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

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Nuclear Data group at Centro Atómico Bariloche

Rolando Granada
Scattering theory and advanced neutron sources

Florence 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

$w_{\text{cont}} = 0.5$

Two Einstein oscillators

$\hbar \nu_1 = 0.205 \text{ eV}$ \hspace{1cm} $w_1 = \frac{1}{6}$

$\hbar \nu_2 = 0.391 \text{ eV}$ \hspace{1cm} $w_2 = \frac{2}{6}$
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

\[
\begin{array}{|c|c|c|}
\hline
\text{hv}_1 &= 0.12 \text{ eV} & \text{(Ring breathing)} \\
\omega_1 &= 0.170 \\
\hline
\text{hv}_2 &= 0.17 \text{ eV} & \text{(C-H stretching in CH}_3\text{ )} \\
\omega_2 &= 0.310 \\
\hline
\text{hv}_3 &= 0.37 \text{ eV} & \text{(C-H stretching in the ring)} \\
\omega_3 &= 0.332 \\
\hline
\end{array}
\]

\[\omega_{\text{const}} = 0.188\]
• 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.

![Graph of Z(E) vs E for crystal and glassy phases.](image1)

<table>
<thead>
<tr>
<th>$h\nu_1$</th>
<th>0.12 eV (Ring breathing)</th>
<th>$h\nu_2$</th>
<th>0.17 eV (C-H stretching in CH$_3$)</th>
<th>$h\nu_3$</th>
<th>0.37 eV (C-H stretching in the ring)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\omega_1$</td>
<td>0.30</td>
<td>$\omega_2$</td>
<td>0.23</td>
<td>$\omega_3$</td>
<td>0.34</td>
</tr>
</tbody>
</table>

$\omega_{cont} = 0.13$

![Graph of Total Cross Section vs E.](image2)
Liquid hydrogen and deuterium

• 2000: for OPAL cold neutron source

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


• 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
Normal Hydrogen

Para-Hydrogen

Ortho-deuterium

Freq.Spec. Collective Excitations
Liquid H₂ & D₂

H₂ - 2016
D₂ - 2016

Scattering Cross Section [b]

Scattering Cross Section per D₂ molecule [b]
Sapphire

- 2008: for the neutronography 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-36 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-36 reactor, Argentina (M. Sztejnberg, 2010)
- Paul Scherer Institute, Switzerland (E. Rantsiou, 2013)
- LAHN (Argentinean Neutron Beams Laboratory Project) (A. Tartaglione, 2017)

**Silicon single crystal at room temperature**

- NJOY calculation with Debye spectrum
- Brugger et al. (1979) [5]

**Sapphire single crystal at room temperature**

- NJOY calculation with Debye spectrum
- CAB experiment

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**Technical note**

*Thermal neutron scattering kernels for sapphire and silicon single crystals*

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

[https://doi.org/10.1016/j.anucene.2015.01.020](https://doi.org/10.1016/j.anucene.2015.01.020)
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