



# CAB Activity Report:

## Thermal Scattering Libraries for non-Traditional Materials

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WPEC SG-42 second meeting

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OECD- Paris

France

## 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  $S(\alpha,\beta)$  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.



## RA-10 Reactor Project

It is a multipurpose 30 MW reactor which includes a cold neutron source.

Our group responded to demands of **thermal scattering libraries** for the design of the reactor and the cold neutron source

We are currently working on a project to strengthen the scientific community and prepare the users for the reactor

Jose Antonio Balseiro School 2015 on Neutron Scattering Techniques.  
We included a workshop on thermal scattering libraries and Monte Carlo simulation

# Paul Scherer Institute

## Joint CAB- PSI Project

### "Neutron Filters cross-section libraries and components for MCNP and McStas simulations"

- McStas School in February 2016 in Bariloche.
- Development of McStas components: filters and monocromators

Seed Money Grant / Latin America 2015 / Application Form



Latin America - Exploratory Mandate

SEED MONEY GRANTS  
APPLICATION FORM

**PART 1: GENERAL INFORMATION**

**1) Basic Data**

<b>Project title</b>	Neutron Filter cross-section libraries and components for MCNP and McStas simulations
<b>Keywords</b>	Neutron filters, MCNP thermal cross-section libraries, McStas filter components, sapphire cross-sections, silicon cross-sections, beryllium cross-sections
<b>Swiss institution</b>	Paul Scherrer Institute (PSI)
<b>Latin American institution</b>	Centro Atómico Bariloche (CNEA)
<b>Partner country</b>	-
<b>Short summary (5 lines)</b>	This project aims to enrich the MCNP code's cross-section library suite with libraries of materials used as neutron filters, and similarly expand the McStas code with neutron filter components.
<b>Total funding requested (in CHF)</b>	22,270CHF

I hereby confirm that all the information given in this application and the attachments is correct to the best of my knowledge

26/05/2015

Emmanouela Rantsiou

Place, date

Swiss Principal Investigator

26/05/2015

Florencia Cantarigi

Place, date

Latin American Principal Investigator



# IAEA-NDS

Participation as a member of INDC

- IAEA supports our participation in WPEC  
2015+2016

INDC meeting in 2014 recommendations

- Inclusion of thermal scattering theory in the ICTP workshops in Trieste  
Lecturer in the ICTP School

"Nuclear Data Measurements for Science and Applications" in 2015

- EXFOR compilation

Participation in the IAEA-NDS Consultancy Meeting "EXFOR  
compilation of thermal neutron scattering data" + implementation



# IAEA-CRP (F12026)

We participate in the IAEA Coordinated Research Project

"Advanced Moderator for Intense Cold Neutron Beams in Materials Research" (2014-2018)

The screenshot shows the IAEA website interface for the Coordinated Research Project F12026. The page is titled "All active CRPs" and lists the following details:

- Title:** Advanced Moderators for Intense Cold Neutron Beams in Materials Research
- CRP Code:** F12026
- AZPS Project:** 1000162
- Status:** Active
- Begin Date:** 2014-02-13
- Expected End Date:** 2018-02-13
- Completed Date:** (blank)
- Participating Countries:** Argentina, Australia, Denmark, France, Hungary, India, Japan, Sweden, United States of America
- Section 1:** IIR - Physics Section
- Division 1:** NARC - Division of Physical and Chemical Sciences
- Summary:** The proposed CRP aims at providing a platform for collaborative research among research reactors of various sizes and accelerator-driven neutron sources from TC eligible and developed countries to increase the cold neutron fluxes available at existing neutron sources. Cold neutrons are ideal tools to study almost all forms of condensed matter through neutron scattering and at the same time they are preferred in neutron imaging or Prompt Gamma Neutron Activation Analysis (PGNAA). As such, they have attracted the interest of many research groups all over the world and the need for intense cold neutron beams is continuously increasing. To date, the major drawbacks in the application of cold neutrons is the very low efficiency in their production via different types of moderators. The need for higher cold neutron fluxes has led to various improvements in moderator shapes and designs. Still, however, a breakthrough in enhancing cold neutron fluxes is still pending and the solution to the problem requires new ideas regarding brand new moderator materials. Making progress in the field will require coordinated research among several institutions, with activities ranging from the development of new simulation tools and associated data libraries to the experimental characterization of the scattering from nano-structured materials and the experimental investigation of candidate designs and materials in test moderators. We anticipate a CRP that includes experts on simulating neutron facilities with modern neutron transport codes from some of the world's premier neutron sources, researchers at research reactors in developing countries who need experience with such codes, and researchers at facilities capable of testing new moderator designs experimentally. It is a key element in the program to identify and characterize the scattering properties of candidate materials, and assessing the influence of processing parameters on those properties. This materials survey task is one that is well suited to smaller research reactor or accelerator facilities in developing countries.

Participation of 16 countries

Argentina -->

Studies on new cold moderators:  
ethane, triphenyl methane

First version of scattering kernels ready

Proposal sent to measure total cross sections (ISIS, 2016)



# Cross section library generation with NJOY

Frequency spectrum (FE)

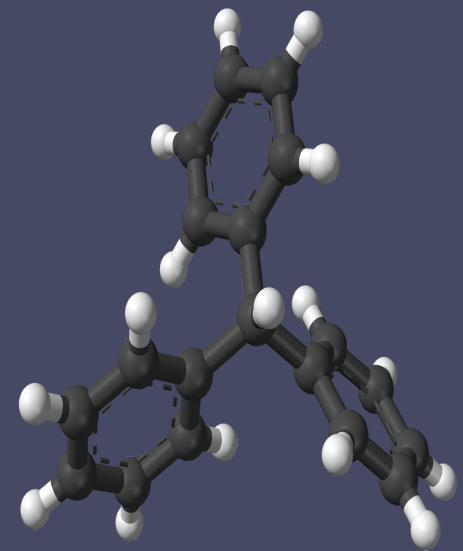
Data from experiments

Data from theory

Combination from both

## Triphenylmethane

FE from neutron spectrometry (Dubna)



# Ethane (C<sub>2</sub>H<sub>6</sub>)

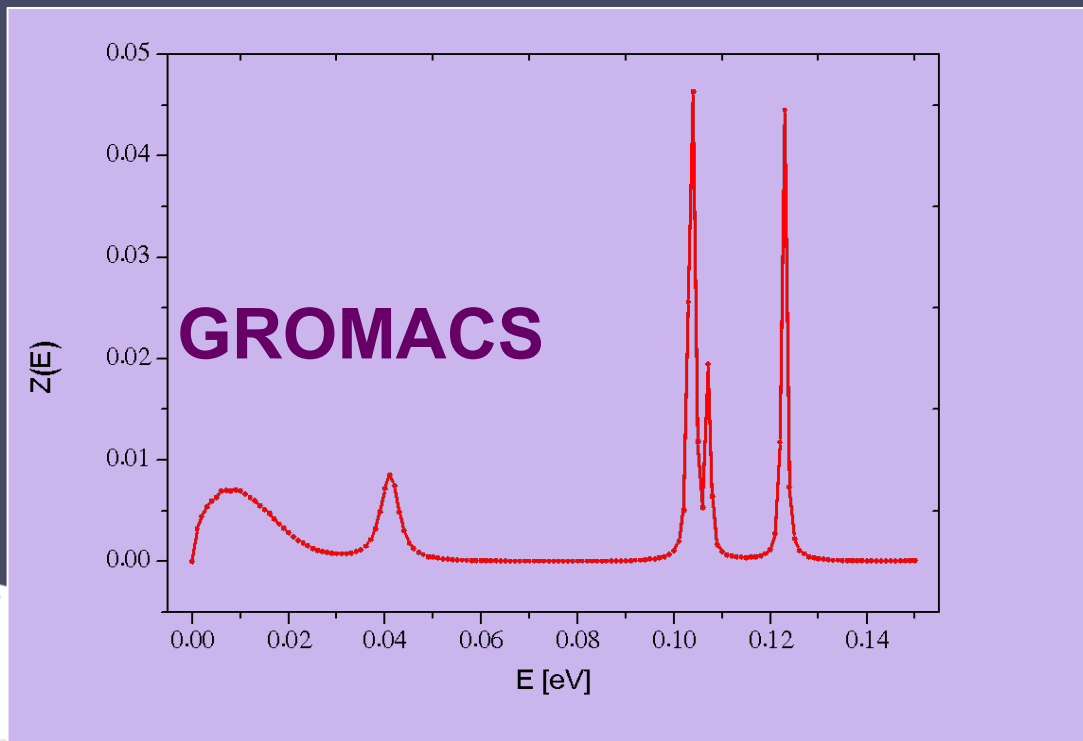
Advantage: liquid from 90 K to 186 K

- Diffusive component calculated Egelstaff-Schofield model

$$m_{\text{diff}} = 3 m_{\text{mol}} = 90 \text{ g/mol and } D = 0.71 \cdot 10^{-5} \text{ cm}^2/\text{s}, \quad w_{\text{traslac}} = 0.0111$$

- Continuous frequency spectrum representing rotations and internal vibrations of the molecule

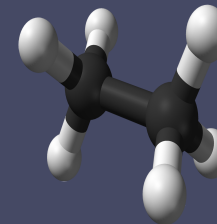
$$w_{\text{cont}} = 0.3859$$



- Two Einstein oscillators

$$h\nu_1 = 0.18 \text{ eV} \quad w_1 = 0.299$$

$$h\nu_2 = 0.37 \text{ eV} \quad w_2 = 0.304$$



(data for ethane @ 100 K)

# Other Applications

- BIOLOGICAL APPLICATIONS

Neutron thermalization for neutron dosimetry in BNCT  
(Ricardo Ramos, Centro Atómico Ezeiza).

- SCIENTIFIC APPLICATIONS

Scattering kernel development for inelastic scattering corrections in  
neutron diffractometry

(Luis Rodríguez Palomino, Centro Atómico Bariloche)

1-Propanol and 1-Butanol in hydrogenated and deuterated variants



# Final Remarks

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

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://www.cab.cnea.gov.ar/nyr/tsl\\_eng.html](http://www.cab.cnea.gov.ar/nyr/tsl_eng.html)

We are also including neutron scattering theory in training courses for graduated and post-graduated students.