Chapter 4

THERMAL SCATTERING DATA

Thermal scattering law data, S(α,β) are included for:

H in H_2O	8 temperatures from 293.6 to 623.6 K
D in D_2O	8 temperatures from 293.6 to 673.6 K
C in graphite	11 temperatures from 293.6 to 3 000 K
Be	8 temperatures from 293.6 to 1 200 K
H in polyethylene	2 temperatures, 293.6 and 350 K

The thermal scattering models are described in JEF Report 2 by J. Keinert and M. Mattes, IKE Stuttgart, "JEF-1 Scattering Law Data" (IKE 6 147, Sept. 1984). New evaluations of the phonon frequency spectra were made for H_2O and D_2O. For graphite and Be the lattice-dynamics model used to derive the phonon frequency spectrum is the same as that used for deriving the ENDF/B-III data.

The S(α,β) values are tabulated on a finer α,β mesh than that used for the ENDF/B thermal scattering data current at the time the evaluations were made. Extensive comparisons have been made with experiments.

Pointwise data have also been produced (using a modified version of NJOY-89.62) for the cold moderators, liquid ortho and para hydrogen at 20.38 K and liquid ortho and para deuterium at 23.65 K. Pointwise data have been produced because the corresponding scattering law data, S(α,β), have three digit exponents and require to be processed on 64 bit computers.

The S(α,β) data are taken from the JEF-1 scattering law data file (or the IKE file in the case of Be) and converted to ENDF-6 format. The number of principal atoms is added, and the principal atom scattering cross-section now agrees with the current general purpose evaluation. The effective temperatures for the principal atom have also been added. The files for H(H_2O,)and D(D_2O) date from November 1990 and those for Be, graphite and polyethylene from July 1991; they were prepared by M. Mattes of IKE Stuttgart.

Thermal scattering law data in the incoherent approximation have been generated using the code GASKET version 2 [5]. A maximum neutron energy transfer of 1.8554 eV was assumed using NMESH = 1 in GASKET-2. If the alpha or beta required is outside the range of the table in File 7, the differential scattering cross-section can be computed with the "short collision time" (SCT) approximation using the corresponding effective scattering temperatures T_{eff}. This is done e.g. in the THERMR module of NJOY [6].

The authors point out that data for intermediate temperatures should be obtained by interpolating between the resulting cross-sections and not by interpolating S(α,β).

H(H_2O)

Thermal neutron scattering law data in MF =7 are given for the temperatures:

T = 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6 K

Incoherent scattering (MT = 4) is represented by the thermal neutron scattering law $S(\alpha,\beta,T)$.

The frequency spectrum of hydrogen bound in water (H_2O) is based on a re-evaluation of the scattering dynamic model given in Refs. [1] and [2] at IKE. The improvements are as follows (Ref. [7]):

- Temperature dependence for the translational mass of H_2O is based on the results of Eucken [3].
- Temperature dependence for the hindered rotational band derived from Haywood and Page [4].
- -The two discrete vibrational modes for the intramolecular oscillations remained unchanged.

With this frequency distribution, thermal scattering law data have been generated for one hydrogen atom in the H_2O molecule in incoherent approximation using the code GASKET-2.

D(D_2O)

Thermal neutron scattering law data in MF = 7 are given for the temperatures:

T = 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 673.6 K

Incoherent scattering (MT = 4) is represented by the thermal neutron scattering law $S(\alpha,\beta,T)$.

The frequency spectrum of deuterium bound in heavy water (D_2O) is based on a re-evaluation of the scattering dynamic model given in [8,9]. The modifications are as follows:

- Upper oscillator frequency increased to 0.338 eV, being consistent with the value for H in H_2O.
- Re-normalisation of the temperature dependent band of hindered rotations derived from the results of Haywood and Page [10].
- Translational mass unit = 20.0 (temperature independent).

With this frequency distribution thermal scattering law data have been generated for one deuterium atom in the D_2O molecule in incoherent approximation with the code GASKET-2.

Beryllium

Thermal neutron scattering law data in MF = 7 are given for the temperatures:

T = 293.6, 400, 500, 600, 700, 800, 1 000, 1 200 K

- Coherent elastic scattering (MT = 2): The quantity actually given in the file is S(E,T), which is conveniently represented as a stair-step function with breaks at the Bragg edges using histogram interpolation. Bragg edges and structure factors are derived from the cross-section.

- Incoherent inelastic scattering (MT = 4) is represented by the thermal neutron scattering law $S(\alpha,\beta,T)$.

The frequency spectrum of polycrystalline beryllium was derived from a central force lattice dynamical model calculation of the unit cell [11,12]. With this frequency distribution the thermal scattering law data have been generated in incoherent approximation with the code GASKET-2.

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Thermal neutron scattering law data in MF = 7 are given for the temperatures:

T = 293.6, 400, 500, 600, 700, 800, 1 000, 1 200, 1 600, 2 000, 3 000 K

- Coherent elastic scattering (MT = 2): The quantity actually given in the file is S(E,T), which is conveniently represented as a stair-step function with breaks at the Bragg edges using histogram interpolation. Bragg edges and structure factors are derived from the cross-section.

- Incoherent inelastic scattering (MT = 4) is represented by the thermal neutron scattering law $S(\alpha,\beta,T)$.

The frequency spectrum for carbon bound in graphite was derived from a central force lattice dynamical model calculation of the graphite unit cell [12,13]. With this frequency distribution the thermal scattering law data have been generated in incoherent approximation with the code GASKET-2.

H in polyethylene

Thermal neutron scattering law data in MF = 7 are given for the temperatures T = 293.6 and 350 K.

- Incoherent elastic scattering (MT = 2) is represented using a bound cross-section and Debye-Waller integral given in the file as $W'(T)$ divided by the atomic mass (1/eV) as a function of temperature (K).

- Incoherent inelastic scattering (MT = 4) is represented by the thermal neutron scattering law $S(\alpha,\beta,T)$.

The phonon frequency spectrum of hydrogen bound in polyethylene was derived by Sprevak and Koppel [14] in calculating the dispersion relations for the infinite chain of CH_2 radicals as well as the polarisation vector for each normal frequency using the set of force constants determined by Lin and Koenig [15]. The weighted frequency spectrum was then calculated using the computed dispersion relations and the computed amplitude vectors.

The $S(\alpha,\beta)$ data are generated for one hydrogen atom in the CH_2 molecule in incoherent approximation for two temperatures with the code GASKET-2.

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