Thermal Cross Section libraries for cold moderators and filters

Florencia Cantargi

cantargi@cab.cnea.gov.ar

Neutron Physics Group
(Centro Atómico Bariloche)
Comisión Nacional de Energía Atómica

Instituto Balseiro
Universidad Nacional de Cuyo

ARGENTINA

Who we are: Thermal scattering nuclear data group at Centro Atomico Bariloche

Rolando Granada
Scattering theory and advanced neutron sources

Florencia Cantargi
Cold moderator materials and neutron filters

Ignacio Marquez
Nuclear reactor applications and benchmarking

The Neutron Physics Department at Centro Atómico Bariloche has more than 40 years of continuous experience working in neutron scattering applied to nuclear data and nuclear engineering.

As part of the Neutron Physics Department, our main activity is the generation of S(α,β) in ENDF format and thermal neutron scattering cross sections in ACE format for our R&D activity or by demand of other groups from Argentina (CNEA and INVAP) and also from other countries.

Material	Users and collaborators
H_2O	Slovak University of Technology in Bratislava, Slovakia (S. Cerba, 2011) CEA Cadarache
D_2O	Chalk River Laboratories, AECL (active collaboration)
CH_2	Chalmers Univeristy of Technology, Department of Reactor Physics, Göteborg, Sweden (Prof. Nils G. Sjöstrand, 1988)
C_6H_6	
Plexiglass	Institute of Nuclear Physics, Division of Applications of Physics and Interdisciplinary Research, Krakow, Poland (Dr. U. Woznicka, 1991)
Ethanol	
Dowtherm	
Metal Hydrides	
Dodecane	Century Research Center Corp., Advanced Technology Dept., Engineering Group, Tokyo, Japan (Dr. H. Kadotani, 1988)
Tributylphosphate	Century Research Center Corp., Advanced Technology Dept., Engineering Group, Tokyo, Japan (Dr. H. Kadotani, 1988)
Graphite	

Cold moderators

Material	Users and collaborators
Liquid H_2	INVAP S.E., Bariloche, Argentina (O. Lovotti, 2000)
Liquid D_2	INVAP S.E., Bariloche, Argentina (O. Lovotti, 2000)
Solid D_2	Paul Scherrer Institute, SINQ, Villegen, Switzerland (M. Daum, 2008)
Liquid & Solid. CH_4	Indiana University, LENS, Bloomington, USA (D. Baxter, 2009)
Water Ice *	• Bhaba Research Centre, DRUVA Reactor, India (S. Basu, 2008) • Hokkaido University, Japan (Y. Kiyanagi, 2011)
Clathrate	JESSICA Collaboration, FZ Juelich, Germany (F. Conrad, 2007)
Mesitylene*	• 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) • LANL, USA (M. Mocko, 2014) • Savannah River National Laboratory (A. Brand, 2015)
Mesityle:Toluene mix *	TRIUNF, Canada (A. Miller, 2013)
Trifenilmethane	Joint Institute of Nuclear Physics, Franck Laboratory, Dubna, Russia (S. Kulikov, 2015)
Ethane	

Neutron filters

Material	Users and collaborators
Silicon *	• RA-10 project, Argentina (A. Cintas, 2013) • Paul Scherrer Institute, Switzerland (E. Rantsiou, 2013)
Sapphire *	• RA-6 reactor, Argentina (F. Sanchez, 2008) • RA-3 6 reactor, Argentina (M. Sztejnberg, 2010) • Paul Scherrer Institute, Switzerland (E. Rantsiou, 2013)
Bismuth	RA-6 reactor, Argentina (F. Sanchez, 2013)
Silica	ORNL, USA (Luiz Leal , 2010)

Frequency spectra

(information about the dynamics of the scattering system)

↓

LEAPR module of
NJOY
Nuclear Data Processing System

↓

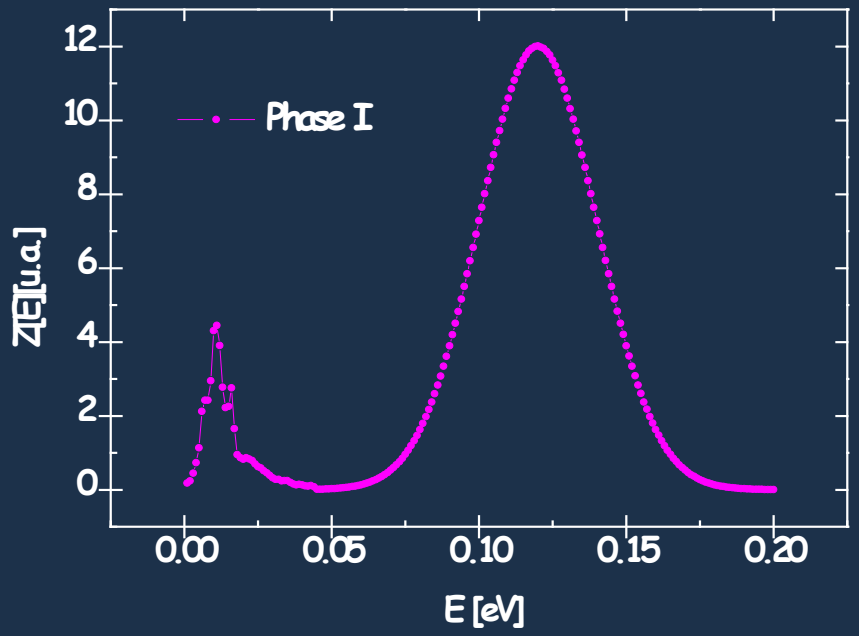
Cross Section Libraries

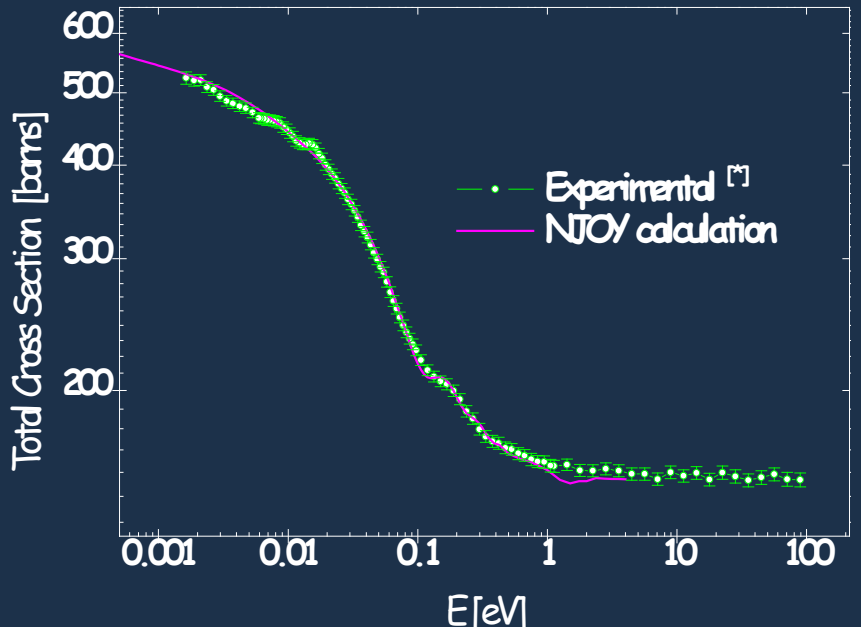
(validated with total cross section measurements from EXFOR or our own measurements at the LINAC of Centro Atómico Bariloche using the TOF technique

EXAMPLES OF MATERIALS STUDIED at NPD of CAB

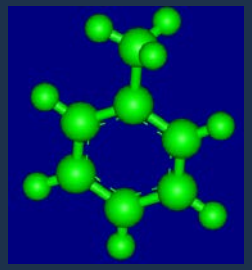
BENZENE (C_6H_6)

Lattice modes	In-plane and out-of-plane modes *(Eg: Ring breathing)*	In-plane modes *(Eg: C-H stretching)*
Experimental information [Natkaniec et al., Proceedings of ICANS XVI, 2003]	Gaussian centered at 0.12 eV	$h\nu_1$= 0.38 eV
w_{cont} = 0.65		w_1 = 0.35

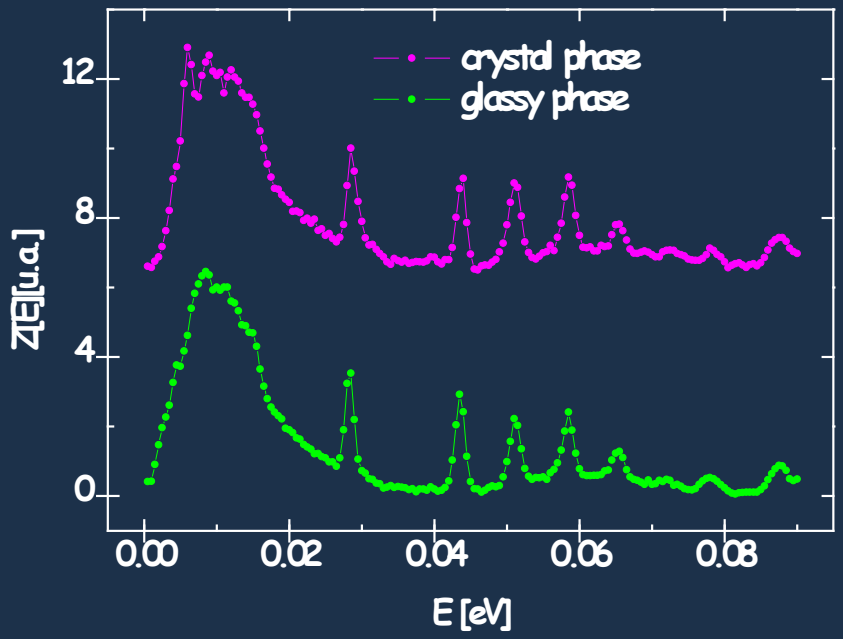


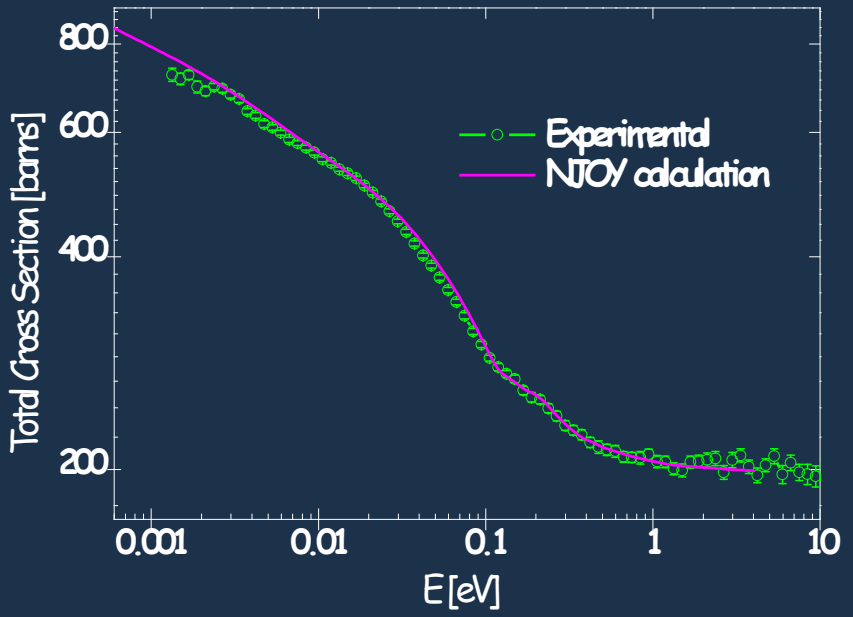


TOLUENE (C_7H_8)

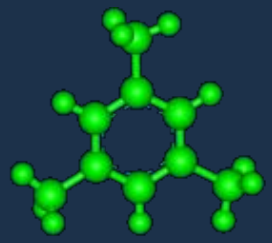


Experimental information [Natkaniec et al., Proceedings of ICANS XVI, 2003]	$h\nu_1$= 0.12 eV (Ring breathing)	$h\nu_2$= 0.17 eV (C-H stretching in CH_3)	$h\nu_3$= 0.37 eV (C-H stretching in the ring)
ω_{cont} = 0.15	ω_1 = 0.378	ω_2 = 0.17	ω_3 = 0.30

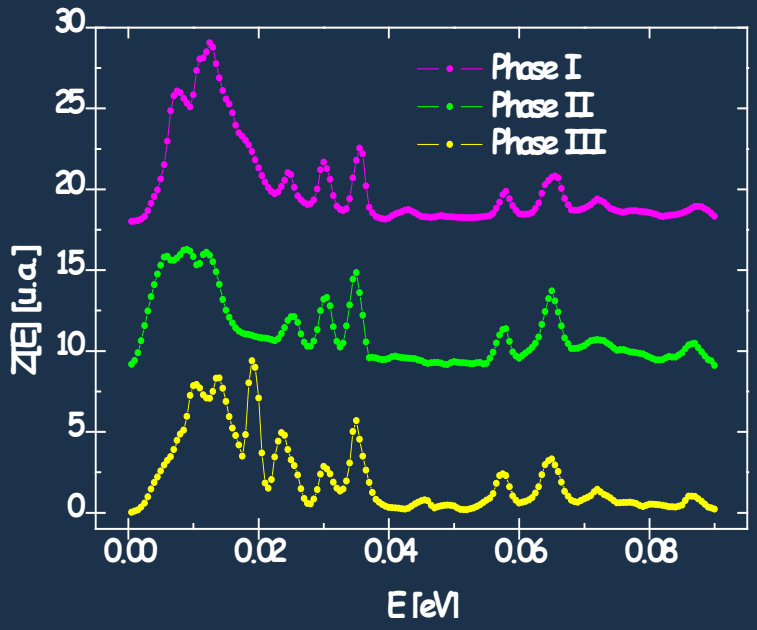


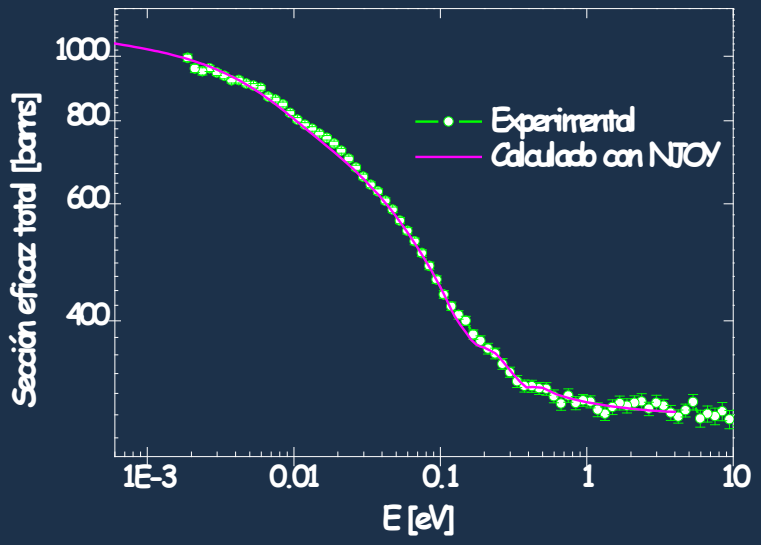


MESITYLENE (C_9H_{12})



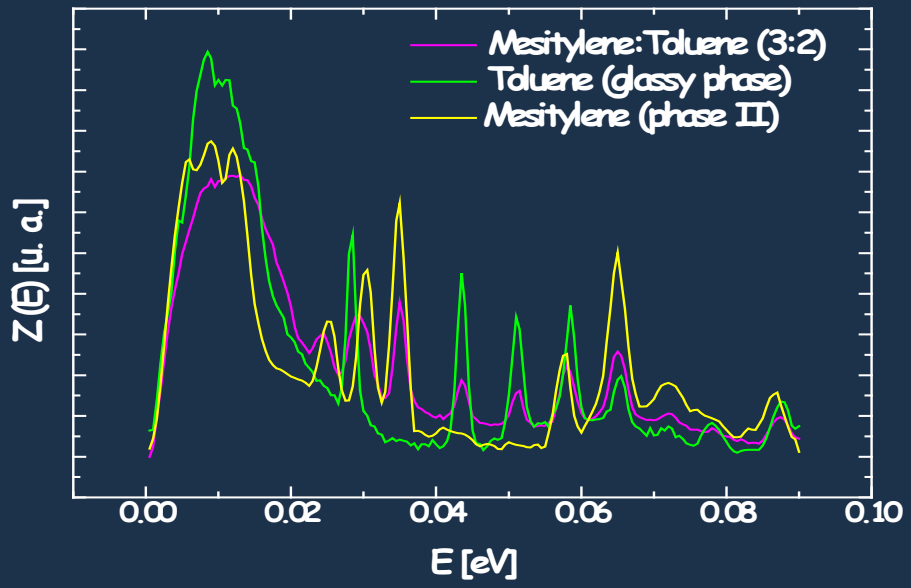
Experimental information [Natkaniec et al., Proceedings of ICANS XVI, 2003]	$h\nu_1$= 0.12 eV (Ring breathing)	$h\nu_2$= 0.17 eV (C-H stretching in CH_3)	$h\nu_3$= 0.37 eV (C-H stretching in the ring)
ω_{cont} = 0.252	ω_1 = 0.1505	ω_2 = 0.341	ω_3 = 0.2565

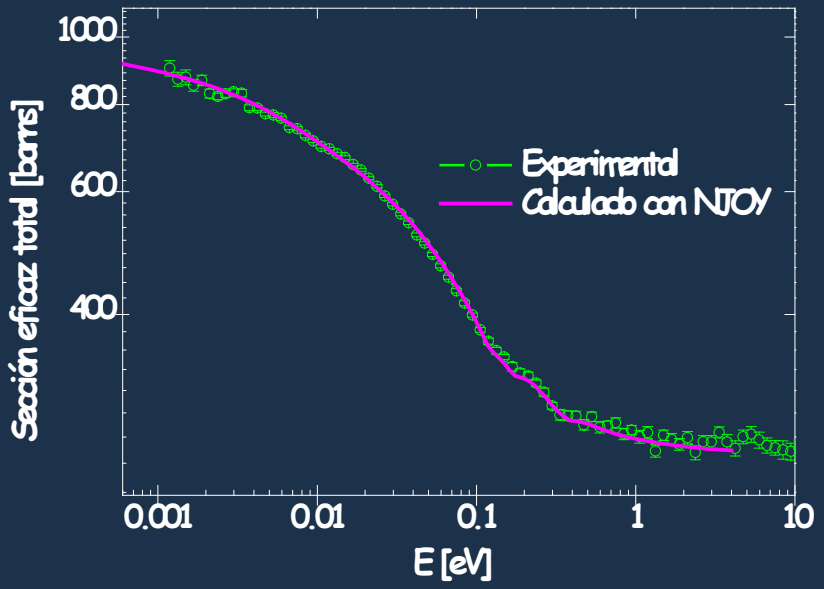




SOLUTION MESITYLENE : TOLUENE 3:2 by volume

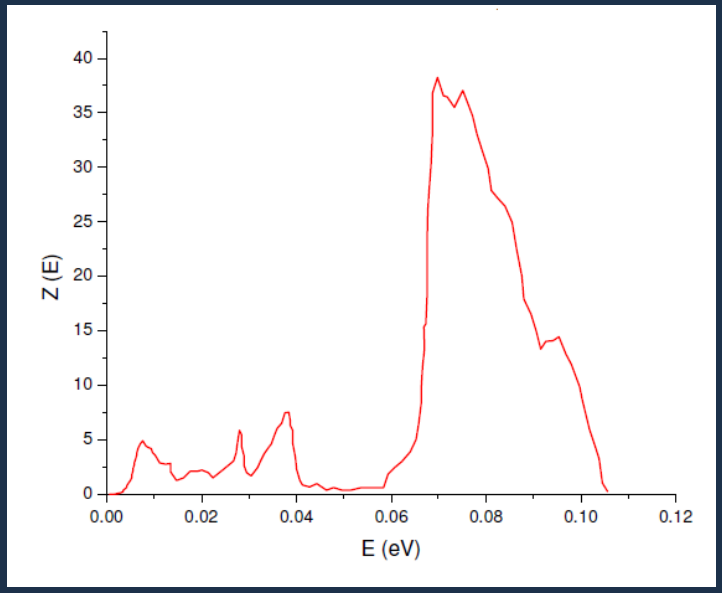
Experimental information [Natkaniec et al., Proceedings of ICANS XVI, 2003]	$h\nu_1$ = 0.12 eV (Ring breathing)	$h\nu_2$ = 0.17 eV (C-H stretching of CH_3)	$h\nu_3$ = 0.37 eV (C-H stretching in the ring)
w_{cont} = 0.167	w_1 = 0.217	w_2 = 0.281	w_3 = 0.335

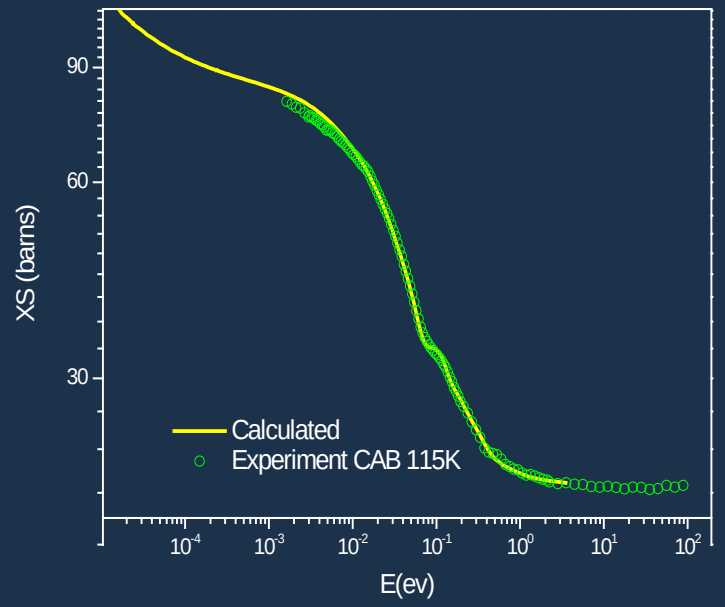




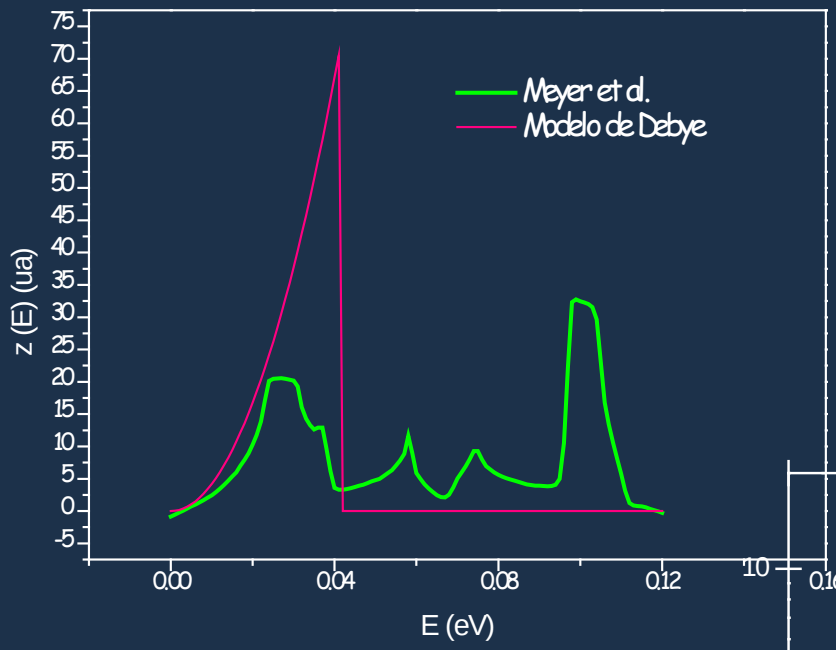
LIGHT WATER ICE

Experimental information [Kolesnikov et al., J.Phys.: Condens. Matter 6 , 375 (1994)]	hn_1 = 0.203 eV	hn_2 = 0.408 eV
w_{cont} = 0.5	w_1 = 1/6	w_2 = 2/6

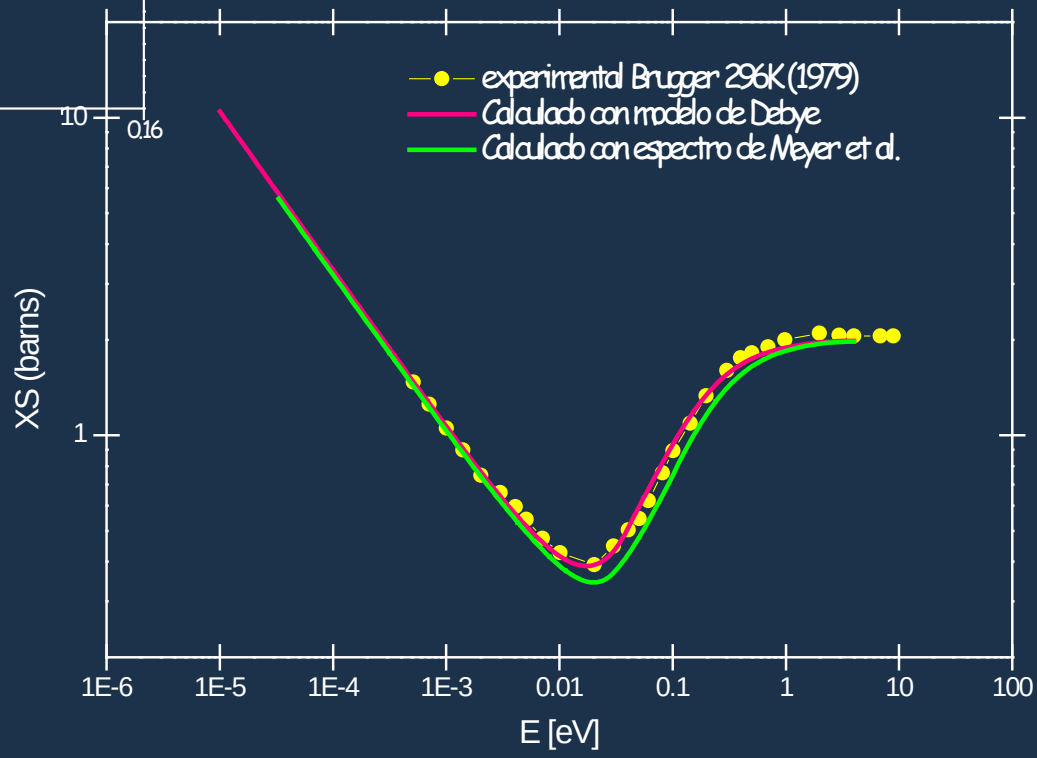




SILICON SINGLE CRYSTAL

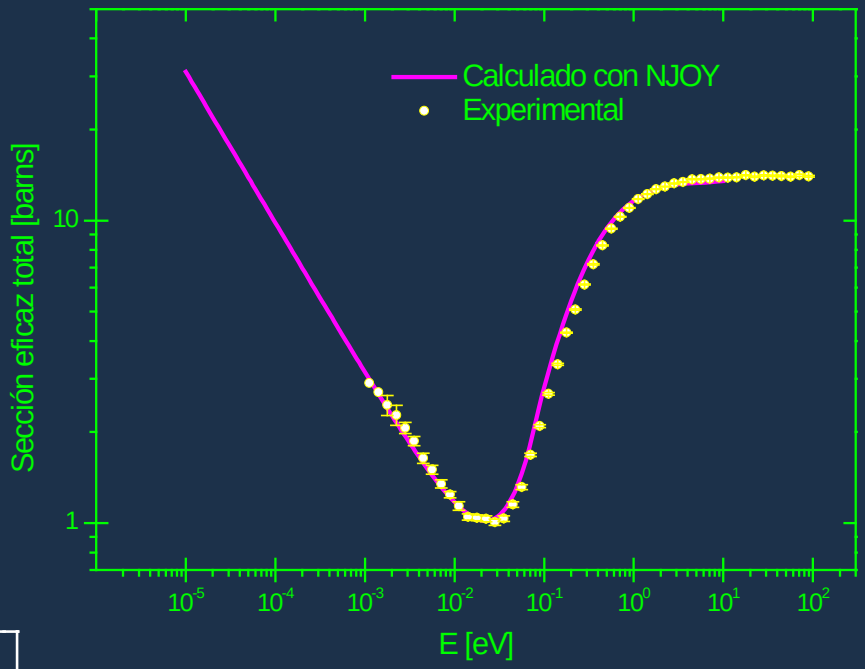


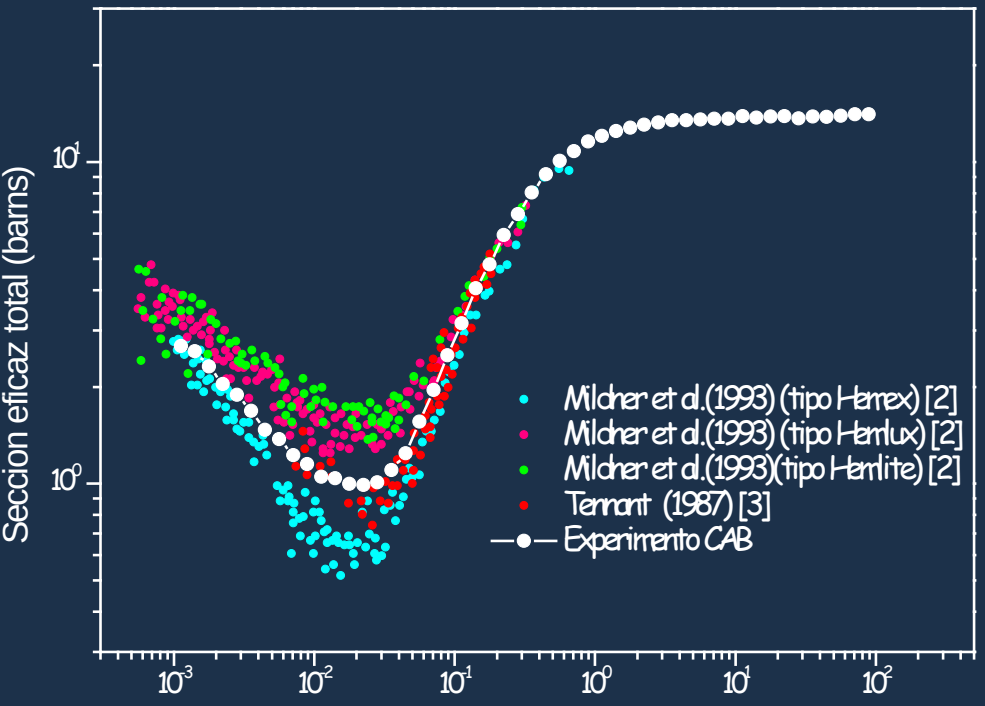
Debye spectrum
with T_D=485 K



SAPPHIRE SINGLE CRYSTAL

Debye spectrum
with T_D=1032 Kc





HEMEX (premium grade)

HEMLUX (superior grade)

HEMLITE (standard optical grade)

FINAL REMARKS

At the Neutron Physics Department (Centro Atómico Bariloche), the thermal scattering data group has the capability of producing S(α,β) in ENDF format and thermal neutron scattering cross sections in ACE format.

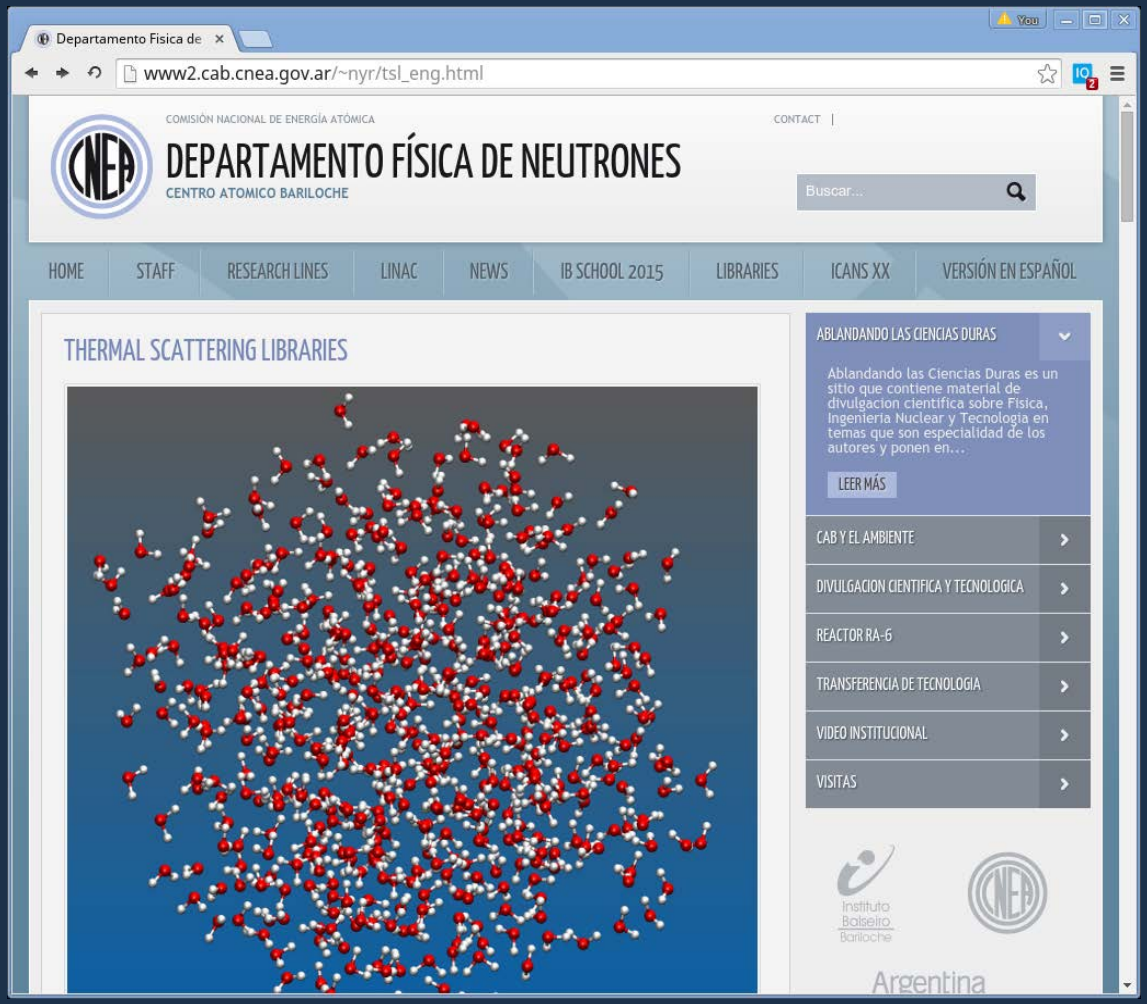
A good representation of the frequency spectrum (FS) of the studied material should be found

If available and trustable ⟶ experimental data for FS

Validation: cross sections are compared with experimental data from EXFOR or from our own measurements at the e-LINAC at Centro Atómico Bariloche

Our cross section libraries are available in ENDF-6 and ACE format in the webpage of the Neutron Physics Department

http://www2.cab.cnea.gov.ar/~nyr/tsl_eng.html



THANKS FOR YOUR ATTENTION

We can also measure total cross sections at the 25 MeV e-LINAC at Centro Atómico Bariloche

- It started operating in 1969 (45 years ago)
- It is a pulsed accelerator which uses a microwave of 2856 MHz to accelerate electrons upto 25 MeV.
- Electron pulses can be extended upto μs, with a repetition frequency upto 150 pps.
- The LINAC reaches its maximum neutron production operating at 100 pps (~ 10^{11} n/s) and 25 mA mean current.
- It is situated at the Neutron Physics Department (Centro Atómico Barilohe). It belongs to National Commission of Atomic Energy.
- It is normally used for researh, development and trainning .

By means of transmission and time-of-flight techniques, total cross section of almost any material can be measured at the Bariloche e-LINAC from room temperature down to 32 K

These measurements are used to validate the cross section libraries that we model