Contribution of Thermal Scattering Libraries to JEFF from the Nuclear Data Group at Centro Atómico Bariloche

J

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Argentina

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OECD- Paris
France

Nuclear Data group at Centro Atómico Bariloche

Rolando Granada
Scattering theory and advanced neutron sources

Florencia Cantargi
Cold moderator materials and neutron filters

Christian Helman
Solid state physics and ab initio methods

Ignacio Marquez
Nuclear reactor applications and benchmarking

Past members: Monica Sbaffoni (currently at IAEA), Victor Gillette (currently at University of Sharjah, U.A.E).

2016: Agreement with OECD/NEA to supply thermal scattering libraries to JEFF

Filters: Silicon and sapphire

Cold moderators: liquid hydrogen, liquid deuterium, mesitylene, toluene and light water ice

Thermal moderators: light and heavy water

Light water ice

- 2002: First studied as cold moderator together with methane clathrate using the synthetic model (ACoM6 Proceedings, Jülich 2002)

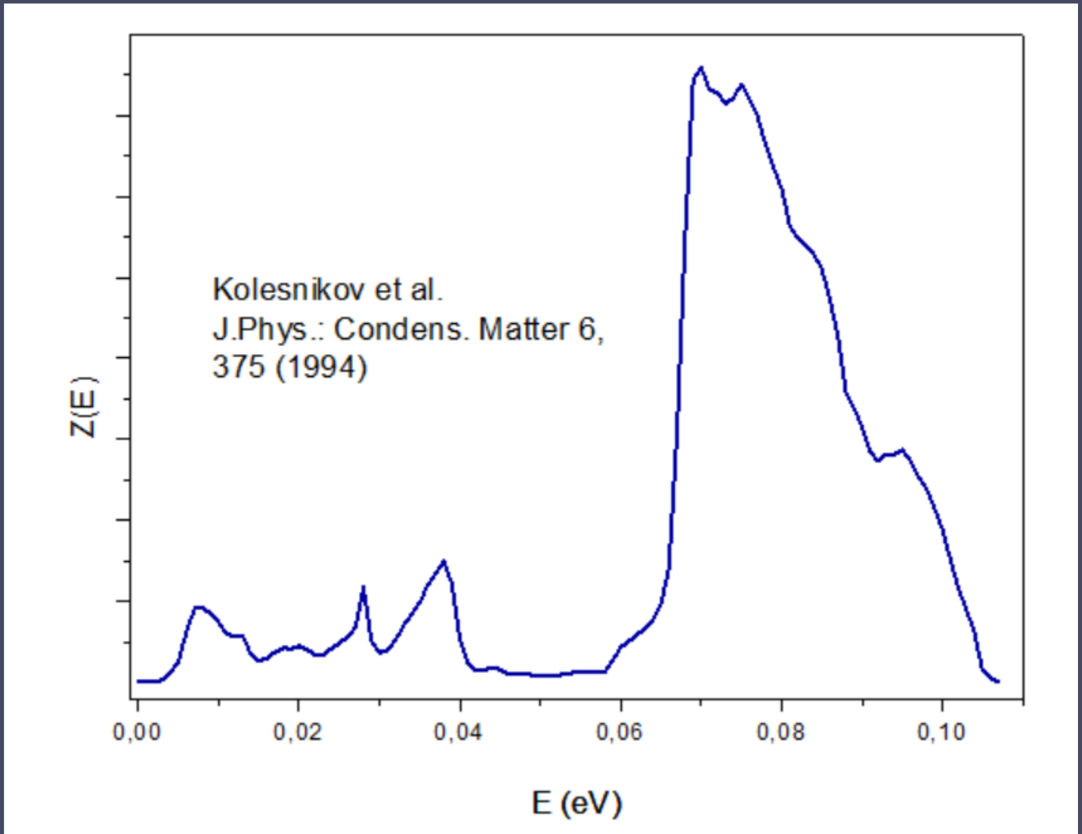
- 2008: Reviewed for IAEA-CRP and delivered to S. Basu (Bhaba Research Centre, DRUVA Reactor, India)

- 2011: Reviewed and delivered to Y. Kiyanagi (Hokkaido University)

- 2012: Used for calculations at our LINAC cold neutron source to compute the ice layer formed around the container

- 2016: Reviewed and validated for JEFF (see Oscar Cabellos presentation)

H bound in light water ice



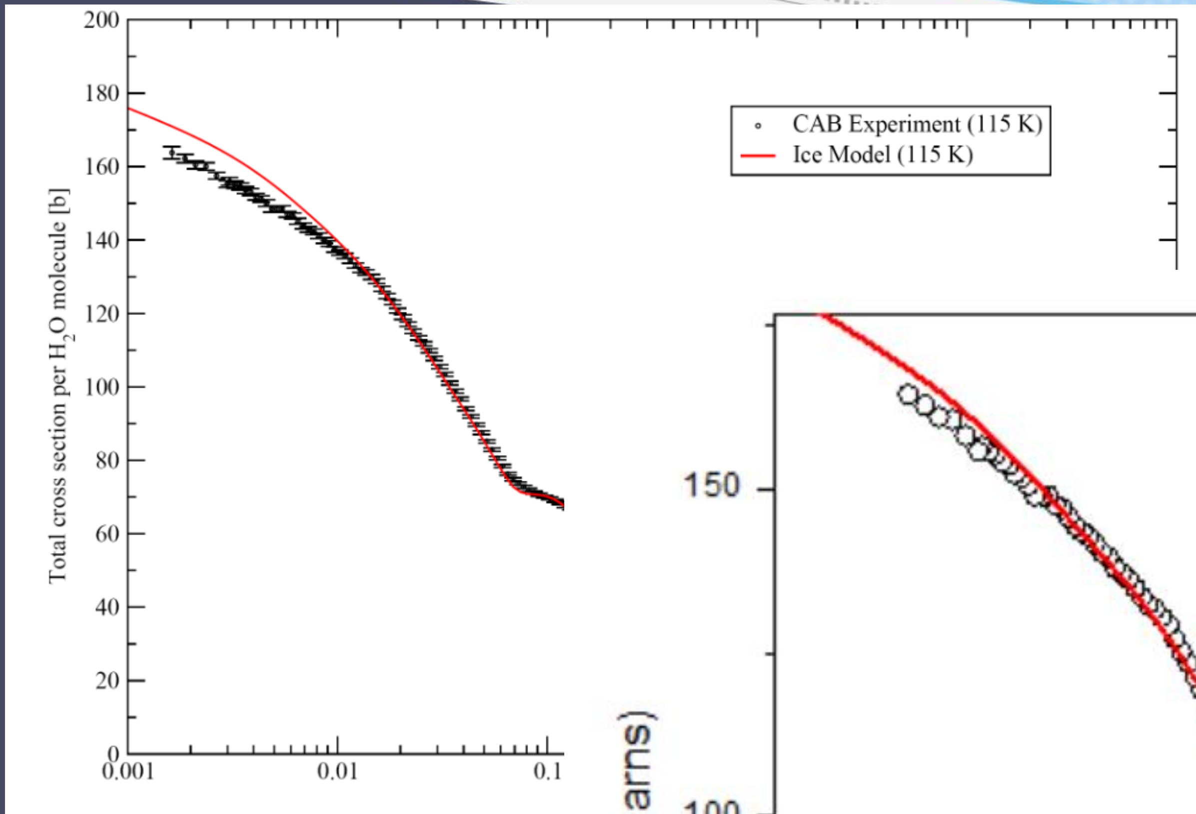
Continuous frequency spectrum representing rotations and internal vibrations of the molecule

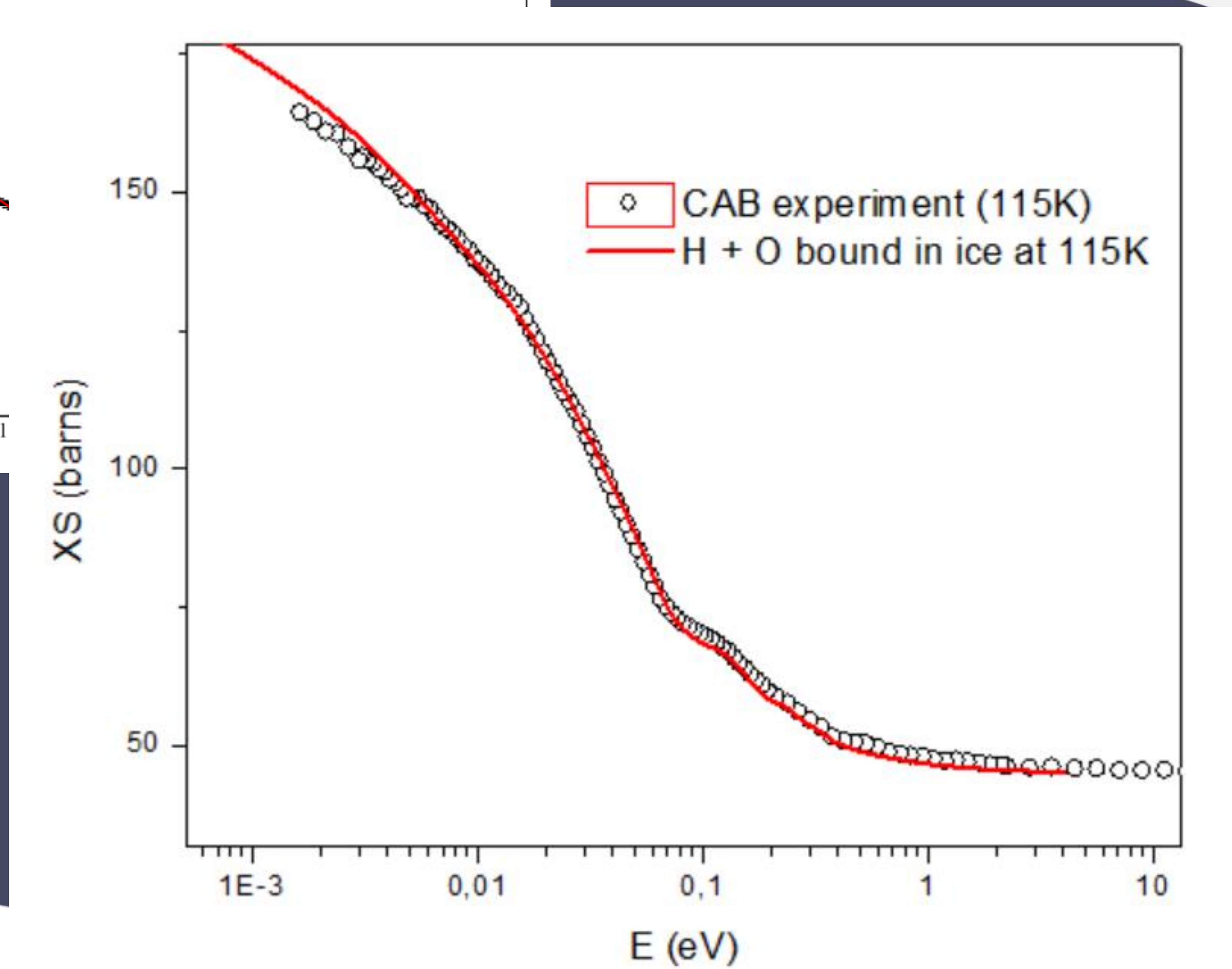
w_{cont}=0.5

Two Einstein oscilllators

$h\nu_1$= 0.205 eV w_1= 1/6

$h\nu_2$=0.391 eV w_2= 2/6


CAB Experiment (115 K)
Ice Model (115 K)
Total cross section per H2O molecule [b]
200
180
160
140
120
100
80
60
40
20
0
0.001
0.01
0.1


CAB experiment (115K)
H + O bound in ice at 115K
XS (barns)
150
100
50
1E-3
0,01
0,1
1
10
E (eV)

Mesitylene

- Already used as cold moderator at two low power facilities:

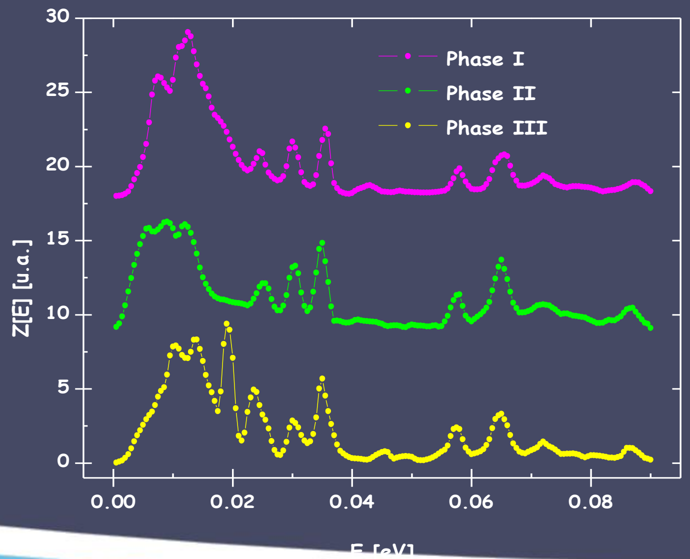
the pulsed source of Kyoto University and the Cornell 500 kW TRIGA reactor

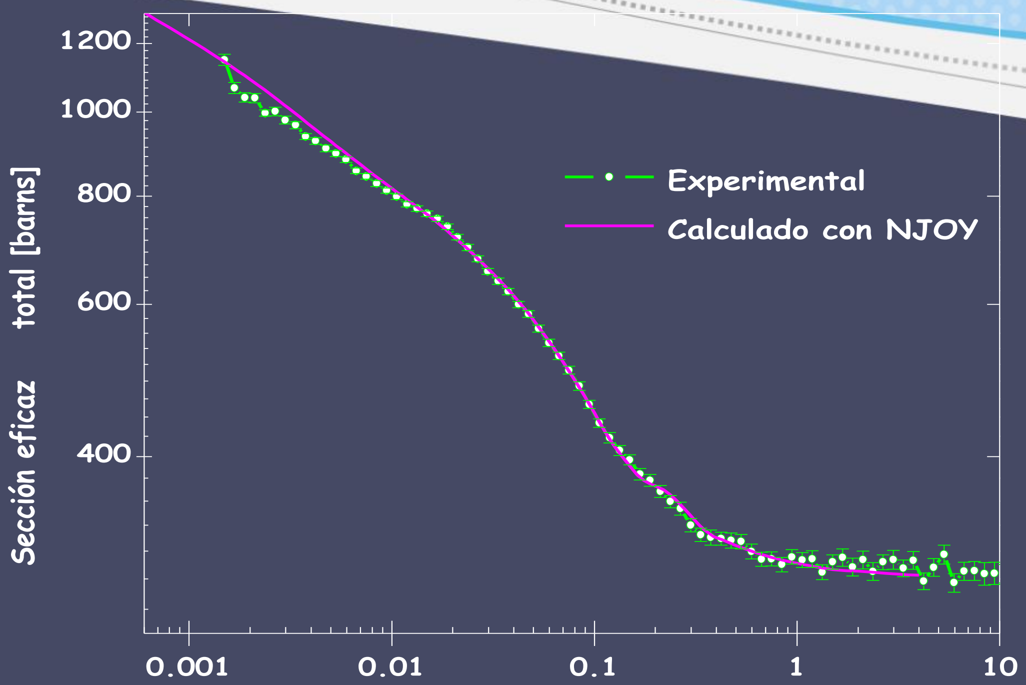
- 2003: Frequency spectrum measurements performed and presented at **ICANS XVI** by Natkaniec et al., Joint Institute for Nuclear Research , Dubna)

- 2004-2007: Frequency spectrum built for NJOY calculations using experimental information from Natkaniec + 3 Einstein oscillators. First mesitylene cross section library developed and validated with our own measurements at CAB

$h\nu_1$= 0.12 eV (Ring breathing)	$h\nu_2$= 0.17 eV (C-H stretching in CH_3)	$h\nu_3$= 0.37 eV (C-H stretching in the ring)
ω_1 = 0.170	ω_2 = 0.310	ω_3 = 0.332

ω_{cont} = 0.188





Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms
Volume 268, Issue 16, 15 August 2010, Pages 2487–2491

Thermal neutron cross-section libraries for aromatic hydrocarbons

F. Cantargi[a, b], J.R. Granada[a, b, c]
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https://doi.org/10.1016/j.nimb.2010.04.030
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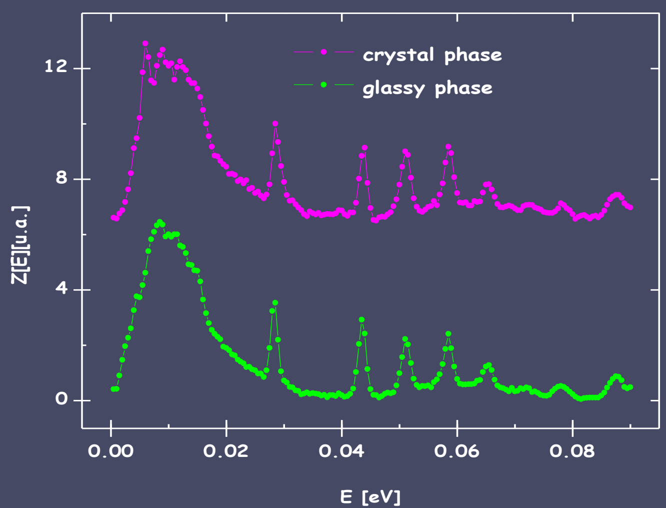
- Libraries delivered to :
  - Joint Institute of Nuclear Physics, Franck Laboratory, Dubna, Russia (E. Shabalin, S. Kulikov, 2006)
  - JESSICA Collaboration, FZ Juelich, Germany (F. Conrad, 2007)
  - Hokkaido University, Japan (Y. Kiyanagi, 2007)
  - TRIUNF, Canada (A. Miller, 2013)
  - Paul Scherrer Institute, Switzerland (V. Talanov, 2013)
  - LANL, USA (M. Mocko, 2014)
  - Savannah River National Laboratory (A. Brand, 2015)

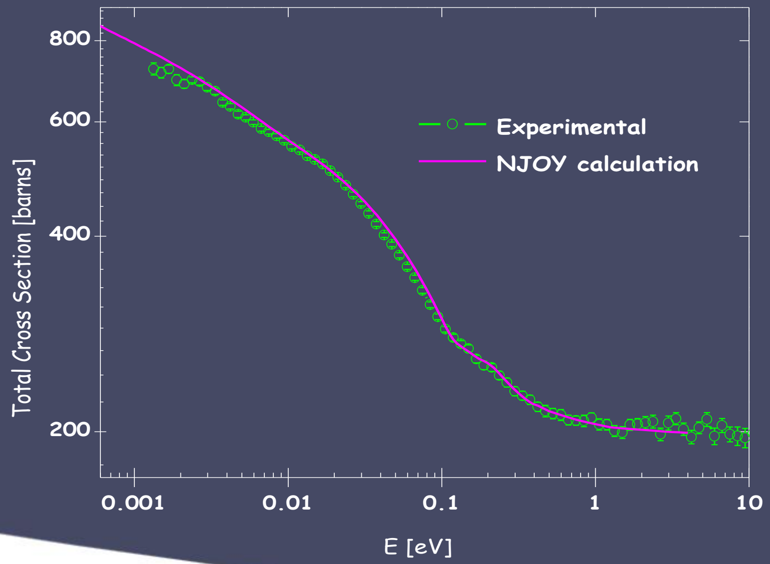
Toluene

- Similar behavior as mesitylene. Not used alone. Useful when mixed with mesitylene



$h\nu_1$= 0.12 eV (Ring breathing)	$h\nu_2$= 0.17 eV (C-H stretching in CH_3)	$h\nu_3$= 0.37 eV (C-H stretching in the ring)
ω_1 = 0.30	ω_2 = 0.23	ω_3 = 0.34

ω_{cont} = 0.13



Liquid hydrogen and deuterium

- 2000: for OPAL cold neutron source

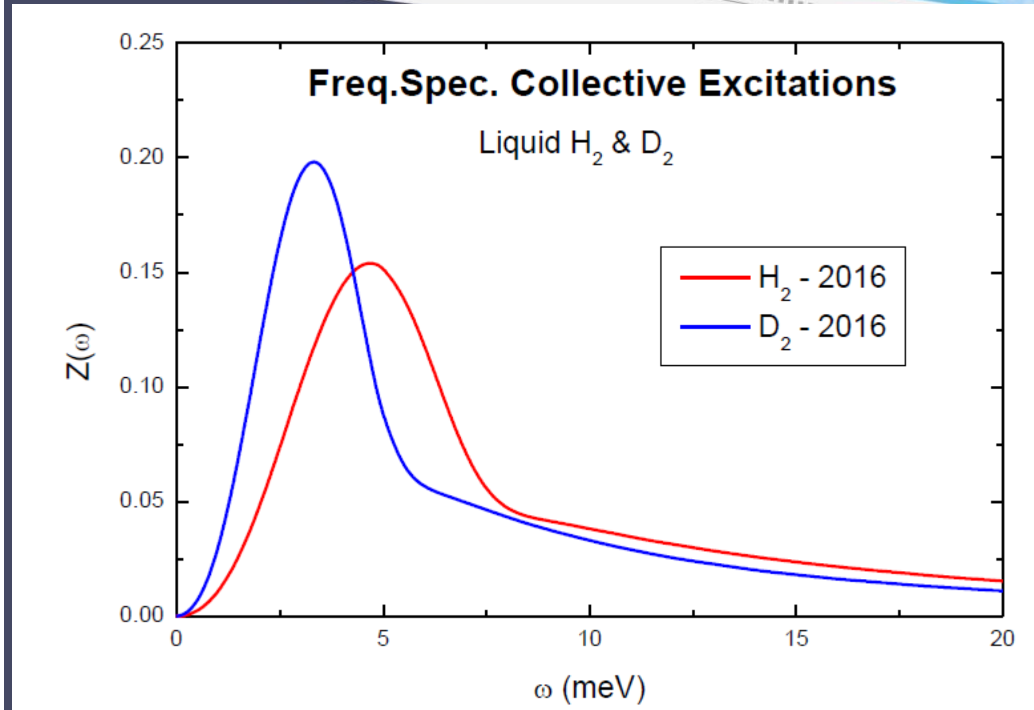
  INVAP S.E., Bariloche, Argentina (O. Lovotti, 2000)

  2004: published in Journal of Neutron Research, vol. 11, no. 1, 2, pp. 25-40, 2003 and Physica B: Condensed Matter Volume 348, Issues 1–4, 1 May 2004, Pages 6–14

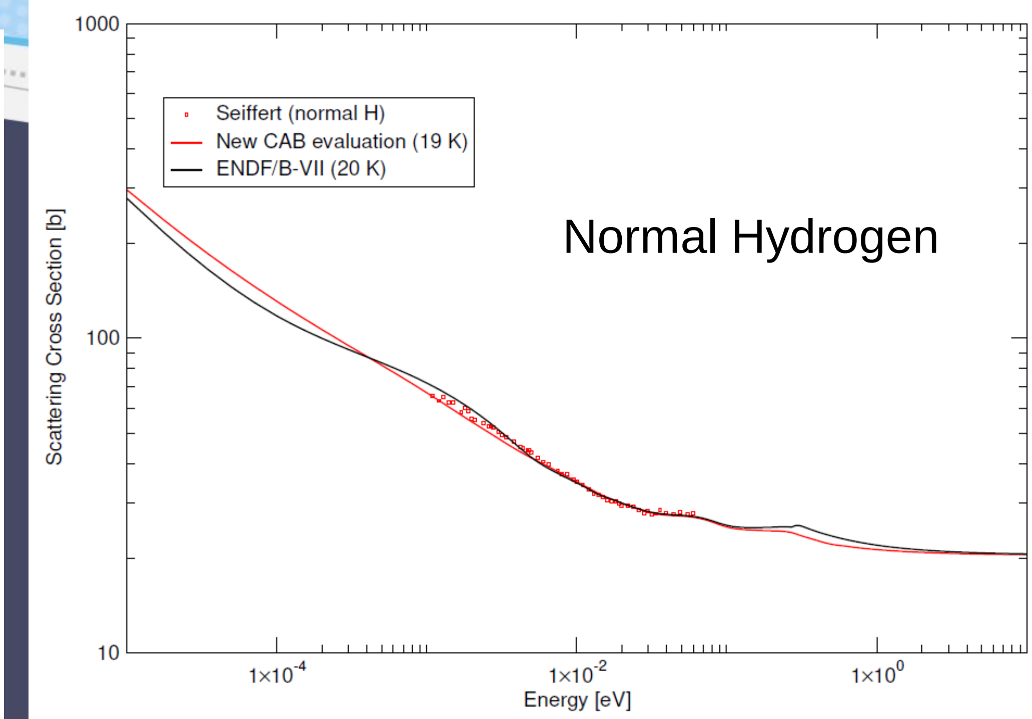
- 2014: cross section libraries delivered to RA-10 project

  RA-10 project, Argentina (F. Sánchez-A. Márquez, 2014)

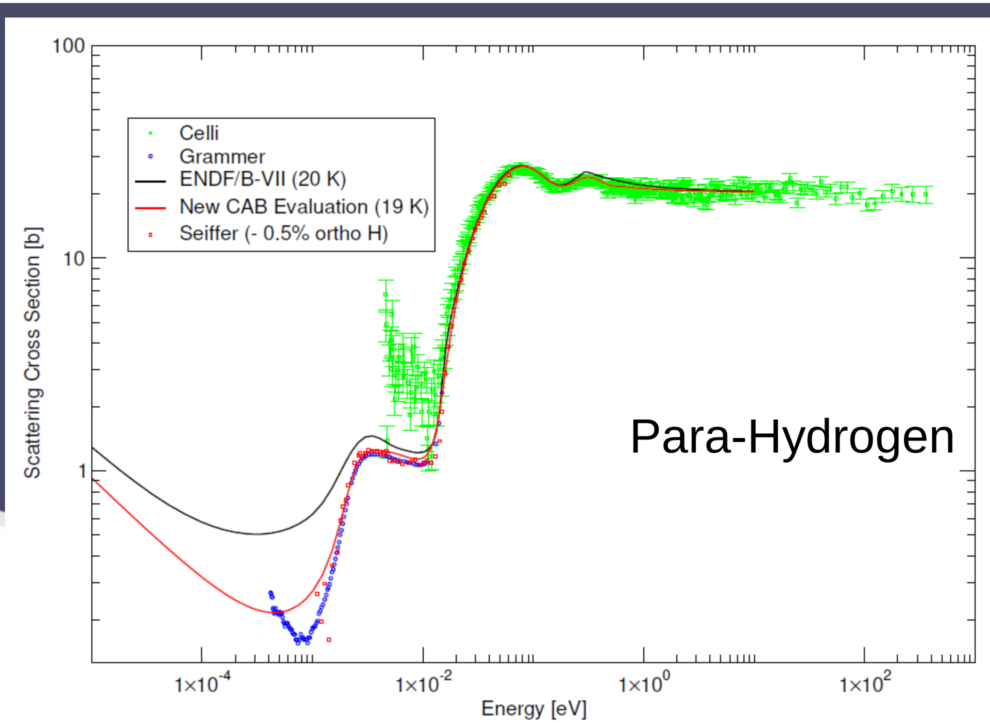
- 2016: update kernels. Modification in LEAPR module of NJOY: Sköld correction instead of Vineyard + revision of frequency spectra and structure factors



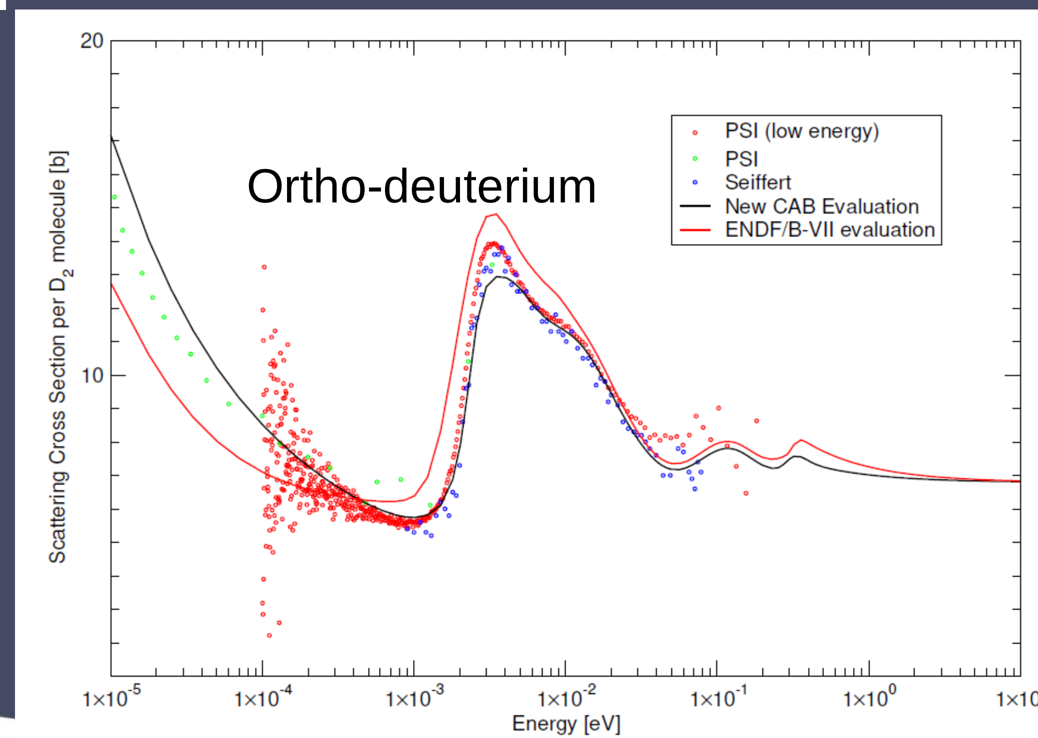
Freq.Spec. Collective Excitations
Liquid H2 & D2
H2 - 2016
D2 - 2016
Z(ω)
ω (meV)
0.25
0.20
0.15
0.10
0.05
0.00
0
5
10
15
20



Normal Hydrogen
Seiffert (normal H)
New CAB evaluation (19 K)
ENDF/B-VII (20 K)
Scattering Cross Section [b]
Energy [eV]
1000
100
10
1×10^-4
1×10^-2
1×10^0



Para-Hydrogen
Celli
Grammer
ENDF/B-VII (20 K)
New CAB Evaluation (19 K)
Seiffer (- 0.5% ortho H)
Scattering Cross Section [b]
Energy [eV]
100
10
1
1×10^-4
1×10^-2
1×10^0
1×10^2



Ortho-deuterium
PSI (low energy)
PSI
Seiffert
New CAB Evaluation
ENDF/B-VII evaluation
Scattering Cross Section per D2 molecule [b]
Energy [eV]
20
10
1×10^-5
1×10^-4
1×10^-3
1×10^-2
1×10^-1
1×10^0
1×10^1

Sapphire

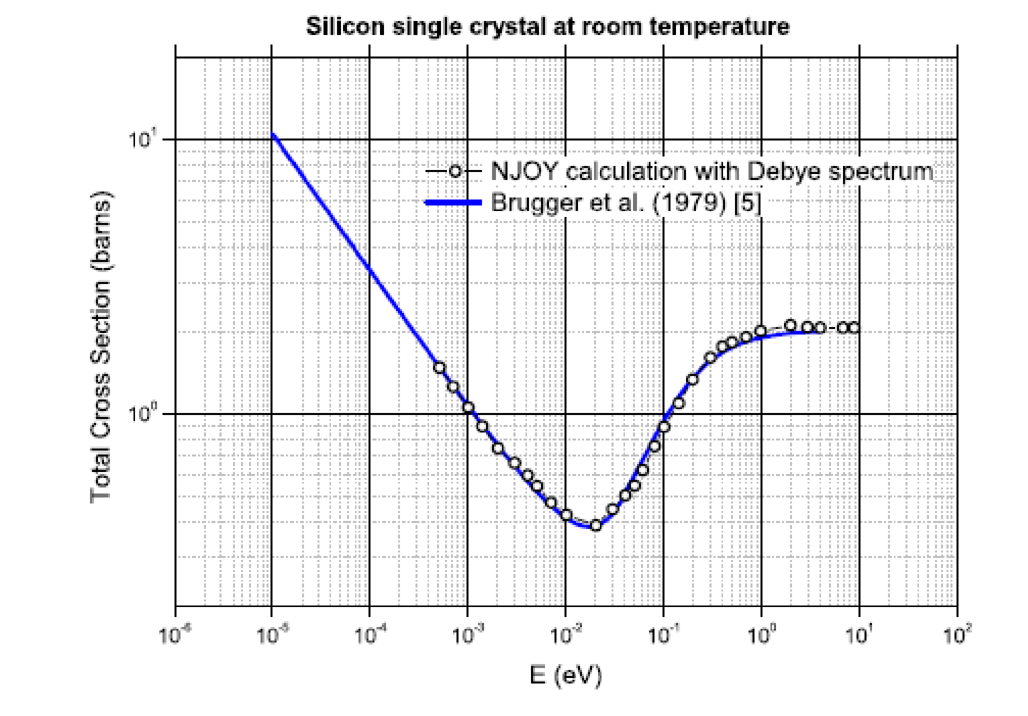
- 2008: for the neutrography facility of RA-6 nuclear reactor. Cross section libraries generated and validated with our own measurements at CAB. Debye model with T_D= 485K was used as a good representation of the frequency spectrum

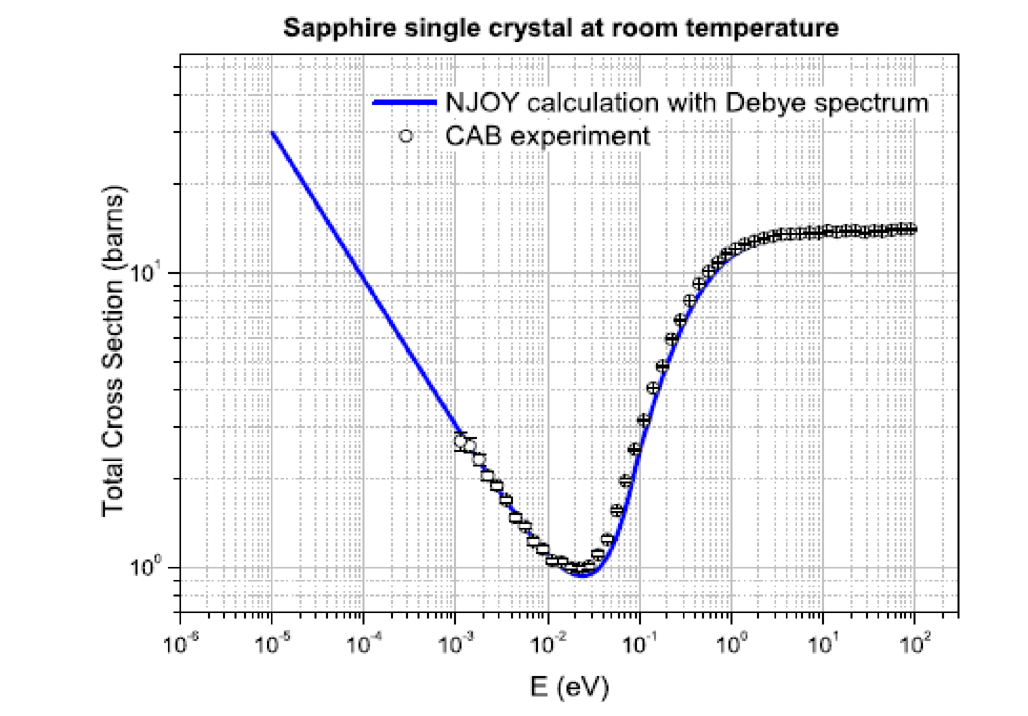
    - RA-6 reactor, Argentina (F. Sanchez, 2008)
    - RA-3 6 reactor, Argentina (M. Sztejnberg, 2010)
    - Paul Scherer Institute, Switzerland (E. Rantsiou, 2013)
    - LAHN (Argentinean Neutron Beams Laboratory Project) (A. Tartaglione, 2017)

Silicon

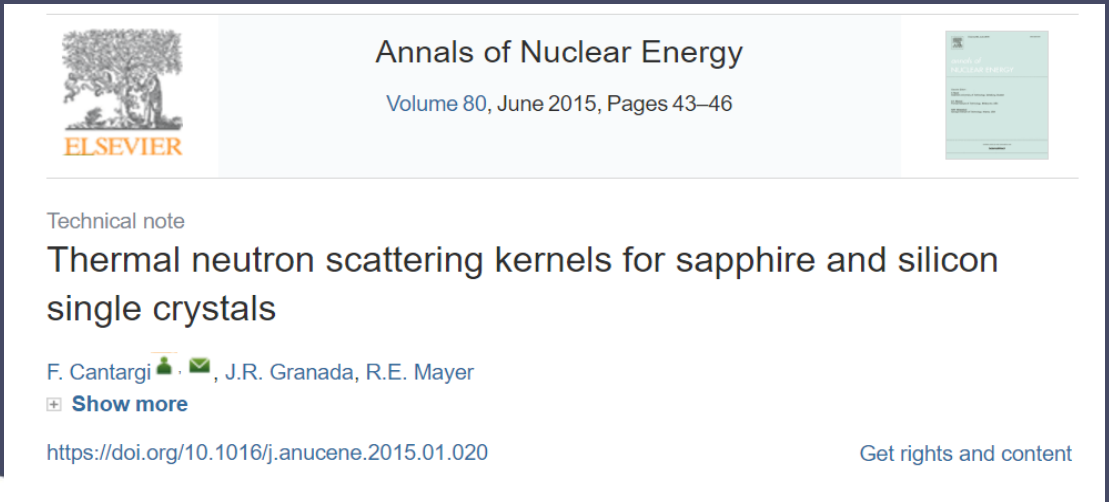
2013: for Neutron Transmutation Doping at RA-10 nuclear reactor. Debye model with T_D= 1032K was used as a good representation of the frequency spectrum

- RA-10 project, Argentina (A. Cintas, 2013)
- RA-3 6 reactor, Argentina (M. Sztejnberg, 2010)
- Paul Scherer Institute, Switzerland (E. Rantsiou, 2013)
- LAHN (Argentinean Neutron Beams Laboratory Project) (A. Tartaglione, 2017)





[5] Brugger, R., Fluharty, R., Lisowski, P., Olsen, C.E., 1979. The neutron total cross section of single crystal silicon at 21k. In: International Conference on Nuclear Cross Sections for Technology


Annals of Nuclear Energy
Volume 80, June 2015, Pages 43–46

Technical note

Thermal neutron scattering kernels for sapphire and silicon single crystals

F. Cantargi, J.R. Granada, R.E. Mayer

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https://doi.org/10.1016/j.anucene.2015.01.020

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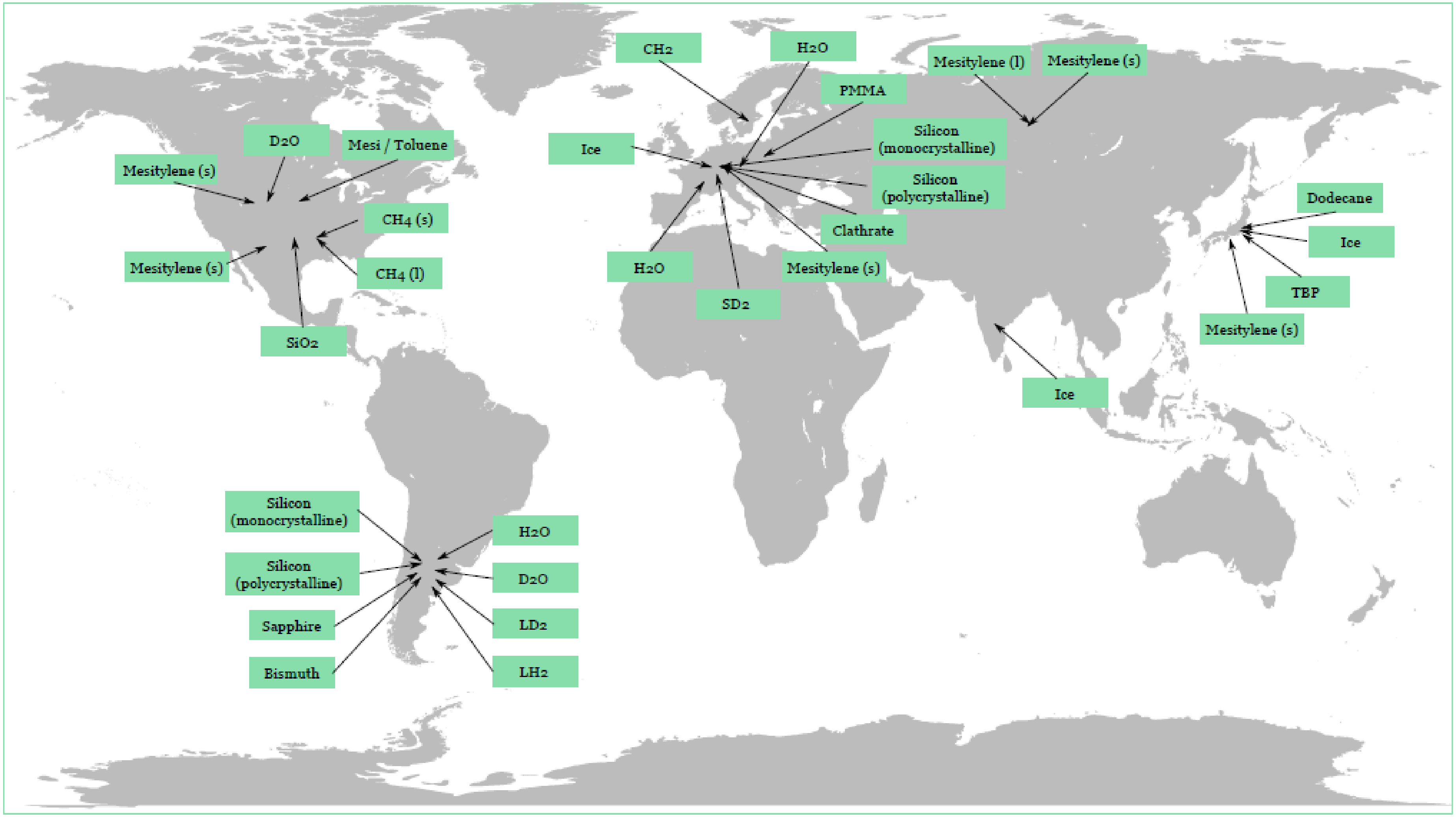
Final Remarks



At the Nuclear Data Group of the Neutron Physics Department (Centro Atómico Bariloche), we have the capability of producing $S(\alpha,\beta)$ in ENDF format and thermal neutron scattering cross sections in ACE format.

Our cross section libraries are available in ENDF-6 and ACE format on demand

Most of them, will also be available in the next release of JEFF

Thanks for your attention