Nuclear Data Testing and Evaluation at CNL and CAB

D. Roubtsov

Canadian Nuclear Laboratories, Chalk River, Canada

www.cnl.ca

J. I. Márquez Damián

Neutron Physics Department, Centro Atomico Bariloche, Argentina

CSEWG 2015, BNL, USA

$S(\alpha,\beta)$ for light & heavy water

WPEC Subgroup 42 (SG42)

Thermal Scattering Kernel S(α,β): Measurement, Evaluation and Application

https://www.oecd-nea.org/science/wpec/sg42/

Meeting: May 2015 (NEA, Paris)

16 presentations available:

https://www.oecd-nea.org/science/wpec/sg42/Meetings/2015_May/index.html

Main news (CSEWG 2015):

new $S(\alpha,\beta)$ evaluations for light and heavy water (liquid H_2O / D_2O) are available for testing and comments via BNL *gforge*,

USNDP/CSEWG GForge Collaboration Server

Home > Projects > ENDF/B-VII > SVN > trunk > endf7 > thermal_scatt

NEW $S(\alpha,\beta)$ for light & heavy water

Main news:

new $S(\alpha,\beta)$ evaluations (MF7) for light and heavy water are available for testing and comments via BNL *gforge*,

USNDP/CSEWG GForge Collaboration Server

Home > Projects > ENDF/B-VII > SVN > trunk > endf7 > thermal_scatt

https://ndclx4.bnl.gov/gf/project/endf/scmsvn/?action=browse&path=%2Ftrunk%2Fendf7%2Fthermal_scatt%2F

tsl-HinH2O.endf

and

tsl-DinD2O.endf ,

tsl-OinD2O.endf

Index of /trunk/endf7/thermal_scatt

Files shown: 26

Directory revision: 669 (of 687)

Sticky Revision: [ ] Set

File	Rev.	Age	Author	Last log entry
Parent Directory				
tsl-013_Al_027.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-026_Fe_056.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-Be-metal.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-BeinBeO.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-CinSiC.endf	625	15 months	dbrown	set EMAX in both evaluations to 5 eV
tsl-DinD2O.endf	669	7 weeks	marquezj	Submitting the TSL for deuterium and oxygen bound in heavy water calculated with...
tsl-HinC5O2H8.endf	658	4 months	dbrown	On behalf of Ayman Hawari: This updated file was generated by running LEAPR usi...
tsl-HinCH2.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-HinH2O.endf	668	7 weeks	marquezj	Submitting the TSL for hydrogen bound in light water calculated with the CAB Mod...
tsl-HinZrH.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-OinBeO.endf	626	15 months	dbrown	set EMAX in the header of all evaluations to the ENDF declared maximum of 5 eV (...
tsl-OinD2O.endf	669	7 weeks	marquezj	Submitting the TSL for deuterium and oxygen bound in heavy water calculated with...

NEW $S(\alpha,\beta)$ for light & heavy water

/trunk/endf7/thermal_scatt/tsl-HinH2O.endf

tsl-HinH2O.endf

Submitting the TSL for hydrogen bound in light water
calculated with the CAB Model

https://ndclx4.bnl.gov/gf/project/endf/scmsvn/?action=browse&path=%2Ftrunk%2Fendf7%2Fthermal_scatt%2Ftsl-HinH2O.endf&view=log

/trunk/endf7/thermal_scatt/tsl-DinD2O.endf

tsl-DinD2O.endf

Submitting the TSL for deuterium and oxygen bound in heavy water
calculated with the CAB Model

https://ndclx4.bnl.gov/gf/project/endf/scmsvn/?action=browse&path=%2Ftrunk%2Fendf7%2Fthermal_scatt%2Ftsl-DinD2O.endf&view=log

/trunk/endf7/thermal_scatt/tsl-OinD2O.endf

tsl-OinD2O.endf

Submitting the TSL for deuterium and oxygen bound in heavy water
calculated with the CAB Model

https://ndclx4.bnl.gov/gf/project/endf/scmsvn/?action=browse&path=%2Ftrunk%2Fendf7%2Fthermal_scatt%2Ftsl-OinD2O.endf&view=log

NEW $S(\alpha,\beta)$ for light & heavy water

Temperature grid (v. of September 2015), in K :

Temperatures = 283.6, **293.6**, 323.6, 350.0, 373.6, 400.0,
423.6, 450.0, 473.6, 500.0,
523.6, 550.0, 573.6, 600.0 K .

Normalization (parameter **B(1)** = $M_0 \times \sigma_{f0}$; $\sigma_{f0} = \boldsymbol{\sigma_{s,th}}$ at T = 0 K, (MF3, MT2))

H-1: 40.87268 b (M_0 = 2)

H-2: 6.7920 b (M_0 = 2) and O-16: 3.750 b (M_0 = 1)

(change to 3.851810 b for ENDF/B-VII.1)

The files were generated using NJOY 99.396 (with our patches for *leapr*).

The files can be processed with NJOY 99.396 .

However, we do processing with our patches for *thermr* and *acer* ;
NJOY updates are available upon request.

NEW $S(\alpha,\beta)$ for light & heavy water
new & improved models → new evaluation

New **evaluation** (in **ENDF-6** format) is based on combining **molecular dynamics** (**MD**) simulations and reliable *experimental data*.

The resulting new **models** are implemented in / are compatible with /

LEAPR module of **NJOY** (nuclear data post-processing code, **NJOY99** → **NJOY 2012**)

The **key points** for building new $S(\alpha,\beta)$ **models** are:

1. use of molecular **(self)diffusion** for translational motion of liquid H_2O / D_2O (instead of free gas approximation (FG) used in **all** evaluated ND libraries);
2. continuous **vibrational spectra** computed from molecular dynamics (**MD**) simulation at a given thermodynamic state of the liquid, (p, T) and density $\rho = \rho(p, T)$, (instead of derived / adjusted spectra from neutron scattering experiments);
3. a more precise description of **the structure of liquid**: *e.g.*, models for D **and** O in D_2O based on **experimental results** (instead of using the incoherent approximation in ENDF/B-VI or the Lennard-Jones **model** for D-D structure in JEFF 3.1 and ENDF/B-VII.0 → ENDF/B-VII.1)
4. better **numerics** (*e.g.*, extended grid(s), α_i, β_j, T_n, and NJOY data processing options revisited, and we use **NJOY with** patches in **leapr** , **thermr** , and **acer** ;)
5. **ACE files** to be generated for **testing / benchmarking** with MCNP**5**, MCNP**6**, and SERPENT

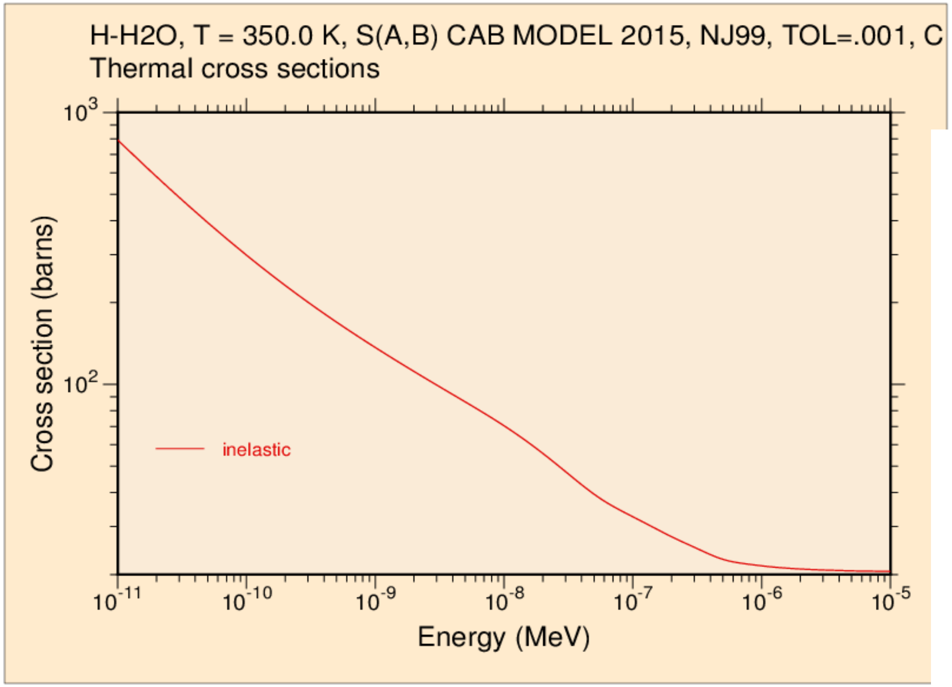
The resulting scattering kernels & cross sections will be an improvement over existing evaluations: **they are compared with measurements** of double differential scattering cross sections, quasi-elastic neutron scattering measurements, angular distributions of out-scattered neutrons, average cosine of the scattering angle (mu-bar), and total cross sections;

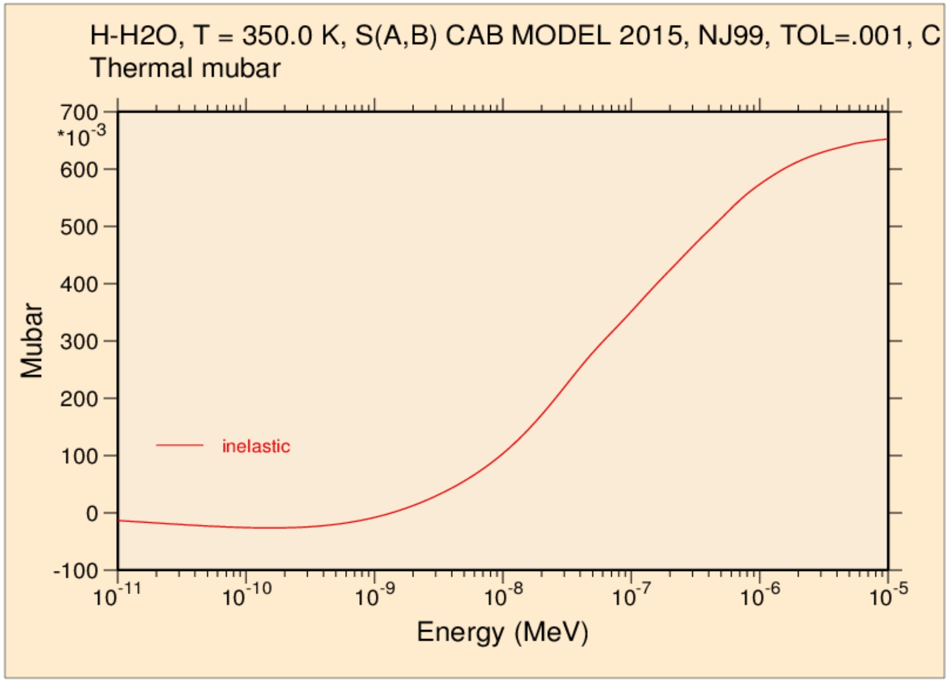
Need more measurements at different (p, T) : not too many experimental data beyond room T.

NEW $S(\alpha,\beta)$ for light water (H_2O)
H-in-H_2O, from MF7 $\rightarrow$ thermal ace files

Processed with NJOY99: check $E \rightarrow 0$ and 'cross-over' ($E \sim$ 5-10eV) asymptotics

$\sigma_s(E)$ and 'Mubar', or $\langle \mu \rangle(E)$

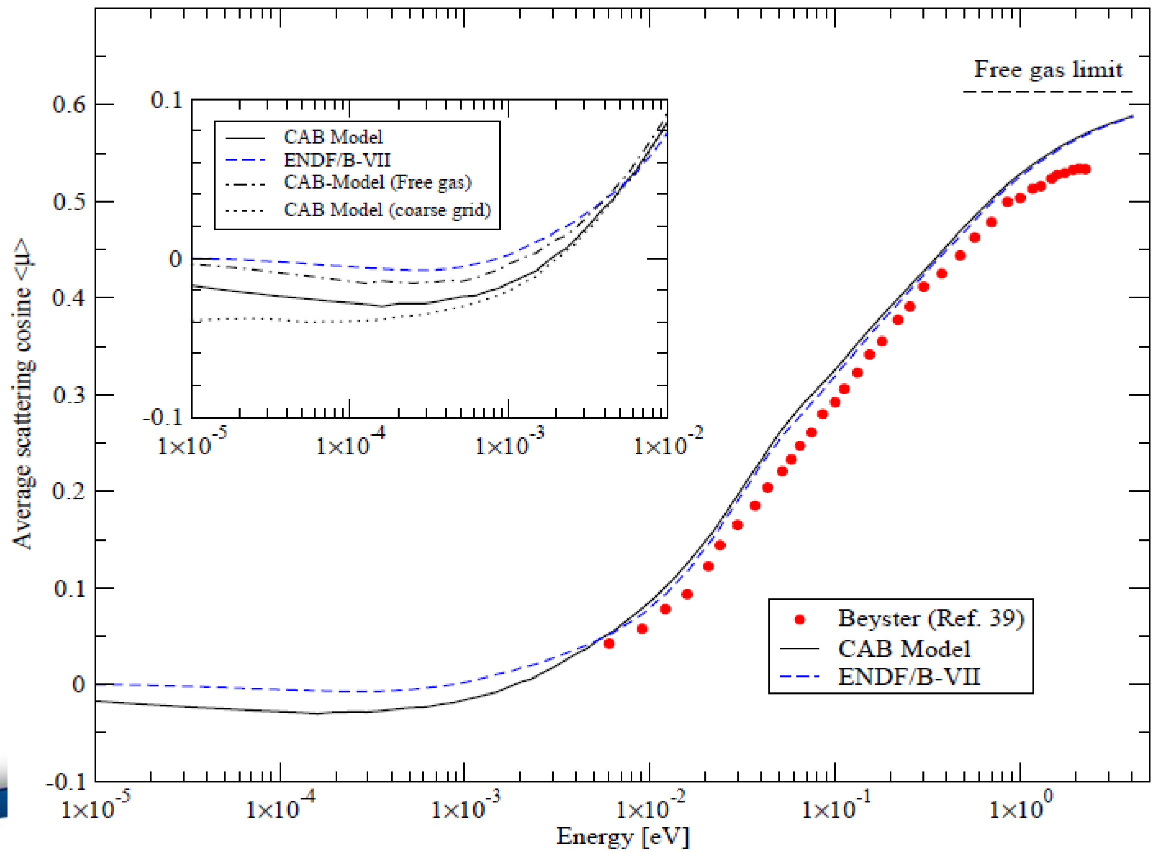




NEW $S(\alpha,\beta)$ for light water (H_2O) H-in-H_2O, from MF7 → thermal ace files

Processed with NJOY99: check $E \to 0$ and 'cross-over' ($E \sim$ 5-10eV) asymptotics

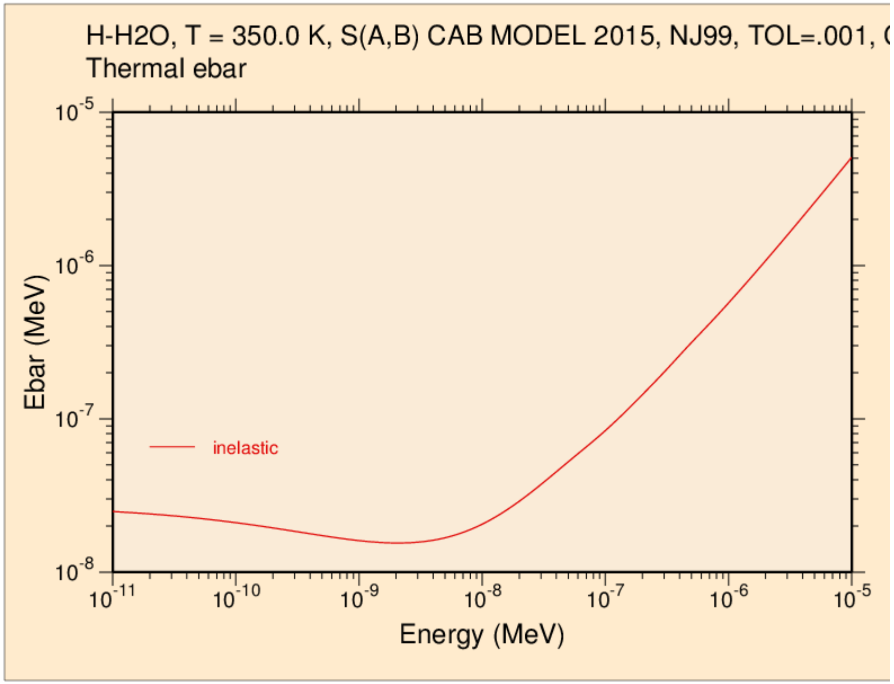
'Mubar', or $\langle \mu \rangle(E)$

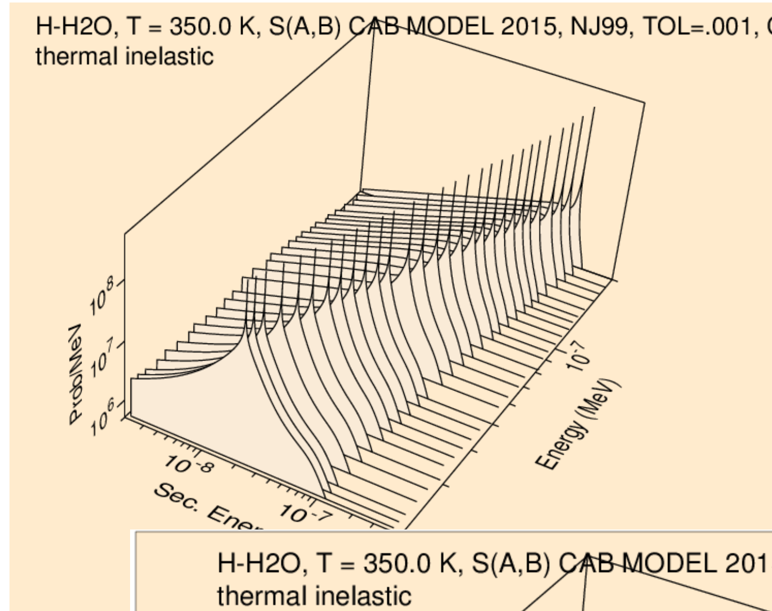


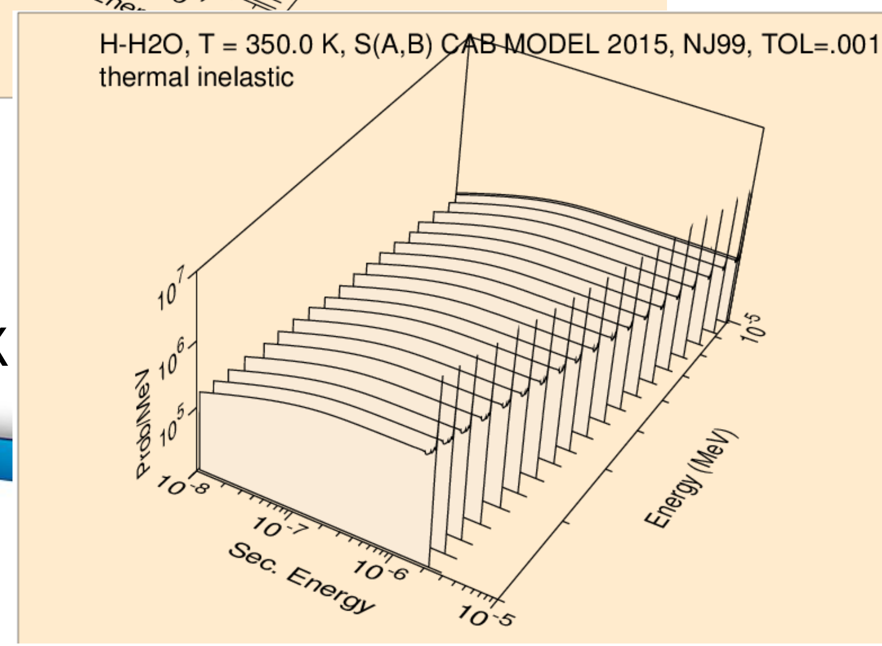
NEW $S(\alpha,\beta)$ for light water (H_2O)

H-in-H_2O, from MF7 → thermal ace files

Processed with NJOY99: check $E \rightarrow 0$ and ‘cross-over’ ($E \sim$ 5-10eV) asymptotics







‘Ebar’, or $\langle E' \rangle(E)$

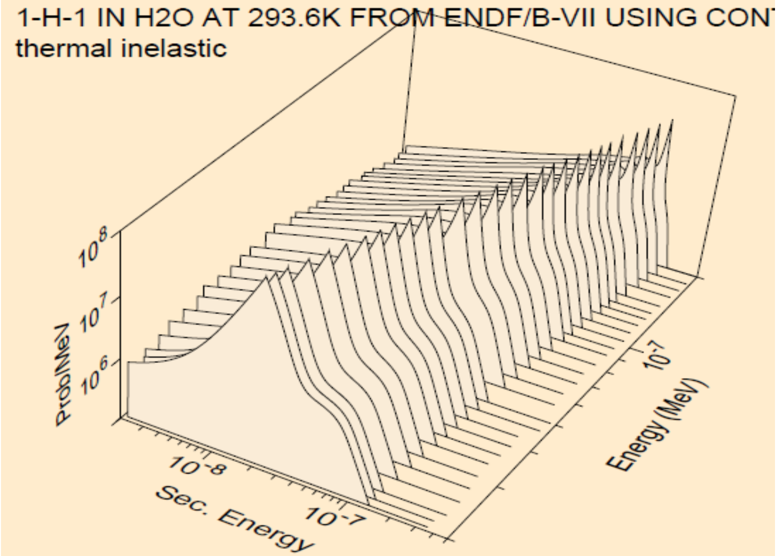
and Prob/MeV , $P_s(E \rightarrow E')$, at T = 350 K

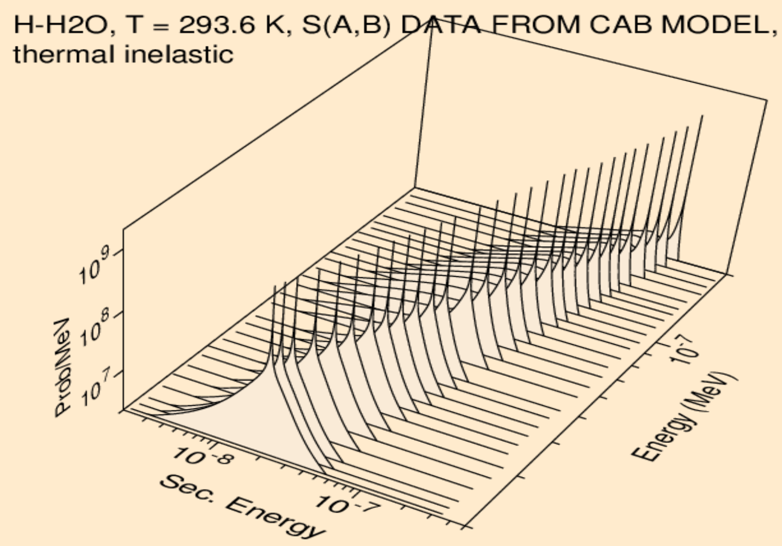
NEW $S(\alpha,\beta)$ for light water (H_2O)

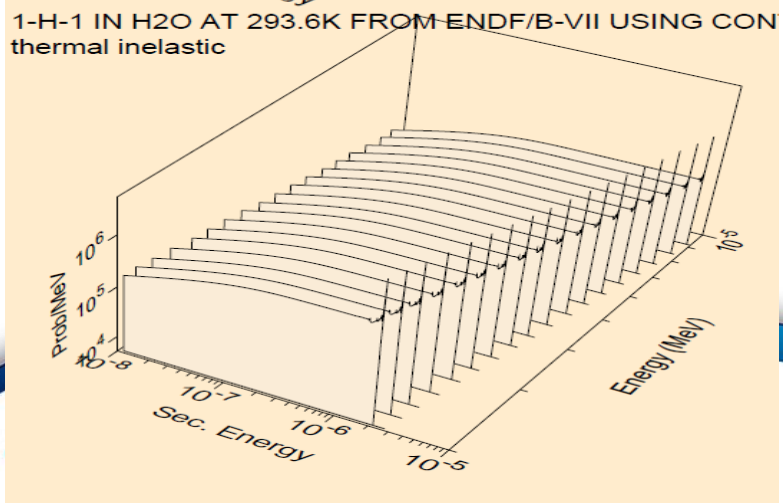
H-in-H_2O, from MF7 → thermal ace files, compare with ENDF/B-VII.0,.1

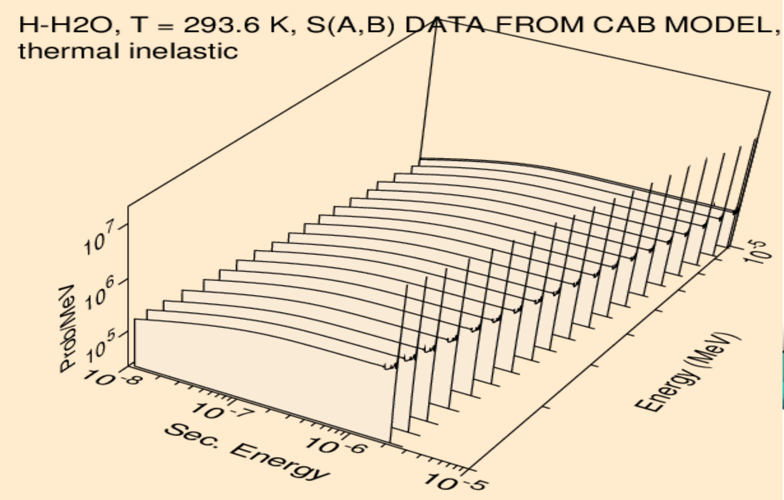
Processed with NJOY99: check $E \rightarrow 0$ and 'cross-over' ($E \sim$ 5-10eV) asymptotics

https://t2.lanl.gov/nis/data/endf/endfvii-thermal.html see view PDF plots





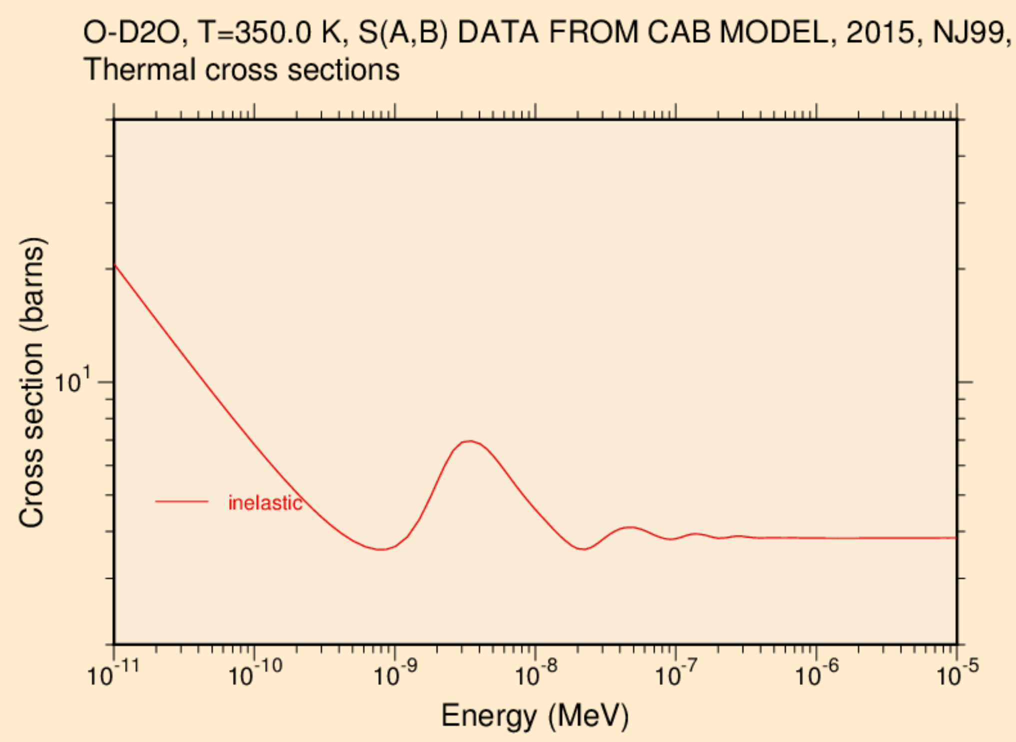


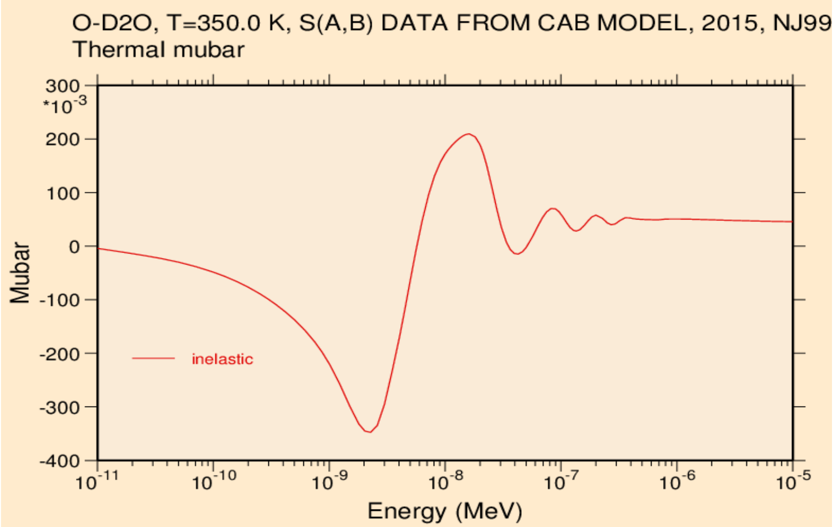


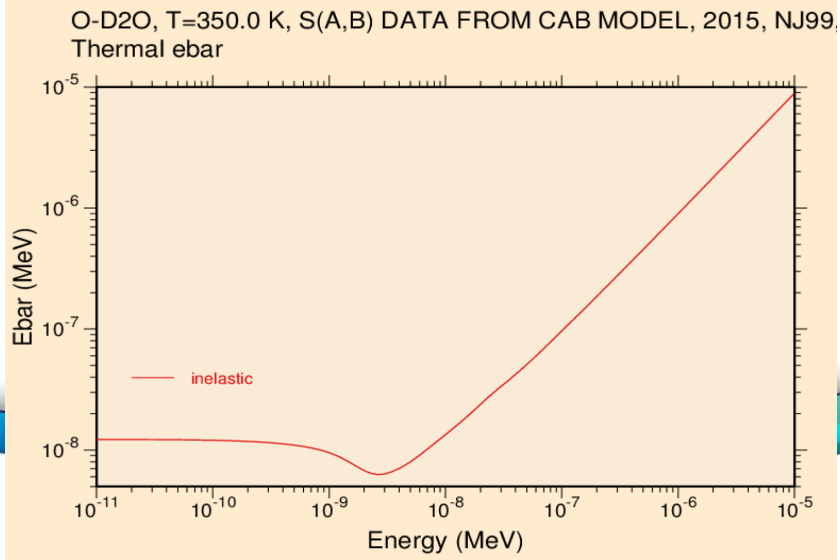
NEW $S(\alpha,\beta)$ for heavy water

O-16-in-D_2O, from MF7 $\rightarrow$ thermal ace files

Processed with NJOY99: check $E \rightarrow 0$ and 'cross-over' ($E \sim$ 5-10eV) asymptotics





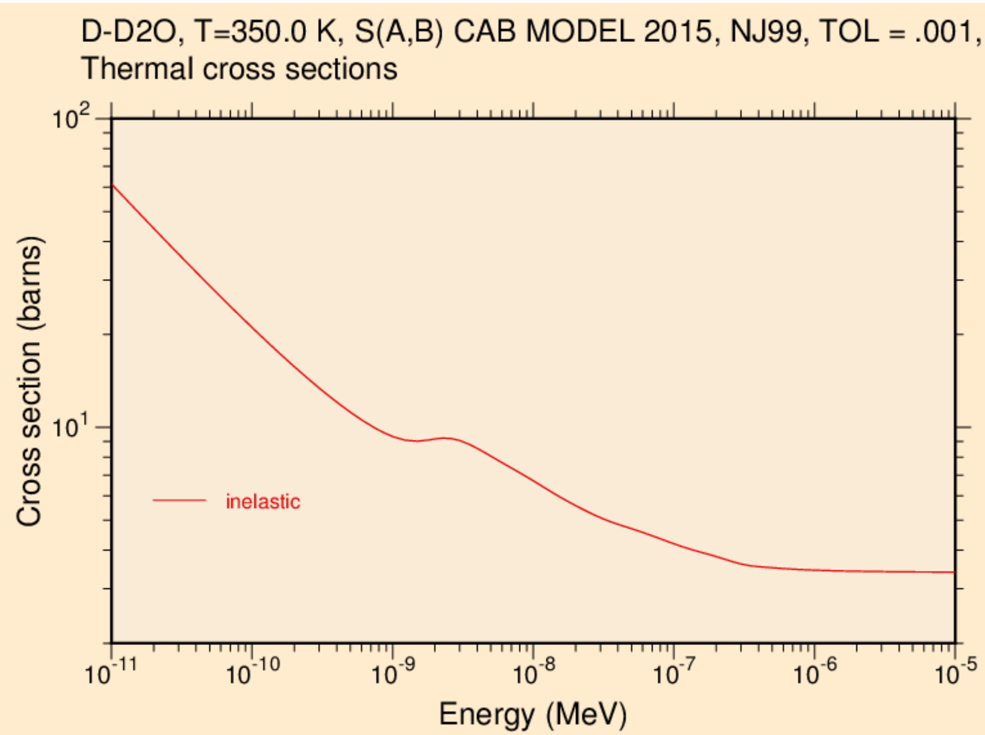


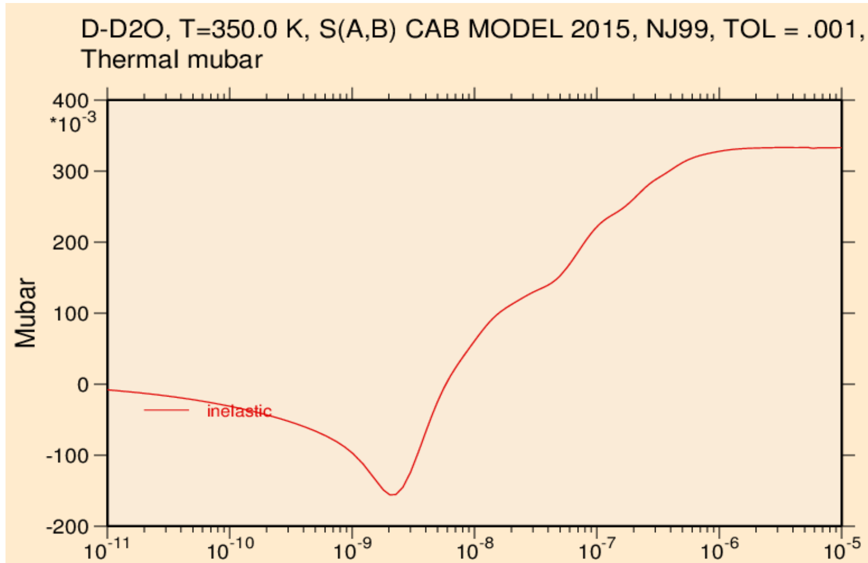
$\sigma_s(E)$, $\langle \mu \rangle(E)$, and $\langle E' \rangle(E)$ at T = 350 K

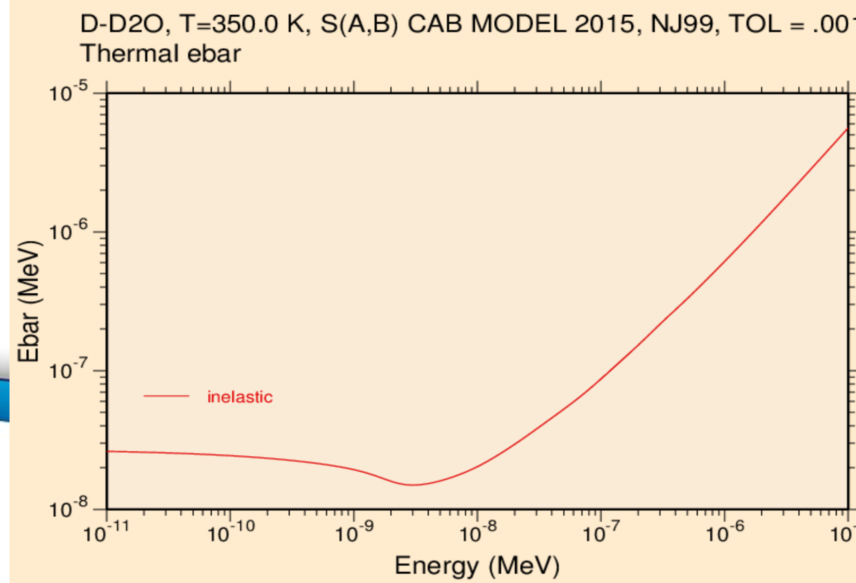
NEW *S*(*α*,*β*) for heavy water

H-2-in-D_2O, from MF7 → thermal ace files

Processed with NJOY99: check $E \to 0$ and ‘cross-over’ ($E \sim$ 5-10eV) asymptotics





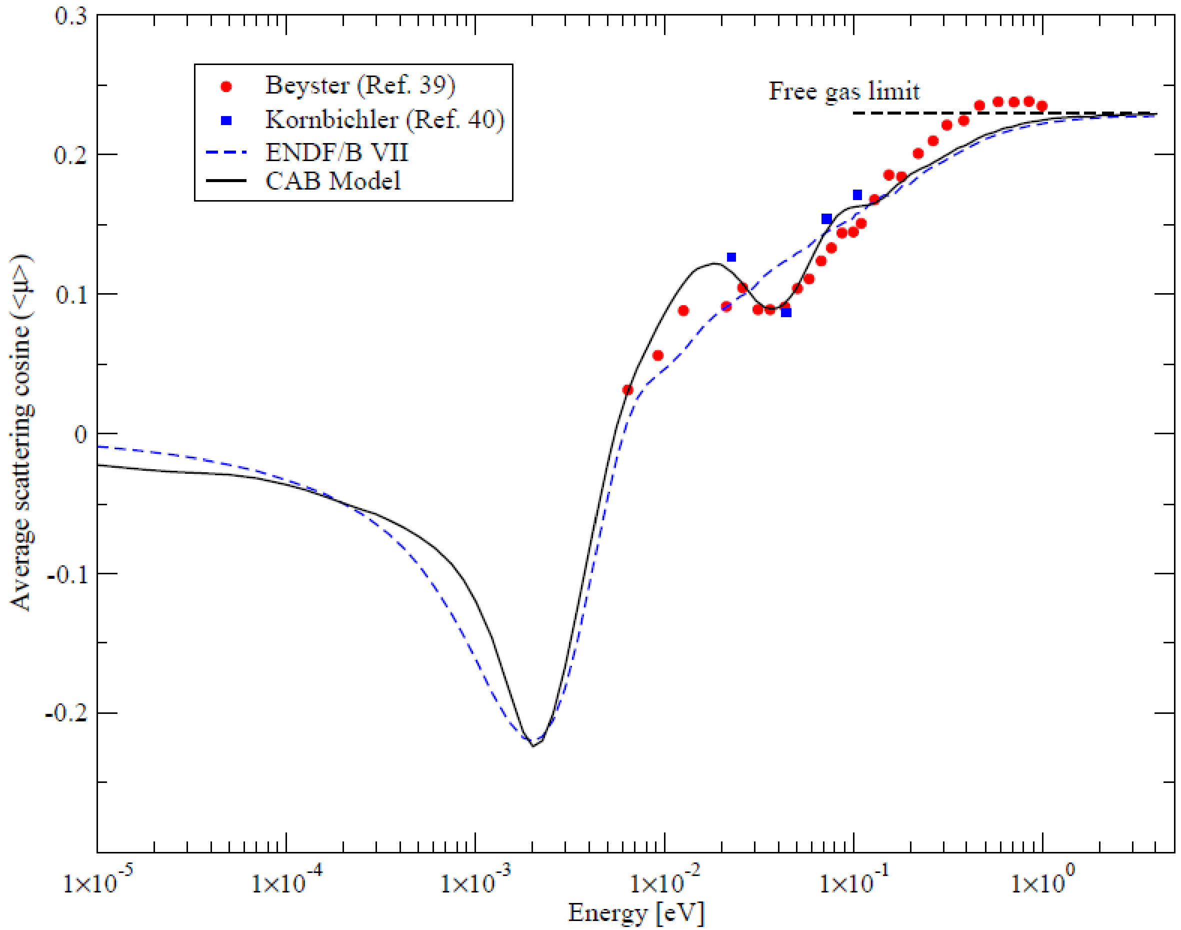


$\sigma_s(E)$, $\langle \mu \rangle(E)$, and $\langle E' \rangle(E)$ at T = 350 K

NEW $S(\alpha,\beta)$ for heavy water

we need H-2-in-D_2O and O-16-in-D_2O to calculate mu-bar per molecule

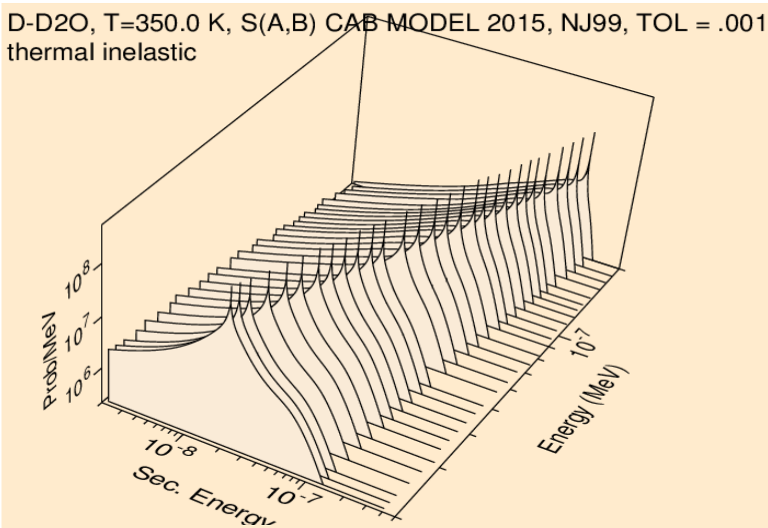
$\langle \mu \rangle (E)$

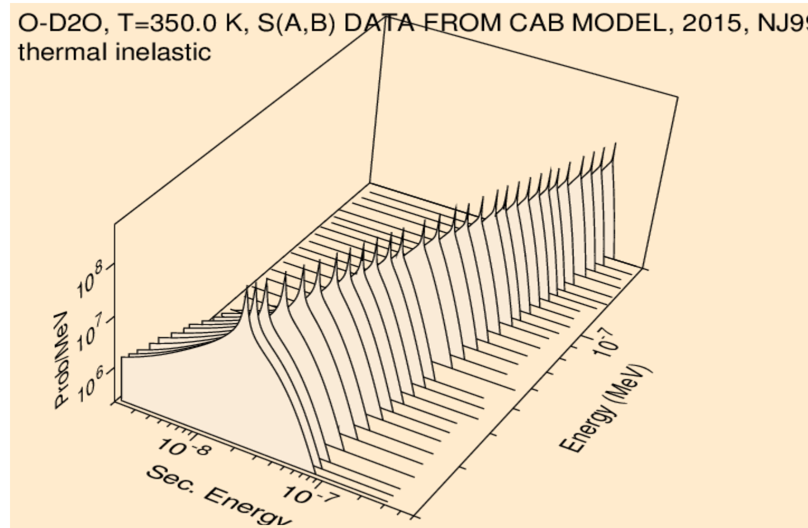


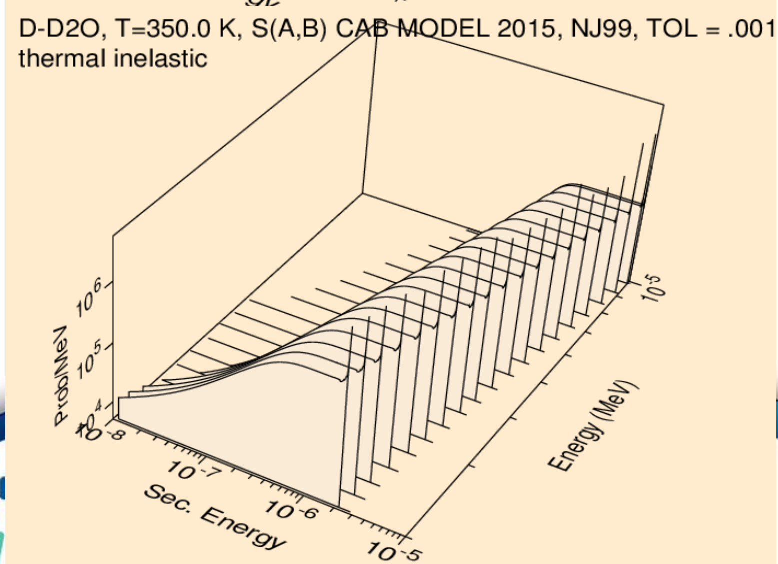
NEW *S*(*α*,*β*) for heavy water

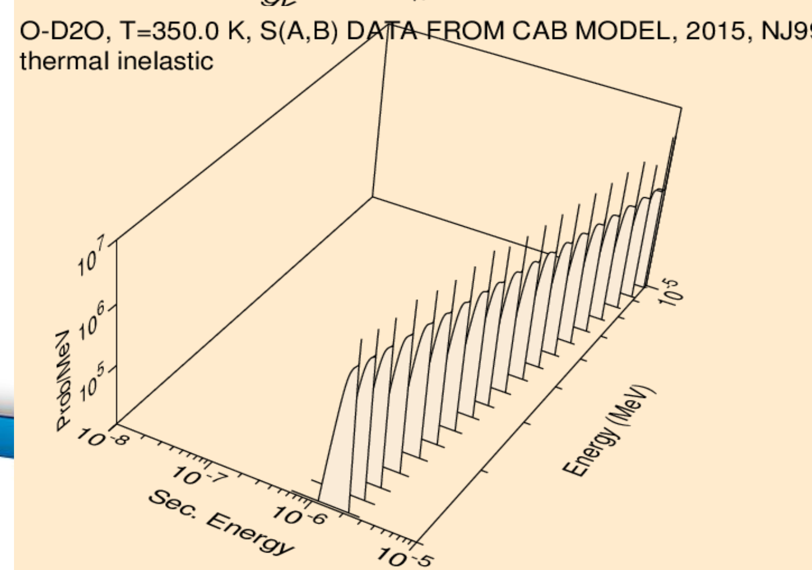
we have H-2-in-D_2O and O-16-in-D_2O to describe n scatt. from D_2O

Processed with NJOY99: $P_s(E \rightarrow E')$, T = 350 K; thermal E and $E \sim$ 5-10 eV





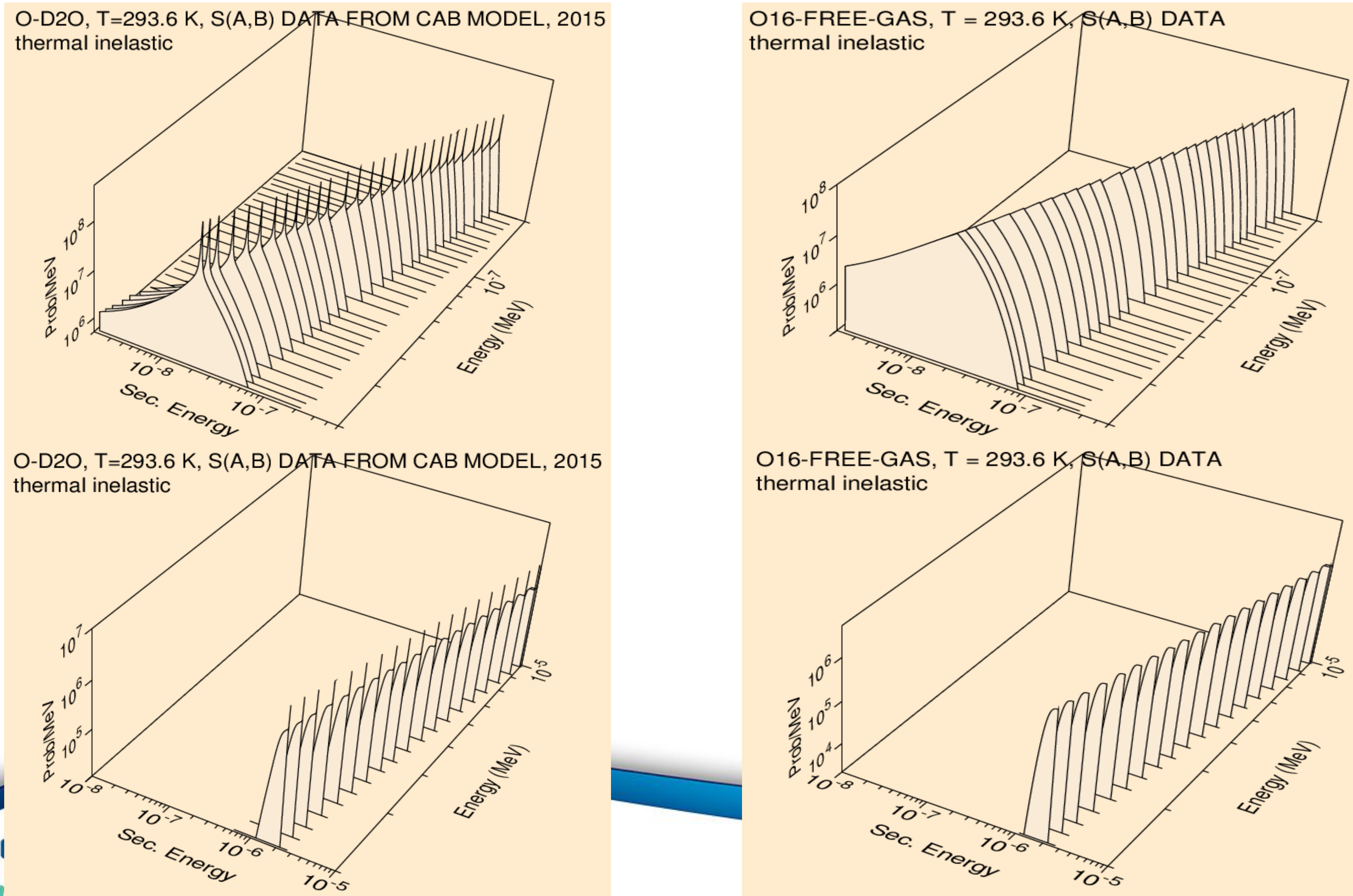




NEW $S(\alpha,\beta)$ for heavy water

O-16-in-D_2O *vs.* O-16 free gas model (at room T)

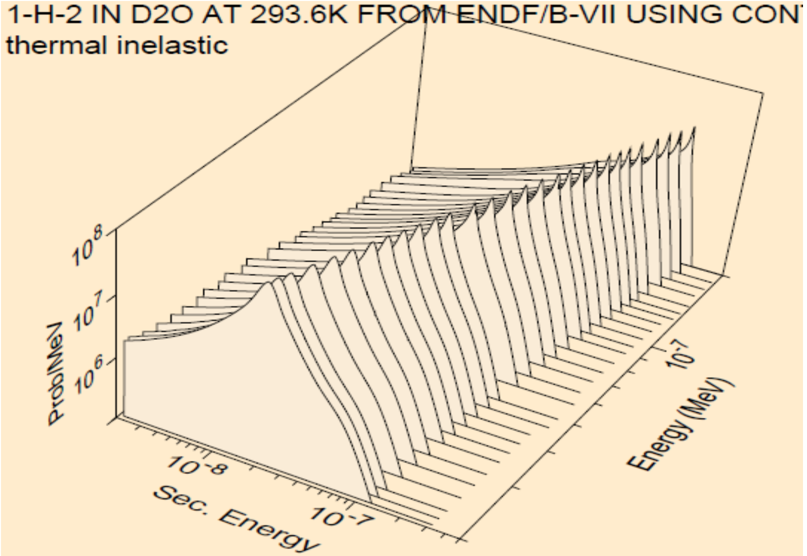
Processed with NJOY99: $P_s(E \rightarrow E')$, T = 293.6 K; thermal E and $E \sim$ 5-10 eV

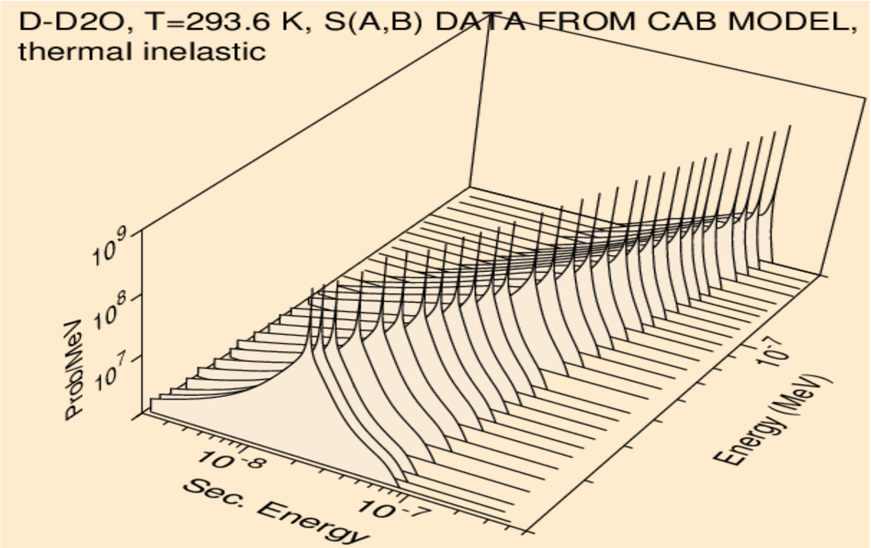


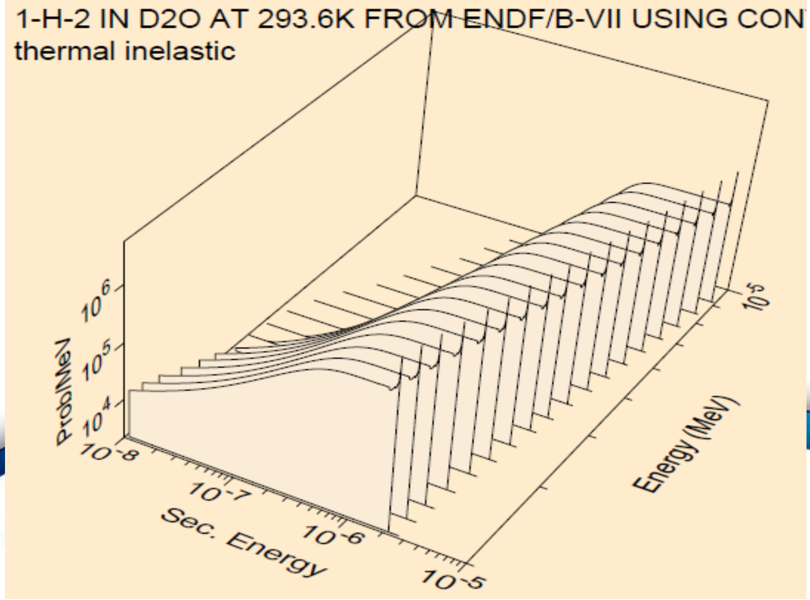
NEW $S(\alpha,\beta)$ for heavy water

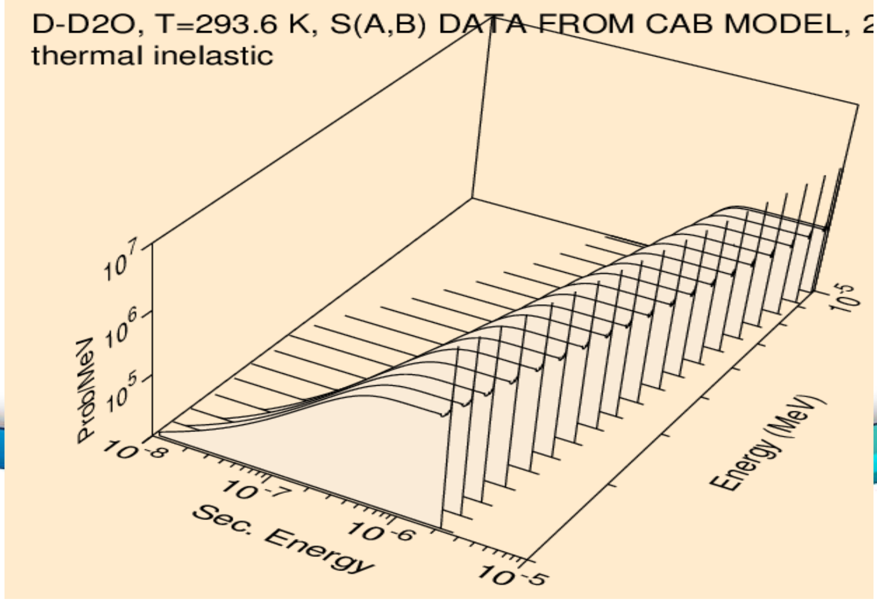
H-2-in-D_2O: compare with ENDF/B-VII.0 (.1), at room T

Processed with NJOY99 : $P_s(E \rightarrow E')$, T = 293.6 K; thermal E and $E \sim$ 5-10 eV







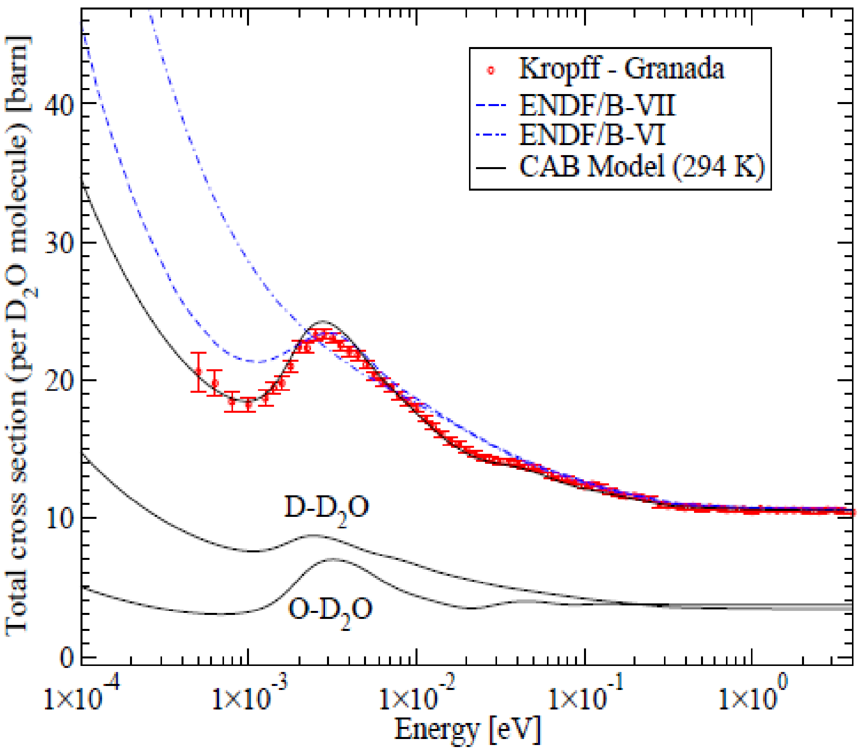


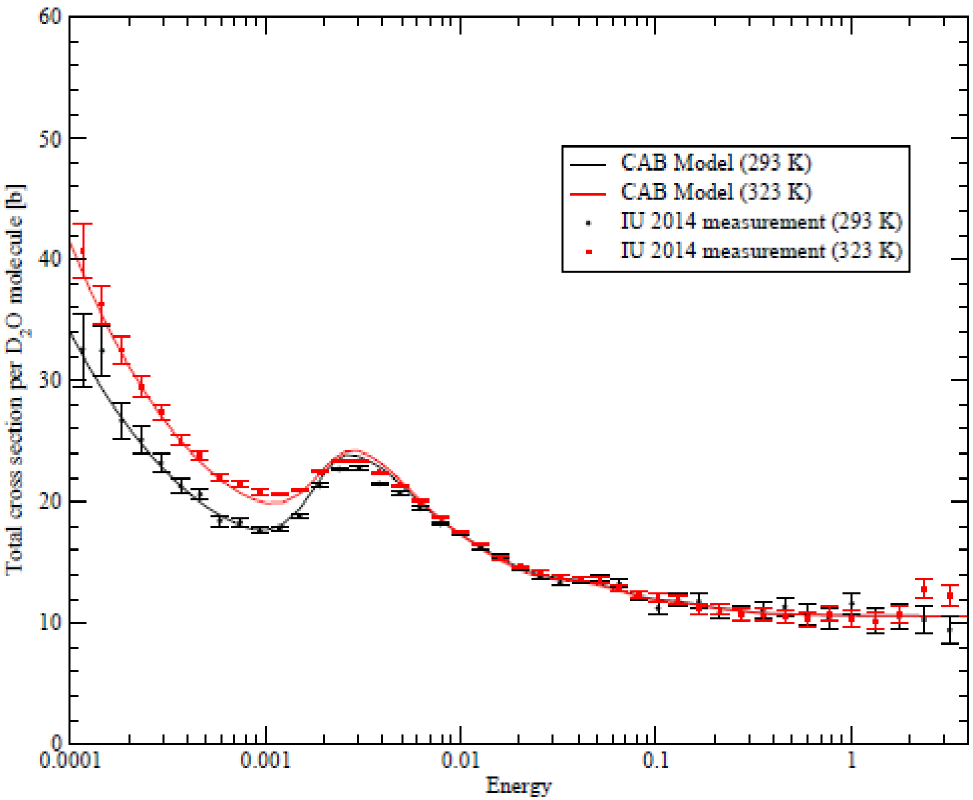
Validation *of* $S(\alpha,\beta)$ for heavy water

we have H-2-in-D_2O and O-16-in-D_2O → σ_{tot} (per molecule) *vs. E*

New experiments in IU with Prof. D. Baxter, (2014), at T = 50 C (~ 323 K)

Room T

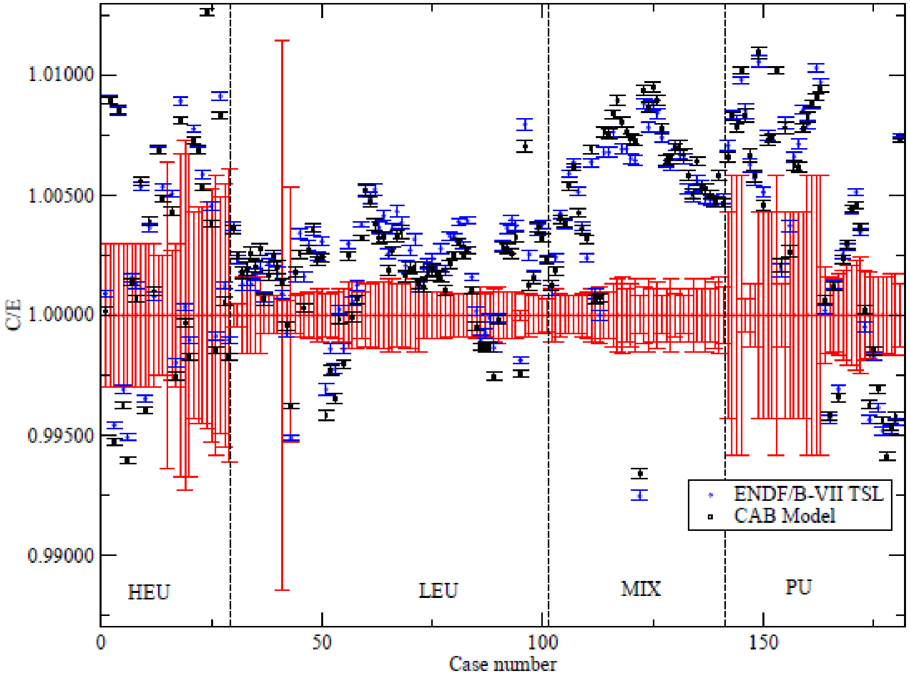




Benchmarking $S(\alpha,\beta)$ for light / heavy water

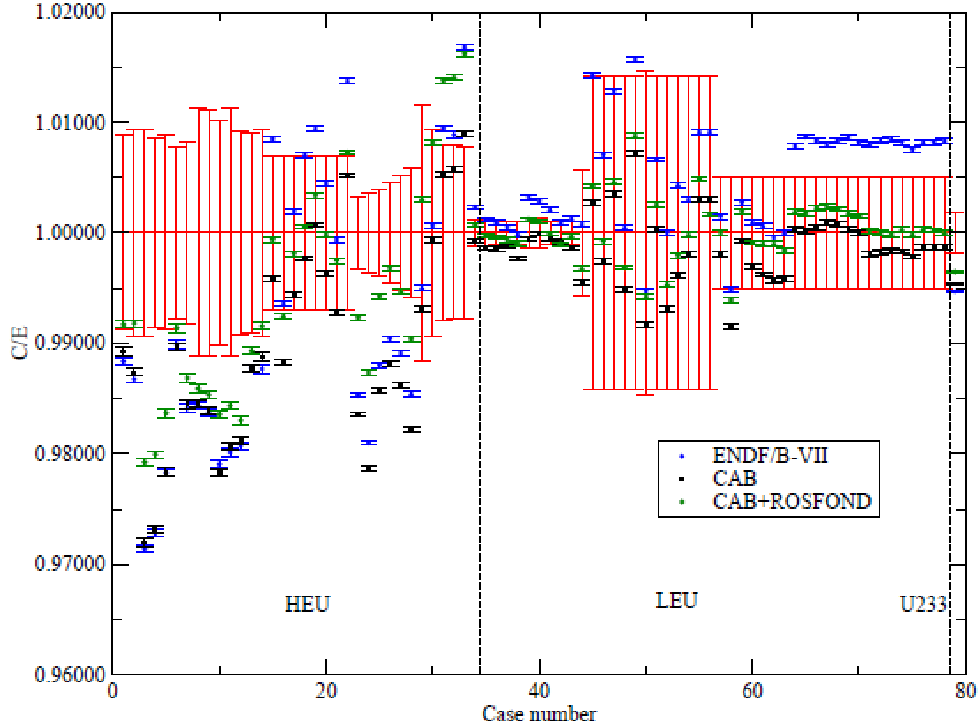
International Handbook of Evaluated Criticality Safety Benchmark Experiments

https://www.oecd-nea.org/science/wpncs/icsbep/



↑ with **new** TSL for H_2O : ?

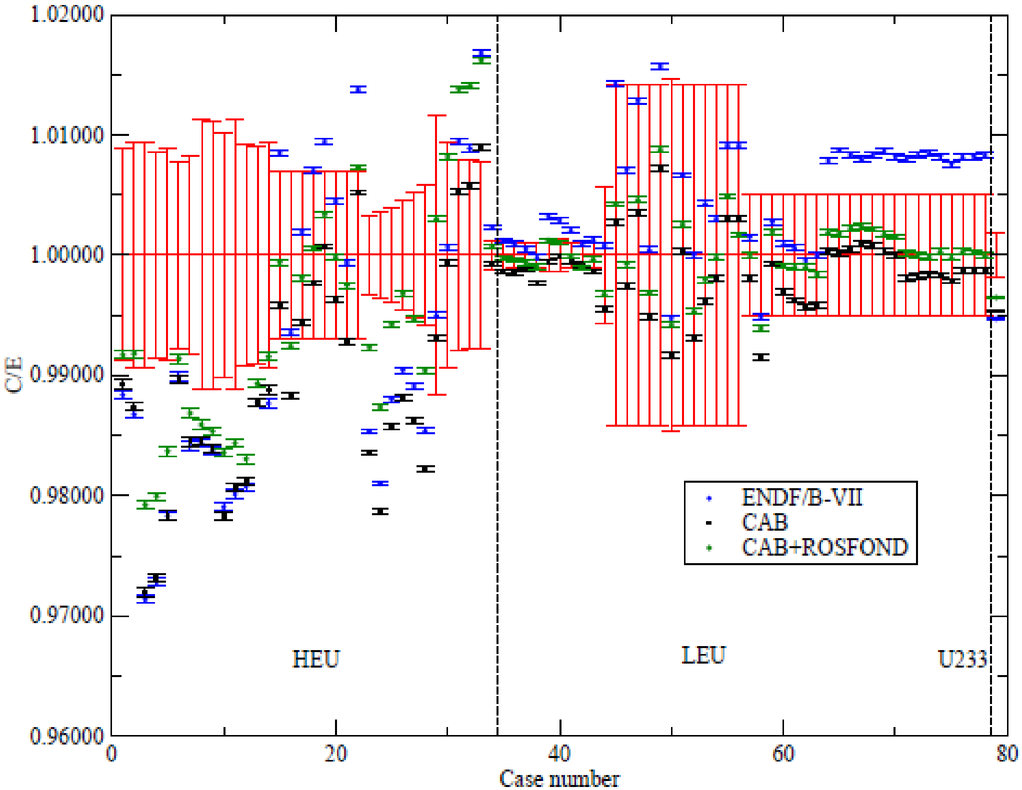
↓ with D_2O, room T : toward better agr. in C/E

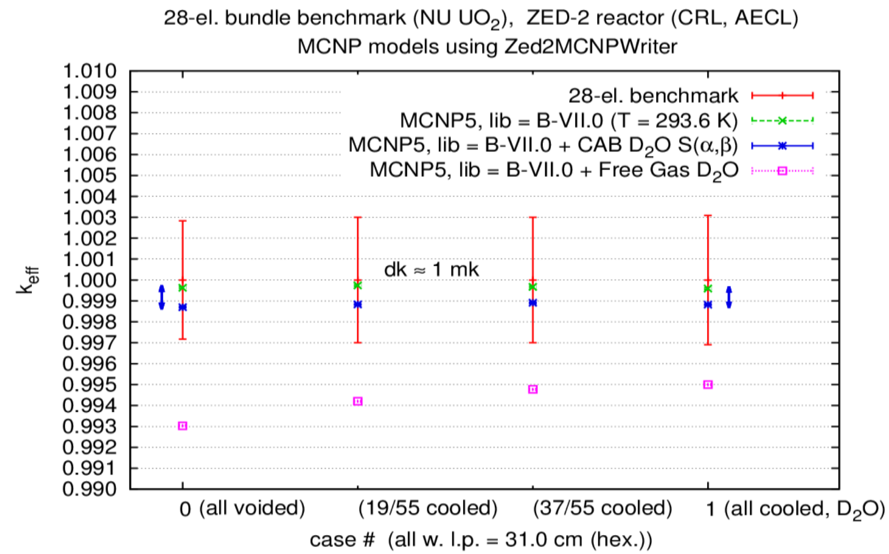


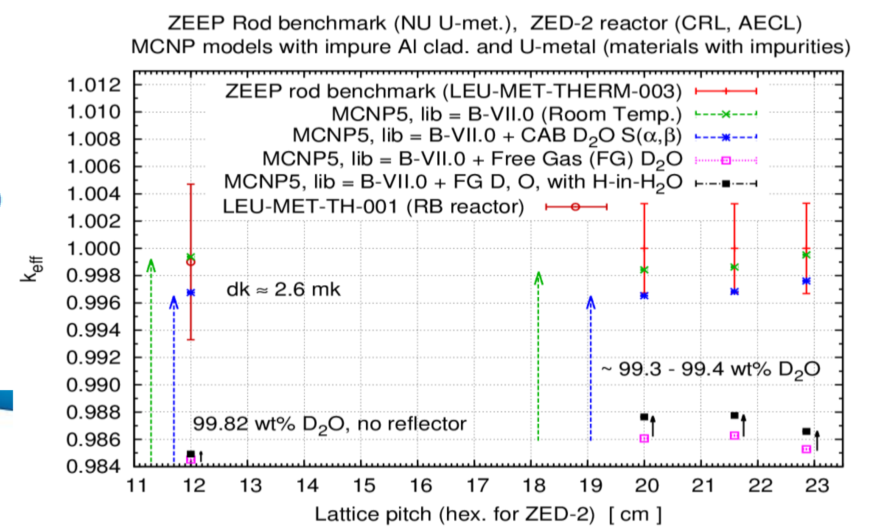
Benchmarking $S(\alpha,\beta)$ for heavy water

International Handbook of Evaluated Criticality Safety Benchmark Experiments

https://www.oecd-nea.org/science/wpncs/icsbep/







with new TSL for D_2O ,
k-eff changes (decreases) by 100-1000 pcm

Canadian Nuclear Laboratories | Laboratoires Nucléaires Canadiens

Conclusion (new TSL for light / heavy water)

- The new TSL evaluations are an improvement over the models of thermal neutron scattering from molecular liquids currently used in the evaluated nuclear data libraries.

- New TSL for H_2O and D_2O are available from testing (some help with NJOY99 processing can be provided).

- The improvements are more important in the case of heavy water

- When we apply these libraries to the calculation of light water moderated critical systems, small changes in the range ±150 pcm are observed. These changes can be traced to a slight hardening of the spectrum.

- In the case of heavy water moderated systems, the differences are more significant, with changes of ~ 1200 pcm. When the new TSL for heavy water is combined with the ROSFOND-2010 evaluation of deuterium, a significant improvement in the calculations is found.

Technical note (NJOY99 and NJOY 2012)

Processing MF7 using E - E' - μ representation: $P(\mu \mid E \to E')$

thermr parameter **nbin** = number of equi-probable bins (angles μ_j)

Each angular bin, prob = 1/nbin, is represented by μ_j, dim(μ_j) = nbin

Suggest enforcing $-1.0 \le \mu_j \le +1.0$,

```
*i thermr.1824
     if ( a(il+jscr) .gt. 1.0D0 ) then
         write(nsyso,'(/
         &    '' ***warning***'',
         &    ''cosine '', f12.8,
         &    '' set to 1.0'')') a(il+jscr)
         a(il+jscr) = 1.0D0
     endif
```

in thermr **and** acer / aceth (if iwt=2 in acer / aceth)

MCNP5 / MCNP6 and other MC codes with <u>thermal ace files</u> with 'wrong' μ_j : any problem (**?**), improve ace files (**?**) ...

REFERENCES

- J.I. Márquez Dámian, J.R. Granada, D.C. Malaspina, *"CAB models for water: A new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format,"* Annals of Nuclear Energy, Vol. **65**, pp. 280-289, **2014** (March); doi:10.1016/j.anucene.2013.11.014 http://www.sciencedirect.com/science/article/pii/S0306454913005987

- J.I. Márquez Dámian, J.R. Granada, D. Roubtsov, *"Improvement on the calculation of D_2O moderated critical systems with new thermal neutron scattering libraries,"* Annals of Nuclear Energy, Vol. **71**, pp. 206-210, **2014** (September); doi:10.1016/j.anucene.2014.03.024 http://www.sciencedirect.com/science/article/pii/S0306454914001467

- J.I. Márquez Damián, J.R. Granada, D. Roubtsov, J.C. Chow, *"From Molecular Dynamics to Reactor Physics: Improvement on the Calculation of D_2O Moderated Critical Systems with New Thermal Neutron Scattering Libraries"*, in Proceedings of XXI Congress of Numerical Methods and Their Applications (**ENIEF 2014**), Bariloche, September 2014, Argentina; http://www.cimec.org.ar/ojs/index.php/mc/article/view/4899

Thank you / *Merci* / Gracias

Questions?

D. Roubtsov
Canadian Nuclear Laboratories, Canada
dan.roubtsov@cnl.ca

J.I. Márquez Damián
Departamento Física de Neutrones
Centro Atomico Bariloche, Argentina
marquezj@cab.cnea.gov.ar