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JEF Report 2

JEF/DOC 41.2

IKE 6-147

JEF-1 SCATTERING LAW DATA

September 1984

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ABSTRACT

This report describes the scattering-law data adopted for the Joint Evaluated File (JEF) for light water, heavy water, graphite and polyethylene. Tests that have been carried out on these data are outlined and comparisons of derived quantities with experimental data are presented in graphical form.

Report prepared at the NEA Data Bank

by M. Mattes and E. Sartori

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I. INTRODUCTION

The scattering law data that are still widely utilised are those released with the version III of ENDF/B. Their use has shown that they are of acceptable quality. New evaluations of the phonon frequency spectra have, however, been carried out since then and comparison with experiment has shown that these give better results especially for light water. In addition the number of points at which the scattering law data were tabulated in ENDF/B has not always been found to be adequate.

The new scattering law data have therefore been calculated on a finer mesh of α and β values. Extensive comparisons with experimental data have also been carried out.

These improved data for the thermal neutron scattering behaviour are adopted for inclusion in the Joint Evaluated File JEF.

II. GENERAL DATA DESCRIPTION

The scattering law $S(\alpha,\beta)$ describes the binding of the scattering atoms in a moderator material.

In ENDF/B notation (1), the thermal incoherent scattering cross section is related to $S(\alpha,\beta)$ as follows:

$$\sigma^{inc}(E\rightarrow E',\mu,T) = \sigma_b/(2kT)\sqrt{\frac{E'}{E}}\, e^{-\frac{\beta}{2}} S(\alpha,\beta,T)$$

where E - initial neutron energy
E' - energy of the scattered neutron
μ - scattering cosine in the laboratory system
σ_b - bound incoherent scattering cross section of the nuclide
k - Boltzmann's constant
T - temperature in Kelvin
β - dimensionless energy transfer = (E'-E)/kT
α - squared dimensionless momentum transfer = $(E'+E-2\mu\sqrt{E'E})/(AkT)$
A - ratio of the scatterer mass to the neutron mass

The bound scattering cross section is related to the free atom scattering cross section as follows:

$$\sigma_b = (A+1)^2/A^2 * \sigma_{free}$$

For binding in liquids and solids, $S(\alpha,\beta,T)$ for several moderator materials has been computed with the GASKET code (2). The data has been produced in ENDF/B-V File 7 format. The scattering law is given as tables of S versus α for various values of β and different temperatures. Any desired value of S for the given temperatures can be obtained by interpolation in α and β. Interpolation in temperature of $S(\alpha,\beta)$ is not recommended. For intermediate temperatures the interpolation should be carried out on the cross sections and <u>not</u> on the $S(\alpha,\beta)$ values.

If the required α or β is outside the range of the table in File 7, the scattering law may be computed using the short collision time approximation for neutron downscattering ($\beta<0$)

$$S(\alpha,\beta,T,T_{eff}) = (4\pi\alpha T_{eff}/T)^{-\frac{1}{2}}\, e^{\frac{\beta}{2}}\, e^{-\frac{T}{4\alpha T_{eff}}(\alpha+\beta)^2}$$

Neutron upscattering can be computed by forcing detailed balance ($S(\alpha,\beta) = S(\alpha,-\beta)$). T_{eff} is the effective temperature of the scatterer; its values are usually larger than the corresponding Maxwellian temperature. T_{eff} is related to the phonon frequency spectrum $\varrho(\omega)$ of the scatterer as follows

$$T_{eff} = \hbar/2k\int_0^\infty \varrho(\omega)*\omega*\coth(\hbar\omega/2kT)d\omega \quad , \quad \hbar\omega = E-E'$$

Another parameter related to $\varrho(\omega)$ is the Debye-Waller integral.

$$W = 1/\hbar\int_0^\infty \varrho(\omega)/\omega*\coth(\hbar\omega/2kT)d\omega$$

It is used in calculating coherent or incoherent elastic scattering cross sections.

III. MODERATORS

1. WATER H_2O, MAT=4001

1.1 Physics of the Neutron-Proton Scattering, Frequency Spectra and Related Parameters

The thermal neutron-proton scattering dynamics for Hydrogen bound in water, H_2O, is characterised by the excitation of the fundamental dynamical modes of the H_2O molecules. For the three modes of motion, the following assumptions are made:

(a) Free translational motion of H_2O molecules clusters. The number of molecules in the water clusters is temperature-dependent (3) as shown in Fig. 1.

The temperature dependent translational masses were derived and are displayed in Fig. 2 and Table 1. This is an improvement compared to ENDF/B (MAT=1002) (4,5) where a single H_2O molecule of mass 18 is used as a translational unit. A better agreement with experiment is achieved for the double-differential scattering cross sections in the quasi-elastic scattering range as shown, in Figs. 5 and 6 for example.

Table 1: Effective temperature-dependent translational masses(amu) of the H_2O molecular clusters

T/K	293.6	323.6	373.6	423.6	473.6	523.6	573.6	623.6
M_t	46	39	31	27	25	23	22	21

(b) The frequency band of hindered rotations (torsional harmonic oscillations of the H_2O molecule) is assumed to be temperature dependent.

By interpolating the two frequency spectra at T = 295K and 550K (Fig. 3) based on the results of Haywood, Page (6) spectra for other temperatures were derived.

(c) The internal vibrations of the H_2O molecule are treated as discrete harmonic oscillations according to Nelkin (7), assuming ω_2=205 meV for the bending vibration. The symmetric and asymmetric stretching vibrations are combined at $\omega_{1,3}$ = 480 meV. The corresponding oscillator masses are assumed as 3 and 6 (see Table 2).

Table 2: Effective masses (amu) related to the H_2O dynamical modes

data base / modes	ENDF/B MAT=1002	JEF-1/IKE MAT=4001
translations	18	46-21
rotations	2.25	2.09-2.21
oscillations		
$\omega_{1,3}$	3	3
ω_2	6	6

The effective scattering temperature of hydrogen bound in water is given in Table 3 and shown in Fig. 4.

Table 3: Integral parameters derived from the frequency spectra of H in H_2O

Temperature (k)	Debye-Waller integral (1/eV)	T_{eff} (K)
293.6	20.68	1398.6
323.6	21.78	1405.1
373.6	23.68	1417.9
423.6	25.66	1433.3
473.6	27.69	1450.9
523.6	29.75	1470.1
573.6	31.82	1491.0
623.6	33.91	1513.2

Thermal neutron scattering in water is dominated by the hydrogen nucleus because of its large free atom scattering cross section and the double atomic density. The hydrogen scatter is essentially incoherent because the coherent scattering cross section is very small and there is little relative order in the liquid phase.

1.2 Data stored in the JEF File

The quantities stored for light water (MAT=4001) are described in the information file MF=1, MT=451 given in Appendix 2.

These are:

$S(\alpha,\beta,T)$ (MF=7,MT=4) for H in H_2O at the following 8 temperatures:

	293.6	323.6	373.6	423.6	473.6	523.6	573.6	623.6	K
i.e.	20	50	100	150	200	250	300	350	C

The data are represented in the temperature-dependent ENDF/B data format (see Appendix F of (1)) at 100 values of α and 150 values of β. The energy limit E_{max} up to which $S(\alpha,\beta,T)$ can be used is 1.8554 eV.

The effective scattering temperatures that are required for the short collision time approximation for higher energy transfers are given in the form of a table in MF=1, MT=451.

The total free atom scattering cross section of Hydrogen is 20.449 b as in ENDF/B-V MAT=1301.

For the neutron scattering by Oxygen, the values for free gas approximation are also stored in file 7.

The molecular absorption cross section is given in MF=3, MT=102.

1.3 Differential Neutron Scattering Data

Comparisons of experimental and derived data from $S(\alpha,\beta,T)$ for double differential and differential neutron scattering cross sections for different incident energies and angles are shown in Figs. 5 through 14. An improvement in the double differential data when compared to ENDF/B can be observed.

1.4 Comparison with Integral Data

The total cross section for water computed from ENDF/B and IKE/JEF-1 data are compared against experimental data in Fig. 15 for room temperature. At lower energies a better agreement with experiment is observed. Fig. 16 shows the comparison at 450 K.

The average cosine of the scattering angle and the neutron diffusion coefficient D(E) for H_2O obtained by processing the JEF data are compared against experimental data at room temperature and at T=200 C in Figs. 17 through 20.

A set of 126 group cross sections derived from the JEF/IKE data was used to calculate the temperature dependence of the diffusion coefficient $\overline{D}$, the neutron diffusion length $\overline{L}$ and the average diffusion constant D_o (their definition is given in the Appendix 1). The obtained results are compared against experiments in Figs. 21, 22, and 23. A good agreement is observed.

1.5 Comparison of Computed and Measured Neutron Flux Spectra

This section shows graphical comparisons of computed and measured neutron flux spectra at different temperatures and different poison concentrations. A 126 thermal-group cross-section library has been used for this purpose (42).

Figs. 24 through 33 show the good agreement that has been obtained with experimental data.

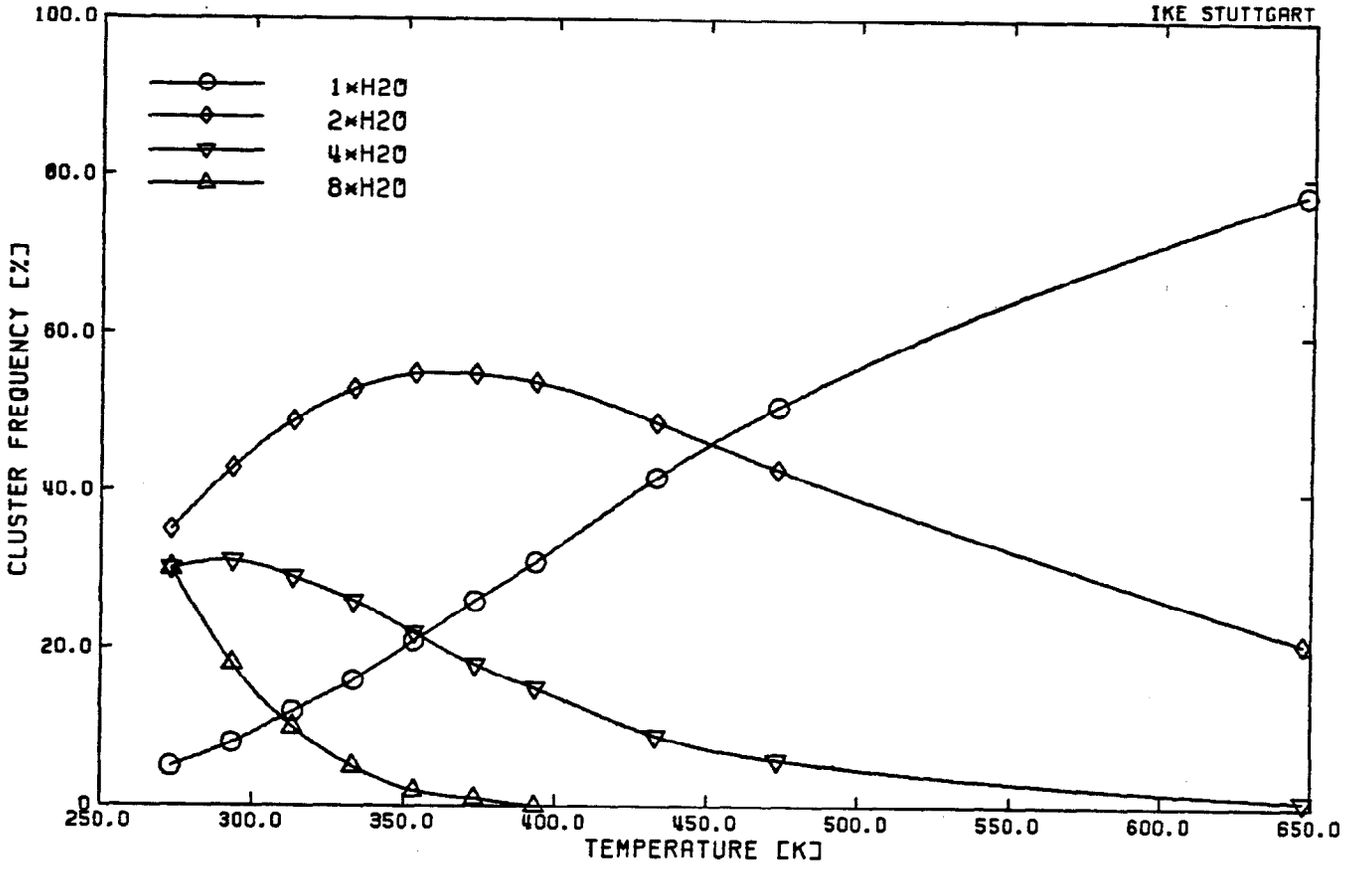

Fig. 1 Cluster Structures of Water (Eucken 1946)

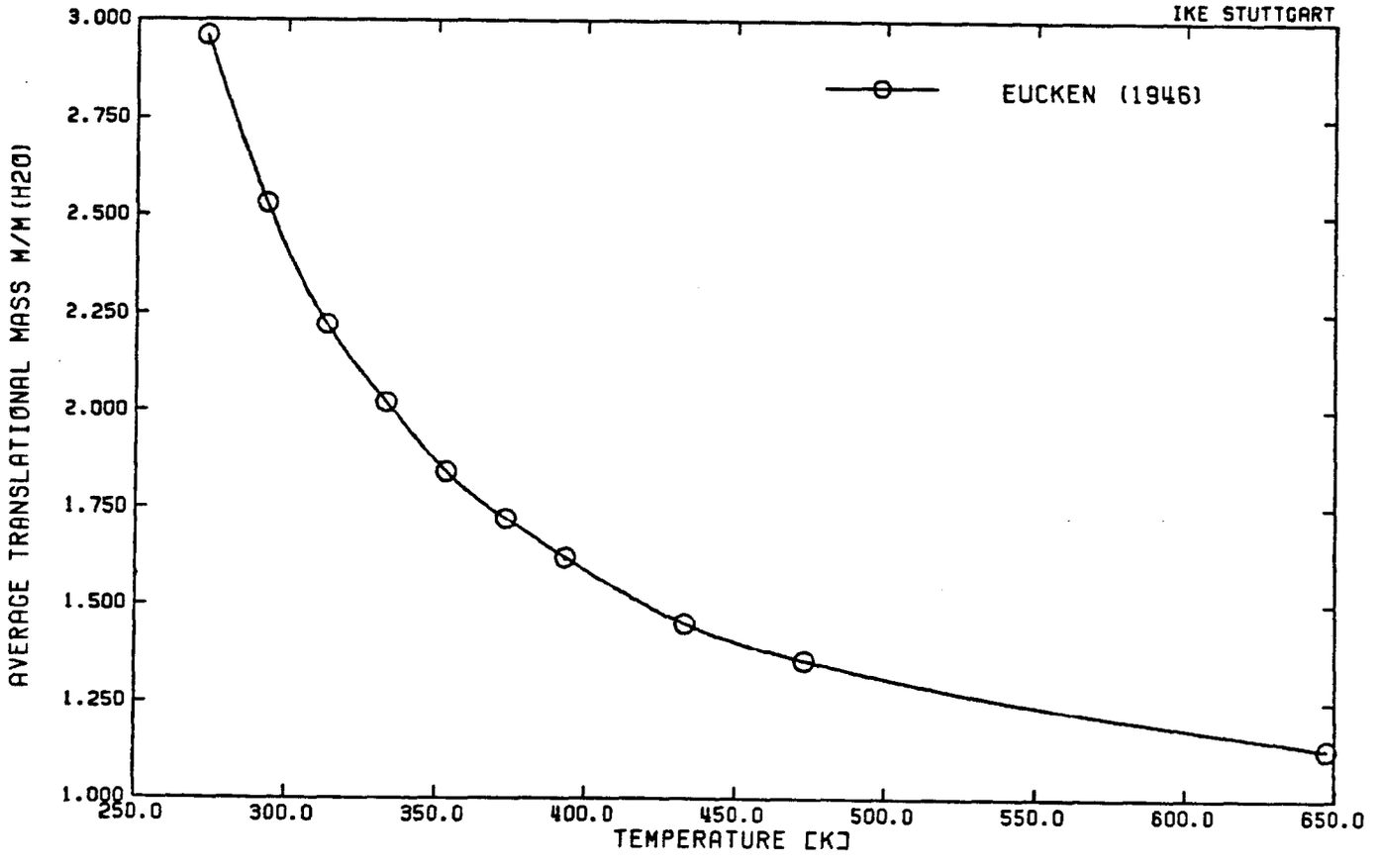

Fig. 2 Translational Masses of Water, H_2O

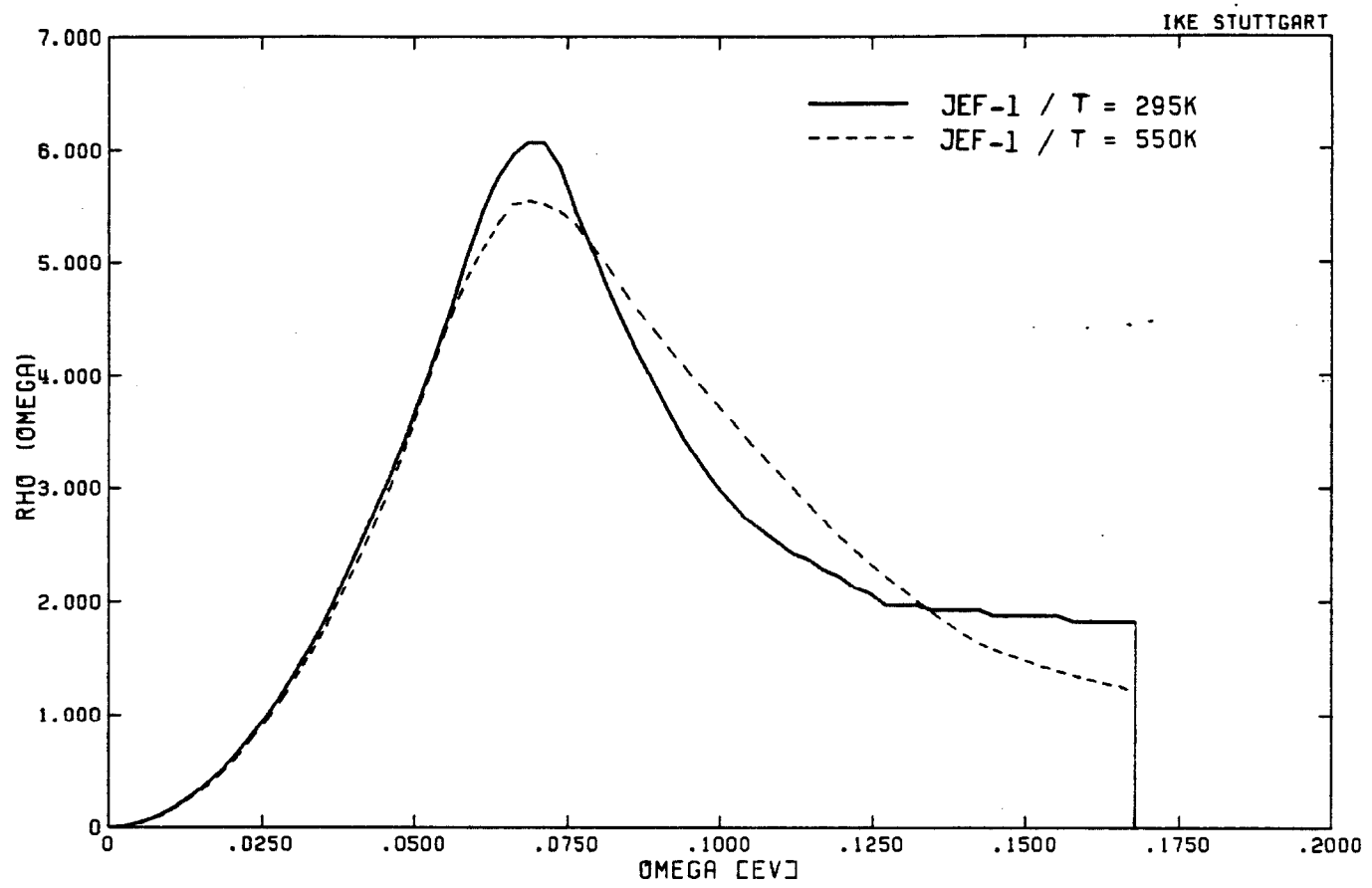

Fig. 3 Phonon Frequency Spectra for the Hindered Rotations of Hydrogen Bound in Liquid Water

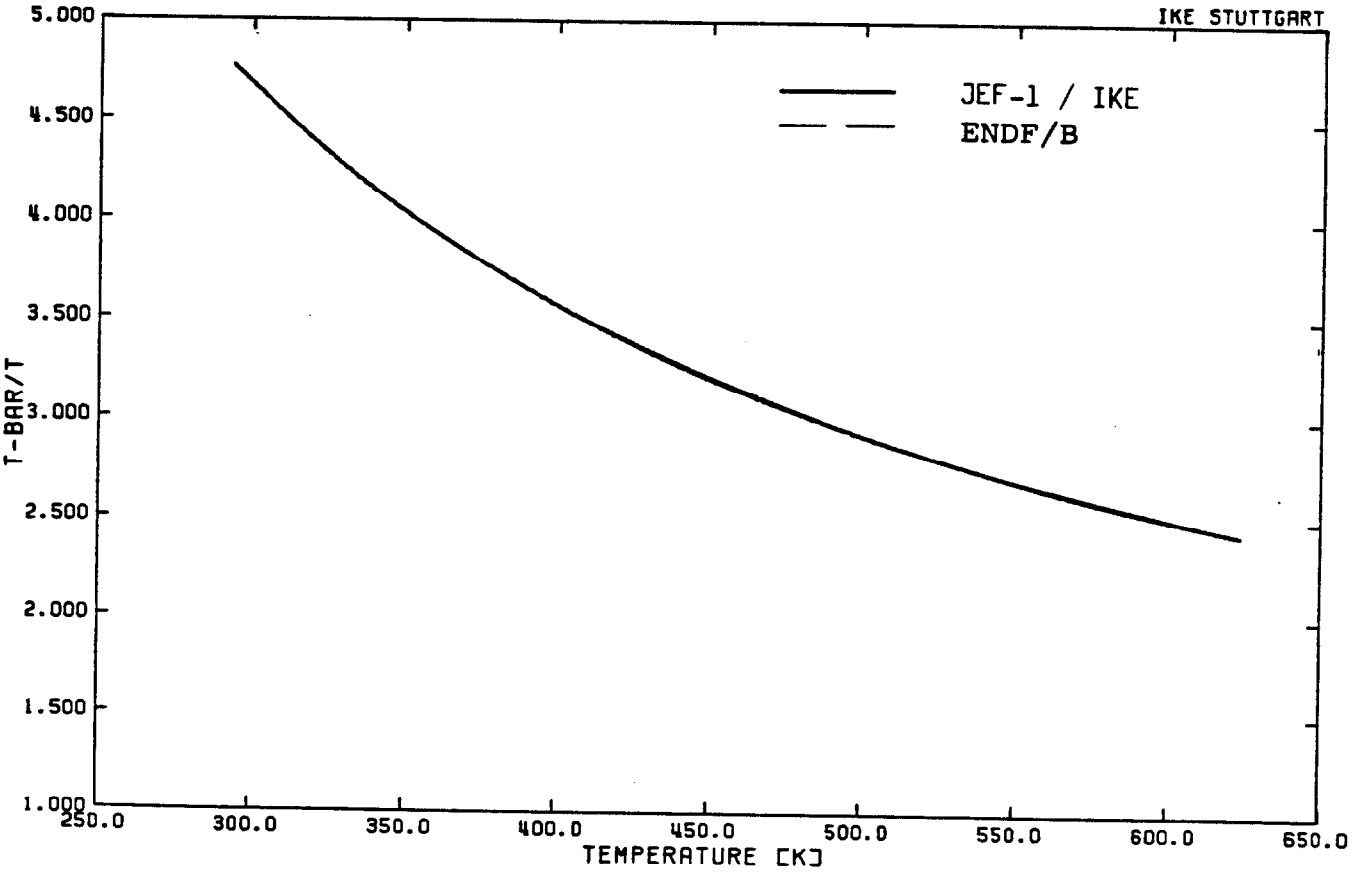

Fig. 4 Effective Scattering Temperature of Hydrogen Bound in Water

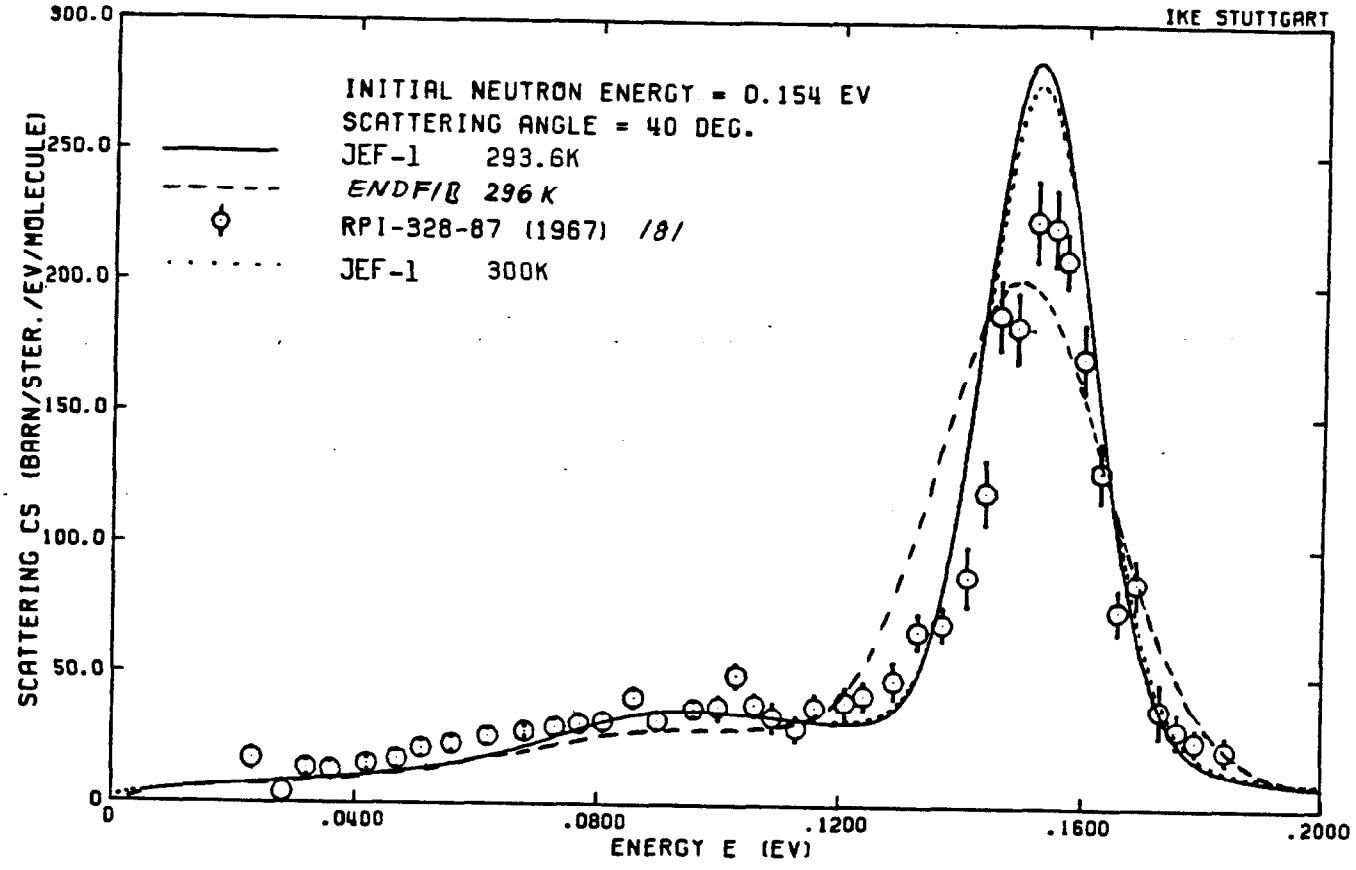

Fig. 5 Double Differential Neutron Scattering Cross Section for Water at 300 K at E = 0.154 eV and 40 degrees

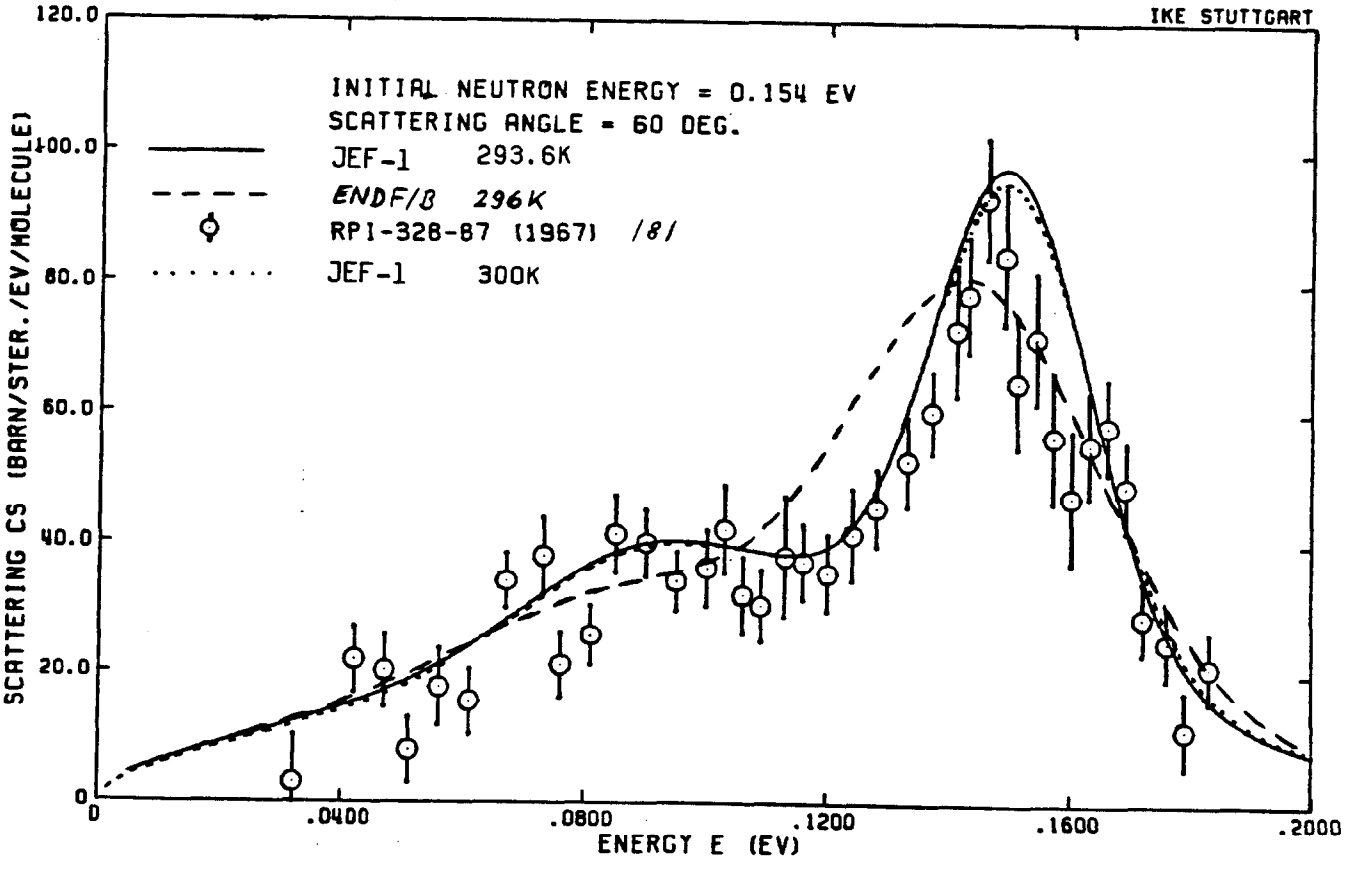

Fig. 6 Double Differential Neutron Scattering Cross Section for Water at 300 K

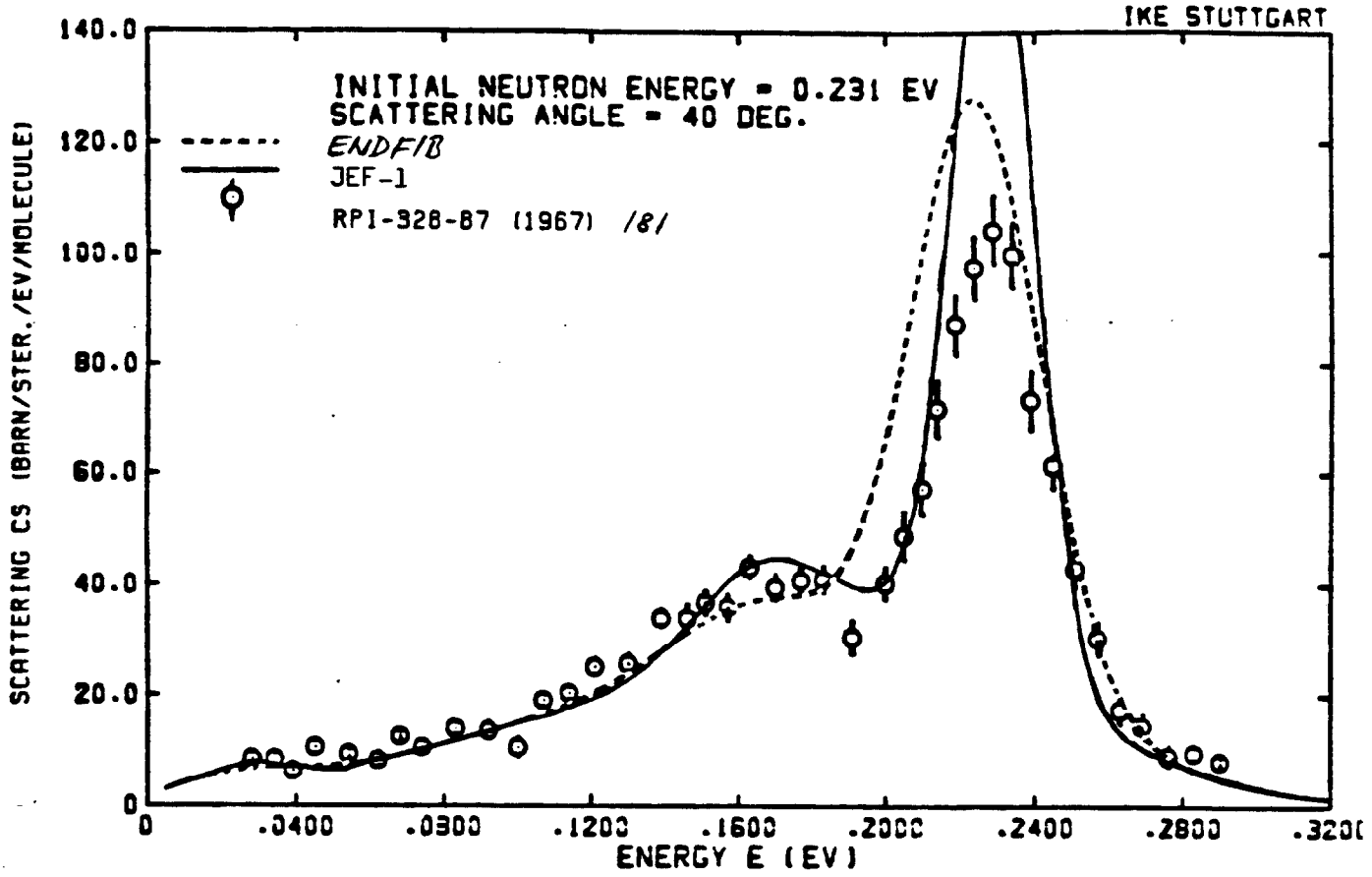

Fig. 7 Double Differential Neutron Scattering Cross Section for Water at 300 K

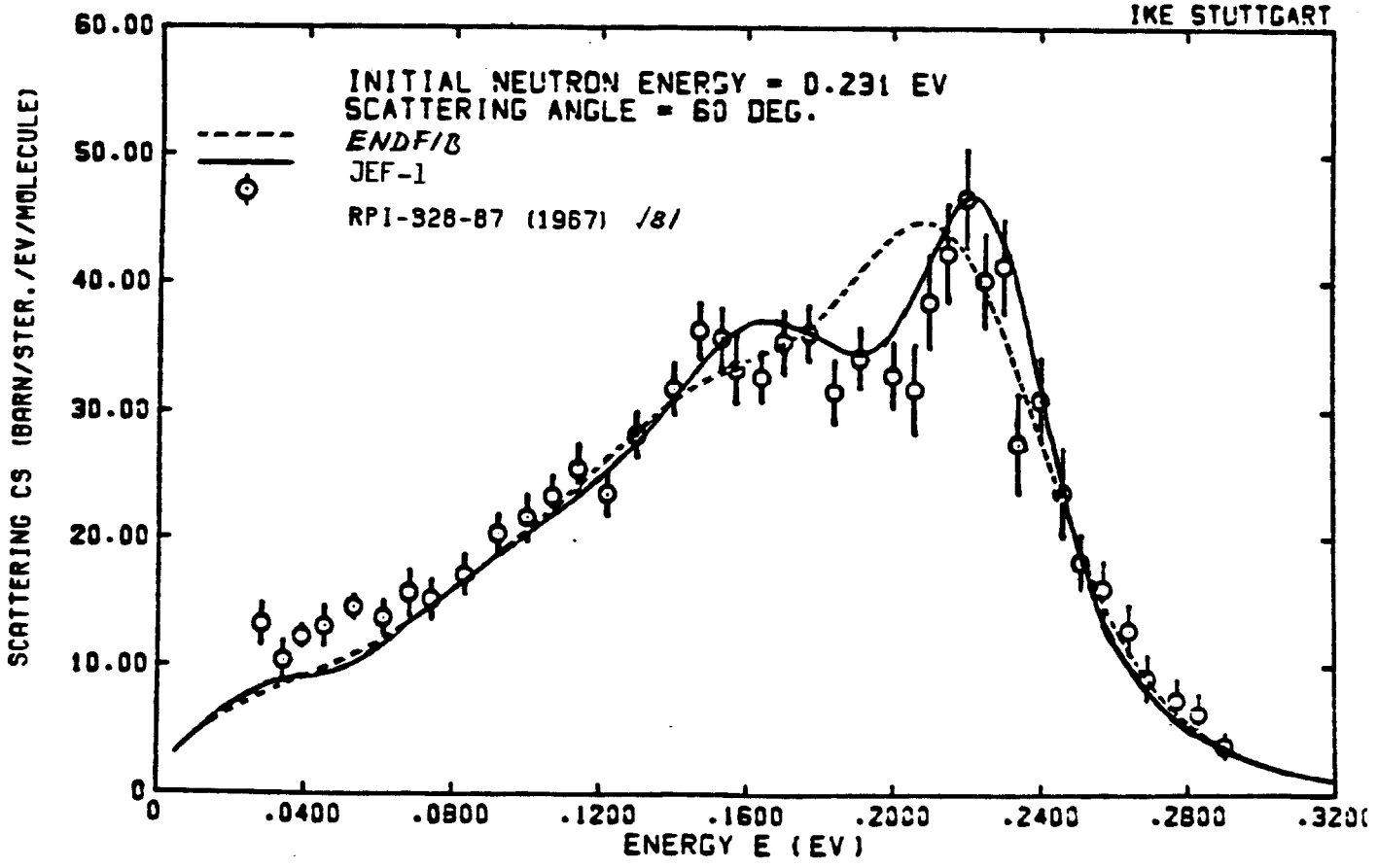

Fig. 8 Double Differential Neutron Scattering Cross Section for Water at 300 K

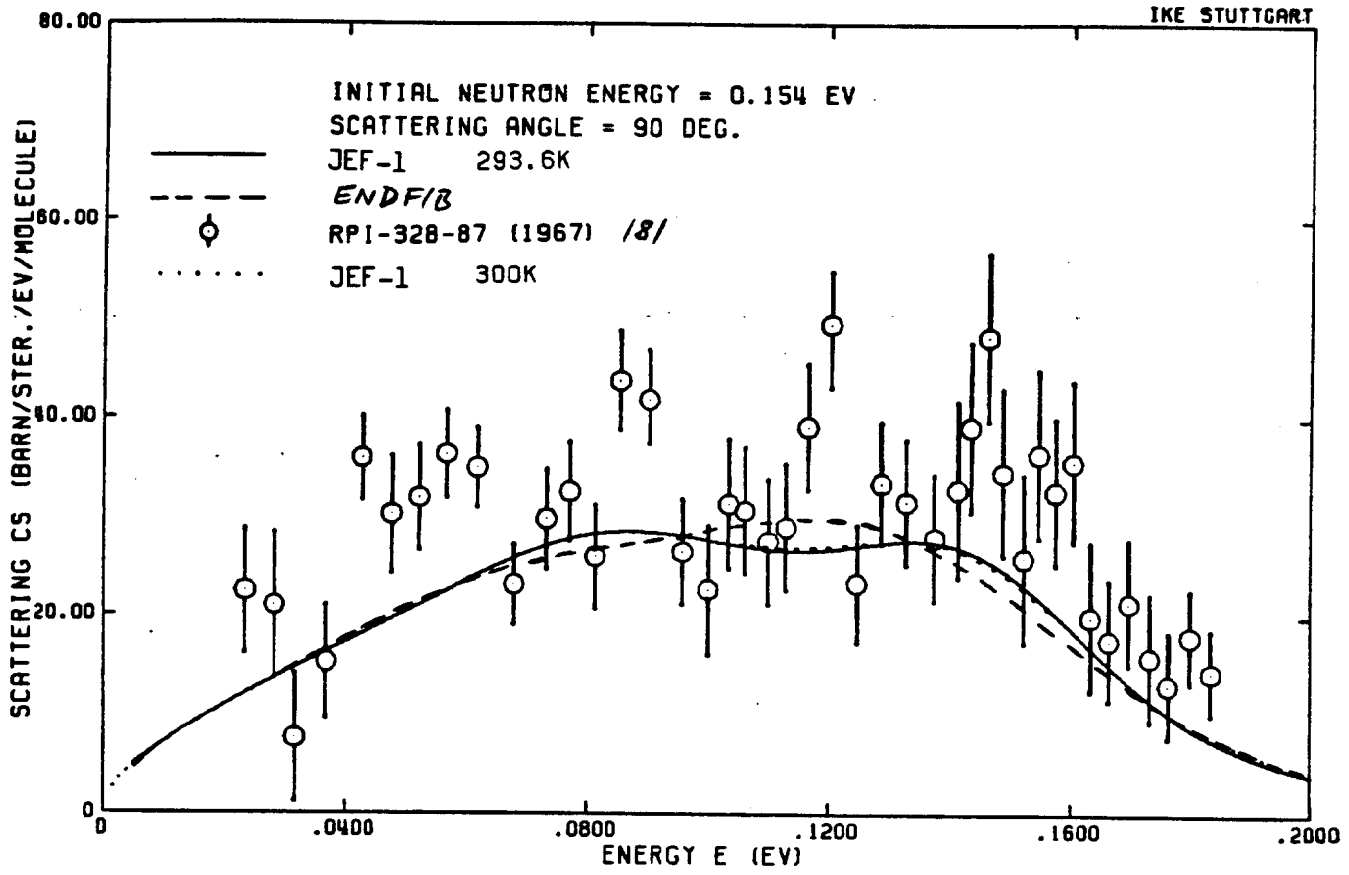

Fig. 9 Double Differential Neutron Scattering Cross Section for Water at 300 K

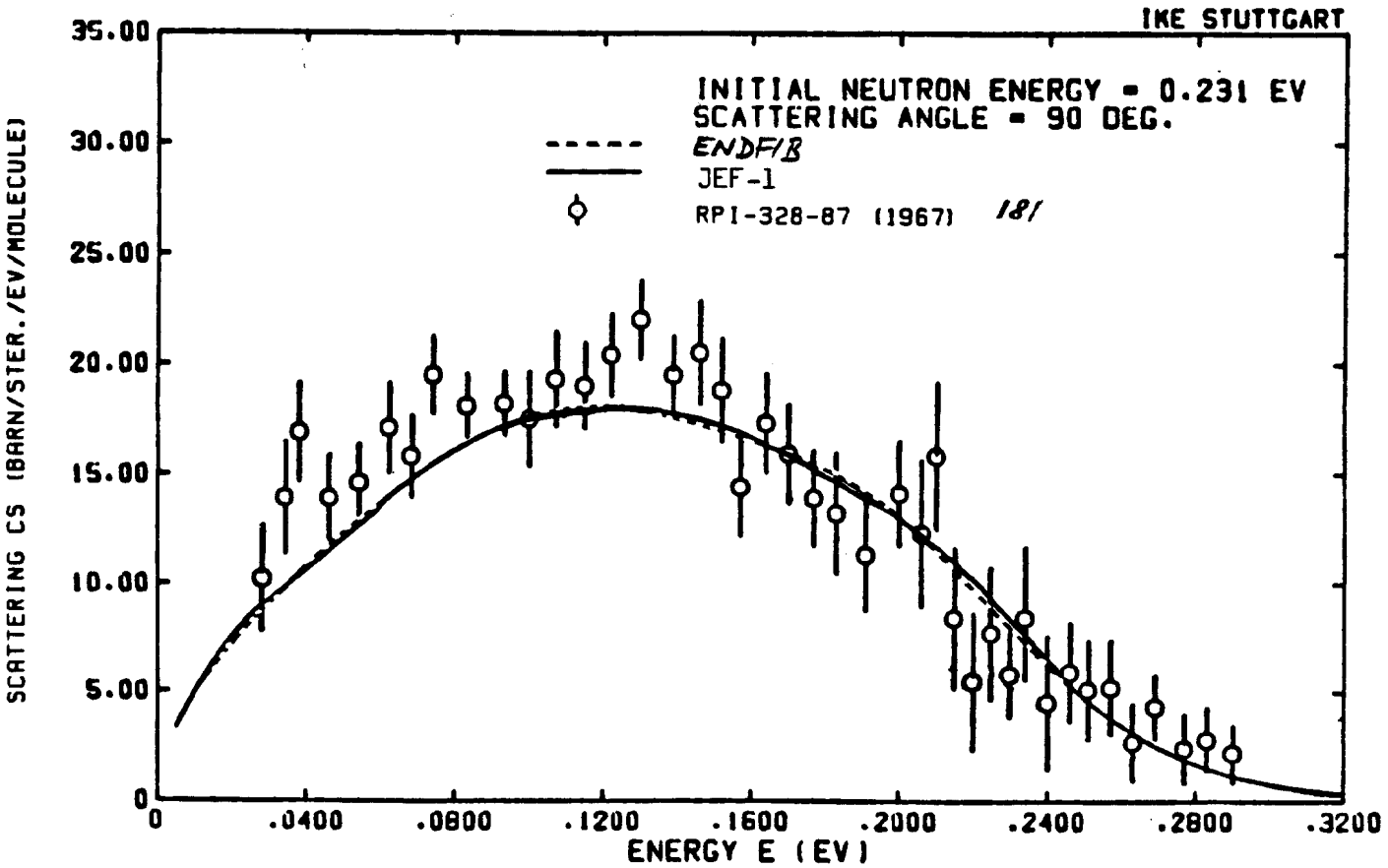

Fig. 10 Double Differential Neutron Scattering Cross Section for Water at 300 K

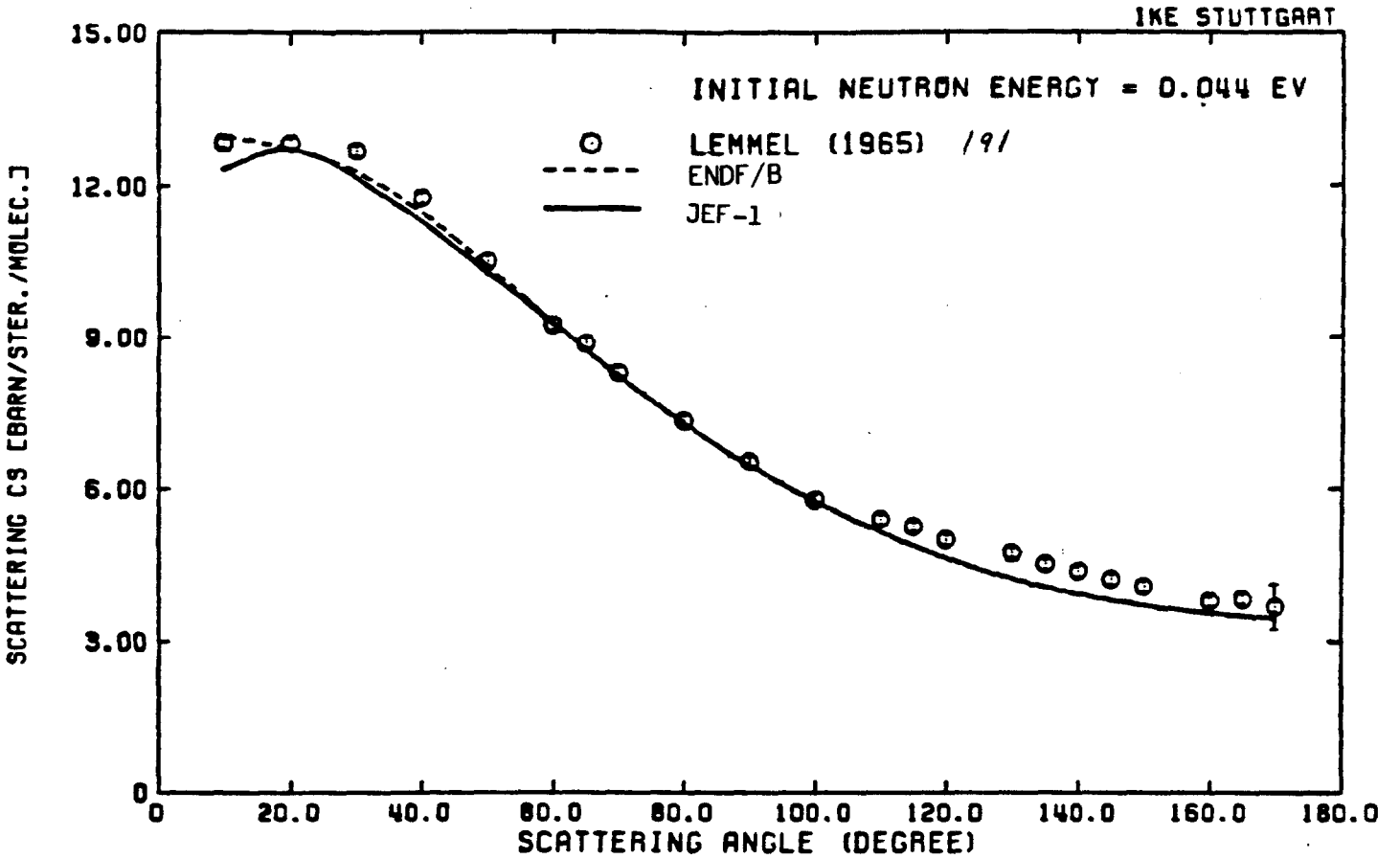

Fig. 11 Differential Neutron Scattering Cross Section of Water at T = 293.6 K

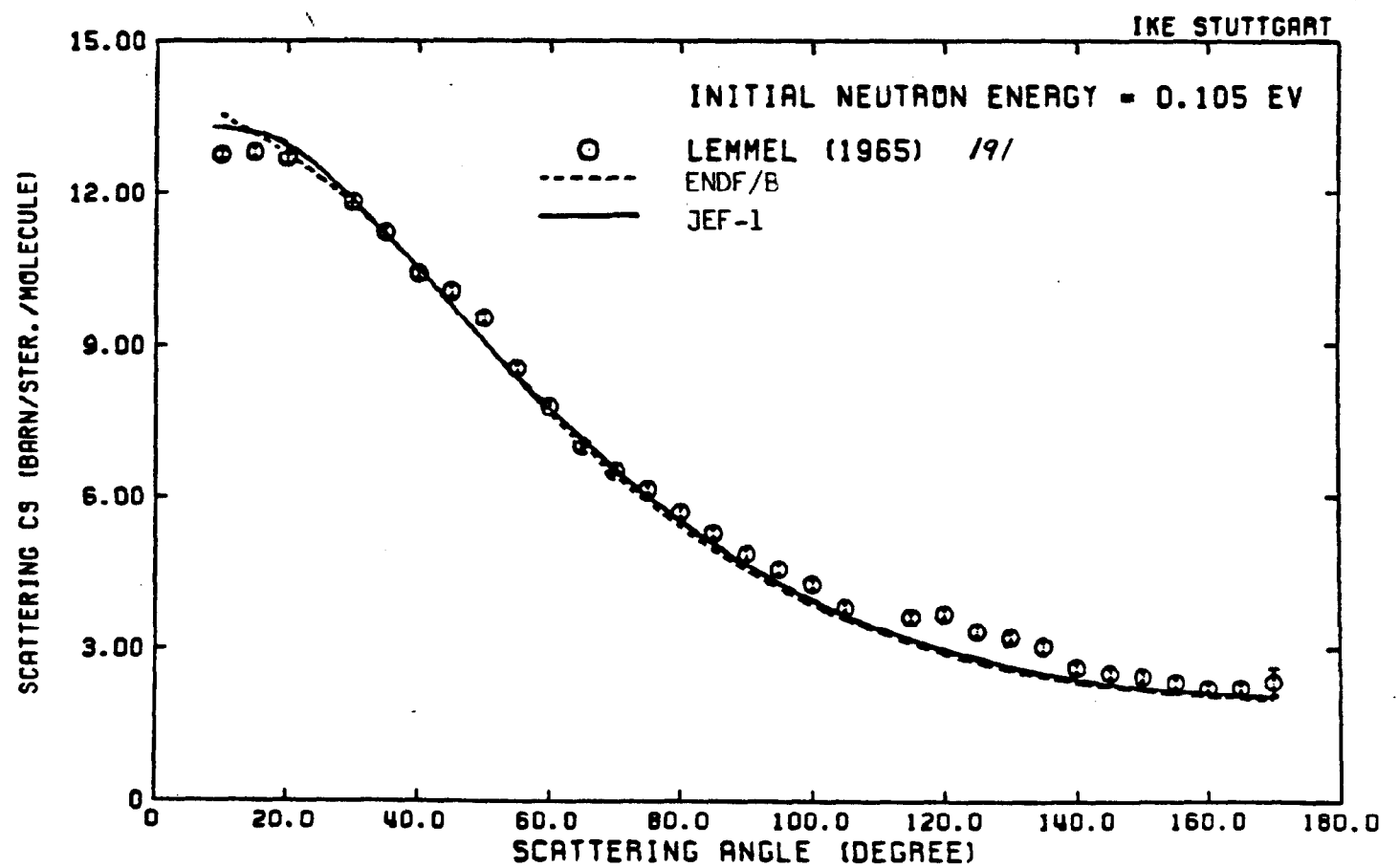

Fig. 12 Differential Neutron Scattering Cross Section of Water at T = 293.6 K

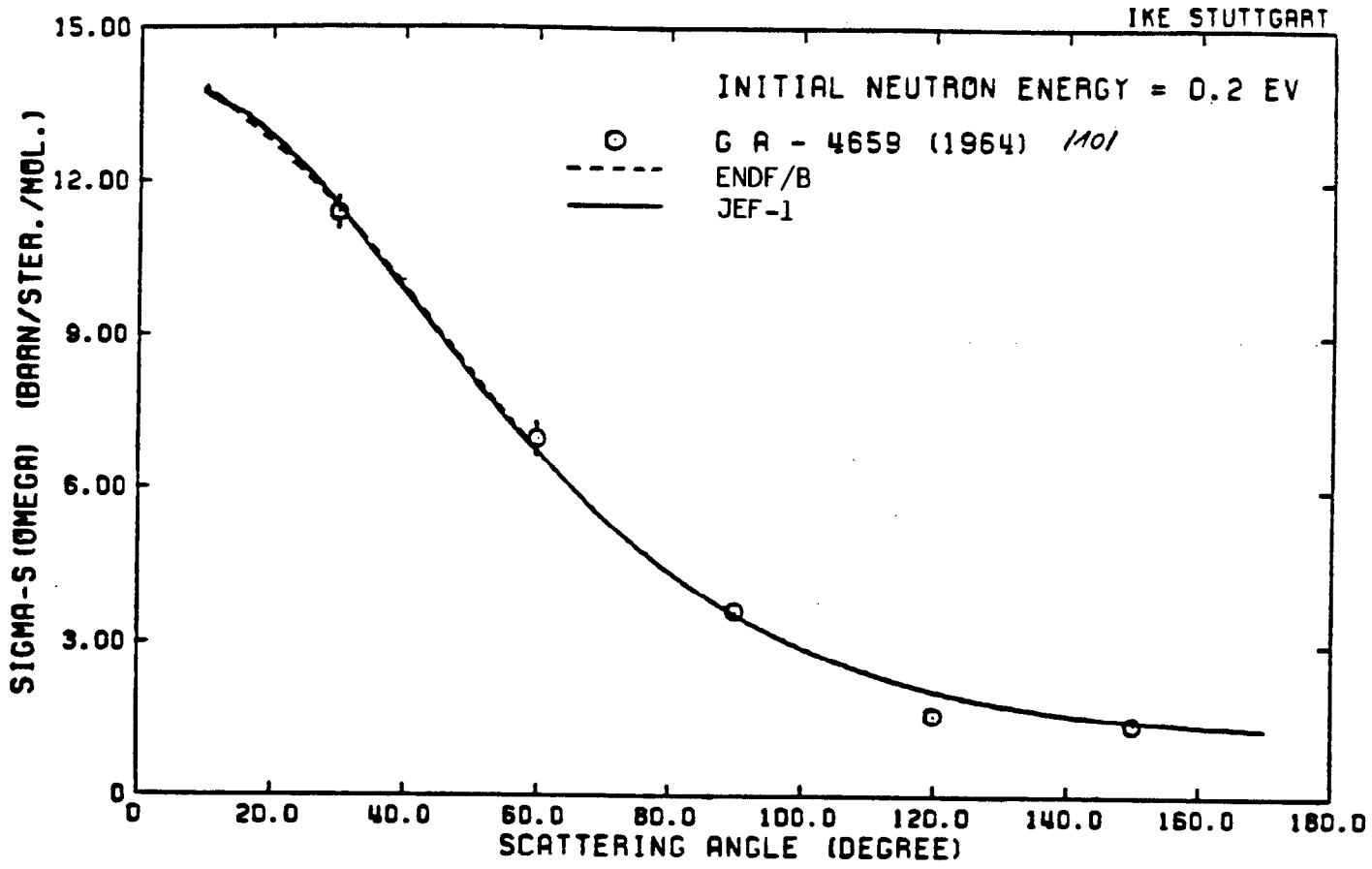

Fig. 13 Differential Neutron Scattering Cross Section of Water at T = 293.6 K

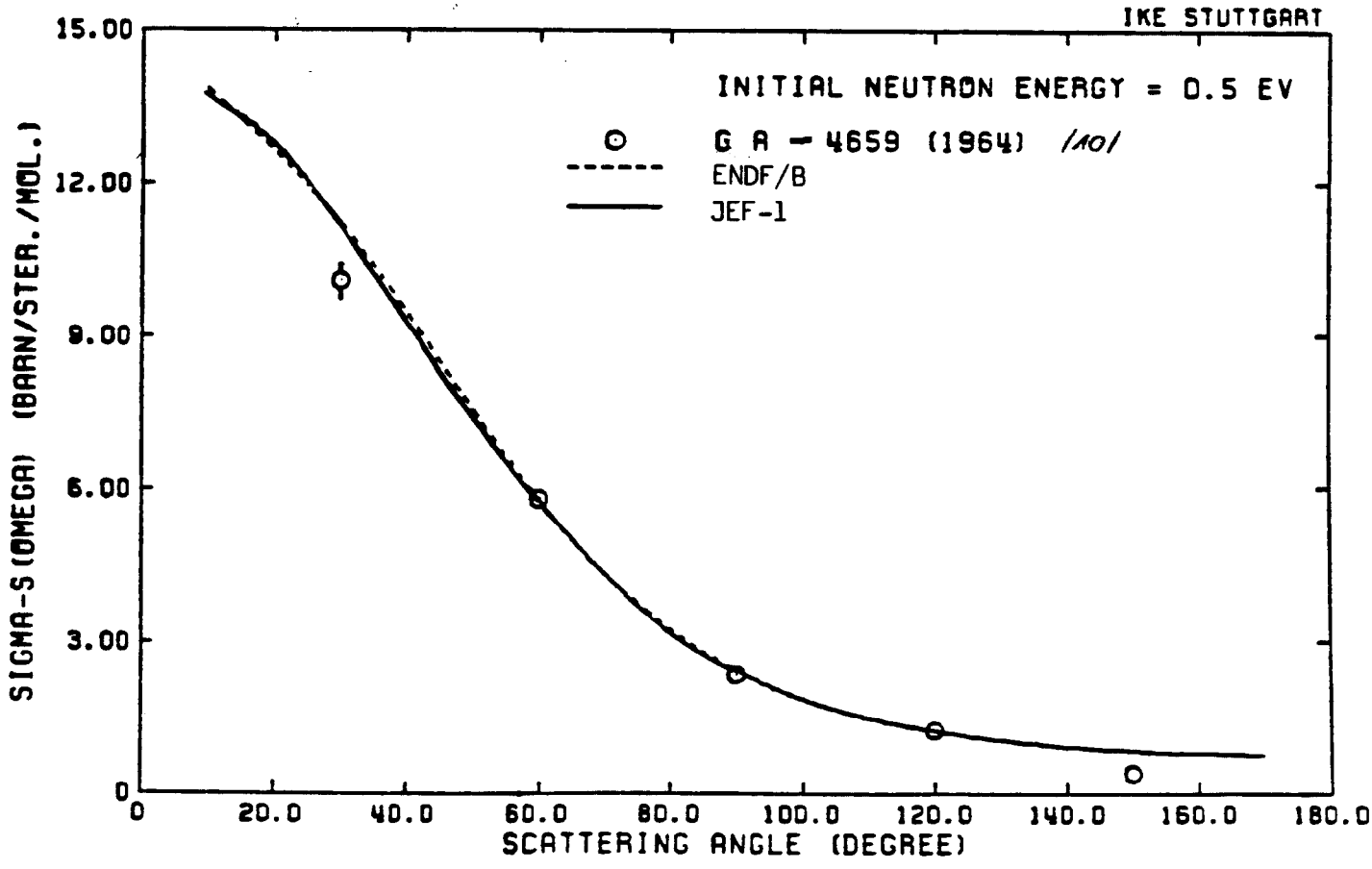

Fig. 14 Differential Neutron Scattering Cross Section of Water at T = 293.6 K

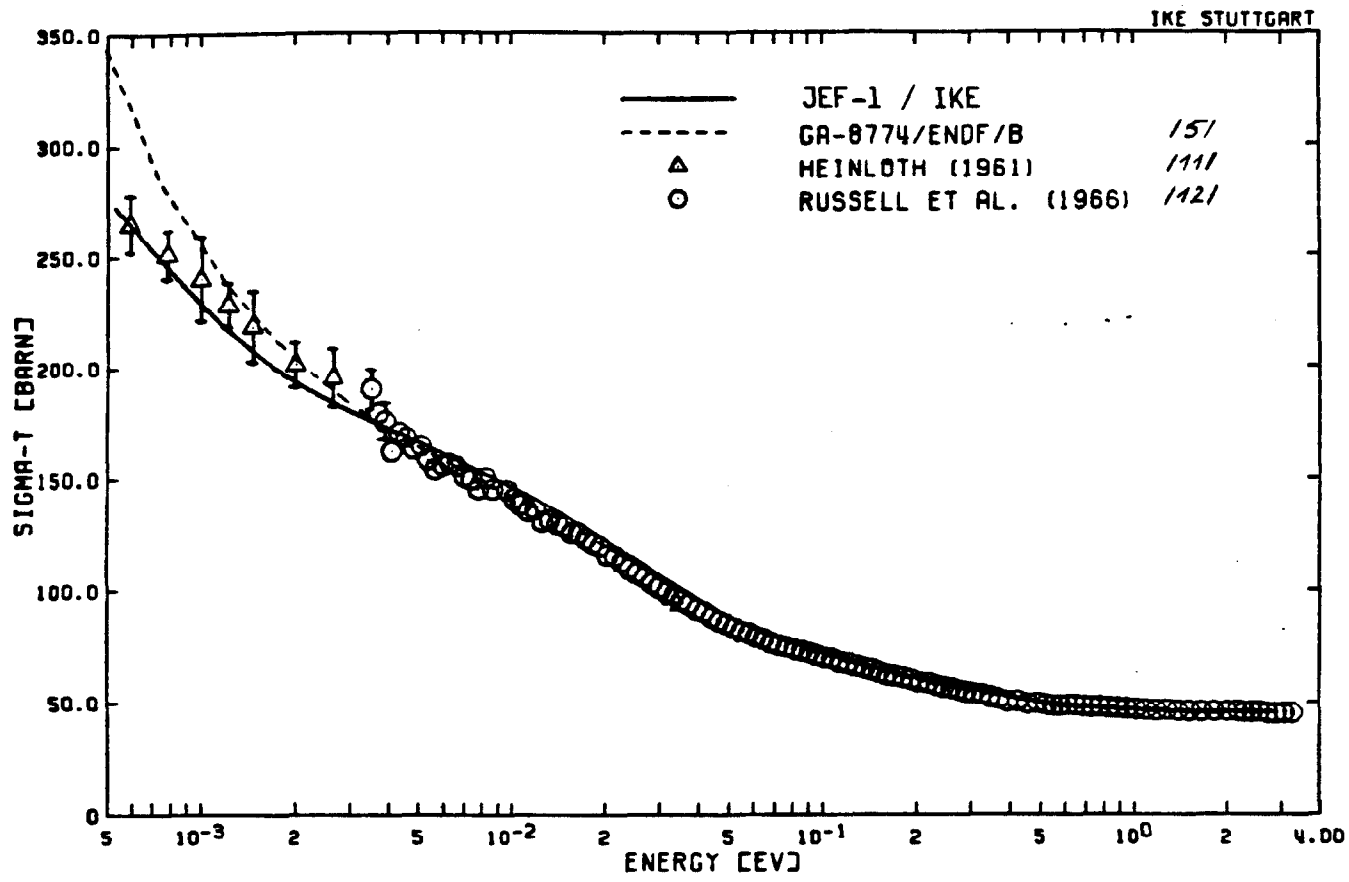

Fig. 15 Total Neutron Cross Section of H_2O at Room Temperature

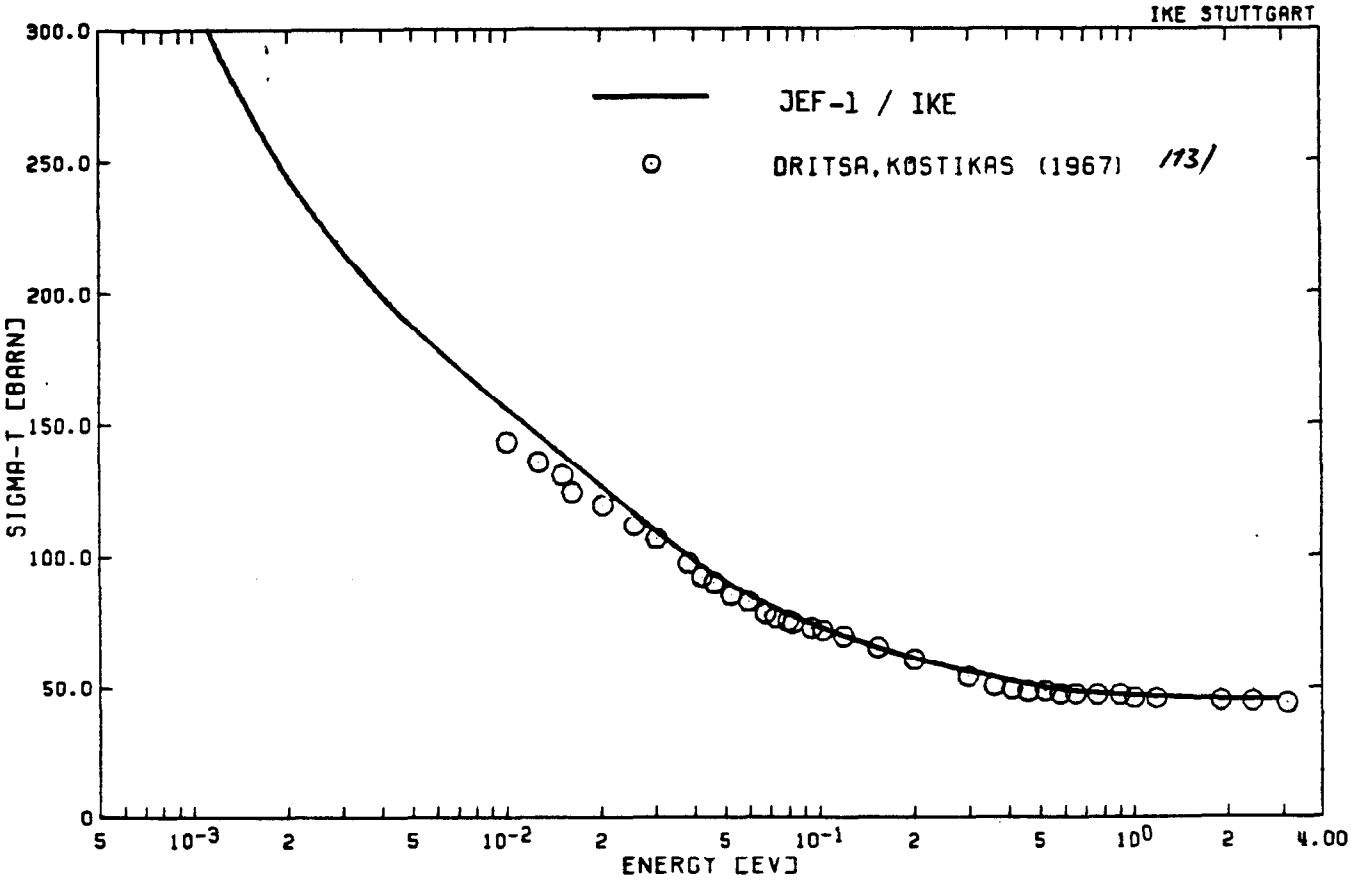

Fig. 16. Total Neutron Cross Section of H_2O at T = 450 K

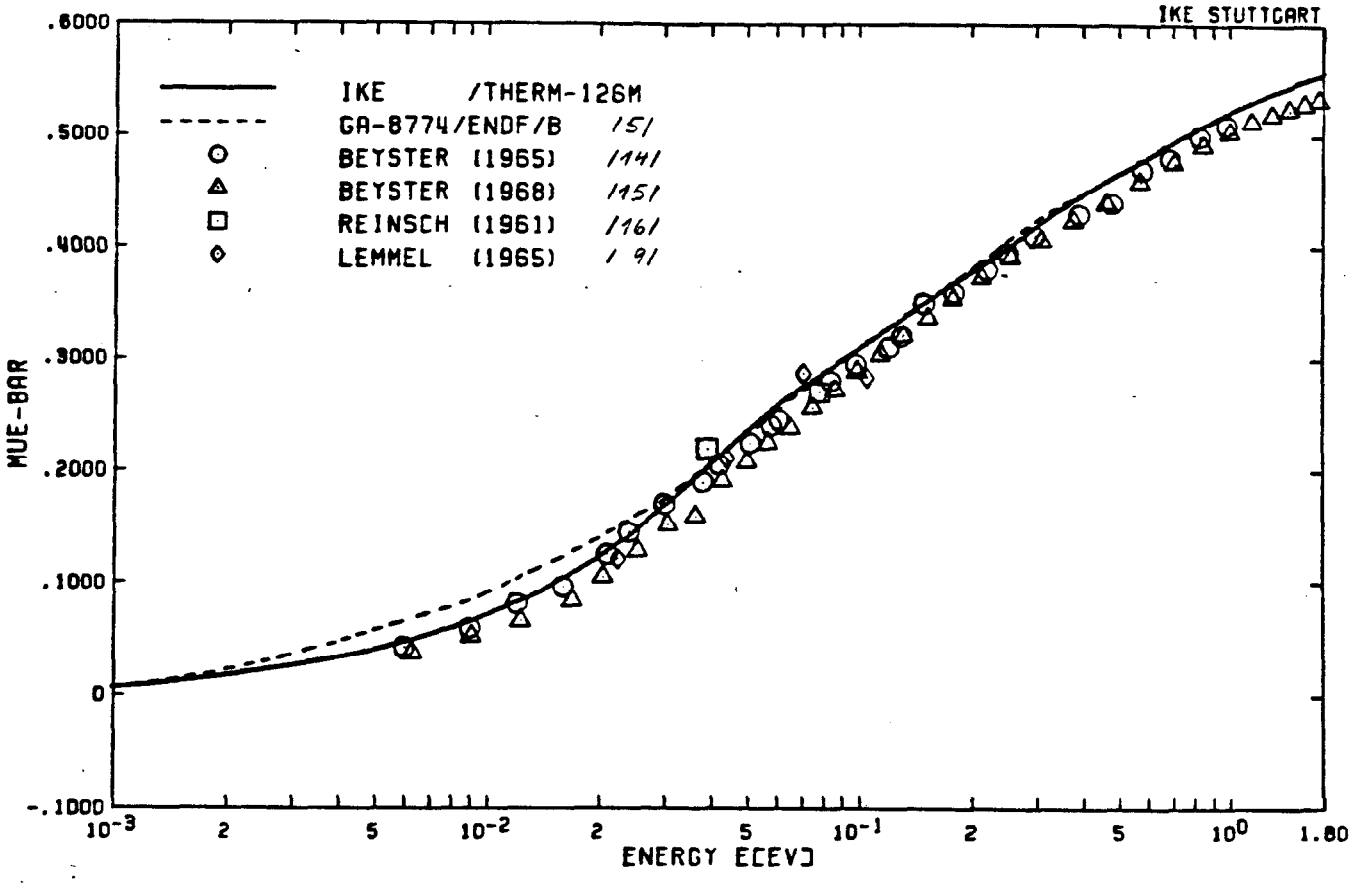

Fig. 17 Average Cosine of the Neutron Scattering Angle for H_2O at Room Temperature

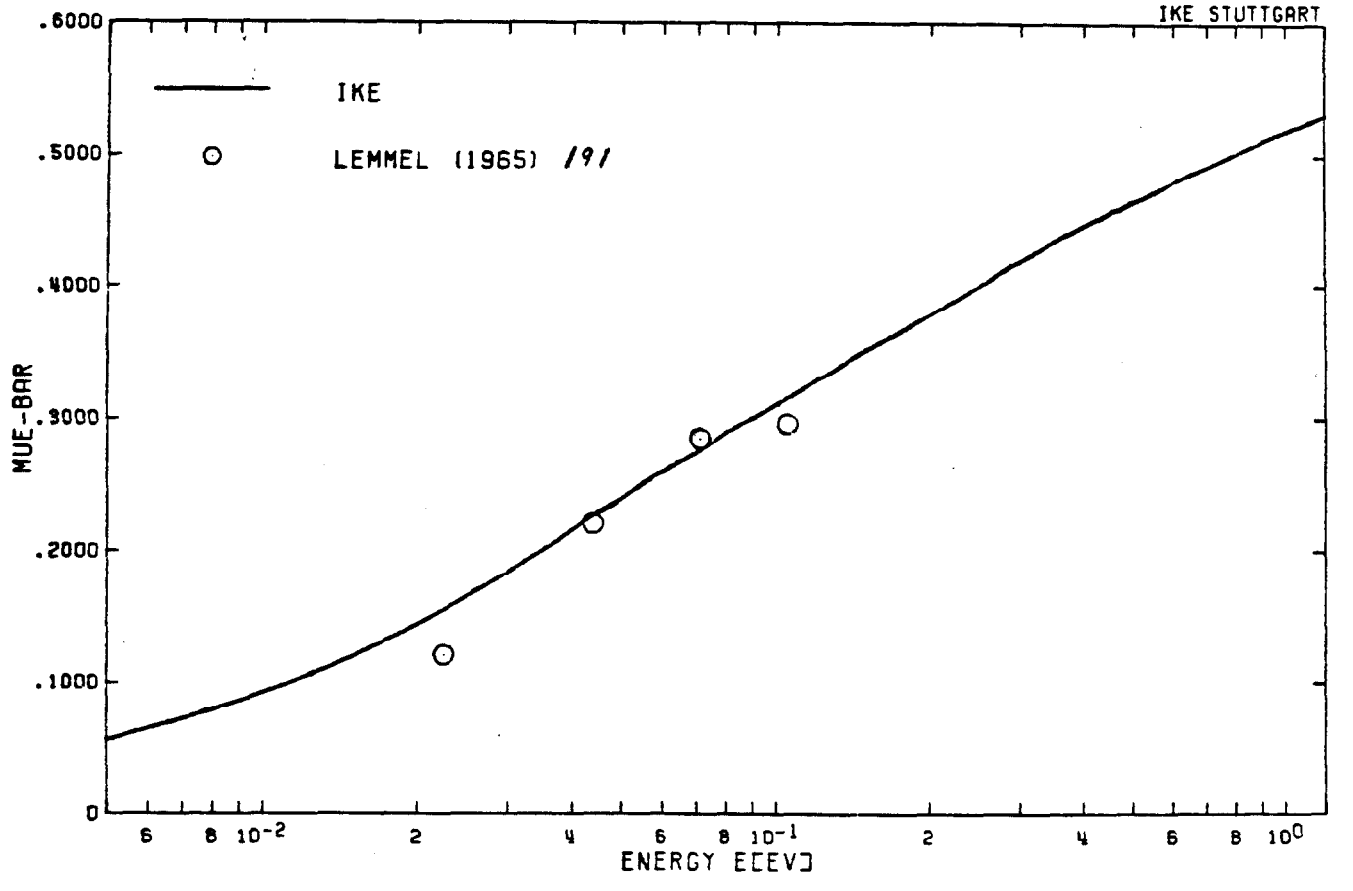

Fig. 18 Average Cosine of the Neutron Scattering Angle for H_2O at T = 200 C

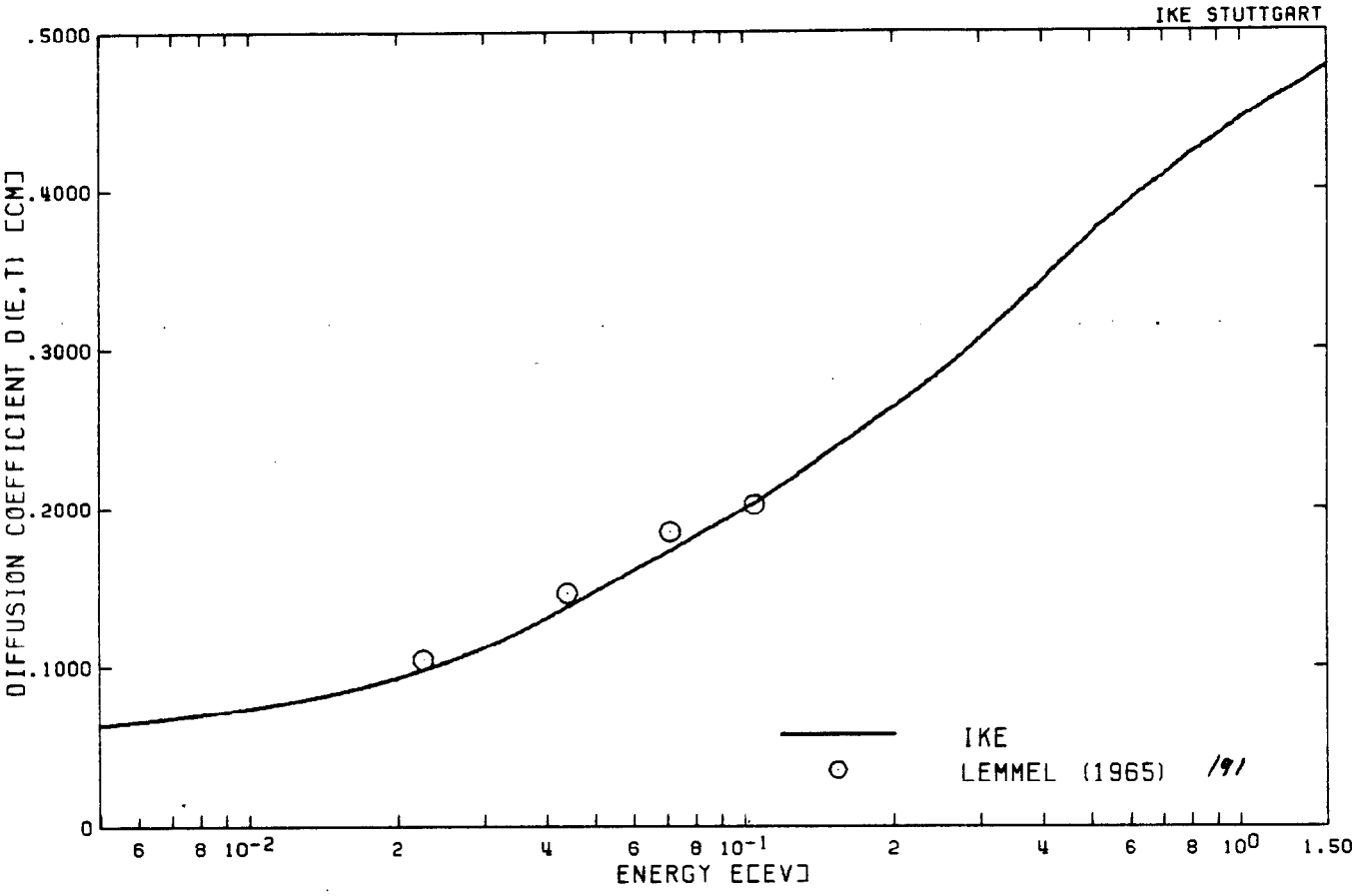

Fig. 19 Neutron Diffusion Coefficient in H_2O at Room Temperature

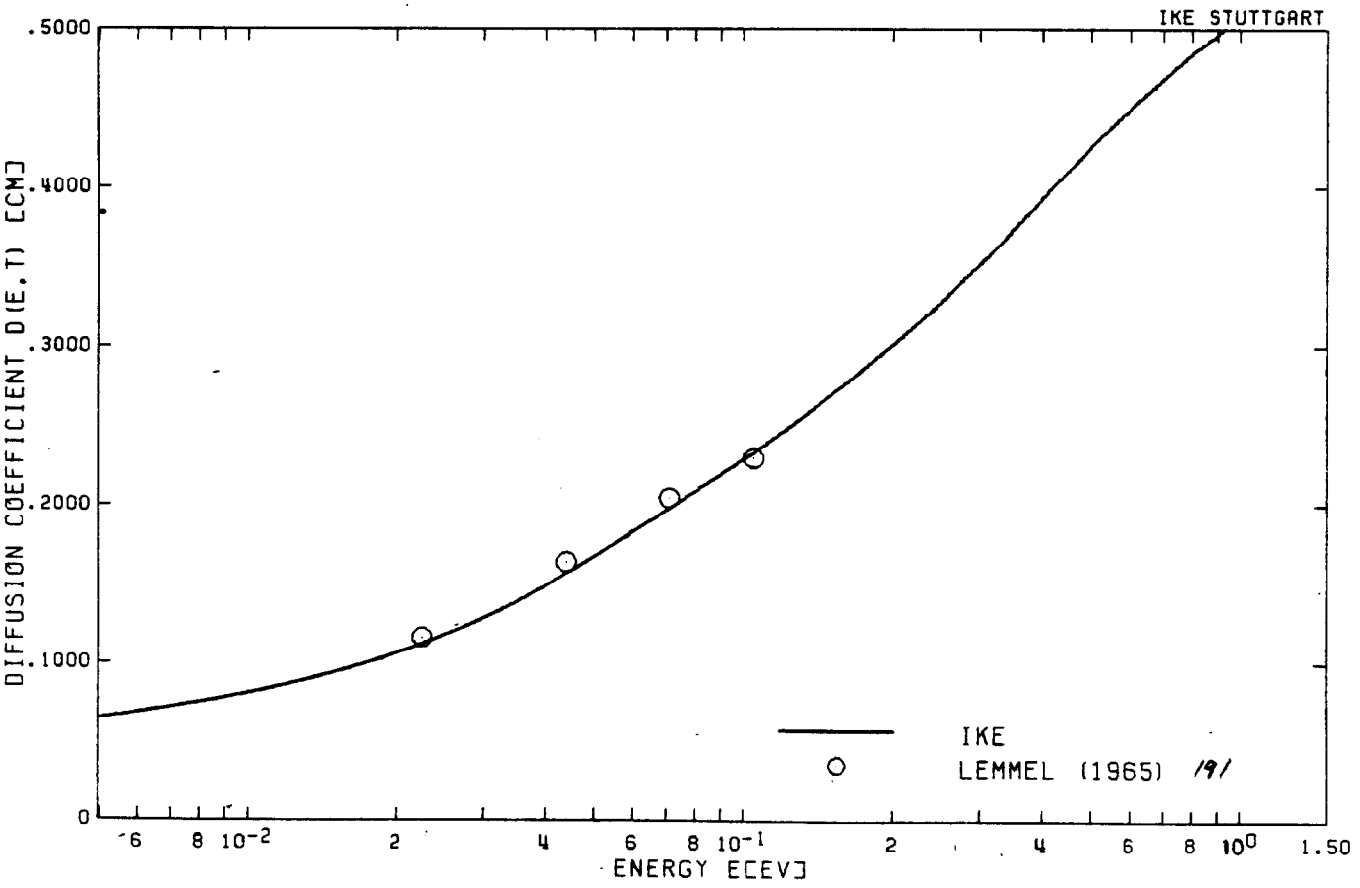

Fig. 20 Neutron Diffusion Coefficient in H_2O at T = 200 C (473 K)

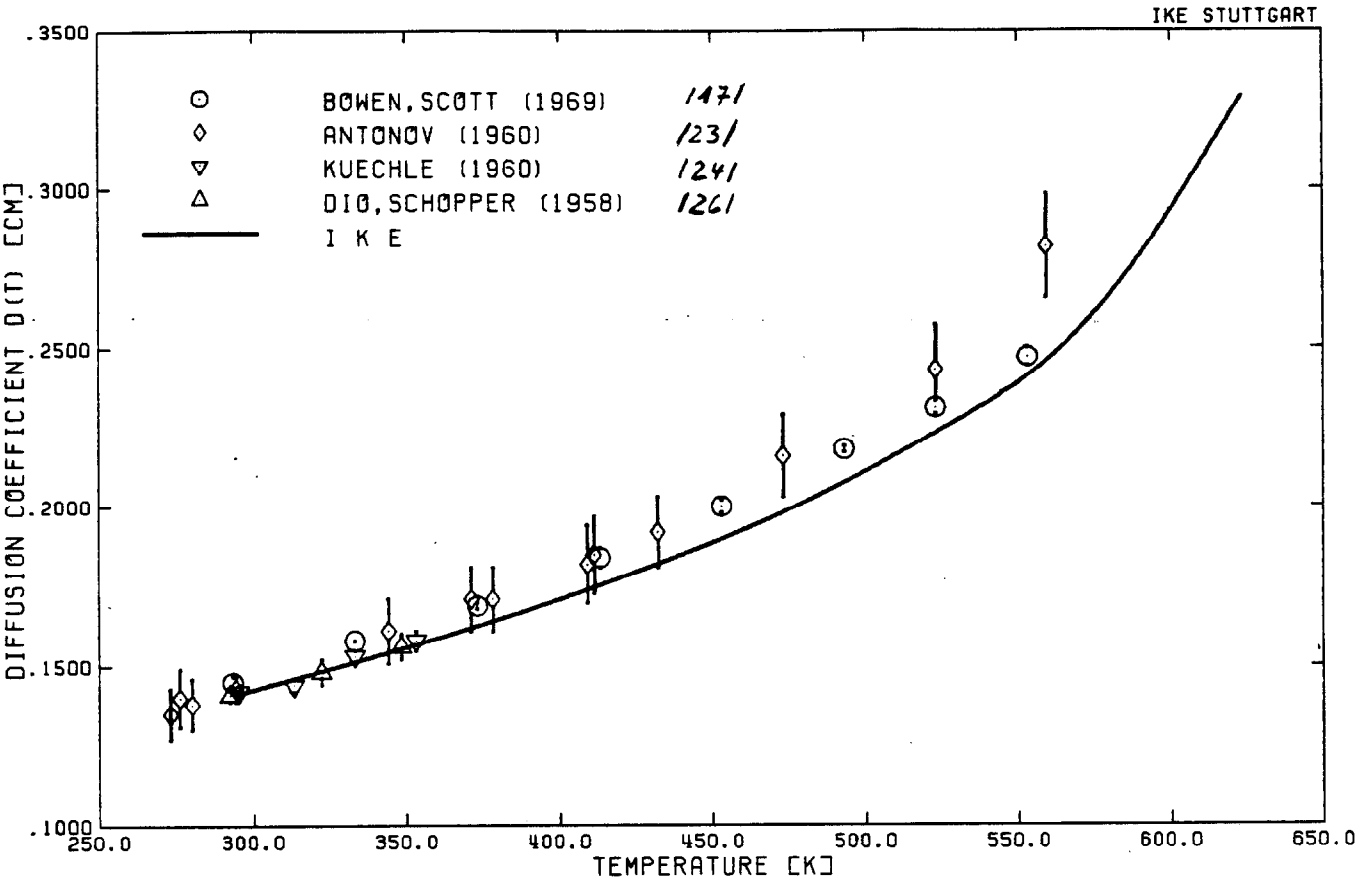

Fig. 21 Neutron Diffusion Coefficient $\bar{D}(T)$ in Water, H_2O

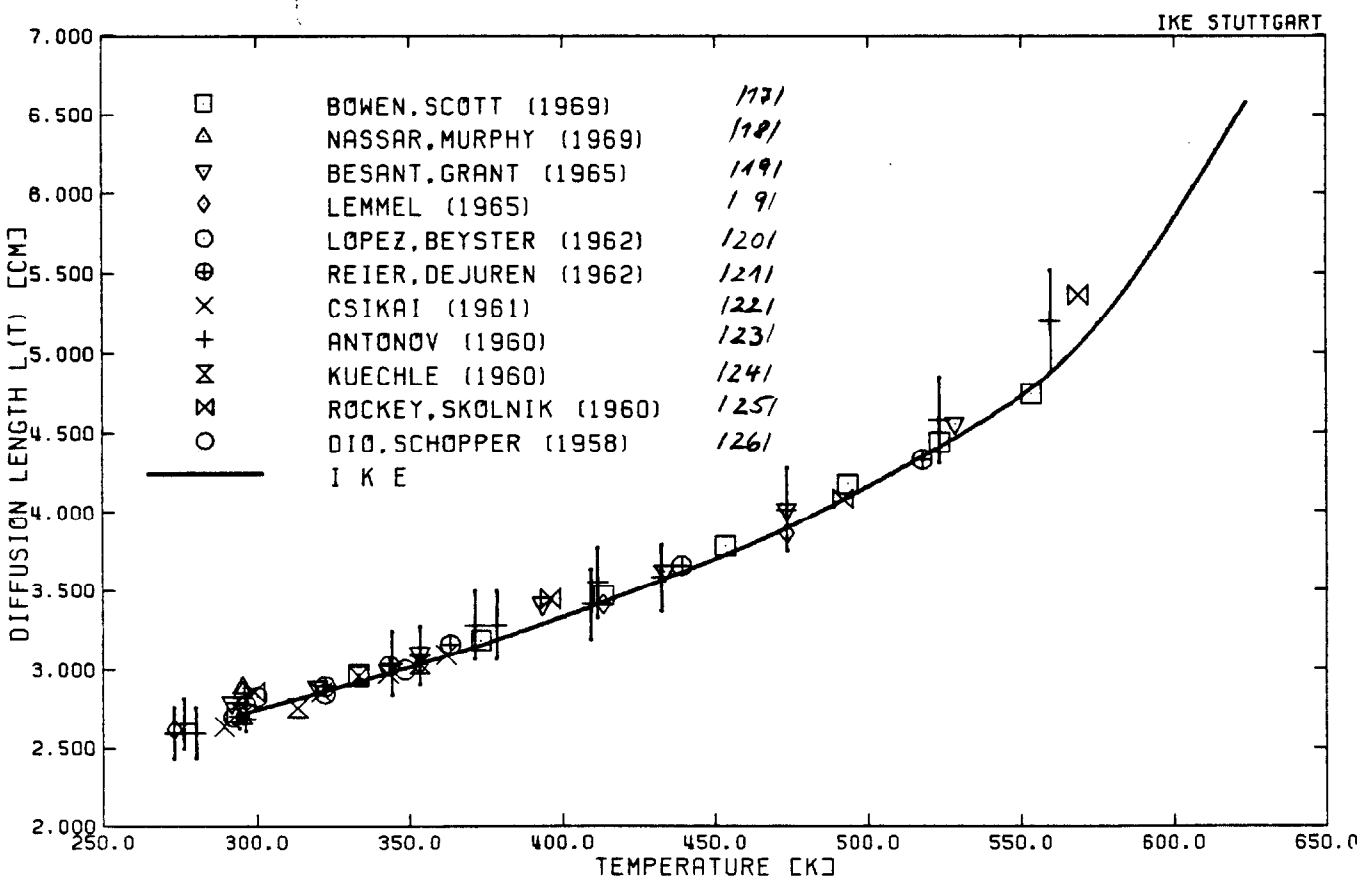

Fig. 22 Neutron Diffusion Length $\bar{L}(T)$ in Water, H_2O

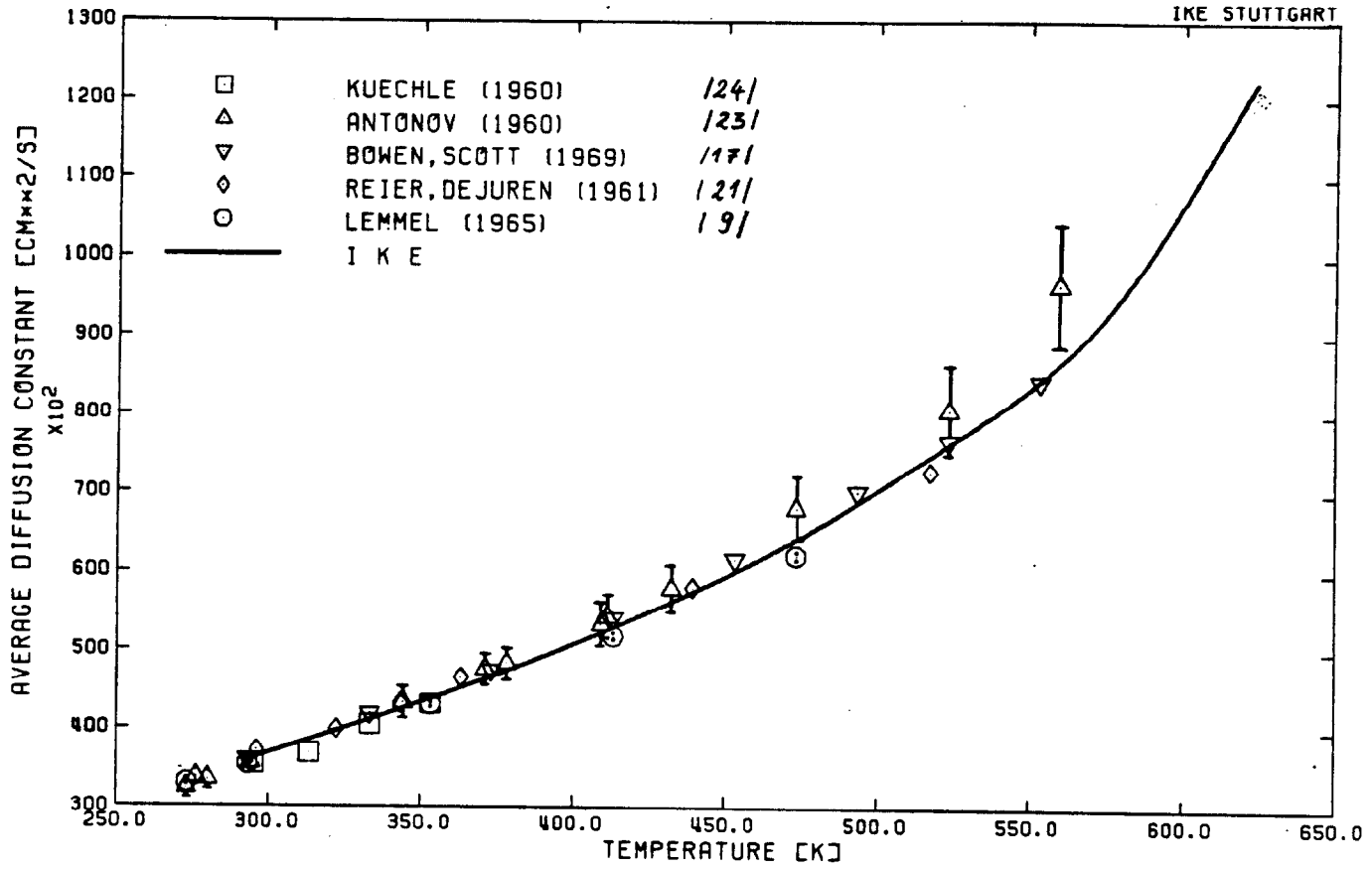

Fig. 23 Average Diffusion Constant $\overline{D^*v}(T)$ in Light Water

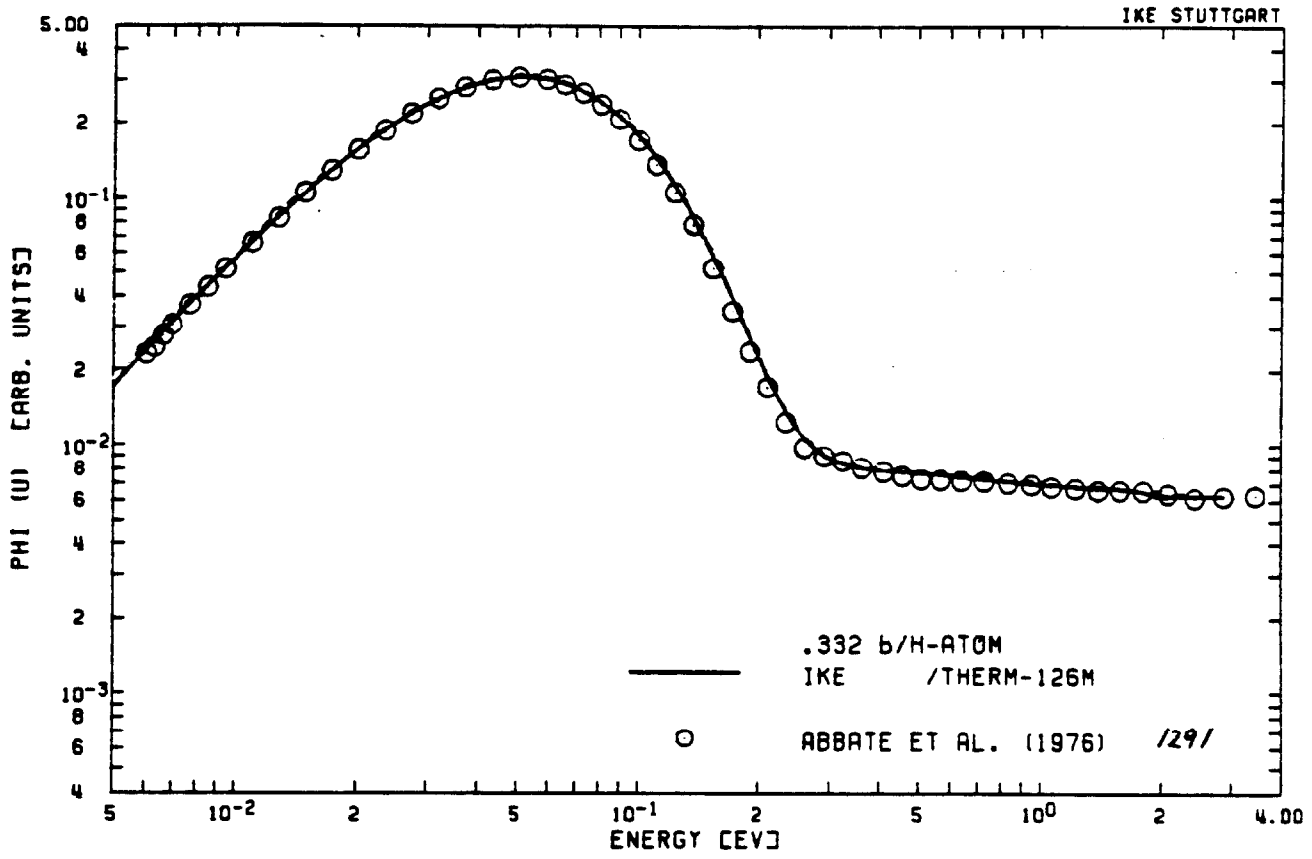

Fig. 24 Infinite Medium Neutron Spectra in Pure Water at T = 23 C

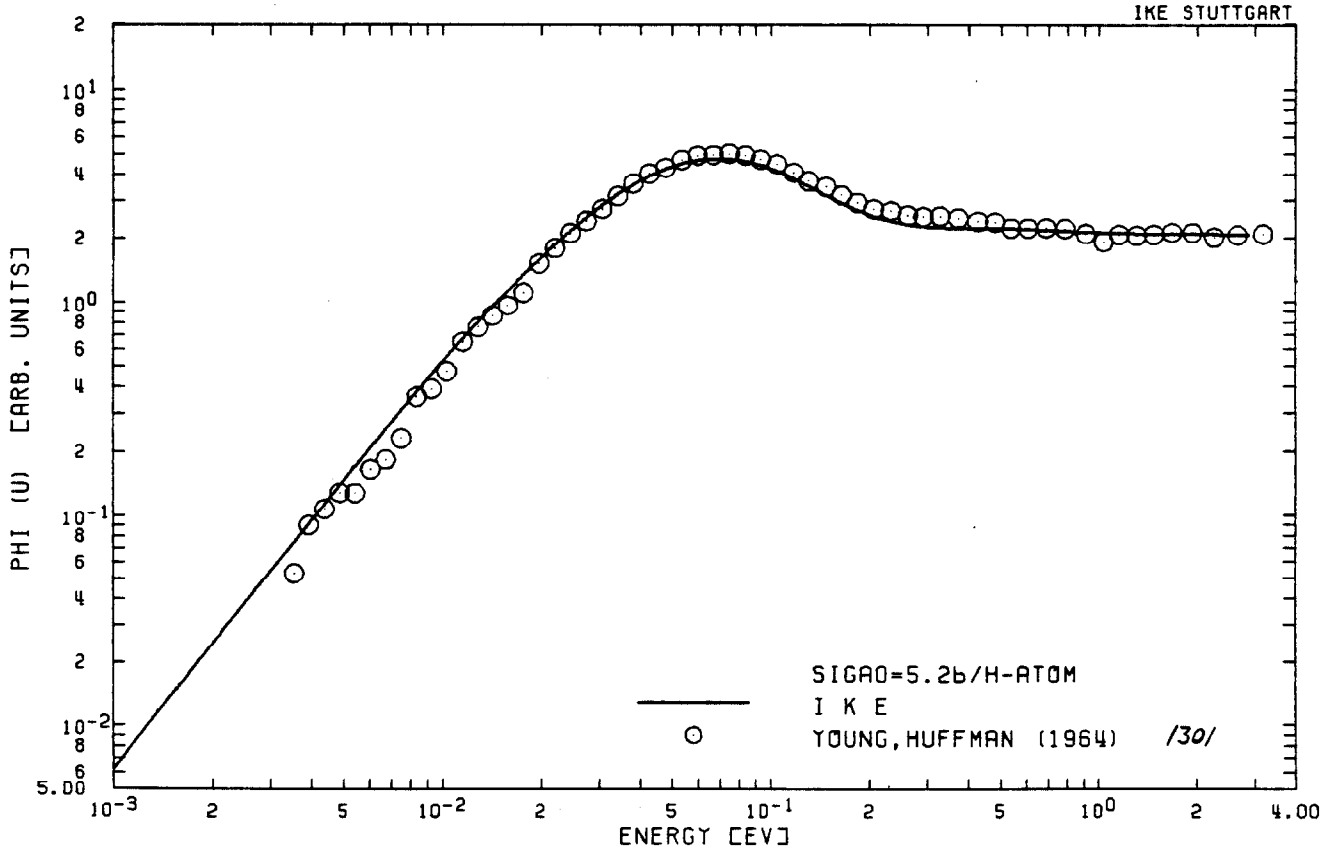

Fig. 25 Infinite Medium Neutron Spectra in Borated Water at Room Temperature

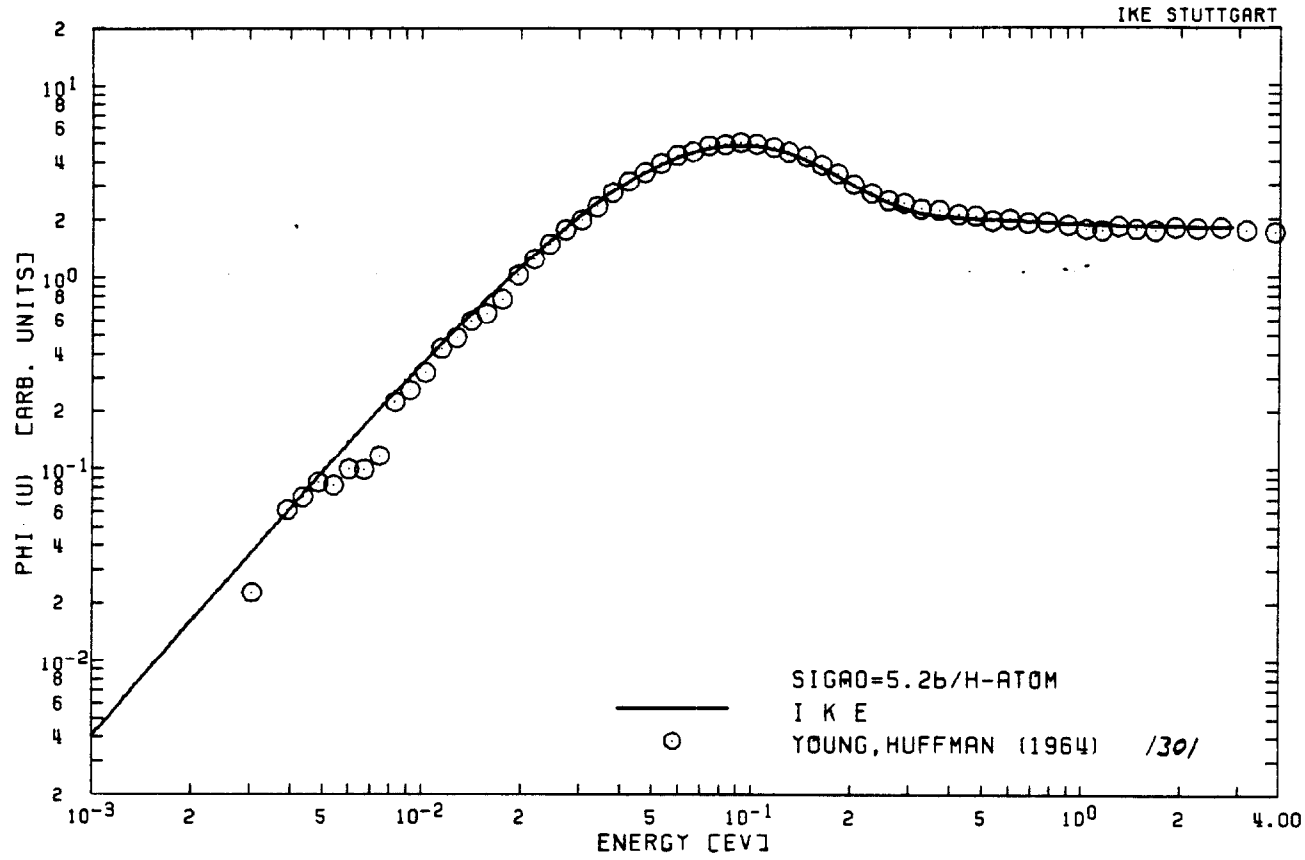

Fig. 26 Infinite Medium Neutron Spectra in Borated Water at T = 150 C

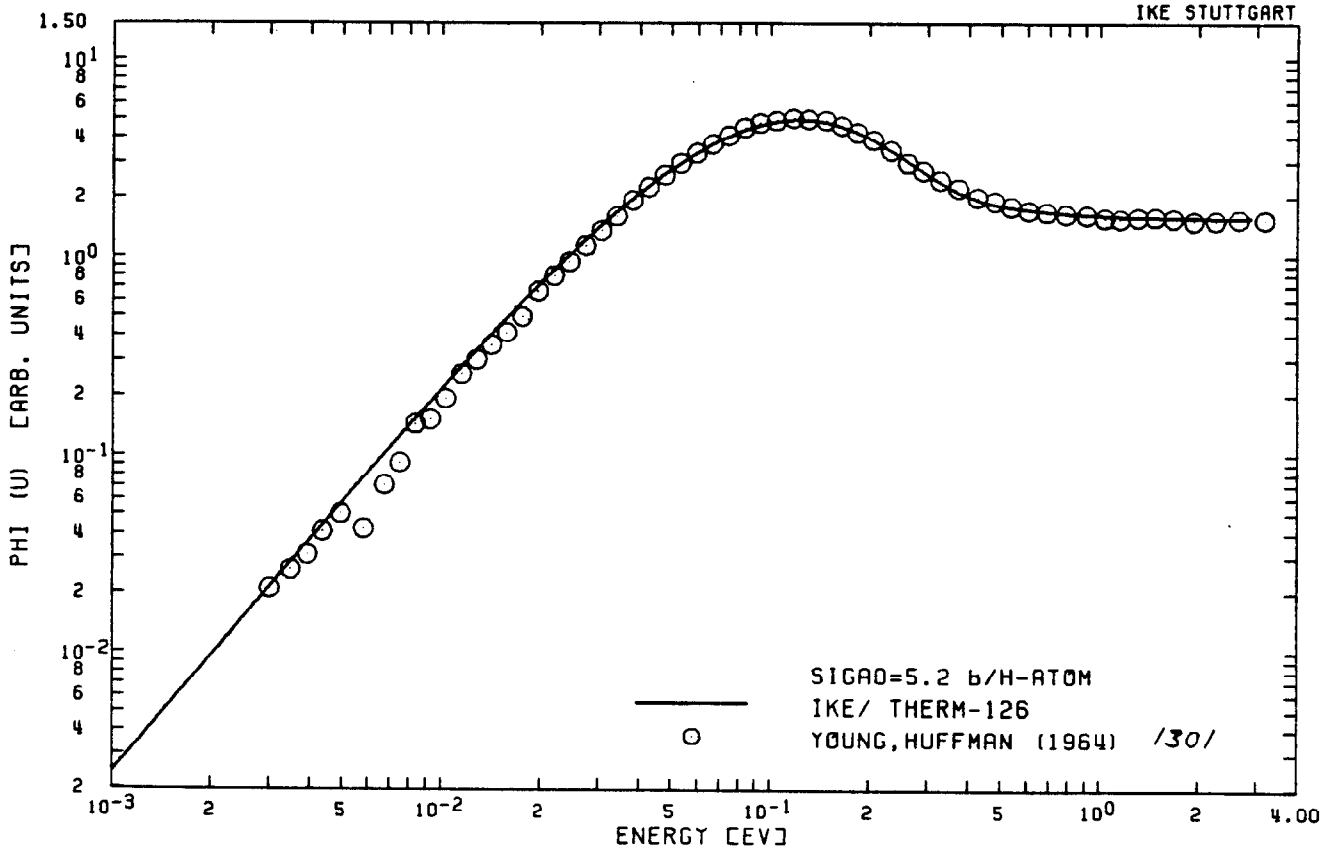

Fig. 27 Infinite Medium Neutron Spectra in Borated Water at T = 316 C

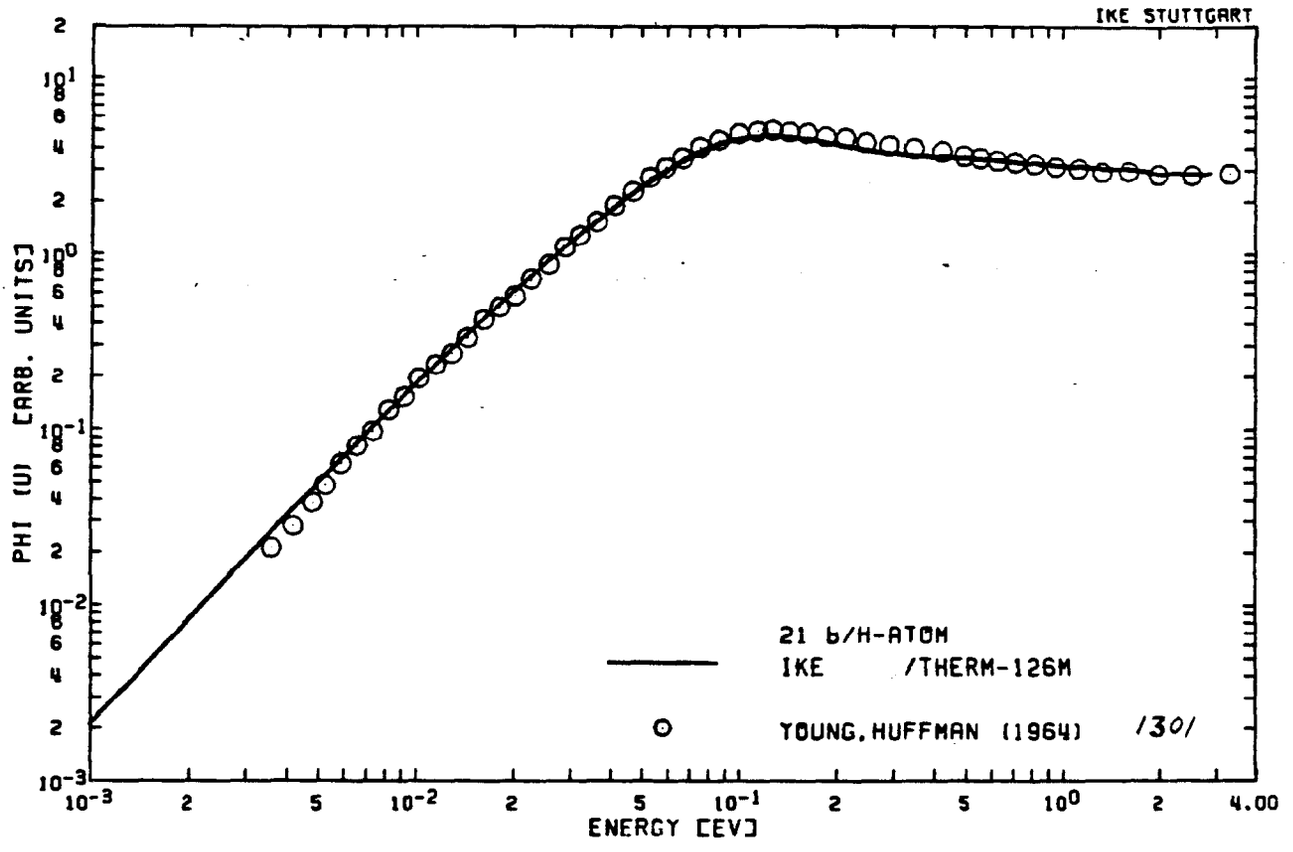

Fig. 28 Infinite Medium Neutron Spectra in Gadolinium Poisoned Water at Room Temperature

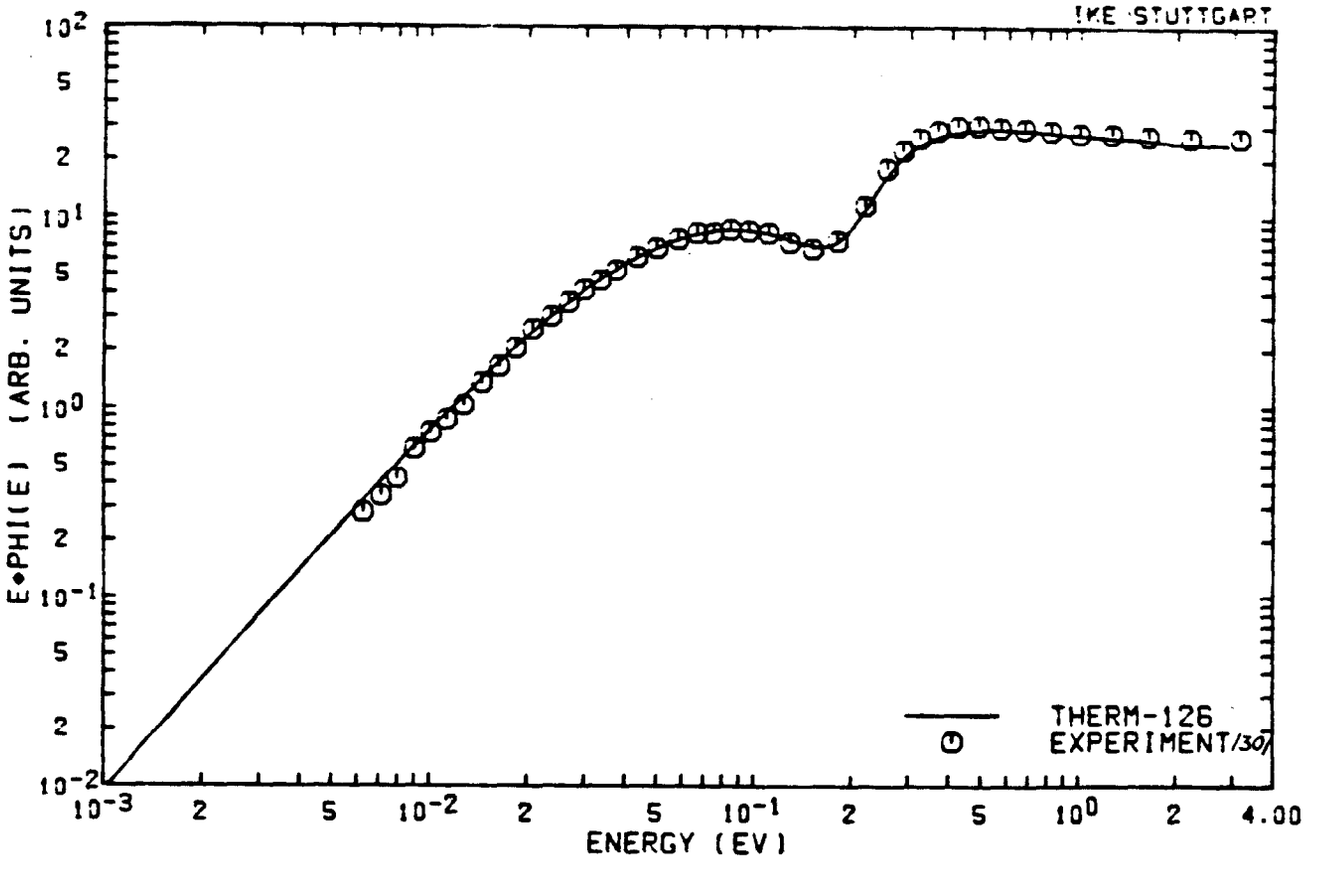

Fig. 29 Infinite Medium Neutron Spectra in Cadmium Poisoned H_2O

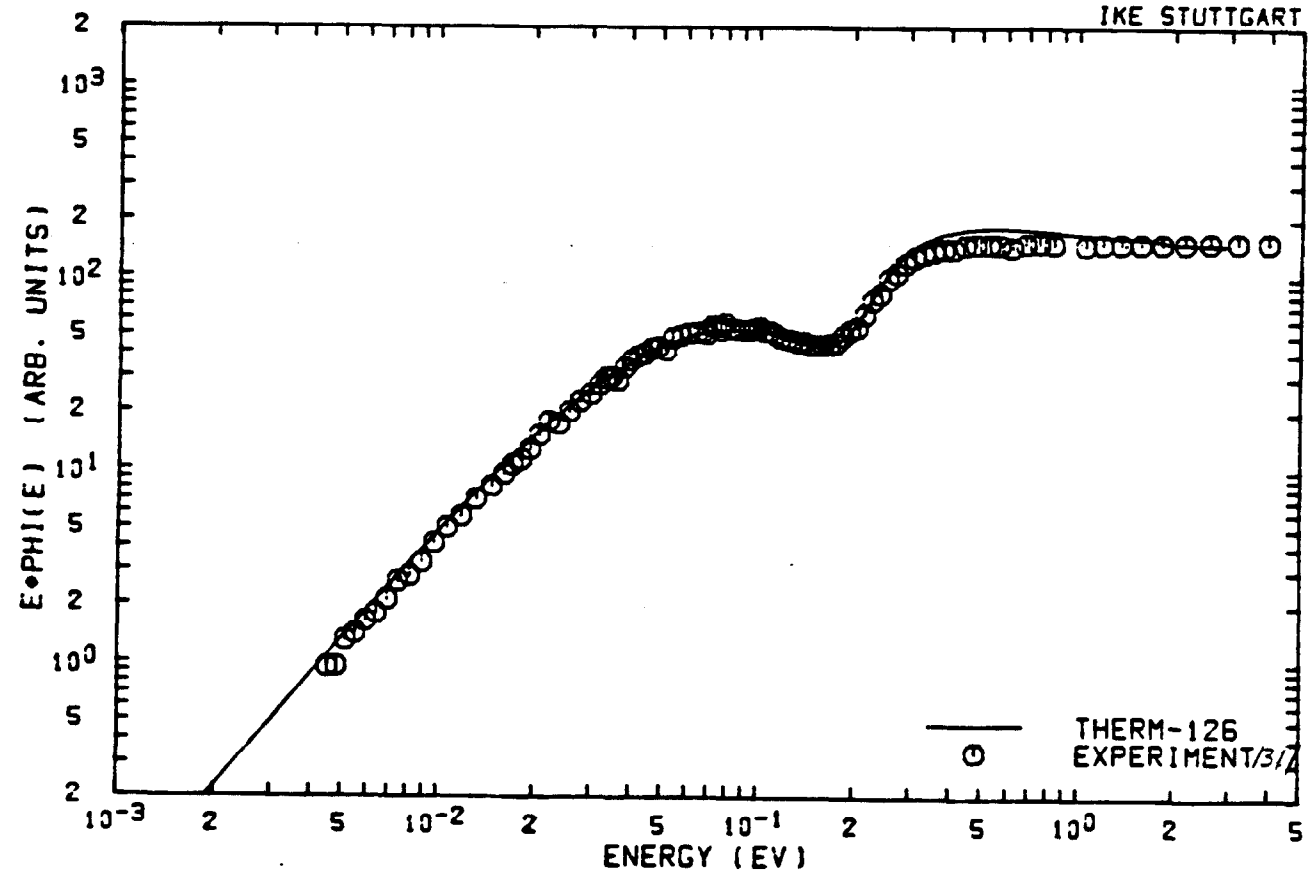

Fig. 30 Perpendicular Surface Leakage Spectrum in Cadmium Poisoned H_2O

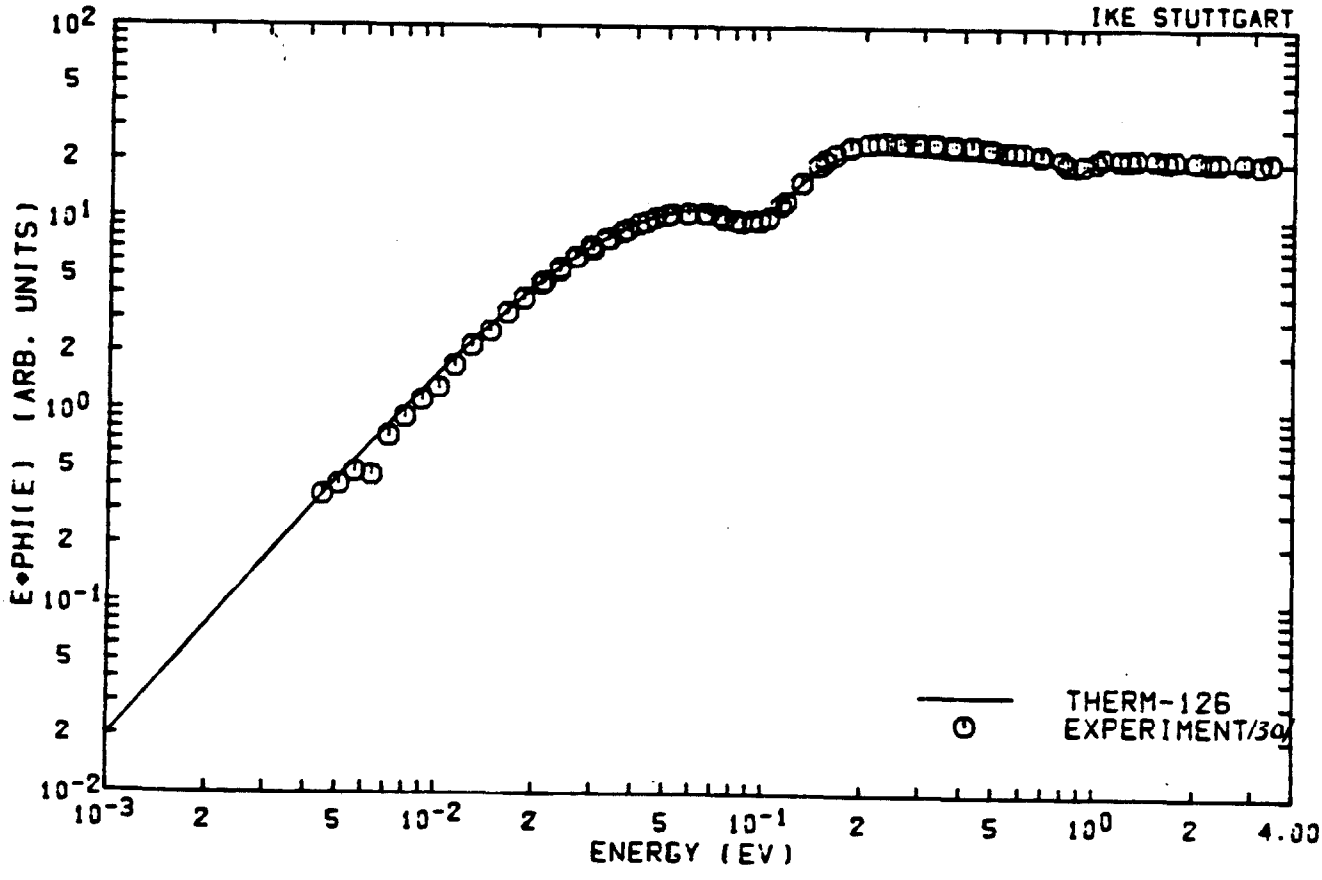

Fig. 31 Infinite Medium Neutron Spectrum in Samarium Poisoned H_2O

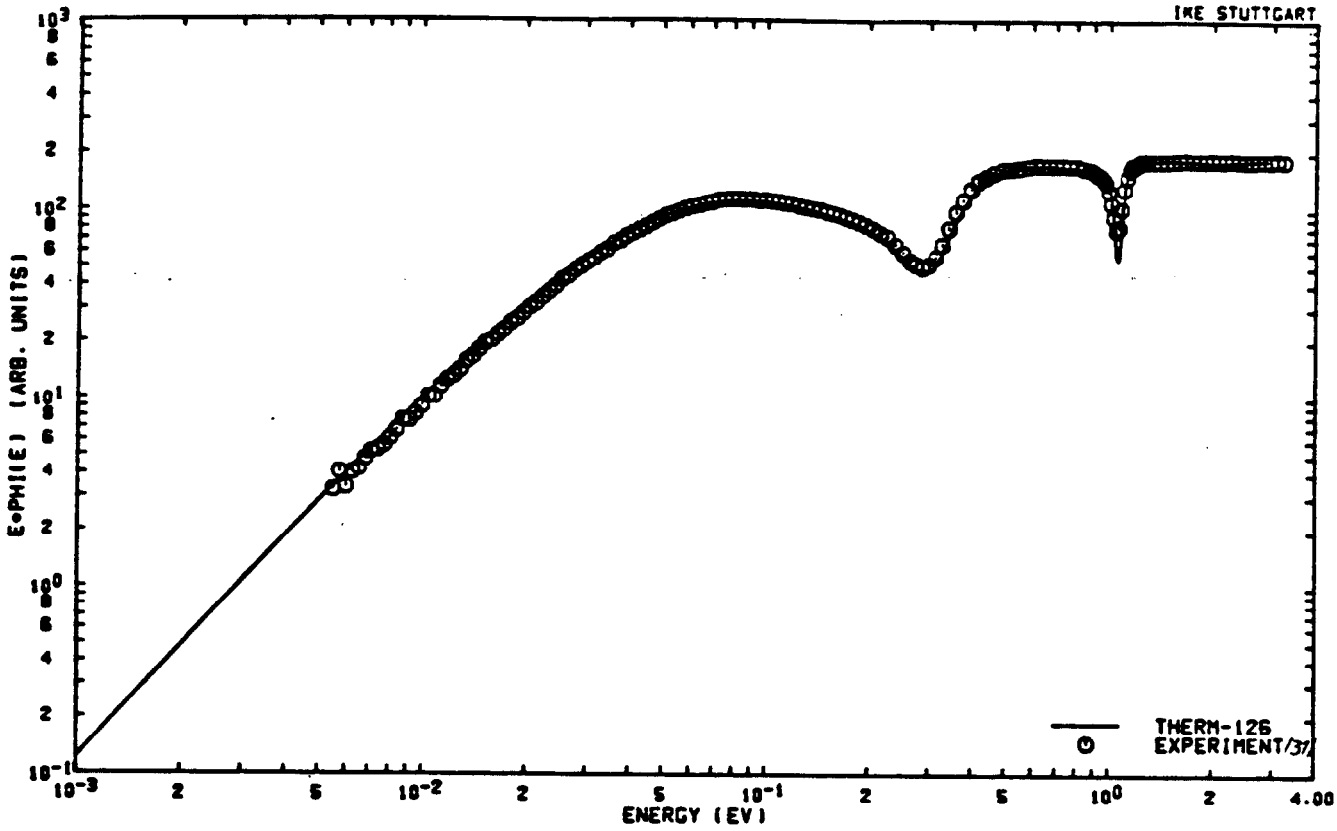

Fig. 32 Infinite Medium Neutron Spectrum in a Plutonium Nitrate Solution (193.4 g Pu/l at 5 wt% Pu-240)

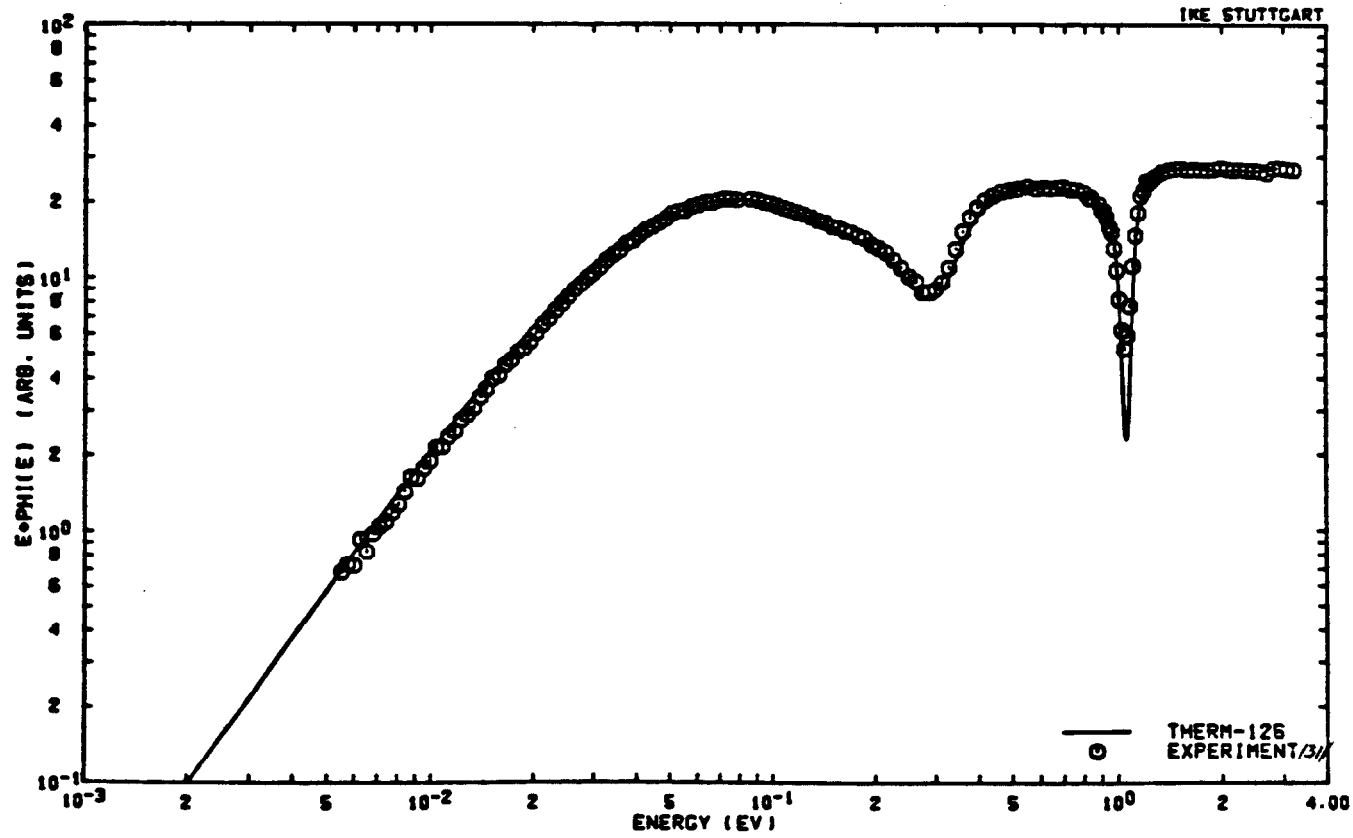

Fig. 33 Infinite medium Neutron Spectrum in a Plutonium Nitrate Solution (197.9 g Pu/l at 23 wt% Pu-240)

2. HEAVY WATER D_2O, MAT=4002

2.1. Physics of the Neutron Deuterium Scattering, Phonon Frequency Spectra and Related Parameters

The molecular structure of D_2O is similar to the one of H_2O and therefore the neutron-deuterium scattering dynamics in some aspects is comparable to the one contained in the model for light water. The frequencies of the internal modes of vibration however are approximately smaller by a factor $1/\sqrt{2}$ because of the mass ratio.

The following fundamental dynamical modes of motion are considered in (32):

- free translational motion of the single D_2O molecule. No temperature dependent translational masses are used. This simplification was also used in producing the ENDF/B scattering law data for D_2O, MAT = 1004 (4,5).

- the hindered rotations of the Deuterium atoms are represented by temperature dependent broad band frequencies, derived from the results of Haywood, Page (33) by inter- and extrapolation. In Fig. 34, the phonon spectra for the lowest and highest considered temperatures are shown.

- the internal vibrations of the Deuterium atoms are represented by discrete harmonic oscillations. The bending vibration frequency is ω_2= 0.145 eV and the symmetric and asymmetric stretching vibrations are localised at $\omega_{1,3}$ = 0.338 eV. The corresponding oscillation masses are 3 and 6.

The same effective masses as in ENDF/B have been used (Table 4). Fig. 35 displays the phonon spectra used for JEF-1/IKE and ENDF/B.

Table 4: Effective masses (amu) of the D_2O dynamical unit

mode \ data base	ENDF/B MAT=1004	IKE/JEF-1 MAT=4002
translations	20.0	20.0
rotations	2.222	2.222
oscillations		
$\omega_{1,3}$	3.0	3.0
ω_2	6.0	6.0

The effective scattering temperature of Deuterium bound in heavy water is given in Table 5 and shown in Fig. 36.

Table 5: Integral parameters derived from the frequency spectra of D in D_2O

Temperature (K)	Debye-Waller integral (1/eV)	T_{eff} (K)
293.6	40.32	1015.60
323.6	42.88	1026.71
373.6	47.11	1046.74
423.6	51.24	1068.50
473.6	55.24	1091.84
523.6	59.10	1116.63
573.6	62.69	1143.10
673.6	69.15	1200.08

Unlike the neutron scattering on Hydrogen bound in H_2O, the scattering on D bound in D_2O is largely coherent. Inter- and intramolecular interference scattering would therefore have to be considered at low energies. For higher energies, however, important cancellation effects in the scattering occur.

For practical applications in the field of neutron thermalisation, the neutron scattering in D_2O can be predicted accurately with the incoherent approximation. In fact large neutron energy transfer is predominant and the quasi-elastic scattering may be neglected.

2.2 Data Stored in the JEF File

The quantities stored for heavy water (MAT=4002) are described in the information file MF=1, MT=451 given in Appendix 3.

These are:

$S(\alpha,\beta,T)$ (MF=7, MT=4) for D in D_2O at the following 8 temperatures:

	293.6	323.6	373.6	423.6	473.6	523.6	573.6	673.6	K
i.e.	20	50	100	150	200	250	300	400	C

The data are represented in the temperature-dependent ENDF/B data format (see Appendix F of (1)) at 100 values of α and 150 values of β. The energy limit E_{max} up to which $S(\alpha,\beta,T)$ can be used is 1.8554 eV.

The effective scattering temperatures that are required for the short collision time approximation for higher energy transfers are given in the form of a table in MF=1, MT=451.

The total free atom cross section of Deuterium is 3.395 b as in ENDF/B-V MAT=1302.

For the neutron scattering by Oxygen, the values for free gas approximation are also stored in file 7.

The molecular absorption cross section is given in MF=3, MT=102.

2.3 Comparison of Calculated and Measured Scattering Law Data

Comparisons of experimental and theoretical $S(\alpha,\beta)$ data for different values of β as a function of α are shown in Figs. 37 and 38 together with the corresponding ENDF/B data.

2.4 Comparison with Integral Data

The total cross section, the average cosine of the scattering angle and the neutron diffusion coefficient for heavy water obtained by processing the JEF data, are compared against experimental data in Fig. 39 through 42.

2.5 Comparison of Computed and Measured Neutron Flux Spectra

A 126 group cross-section library (42) was used for calculating neutron flux spectra at room temperature for two different poisons. These results are compared with experimental data in Figs. 43 and 44.

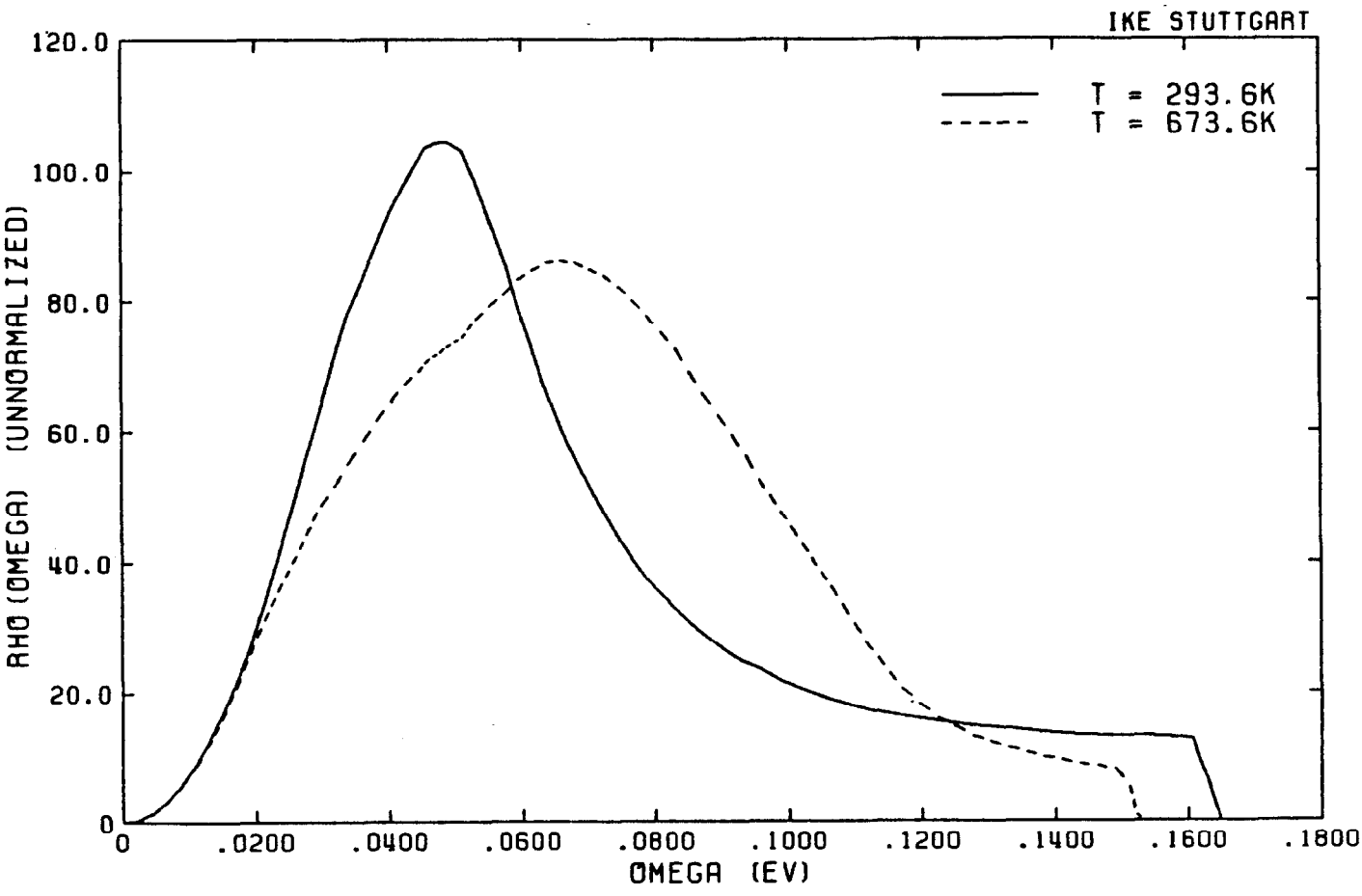

Fig. 34 Temperature Dependence of the Phonon Frequency Spectra for the Hindered Rotations of Deuterium Bound in Heavy Water D_2O

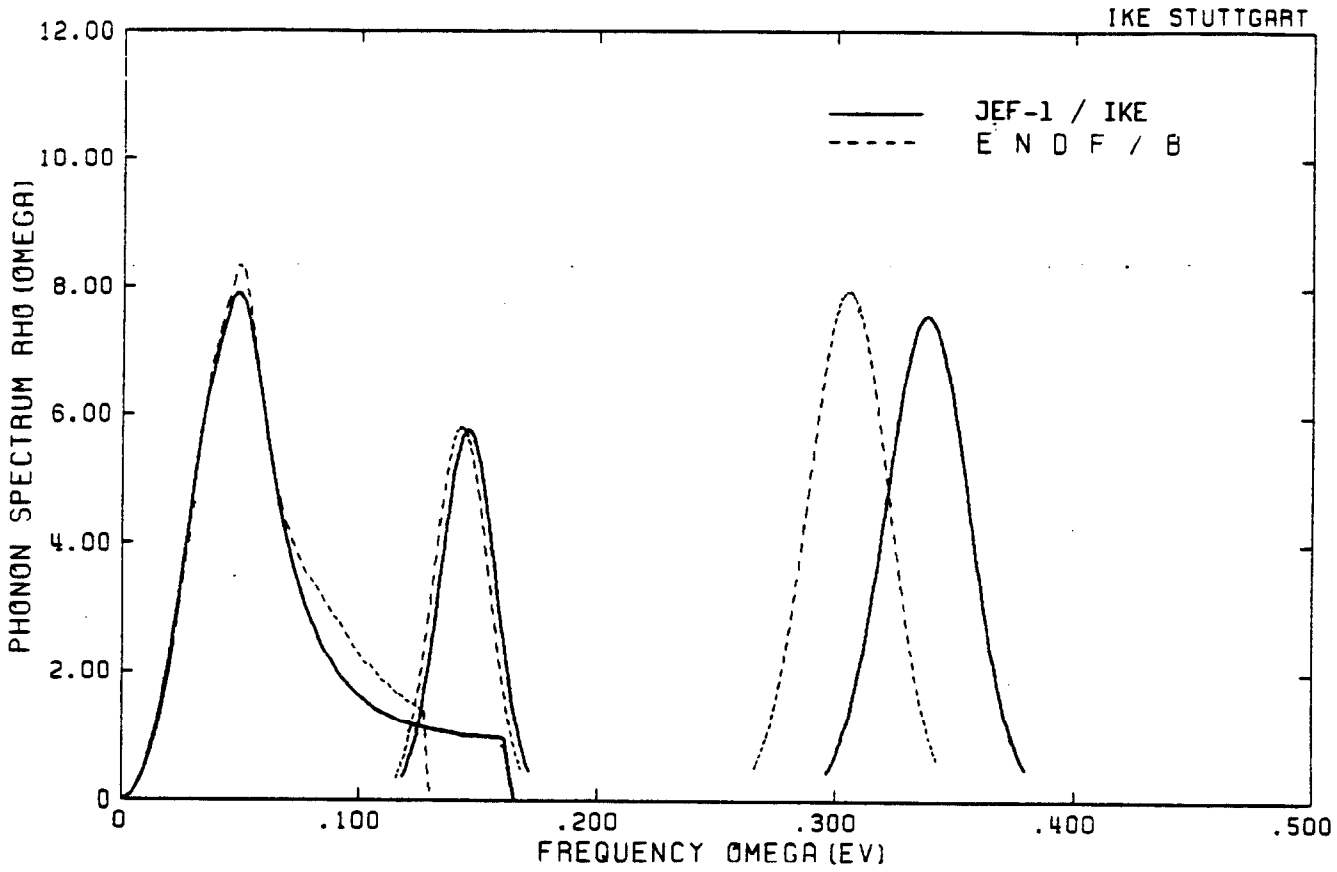

Fig. 35 Phonon Frequency Spectra of Deuterium Bound in Heavy Water

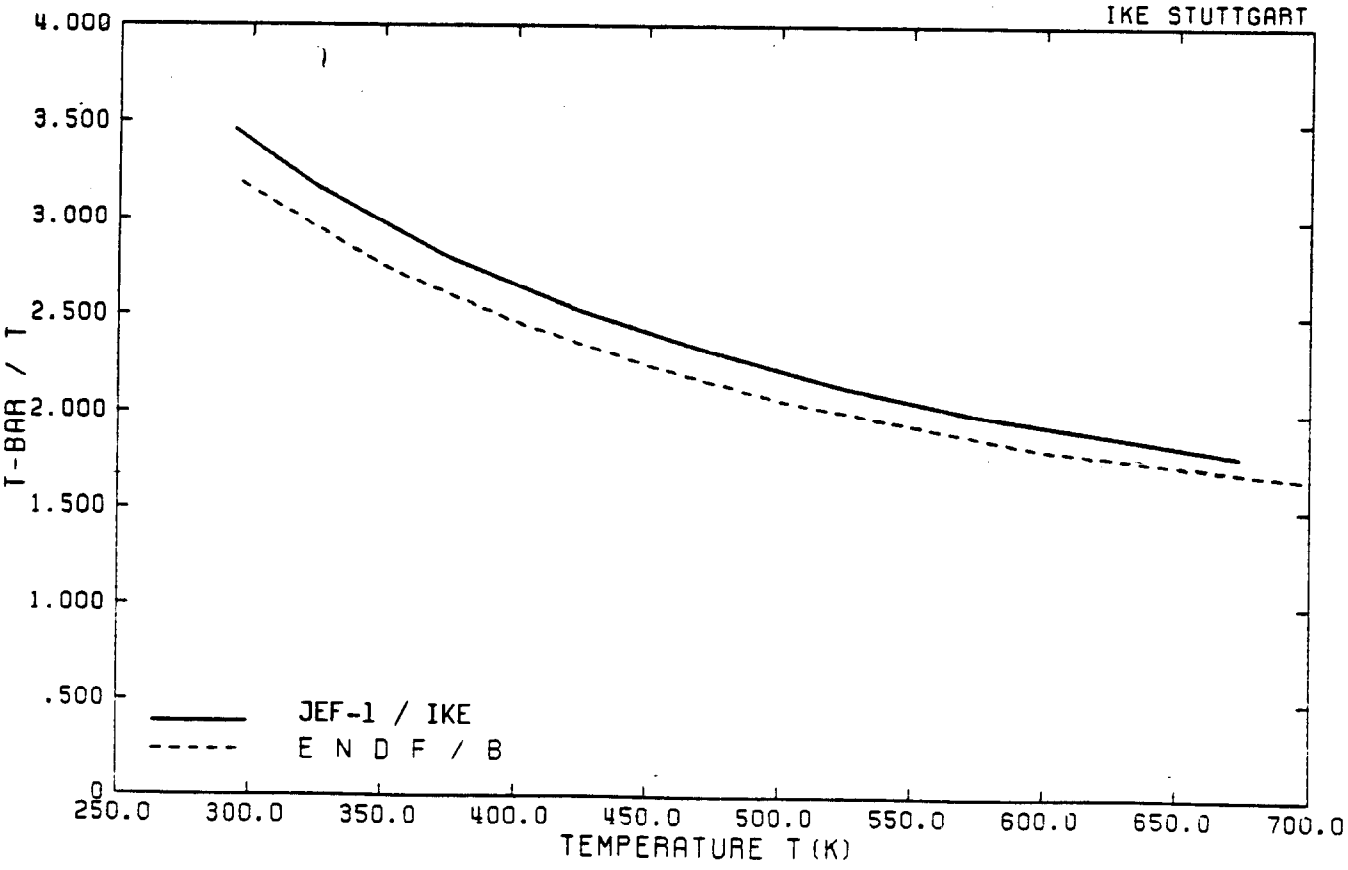

Fig. 36 Effective Scattering Temperature of Deuterium Bound in D_2O

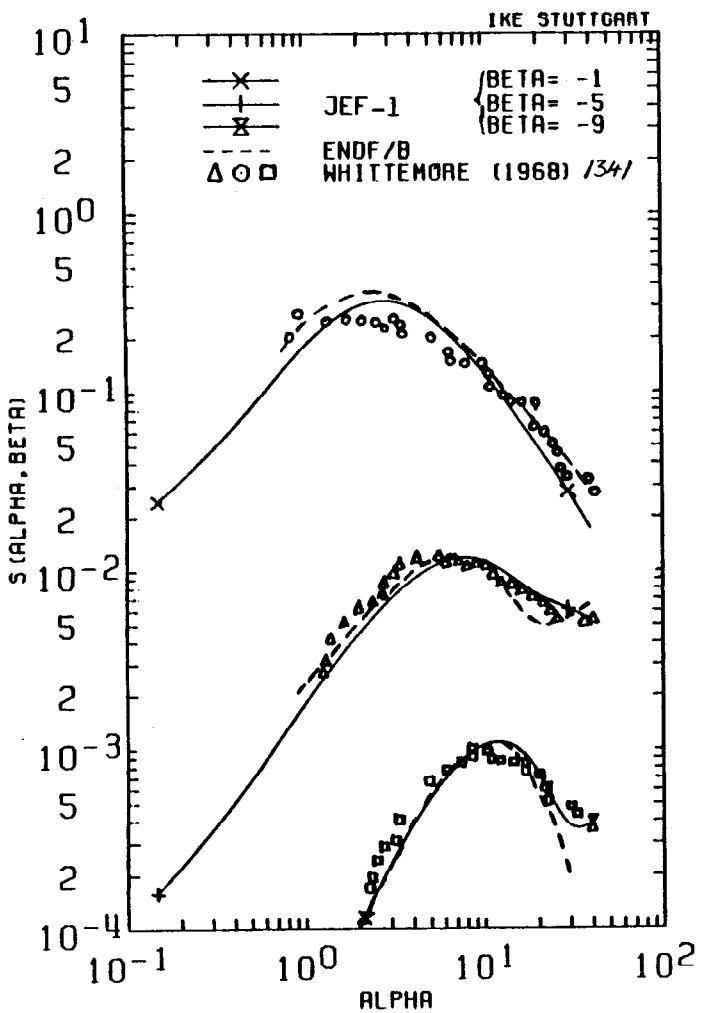

Fig. 37 Scattering Law Data for Heavy Water at T = 300 K

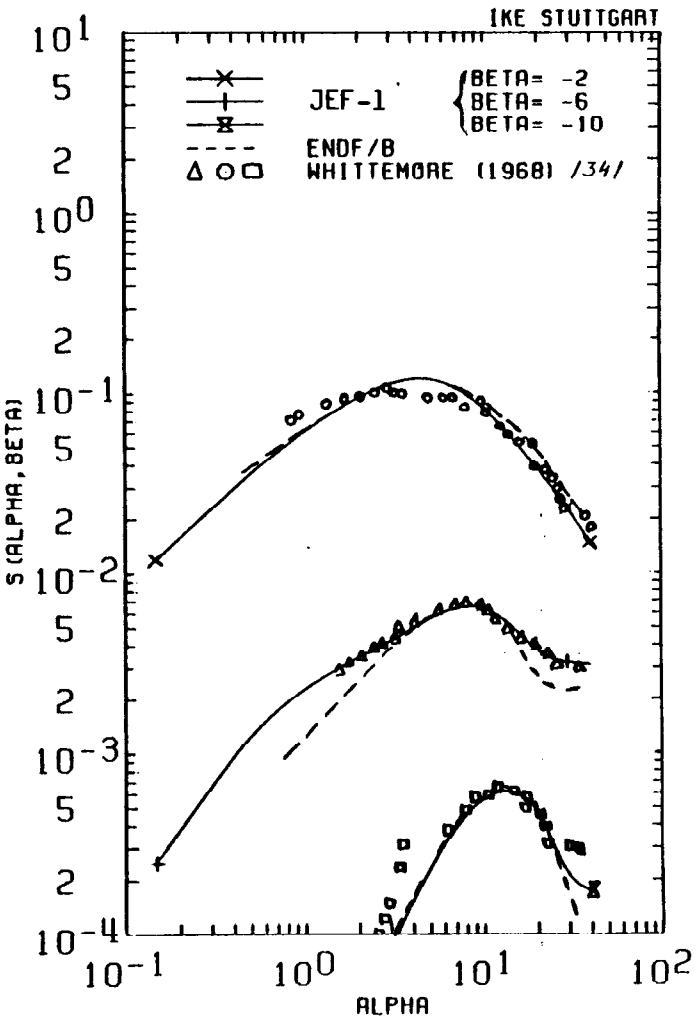

Fig. 38 Scattering Law Data for Heavy Water at T = 300 K

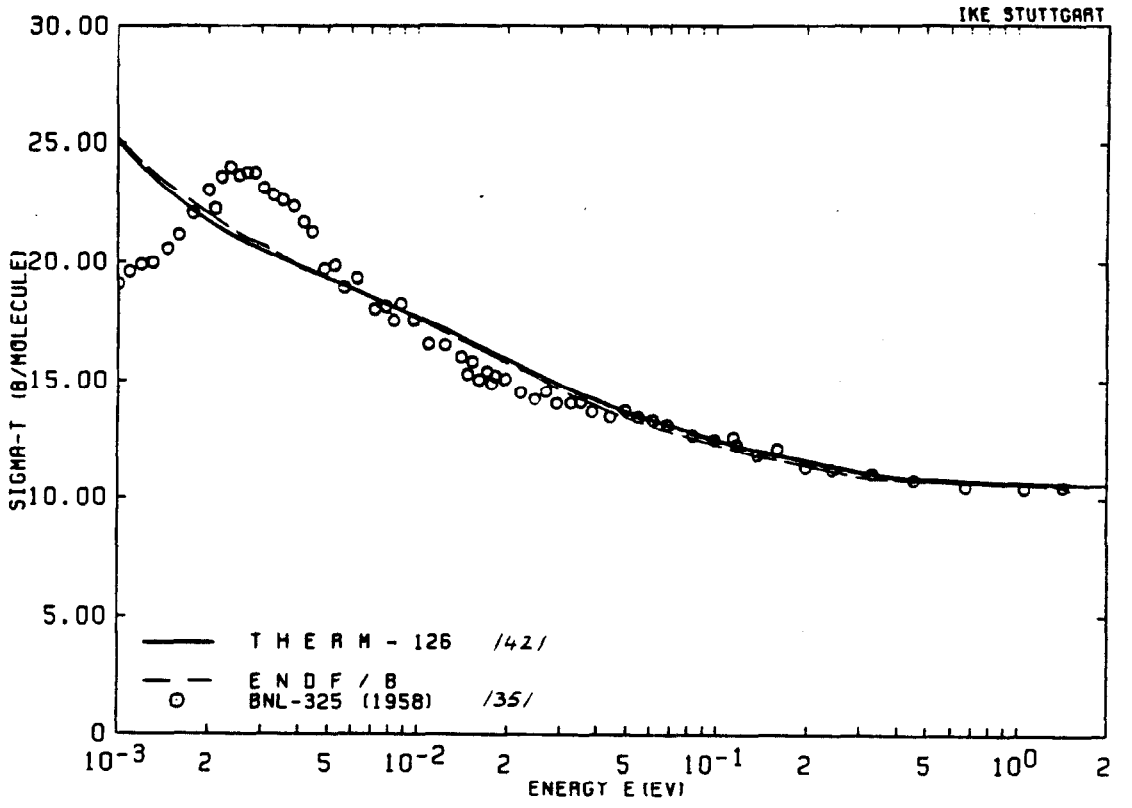

Fig. 39 Total Neutron Cross Sections for Heavy Water at Room Temperature

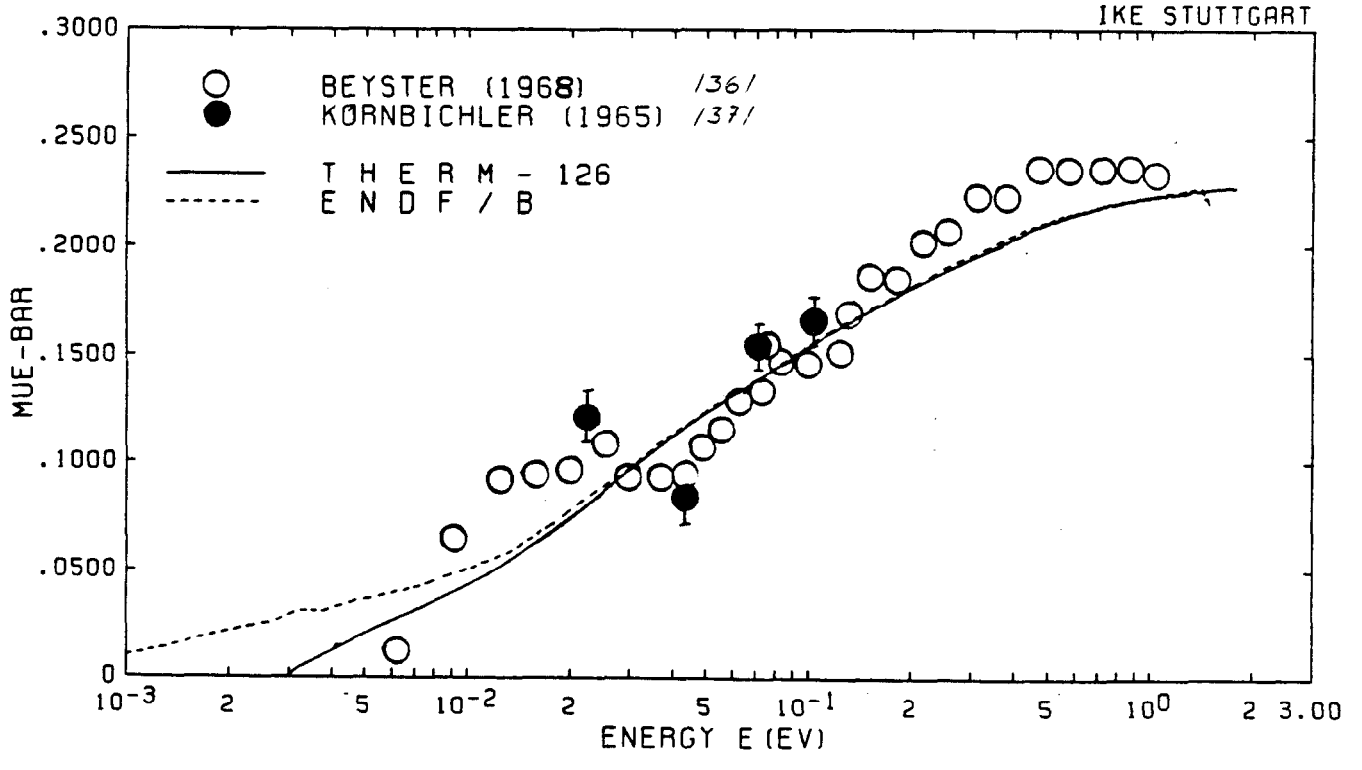

Fig. 40 Average Cosine of the Neutron Scattering Angle for Heavy Water at Room Temperature

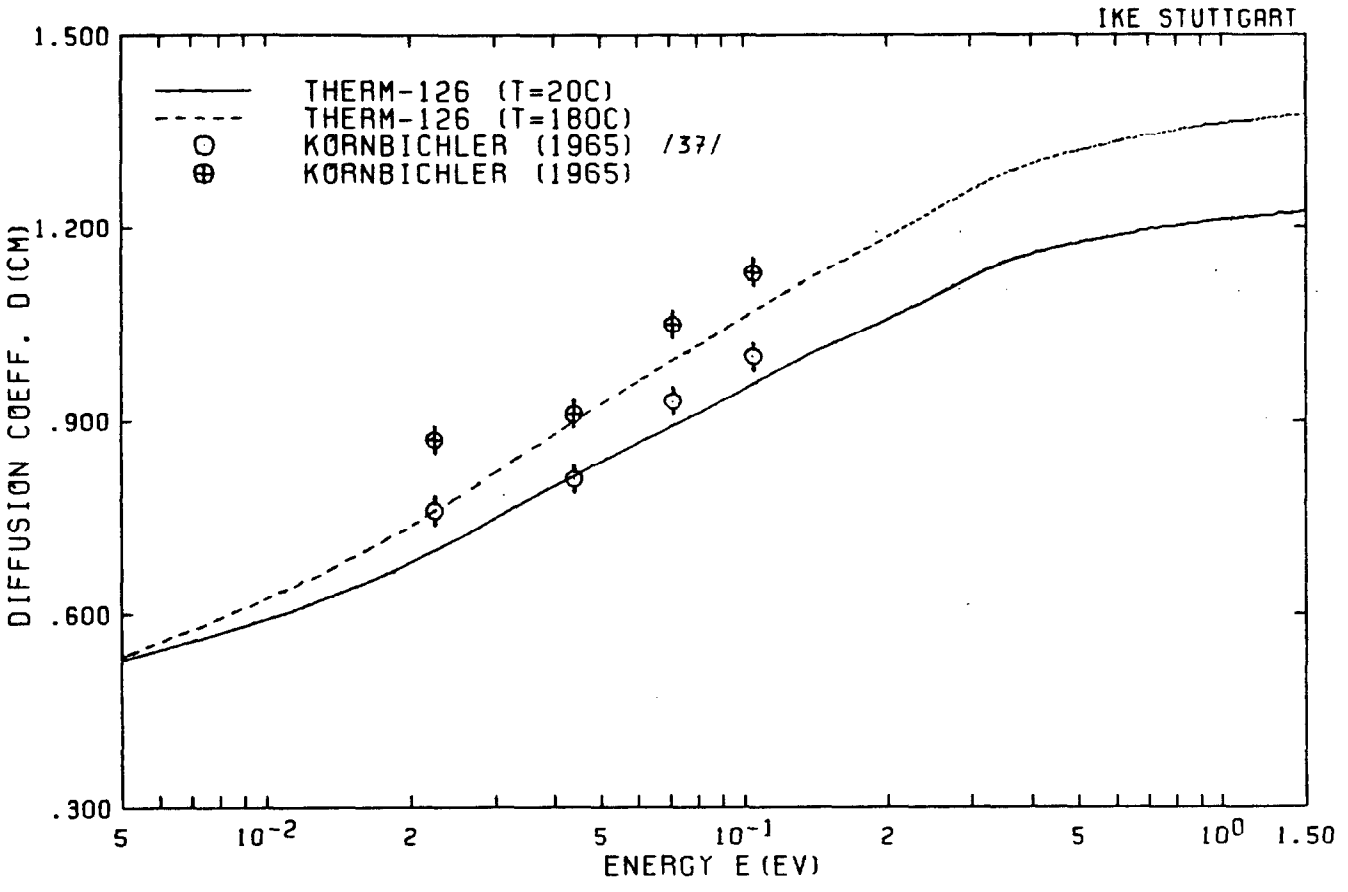

Fig. 41 Neutron Diffusion Coefficient in D_2O

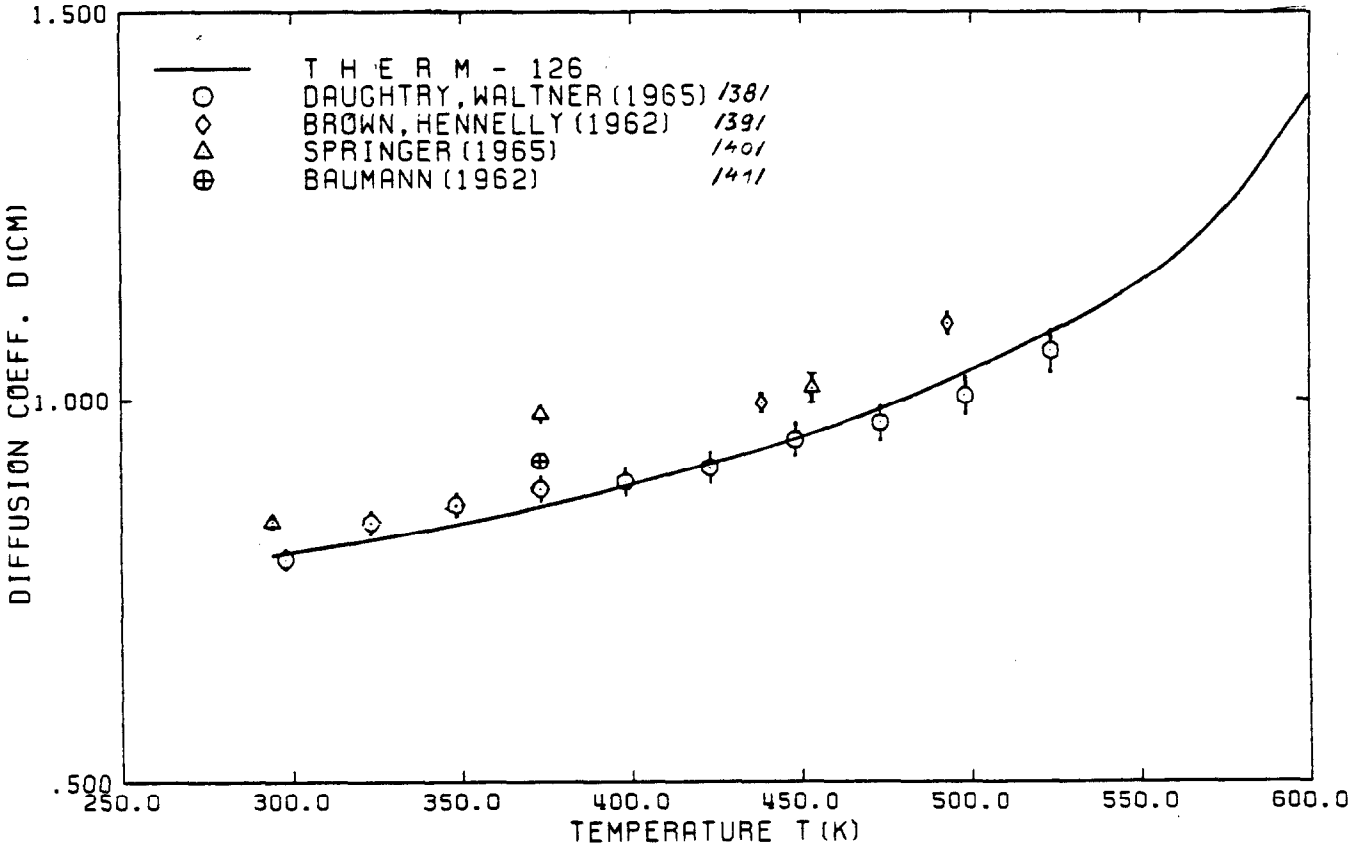

Fig. 42 Neutron Diffusion Coefficient in Heavy Water D_2O

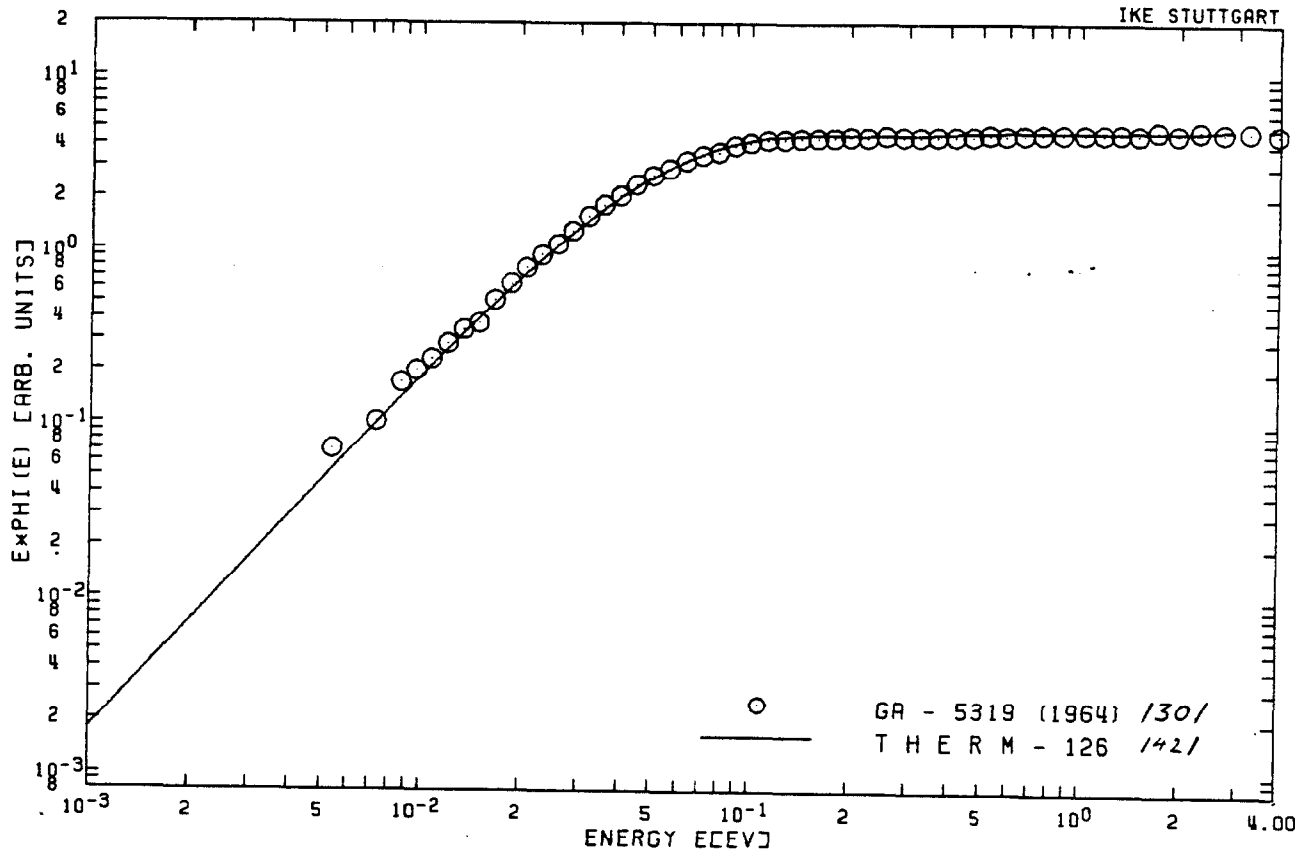

Fig. 43 Neutron Spectrum in Borated D_2O at Room Temperature (2.1 b/D-atom)

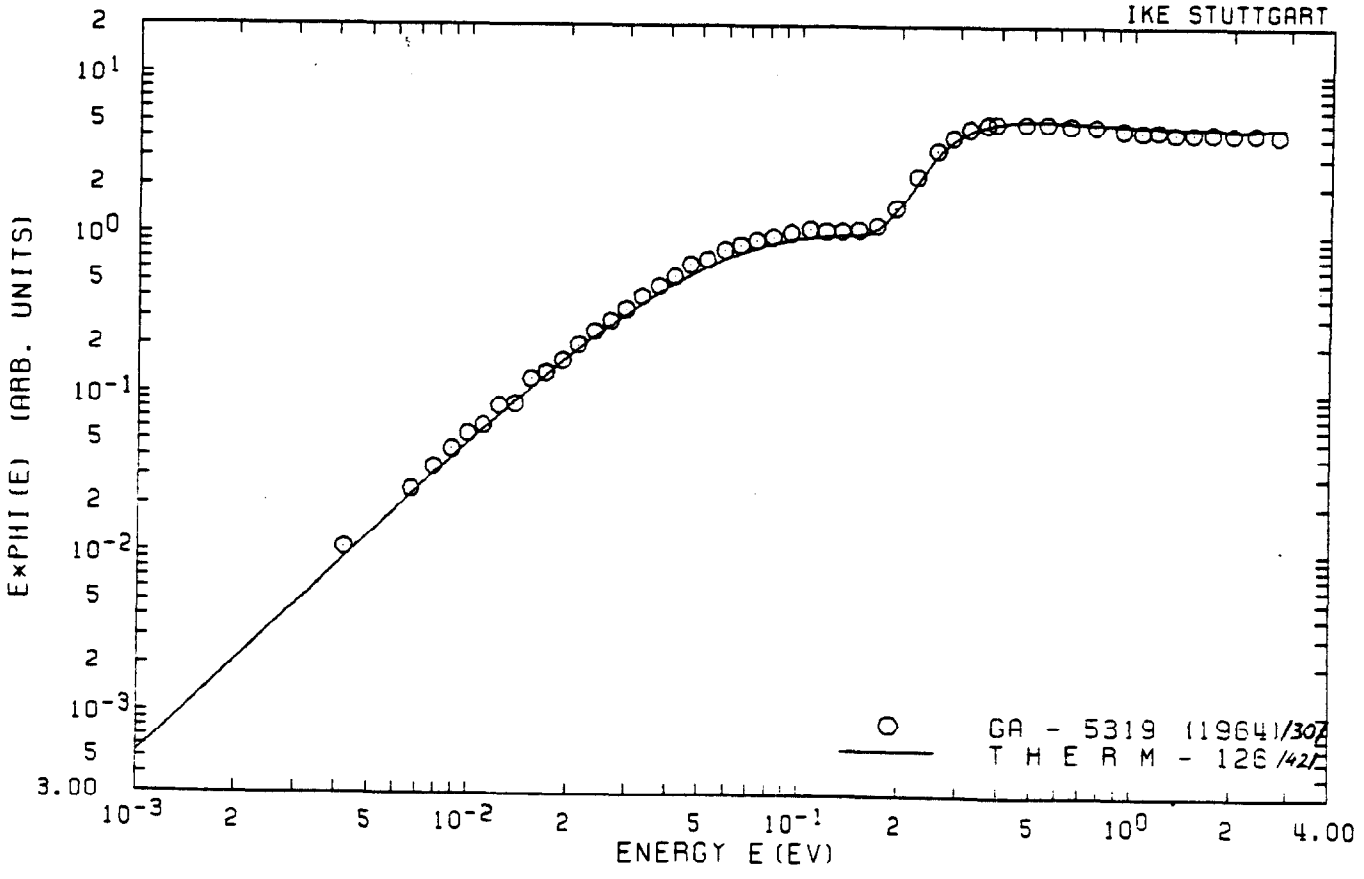

Fig. 44 Neutron Spectrum in D_2O + Cd - Nitrate at Room Temperature (2.4 b/D-atom)

3. GRAPHITE, MAT=4003

3.1 Physics of the Neutron Scattering in Graphite, Phonon Frequency Spectrum, Related Parameters and Specific Heat

A central-force lattice-dynamics model for the graphite unit cell (43,44) was used for deriving the frequency spectrum of Carbon bound in graphite.

This model contains four force constants:

- the nearest neighbour central force which binds two hexagonal planes together;
- a bond-bending force in a hexagonal plane;
- the bond-stretching force between the nearest neighbours in the plane;
- the restoring force against bending of the hexagonal plane.

The force constants are precisely fitted to the high and low temperature specific heat, and to the compressibility of reactor grade graphite.

This model is the same as the one used in deriving the ENDF/B data for MAT=1065 (5,45).

The theoretical phonon frequency spectrum is shown in Fig. 45, together with the phonon spectra derived by Butland (47) and Haywood (48) from experimental data.

Assuming that the vibrational states of the nuclei at a given temperature may be described by a set of harmonic oscillators obeying Bose-Einstein-statistics, and assuming that the phonon frequency spectrum $\varrho(\omega)$ is temperature invariant, it may be shown that the specific heat at constant volume, C_v, is generally given by:

$$\frac{C_v}{3R} = \frac{\hbar^2}{(kT)^2} \int_0^\infty \varrho(\omega) \frac{\omega^2 e^{\frac{\hbar\omega}{kT}}}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2} d\omega$$

R is the gas constant, C_v applies to one mole,

and $\int_0^\infty \varrho(\omega) d\omega = 1.$

The specific heat of graphite as derived from different phonon spectra are shown in Fig. 46. A good agreement with the results of Butland and experimental data is observed.

The effective scattering temperatures and the Debye-Waller integrals for graphite derived from the phonon frequency spectrum are given in Table 6 and shown in Fig. 47.

Table 6: Integral parameters derived from the frequency spectrum of graphite

Temperature (K)	Debye-Waller integral (1/eV)	T_{eff} (K)
293.6	26.06	712.61
400	32.70	754.66
500	39.20	806.65
600	45.88	868.37
700	52.66	937.62
800	59.53	1012.64
1000	73.41	1174.94
1200	87.42	1348.12
1600	115.66	1712.90
2000	144.04	2090.99
3000	215.26	3061.02

3.2 Data Stored in the JEF File

The different quantities stored for graphite, MAT=4003, are described in the information file (MF=1, MT=451) given in Appendix 4.

These are:

$S(\alpha,\beta,T)$ (MF=7,MT=4) for Carbon bound in graphite at the following temperatures:

293.6 400 500 600 700 800 1000 1200 1600 2000 3000 K

The data are represented in the temperature-dependent ENDF/B data format (see Appendix F of (1)) at 100 values of α and 150 values of β. The energy limit E_{max} up to which $S(\alpha,\beta,T)$ can be used is 1.8554 eV.

The effective scattering temperatures that are required for the short collision time approximation for higher energy transfers are given in the form of a table in MF=1, MT=451.

The total free atom scattering cross section of Carbon is 4.74 b.

The coherent elastic cross sections are not given in this file. They should be computed by the method given in HEXSCAT (60) as coded in the THERMR module of NJOY (61). The Debye-Waller integrals required for this purpose are provided for different temperatures in tabular form in MF=1, MT=451.

The numerical values of the phonon spectrum are also given.

3.3 Comparison of Calculated and Measured Scattering Law Data

The JEF/IKE scattering law data for two temperatures are compared against experimental data in Figs. 48 and 49.

3.4 Comparison with Integral Data

The total neutron cross sections for graphite as computed by NJOY (61) using the $S(\alpha,\beta)$ data of JEF-1 are compared against experimental data in Fig. 50.

A set of 126 group cross sections derived from the JEF/IKE data was used to calculate the temperature dependence of the neutron diffusion length $\overline{L}$. The obtained results together with experimental results are shown in Fig. 51.

3.5 Comparison of Computed and Measured Neutron Flux Spectra

The same 126 group cross section library was used for calculating neutron flux spectra at two temperatures for Samarium poisoned graphite. The Figs. 52 and 53 show a good agreement with experimental data.

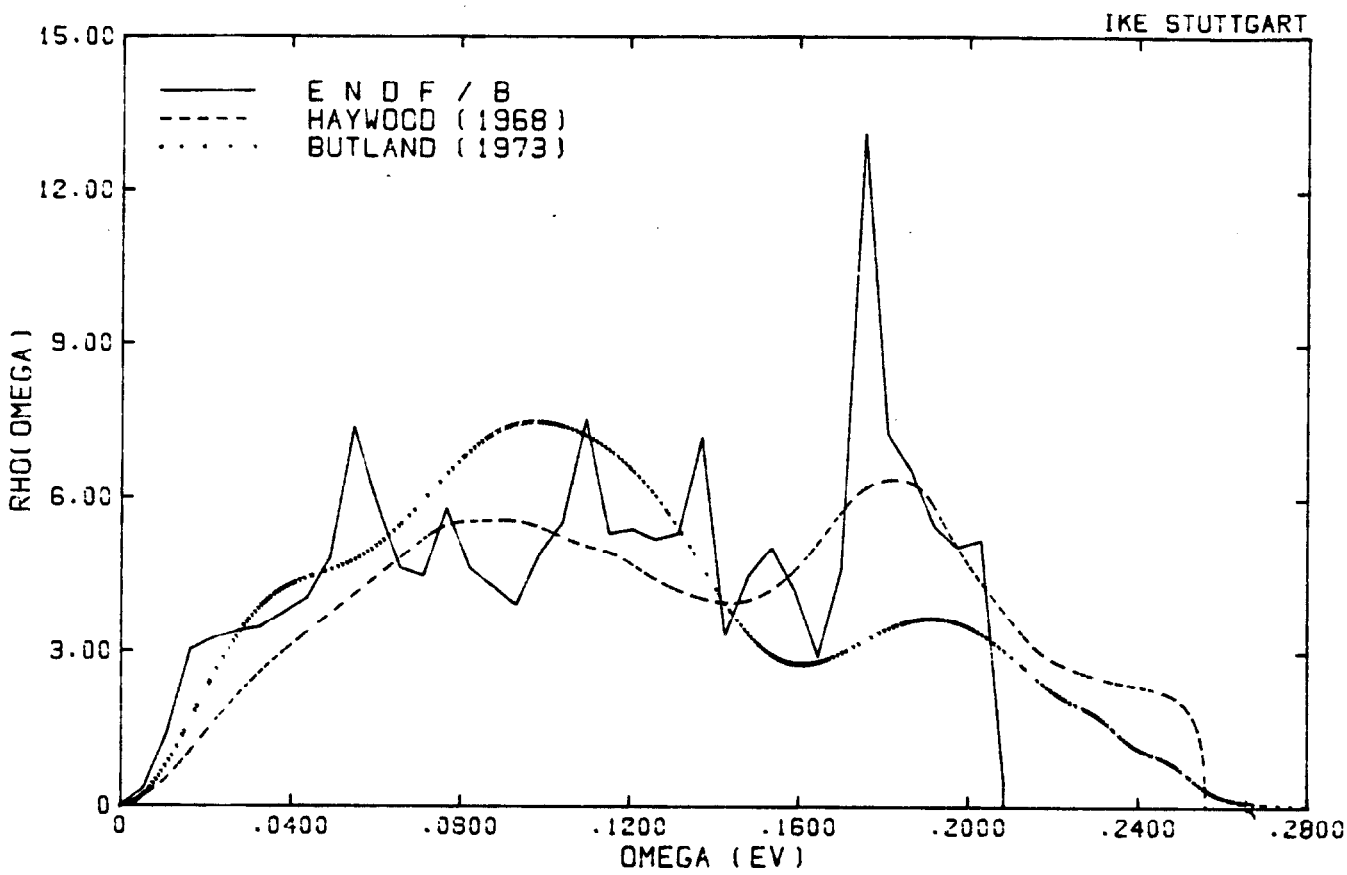

Fig. 45 Comparison of Phonon Frequency Spectra in Graphite

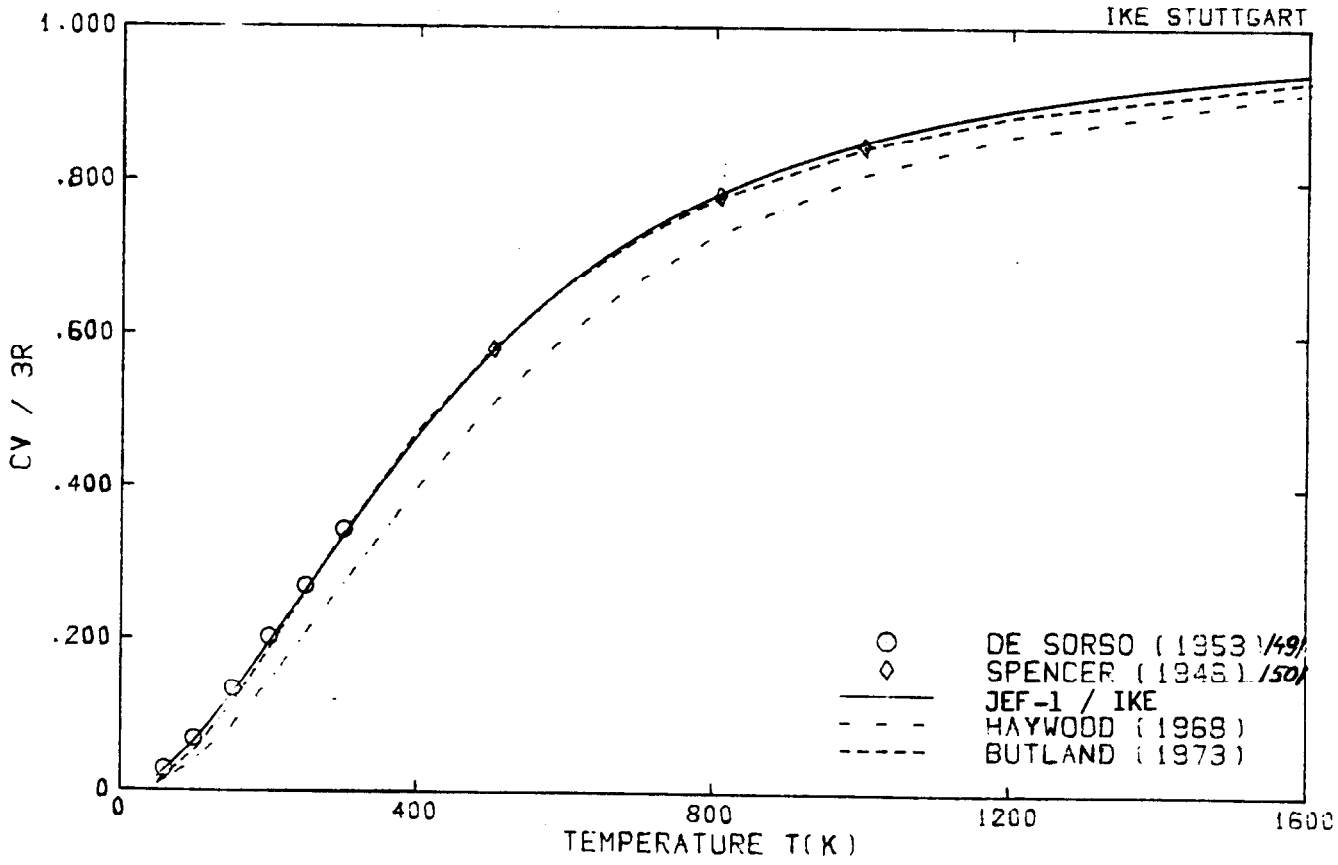

Fig. 46 Specific Heat of Graphite

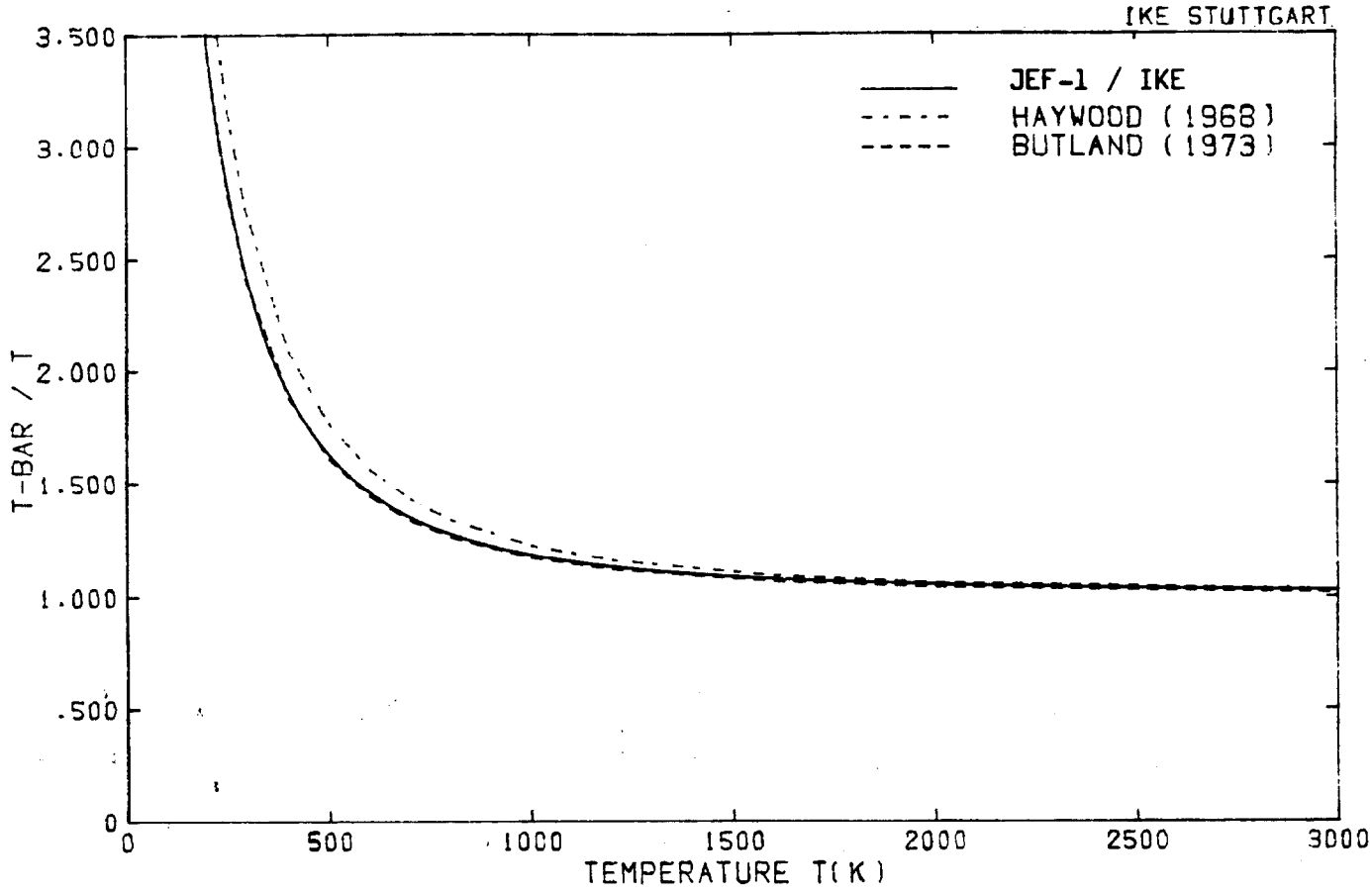

Fig. 47 Effective Scattering Temperature of Graphite

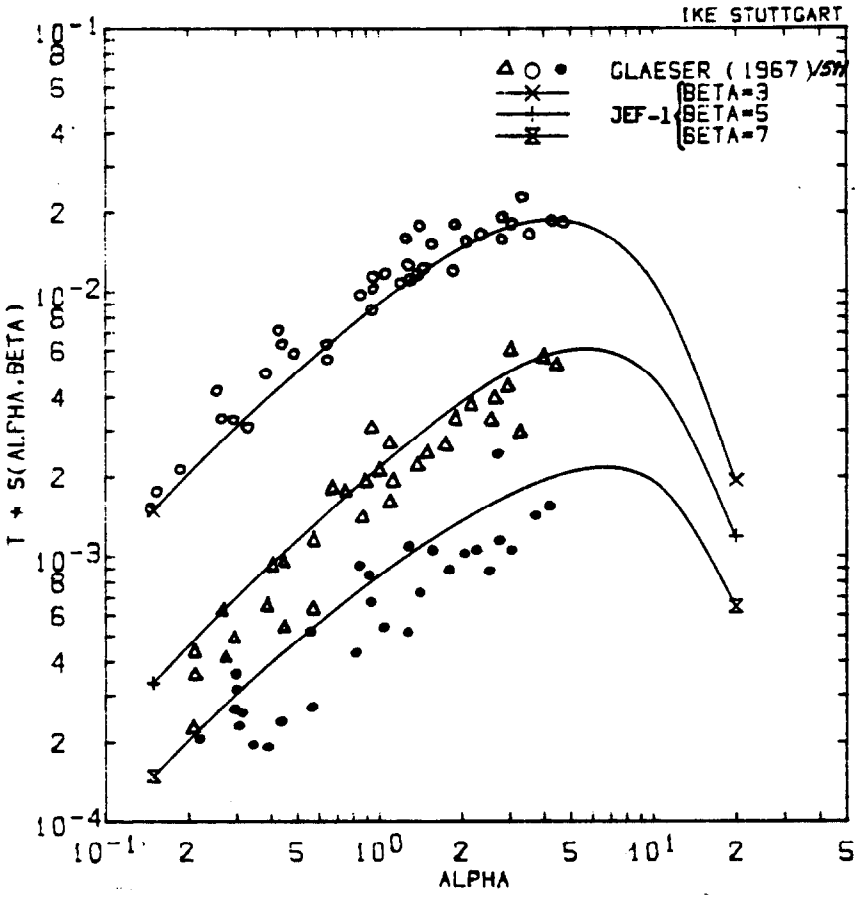

Fig. 48 Scattering Law Data for Graphite at T = 300 K for Different β

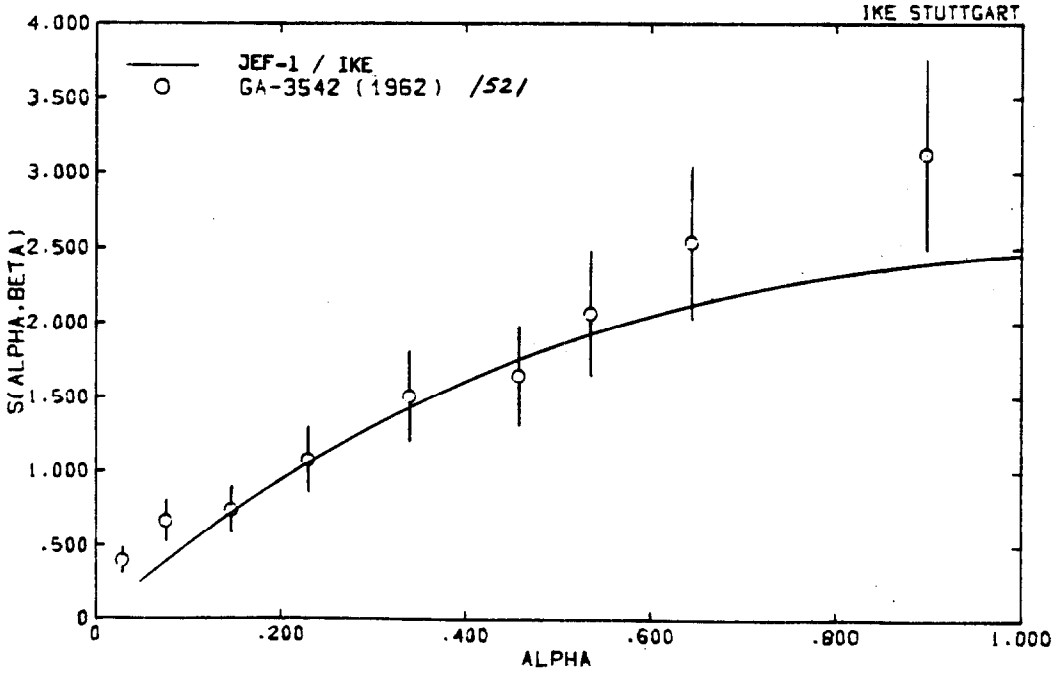

Fig. 49 Scattering Law Data for Graphite at T = 635 K (β = 1.0)

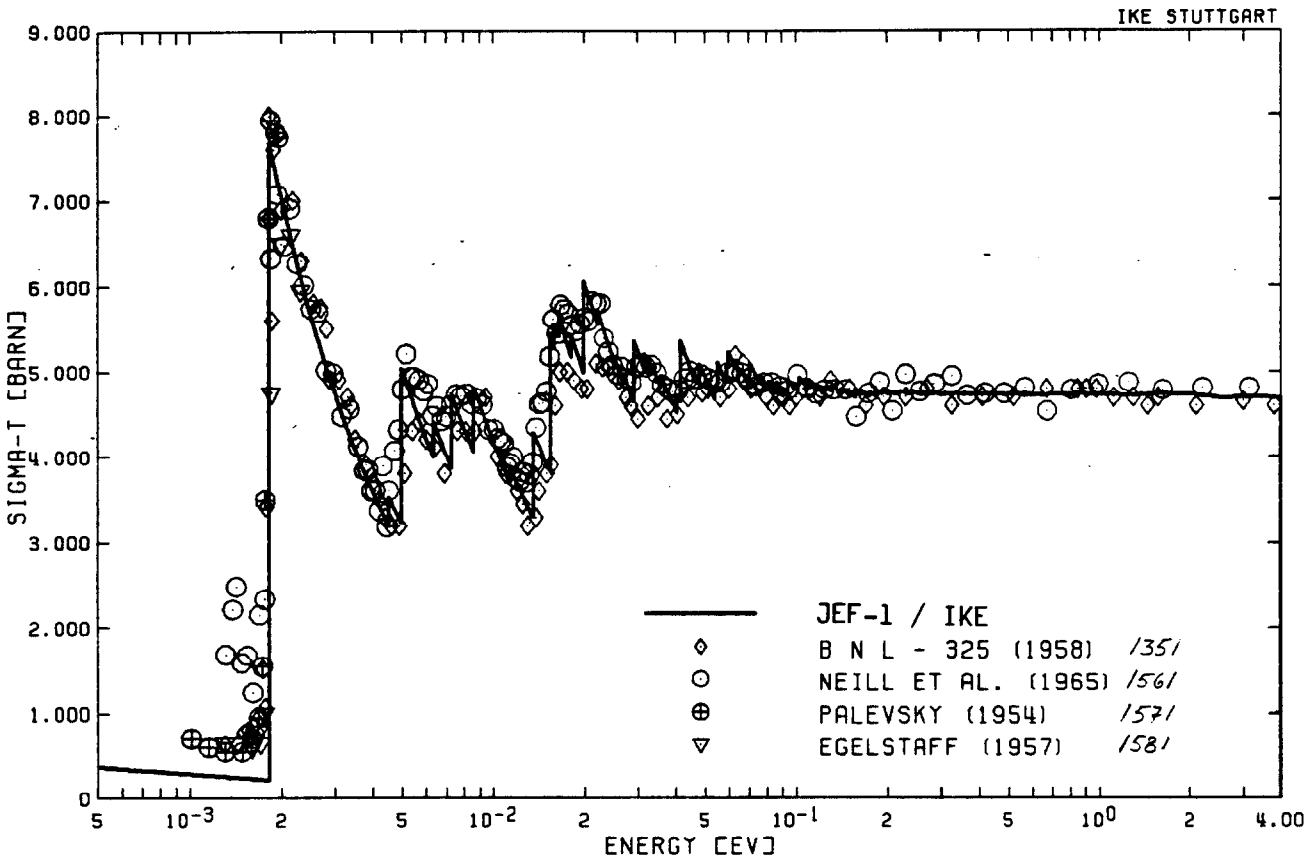

Fig. 50 Total Neutron Cross Section for Graphite at Room Temperature

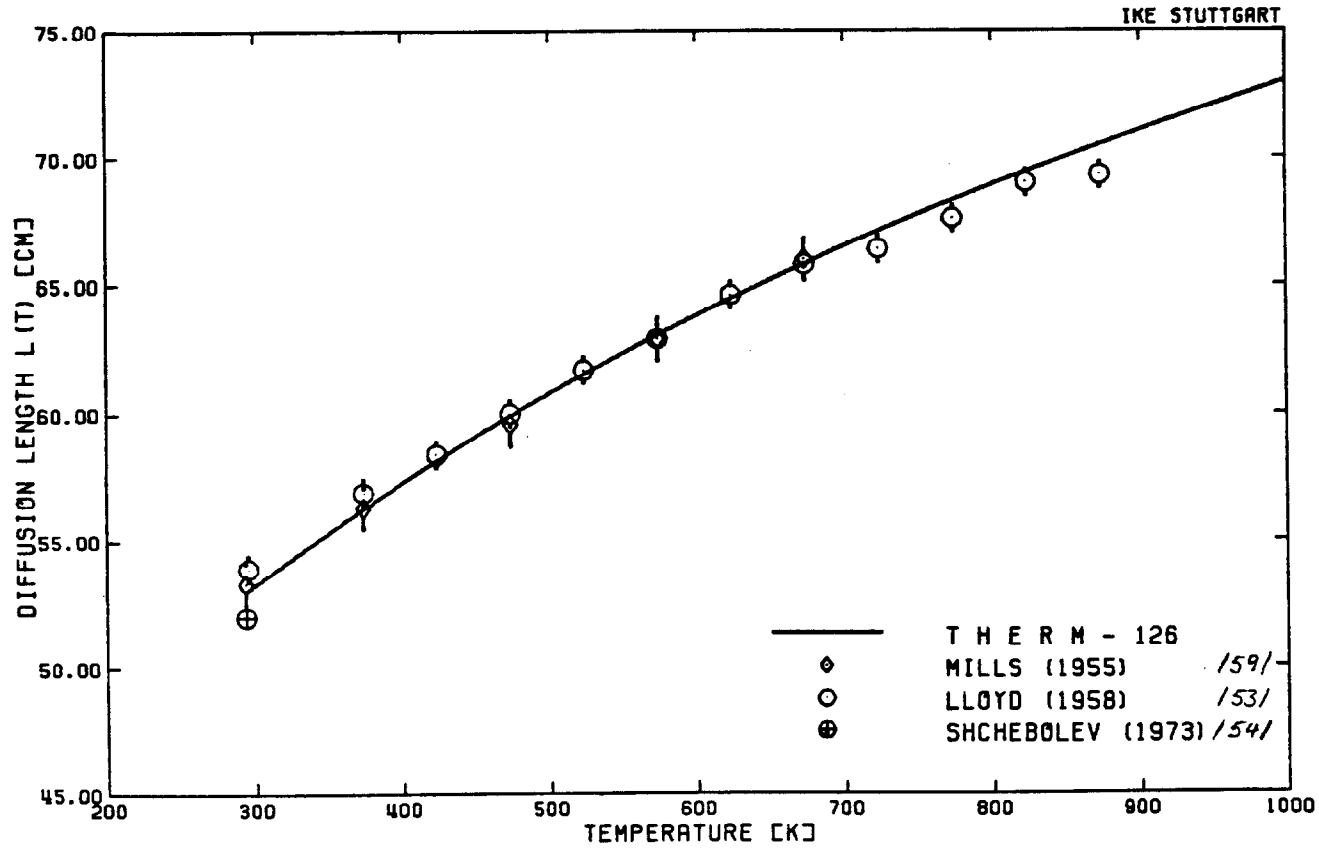

Fig. 51 Neutron Diffusion Length $\overline{L}(T)$ in Graphite

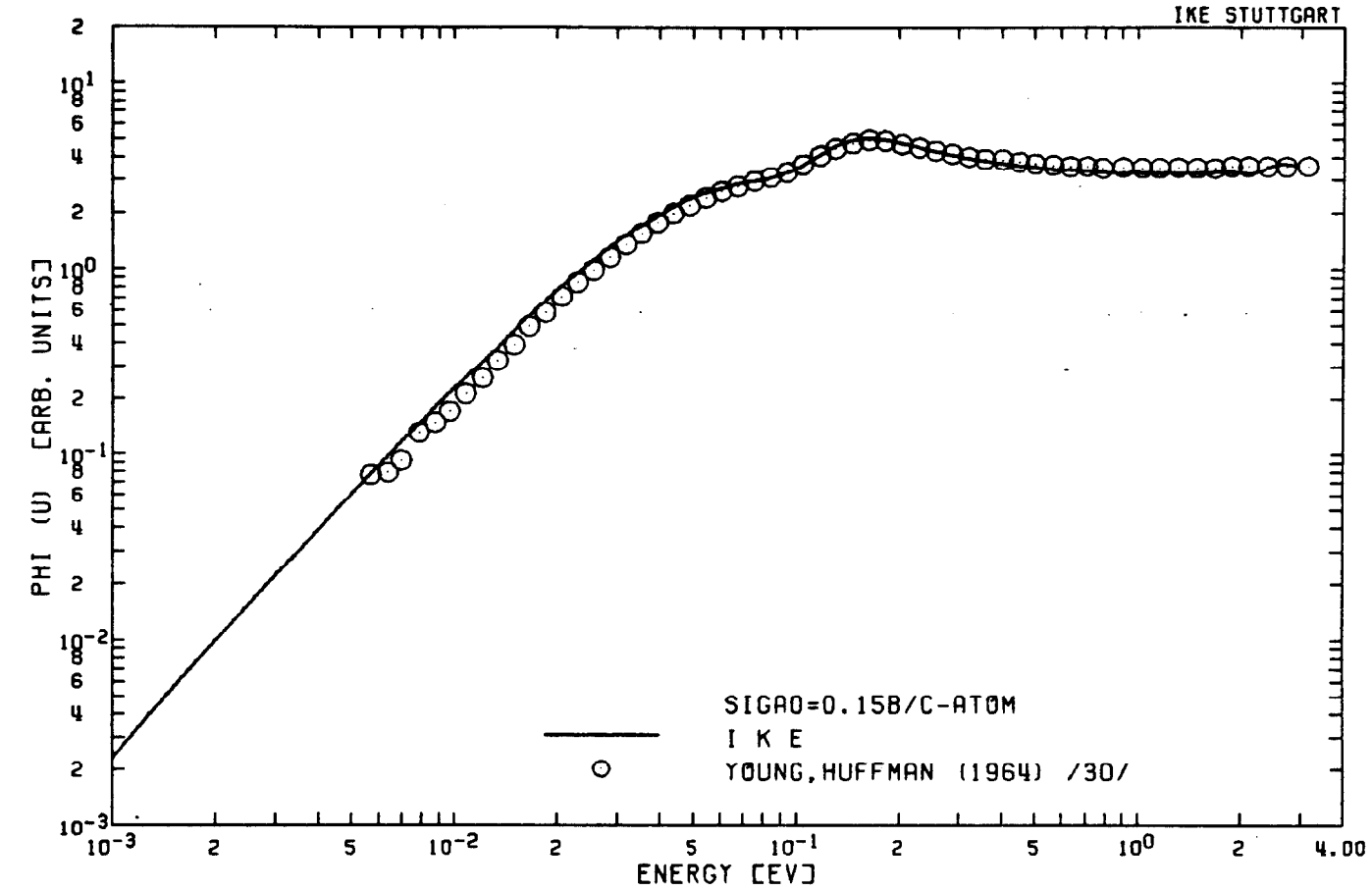

Fig. 52 Neutron Spectrum in Samarium Poisoned Graphite at 300 K

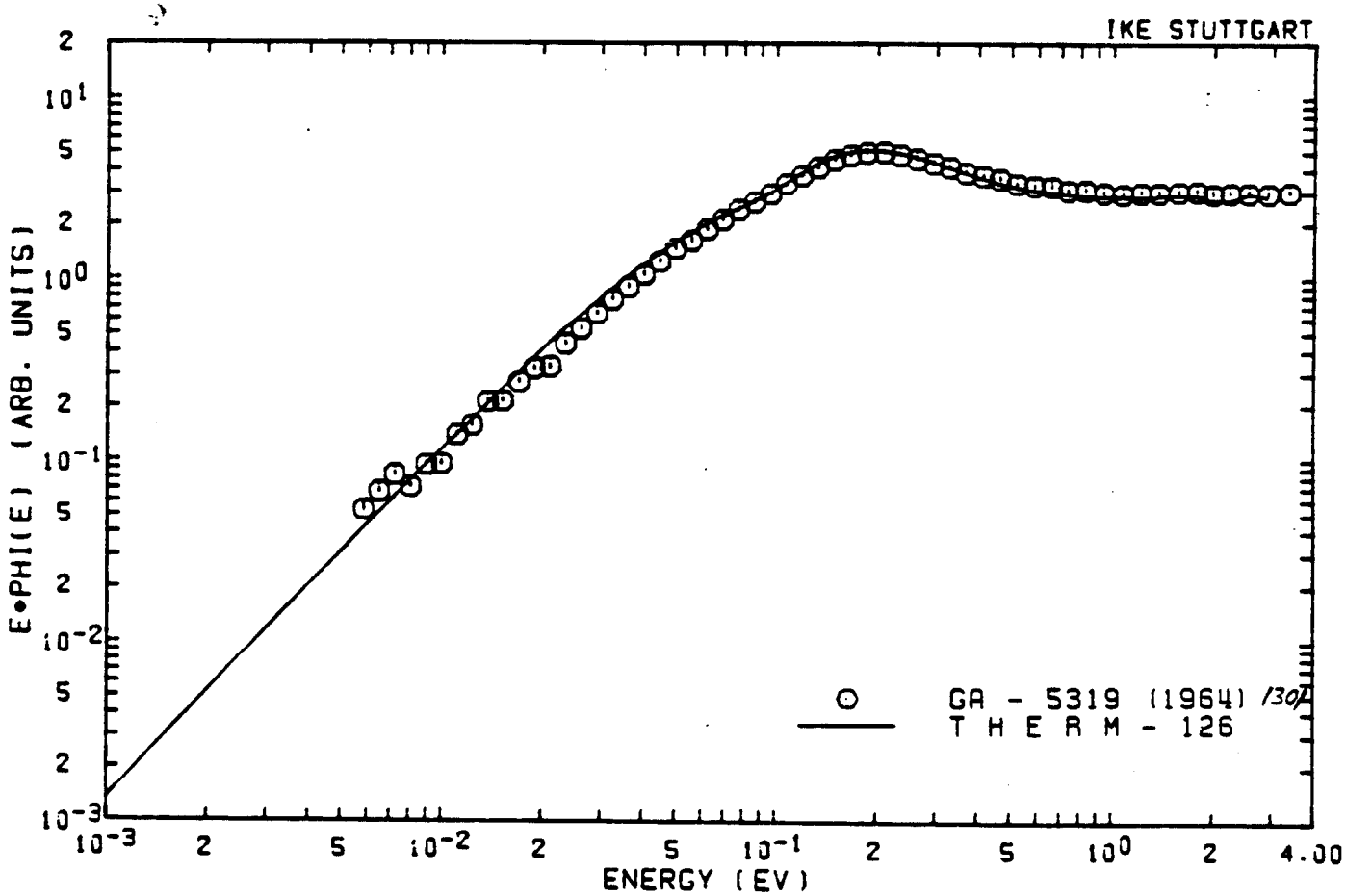

Fig. 53 Neutron Spectrum in Samarium Poisoned Graphite at 600 K

4. POLYETHYLENE $(CH_2)_n$, MAT=4004

4.1 Physics of the Neutron-Proton Scattering, Phonon Frequency Spectrum, Related Parameters and Specific Heat

The phonon frequency spectrum of hydrogen bound in polyethylene has been derived by Sprevak, Koppel (71) on the basis of a model of non-interacting infinite chains of CH_2 radicals originally developed by Lin, Koenig (70). The lattice dynamics of polyethylene shows that nine branches of the dispersion relation are present, the frequencies in each branch being a function of the phase difference of the vibration of corresponding atoms in neighbouring CH_2 units. For some normal modes of vibration the ratio of the amplitude of the hydrogen atom vibrations to the amplitude of the carbon atom vibrations depends strongly on the phase difference.

Sprevak, Koppel (71) calculated the phonon frequency spectrum of hydrogen bound in polyethylene exactly, using the computed frequencies and amplitude vectors. The weighted frequency spectrum used for computing the neutron scattering was first derived in histogram form; then two modifications were made:

- the low frequency part for $\omega < 20$ meV was replaced by a Debye spectrum having the same area;
- to avoid numerical difficulties, the histogram was replaced by Gaussian functions of area equal to the area under each step and centered at the center of each interval in the histogram.

The phonon frequency spectrum of hydrogen bound in polyethylene is represented in Fig. 54. The dynamical modes of vibration of the CH_2 unit are shown in Fig. 55.

The frequency spectrum model is the same as the one used in deriving the ENDF/B data for MAT=1114 (5,45).

The effective scattering temperatures and the Debye-Waller integrals for hydrogen bound in polyethylene are given in Table 7.

Table 7: Integral parameters derived from the frequency spectrum of H in $(CH_2)_n$

Temperature (K)	Debye-Waller integral (1/eV)	T_{eff} (K)
293.6	34.73	1203.87
350	40.29	1214.98

The specific heat of polyethylene as derived from the phonon spectrum is shown in Fig. 56.

4.2 Data Stored in the JEF File

The quantities stored for polyethylene (MAT=4004) are described in the information file MF=1, MT=451 given in Appendix 5.

These are:

$S(\alpha,\beta,T)$ (MF=7,MT=4) for H in $(CH_2)_n$ at the two temperatures:

293.6, 350 K

The data are represented in the temperature-dependent ENDF/B data format (see appendix F of (1)) at 100 values of α and 150 values of β. The energy limit E_{max} up to which $S(\alpha,\beta,T)$ is treated exactly is 1.8554 eV.

The effective scattering temperatures that are required for the short collision time approximation for energy transfers beyond E_{max} are given in the form of a table in MF=1, MT=451.

The same total free atom neutron scattering cross section for hydrogen is used as in ENDF/B-V MAT=1301, namely 20.449 b. The values required for the free gas approximation of the neutron scattering by carbon are also stored in file 7.

The incoherent elastic scattering cross sections are not given explicitly in the file for polyethylene. This contribution to the total scattering should be computed by the THERMR module of NJOY (61). The Debye-Waller integrals required for this purpose are provided for the two temperatures in tabular form in MF=1, MT=451.

The molecular absorption cross section for polyethylene is given in MF=3, MT=102, and has the value of 0.6675 b at 0.0253 eV.

4.3 Differential Neutron Scattering Data

Comparisons with experiment of double differential and differential neutron scattering cross sections derived from $S(\alpha,\beta,T)$ for various incident neutron energies and scattering angles are shown in Figs. 57 through 64.

4.4 Comparison with Integral Data of Polyethylene and Paraffin

The total neutron cross section for polyethylene is compared against experimental data in Fig. 65 for room temperature.

The average cosine of the neutron scattering angle in polyethylene is represented in Fig. 66 where, in addition, a comparison with ENDF/B data (5) is shown.

A set of 126-group cross-sections (42) generated from JEF/IKE data with NJOY was used to calculate the neutron diffusion parameters at room temperature. The results for polyethylene are compared against experiments in Table 8.

For practical purposes, the data derived for polyethylene can also be used for paraffin. Experimental results for paraffin with two different densities are shown in Table 9 together with the computed values.

Table 8: Neutron Diffusion Parameters of Polyethylene at Room Temperature

D (cm)	L (cm)	Reference
0.103	2.12	Calculation (55)
0.103 ± 0.004	2.12 ± 0.04	Measurement (67)

Table 9: Neutron Diffusion Parameters of Paraffin at Room Temperature

D (cm)	L (cm)	Density (g/cm^3)	Reference
0.109 ± 0.004	2.19 ± 0.07	0.87	Measurement (68)
0.1087	2.237		Calculation (55)
0.108 ± 0.002	2.13 ± 0.04	0.89	Measurement (69)
0.1062	2.187		Calculation (55)

4.5 Comparison of Computed and Measured Neutron Flux Spectra in Polyethylene and Paraffin

Graphical comparisons of computed and measured neutron flux spectra in polyethylene are shown for two poison concentrations in Fig. 67 and 68. A 126-group neutron cross-section library (42) has been used to compute these two energy spectra.

In addition the neutron spectrum in a mixture of uranium tetrafluoride and paraffin was calculated using the polyethylene scattering kernel data.

The results are compared against experimental data and presented in Fig. 69. The good agreement shows that the polyethylene data are well suited to describe the neutron thermalisation in paraffin.

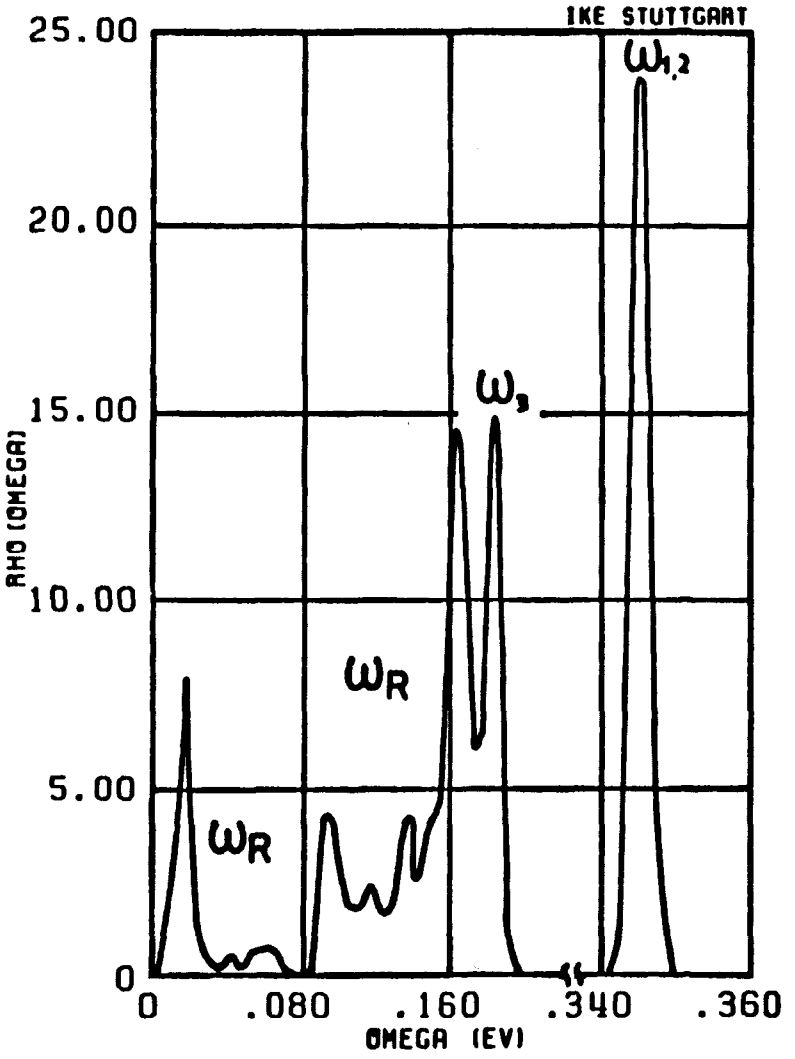

Fig. 54 Phonon Spectrum of Hydrogen Bound in Polyethylene

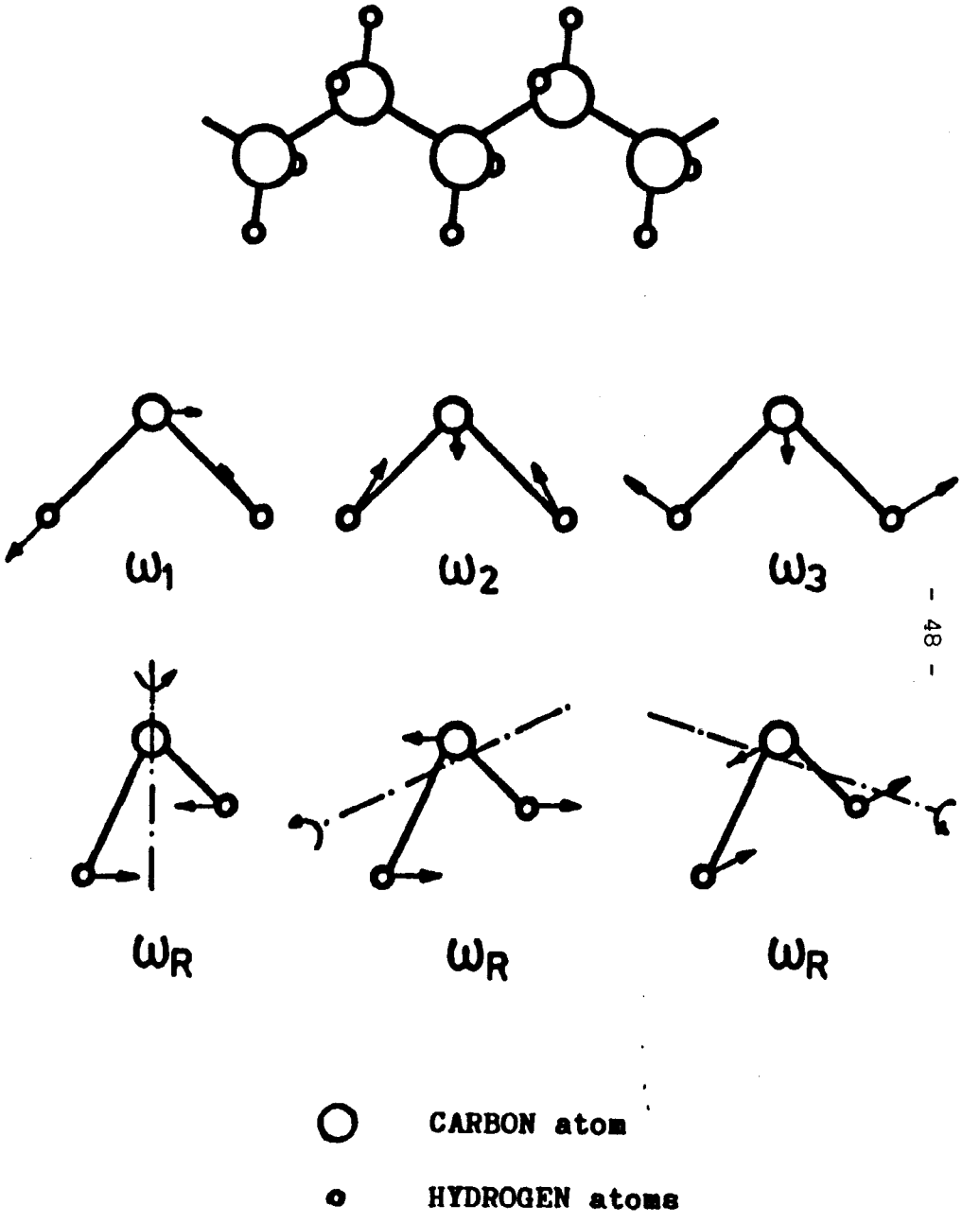

Fig. 55 Structure and Dynamics of Polyethylene

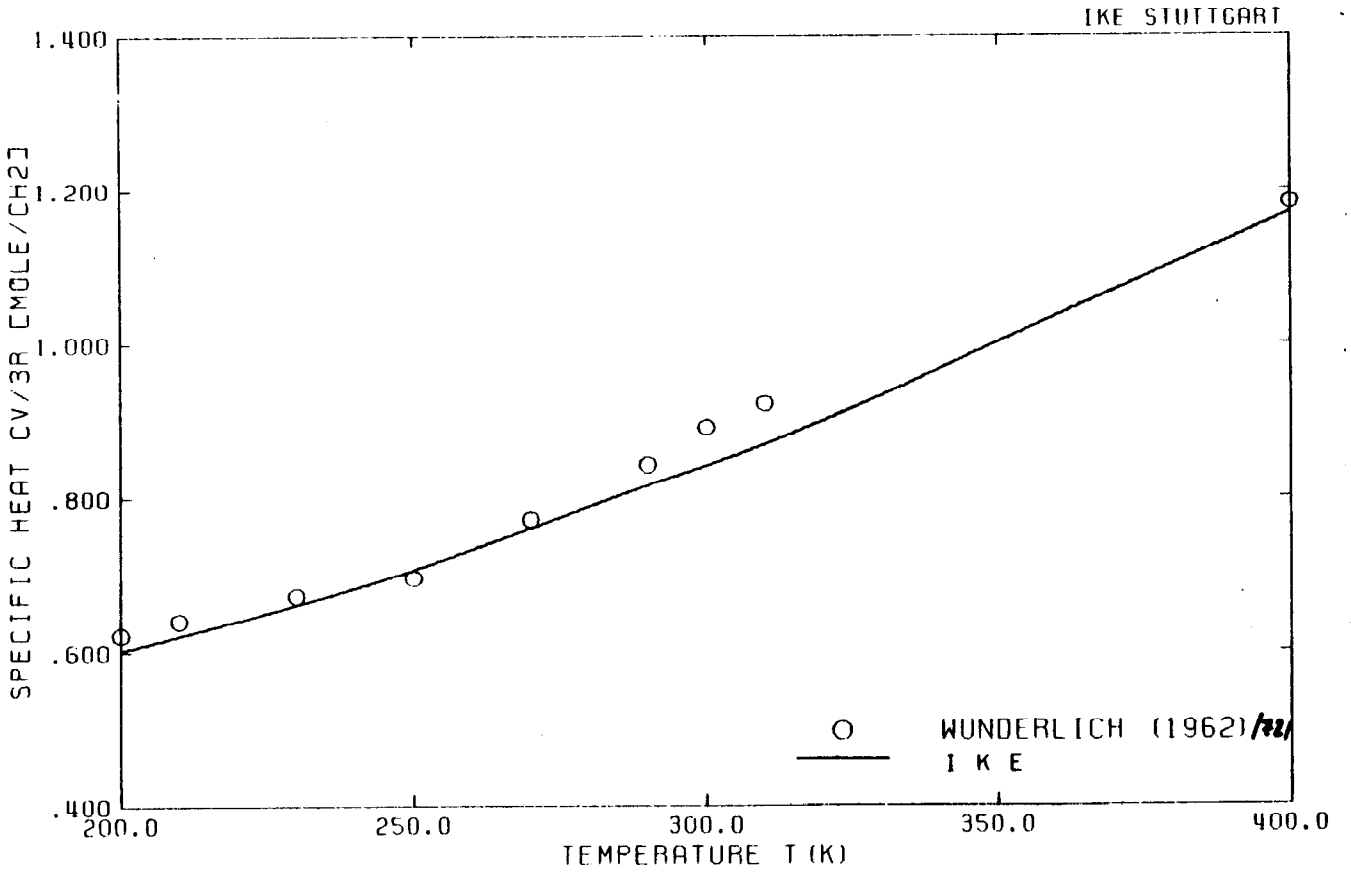

Fig. 56 Specific Heat of Polyethylene

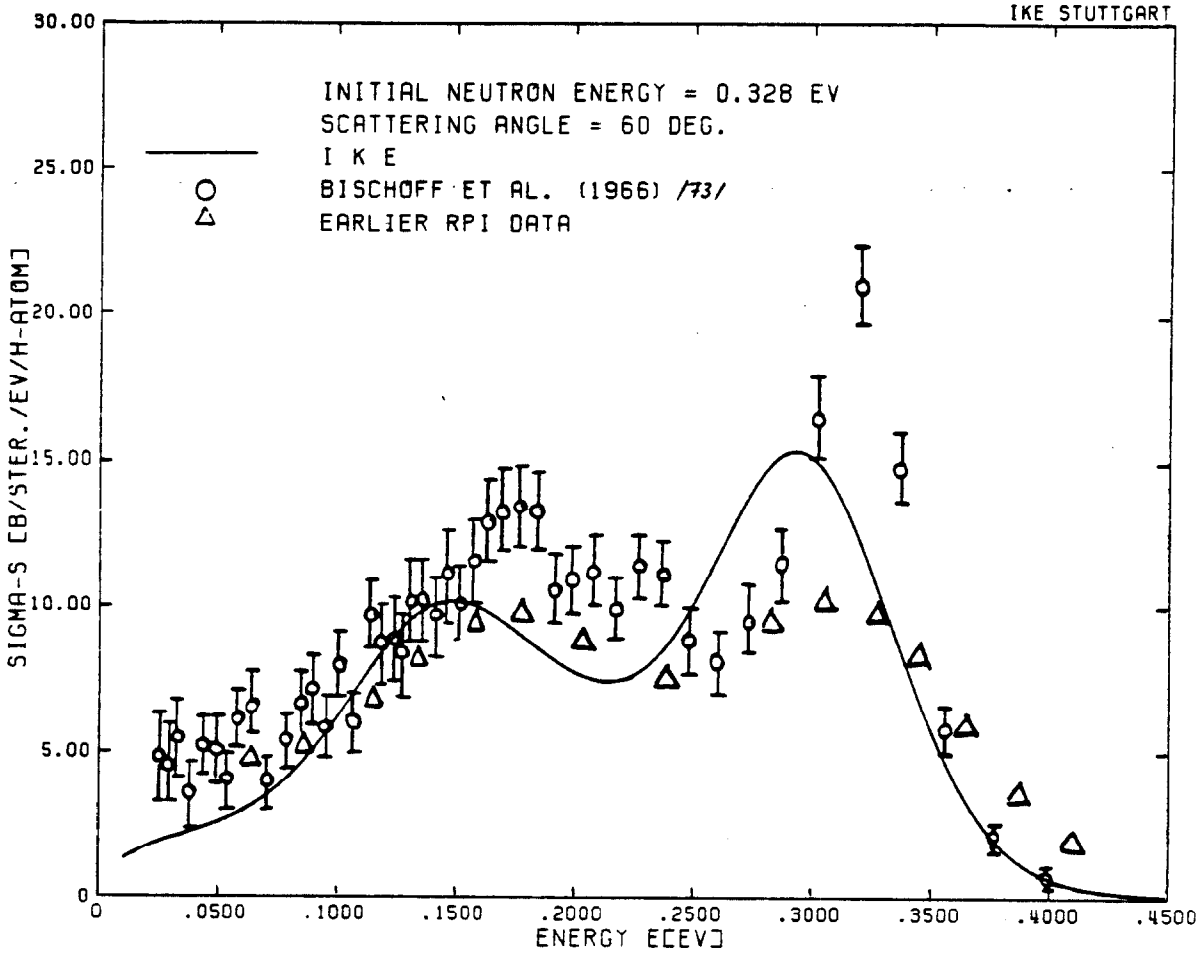

Fig. 57 Double Differential Neutron Cross Section for Polyethylene at Room Temperature at E = 0.328 eV and 60 Degrees

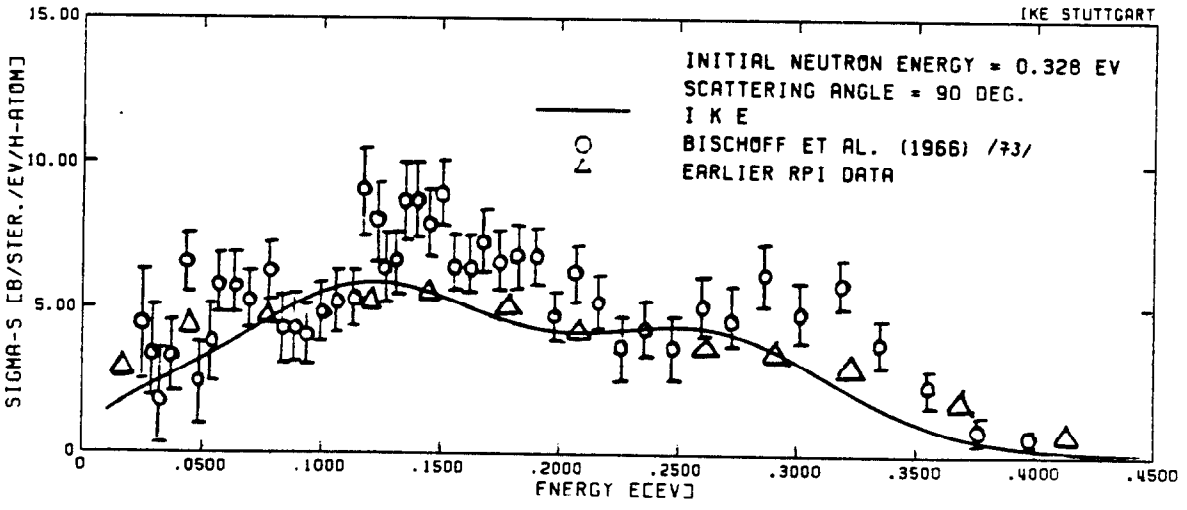

Fig. 58 Double Differential Neutron Cross Section for Polyethylene at Room Temperature at E = 0.328 eV and 90 Degrees

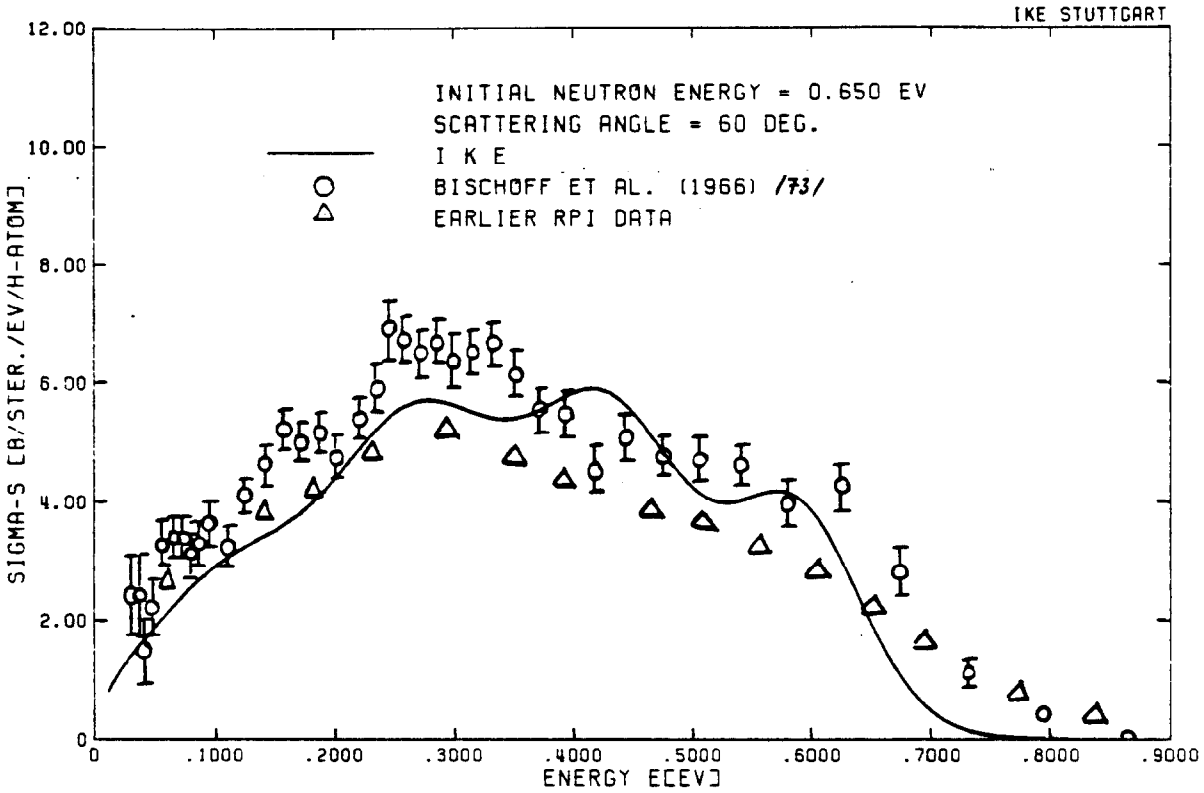

Fig. 59 Double Differential Neutron Cross Section for Polyethylene at Room Temperature at E = 0.65 eV and 60 Degrees

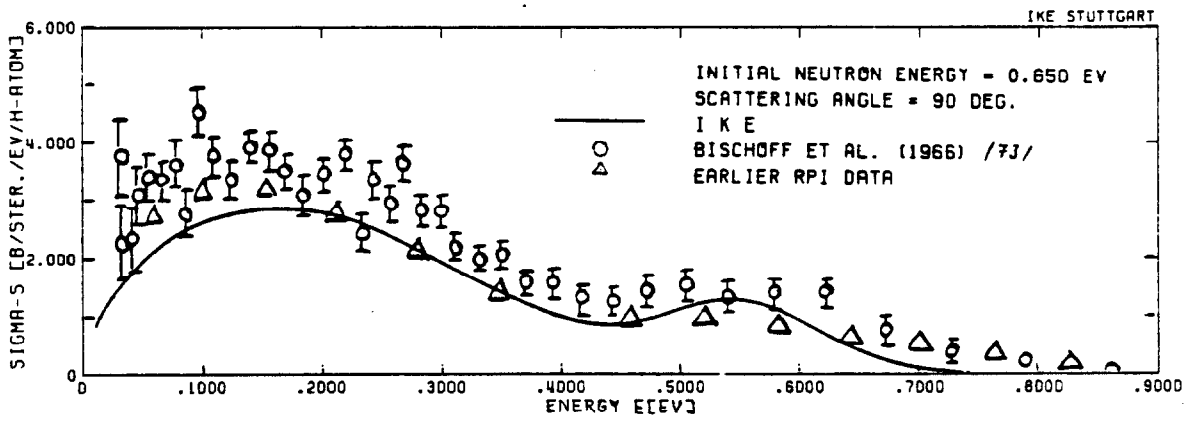

Fig. 60 Double Differential Neutron Cross Section for Polyethylene at Room Temperature at E = 0.65 eV and 90 Degrees

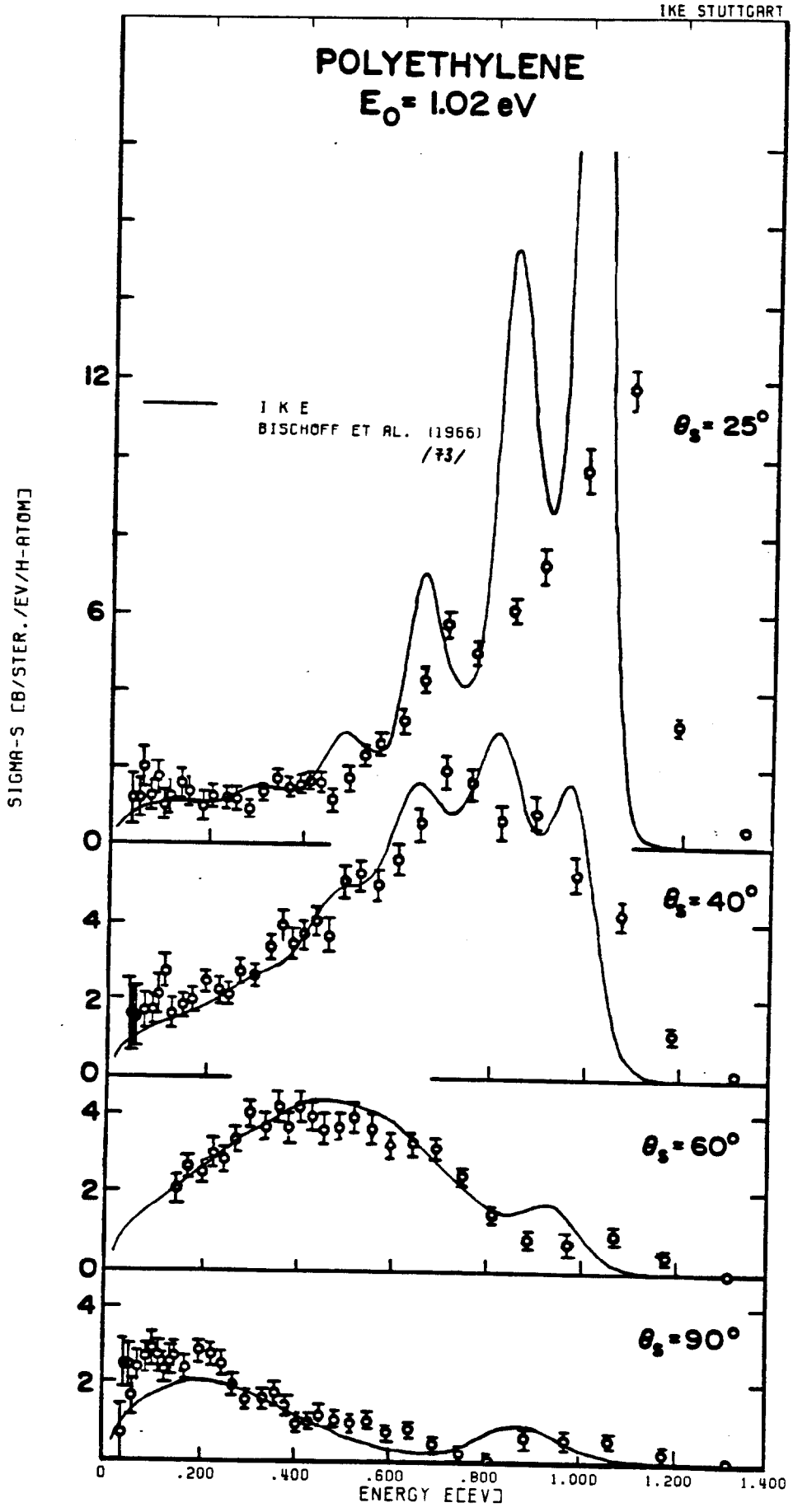

Fig. 61 Double Differential Neutron Cross Section for Polyethylene at Room Temperature at E = 1.02 eV for Different Angles

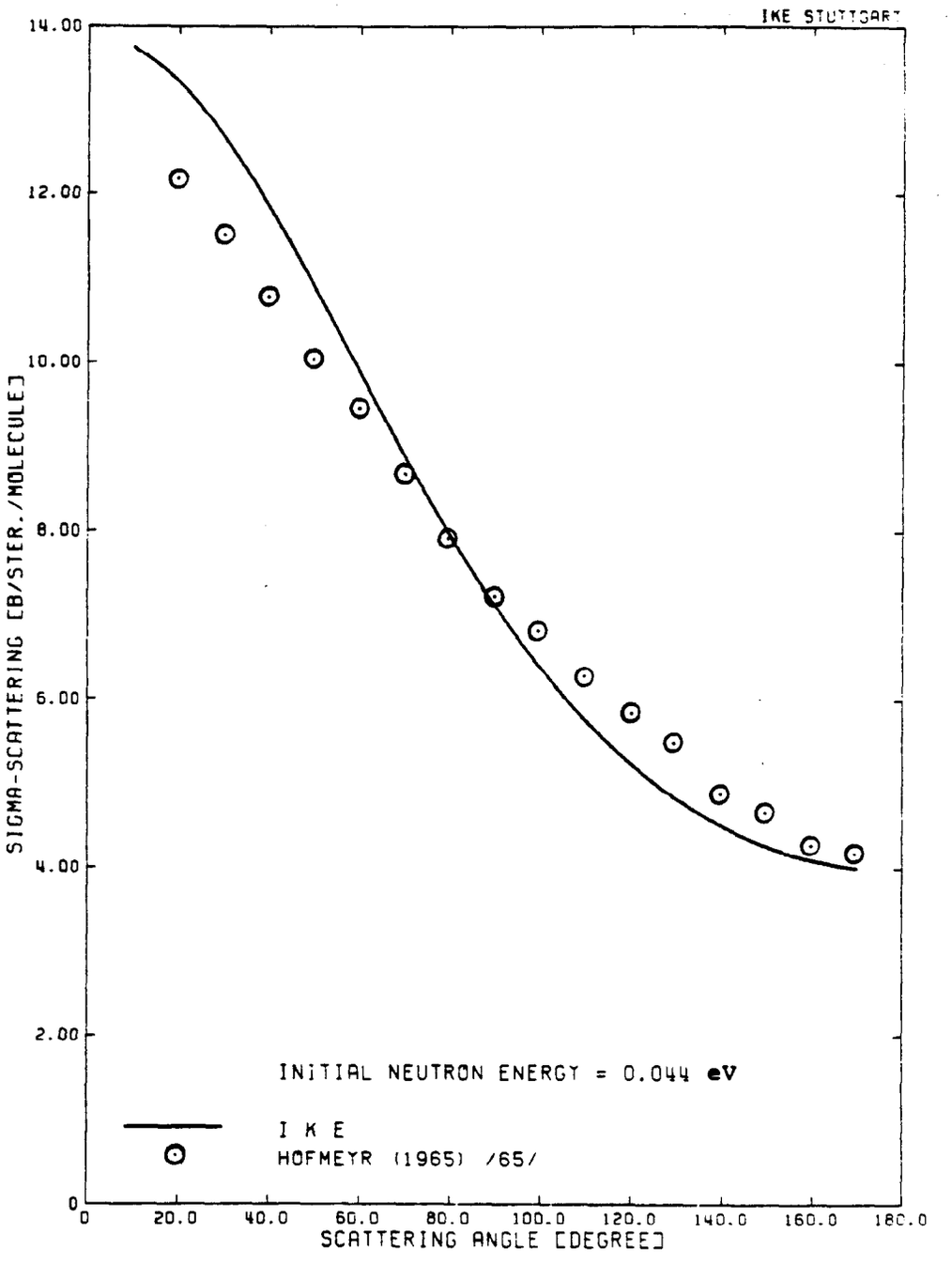

Fig. 62 Differential Neutron Scattering Cross Section of Polyethylene at Room Temperature at E = 0.044 eV

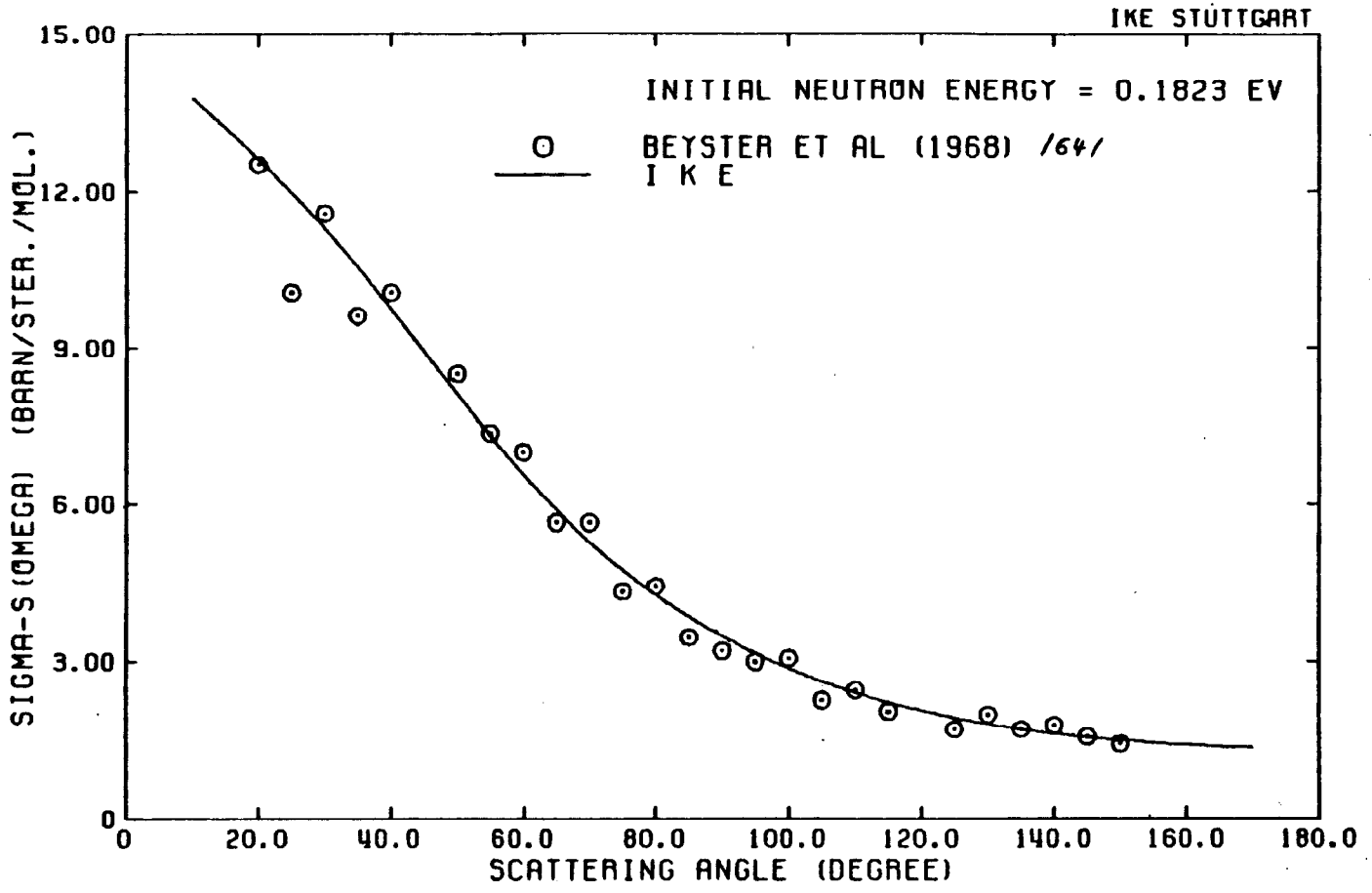

Fig. 63 Differential Neutron Scattering Cross Section of Polyethylene at Room Temperature at E = 0.1823 eV

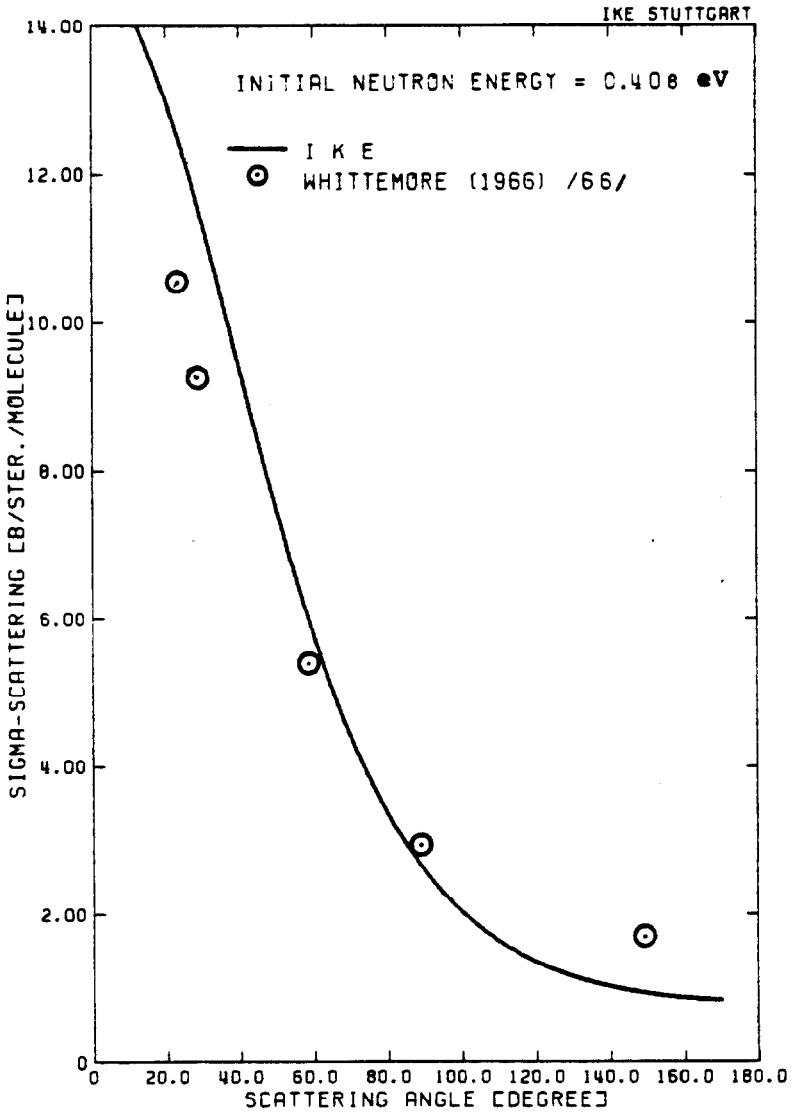

Fig. 64 Differential Neutron Scattering Cross Section of Polyethylene at Room Temperature at E = 0.408 eV

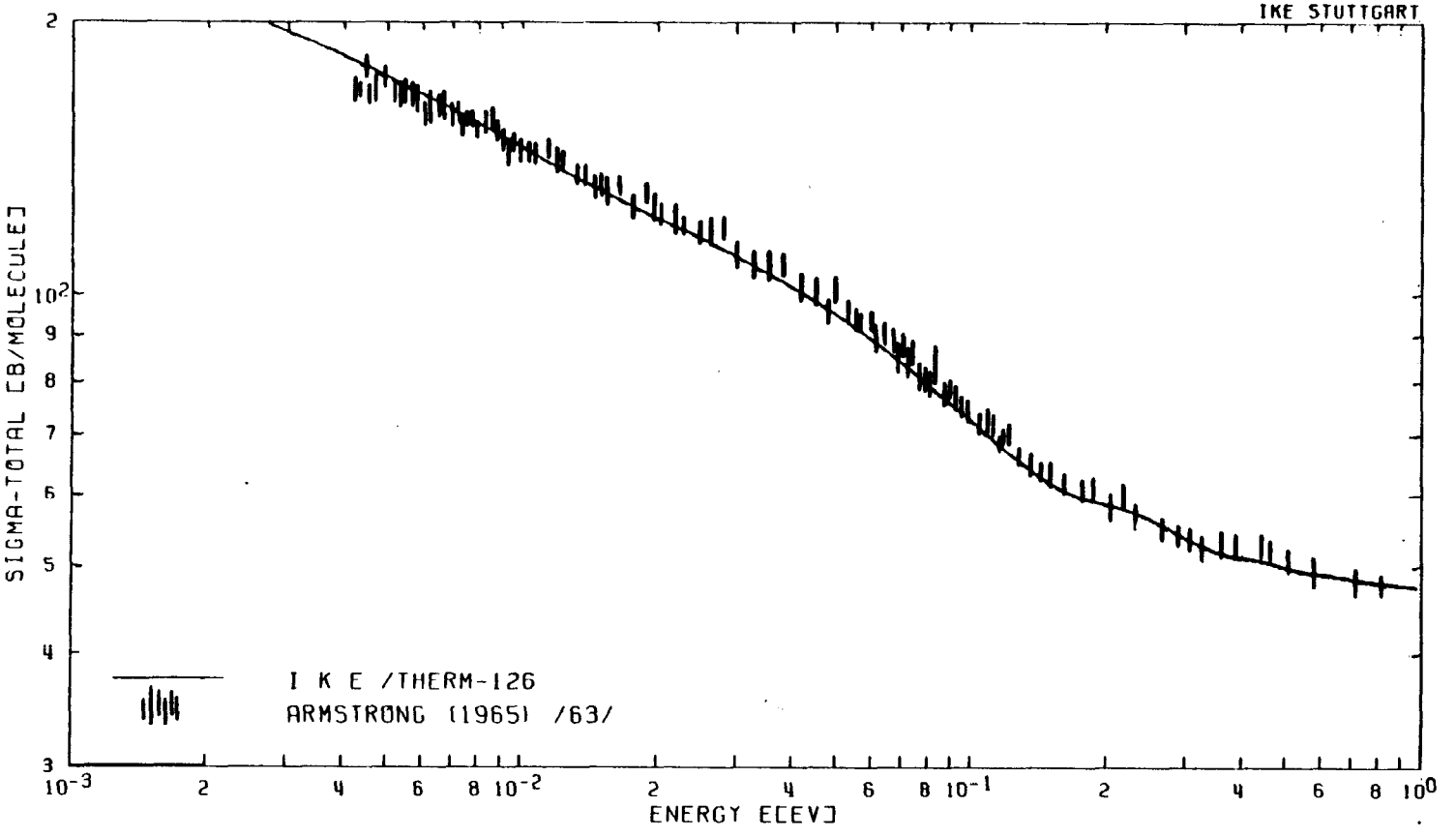

Fig. 65 Total Neutron Cross Section of Polyethylene at Room Temperature

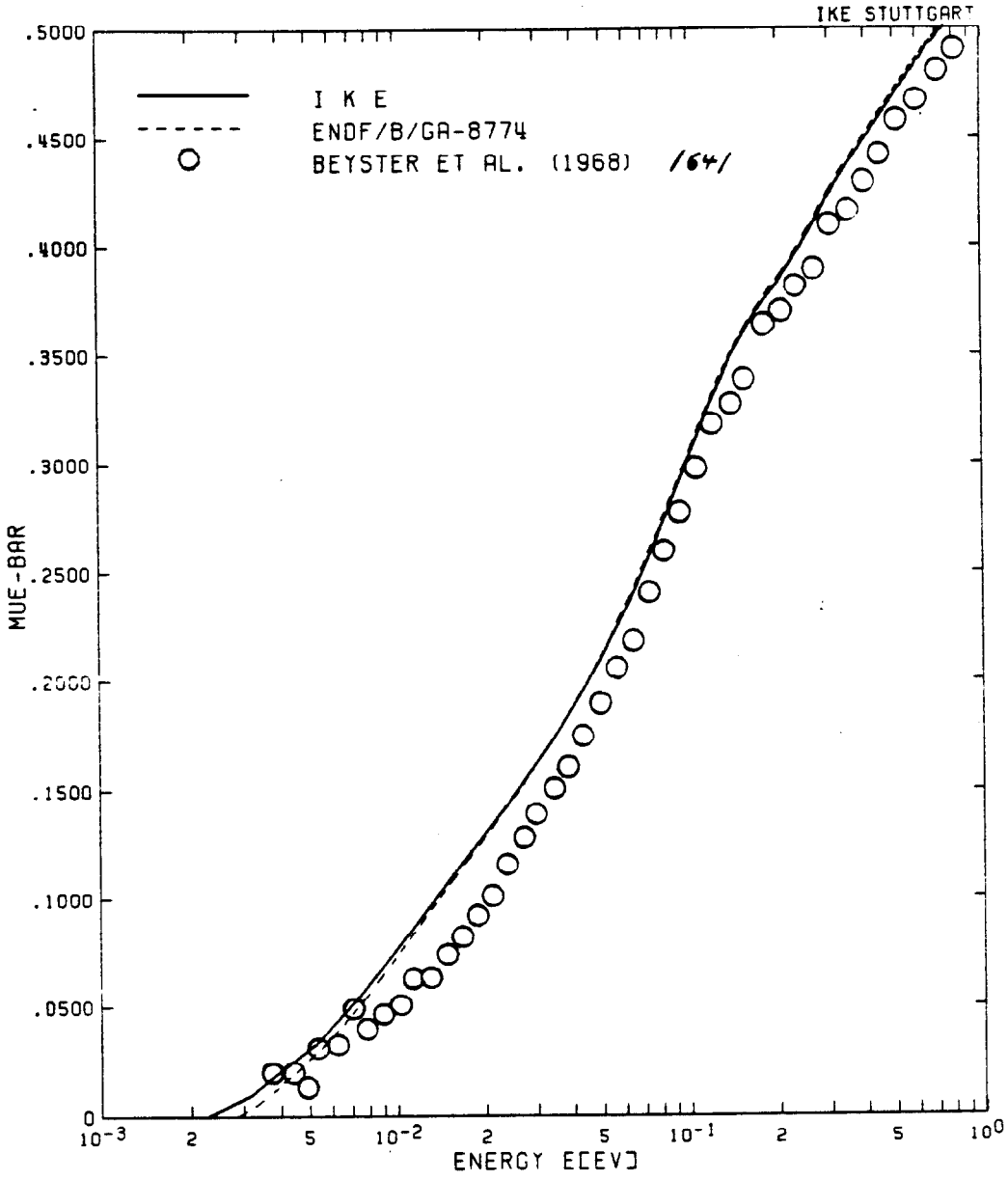

Fig. 66 Average Cosine of the Neutron Scattering Angle in Polyethylene at Room Temperature

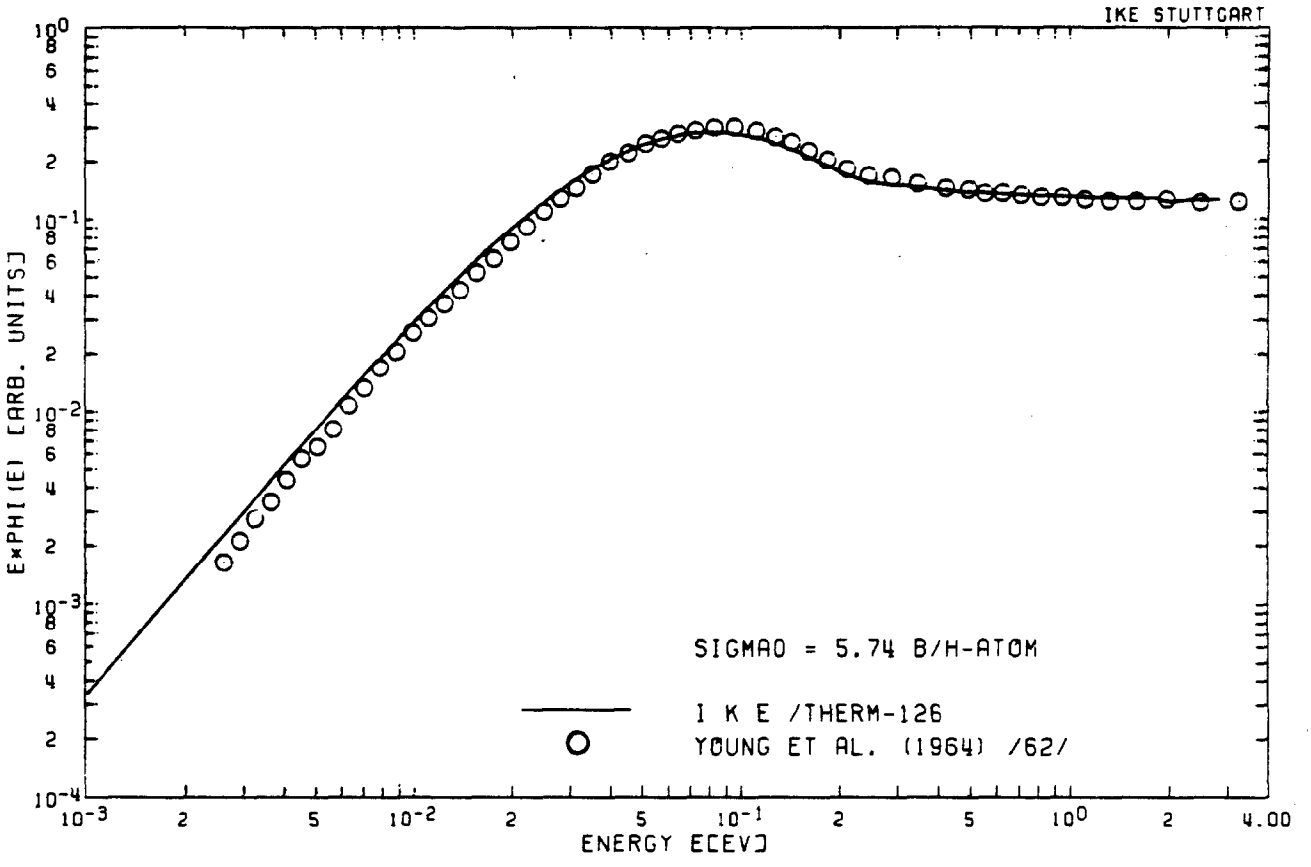

Fig. 67 Infinite Medium Neutron Spectrum in Borated Polyethylene at Room Temperature (σ_A = 5.74 b/H-atom)

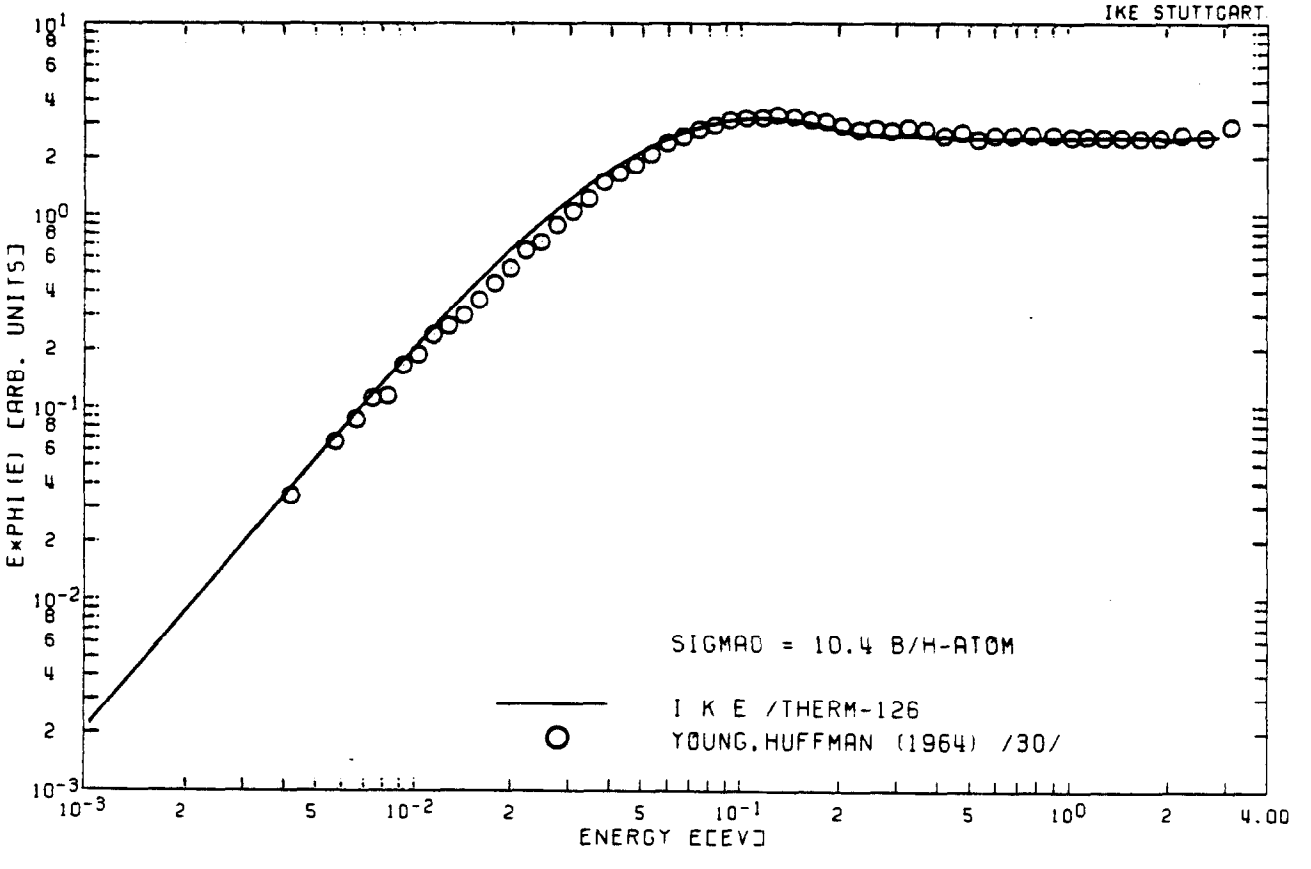

Fig. 68 Infinite Medium Neutron Spectrum in Borated Polyethylene at Room Temperature (σ_A = 10.6 b/H-atom)

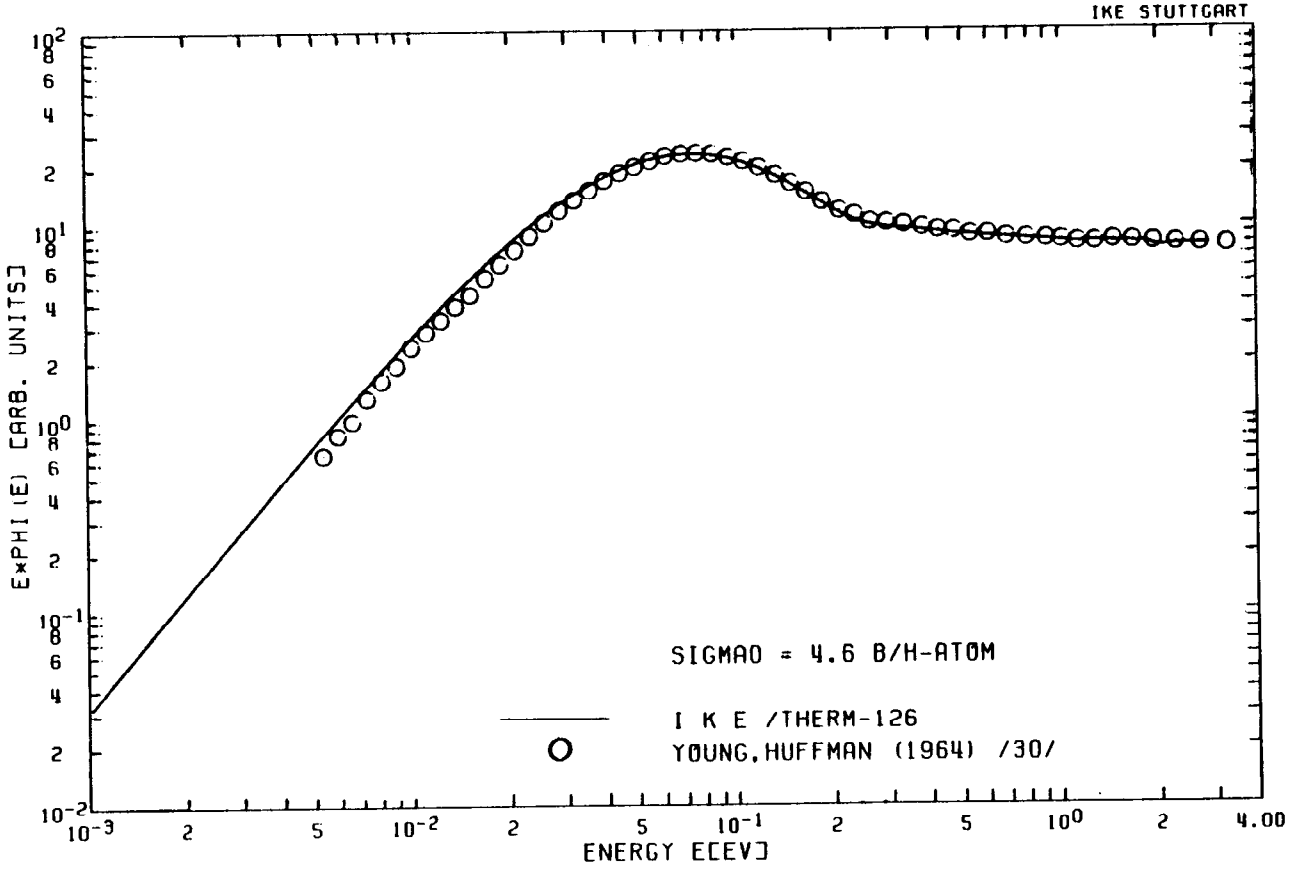

Fig. 69 Infinite Medium Neutron Spectrum in UF_4 + Paraffin at Room Temperature

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Appendix 1

Definition of the Maxwellian Averaged Thermal Neutron Diffusion Coefficient $\overline{D}(T)$, Diffusion Length $\overline{L}(T)$, and the Diffusion Constant $D_o(T)$ for the Temperature T of the Medium.

In the multigroup representation $\overline{D}$ is defined by:

$$\overline{D} = 1/3\overline{\Sigma}_{tr}$$

where

$$\overline{\Sigma}_{tr} = \overline{\Sigma}_A + 1 \Big/ \sum_g \frac{\Phi_g}{\Sigma^g_{So} - \frac{1}{3}\Sigma^g_{S1}}$$

$$\Sigma_A = \sum_g \Phi_g \Sigma^g_A$$

$$\sum_g \Phi_g = 1, \quad \Phi_g = \int_{E_g}^{E_{g-1}} \frac{E}{(kT_n)^2} \exp\left(-E/kT_n\right) dE$$

where T_n is the neutron temperature.

The thermal neutron diffusion length is related to the thermal neutron diffusion coefficient by:

$$\overline{L}(T) = \sqrt{\overline{D}(T)/\overline{\Sigma}_A(T)}$$

The neutron diffusion "constant", $D_o(T)$, of a homogeneous medium and the diffusion coefficient, $\overline{D}(T)$, are related by

$$D_o(T) = 2\,\overline{D}(T)\, v_p(T_n)/\sqrt{\pi}$$

where $v_p(T_n)$ is the most probable neutron velocity for a Maxwellian spectrum at the neutron temperature T_n.

The neutron temperature T_n is slightly higher than the temperature T of the medium. The constant c that proportionally relates these two quantitites (T_n=cT) has approximately the following values:

Moderator	c
light water	1.056
heavy water	1.001
graphite	1.015
polyethylene	1.056

Appendix 2

```
SCATTERING LAW DATA AND C/S FOR H(H2O) FROM IKE STUTTGART          1 0  0    0
1.00000+ 2 1.78606+ 1          0          0          0          14001 1451    1
0.00000+ 0 0.00000+ 0          0          0          0          04001 1451    2
0.00000+ 0 0.00000+ 0          0          0         73          34001 1451    3
H(H2O)    IKE        EVAL-AUG71 J.KEINERT                       4001 1451    4
JEF/DOC-41 IKE 6-147 DIST-SEP83 REV1 JUN82                      4001 1451    5
                                                                4001 1451    6
REEVALUATION OF THE SCATTERING DYNAMIC MODEL GIVEN IN /2,3/ AT   4001 1451    7
IKE. THE FREQUENCY SPECTRUM OF HYDROGEN BOUND IN WATER (H2O) WAS 4001 1451    8
IMPROVED AS FOLLOWS                                             4001 1451    9
                                                                4001 1451   10
  - TEMPERATURE DEPENDENCE FOR THE TRANSLATIONAL MASS OF H2O     4001 1451   11
    BASED ON THE RESULTS OF EUCKEN /5/                          4001 1451   12
                                                                4001 1451   13
  - TEMPERATURE DEPENDENCE FOR THE HINDERED ROTATIONAL BAND      4001 1451   14
    DERIVED FROM HAYWOOD,PAGE /4/                               4001 1451   15
                                                                4001 1451   16
THE TWO DISCRETE VIBRATIONAL MODES FOR THE INTRAMOLECULAR        4001 1451   17
OSCILLATIONS REMAINED UNCHANGED..                               4001 1451   18
                                                                4001 1451   19
                    * * * * *                                   4001 1451   20
DATA TRANSLATED INTO ENDF/B-V FORMAT BY M.MATTES (IKE) AUG.1983  4001 1451   21
                                                                4001 1451   22
IN ADDITION DATA NECESSARY FOR THE CALCULATION OF THERMAL NEUTRON4001 1451   23
CROSS SECTIONS FOR H2O (LIGHT WATER) ARE STORED IN MF=3 AND MF=7 4001 1451   24
(FREE GAS APPROXIMATION FOR OXYGEN). THE GIVEN AWR VALUE         4001 1451   25
CORRESPONDS TO THE MOLECULAR MASS OF 18.0154. THE SIGMA-SFREE    4001 1451   26
VALUES ARE 20.449 BARN FOR HYDROGEN AS IN ENDF/B-V MAT=1301      4001 1451   27
      AND 3.761 BARN FOR OXYGEN /6/.                            4001 1451   28
                                                                4001 1451   29
                    * * * * *                                   4001 1451   30
                                                                4001 1451   31
MF = 3    MT = 102                                              4001 1451   32
       SIGMA AT 0.0253 EV = 0.6642 BARN FOR THE H2O-MOLECULE    4001 1451   33
                                                                4001 1451   34
MF = 7    MT = 4                                                4001 1451   35
                                                                4001 1451   36
THE THERMAL SCATTERING LAW DATA ARE COMPUTED FOR ONE HYDROGEN    4001 1451   37
ATOM IN THE H2O MOLECULE IN INCOHERENT APPROXIMATION FOR         4001 1451   38
8 TEMPERATURES WITH THE GASKET CODE /1/. A MAXIMUM NEUTRON ENERGY4001 1451   39
TRANSFER OF 1.8554 EV WAS USED.                                  4001 1451   40
HIGHER ENERGY TRANSFERS CAN BE COMPUTED WITH THE SHORT COLLISION 4001 1451   41
TIME APPROXIMATION USING THE CORRESPONDING EFFECTIVE SCATTERING  4001 1451   42
TEMPERATURE TEFF.                                                4001 1451   43
                                                                 4001 1451   44
                        DEBYE-WALLER      EFFECTIVE              4001 1451   45
   TEMPERATURE          INTEGRAL          SCATTERING             4001 1451   46
       K                  1/EV            TEMPERATURE            4001 1451   47
                                              K                  4001 1451   48
   ------------------------------------------------             4001 1451   49
      293.6               20.68            1398.6               4001 1451   50
      323.6               21.78            1405.1               4001 1451   51
      373.6               23.68            1417.9               4001 1451   52
      423.6               25.66            1433.3               4001 1451   53
      473.6               27.69            1450.9               4001 1451   54
      523.6               29.75            1470.1               4001 1451   55
      573.6               31.82            1491.0               4001 1451   56
      623.6               33.91            1513.2               4001 1451   57
   ------------------------------------------------             4001 1451   58
                                                                4001 1451   59
*****************************************************************4001 1451   60
* INTERMEDIATE TEMPERATURES SHOULD BE OBTAINED BY INTERPOLATING *4001 1451   61
* BETWEEN THE RESULTING CROSS SECTIONS AND NOT BY INTERPOLATING *4001 1451   62
* S(ALPHA,BETA).                                               *4001 1451   63
*****************************************************************4001 1451   64
                                                                4001 1451   65
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        (1946)                                                  4001 1451   73
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        SECTIONS, VOL.1,PART A, ACADEMIC PRESS (1981)           4001 1451   75
                                                                4001 1451   76
                                1          451         79       04001 1451   77
                                3          102          4       04001 1451   78
                                7            4      24306       04001 1451   79
 0.0          0.0               0            0          0       04001 1  0   80
 0.0          0.0               0            0          0       04001 0  0   81
```

Appendix 3

```
SCATTERING LAW DATA AND CS FOR D(D2O) FROM IKE STUTTGART          2 0  0    0
 1.01000+ 2 1.98556+ 1          0          0          0        14002 1451    1
 0.00000+ 0 0.00000+ 0          0          0          0        04002 1451    2
 0.00000+ 0 0.00000+ 0          0          0         70        34002 1451    3
 D(D2O)    IKE        EVAL-JUL71 J.KEINERT                      4002 1451    4
 JEF/DOC-41 IKE 6-147 DIST-JAN84 REV1 AUG81                     4002 1451    5
                                                                4002 1451    6
 SCATTERING LAW DATA FOR D IN D2O STORED IN MF= 7 ARE BASED ON THE4002 1451    7
 REEVALUATION OF THE SCATTERING DYNAMIC MODEL AT IKE /1,2/.      4002 1451    8
 THE FREQUENCY SPECTRUM OF DEUTERIUM BOUND IN HEAVY WATER (D2O)  4002 1451    9
 WAS MODIFIED AS FOLLOWS                                        4002 1451   10
                                                                4002 1451   11
   - UPPER OSCILLATOR FREQUENCY INCREASED TO 0.338 EV, BEING     4002 1451   12
     CONSISTENT WITH THE VALUE FOR H IN H2O                     4002 1451   13
                                                                4002 1451   14
   - RENORMALIZATION OF THE TEMPERATURE DEPENDENT BAND OF HINDERED4002 1451   15
     ROTATIONS DERIVED FROM THE RESULTS OF HAYWOOD,PAGE /3/.    4002 1451   16
                                                                4002 1451   17
   - TRANSLATIONAL MASS UNIT = 20.0 (TEMPERATURE INDEPENDENT)   4002 1451   18
                                                                4002 1451   19
                        * * * * *                               4002 1451   20
 DATA TRANSLATED INTO ENDF/B-V FORMAT BY M.MATTES (IKE) NOV.1983 4002 1451   21
                                                                4002 1451   22
 IN ADDITION DATA NECESSARY FOR THE CALCULATION OF THERMAL NEUTRON4002 1451   23
 CROSS SECTIONS FOR D2O (HEAVY WATER) ARE STORED IN MF=3 AND MF=7 4002 1451   24
 (FREE GAS APPROXIMATION FOR OXYGEN). THE GIVEN AWR VALUE        4002 1451   25
 CORRESPONDS TO THE MOLECULAR MASS OF 20.02761. THE SIGMA-SFREE  4002 1451   26
 VALUES ARE 3.395 BARN FOR DEUTERIUM AS IN ENDF/B-V MAT=1302     4002 1451   27
        AND 3.761 BARN FOR OXYGEN /5/.                          4002 1451   28
                                                                4002 1451   29
                        * * * * *                               4002 1451   30
                                                                4002 1451   31
 MF = 3    MT = 102                                             4002 1451   32
         SIGMA AT 0.0253EV=0.001312 BARN FOR THE D2O-MOLECULE   4002 1451   33
                                                                4002 1451   34
 MF = 7    MT = 4                                               4002 1451   35
                                                                4002 1451   36
 THE THERMAL SCATTERING LAW DATA ARE COMPUTED FOR ONE DEUTERIUM  4002 1451   37
 ATOM IN THE D2O MOLECULE IN INCOHERENT APPROXIMATION FOR        4002 1451   38
 8 TEMPERATURES WITH THE GASKET CODE /4/. A MAXIMUM NEUTRON ENERGY4002 1451   39
 TRANSFER OF 1.8554 EV WAS USED.                                4002 1451   40
 HIGHER ENERGY TRANSFERS CAN BE COMPUTED WITH THE SHORT COLLISION 4002 1451   41
 TIME APPROXIMATION USING THE CORRESPONDING EFFECTIVE SCATTERING 4002 1451   42
 TEMPERATURE TEFF.                                              4002 1451   43
                                                                4002 1451   44
                        DEBYE-WALLER      EFFECTIVE             4002 1451   45
          TEMPERATURE      INTEGRAL       SCATTERING            4002 1451   46
             K              1/EV        TEMPERATURE  K         4002 1451   47
         ------------------------------------------------       4002 1451   48
            293.6          40.32          1015.60               4002 1451   49
            323.6          42.88          1026.71               4002 1451   50
            373.6          47.11          1046.74               4002 1451   51
            423.6          51.24          1068.50               4002 1451   52
            473.6          55.24          1091.84               4002 1451   53
            523.6          59.10          1116.63               4002 1451   54
            573.6          62.69          1143.10               4002 1451   55
            673.6          69.15          1200.08               4002 1451   56
         ------------------------------------------------       4002 1451   57
                                                                4002 1451   58
 ***************************************************************4002 1451   59
 * INTERMEDIATE TEMPERATURES SHOULD BE OBTAINED BY INTERPOLATING *4002 1451   60
 * BETWEEN THE RESULTING CROSS SECTIONS AND NOT BY INTERPOLATING *4002 1451   61
 * S(ALPHA,BETA).                                               *4002 1451   62
 ***************************************************************4002 1451   63
                                                                4002 1451   64
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    /5/ S.F.MUGHAGHAB,M.DIVADEENAM,N.E.HOLDEN: NEUTRON CROSS    4002 1451   71
        SECTIONS, VOL.1,PART A, ACADEMIC PRESS (1981)           4002 1451   72
                                                                4002 1451   73
                          1        451          76         0 4002 1451   74
                          3        102           4         0 4002 1451   75
                          7          4       24302         0 4002 1451   76
                                                             4002 1  0   77
                                                             4002 0  0   78
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SCATTERING LAW DATA FOR GRAPHITE FROM IKE STUTTGART                    3 0  0    0
 2.41000+ 2 1.19080+ 1          0          0          0          14003 1451    1
 0.00000+ 0 0.00000+ 0          0          0          0          04003 1451    2
 0.00000+ 0 0.00000+ 0          0          0         77          24003 1451    3
 GRAPHITE  IKE        EVAL-SEP72 J.KEINERT                       4003 1451    4
 JEF/DOC-41 IKE 6-147 DIST-JAN84 REVO                            4003 1451    5
                                                                 4003 1451    6
 DATA TRANSLATED INTO ENDF/B-V FORMAT BY M.MATTES (IKE) JAN.1984 4003 1451    7
                                                                 4003 1451    8
 MF=7, MT=4   THERMAL NEUTRON SCATTERING LAW DATA  S(ALPHA,BETA) 4003 1451    9
              SIGMA-SFREE = 4.74 BARN /1/                        4003 1451   10
                                                                 4003 1451   11
 THE FREQUENCY SPECTRUM OF CARBON BOUND IN GRAPHITE WAS DERIVED  4003 1451   12
 FROM A CENTRAL FORCE LATTICE DYNAMICAL MODEL CALCULATION OF THE 4003 1451   13
 GRAPHITE UNIT CELL /4,5/. THE NUMERICAL VALUES ARE LISTED BELOW 4003 1451   14
 AS PAIRS OF OMEGA AND RHO(OMEGA) (TAB1 RECORD):                 4003 1451   15
 0.0          0.0               0          0          1         404003 1451   16
        40           2                                          4003 1451   17
 0.           0.        5.48470-03 3.46610-01 1.09690-02 1.41350+004003 1451   18
 1.64540-02 3.03320+00 2.19390-02 3.25900+00 2.74240-02 3.38470+004003 1451   19
 3.29080-02 3.48270+00 3.83930-02 3.76400+00 4.38780-02 4.05030+004003 1451   20
 4.93630-02 4.84700+00 5.48470-02 7.35740+00 6.03320-02 5.88220+004003 1451   21
 6.58170-02 4.63260+00 7.13020-02 4.48290+00 7.67860-02 5.80640+004003 1451   22
 8.22710-02 4.63800+00 8.77560-02 4.28500+00 9.32410-02 3.92080+004003 1451   23
 9.87250-02 4.91350+00 1.04210-01 5.53840+00 1.09690-01 7.51080+004003 1451   24
 1.15180-01 5.31650+00 1.20660-01 5.40530+00 1.26150-01 5.20380+004003 1451   25
 1.31630-01 5.32760+00 1.37120-01 7.17250+00 1.42600-01 3.31810+004003 1451   26
 1.48090-01 4.50130+00 1.53570-01 5.04660+00 1.59060-01 4.20890+004003 1451   27
 1.64540-01 2.91990+00 1.70030-01 4.65110+00 1.75510-01 1.31320+014003 1451   28
 1.81000-01 7.25020+00 1.86480-01 6.56620+00 1.91970-01 5.47180+004003 1451   29
 1.97450-01 5.06140+00 2.02940-01 5.19810+00 2.08420-01 4.57090-014003 1451   30
 2.08430-01 0.                                                   4003 1451   31
                                                                 4003 1451   32
 WITH THIS FREQUENCY DISTRIBUTION THE THERMAL SCATTERING LAW DATA 4003 1451   33
 HAVE BEEN GENERATED IN INCOHERENT APPROXIMATION WITH THE GASKET  4003 1451   34
 CODE /6/ FOR 11 TEMPERATURES FROM ROOM TEMPERATURE UP TO 3000K.  4003 1451   35
 A MAXIMUM NEUTRON ENERGY TRANSFER OF 1.8554 EV WAS USED. GREATER 4003 1451   36
 ENERGY TRANSFERS CAN BE COMPUTED WITH THE SHORT COLLISION        4003 1451   37
 TIME APPROXIMATION USING THE CORRESPONDING EFFECTIVE             4003 1451   38
 SCATTERING TEMPERATURE TEFF.                                    4003 1451   39
                                                                 4003 1451   40
                        DEBYE-WALLER      EFFECTIVE              4003 1451   41
          TEMPERATURE     INTEGRAL        SCATTERING             4003 1451   42
              K            1/EV          TEMPERATURE  K         4003 1451   43
         ------------------------------------------------        4003 1451   44
            293.6          26.06          712.61                 4003 1451   45
              400          32.70          754.66                 4003 1451   46
              500          39.20          806.65                 4003 1451   47
              600          45.88          868.37                 4003 1451   48
              700          52.66          937.62                 4003 1451   49
              800          59.53         1012.64                 4003 1451   50
             1000          73.41         1174.94                 4003 1451   51
             1200          87.42         1348.12                 4003 1451   52
             1600         115.66         1712.90                 4003 1451   53
             2000         144.04         2090.99                 4003 1451   54
             3000         215.26         3061.02                 4003 1451   55
         ------------------------------------------------        4003 1451   56
                                                                 4003 1451   57
                                                                 4003 1451   58
 FOR GRAPHITE THE THERMAL SCATTERING CROSS SECTIONS GENERATED FROM4003 1451   59
 S(ALPHA,BETA) MUST BE SUPPLEMENTED BY THE COHERENT ELASTIC CROSS 4003 1451   60
 SECTIONS USING THE METHOD OF HEXSCAT /2/. THIS IS DONE E.G. IN  4003 1451   61
 THE THERMR MODULE OF THE NJOY NUCLEAR DATA PROCESSING SYSTEM /3/.4003 1451   62
                                                                 4003 1451   63
 ************************************************************** 4003 1451   64
 * INTERMEDIATE TEMPERATURES SHOULD BE OBTAINED BY INTERPOLATING * 4003 1451   65
 * BETWEEN THE RESULTING CROSS SECTIONS AND NOT BY INTERPOLATING * 4003 1451   66
 * S(ALPHA,BETA).                                               * 4003 1451   67
 ************************************************************** 4003 1451   68
                                                                 4003 1451   69
    REFERENCES                                                   4003 1451   70
                                                                 4003 1451   71
       /1/ S.F.MUGHABGHAB,M.DIVADEENAM,N.E.HOLDEN: NEUTRON CROSS 4003 1451   72
           SECTIONS,VOL. 1, PART A, ACADEMIC PRESS (1981)        4003 1451   73
       /2/ Y.D.NALIBOFF,J.U.KOPPEL: GA-6026 (1964)               4003 1451   74
       /3/ R.E.MACFARLANE,D.W.MUIR,R.M.BOICOURT:   LA-9303-M     4003 1451   75
           (ENDF-324) (1982)                                     4003 1451   76
       /4/ J.A.YOUNG,N.F.WIKNER,D.E.PARKS, NUKLEONIK 7,295 (1965) 4003 1451   77
       /5/ J.U.KOPPEL,D.H.HOUSTON, GA-8774 (1968)                4003 1451   78
       /6/ J.U.KOPPEL,J.R.TRIPLETT,Y.D.NALIBOFF, GA-7417 (1966)  4003 1451   79
                                                                 4003 1451   80
                              1        451         82            04003 1451   81
                              7          4      32406            04003 1451   82
 0.0          0.0             0          0          0            04003 1  0   83
 0.0          0.0             0          0          0            04003 0  0   84
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Appendix 5

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SCATTERING LAW DATA AND C/S FOR H(CH2) FROM IKE STUTTGART          4 0 0    0
2.05000+ 2 1.39063+ 1          0          0          0          14004 1451    1
0.00000+ 0 0.00000+ 0          0          0          0          04004 1451    2
0.00000+ 0 0.00000+ 0          0          0         66          34004 1451    3
H(CH2)     IKE          EVAL-MAY71 J.KEINERT                     4004 1451    4
JEF/DOC-41 IKE 6-147 DIST-APR84 REV1 SEP81                      4004 1451    5
                                                                4004 1451    6
THE PHONON FREQUENCY SPECTRUM OF HYDROGEN BOUND IN POLYETHYLENE  4004 1451    7
WAS DERIVED BY SPREVAK,KOPPEL /1/ IN CALCULATING THE DISPERSION  4004 1451    8
RELATIONS FOR THE INFINITE CHAIN OF CH2 RADICALS AS WELL AS THE  4004 1451    9
POLARIZATION VECTOR FOR EACH NORMAL FREQUENCY USING THE SET OF   4004 1451   10
FORCE CONSTANTS DETERMINED BY LIN,KOENIG /2/. THE WEIGHTED       4004 1451   11
FREQUENCY SPECTRUM WAS THEN CALCULATED USING THE COMPUTED        4004 1451   12
DISPERSION RELATIONS AND THE COMPUTED AMPLITUDE VECTORS.         4004 1451   13
                                                                4004 1451   14
                      * * * * *                                 4004 1451   15
DATA TRANSLATED INTO ENDF/B-V FORMAT BY M.MATTES (IKE) APR.1984  4004 1451   16
                                                                4004 1451   17
IN ADDITION DATA NECESSARY FOR THE CALCULATION OF THERMAL NEUTRON4004 1451   18
CROSS SECTIONS FOR CH2 (POLYETHYLENE) ARE STORED IN MF=3 AND MF=74004 1451   19
(FREE GAS APPROXIMATION FOR CARBON). THE GIVEN AWR VALUE         4004 1451   20
CORRESPONDS TO THE MOLECULAR MASS OF 14.0268. THE SIGMA-SFREE    4004 1451   21
VALUES ARE 20.449 BARN FOR HYDROGEN AS IN ENDF/B-V MAT=1301      4004 1451   22
      AND 4.74 BARN FOR CARBON /3/.                             4004 1451   23
                                                                4004 1451   24
                      * * * * *                                 4004 1451   25
                                                                4004 1451   26
MF = 3    MT = 102                                              4004 1451   27
       SIGMA AT 0.0253 EV = 0.6675 BARN FOR THE CH2-MOLECULE    4004 1451   28
                                                                4004 1451   29
MF = 7    MT = 4                                                4004 1451   30
                                                                4004 1451   31
THE THERMAL SCATTERING LAW DATA ARE COMPUTED FOR ONE HYDROGEN    4004 1451   32
ATOM IN THE CH2 MOLECULE IN INCOHERENT APPROXIMATION FOR         4004 1451   33
2 TEMPERATURES WITH THE GASKET CODE /4/. A MAXIMUM NEUTRON ENERGY4004 1451   34
TRANSFER OF 1.8554 EV WAS USED.                                  4004 1451   35
HIGHER ENERGY TRANSFERS CAN BE COMPUTED WITH THE SHORT COLLISION  4004 1451   36
TIME APPROXIMATION USING THE CORRESPONDING EFFECTIVE SCATTERING   4004 1451   37
TEMPERATURE TEFF.                                                4004 1451   38
                                                                4004 1451   39
                        DEBYE-WALLER      EFFECTIVE              4004 1451   40
   TEMPERATURE           INTEGRAL         SCATTERING             4004 1451   41
      K                    1/EV          TEMPERATURE            4004 1451   42
                                             K                  4004 1451   43
   ------------------------------------------------             4004 1451   44
     293.6                34.73            1203.9               4004 1451   45
     350.0                40.29            1215.0               4004 1451   46
   ------------------------------------------------             4004 1451   47
                                                                4004 1451   48
FOR POLYETHYLENE THE INCOHERENT ELASTIC SCATTERING CROSS SECTION 4004 1451   49
SHOULD BE CALCULATED SEPARATELY AND ADDED TO THE INCOHERENT       4004 1451   50
CROSS SECTION GENERATED FROM S(ALPHA,BETA). THIS CAN BE DONE     4004 1451   51
E.G.BY THE THERMR MODULE OF NJOY /5/.                            4004 1451   52
                                                                4004 1451   53
*****************************************************************4004 1451   54
 INTERMEDIATE TEMPERATURES SHOULD BE OBTAINED BY INTERPOLATING *  4004 1451   55
 BETWEEN THE RESULTING CROSS SECTIONS AND NOT BY INTERPOLATING *  4004 1451   56
 S(ALPHA,BETA).                                               *  4004 1451   57
*****************************************************************4004 1451   58
                                                                4004 1451   59
REFERENCES                                                      4004 1451   60
                                                                4004 1451   61
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   /2/ T.P.LIN,J.L.KOENIG, J.MOLEC.SPECTRA 9,228 (1962)         4004 1451   63
   /3/ S.F.MUGHABGHAB,M.DIVADEENAM,N.E.HOLDEN: NEUTRON CROSS    4004 1451   64
       SECTIONS, VOL.1,PART A, ACADEMIC PRESS (1981)            4004 1451   65
   /4/ J.U.KOPPEL,J.R.TRIPLETT,Y.D.NALIBOFF, GA-7417 (1966)     4004 1451   66
   /5/ R.E.MACFARLANE,D.W.MUIR,R.M.BOICOURT:  LA-9303-M         4004 1451   67
       (ENDF-324) (1982)                                        4004 1451   68
                                                                4004 1451   69
                          1        451          72              04004 1451   70
                          3        102           4              04004 1451   71
                          7          4        8106              04004 1451   72
                                                                4004 1 0    73
                                                                4004 0 0    74
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ACKNOWLEDGEMENT

The data discussed in this report were generated with the support of IKE Stuttgart and BMFT/GID/FIZ. The authors wish to acknowledge this contribution, and the permission of the sponsors to release these data for incorporation in the Joint Evaluated File.