Part II

Photo-Atomic Interaction Data (NSUB=3)

Evaluation: **Photo-Atomic Interaction Sublibrary, Release** 0
Energy: 10 eV to 100GeV
Files: 1, 23, 27
Evaluators: D. R. Cullen, et al. (LLNL)

Photon interaction cross sections and atomic form factors or scattering functions for 100 materials have been converted from the Livermore Evaluated Photon Data Library (EPDL) Library [1].

From 1 eV to 1 MeV, the photon interaction cross section is based on the total photoelectric cross sections of Scofield [2,3]; from 1 MeV to 100 GeV, the cross sections of Hubbell [4,5] are used. The sets were joined at 1 MeV, where the total photoelectric cross sections from both sources are identical.

The coherent and incoherent form factors are taken from the nonrelativistic data of Hubbell [4,5].

REFERENCE

1. D. E. Cullen, et al., **UCRL-50400**, Vol. 6, Rev. 4, Parts A and B (1989) Lawrence Livermore National Laboratory
2. J. H. Scofield, **UCRL-51326** (1973) Lawrence Livermore National Laboratory
3. E. B. Saloman, J. H. Hubbell, and J. H. Scofield, ***At. Data Nucl. Data Tables*** **38**, 1 (1988)
4. J. H. Hubbell, H. M. Gerstenberg, and E. B. Saloman, **NBSIR 86-3461** (1986) National Bureau of Standards
5. M. J. Berger and J. H. Hubbell, XCOM: *Photon Cross Sections on a Personal Computer*, **NBSIR 87-3597**[1] (1987) National Bureau of Standards

[1] The XCOM data is available through the NNDC Online Service XRAY database.

Part III

Radioactive Decay Data (NSUB=4)

The Radioactive Decay Data Sublibrary contains evaluations for 799 materials, which were distributed in Release 1. A modification to ^{98}Tc was distributed in Release 2 to correct the MAT number.

Most evaluations were contributed by C. W. Reich (INEL), F. Mann and F. Schmittroth (HEDL), and T. England (LANL, with contributions from B. Magurno (BNL), W. Mannhart (PTB), and R. Schenter (HEDL). See individual evaluations for more detail.

Part IV

Spontaneous Fission Product Yields (NSUB=15)

Evaluation: **Spontaneous Fission-Product Yields, Release 1,2**
Energy: Spontaneous fission
Files: 1, 8
Evaluators: T. R. England and B. F. Rider (LANL)

Independent and cumulative yield data are given for 9 materials in Release 1 and 2. See England and Rider [1] for complete documentation.

Yields are given for: ^{238}U, ^{244,246,248}Cm, ^{250,252}Cf, ^{253}Es, ^{254,256}Fm.

REFERENCE

1. T. R. England and B. F. Rider, **LA-UR-94-3106** (**ENDF-349**) (1994) Los Alamos National Laboratory

Part V

Neutron-Induced Fission Product Yields (NSUB=11)

Evaluation:	**Neutron Induced Fission-Product Yields, Release 1,2,3**
Energy:	Thermal, Fission Spectrum, 14-MeV
Files:	1, 8
Evaluators:	T. R. England and B. F. Rider (LANL)

Independent and cumulative yield data are given for 51 materials at energies in the thermal range, fission spectrum range, and at 14 MeV in Release 1 and 2. See England and Rider [1] for complete documentation.

An update for ^{241}Pu was made in Release 3 to correct for missing yields.

Thermal yields are given for: ^{227,229}Th, ^{232,233,235}U, ^{237}Np, ^{239,240,242}Pu, ^{241,242m}Am, ^{243,245}Cm, ^{249,251}Cf, ^{254}Es, ^{255}Fm.

Fission spectrum yields are given for: ^{232}Th, ^{233,2345,235,236,237,238}U, ^{237,238}Np, ^{238,239,240,241,242}Pu, ^{241,243}Am, ^{242,243,244,246,248}Cm.

Yields at 14 MeV are given for: ^{232}Th, ^{233,234,235,236,238}U, ^{237}Np, ^{239,240,242}Pu, ^{241}Am.

REFERENCE

1. T. R. England and B. F. Rider, **LA-UR-94-3106** (**ENDF-349**) (1994) Los Alamos National Laboratory

Part VI

Thermal Neutron Scattering Sublibrary (NSUB=12)

All materials in the thermal neutron scattering sublibrary are documented here, including those issued in Release 0, since they have not been documented previously.

Evaluation: **H (H_2O) Thermal Neutron Scattering Sublibrary, Release 3 (MAT 1)**
Temperatures: 296 350 400 450 500 600 800 1000 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

This evaluation was generated using the LEAPR module of NJOY [4]. The physical model is very similar to the one used at General Atomic to produced the original ENDF/B-III evaluations [1]. The α and β grids were extended, and the constants were changed to match the values in the previous ENDF/B-VI evaluation.

Water is represented by freely recoiling H_2O molecules of mass 18. Each molecule can undergo torsional harmonic oscillations (hindered rotations) with a broad spectrum of distributed modes. Between 0.04 and 0.165 eV, the rotation spectrum is taken from the work of Haywood and Thorson [2] joined to a quadratic law below 0.04 eV. In addition, there are two internal vibrations at frequencies of 0.205 and 0.48 eV taken over from the Nelkin model [3] with slightly readjusted masses of 6 and 3, respectively. The torsional band is normalized to a mass of 18/8. The scattering by the oxygen atoms is not included in the tabulated scattering law data. It should be taken into account by adding the scattering for free oxygen of mass 16.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic; revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. B. C. Haywood and J. M. Thorson, Neutron Thermalization Conference, **BNL-719** (1962) Brookhaven National Laboratory
3. M. Nelkin, ***Phys. Rev.*** **119**, 741 (1960)
4. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation:	**Liquid Para Hydrogen Thermal Neutron Scattering Sublibrary, Release 3 (MAT 2)**
Temperatures:	20 ˚K
Files:	1, 7
Evaluators:	R. E. MacFarlane (LANL)

Liquid para hydrogen at 20 ˚K computed using the LEAPR module of NJOY [1]. The scattering law is based on the model of Keinert and Sax [2], which includes spin correlations from the Young and Koppel model [3], diffusion and local hindered motions from an effective translational scattering law based on a frequency distribution, and intermolecular coherence after Vinyard [4].

REFERENCES

1. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory
2. J. Keinhert and J. Sax, ***Kerntechnik*** **51**, 19 (1987)
3. J. A. Young and J. U. Koppel, ***Phys. Rev.*** **135**, A603 (1964)
4. G. H. Vineyard, ***Phys. Rev.*** **110**, 999 (1958)

Evaluation: **Liquid Ortho Hydrogen Thermal Neutron Scattering Sublibrary, Release 3 (MAT 3)**
Temperatures: 20 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

Liquid ortho hydrogen at 20 ˚K computed using the LEAPR module of NJOY [1]. The scattering law is based on the model of Keinert and Sax [2], which includes spin correlations from the Young and Koppel model [3], diffusion and local hindered motions from an effective translational scattering law based on a frequency distribution, and intermolecular coherence after Vinyard [4].

REFERENCES

1. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory
2. J. Keinhert and J. Sax, ***Kerntechnik*** **51**, 19 (1987)
3. J. A. Young and J. U. Koppel, ***Phys. Rev.*** **135**, A603 (1964)
4. G. H. Vineyard, ***Phys. Rev.*** **110**, 999 (1958)

Evaluation: **H (ZrH) Thermal Neutron Scattering Sublibrary, Release 3 (MAT 7)**
Temperatures: 296 400 500 600 700 800 1000 1200 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

This evaluation was generated using the LEAPR module of NJOY [3]. The physical model is very similar to the one used at General Atomic to produced the original ENDF/B-III evaluations [1]. The α and β grids were extended lightly, and the constants were changed to match the values in the previous ENDF/B-VI evaluation.

The lattice dynamics of ZrH were computed from a central force model. The slightly tetragonal lattice of ZrH_2 was approximated by a face-centered-cubic lattice. Four force constants (μ, γ, ν, and δ) were introduced describing respectively the interaction of a zirconium atoms with its nearest neighbors (8 H atoms) and its next nearest neighbors (12 Zr atoms), and the interaction of a hydrogen atom with its next nearest neighbors (6 H atoms) and its third nearest atoms (12 H atoms). Eigenvalues and eigenvectors of the dynamical matrix were calculated, and a phonon frequency spectrum was obtained by means of a root sampling technique. Weighted frequency spectra for hydrogen in ZrH were then obtained by appropriate use of the dynamical matrix eigenvectors [2].

The final values of the four force constants were obtained by fitting both specific heat and neutron data. The position of an optical peak observed by neutron scattering techniques to be centered roughly around 0.14 eV determines the constant μ, while the overall width and shape of this peak determine ν and δ respectively. Existing neutron data are not sufficiently precise to confirm the structure predicted in the optical peak by the central force model. Specific heat data were used to determine the force constant γ, which primarily determines the upper limit on the phonon energies associated with acoustic modes.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic; revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. E. L. Slaggie, **GA-8132** (1967) General Atomic
3. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation: **D (D_2O) Thermal Neutron Scattering Sublibrary, Release 0 (MAT 11)**
Temperatures: 296 350 400 450 500 600 800 1000 ˚K
Files: 1, 7
Evaluators: J. U. Koppel and D. H. Houston (GA)

This evaluation was produced at General Atomic in 1969 using the GA code gasket [1]. It was converted to ENDF-6 format at Los Alamos in 1989. The only changes made to the contents were adjustments of cross sections to match the ENDF/B-VI values.

Whereas hydrogen is nearly a completely incoherent neutron scatterer, the scattering from deuterium is largely coherent. Although it would appear that due to this fact a treatment of D_2O analogous to the one used for H_2O would be inadequate, calculations [2] have shown that because of a great deal of cancellation between inter and intra-molecular interference scattering, integral quantities like the total cross section or thermal neutron spectra can actually be predicted quite accurately with an incoherent model.

Therefore, the scattering law for D_2O is based on a model quite similar to the one used for the General Atomic evaluation of H_2O; namely, freely recoiling D_2O molecules of mass 20. Each molecule can undergo torsional harmonic oscillations (hindered rotations) with a broad spectrum of distributed modes. Between 0.025 and 0.127 eV, the rotation spectrum is taken from the work of Haywood [3] joined to a quadratic law below 0.025 eV. In addition, there are two internal vibrations at frequencies of 0.142 and 0.305 eV (the frequencies are approximately $1/\sqrt{2}$ times the corresponding frequencies for H_2O as expected from the mass ratio) with masses of 6 and 3, respectively. The torsional band is normalized to a mass of 20/9. The scattering by the oxygen atoms is not included in the tabulated scattering law data. It should be taken into account by adding the scattering for free oxygen of mass 16.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic; revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. J. U. Koppel and J. A. Young, ***Nukleonik*** **7**, 408 (1965).
3. B. C. Haywood, **Pulsed Neutron Research**, Symposium, Karlsruhe, 10-14 May 1965, Vol. I, p.434 (1965)

Evaluation: **Para Deuterium Thermal Neutron Scattering Sublibrary, Release 3 (MAT 12)**
Temperatures: 19 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

Liquid para deuterium at 19 ˚K was computed using the LEAPR module of NJOY [1]. The scattering law is based on the model of Keinert and Sax [2], which includes spin correlations from the Young and Koppel model [3], diffusion and local hindered motions from an effective translational scattering law based on a frequency distribution, and intermolecular coherence after Vinyard [4].

REFERENCES

1. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory
2. J. Keinhert and J. Sax, ***Kerntechnik*** **51**, 19 (1987)
3. J. A. Young and J. U. Koppel, ***Phys. Rev.*** **135**, A603 (1964)
4. G. H. Vineyard, ***Phys. Rev.*** **110**, 999 (1958)

Evaluation: **Ortho Deuterium Thermal Neutron Scattering Sublibrary, Release 3 (MAT 13)**
Temperatures: 19 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

Liquid ortho deuterium at 19 ˚K was computed using the LEAPR module of NJOY [1]. The scattering law is based on the model of Keinert and Sax [2], which includes spin correlations from the Young and Koppel model [3], diffusion and local hindered motions from an effective translational scattering law based on a frequency distribution, and intermolecular coherence after Vinyard [4].

REFERENCES

1. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory
2. J. Keinhert and J. Sax, ***Kerntechnik*** **51**, 19 (1987)
3. J. A. Young and J. U. Koppel, ***Phys. Rev.*** **135**, A603 (1964)
4. G. H. Vineyard, ***Phys. Rev.*** **110**, 999 (1958)

Evaluation: **Be metal Thermal Neutron Scattering Sublibrary, Release 3 (MAT 26)**
Temperatures: 296, 400, 500, 600, 700, 800, 1000, 1200 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

This evaluation was generated using the LEAPR module of NJOY [3]. The physical model is very similar to the one used at General Atomic to produced the original ENDF/B-III evaluations [1]. Tighter grids and extended ranges for α and β were used. A slightly more detailed calculation of the coherent inelastic scattering was generated. The various constants were updated to agree with the ENDF/B-VI evaluation of Be.

The phonon dispersion curves were fitted by Schmunk, et al. [2], using a model of central forces that extend to the fifth nearest neighbors. The phonon spectrum corresponding to this model was calculated by the root sampling method, and then used to compute $S(\alpha,\beta)$. The coherent elastic scattering cross section was computed using the known lattice structure (hexagonal close-packed) and the Debye-Waller integrals from the lattice dynamics model.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic; revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. R. E. Schmunk, et al., ***Phys. Rev.*** **128**, 562 (1962)
3. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation: **BeO Thermal Neutron Scattering Sublibrary, Release 3 (MAT 27)**
Temperatures: 296 400 500 600 700 800 1000 1200 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

This evaluation was generated using the LEAPR module of NJOY [3]. The physical model is very similar to the one used at General Atomic to produced the original ENDF/B-III evaluations [1]. Tighter grids and extended ranges for α and β were used. A slightly more detailed calculation of the coherent inelastic scattering was generated. The various constants were updated to agree with the ENDF/B-VI evaluation of Be and oxygen.

Beryllium oxide consists of two interpenetrating hexagonal close-packed structures with four atoms per unit cell. The lattice dynamics [2] is described using a shell model whose parameters have been adjusted to fit the elastic constants, the measured Raman frequencies, and preliminary dispersion relations measured by neutron scattering [3]. Only the negative ions are assumed to be polarizable, and short-range repulsive forces are used for the first and second neighbors. The frequency spectra weighted by the squares of the amplitude vectors were computed separately for beryllium and oxygen and used to calculate separate scattering laws with GASKET. The scattering laws were then combined and adjusted to be used with the beryllium free-atom cross section. The oxygen free-atom cross section has been provided for use with the short-collision-time approximation (SCT). Thus, the thermal cross section computed from either $S(\alpha,\beta)$ or by the SCT approximation gives an asymptotic limit of approximately 6.15 ± 3.75 barns. The elastic part of the scattering was calculated using the average of the Debye-Waller factors for beryllium and oxygen.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic; revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. G. Borgonovi, **GA-8758** (1968) General Atomic
3. R. M. Brugger, K. A. Strong, and J. M. Carpenter, ***J. Phys. Chem. Solids*** **28**, 249 (1967)
4. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation: **Graphite Thermal Neutron Scattering Sublibrary, Release 3 (MAT 31)**
Temperatures: 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

This evaluation was generated using the LEAPR module of NJOY [3]. The physical model is very similar to the one used at General Atomic to produced the original ENDF/B-III evaluations [1]. Tighter grids and extended ranges for α and β were used. A slightly more detailed calculation of the coherent inelastic scattering was generated. The various constants were updated to agree with the ENDF/B-VI evaluation of natural carbon.

Graphite has an hexagonal close-packed crystal structure. The lattice dynamics is represented using a model with four force constants [2,3]. One force constant is used to describe a nearest-neighbor central force that binds two hexagonal planes together, another describes a bond-bending force in an hexagonal plane, the third is for bond-stretching between nearest neighbors in a plane, and the fourth corresponds to a restoring force against bending of the hexagonal plane. The force constants were evaluated numerically using a very precise fit to the high and low temperature specific heat and compressibility of reactor grade graphite. The phonon spectrum was computed from this model using the root sampling method, and then used to compute $S(\alpha,\beta)$. The coherent elastic scattering cross section was computed using the known lattice structure and the Debye-Waller integrals from the lattice dynamics model.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic; revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. J. A. Young, N. F. Wilkner, and D. E. Parks, ***Nukleonik*, 7**, 295 (1965)
3. J. A. Young and J. U. Koppel, ***J. Chem. Phys.*** **42**, 357(1965).
4. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation: **Liquid Methane Thermal Neutron Scattering Sublibrary, Release 3 (MAT 33)**
Temperatures: 100 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

Liquid methane (CH_4) at 100 ˚K was generated using the model of Agrawal and Yip [1] as implemented by Picton [2], modified to include a diffusive component. Optical measurements of methane in the gas phase show four fairly well defined vibrational modes at 162, 190, 361, and 374 meV. These have been included in this model as discrete oscillators and were used to calculate $S(\alpha,\beta)$ using the LEAPR module of NJOY [3].

1. A. K. Agrawal and S. Yip, ***Nucl. Sci. Eng.*** **37**, 368 (1969)
2. D. J. Picton, Ph.D. Thesis
3. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation: **Solid Methane Thermal Neutron Scattering Sublibrary, Release 3 (MAT 33)**
Temperatures: 22 ˚K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

Solid methane (CH_4) at 22 ˚K was generated using the model of Picton [1] and the spectrum of Harker and Brugger [2]. Optical measurements of methane in the gas phase show four fairly well defined vibrational modes at 162, 190, 361, and 374 meV. These have been included in this model as discrete oscillators and were used to calculate $S(\alpha,\beta)$ using the LEAPR module of NJOY [3].

1. D. J. Picton, Ph.D. Thesis
2. Y. D. Harker and R. M. Brugger, ***J. Chem. Phys.*** **42**, 275 (1965)
3. R. E. MacFarlane, **LA-12639-MS** (**ENDF-356**) (1994) Los Alamos National Laboratory

Evaluation: **H (Polyethylene) Thermal Neutron Scattering Sublibrary, Release 0 (MAT 37)**
Temperatures: 296 350 ˚K
Files: 1, 7
Evaluators: J. U. Koppel, D. H. Houston, and D. Sprevak (GA)

This evaluation was produced at General Atomic in 1969 using the code GASKET [1]. It was converted to ENDF-6 format at Los Alamos in 1989. The only changes made to the contents were adjustments of cross sections to match the ENDF/B-VI values.

Polyethylene is represented using a model of non-interacting chains of CH_2 radicals originally developed by Lin and Koenig [2]. The dispersion relation of polyethylene shows nine branches, the frequency in each branch being a function of the phase difference of the vibrations of corresponding atoms in neighboring CH_2 units. For some normal modes, the ratio of the amplitude of the hydrogen atom vibrations to the amplitude of the carbon atom vibrations also depends strongly on the phase difference. Using this model, the frequency spectrum was computed exactly for the hydrogen atoms in histogram form [3]. The low frequency part of the histogram (below 0.02 eV) was then replaced by a Debye spectrum having the same area, and the other elements of the histogram distribution were replaced by Gaussian functions of appropriate area centered at the center of each interval of the histogram. GASKET was then used to obtain $S(\alpha,\beta)$. The elastic part of the scattering law is represented using the incoherent approximation with Debye-Waller integrals from the GASKET calculation [1]. This evaluation only gives the scattering from the hydrogen in polyethylene. The carbon should be treated as a free gas with mass 12.011 amu.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic
2. T. P. Lin and J. L. Koenig, ***J. Molec. Spectra*** **9**, 228 (1962).
3. D. Sprevak and J. U. Koppel, ***Nucleonik*** **12**, 87 (1969).

Evaluation: **Benzene Thermal Neutron Scattering Sublibrary, Release 0 (MAT 40)**
Temperatures: 296 350 400 450 500 600 800 1000 ˚K
Files: 1, 7
Evaluators: J. U. Koppel, D. H. Houston, and G. M. Borgonovi (GA)

This evaluation was produced at General Atomic in 1969 using the code GASKET [1]. It was converted to ENDF-6 format at Los Alamos in 1989. The only changes made to the contents were adjustments of cross sections to match the ENDF/B-VI values.

The benzine molecule has an hexagonal planar structure with symmetry D6H, carbon-carbon bond length of 1.39 Å, and carbon-hydrogen bond length of 1.08 Å. In constructing a model for the atomic vibrations, it was assumed [2] that there is no interaction between vibrational and rotational states of the molecule, and that the hindered rotations that describe the interactions of molecules in the liquid can be represented by translations of the whole molecule with an effective mass. Continuous frequency distributions were then obtained for the hydrogen and carbon atoms using methods described in [3]. The cluster of frequencies closely spaced around 0.38 eV was lumped into a single oscillator. The GASKET code was then used to compute separate $S(\alpha,\beta)$ functions for hydrogen and carbon. The scattering laws were combined and adjusted to be used with the hydrogen free-atom cross section. The carbon free-atom cross section has been provided for use with the short-collision-time approximation (SCT). Thus, the thermal cross section computed from either $S(\alpha,\beta)$ or by the SCT approximation gives an asymptotic limit of approximately $6*20+6*4.7$ barns.

REFERENCES

1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic
2. D. Sprevak and J. U. Koppel, ***Nucleonik*** **12**, 87 (1969).
3. D. Sprevak, G. M. Borgonovi, G. W. Carriveau, and J. M. Neill, **GA-8185** (1967) General Atomics

Evaluation: **Zr (ZrH) Thermal Neutron Scattering Sublibrary, Release 3 (MAT 58)**
Temperatures: 296 400 500 600 700 800 1000 1200 °K
Files: 1, 7
Evaluators: R. E. MacFarlane (LANL)

This evaluation was generated using the LEAPR module of NJOY [3]. The physical model is very similar to the one used at General Atomic to produced the original ENDF/B-III evaluations [1]. The α and β grids were extended lightly, and the constants were changed to match the values in the previous ENDF/B-VI evaluation.

The lattice dynamics of ZrH were computed from a central force model. The slightly tetragonal lattice of ZrH_2 was approximated by a face-centered-cubic lattice. Four force constants (μ, γ, ν, and δ) were introduced describing respectively the interaction of a zirconium atoms with its nearest neighbors (8 H atoms) and its next nearest neighbors (12 Zr atoms), and the interaction of a hydrogen atom with its next nearest neighbors (6 H atoms) and its third nearest atoms (12 H atoms). Eigenvalues and eigenvectors of the dynamical matrix were calculated, and a phonon frequency spectrum was obtained by means of a root sampling technique. Weighted frequency spectra for hydrogen in ZrH were then obtained by appropriate use of the dynamical matrix eigenvectors [2].

The final values of the four force constants were obtained by fitting both specific heat and neutron data. The position of an optical peak observed by neutron scattering techniques to be centered roughly around 0.14 eV determines the constant μ, while the overall width and shape of this peak determine ν and δ respectively. Existing neutron data are not sufficiently precise to confirm the structure predicted in the optical peak by the central force model. Specific heat data were used to determine the force constant γ, which primarily determines the upper limit on the phonon energies associated with acoustic modes.

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1. J. U. Koppel and D. H. Houston, **GA-8774** General Atomic
   revised and reissued as **ENDF-269** (1978) National Nuclear Data Center
2. E. L. Slaggie, **GA-8132** (1967) General Atomic
3. R. E. MacFarlane, **LA-12639-MS (ENDF-356)** (1994) Los Alamos National Laboratory

Part VII

Incident Proton Sublibrary (NSUB=10010)

Evaluation: **^{1}H Incident Proton Sublibrary, Release 1 (MAT 125)**
Energy Range: 0 to 100 MeV
Files: 1, 3, 6
Evaluators: D. Dodder (LANL)

ENDF/B-VI MOD 1 EVALUATION (D. Dodder, LANL, October 1987)

The p-p elastic cross sections were calculated using an R-matrix analysis of the p-p cross section and polarization data over the energy range evaluated. The maximum nuclear partial wave allowed in the fit is L=6, and the resulting chi-squared per degree of freedom is 0.793.

Evaluation: **^{3}He Incident Proton Sublibrary, Release 1 (MAT 225)**
Energy Range: 1 keV to 20 MeV
Files: 1, 3, 6
Evaluators: G. Hale (LANL)

ENDF/B-VI MOD 1 EVALUATION (G. Hale, LANL, October 1983)

The p-^{3}He elastic and ^{3}He(p,2p)D cross sections and scattering distributions were calculated using an R-matrix analysis with code EDA. The energy-angle distributions for MT=111 are assumed to follow a 3-body phase-space law.

Part VIII

Incident Deuteron Sublibrary (NSUB=10020)

Evaluation: **^{2}H Incident Deuteron Sublibrary, Release 1 (MAT 128)**
Energy Range: 332.5 eV to 30 MeV
Files: 1, 3
Evaluators: R. M. White, D. A. Resler (LLNL)

ENDF/B-VI MOD 1 EVALUATION (R. M. White, D. A. Resler, LLNL, May 1991)

The D(d,n)^{3}He and D(d,p)^{3}H cross sections are evaluated based on all known experimental data published between 1946 and 1990. See White and Resler [1] for more information on evaluation.

REFERENCE

1. R. M. White and D. A. Resler, **Nuclear Data Evaluation Methodology**, Symposium, Brookhaven, NY, 12-16 October 1992 (World Scientific, 1993)

Evaluation: **^{3}H Incident Deuteron Sublibrary, Release 1 (MAT 131)**
Energy Range: 285 eV to 30 MeV
Files: 1, 3
Evaluators: R. M. White, D. A. Resler (LLNL)

ENDF/B-VI MOD 1 EVALUATION (R. M. White, D. A. Resler, LLNL, May 1991)

The ^{3}H(d,n)^{4}He cross section is evaluated based on all known experimental data published between 1946 and 1990. See White, et al. [1] for more information on evaluation.

REFERENCE

1. R. M. White, D. A. Resler, and S. I. Warshaw, **Nuclear Data for Science and Technology**, Conference, Jülich, Germany, 13-17 May 1991 (Springer-Verlay, 1992)

Evaluation: **^{3}He Incident Deuteron Sublibrary, Release 1 (MAT 225)**
Energy Range: 118.75 eV to 30 MeV
Files: 1, 3
Evaluators: R. M. White, D. A. Resler (LLNL)

ENDF/B-VI MOD 1 EVALUATION (R. M. White, D. A. Resler, LLNL, May 1991)

The $^{3}He(d,p)^{4}He$ cross section is evaluated based on all known experimental data published between 1946 and 1990. See White, et al. [1] for more information on evaluation.

REFERENCE

1. R. M. White, D. A. Resler, and S. I. Warshaw, **Nuclear Data for Science and Technology**, Conference, Jülich, Germany, 13-17 May 1991 (Springer-Verlay, 1992)

Part IX

Incident Triton Sublibrary (NSUB=10030)

Evaluation: **^{3}H Incident Triton Sublibrary, Release 1 (MAT 131)**
Energy Range: 475 eV to 30 MeV
Files: 1, 3
Evaluators: R. M. White, D. A. Resler (LLNL)

ENDF/B-VI MOD 1 EVALUATION (R. M. White, D. A. Resler, LLNL, May 1991)

The $^{3}H(t,2n)^{4}He$ cross section is evaluated based on all known experimental data published between 1946 and 1990. See White, et al. [1] for more information on evaluation.

REFERENCE

1. R. M. White, D. A. Resler, and S. I. Warshaw, **Nuclear Data for Science and Technology**, Conference, Jülich, Germany, 13-17 May 1991 (Springer-Verlay, 1992)