Evaluations of Fission Products

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Presentation at the CSEWG Annual Meeting
BNL, November 4-6, 2003

Brookhaven Science Associates
U.S. Department of Energy

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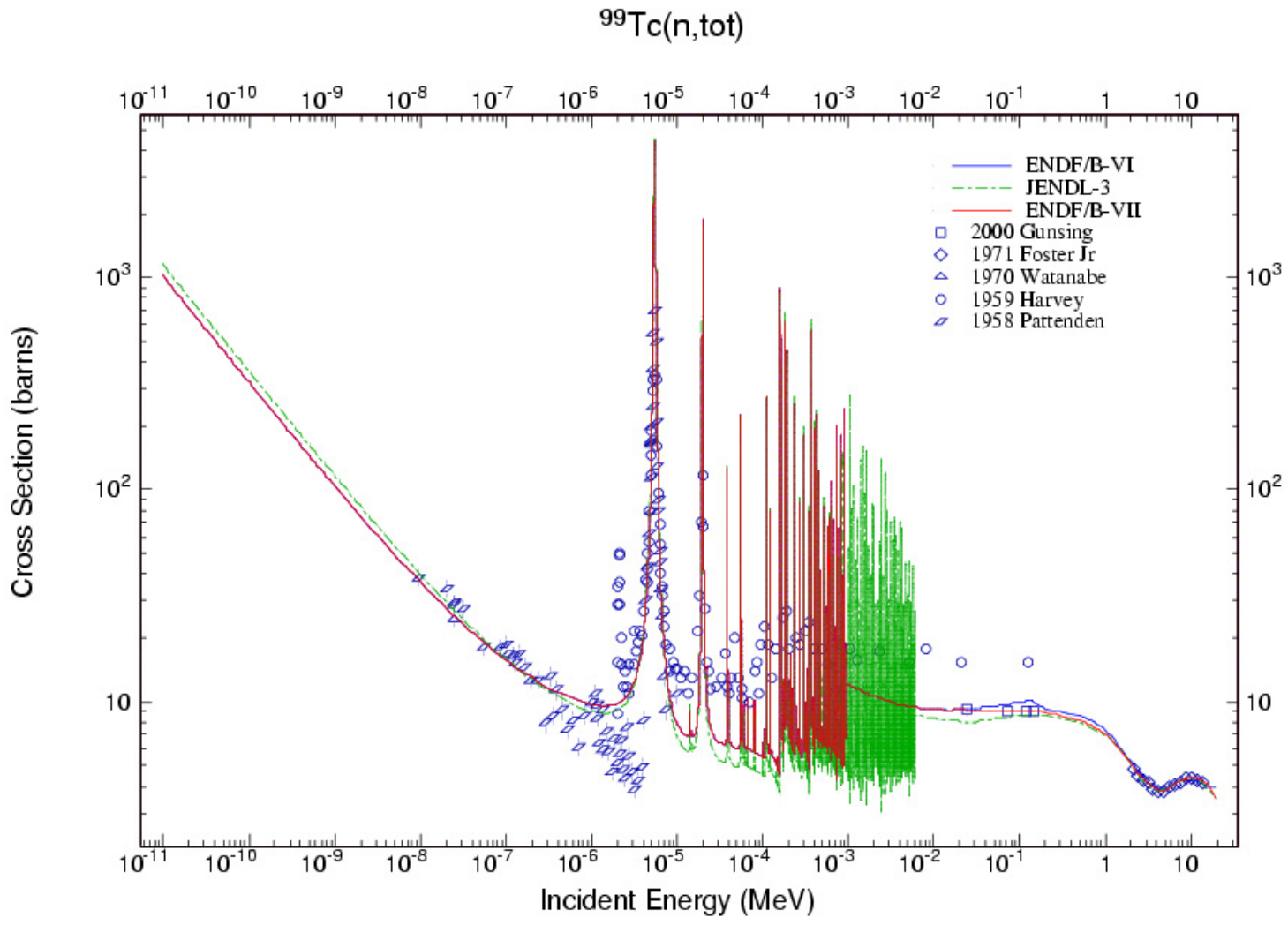
Evaluations of Fission Products: Overview

- **19 materials evaluated by KAERI-BNL collaboration**
  - Submitted to ENDF/B-VII
- **Other materials**
  - 200 fission products in ENDF/B-VI, most of them old and obsolete
  - Bulk of fission products evaluations addressed by WPEC Subgroup 21
- **New BNL-325 evaluations**
  - Systematic re-evaluation of neutron resonance parameters
  - Presentation by Said Mughabghab, BNL

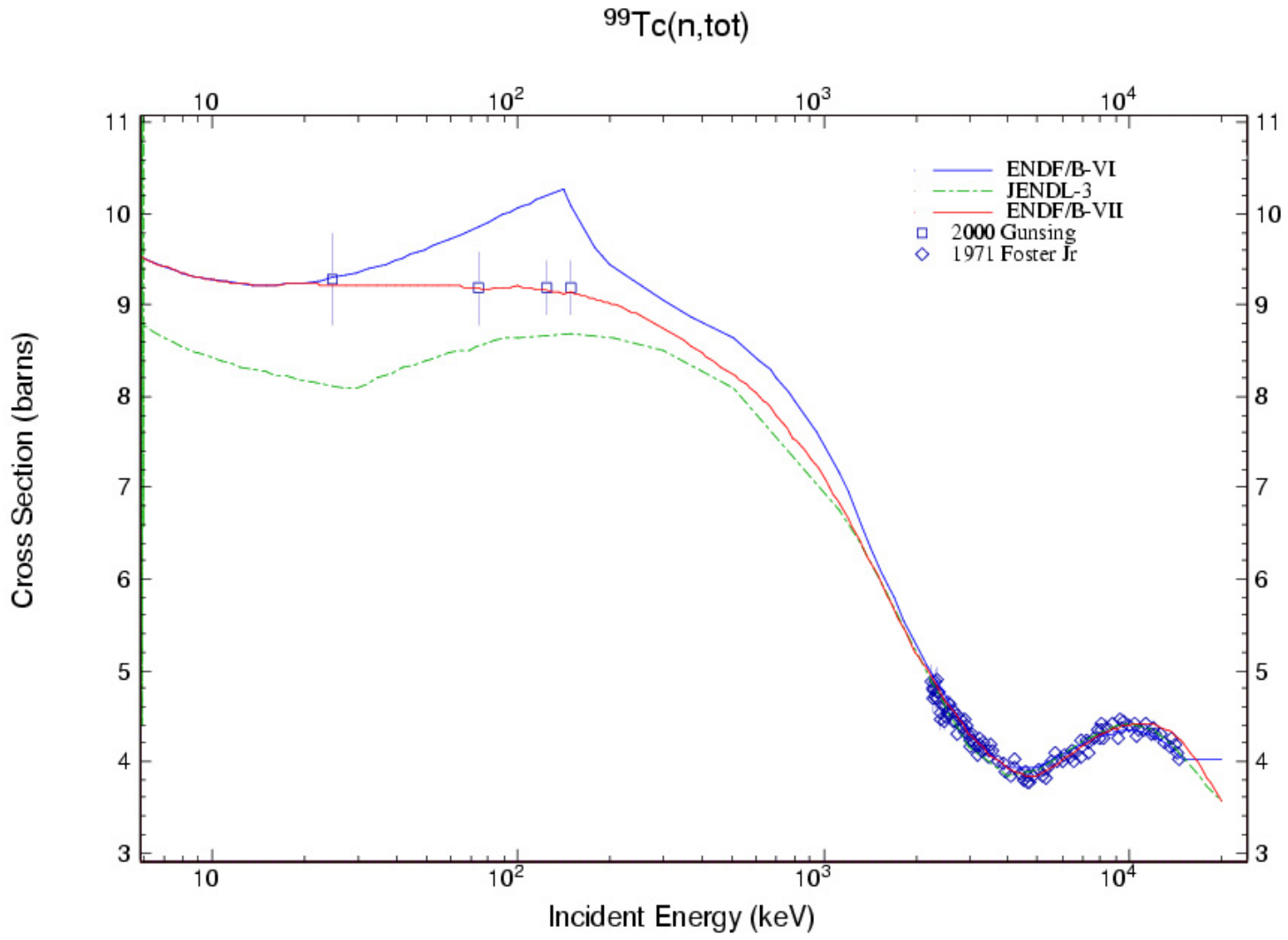
Evaluations of Fission Products: KAERI-BNL collaboration

- **19 priority materials**
  - ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{105}Pd, ^{109}Ag, ^{131}Xe, ^{133}Cs, ^{141}Pr, ^{143,145}Nd, ^{147,149,150,151,152}Sm, ^{153}Eu, ^{155,157}Gd
- **Low energy neutrons (thermal, resolved resonances, URR)**
  - Completed in 1999 and 2000 (Oh, Mughabghab)
  - Included into ENDF/B-VI, release 8, October 2001
- **Fast neutrons**
  - Code EMPIRE employed
  - Completed in 2002 (Lee, Oblozinsky)
- **Creation of complete files**
  - 3 files prepared by BNL (^{99}Tc, ^{153}Eu and ^{157}Gd)
  - 16 files prepared by KAERI, format problems, ok for 10 files now

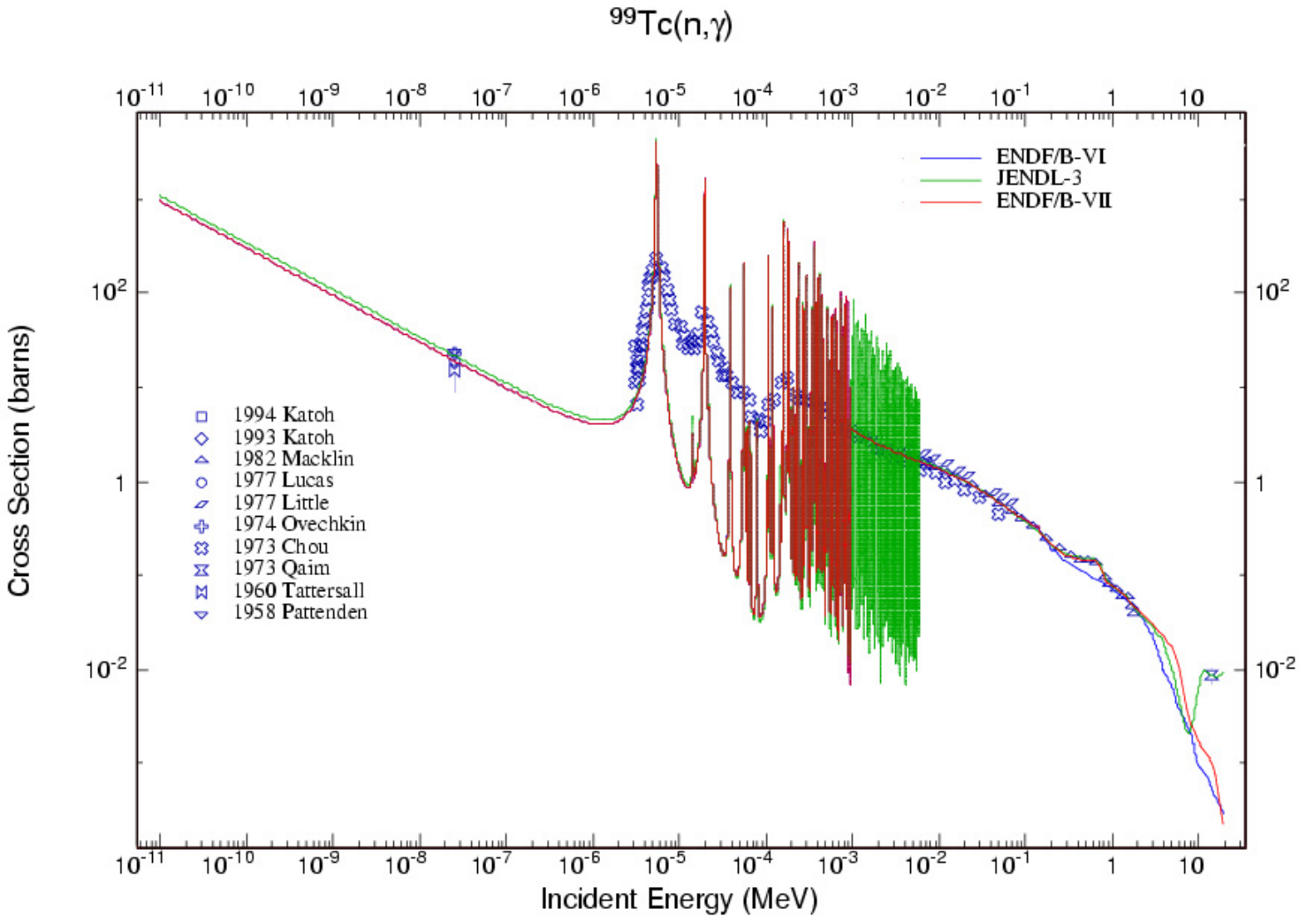
BNL-KAERI Collaboration: ^{99}Tc(n,tot)



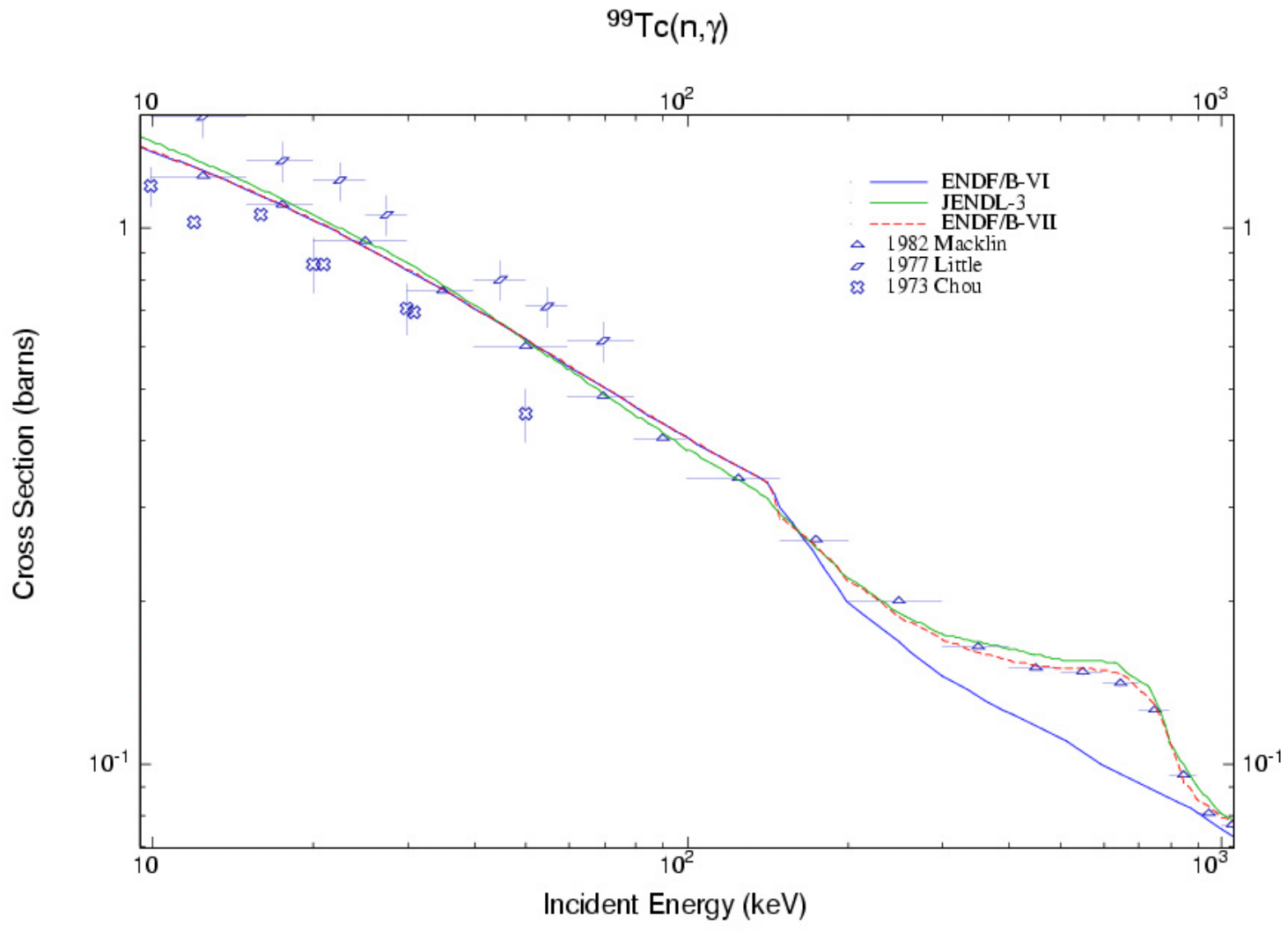
BNL-KAERI Collaboration: ^{99}Tc(n,tot)



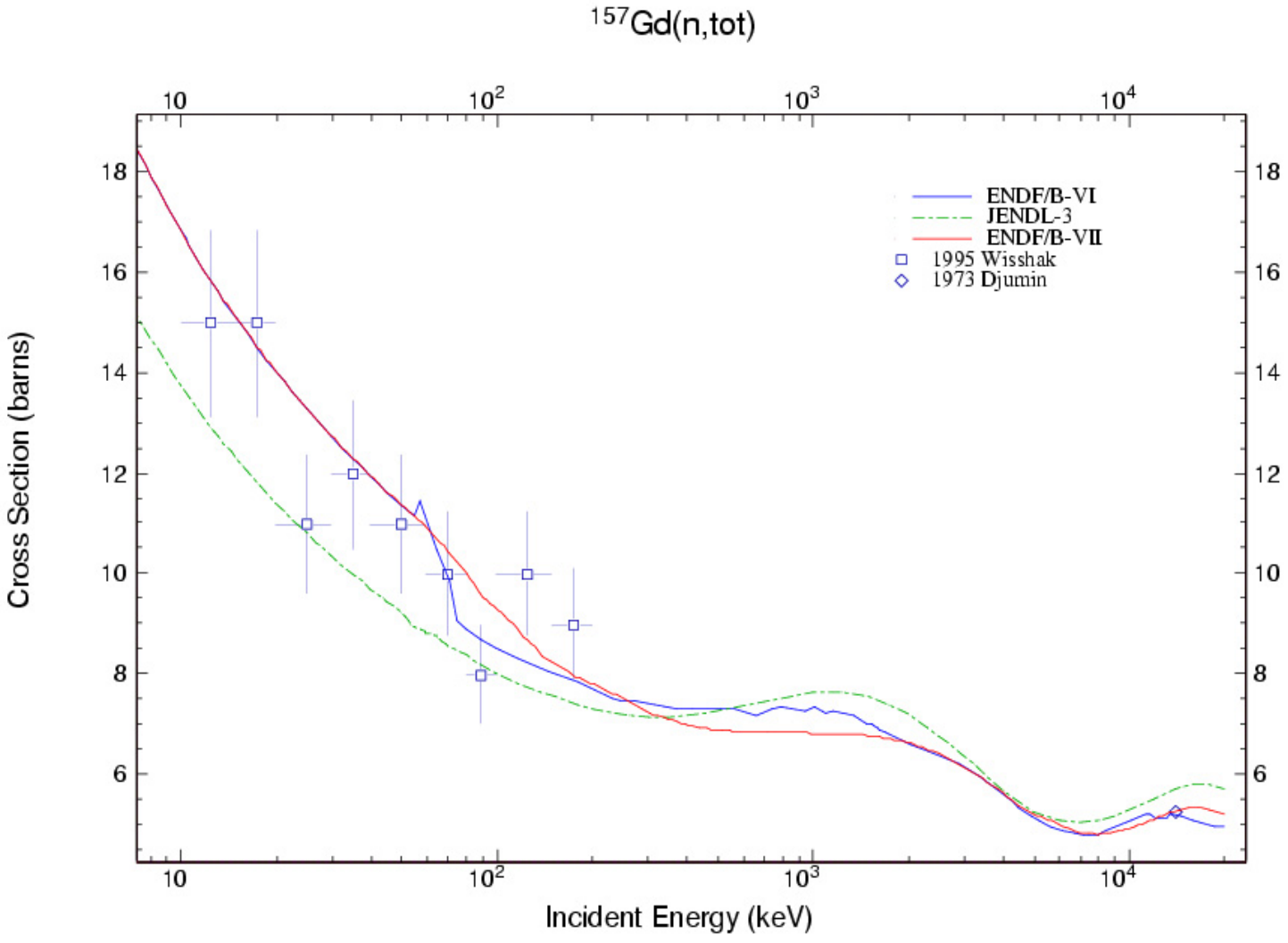
BNL-KAERI Collaboration: $^{99}Tc(n,\gamma)$



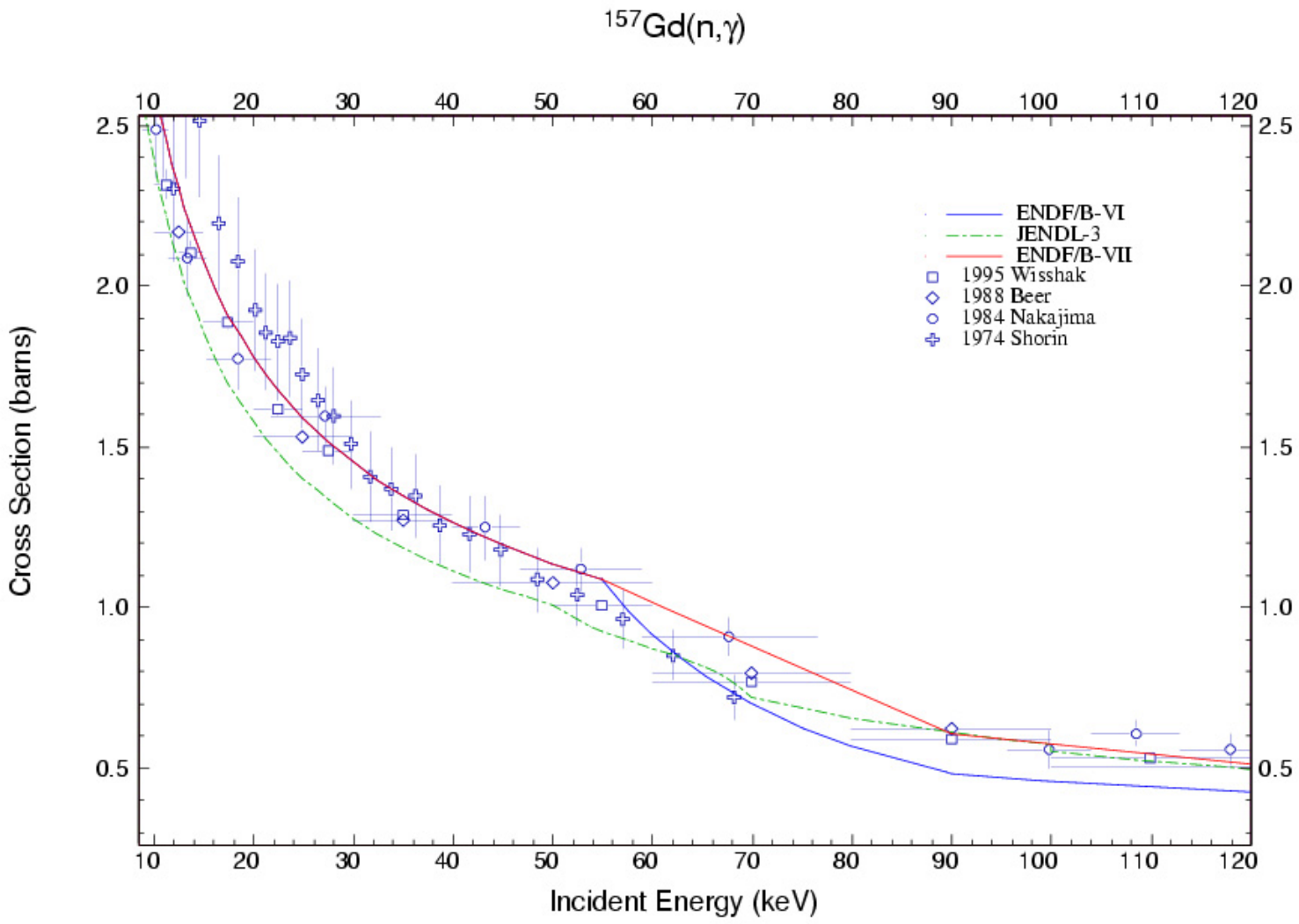
BNL-KAERI Collaboration: $^{99}Tc(n,\gamma)$



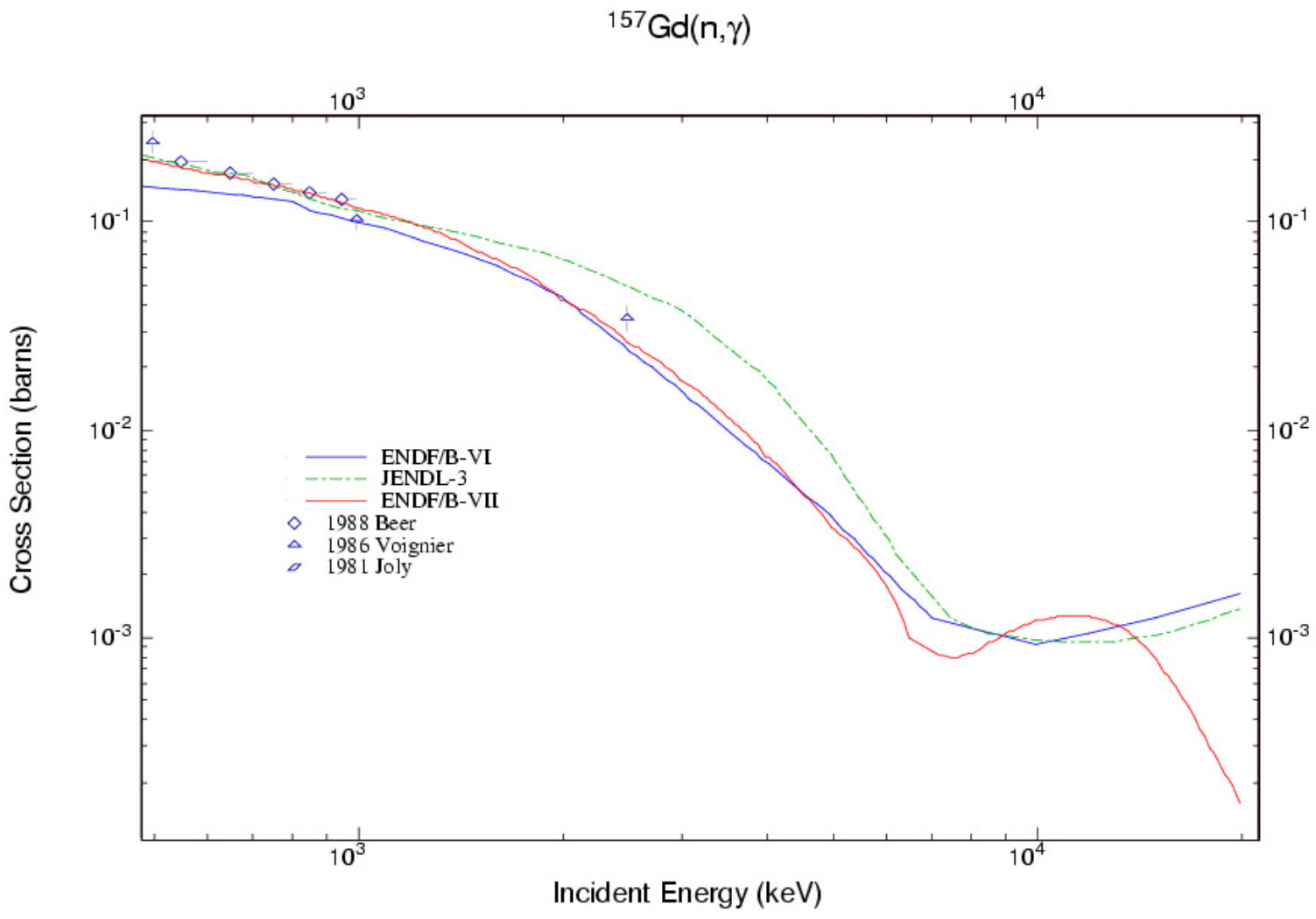
BNL-KAERI Collaboration: ^{157}Gd(n,tot)



BNL-KAERI Collaboration: $^{157}Gd(n, \gamma)$



BNL-KAERI Collaboration: $^{157}Gd(n, \gamma)$



Other Fission Products: Motivation for WPEC Subgroup 21

- Fission products
  - Altogether 211 nuclei in range Z = 31 – 68 in 5 evaluated libraries
  - ~ 20-40 priority materials depending on application
  - ~ 170 lower priority materials, bulk of fission products

- In ENDF/B-VI, release 8 (October 2001)
  - 200 FPs out of 325 materials
  - 65% evaluations more than 20-25 years old
  - 55% evaluations use isotopic elastic angular distribution
  - 30% evaluations use outdated point-wise data in resistance region
  - 30% evaluations use outdated single-level Breit-Wigner representation in resonance region

SG21: Assessment of Neutron Cross-Section Evaluations for the Bulk of Fission Products

- WPEC Subgroup 21
  - Established in April 2001
  - Review and asses evaluations, no validation
  - Focus on bulk of fission products (~ 170 out of 211)
- Participants: 14 members, 11 active reviewers
  - Chairman: P. Oblozinsky (BNL)
  - ENDF: M. Herman (BNL), I. Sirakov (BNL and INRNE), R.E. MacFarlane (LANL), J. Chang (KAERI)
  - JENDL: T. Nakagawa (JAERI), K. Shibata (JAERI), M. Igashira (TIT), M. Kawai (KEK)
  - BROND: A.V. Ignatyuk (IPPE), V. Pronyaev (IAEA), V. Zerkin (IAEA)
  - CENDL: S. Qingbiao (CNDC), Z. Youxiang (CNDC)

WPEC Subgroup21: Review Methodology

1. **Review files**: Summarize available evaluations, origin and updates

2. **Review thermal and resonance region**
   - Review evaluations in thermal, resolved resonance region, unresolved resonance region
   - Consider additional information (new Mughabghab etc)

3. **Review fast energy region**
   - Assess evaluation methodology
   - Review evaluations, compare with experimental data (MT = 1, 2, 4, 16, 102, 103, 107)

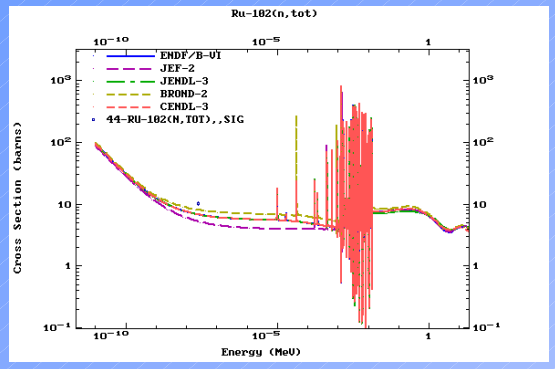
4. **Write short report**
   - Describe review procedure, list findings
   - Make recommendation for thermal & resonance, and for fast region

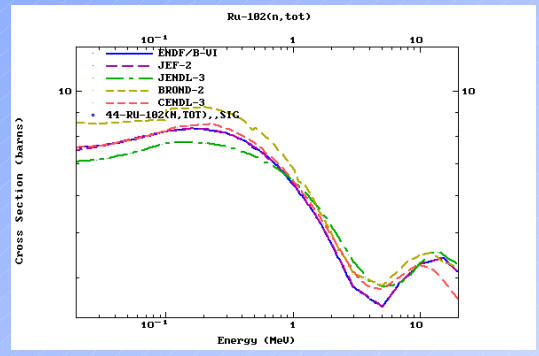
WPEC Subgroup21: Website

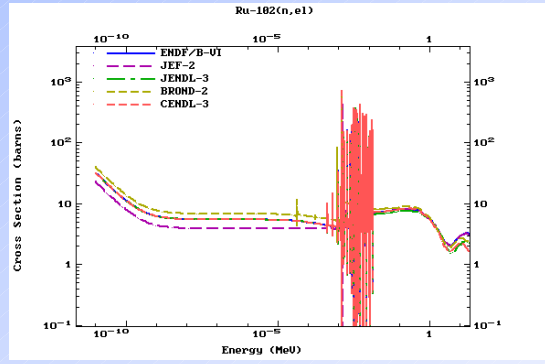
- **SG21 Website**
  - www.nndc.bnl.gov/sg21/
  - Contains all SG 21 documents
  - Contains support information for reviewers
    - S. Mughabghab, Thermal neutron capture cross sections, resonance integrals and g-factors, Report INDC(NDS)-440, Feb 2003
    - Priority list of 130 fission products, taken from the Final Report of SG17: “Status of pseudo-fission-product cross-sections for fast reactors”, 1998
    - One-group capture cross- sections for 211 fission products, calculated by BNL using the methodology of SG17, fast reactor spectrum
  - Inter-comparison plots for all 211 FPs
    - ~1900 plots
    - Links to evaluated files in 5 libraries
    - Links to EXFOR files
  - Review reports (currently for 107 FPs)

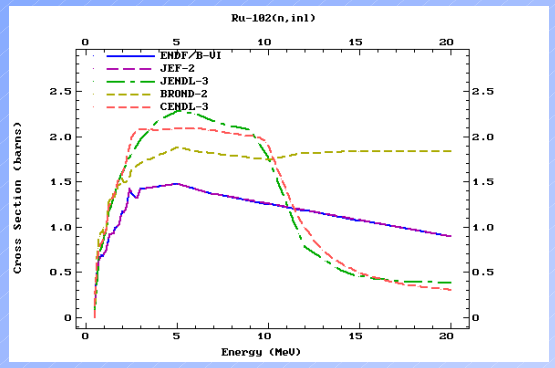
SG21: Example of Intercomparison Plots
(Prepared for all 211 Fission Products)

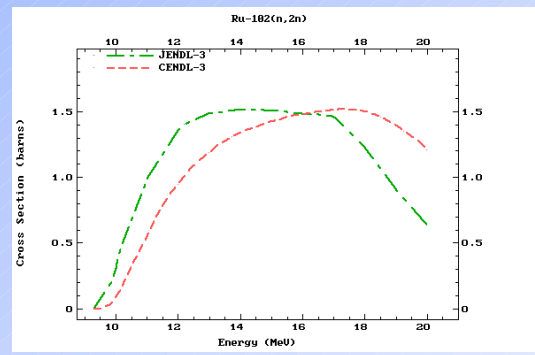
44-Ru-102

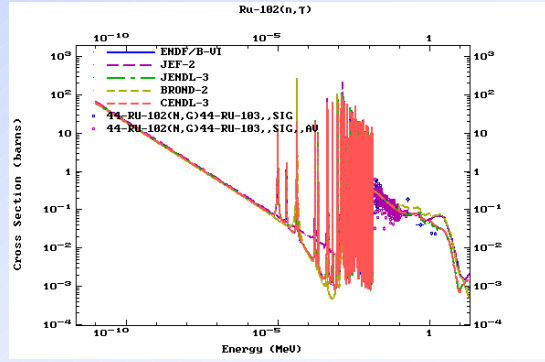


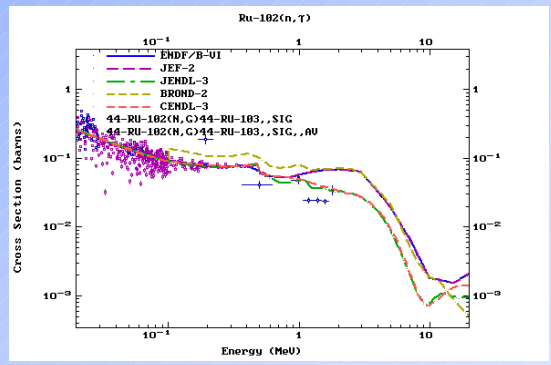


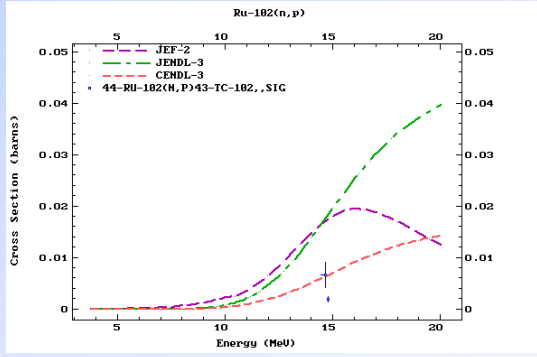


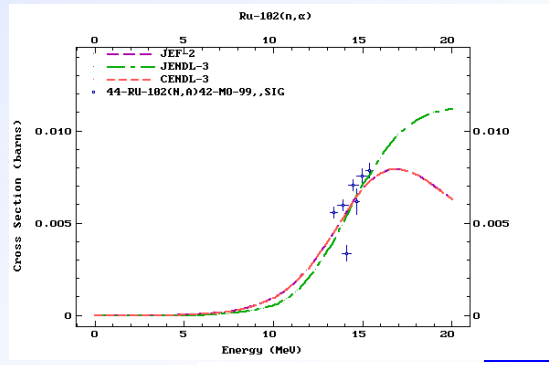












SG21: Priority List of Fission Products

List of 211 fission products marked according to their priority for fast reactor applications and showing the status of reviews. Notation: Underline - already reviewed (107 nuclides), red - first 40 nuclides (p. 28 of SG17 report), blue - next 45 nuclides (p. 29 of SG17 report) and green - last 45 nuclides (p. 30 of SG17 report).

31-Ga- 69, 71
32-Ge- 70, 72, 73, 74, 76
33-As- 75
34-Se- 74, 76, 77, 78, 79, 80, 82
35-Br- 79, 81
36-Kr- 78, 80, 82, 83, 84, 85, 86
37-Rb- 85, 86, 87
38-Sr- 84, 86, 87, 88, 89, 90
39-Y - 89, 90, 91
40-Zr- 90, 91, 92, 93, 94, 95, 96
41-Nb- 93, 94, 95
42-Mo- 92, 94, 95, 96, 97, 98, 99, 100
43-Tc- 99
44-Ru- 96, 98, 99, 100, 101, 102, 103, 104, 105, 106
45-Rh-103, 105
46-Pd-102, 104, 105, 106, 107, 108, 110
47-Ag-107, 109, 110m,111
48-Cd-106, 108, 110, 111, 112, 113, 114, 115m,116
49-In- 113, 115

SG21: Priority List of Fission Products, ctn'd

50-Sn-112, 114, 115, 116, 117, 118, 119, 120, 122, 123, 124, 125, 126
51-Sb-121, 123, 124, 125, 126
52-Te-120, 122, 123, 124, 125, 126, 127m,128, 129m,130, 132
53-I - 127, 129, 130, 131, 135
54-Xe-123, 124, 126, 128, 129, 130, 131, 132, 133, 134, 135, 136
55-Cs-133, 134, 135, 136, 137
56-Ba-130, 132, 134, 135, 136, 137, 138, 140
57-La-138, 139, 140
58-Ce-136, 138, 140, 141, 142, 143, 144
59-Pr- 141, 142, 143
60-Nd-142, 143, 144, 145, 146, 147, 148, 150
61-Pm-147, 148, 148m,149, 151
62-Sm-144, 147, 148, 149, 150, 151, 152, 153, 154
63-Eu-151, 152, 153, 154, 155, 156, 157
64-Gd-152, 154, 155, 156, 157, 158, 160
65-Tb-159, 160
66-Dy-160, 161, 162, 163, 164
67-Ho-165
68-Er- 162, 164, 166, 167, 168, 170

SG21: Example of Detailed Review

Ru-101

Reviewed by T. Nakagawa, JAERI, December 2002

1. Files

ENDF/B-VI: Original evaluation was made by Schenter et al. in 1980 for ENDF/B-V. Those data were carried over to ENDF/B-VI. In 1991, the resonance parameters and capture cross section were updated. Recently, the resonance parameters were revised again by Oh et al. [Oh00] for ENDF/B-VI.8

JENDL-3.3: In 1984, the evaluation was made by JNDC FPND working group for JENDL-2. The data were revised in 1990 for JENDL-3.1, and in 1993 for JENDL-3.2. JENDL-3.3 is basically the same as JENDL-3.2.

JEFF-3.0: RCN-4 evaluation made by Gruppelaar and Van der Kamp was adopted for JEF-2. JEFF-3.0 is the same as JEF-2.2.

CENDL-3: Evaluation was performed by Zhang et al. in 1999. The data were revised in 2001.

BROND-2: Evaluation was made by Ignatyuk et al. in 1984.

SG21: Example of Detailed Review, ctn'd

2. Thermal and resonance region

ENDF/B-VI
The resolved resonance region is up to 1.0354 keV. Resonance parameters were determined on the basis of the data of Mughabghab et al. [Mu81] and Anufriev et al. [An85] Unresolved resonance parameters are given up to 128.49 keV.

JENDL-3.3
The resolved resonance region is up to 1.06 keV. Parameters were determined from experimental data of Priesmeyer and Jung [Pr72], Popov et al. [Po79] and Anufriev et al. [An85]. Unresolved resonance parameters were given in the energy range from 1.06 to 100 keV, which were determined so as to reproduce the capture cross section of Macklin et al. [Ma79, Ma81]

JEFF-3.0
Resolved resonance parameters were taken from Mughabghab et al. [Mu81] Unresolved resonance parameters up to 25 keV were based on the strength functions [Ma80], D-obs adjusted to STEK and PHENIX integral data, s-wave capture width of 0.18 eV [Mu81] and p-wave capture width of 0.19 eV.

CENDL-3
ENDF/B-VI.2 was adopted for the resolved and unresolved resonance parameters. The resolved resonance parameters were based on the recommendation by Mughabghab et al. [Mu81]. The unresolved ones were determined so as to reproduce the average capture cross section of Macklin et al. [Ma79]

BROND-2
Resolved resonance parameters up to 1 keV were based on the recommendation of Mughabghab et al. [Mu81] Unresolved resonance parameters were given up to 120 keV.

Table 2 shows thermal cross sections and resonance integral of capture cross section. The capture cross section of 3.4±0.9 b recommended by Mughabghab et al. [Mu81] is reproduced well by the current evaluations. However, the origin of this value is not certain. Halperin et al. [Ha64] reported a value of 3.1±0.9 b as an average cross section in a reactor spectrum. Did they adopt this value?

The total cross section of 11.2±0.4 [An85] at 0.0253 eV is not reproduced by any evaluations.

Concerning the resonance integral of capture cross section, evaluated data are in good agreement with the data of Mughabghab et al. and Anifriev et al. However, the data of Anufriev et al. is a calculation from resonance parameters which they analyzed. Therefore, the resonance integral is also uncertain.

SG21: Example of Detailed Review, ctn'd

Summary for Resolved and Unresolved Resonance Region: Ru-101

Library	RR Region	UR Region	Remarks
ENDF/B-VI	1.0354 keV MLBW	128.49 keV	
JENDL-3.3	1.06 keV MLBW	100 keV	
JEFF-3.0	1.04426 keV MLBW	25 keV	Background sig given to URP
CENDL-3	1.0 keV MLBW	100 keV	Taken from ENDF/B-VI.2
BROND-2	1.0 keV MLBW	120 keV	

SG21: Example of Detailed Review, ctn'd

Thermal Cross Sections and Resonance Integral (barns): Ru-101

Library/Experiment	Total	Elastic	Capture	Res.Integ.
ENDF/B-VI	7.922	4.473	3.449	112
JENDL-3.3	7.100	3.741	3.359	100
JEFF-3.0	8.467	5.054	3.414	111
CENDL-3	6.629	3.216	3.413	112
BROND-2	7.688	4.289	3.400	112
Mughabghab [Mu81, Mu01]			3.4±0.9	100±20
Halperin [Ha65]			5.23±25%	79.1±10%[a)]
Anufriev [An85]	11.2±0.4			108±15[b)]

a) E-cutoff = 0.54 eV

b) Calculated from resonance parameters.

Recommendation/conclusion for the thermal & resonance region:

ENDF/B-VI.8 is recommended.

Modification needed to reproduce measured thermal cross sections, new experiments desirable to determine more accurate thermal cross sections and resonance integral.

SG21: Example of Detailed Review, ctn'd

3. Fast neutron region

(1) Methodology

ENDF/B-VI
Theoretical calculation was performed using the optical potential parameters of Moldauer. Inelastic scattering cross sections were calculated with the COMNUC-3 code considering 19 discrete levels. The capture cross section was calculated with the NCAP code, and revised to reproduce the data of Macklin et al. [Ma79]. No threshold reaction cross sections were considered.

The angular distributions of elastically scattered neutrons were calculated from Moldauer potential. Those of inelastic scattering were assumed to be isotropic in the laboratory system.

Evaporation spectra were given to the continuum inelastic scattering.

JENDL-3.3
The total, elastic and inelastic scattering, and capture cross sections were calculated with the spherical optical model and statistical model code CASTHY. The gamma-ray strength function was adjusted to the capture cross section of 500 mb at 100 keV [Ma79, Ma81]. For the inelastic scattering, 28 levels were considered. No direct process was considered. The direct/semi-direct capture was calculated from a simple formula of Benzi and Reffo [Be69]

Other reaction cross sections were calculated with the preequilibrium and multi-step evaporation code PEGASUS. The (n,p) and (n,a) reaction cross sections were normalized to the systematics of Forrest [Fo86] at 14.5 MeV. Sum of the threshold reaction cross sections were considered as a competing reaction cross sections in the CASTHY calculation.

Angular distributions of elastic and inelastic scattering were calculated with the CASTHY code. Isotropic distributions were assumed to the other reactions.

The energy distributions were calculated with the PEGASUS code.

JEFF-3.0
Below 127 keV, cross sections were calculated from strength functions. Above this energy, the statistical model code SASSI-ECN and precompound model code PREANG were used for the calculation.

CENDL-3
Based on experimental data and theoretical calculations with the SUNF and DWUCK codes. The optical model parameters were obtained with the APMN code.

BROND-2
The data above 120 keV were taken from ENDF/B-V. The capture cross section was modified by adding a direct and semi-direct capture cross section.

SG21: Example of Detailed Review, ctn'd

(2) Total cross section (MT=1)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt1 and Fig. A1

The evaluated data are compared with experimental data of natural Ru in Fig. A1. *CENDL-3* reproduces well the experimental data.

(3) Capture cross section (MT=102)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt102 and Fig. A2

All evaluated data are in good agreement with experimental data of Macklin and Halperin [Ma80] and with each other below about 1 MeV, including the resonance region. Discrepancies among the evaluated data are found in the MeV region.

(4) Elastic scattering cross section (MT=2)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt2 and Fig. A3

This cross section was obtained as (the total cross section – sum of partial cross sections). Figure A3 shows the evaluated elastic scattering cross sections from the thermal energy to 20 MeV. Discrepancies are large below 100 keV and above 10 MeV.

(5) Inelastic scattering cross section (MT=4, 51 – 91)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt4

Discrete levels considered in the evaluations are as follows:

ENDF/B-VI, BROND-2	19 levels up to 0.9901 MeV
JENDL-3.3	28 levels up to 1.169 MeV
JEFF-3.0	15 levels up to 0.684 MeV
CENDL-3	28 levels up to 1.169 MeV

Direct inelastic was considered in *CENDL-3.3*. The shape of *ENDF/B-VI* and *BROND-2* is not reasonable. Other evaluations are almost the same.

SG21: Example of Detailed Review, ctn'd

(6) (n,2n) reaction cross section (MT=16)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt16

JENDL-3.3, JEFF-3.0 and *CENDL-3* give the (n,2n) reaction cross section.

(7) (n,p) reaction cross section (MT=103)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt103

JENDL-3.3, *CENDL-3* and *JEFF-3.0* give this reaction cross section. *JENDL-3.3* is in a very good agreement with experimental data of Kasugai et al. [Ka98]

(8) (n,a) reaction cross section (MT=107)
See Fig: http://www.nndc.bnl.gov/sg21/fp21/htm/Ru101.htm#mt107

JENDL-3.3, *CENDL-3* and *JEFF-3.0* give this reaction cross section. No experimental data are available.

(9) Other reactions

The following reaction cross sections are given:

ENDF/B-VI	no threshold reactions
JENDL-3.3	(n,3n), (n,na), (n,np), (n,nd), (n,d), (n,t), (n,^{3}He)
JEFF-3.0	(n,3n), (n,na), (n,np)
CENDL-3	(n,3n), (n,na), (n,np), (n,d), (n,t), (n,2p)
BROND-2	no threshold reactions

SG21: Example of Detailed Review, ctn'd

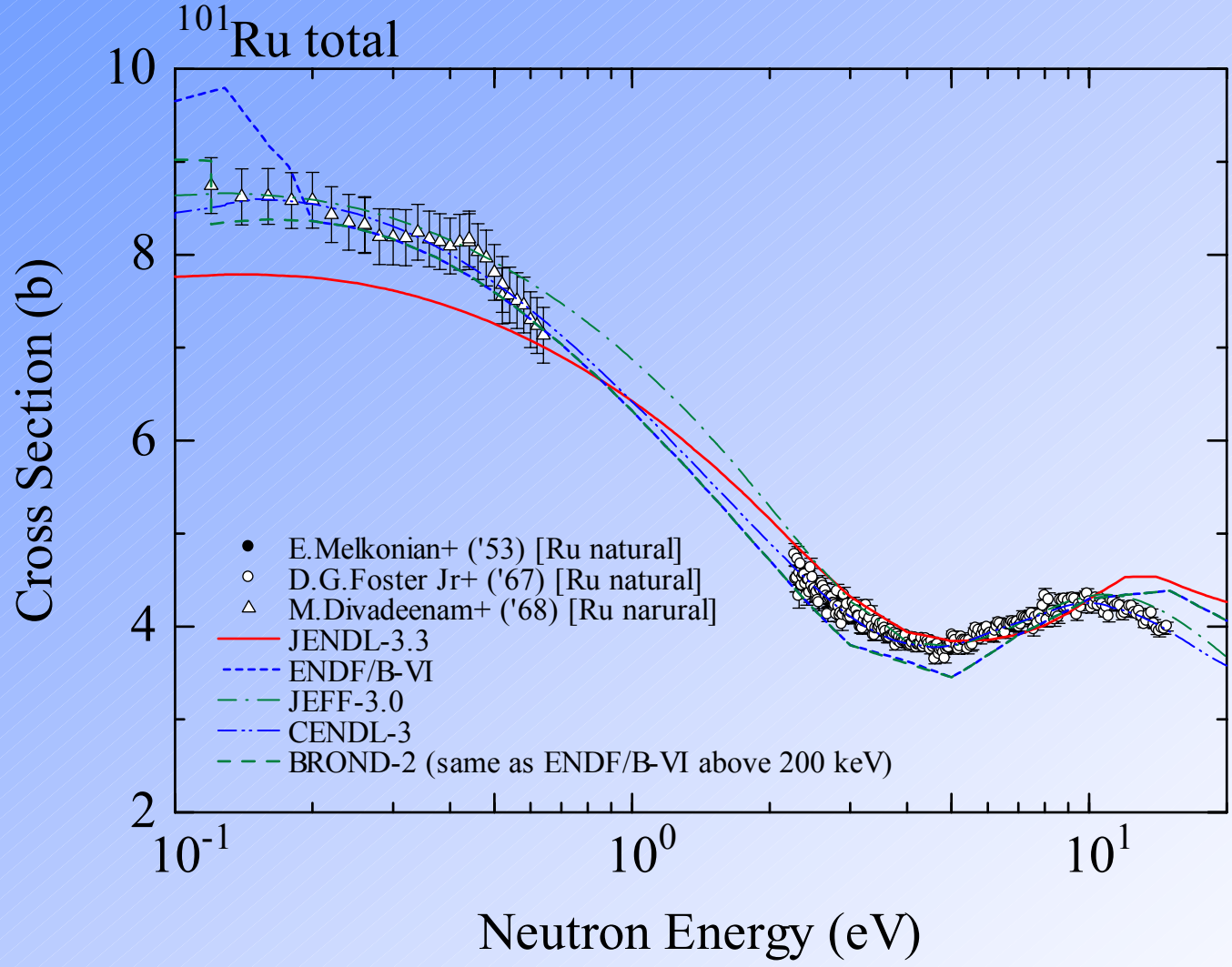


Fig. A1: Ru-101 total cross section

SG21: Example of Detailed Review, ctn'd

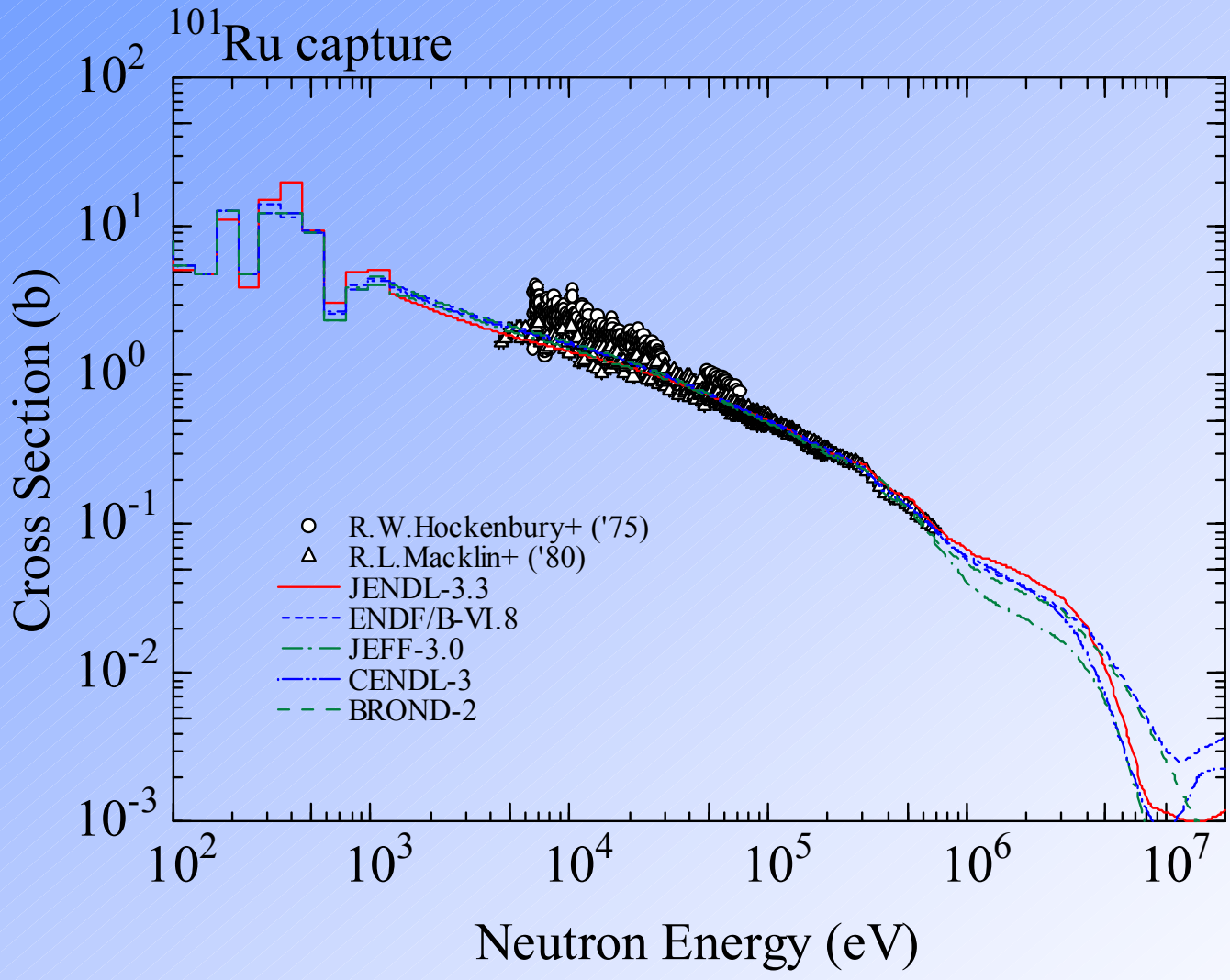


Fig. A2: Ru-101 capture cross section (100 eV to 20 MeV)

SG21: Example of Detailed Review, ctn'd

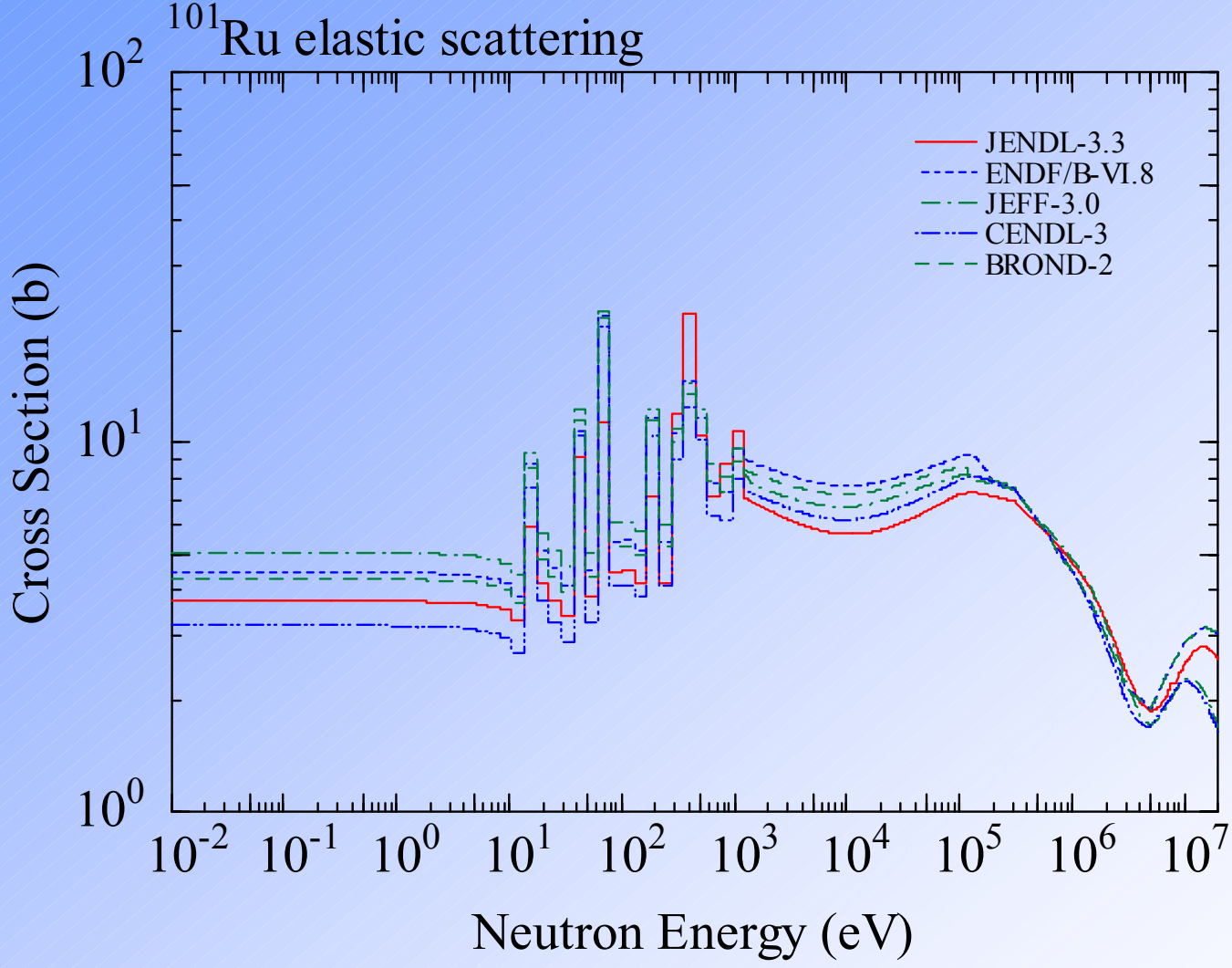


Fig. A3: Ru-101 Elastic scattering cross section

SG21: Example of Detailed Review, ctn'd

Recommendation/conclusion for the fast energy region (Ru-101):
***CENDL-3* is recommended.**

References

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WPEC Subgroup 21: Summary of Recommendations for Fission Products Evaluations

Library	Thermal & Res. Region	Fast Energy Region	Comment
ENDF/B-VI	32	13	Mostly ENDF/B-V, 19 new evaluations in th&res region
JENDL-3	59	45	New evaluations completed 10-12 year ago
CENDL-3	6	39	Most recent evaluations in fast energy region, released 2001
JEF-2	3	5	Mostly ENDF/B-V
BROND-2	2	4	FBROND-2 contains few FP evaluations only
Other	5	1	New Mughabghab (5) and ENDF/B-VII (1) recommended
Total # of materials	**107**	**107**	**18 reviewed in 2001/02, 89 in 2002/03**

WPEC Subgroup 21: Remaining Work

- **Remaining reviews**
  - 104 materials distributed to 11 reviewers in October 2003
  - Deadline for reviews is spring 2004
  - Concluding SG21 Workshop under consideration (April 19-23, 2004 at BNL)

- **Final product**
  - Review report for each FP material
  - Recommendations for best FP evaluations
  - Deadline May 2004

- **Open issues**
  - Creation of actual files for ~170 materials
  - Validation of selected materials
  - Organization of work, funding, timing?

Evaluations of Fission Products: Summary

- **Priority materials**
  - 19 materials by KAERI-BNL collaboration
    - Submitted to ENDF/B-VII
    - Format problems in some files from KAERI
  - Gd isotopes by ORNL ?
- **Other materials**
  - Reviewed by WPEC Subgroup 21
  - Final document with recommendations for all 211 FPs expected in May 2004
- **Open issues**
  - Creation of actual files for ~170 materials
  - Validation of selected materials
  - Organization of work, funding, timing?