UCANS V
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Analysis of the premoderator temperature effect on the Moderator Brightness of a simple TMR model system

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MOTIVATING IDEAS

Journal of Neutron Research 17 (2014) 101–105
DOI 10.3233/JNR-140013
IOS Press

Low dimensional neutron moderators for enhanced source brightness

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Abstract. In a recent numerical optimization study we have found that liquid para-hydrogen coupled cold neutron moderators deliver 3–5 times higher cold neutron brightness at a spallation neutron source if they take the form of a flat, quasi 2-dimensional disc, in contrast to the conventional more voluminous shapes used by now. In the present paper we describe a simple theoretical explanation of this unexpected behavior, which is based on the large difference in para-hydrogen between the values of the scattering mean free path for thermal neutrons (in the range of 1 cm) and its much larger equivalent for cold neutrons. This model leads to the conclusions that the optimal shape for high brightness para-hydrogen neutron moderators is the quasi 1-dimensional tube and these low dimensional moderators can also deliver much enhanced cold neutron brightness in fission reactor neutron sources, compared to the much more voluminous liquid D_2 or H_2 moderators currently used. Neutronic simulation calculations confirm both of these theoretical conclusions.

Keywords: Neutron source, research reactor, spallation source, neutron moderator, cold source, neutron scattering, para-hydrogen

NEUTRON PHYSICS

BY

K. H. BECKURTS and K. WIRTZ

KERNFORSCHUNGSZENTRUM KARLSRUHE

Translated by: L. Dresner, *Oak Ridge National Laboratory*

WITH 293 FIGURES

Springer-Verlag Berlin Heidelberg GmbH
1964

BASIC CONCEPTS

6.2. Solution of the Diffusion Equation in Simple Cases

6.2.1. Simple Symmetrical Sources in Infinite Media

Point Source: See Sec. 6.1.3.

Plane Source: Let the source, which lies in the (x, y)-plane, emit Q neutrons per cm² per second. Then for $z \neq 0$,

$$\frac{d^2\Phi}{dz^2} - \frac{1}{L^2}\Phi = 0.$$

This equation has the solution

$$\Phi(z) = A\,e^{-z/L} \quad \text{for} \quad z > 0$$

Nuclear Instruments and Methods 192 (1982) 129–136
North-Holland Publishing Company

OLD KNOWLEDGE

AN ACCELERATOR-BASED COLD NEUTRON SOURCE

K. INOUE, Y. KIYANAGI and H. IWASA
Department of Nuclear Engineering, Hokkaido University, Sapporo, 060 Hokkaido, Japan

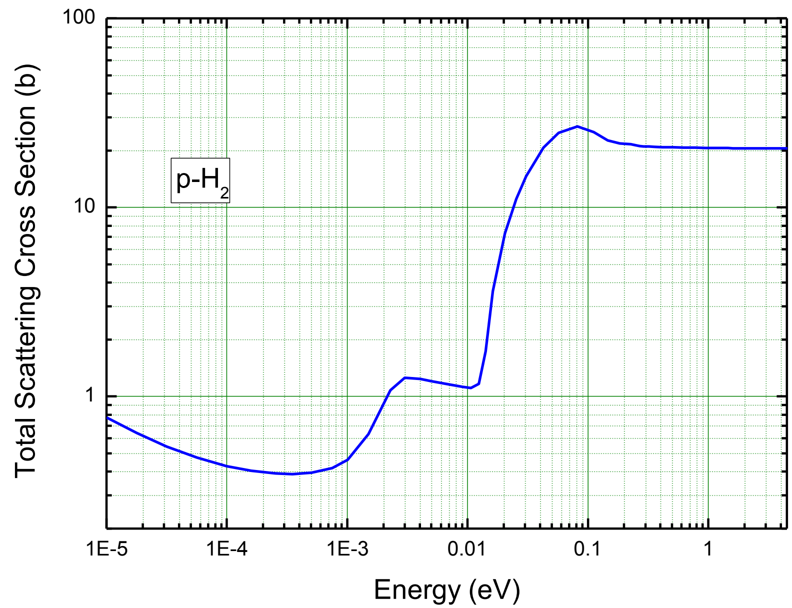
Received 14 July 1981

"…..the thermal or cold neutron intensity emanating from the moderator surface is mainly determined by the slowing down neutron spatial distribution"

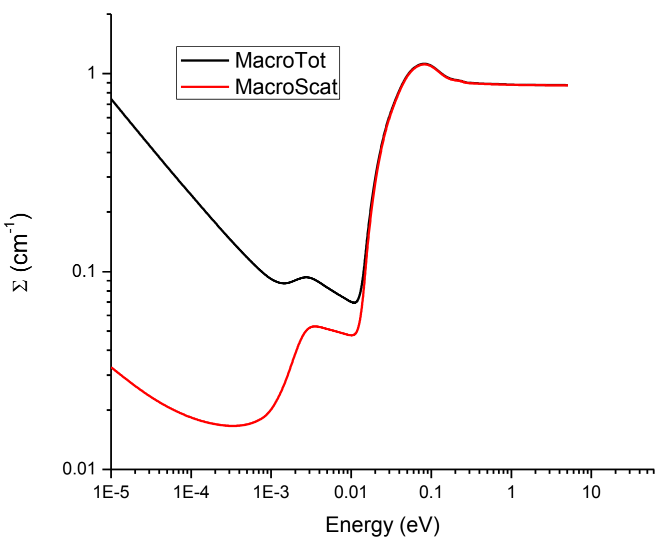
$$\Phi_{COLD} \propto \Phi_{INCOM} \cdot \sigma\,(\text{incom} \rightarrow \text{cold})$$

Liquid Para-Hydrogen

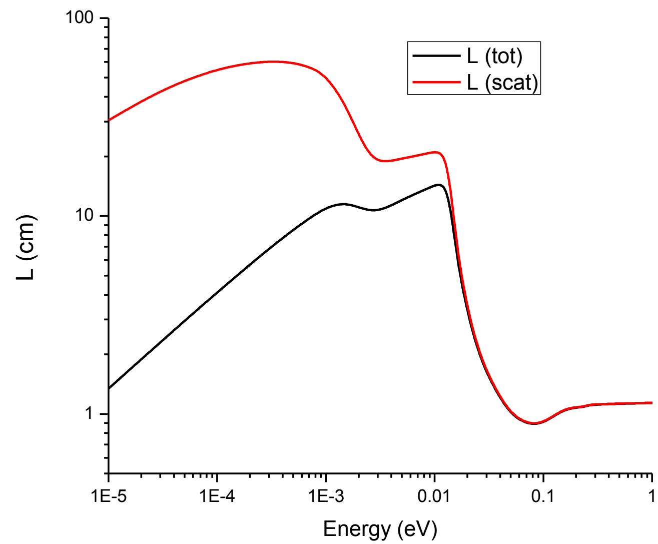
J.R. Granada and V.H. Gillette
Physica **B 348**, 6 (2004)



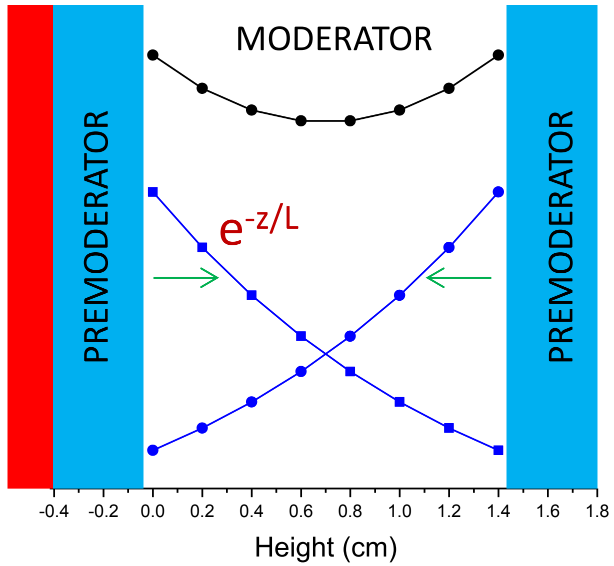
Macroscopic X-sections

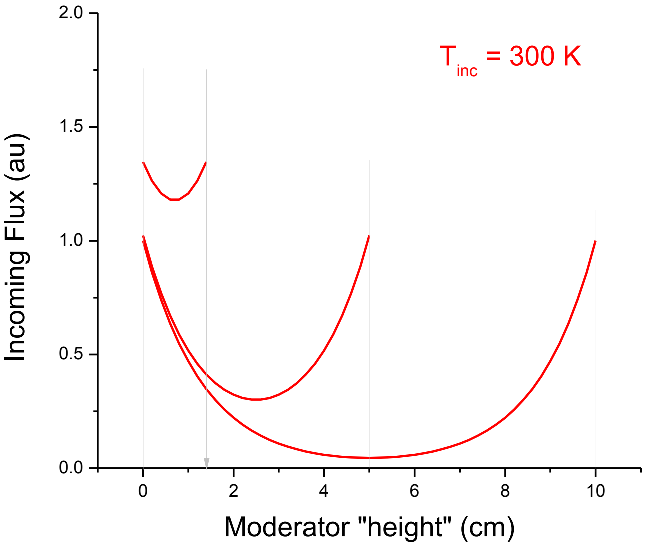


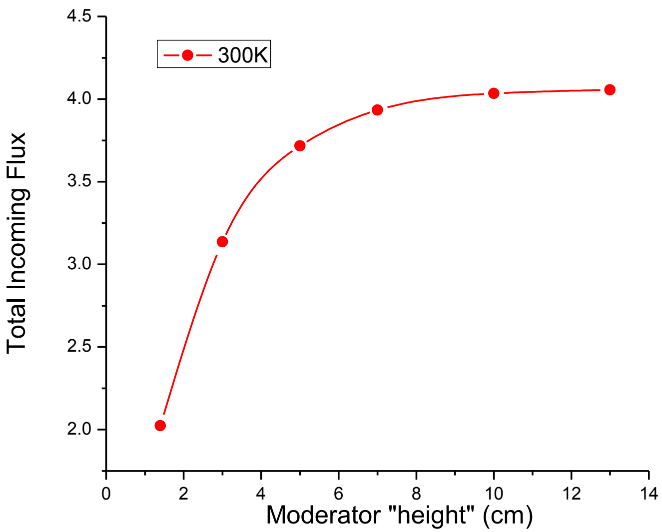
Mean free-paths

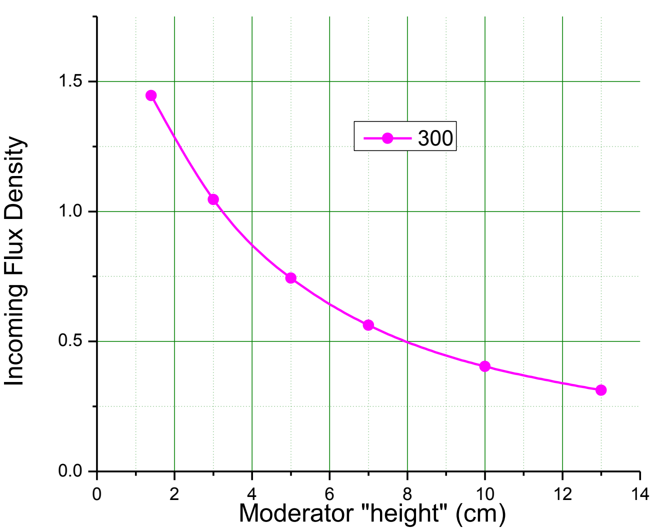


ONE-DIMENSIONAL SYSTEM

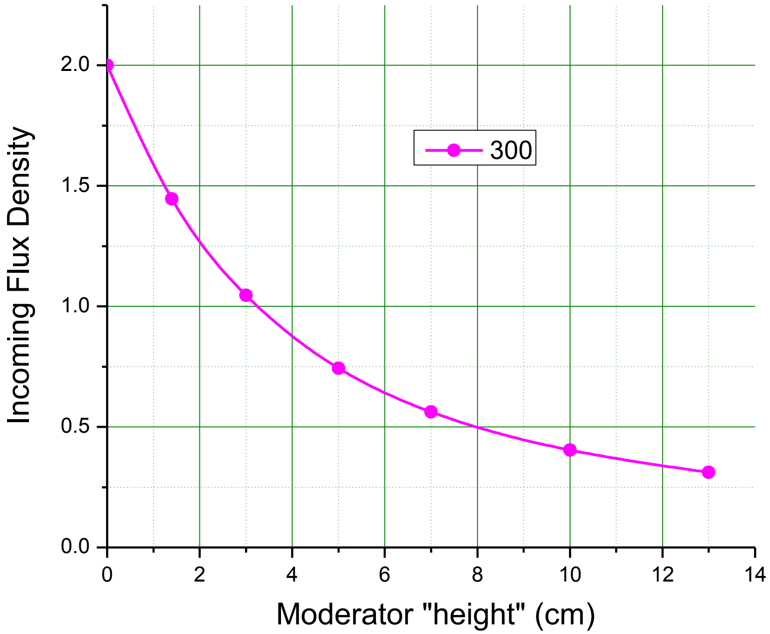




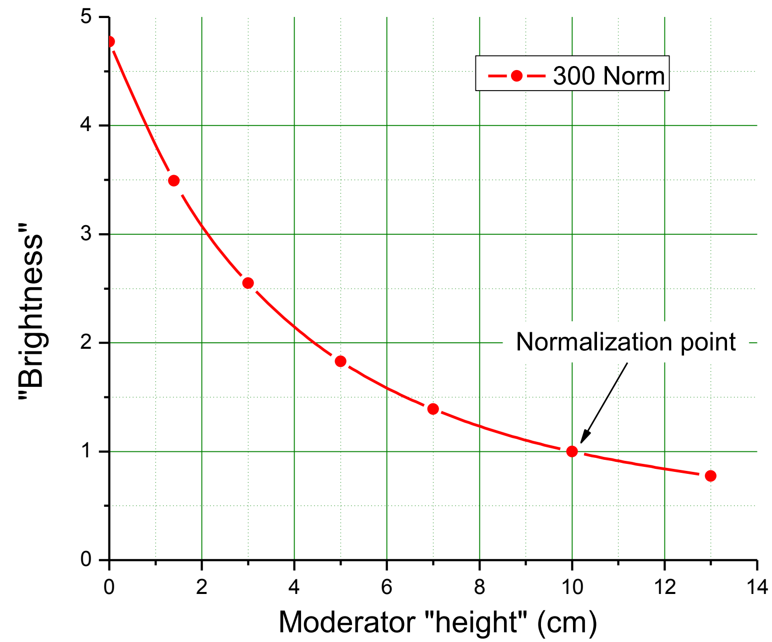




ONE DIMENSIONAL, TWO-ENERGY GROUPS, SINGLE COLLISION MODEL



$* \ \Sigma_{1\to 2}$



Incoming Flux Density: $\Phi_1(z)$

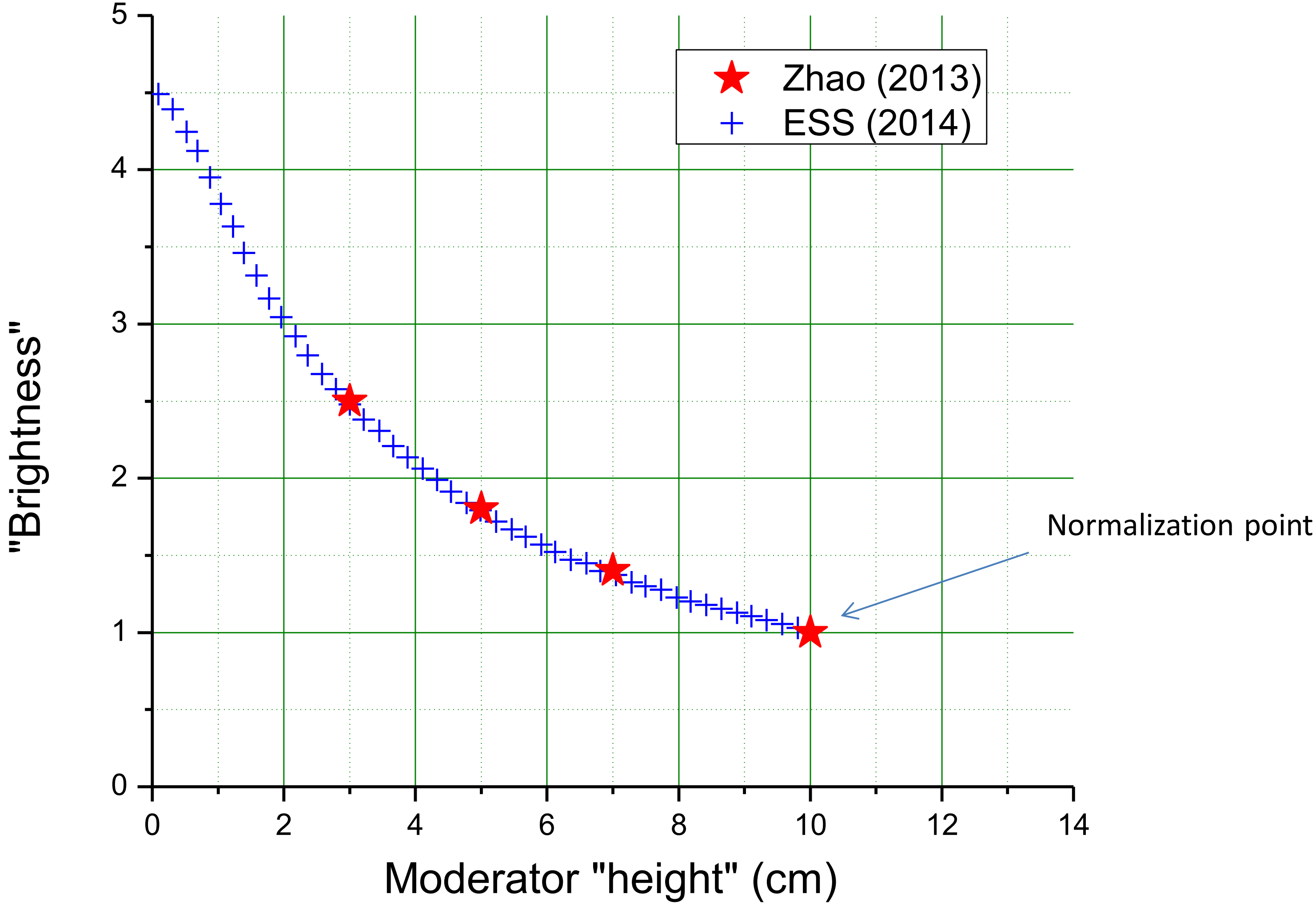
Probability Cold Neutron Production: $\Sigma_{1\to 2}$

Reaction Rate: $dR_{1\to 2}(z) = \Phi_1(z) \,.\, \Sigma_{1\to 2}\, dz$

<u>Brightness:</u> $dR_{1\to 2}(z)/dz = \mathbf{\Phi_1(z) \,.\, \Sigma_{1\to 2}}$

Outcoming Flux: $\int dR_{1\to 2}(z)$

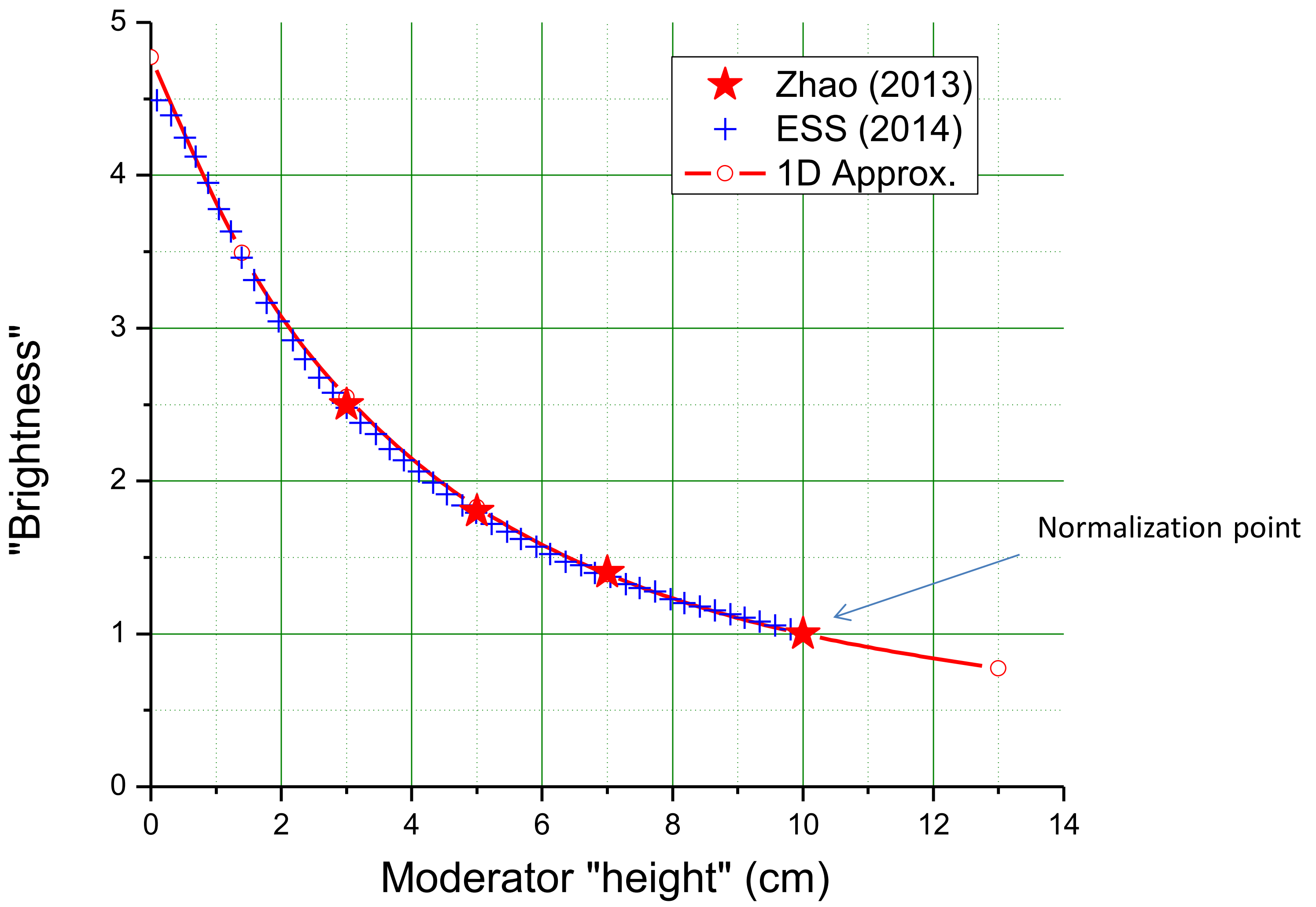
MONTE CARLO CALCULATIONS



★ J.K. Zhao *et al.,* Review of Scientific Instruments **84**, 125104 (2013)

✚ http://europeanspallationsource.se/higher-neutron-brightness-innovative-pancake-moderators

MONTE CARLO CALCULATIONS…AND ONE-DIMENSIONAL APPROX.



★ J.K. Zhao *et al.,* Review of Scientific Instruments **84**, 125104 (2013)

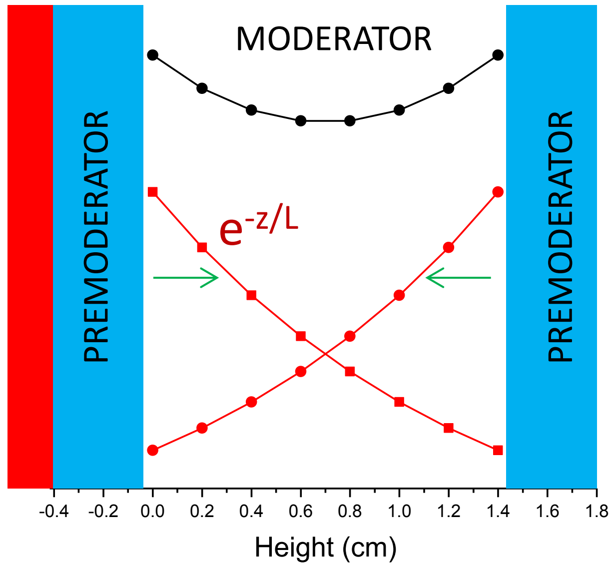
✚ http://europeanspallationsource.se/higher-neutron-brightness-innovative-pancake-moderators

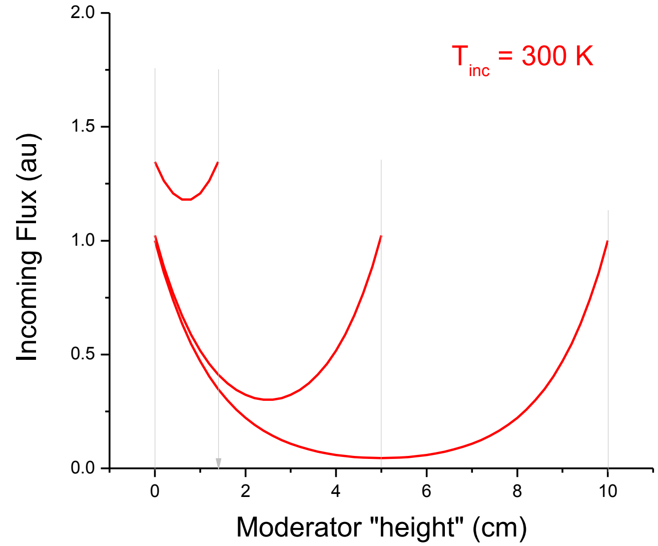
WHAT WE PROPOSED TO STUDY:

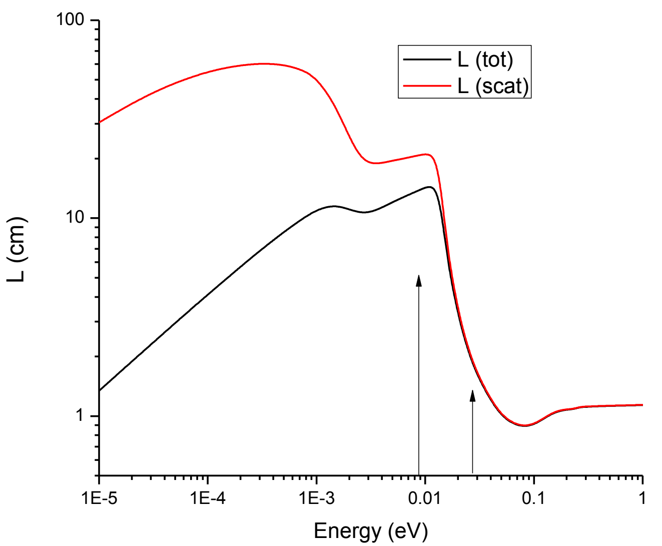
Abstract

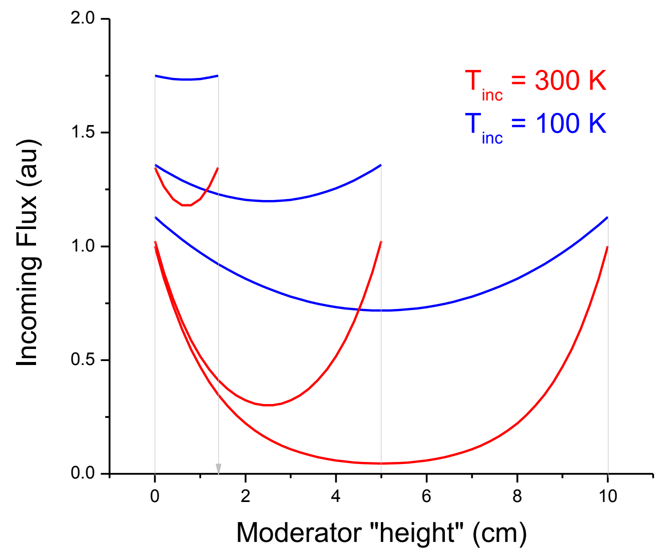
The performance of the cold neutron moderator of a TMR system of simple geometry was studied by means of Monte Carlo calculations. The brightness was determined over the side surface of a cylindrical para-hydrogen moderator of fixed diameter, with a given target, premoderator and reflector configuration, while the height of the moderator was changed. We compare the brightness behavior as a function of **premoderator temperature**, using room temperature water and liquid methane as typical examples.

CHANGING THE PREMODERATOR TEMPERATURE

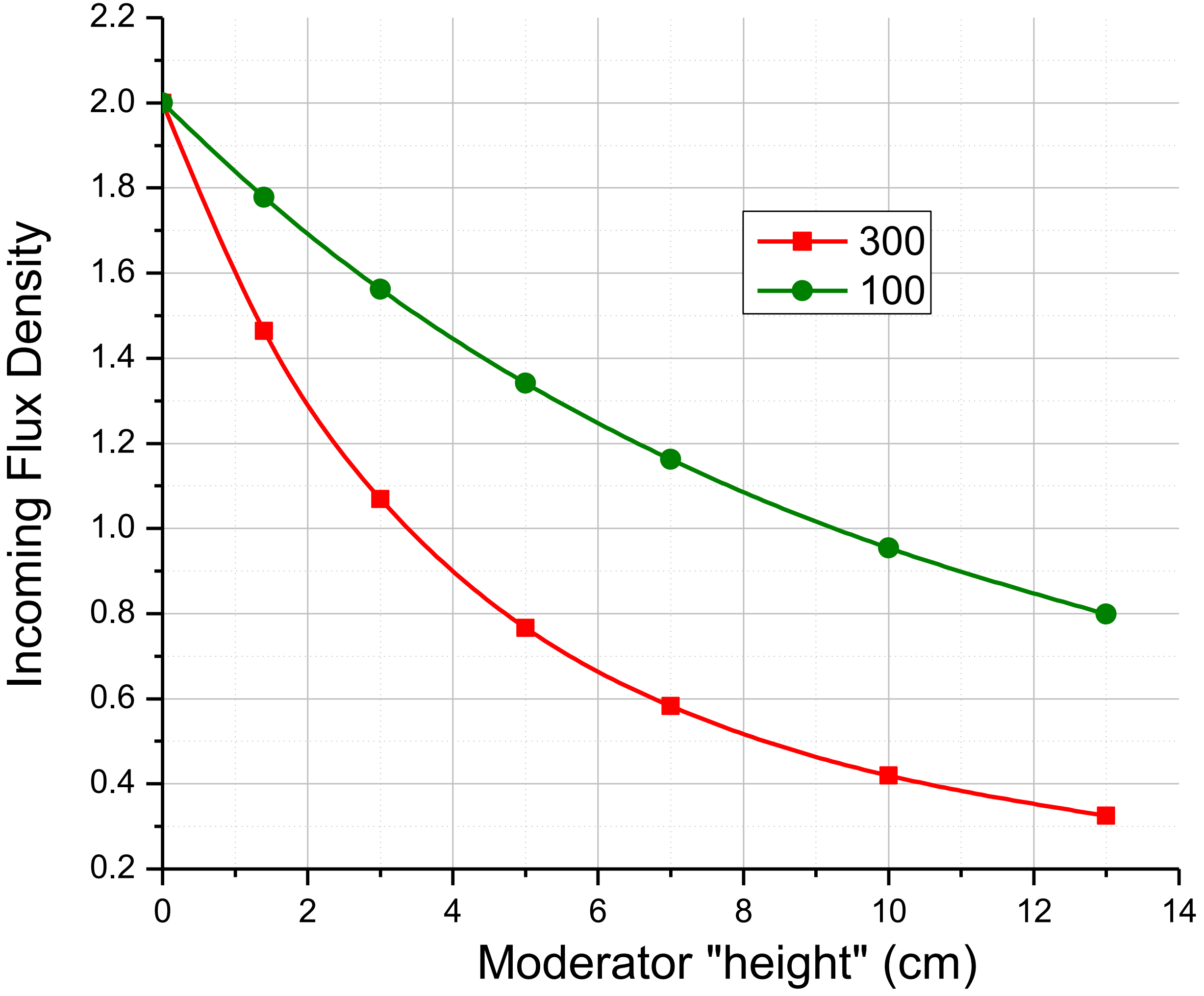




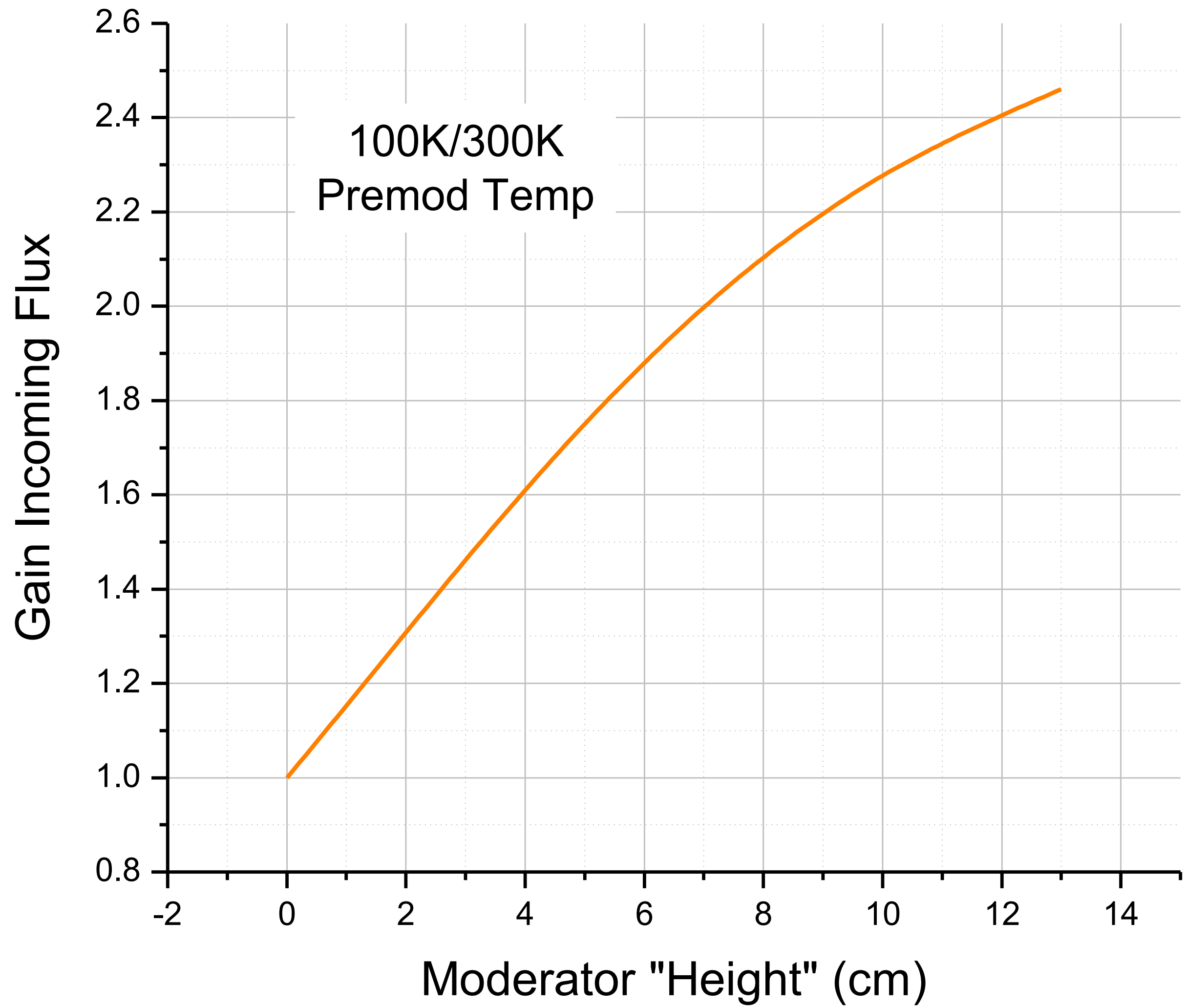




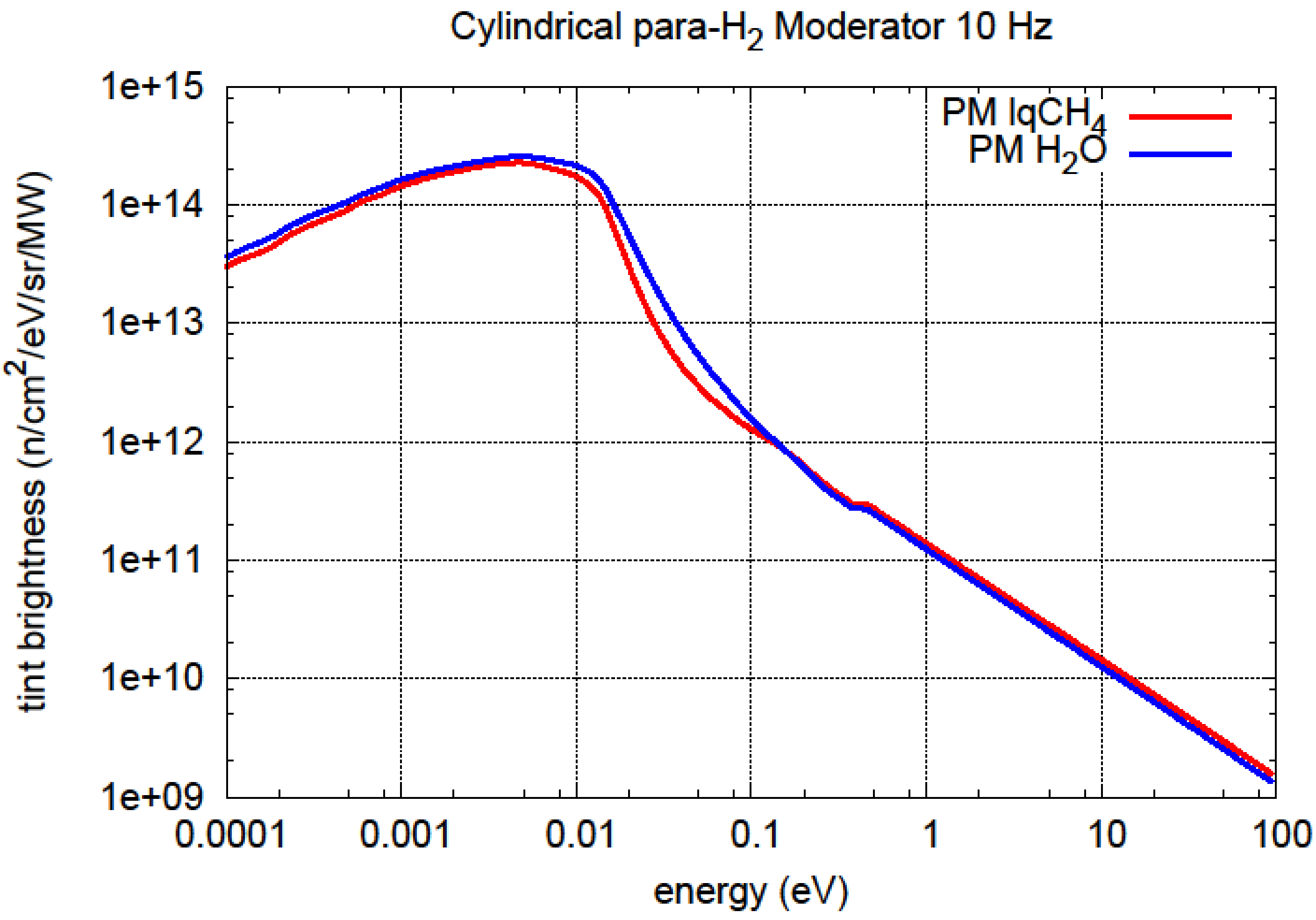
BRIGTHNESSES FOR DIFFERENT PREMOD TEMPS.



GAIN IN BRIGTHNESSES FOR DIFFERENT PREMOD TEMPS.



ACTUAL CALC. RESULTS FOR DIFFERENT PREMOD TEMPS. !!!



(Franz Gallmaier, private communication, 2015)

We confirmed the results obtained by Gallmaier, and found that for such a coupled system (as indicated below), the neutron moderation process is greatly controlled by the large Be reflector rather than by the premoderator. In this situation, the enhanced intensity of the incoming neutron field is accompanied by an enlarged neutron pulse.

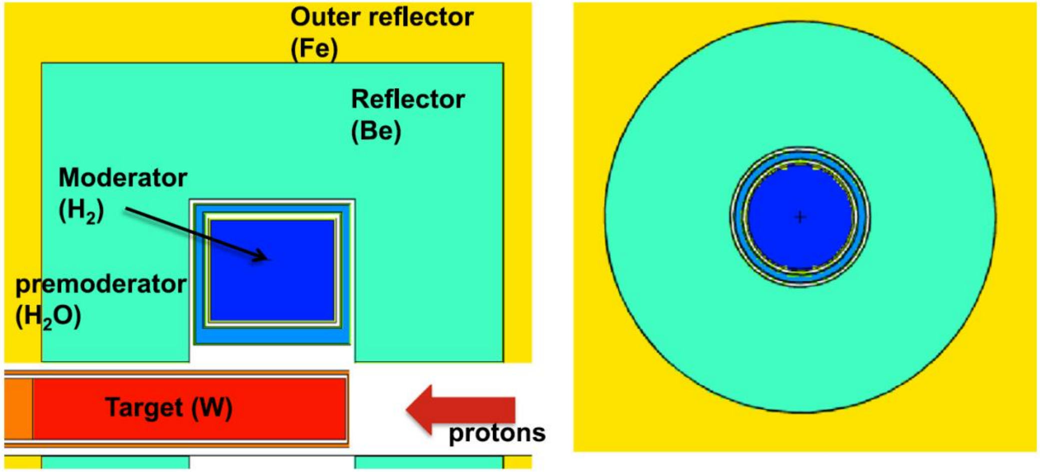
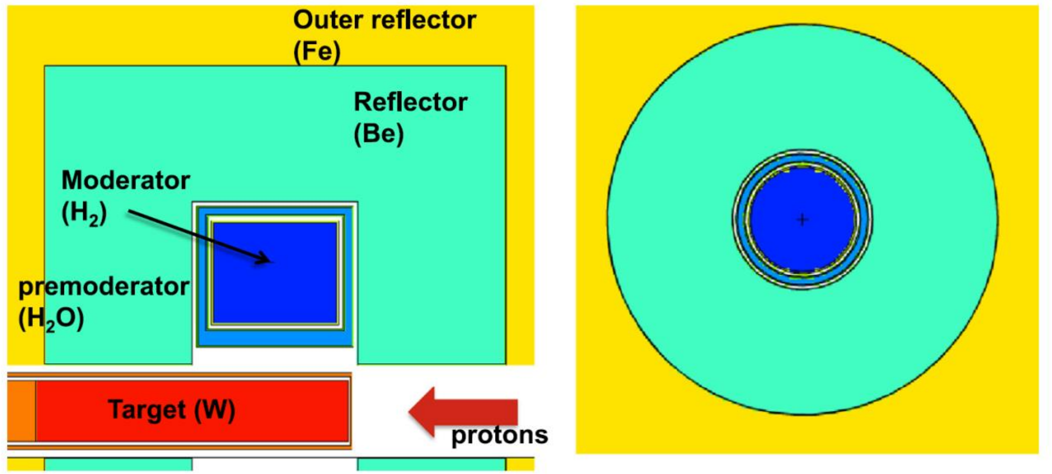


Fig. 1. Side view MCNPX model of the unperturbed moderator (left). Top view of the unperturbed moderator (right).

We then returned to study a TMR system of “UCANS type”

I C A N S



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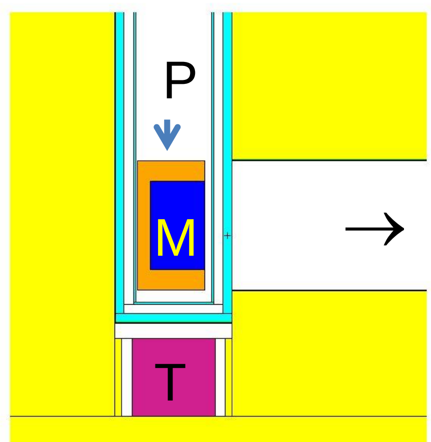
U C A N S



P: premoder.

M: moderator 12x12 cm^2

Moderator Issues

- When neutrons are released from matter their energy is much too high to be useful for most purposes, especially neutron scattering.
- They must therefore be slowed down by many orders of magnitude in energy to serve as probes for solid state research.
- The standard moderator used in reactors are (light or) heavy water for room temperature and liquid hydrogen (mostly D_2) for cryogenic moderators.
- For pulsed sources deuterium is not optimal because it produces long pulses due to its low energy transfer per collision.

Why Cold Neutron Moderators?

- Cold (long wavelength) neutrons are used in neutron scattering to
  - investigate large structures
  - examine slow motions
  - i.e. work at small momentum transfer
- Cold moderators also produce narrower line widths in pulsed sources down to lower energies than ambient temperature ones
  - better resolution
- However, with the exception of Hydrogen down to 15 K all potential moderator materials become solid.
- It would be desirable to have an even lower moderator temperature to take advantage of unoccupied states.

J.M. Carpenter & W.B. Yelon, in *Methods of Experimental Physics,* Vol.23 A, Ch.2 Neutron Sources, Academic Press (1986)

"MODERATION RANGE"

In the Grueling–Goertzel approximation,

$$I(E,t) = \left(\frac{K}{E}\right)\frac{\xi\Sigma_s v}{2\Gamma(2/\gamma)}\left(\frac{\xi\Sigma_s vt}{\gamma}\right)^{2/\gamma}\exp\left(-\frac{\xi\Sigma_s vt}{\gamma}\right). \tag{2.56}$$

This is a differential χ^2 distribution with $2 + 4/\gamma$ degrees of freedom (which is useful to know for purposes of calculations), and is called the "slowing-down time" distribution. Γ is the gamma function. In monatomic materials, ξ is the mean logarithmic energy change per collision,

$$\xi = 1 - \frac{\alpha_0 \varepsilon}{1-\alpha_0} \approx \frac{2}{A} \qquad \text{and} \qquad \varepsilon = \ln\left(\frac{1}{\alpha_0}\right), \tag{2.57}$$

where

$$\alpha_0 = (A-1)^2/(A+1)^2, \tag{2.58}$$

and $2\xi\gamma$ is the mean-*squared* logarithmic energy change per collision,

$$\gamma = 1 - \frac{\alpha_0 \varepsilon^2/2}{1-\alpha_0-\alpha_0\varepsilon} \approx \frac{4}{3A}, \tag{2.59}$$

and Σ_s is the macroscopic scattering cross section of the medium, and A is the mass number of the scatterer. In mixtures, the quantities ξ and $2\xi\gamma$ are averages weighted with respect to the macroscopic scattering cross sections of

J.M. Carpenter & W.B. Yelon, in *Methods of Experimental Physics,* Vol.23 A, Ch.2 Neutron Sources, Academic Press (1986)

The average slowing-down time and the standard deviation of the slowing-down time distribution at energy E (speed v) are

$$\bar{t} = (1 + 2/\gamma)\gamma/(\xi\Sigma_s v), \qquad \sigma_t = \sqrt{1 + 2/\gamma}\,\gamma/(\xi\Sigma_s v). \tag{2.60}$$

When the cross sections and slowing-down parameters are independent of energy, $v\bar{t}$ and $v\sigma_t$ are independent of energy. Indeed, the distribution $EI(E, t)$ is a function of the variable vt only, and invariant with E, a fact that is sometimes useful in connection with numerical calculations and the presentation of data.

The full width $\Delta t(f)$ at fraction f of the maximum of the slowing-down function is given by the difference Δy between the two solutions of the equation

$$ye^{(1-y)} = f^{\gamma/2}, \tag{2.65}$$

where

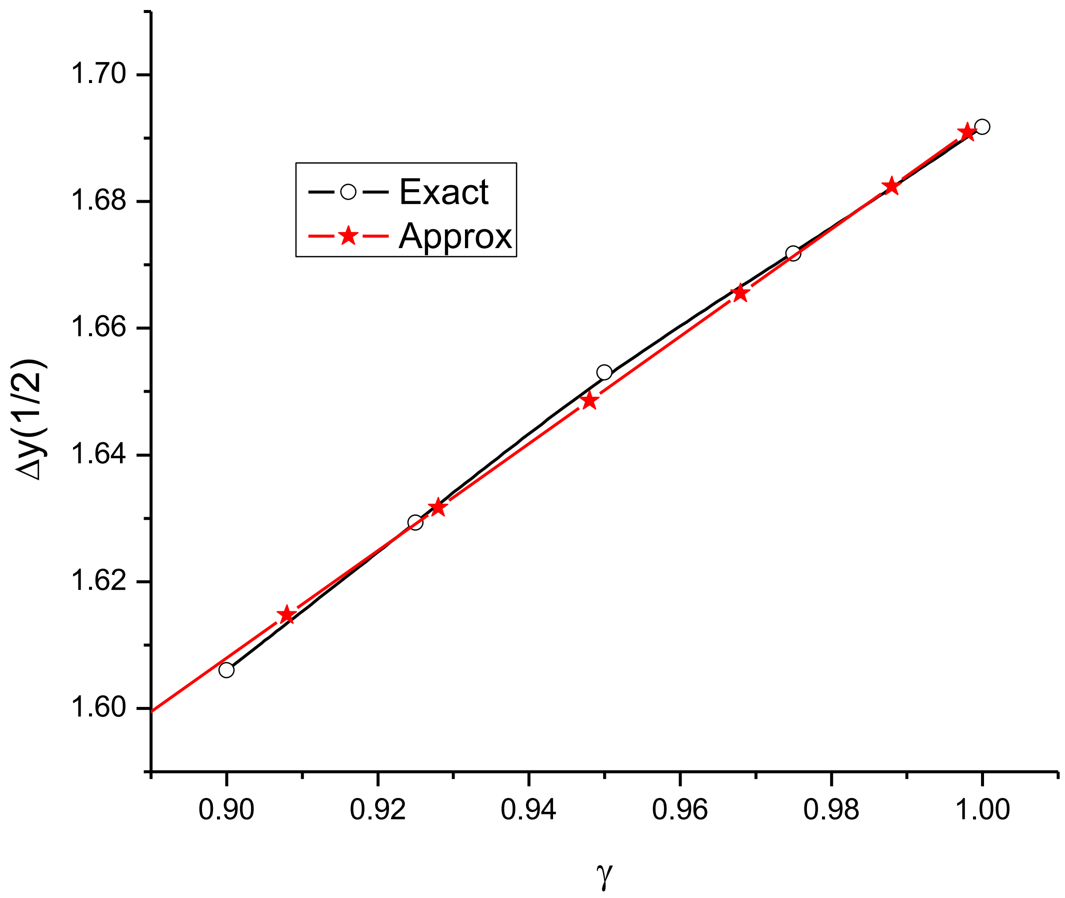
$$y = \frac{\xi\Sigma_s vt}{2}. \tag{2.66}$$

The time widths are

$$\Delta t(f) = 2\Delta y(f)/(\xi\Sigma_s v).$$

A useful approximation for the HWHM of the neutron pulse in hydrogeneus materials

$$\Delta y(1/2) \cong 3\,(1+\gamma)\,/(2\,\pi^{1/2})$$



J.M. Carpenter & W.B. Yelon, in *Methods of Experimental Physics,* Vol.23 A, Ch.2 Neutron Sources, Academic Press (1986)

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The time widths are

($f = ½$) $\quad \Delta t_{1/2} = 3\pi^{-1/2}(1 + \gamma) / (\xi\Sigma_s v)$

Error ≤ 2 ‰
$0.9 \le \gamma \le 1$

(J.R. Granada, 2015)

Neutronic Properties of some Moderators

Parameter	H_2O 293 K	$(CH_2)_n$ 293 K	CH_4 20 K	CH_4 100 K	C_2H_6 100 K	C_2H_6 180 K
σ_{free} (barn)	44.749	45.73	86.73	86.73	132.46	132.46
ρ (g/cm^3)	1	0.94	0.510	0.4392	0.641	0.550
N^{molec} (10^{24}/cm^3)	0.0335	0.0404	0.0192	0.0165	0.0129	0.0110
N^H (10^{22}/cm^3)	6.69	8.09	7.68	6.61	7.72	6.63
D (10^{-5} cm^2/s)	2.3	---	---	5.2	0.82	5.51
Σ_{free} (cm^{-1})	1.5	1.849	1.665	1.431	1.705	1.463
ξ	0.926	0.913	0.954	0.954	0.940	0.940
$\xi\,\Sigma_{free}$ (cm^{-1})	1.39	1.69	1.59	1.37	1.60	1.38
γ	0.924	0.908	0.951	0.951	0.936	0.936
$v\,t_s$ (cm)	2.105	1.723	1.858	2.162	1.832	2.135
$v\,\Delta t_s$ (cm)	1.183	0.963	1.055	1.227	1.034	1.205
$v\,\Delta t_{1/2}$ (cm)	2.346	1.915	2.080	2.421	2.046	2.383

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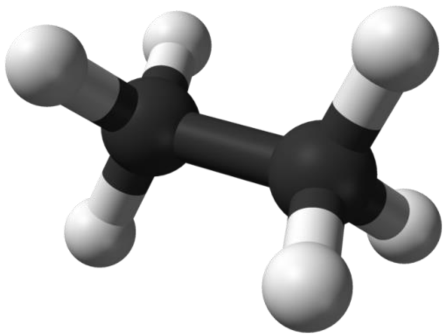
solids

AN INTERESTING "COOL" MODERATOR:

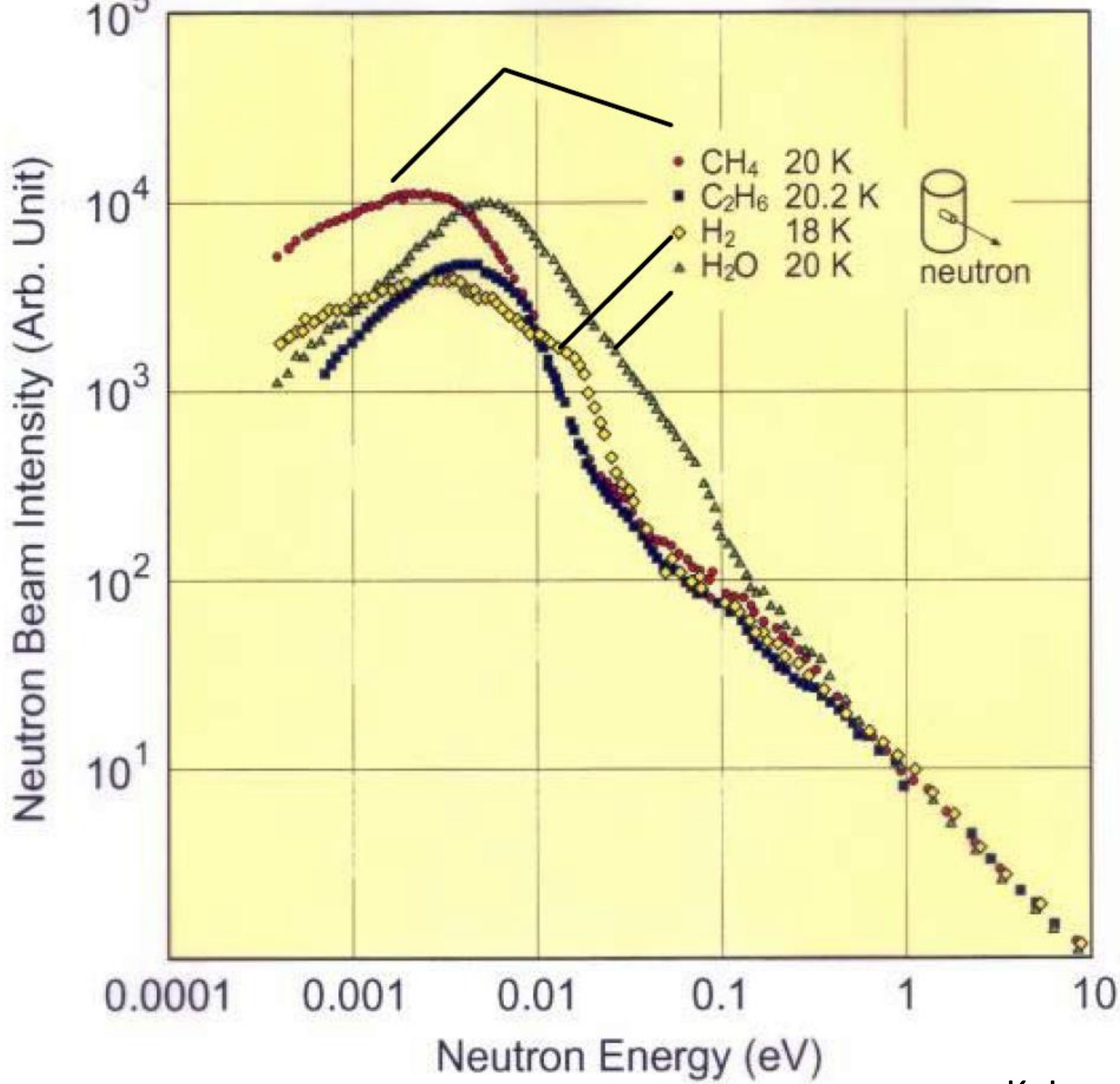


ETHANE

C_2H_6

http://en.wikipedia.org/wiki/Ethane

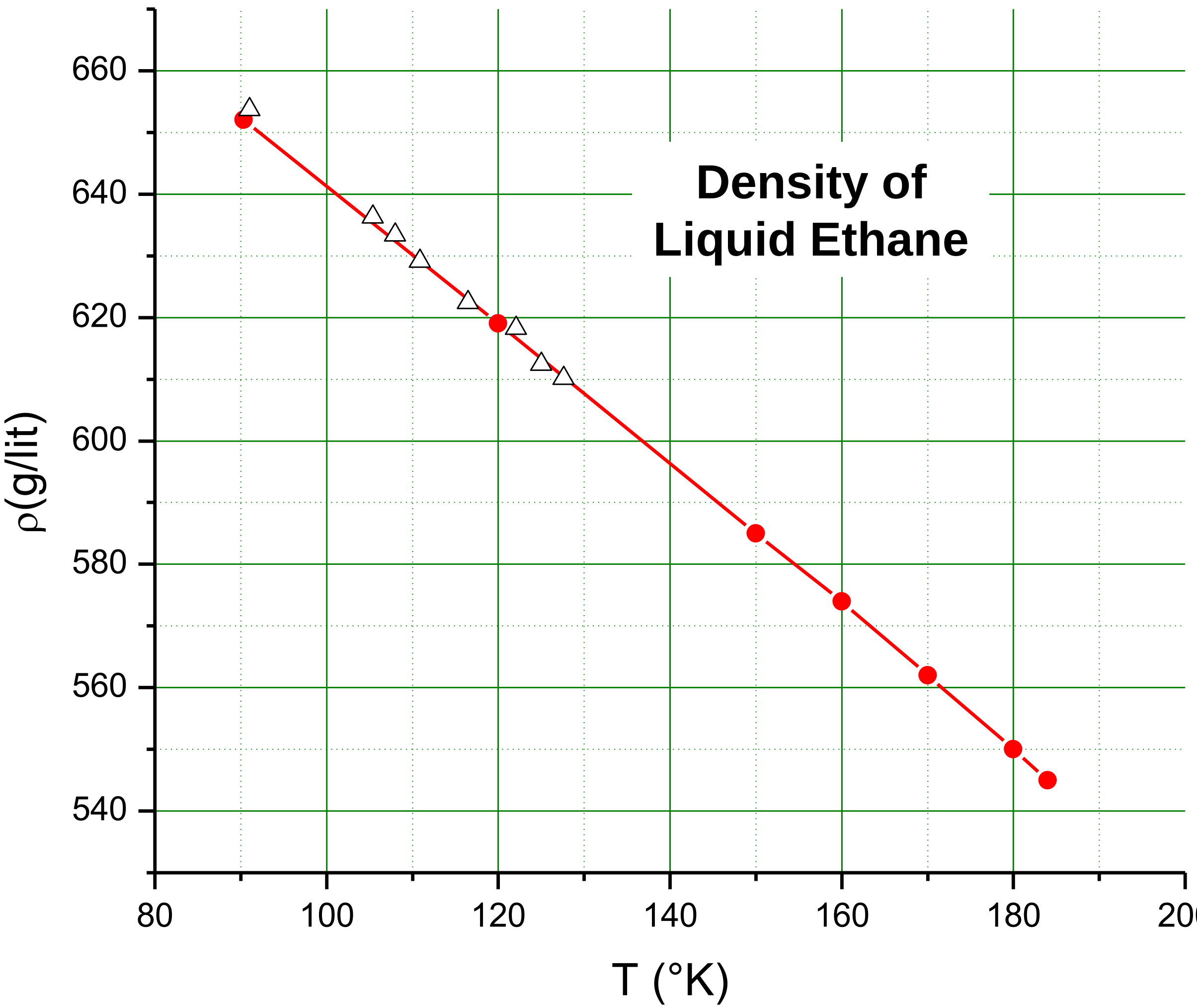
Properties	
Molecular formula	C_2H_6
Molar mass	30.07 g·mol^{-1}
Appearance	Colorless gas
Odor	Odorless
Density	•1.3562 mg cm^{-3} (at 0 °C)[1] •0.5446 g cm^{-3} (at 184 K)[2]
Melting point	−182.8 °C; −296.9 °F; 90.4 K
Boiling point	−88.5 °C; −127.4 °F; 184.6 K



10^5
10^4
10^3
10^2
10^1
Neutron Beam Intensity (Arb. Unit)
0.0001
0.001
0.01
0.1
1
10
Neutron Energy (eV)
CH_4 20 K
C_2H_6 20.2 K
H_2 18 K
H_2O 20 K
neutron

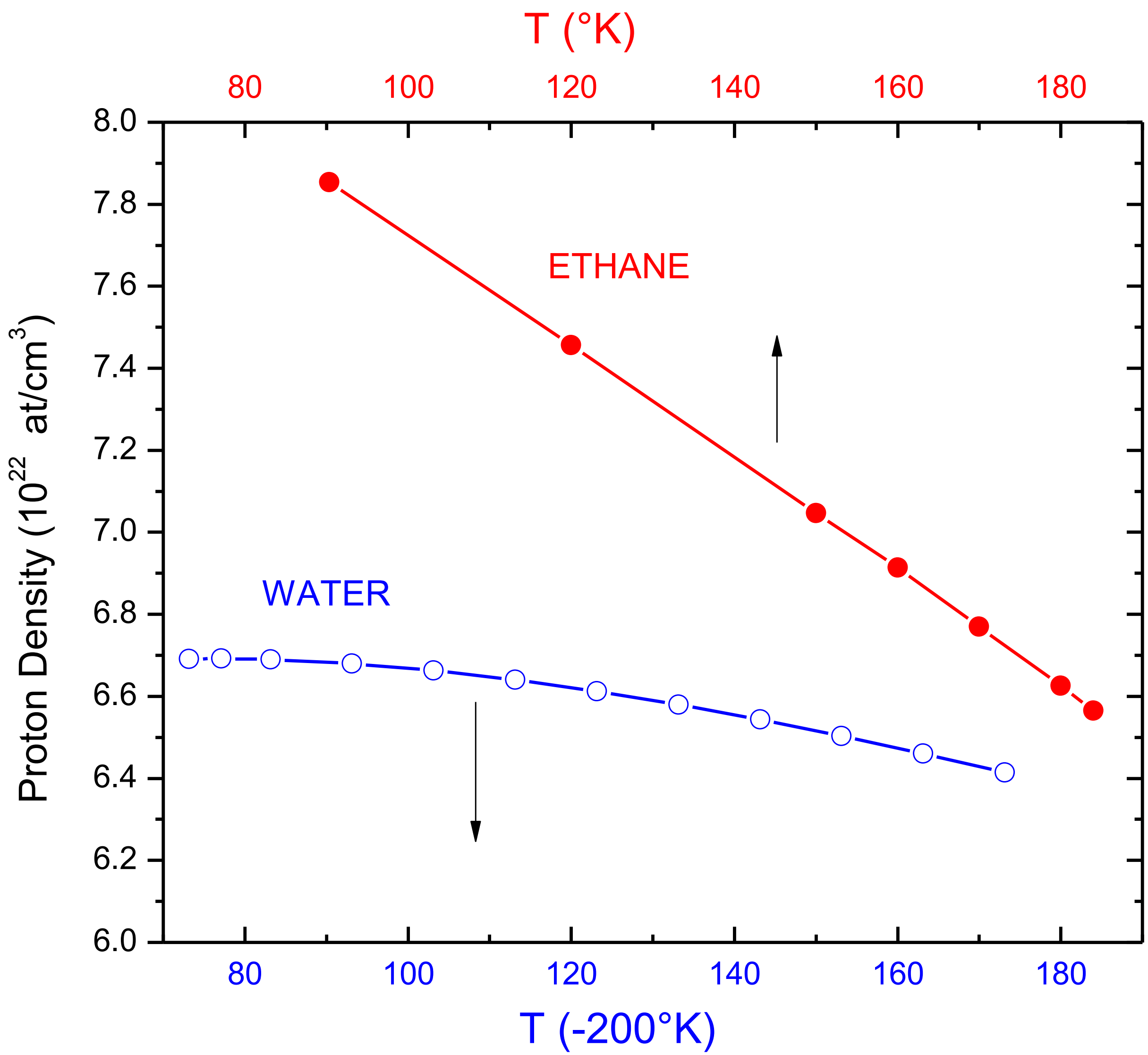
K. Inoue (1979)

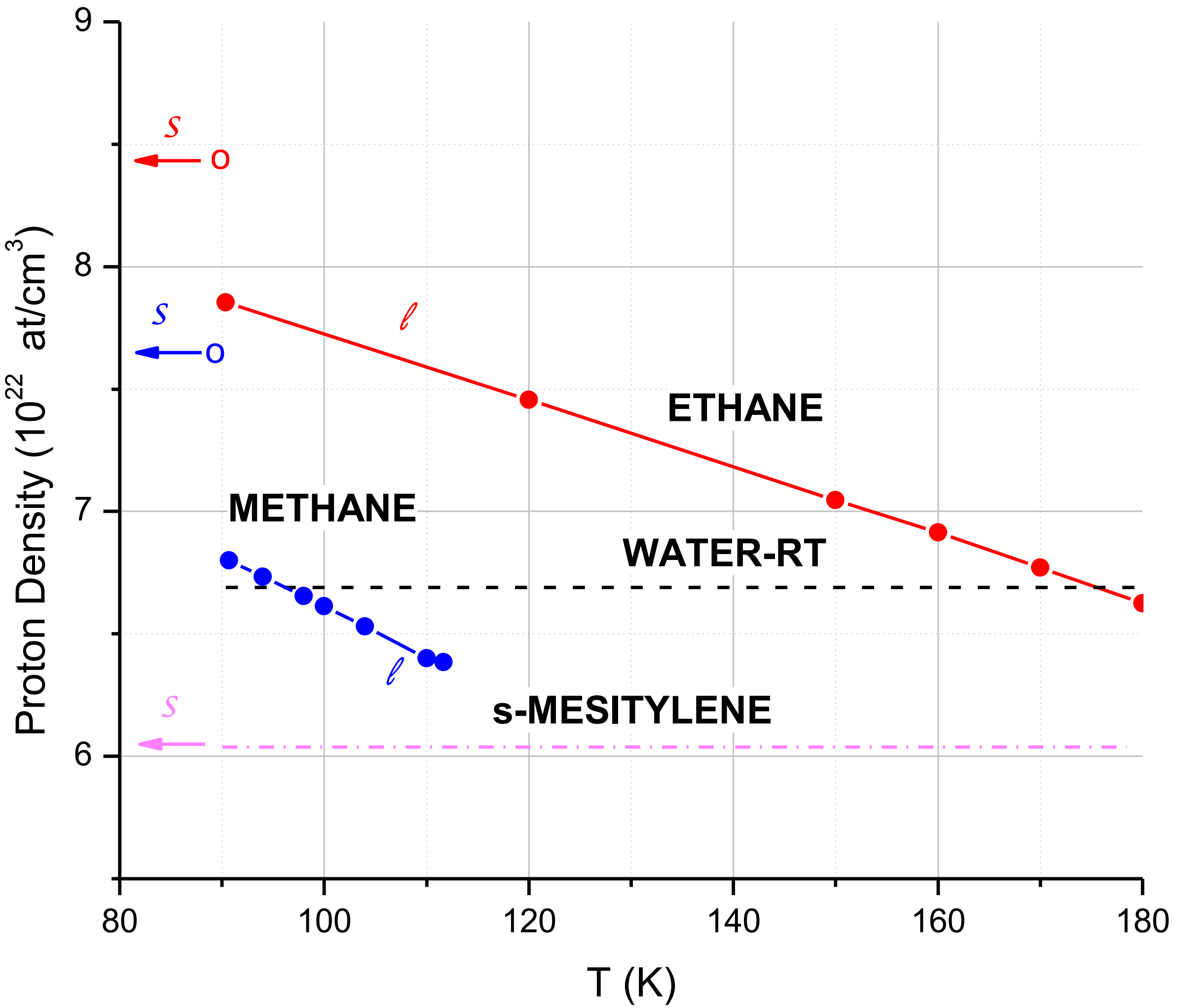
Liquid Ethane exists over a large temp range



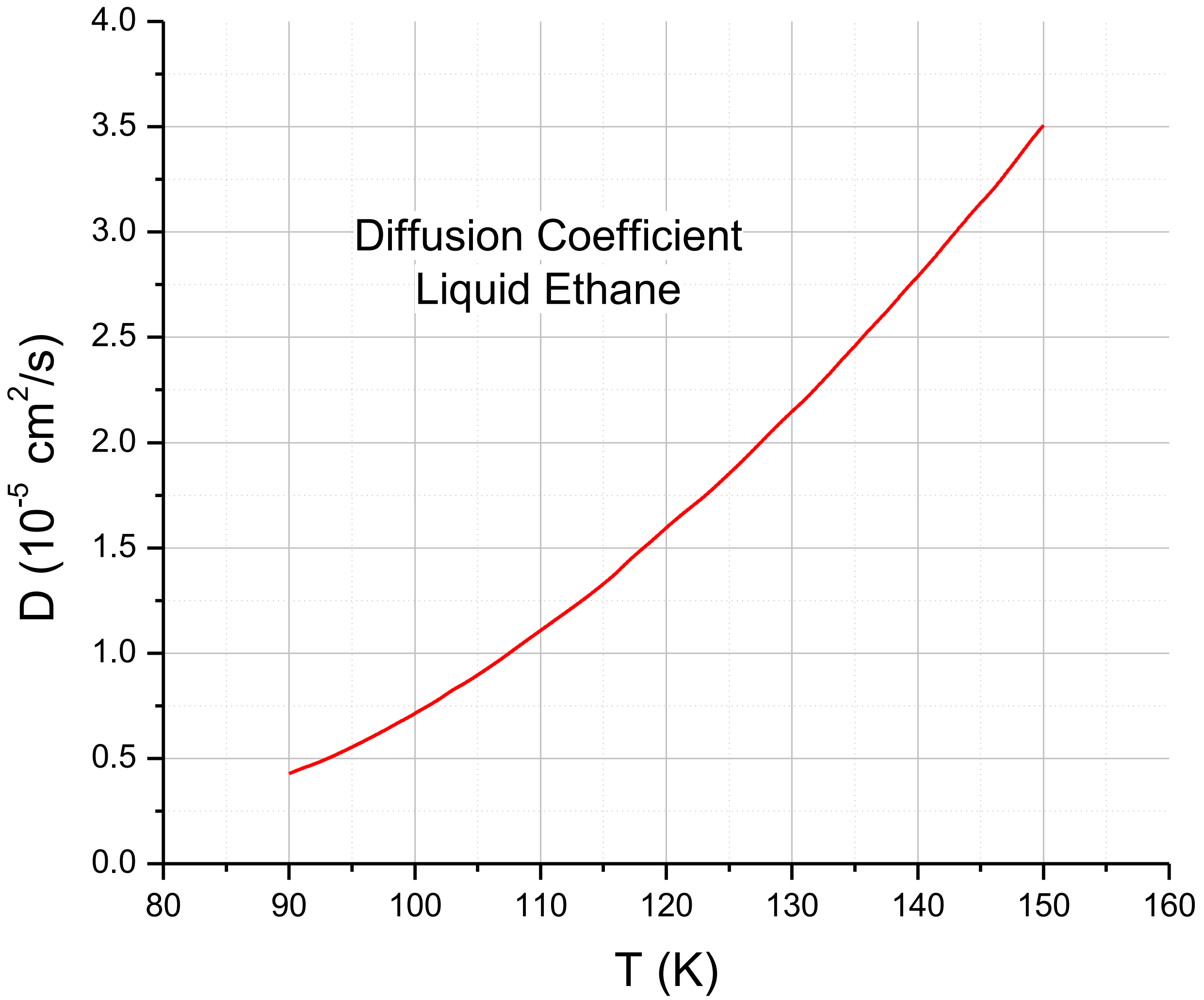
http://www.engineeringtoolbox.com/ethane-thermal-properties-d_1761.html

....and it has a large protonic density





http://www.engineeringtoolbox.com/ethane-thermal-properties-d_1761.html

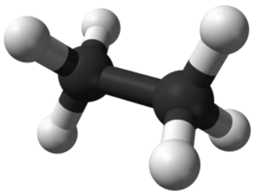


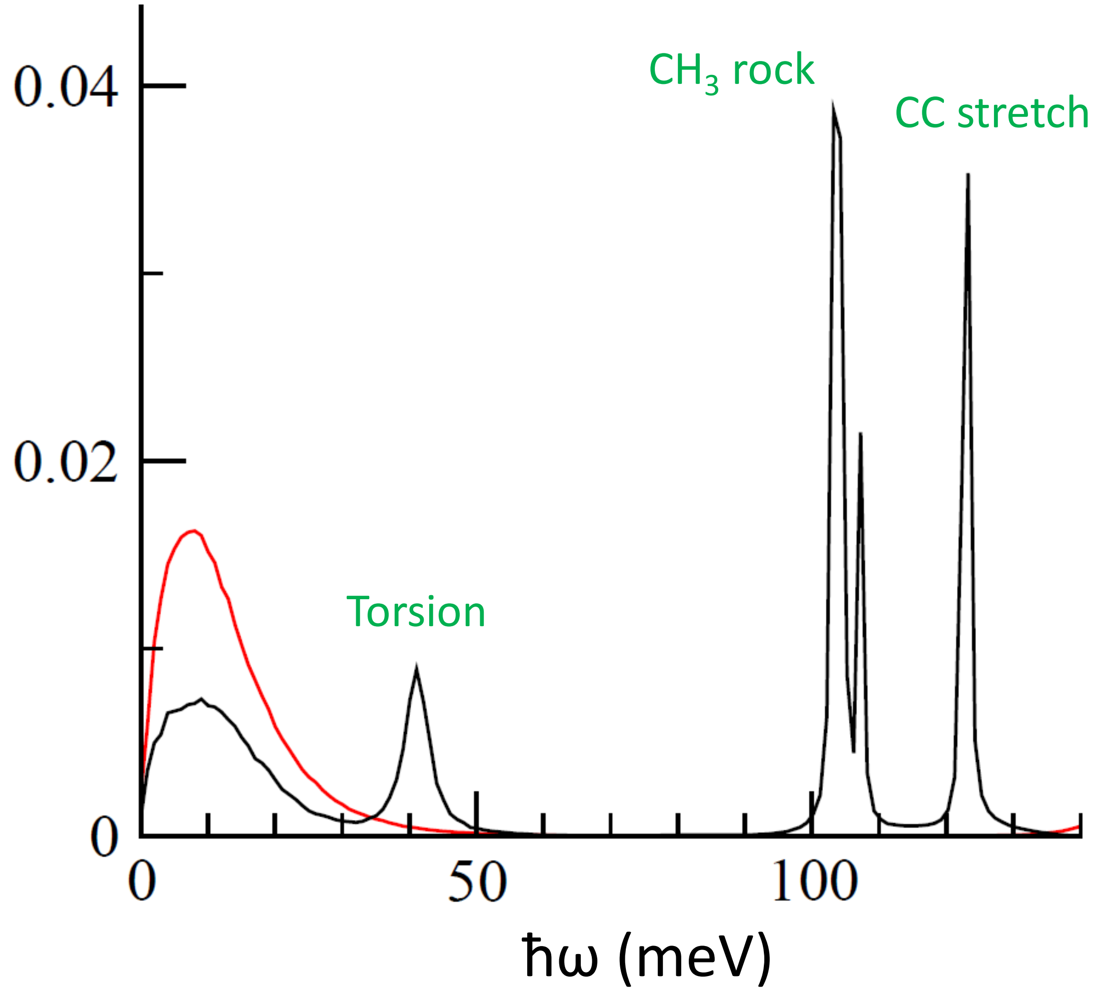
J.F. Harmon & B.H. Muller, Phys.Rev. **182**, 400 (1969)

OUR MODEL FOR LIQUID ETHANE

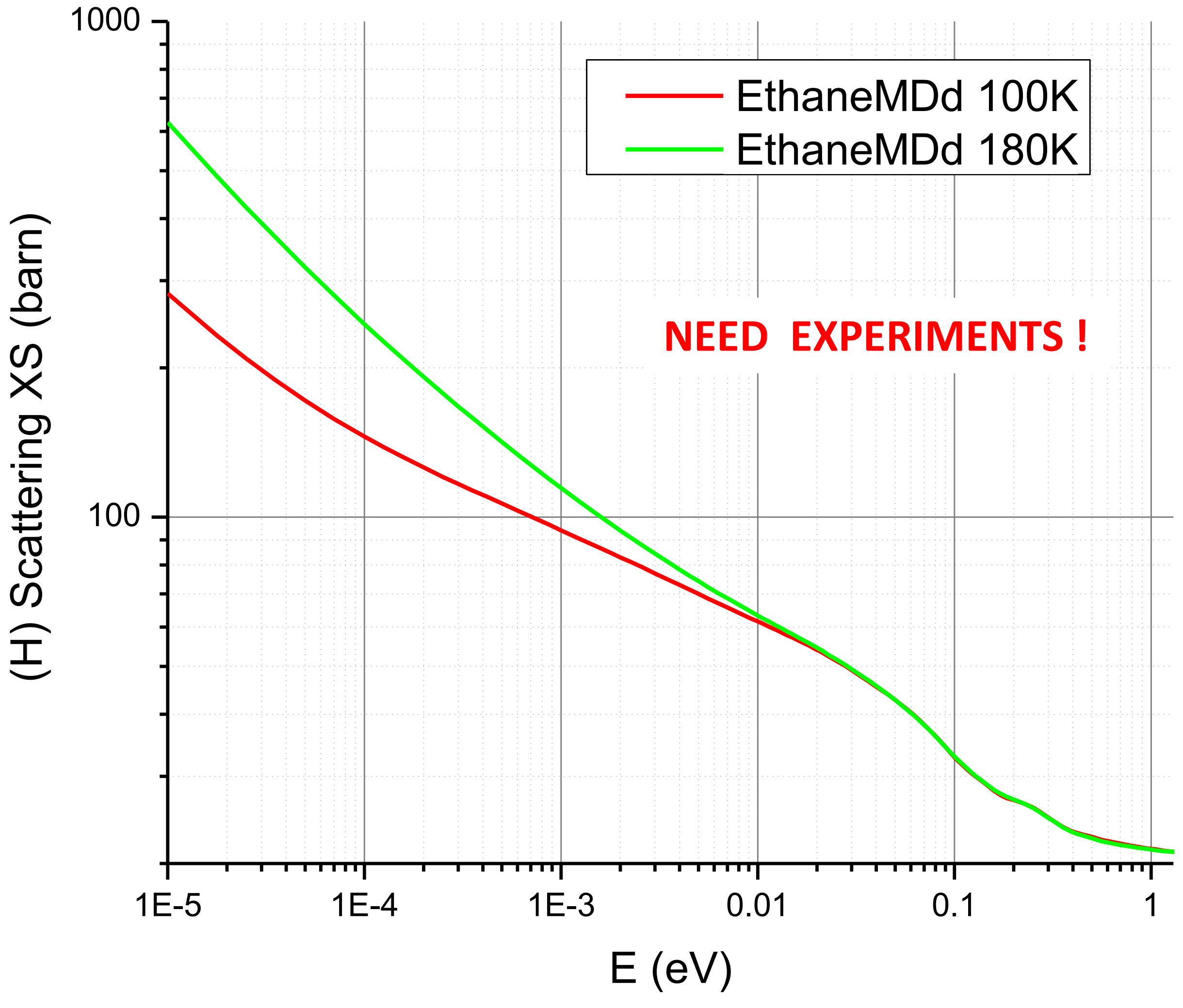
ETHANE (100K)

Frequency Spectrum from MD (lower part)

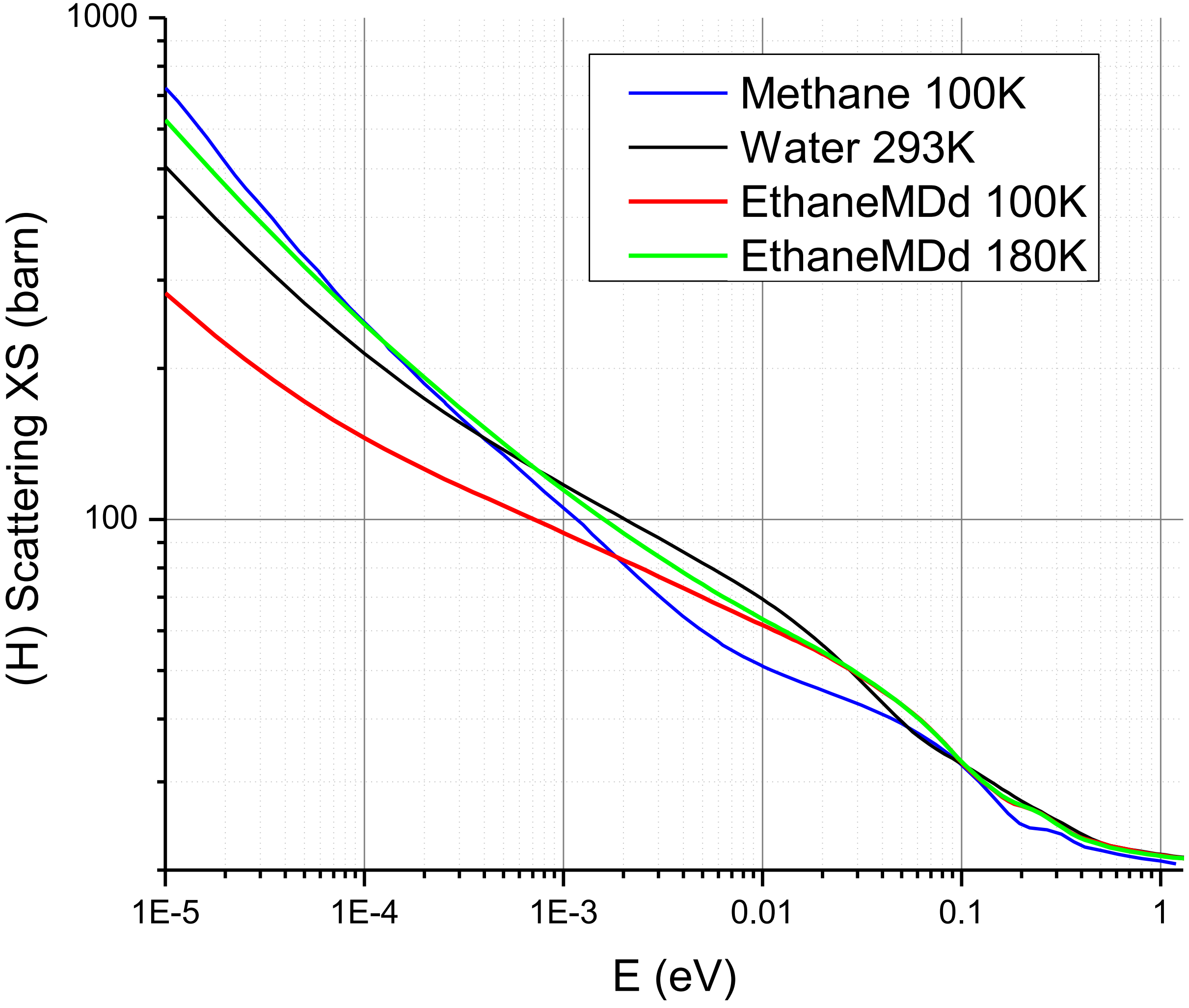




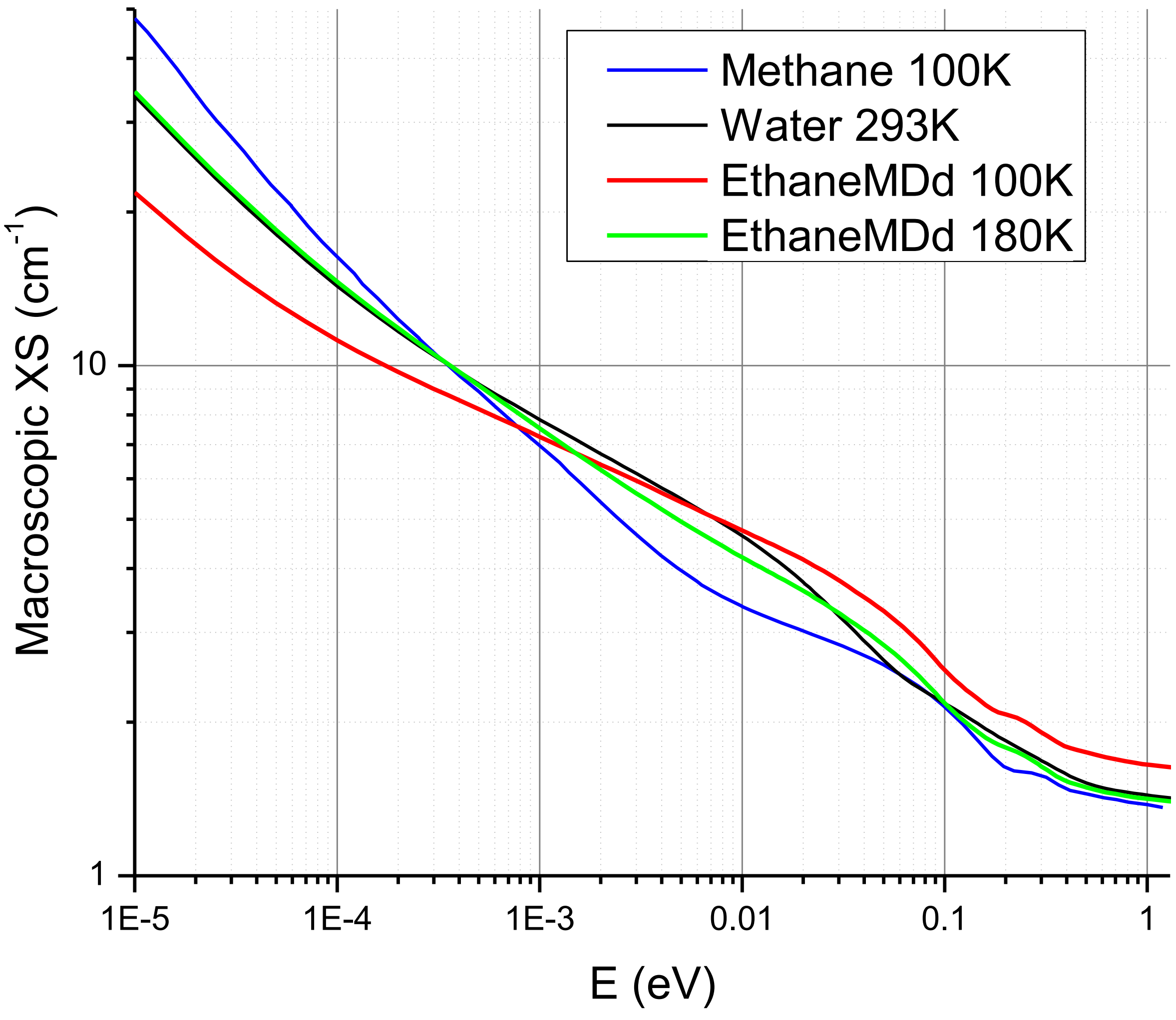
Predicted X-Section for H in Ethane over the liquid range



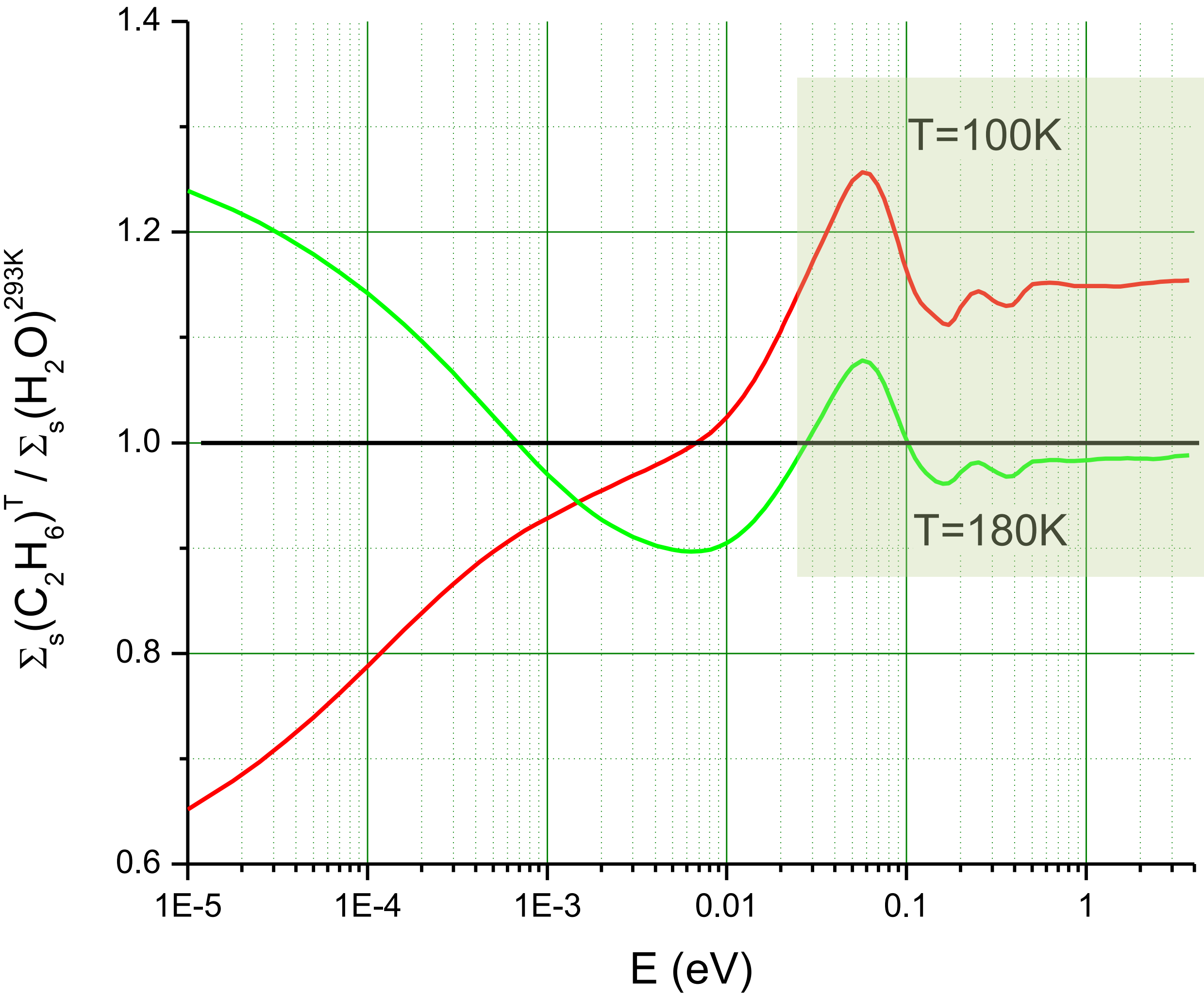
Predicted X-Section for H in Ethane and traditional liq. Mods.



Predicted Macrosc X-Section for H in Ethane and traditional liq. Mods.

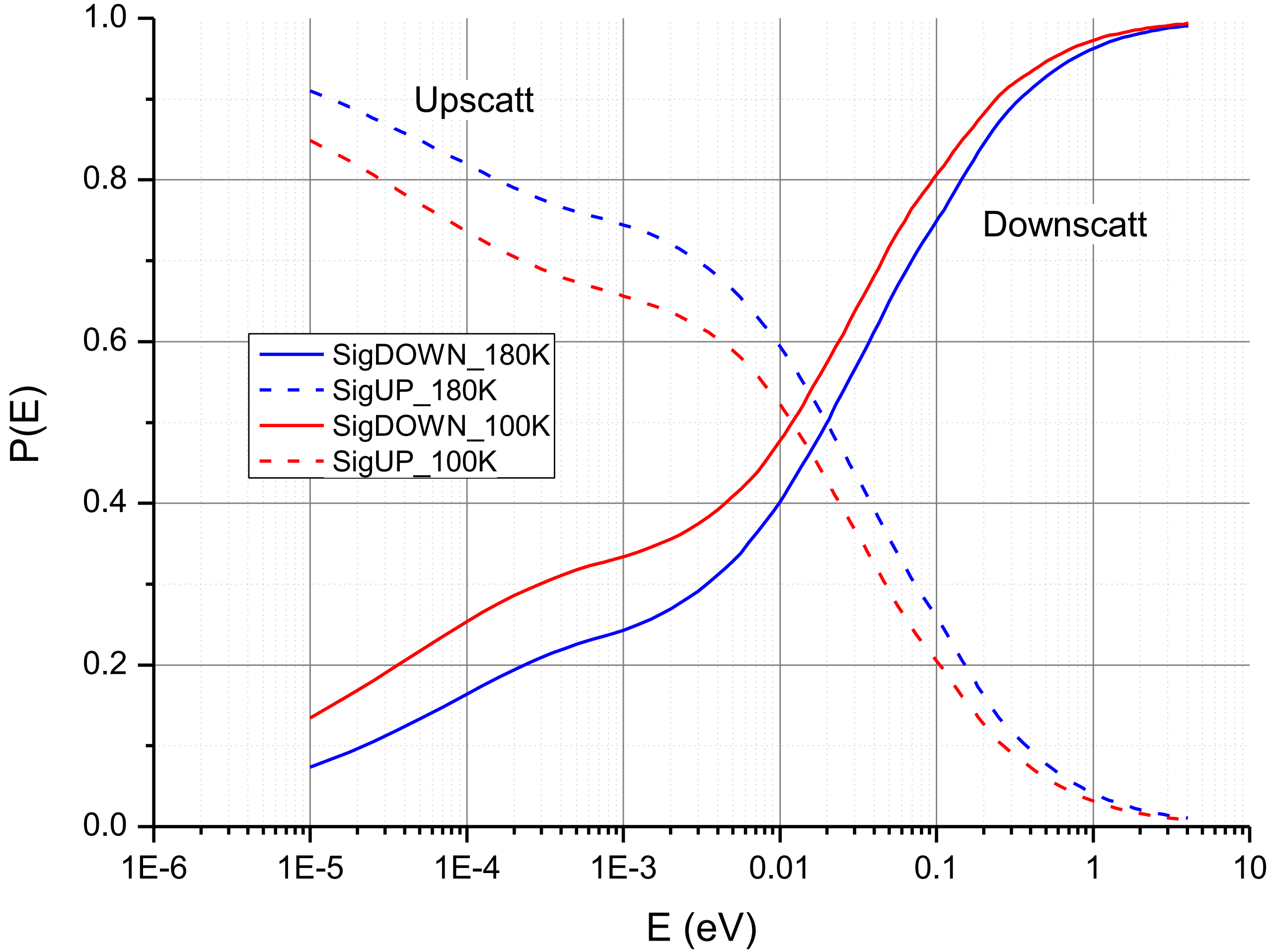


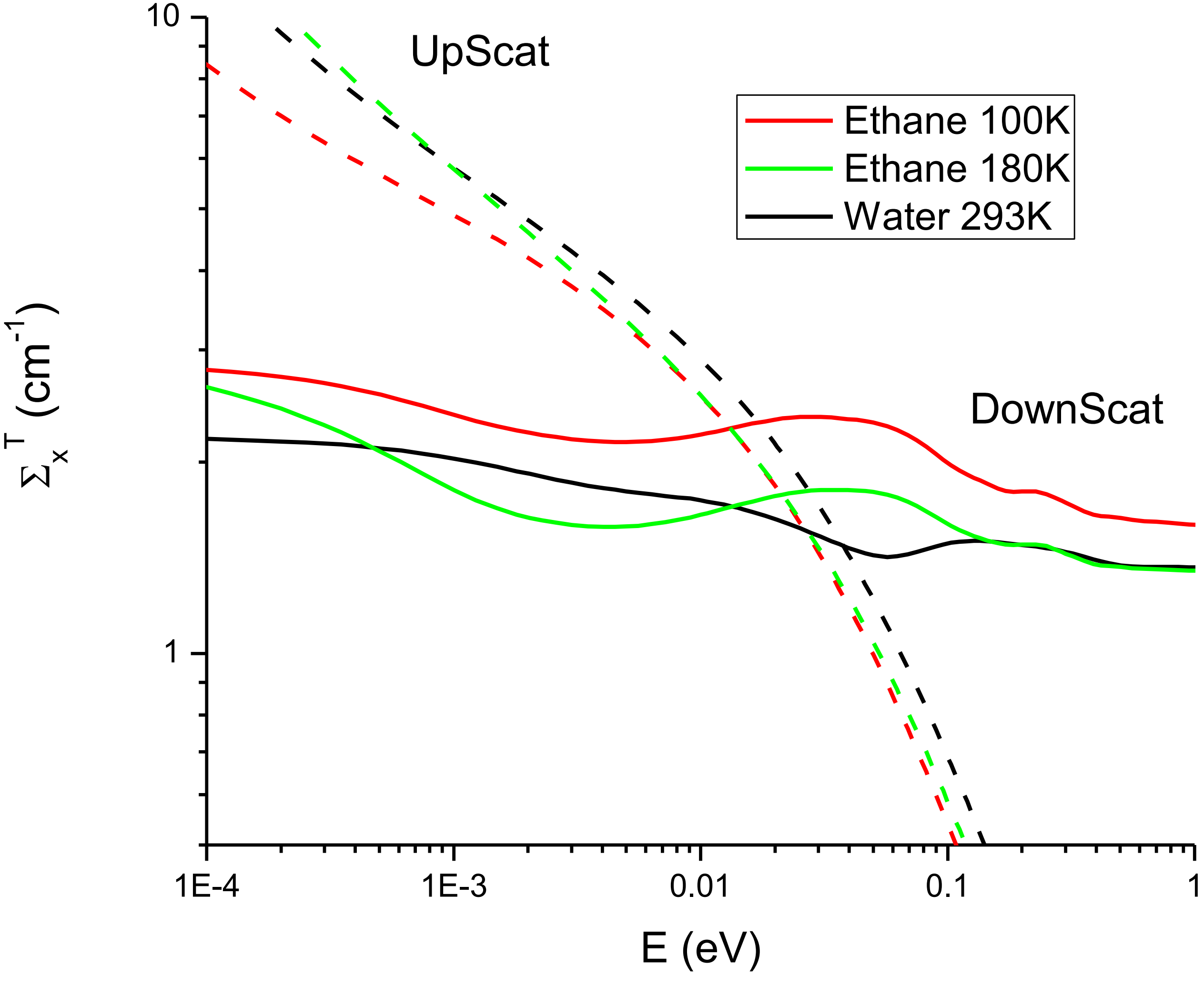
Ratio of Macrosc X-Section of Ethane and Water



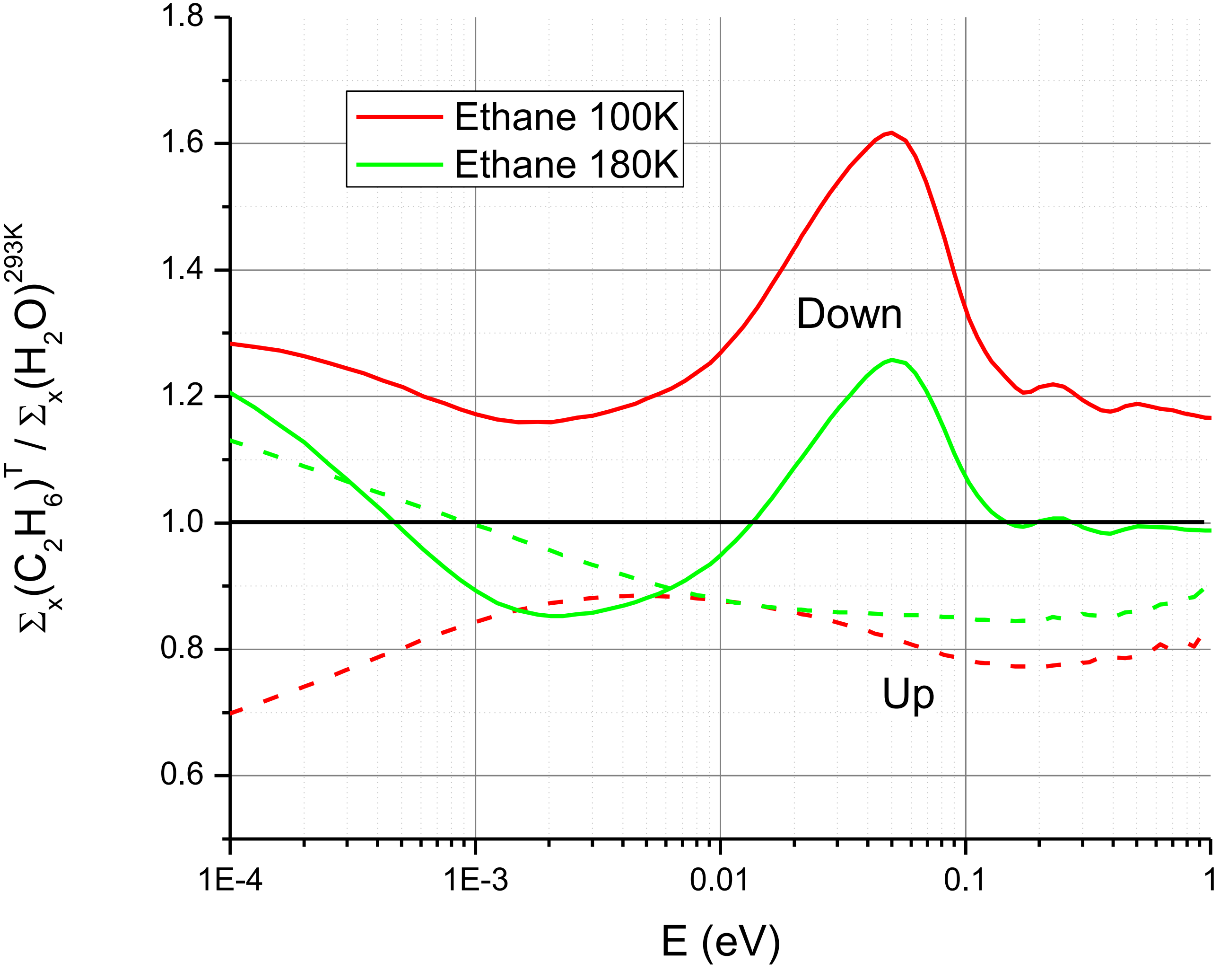
$$P(E) = \int \sigma(E \rightarrow E') \, dE' \;/\; \sigma(E)$$

UpScatt: $E' > E$, DownScatt: $E' < E$

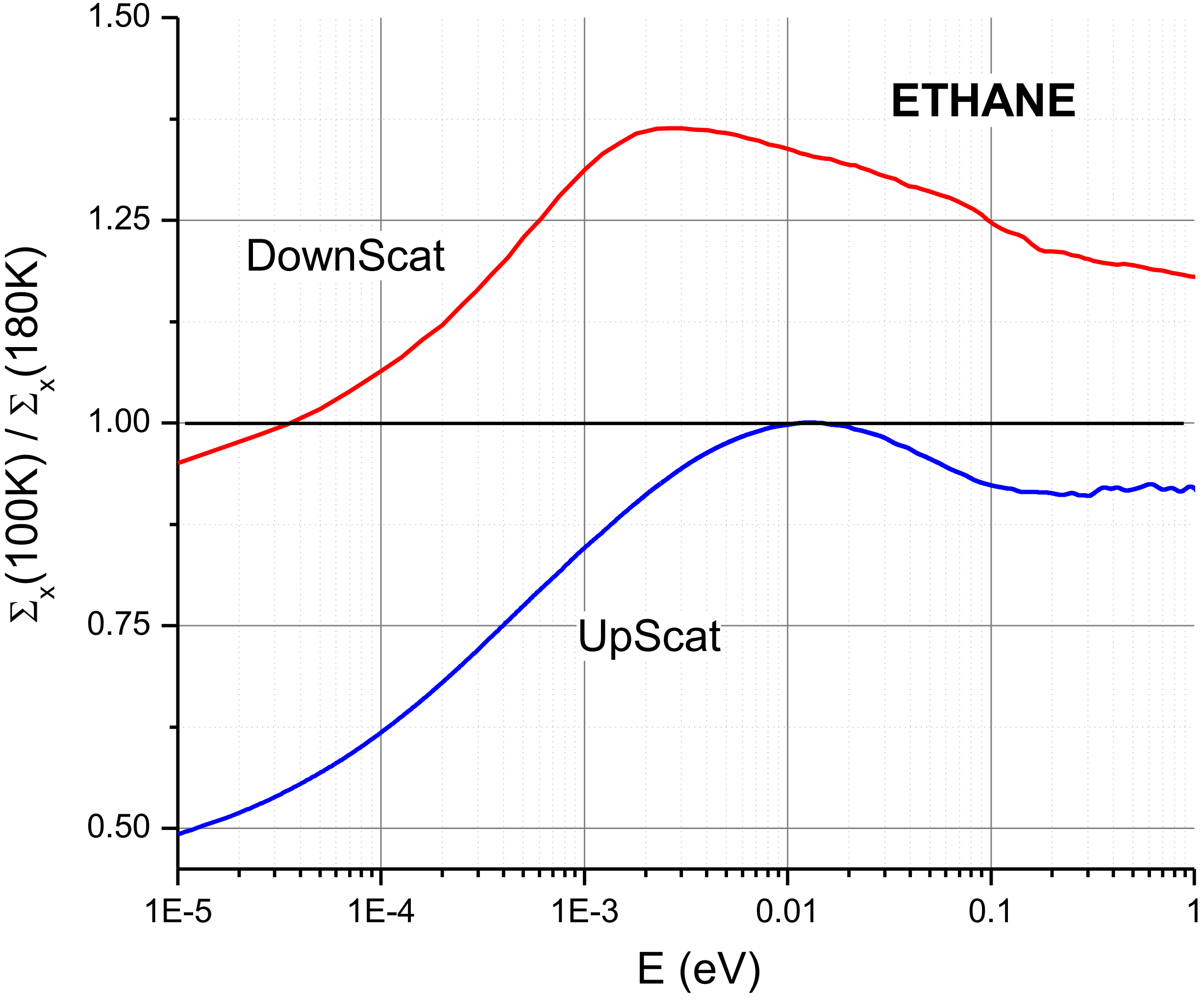




UpScat
DownScat
Ethane 100K
Ethane 180K
Water 293K
10
1
1E-4
1E-3
0.01
0.1
1
E (eV)
Σx T (cm-1)

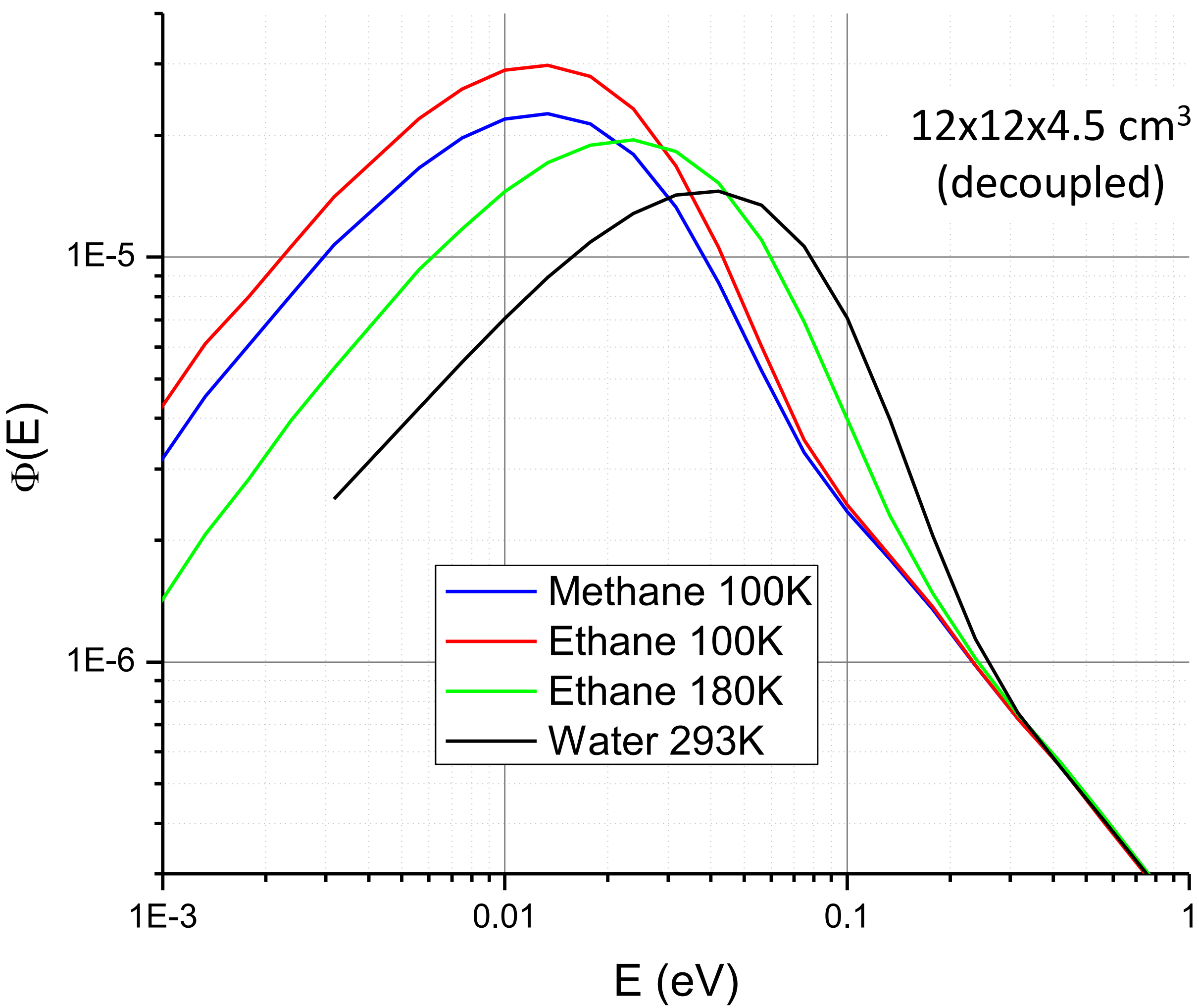


Ethane 100K
Ethane 180K
Down
Up
1.8
1.6
1.4
1.2
1.0
0.8
0.6
1E-4
1E-3
0.01
0.1
1
E (eV)
$\Sigma_x(C_2H_6)^T / \Sigma_x(H_2O)^{293K}$

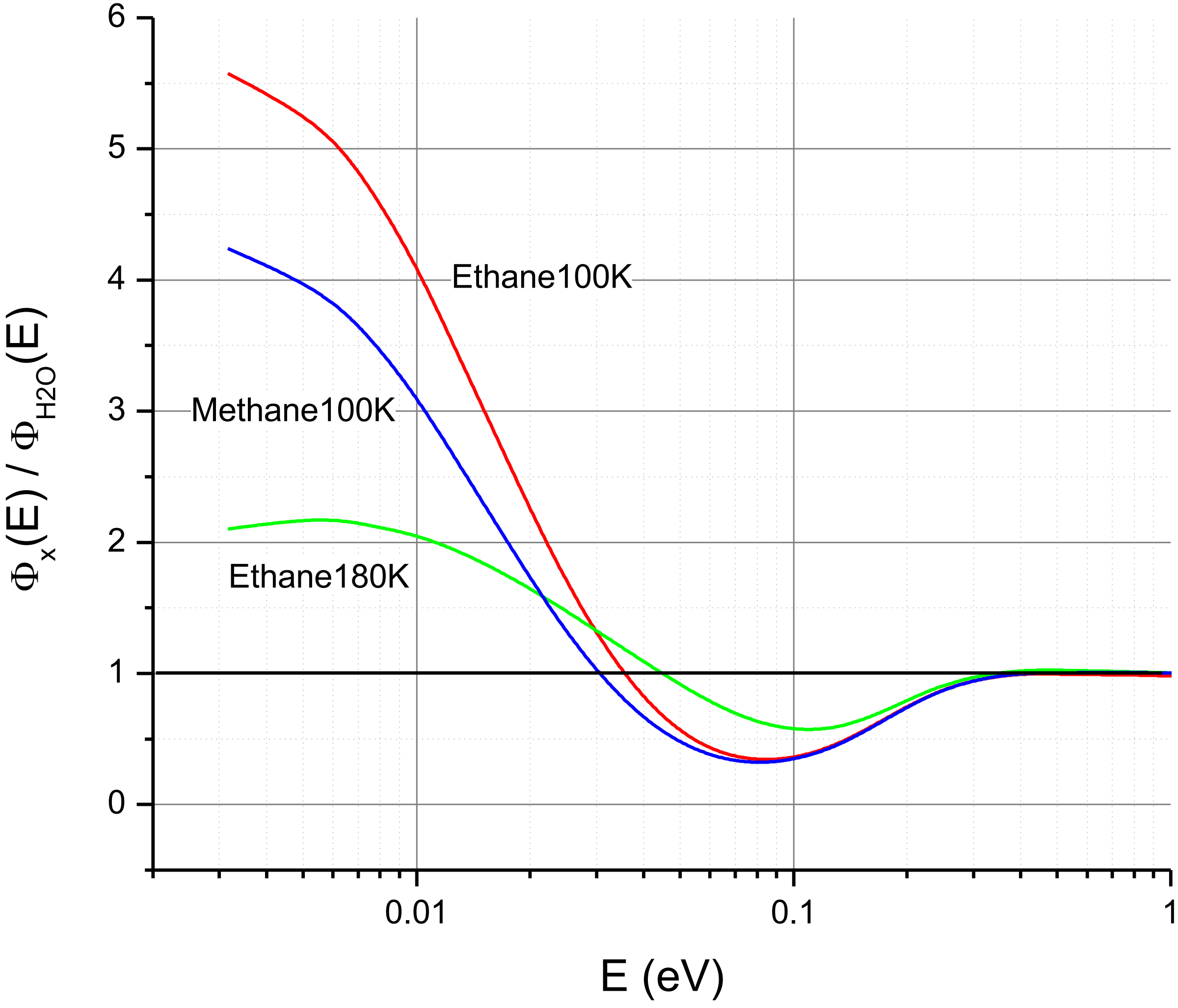


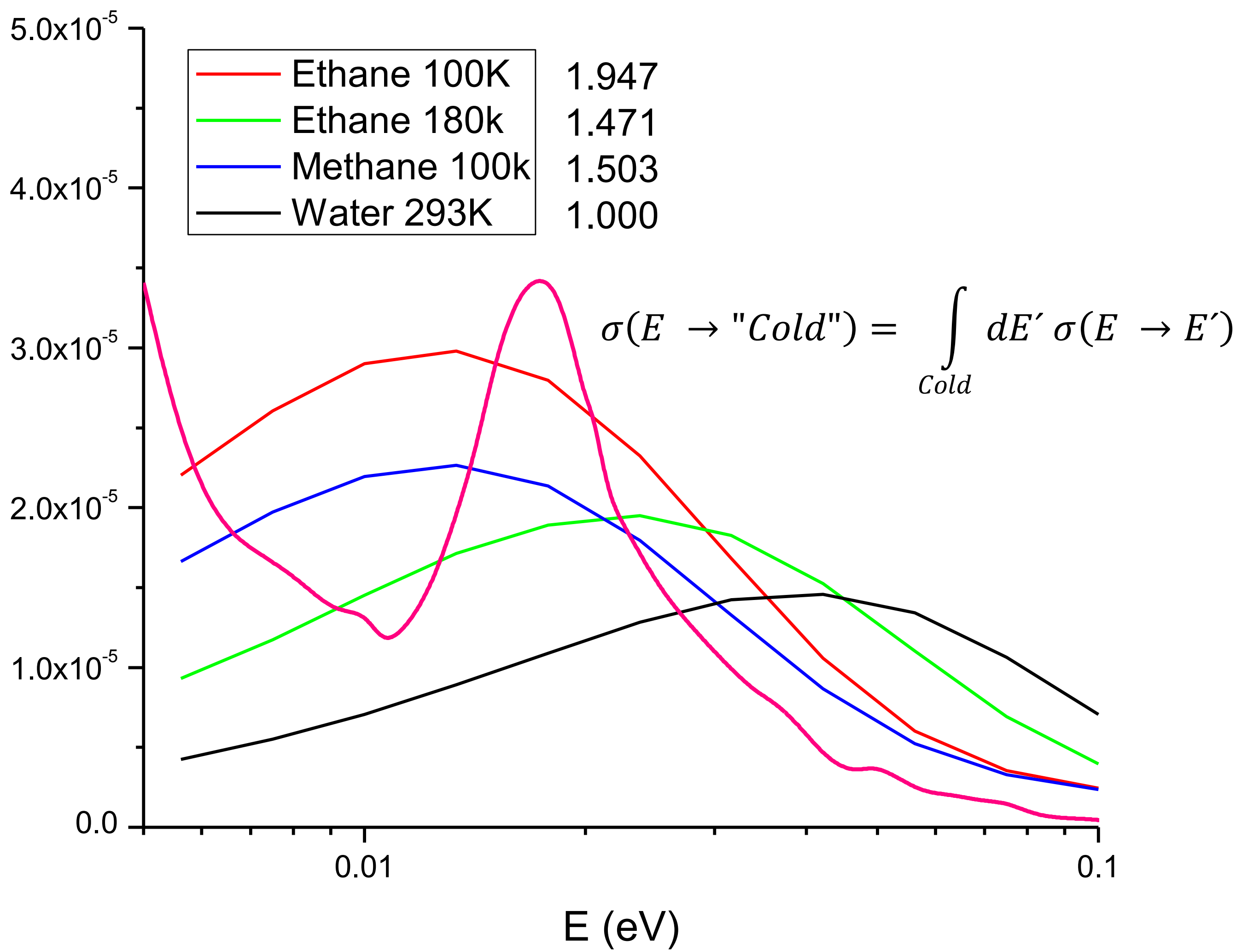
ETHANE
DownScat
UpScat
1.50
1.25
1.00
0.75
0.50
Σx(100K) / Σx(180K)
1E-5
1E-4
1E-3
0.01
0.1
1
E (eV)

Neutron Spectra from Ethane and traditional liq. Mods.



Ratio of Neutron Spectra from Ethane and Water





5.0x10^-5
4.0x10^-5
3.0x10^-5
2.0x10^-5
1.0x10^-5
0.0
Ethane 100K 1.947
Ethane 180k 1.471
Methane 100k 1.503
Water 293K 1.000
$\sigma(E \rightarrow \text{"Cold"}) = \int_{Cold} dE' \, \sigma(E \rightarrow E')$
0.01
0.1
E (eV)

THERMAL SCATTERING LAWS EVALUATED BY OUR GROUP:

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