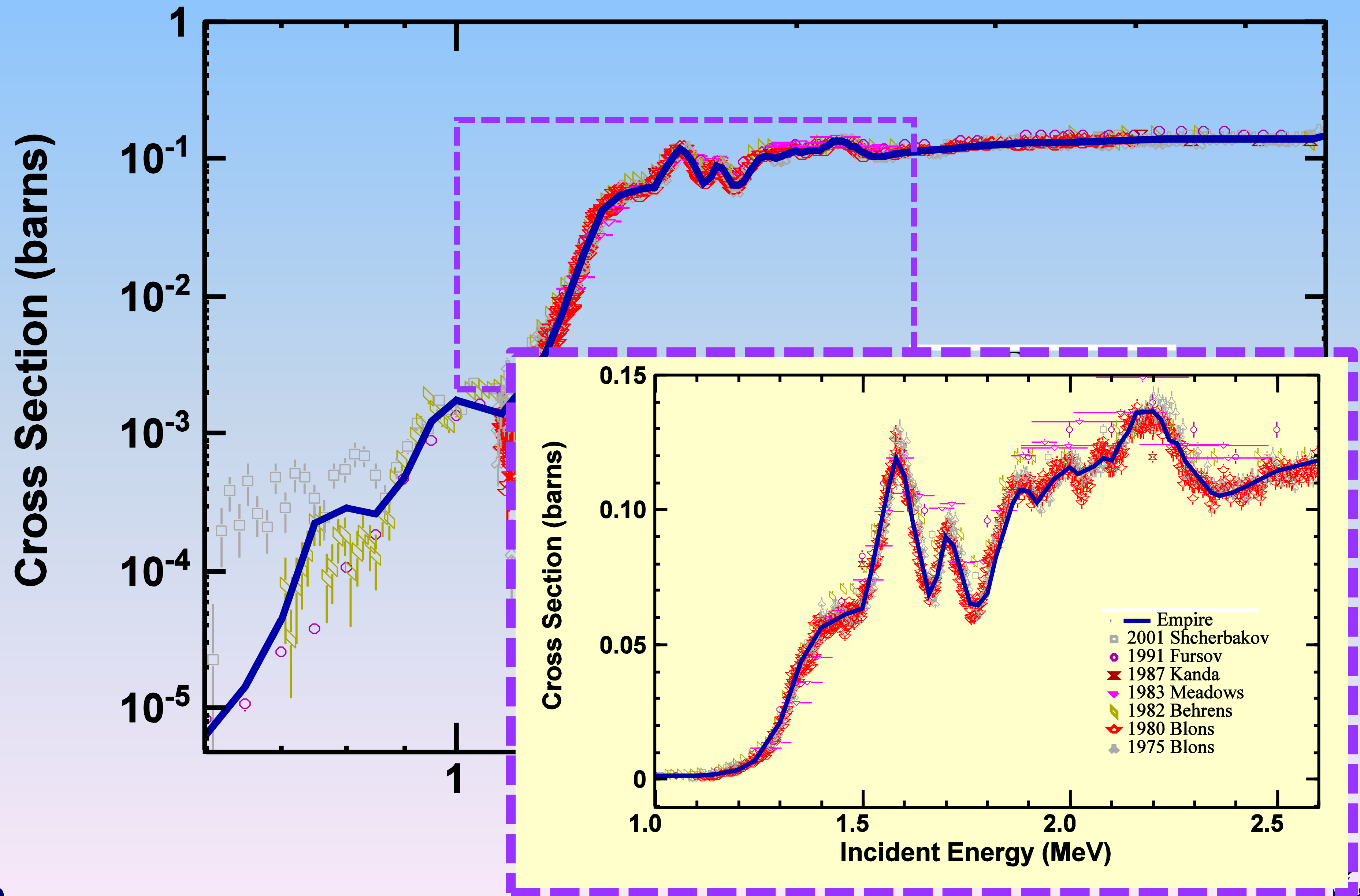

Cross Section (barns)
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
1
Cross Section (barns)
0.15
0.10
0.05
0
1.0
1.5
2.0
2.5
Incident Energy (MeV)
Empire
2001 Shcherbakov
1991 Fursov
1987 Kanda
1983 Meadows
1982 Behrens
1980 Blons
1975 Blons

Using integral data (k_{eff}) in the evaluation

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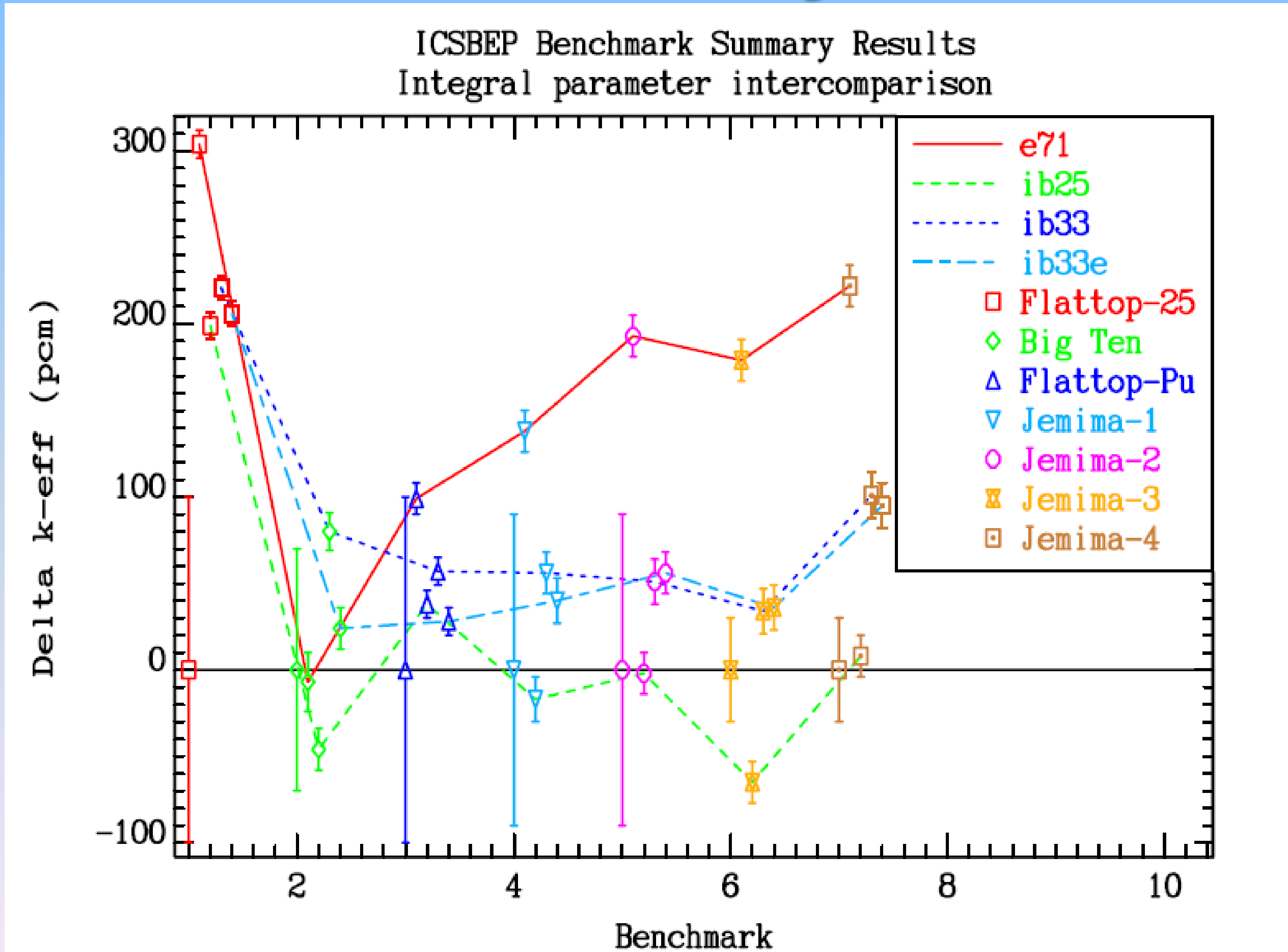
NEA ICSBEP criticality benchmarks



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Using quasi-differential data in the evaluation

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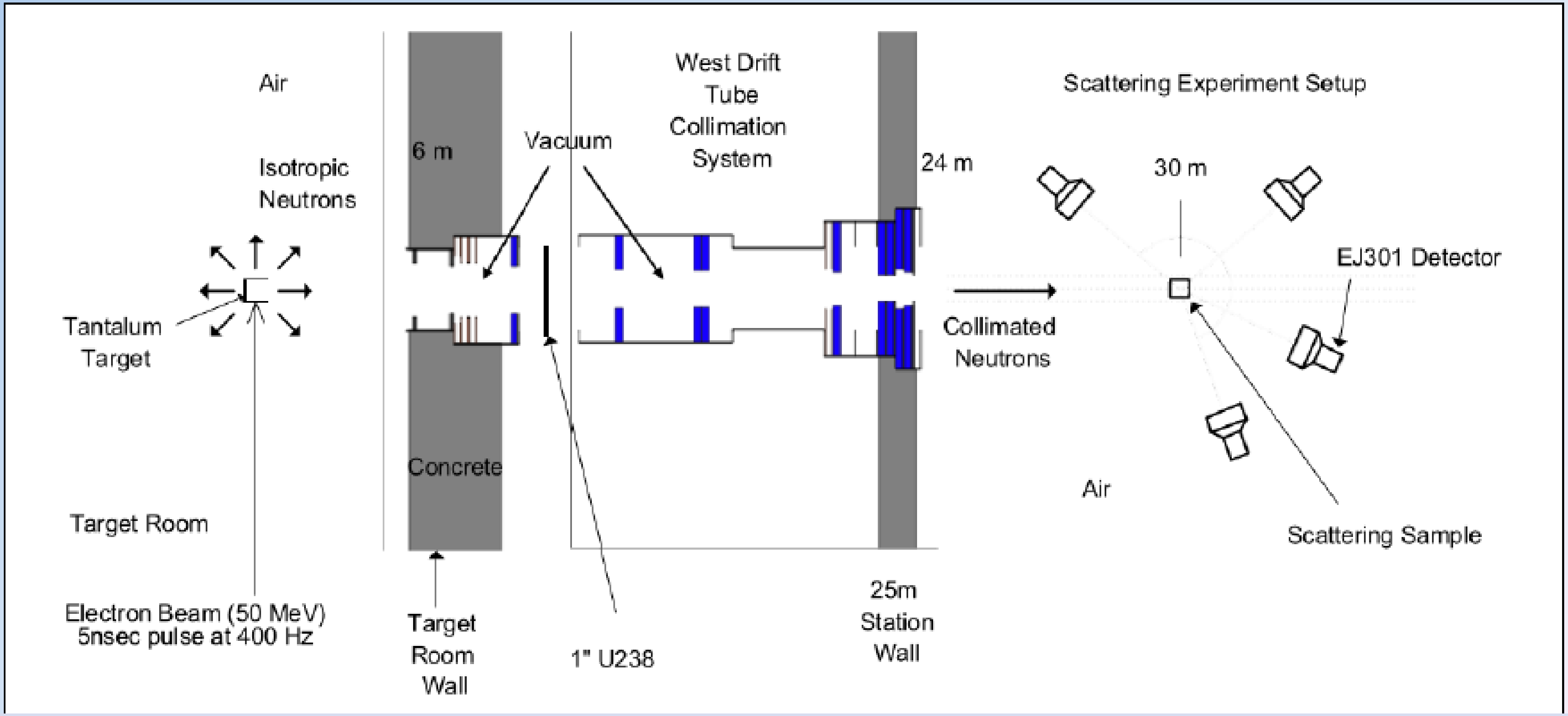
RPI experimental setup



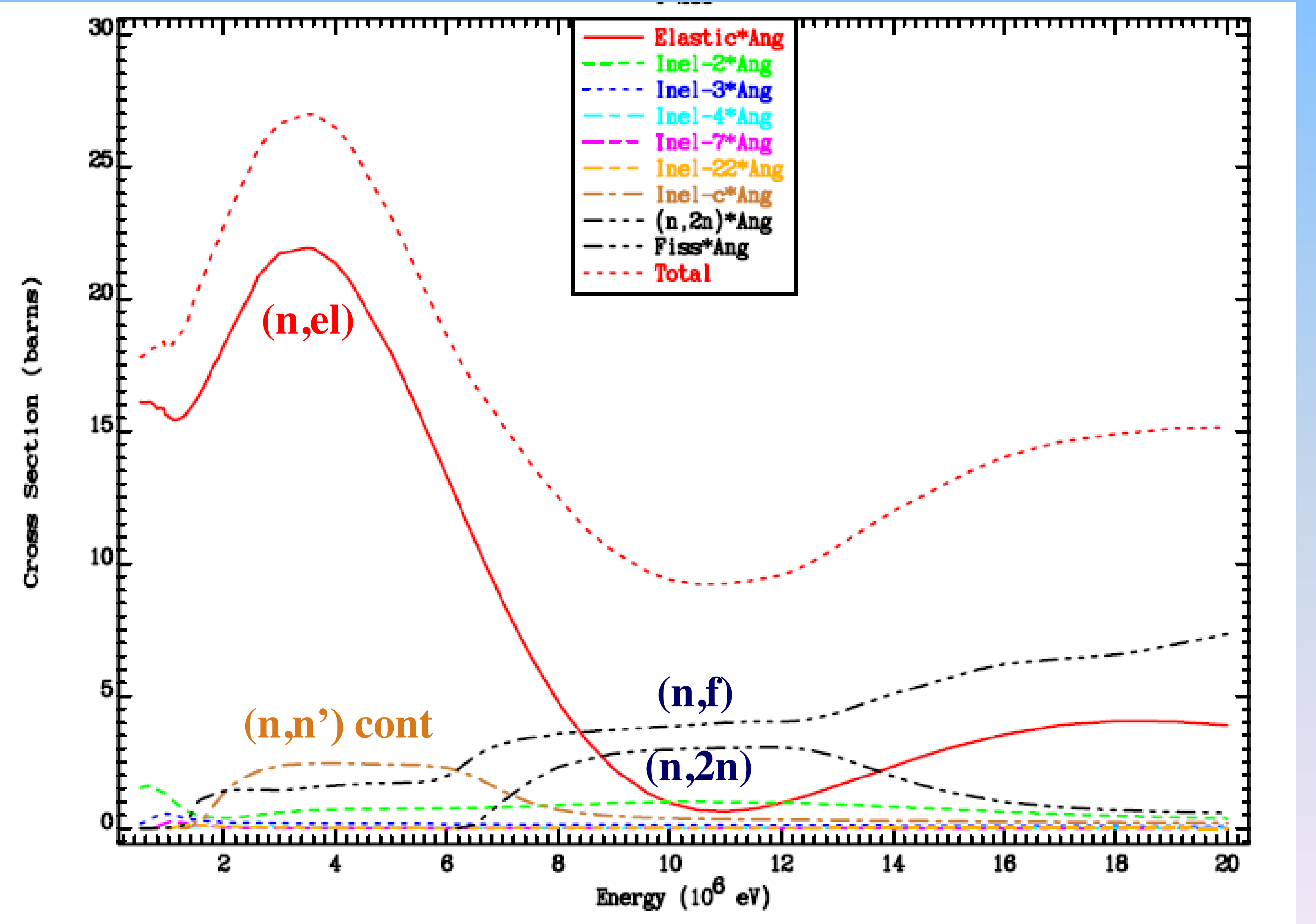
simple & easy to model geometry

Rensselaer
Mechanical, Aerospace and Nuclear Engineering

linac The Gaertner LINAC Center 7

International Workshop on Elastic and Inelastic Scattering, WINS2012, Boston, 17-19 Sept. 2012

Angle dependent cross sections: 29^0



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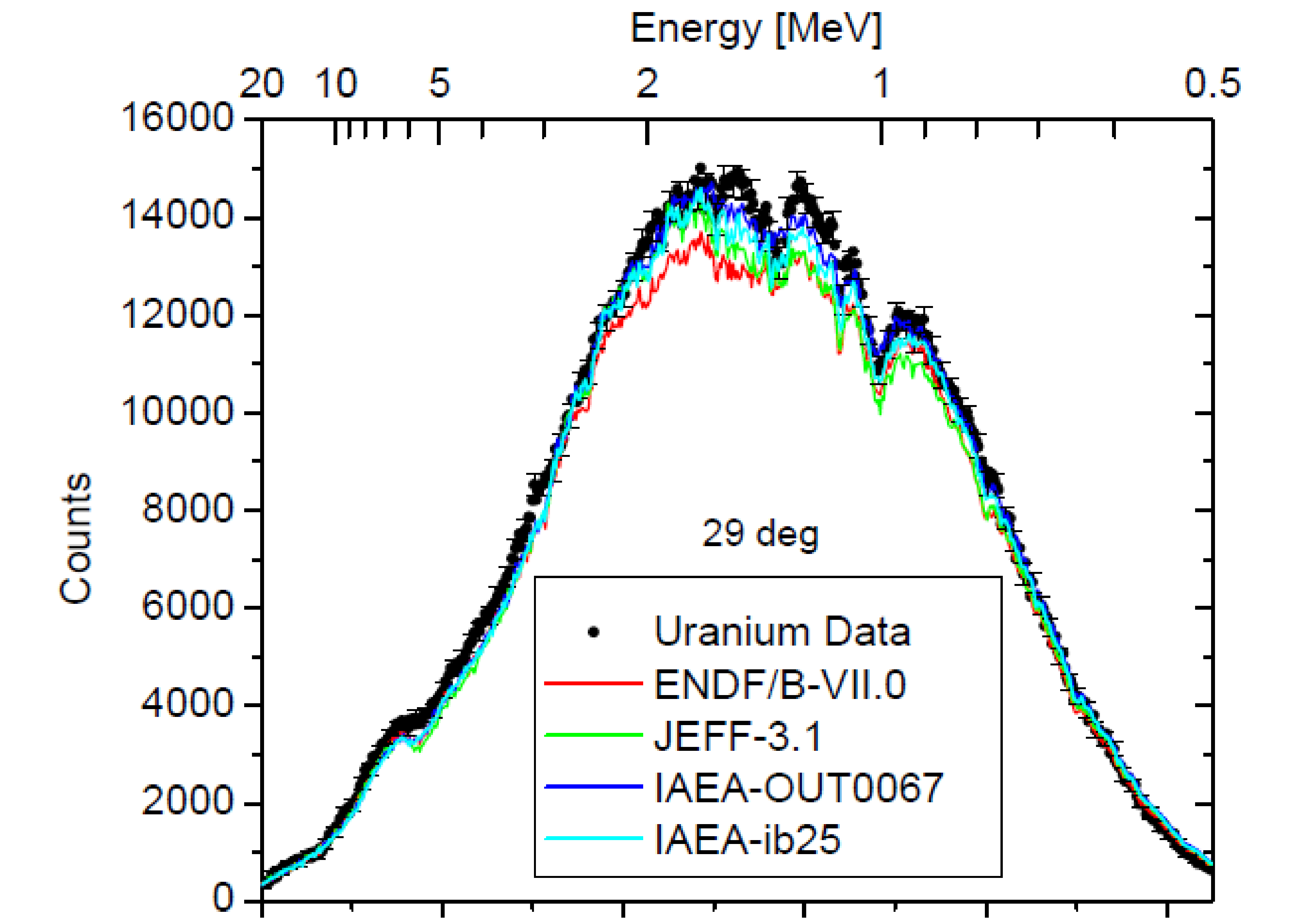
RPI benchmark: 29^0



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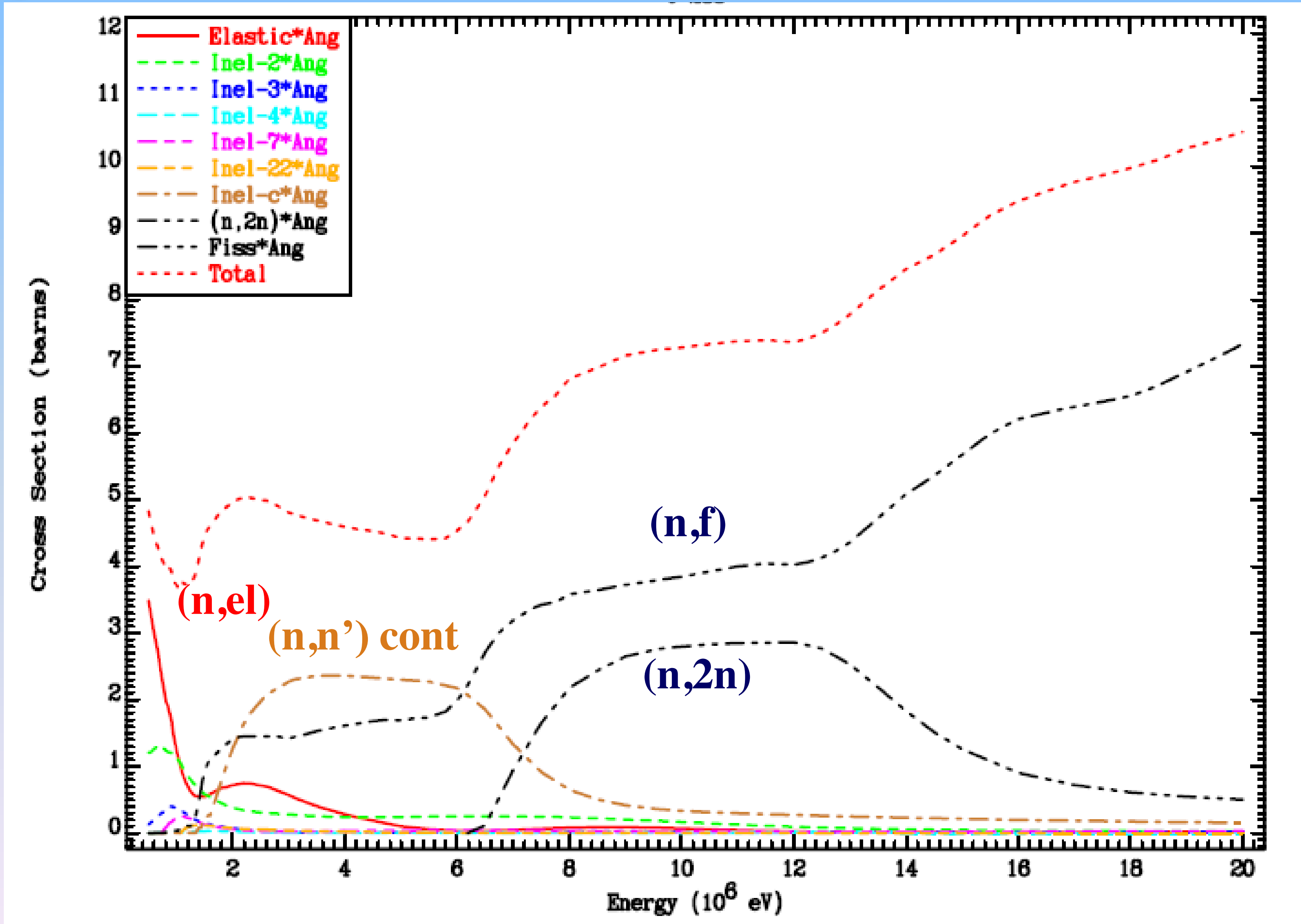
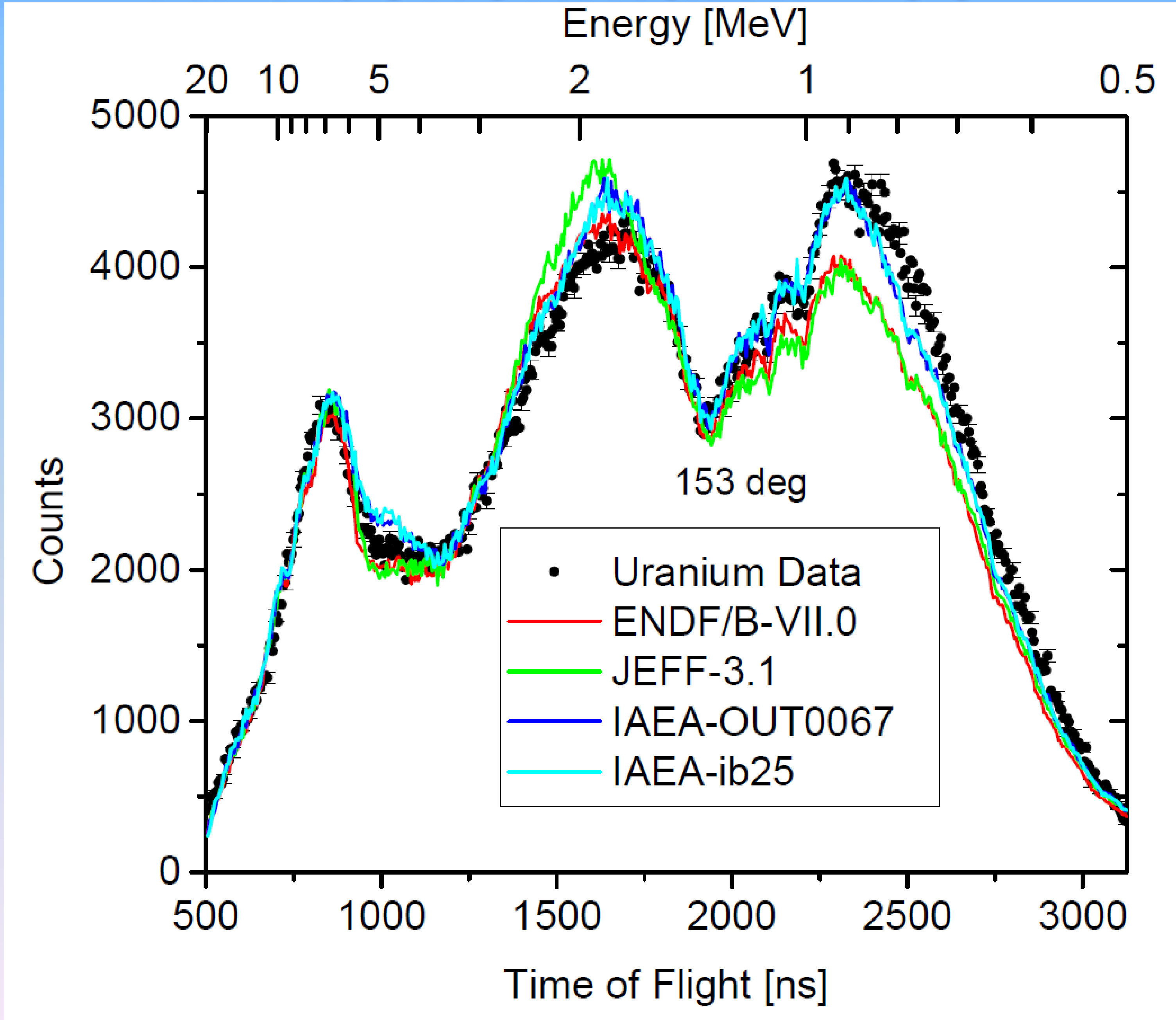
Angle dependent cross sections:153⁰



RPI benchmark: 153^0



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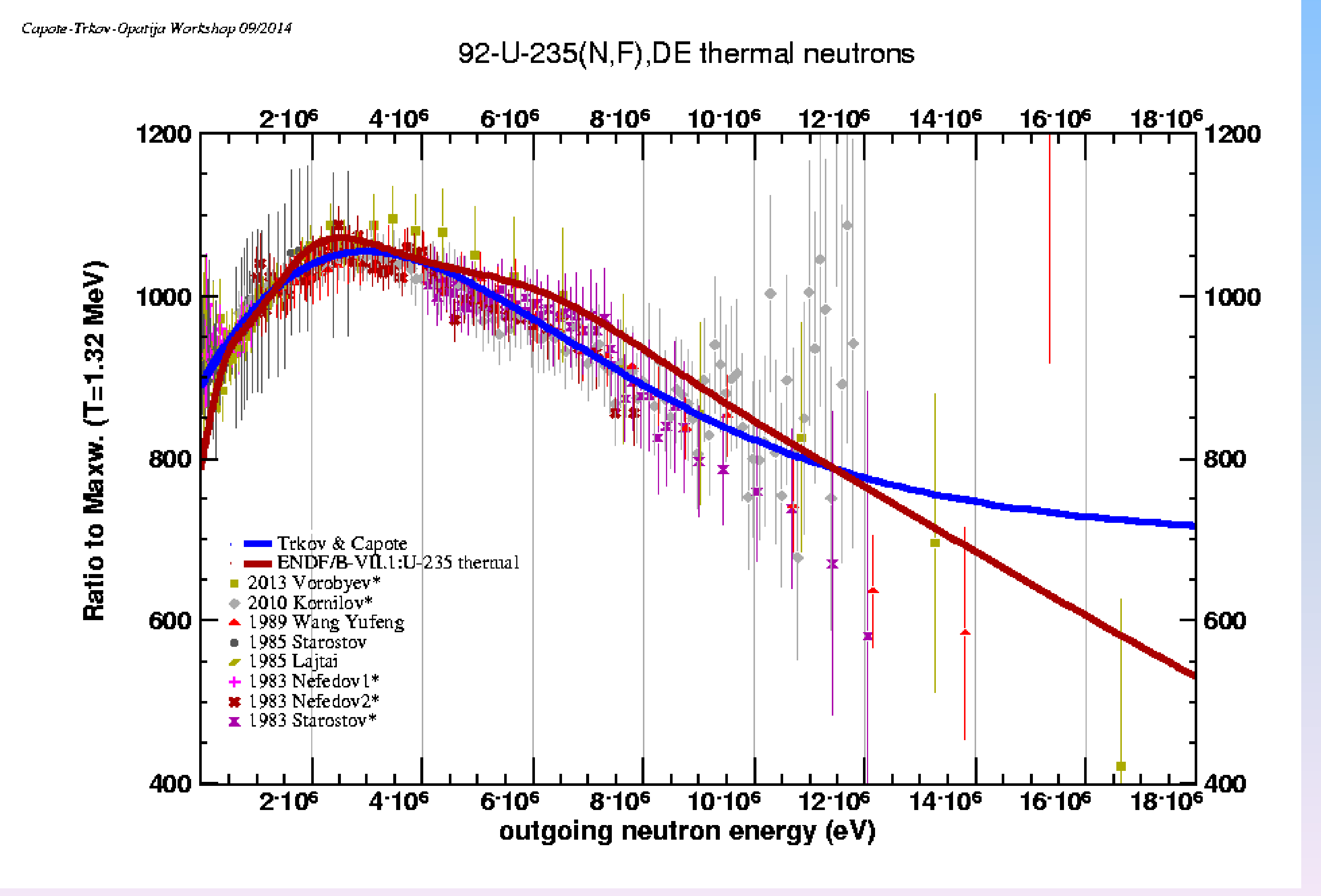
OTHER CHALLENGES: PFNS



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OTHER CHALLENGES: ^{235}U th.nubar

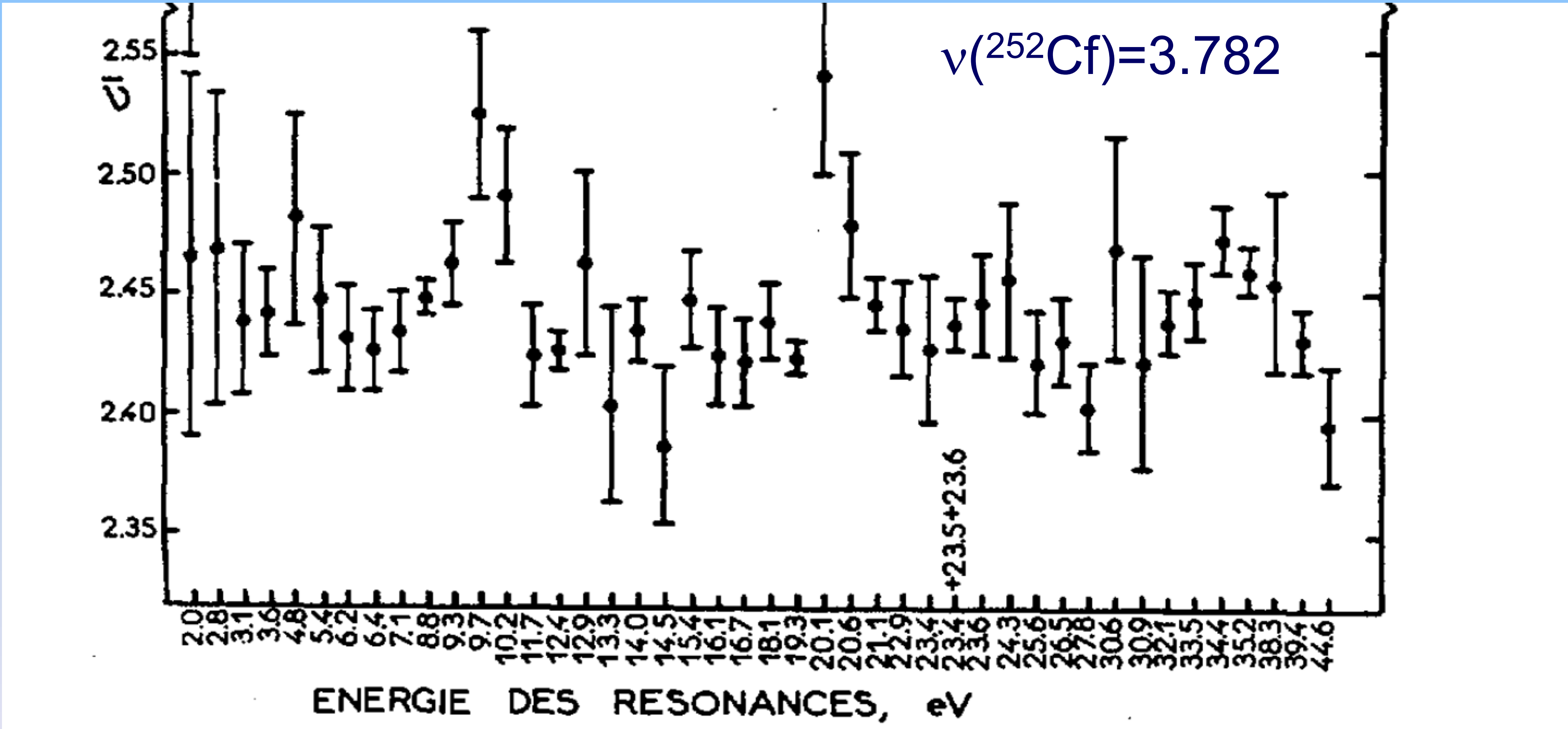

FIG.2. Valeurs de $\bar{\nu}$ e ... pour les résonances de ^{235}U.

Frehaut & Shackleton p.201

www-nds.iaea.org/publications/proceedings/Physics-and-Chemistry-of-Fission-1973-Vol-II.pdf

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SUMMARY

- Reaction modelling of neutron scattering on ^{238}U nucleus
- Dispersive CC OMP coupling all levels up to E_n=1 MeV
- Use of integral and quasi-differential benchmarks as part of the evaluation process
- EMPIRE advanced Hauser-Feshbach treatment includes:
  - Dispersive coupled-channel optical models
  - CN anisotropy
  - Direct effects on the CN emission
  - Multi-humped fission barrier with absorption

- Additional data challenges: PFNS and nubar

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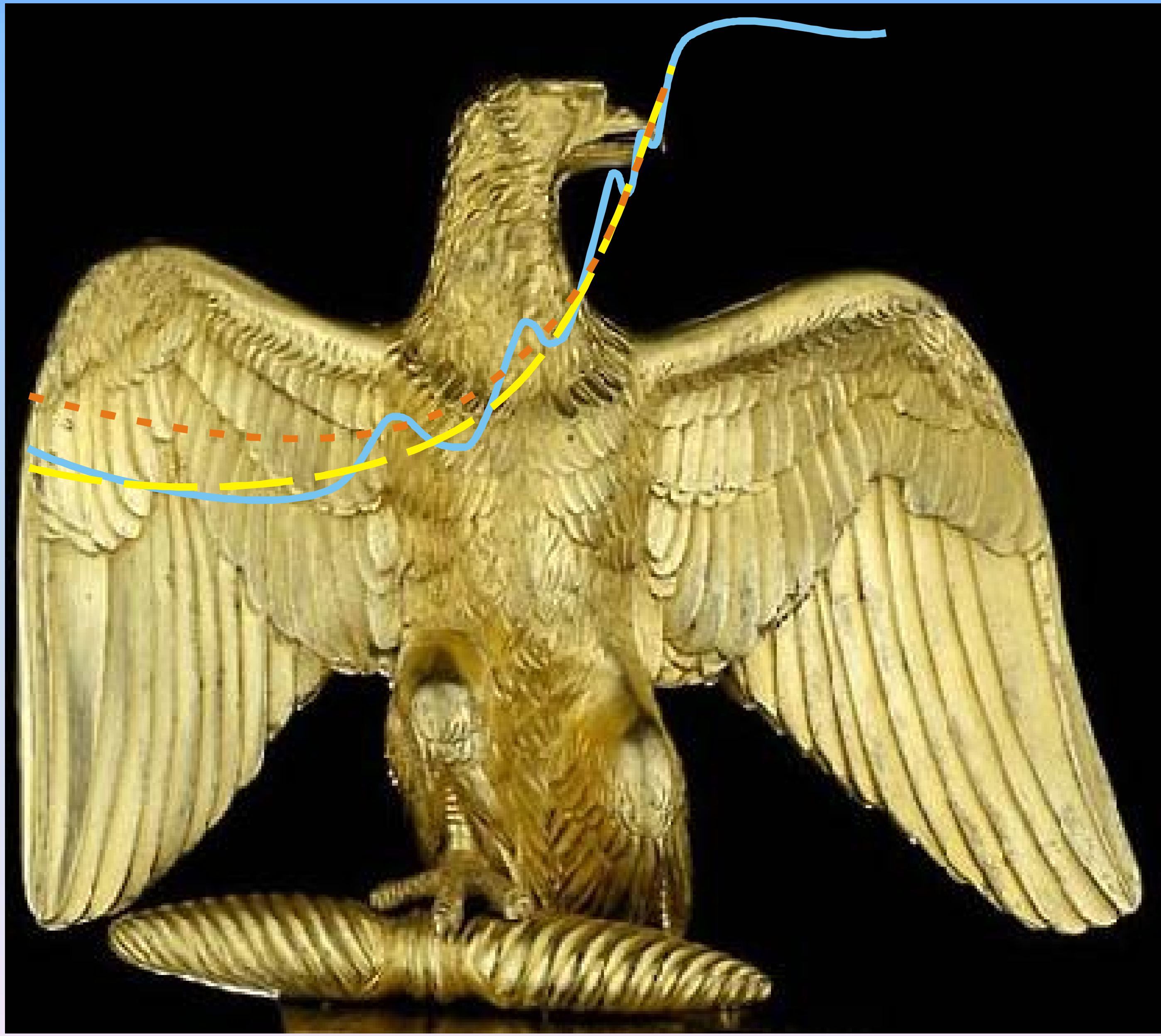

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