WPEC Subgroup 48

Advances in Thermal Scattering Law Analysis

Ayman Hawari, Gilles Noguere

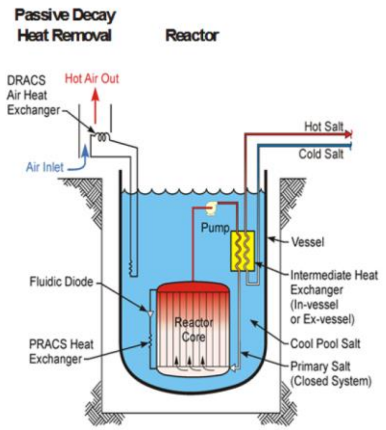
32nd Meeting of the
NEA Working Party on International Nuclear Data Evaluation Co-operation
May 11 – 15, 2019 • WebEx Meeting

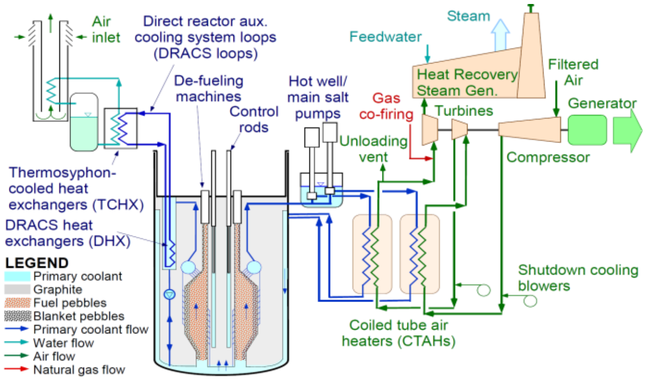
WPEC Subgroup 48
Agenda

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:20	04:30	**13:30**	20:30	Welcome	A. Hawari, G. Noguère
00:20	04:50	**13:50**	20:50	Status of the TSL activities in the framework of the Nausicaa collaboration	G. Noguère
00:20	05:10	**14:10**	21:10	TSL measurement capabilities at ISIS	S. Lilley
00:20	05:30	**14:30**	21:30	Effect of thermal resonant treatment on keV scattering cross sections	R. Dagan
00:20	05:50	**14:50**	21:50	**Short break**	
00:20	06:10	**15:10**	22:10	The impact of uncertainty in thermal scattering on nuclear reactor parameters	L. Snoj
00:20	06:30	**15:30**	22:30	TSL Research at NSCU	A. Hawari
00:20	06:50	**15:50**	22:50	Validation of Thermal Scattering Laws for Light Water at Elevated Temperatures with Diffusion Experiments	J. Holmes
00:30	07:10	**16:10**	23:10	Discussion	
	07:40	**16:40**	23:40	Close	

Motivation – Neutronic Systems

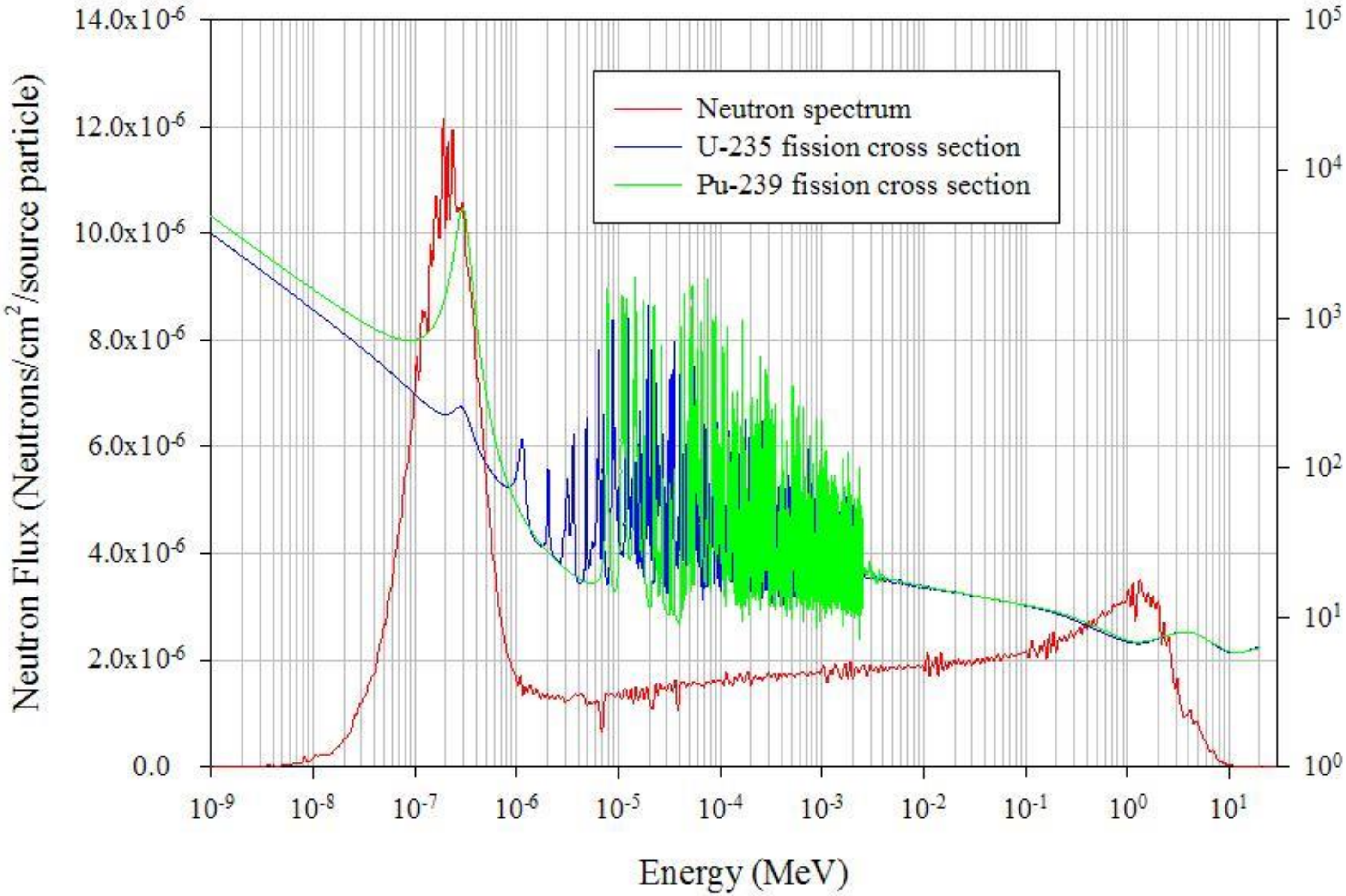
- Current and advanced thermal reactors have been proposed including the LWR, AHTR and FHR
  - The core is dominated by light water, graphite, molten salt, etc. moderators





- Criticality safety applications
- Neutron sources (research reactors and spallation sources) and applications

Neutronic Characteristics



NEA
Nuclear Energy Agency

Neutron Thermalization

Using first Born approximation combined with Fermi pseudopotential, it can be shown that the double differential scattering cross section has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\sqrt{\frac{E'}{E}}\left\{\sigma_{coh} S(\vec{\kappa},\omega) + \sigma_{incoh} S_s(\vec{\kappa},\omega)\right\}$$

The scattering law $S(\vec{\kappa},\omega)$ is composed of two parts

$$S(\vec{\kappa},\omega) = S_s(\vec{\kappa},\omega) + S_d(\vec{\kappa},\omega)$$

Van Hove’s space-time formulation

$$I(\vec{\kappa},t) = \int G(\vec{r},t)\exp(i\vec{\kappa}\cdot\vec{r})d\vec{r}$$

$$S(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\vec{r},t)e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}d\vec{r}dt$$

where $G(\vec{r},t)$ is the *dynamic pair correlation function* and can be expressed in terms of time dependent atomic positions.

Since 1960s

$$S_s(\alpha,\beta) = k_B T \cdot S_s(\vec{\kappa},\omega)$$

$$\left.\frac{d^2\sigma}{d\Omega dE'}\right|_{inelastic} = \frac{\sigma}{2k_B T}\sqrt{\frac{E'}{E}}S_s(\alpha,\beta)$$

$\beta = \frac{E - E'}{k_B T}$ Energy transfer

$\alpha = \frac{(E + E' - 2\sqrt{EE'}\cos\theta)}{k_B T}$ Momentum transfer

The scattering law (TSL) is the Fourier transform of a Gaussian correlation function

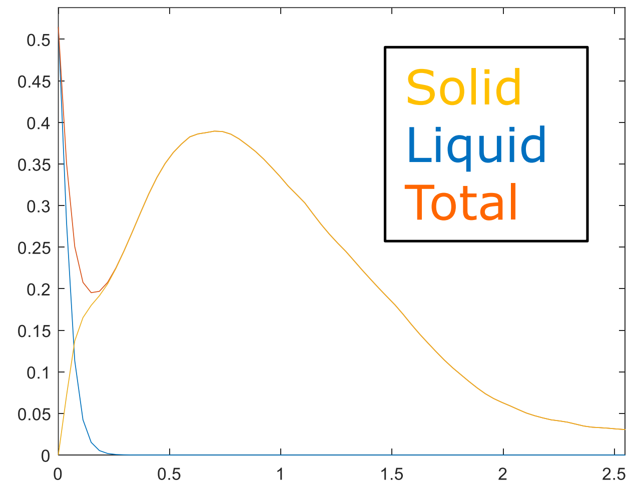
$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\beta t} e^{-\gamma(t)} dt$$

$$\gamma(t) = \frac{\alpha}{2}\int_{-\infty}^{\infty} \frac{\rho(\beta)}{\beta \sinh(\beta/2)}\left[1 - e^{-i\beta t}\right] e^{\beta/2} d\beta$$

$\rho(\beta)$ – density of states (e.g., phonon frequency distribution)

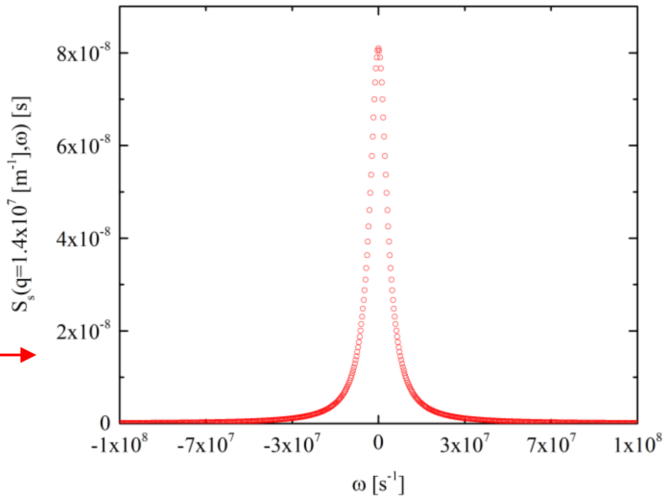
Thermalization in Liquids

- **Separation** of the diffusive DOS from the continuous (solid) DOS



- **Convolution** of the solid like and liquid TSL components

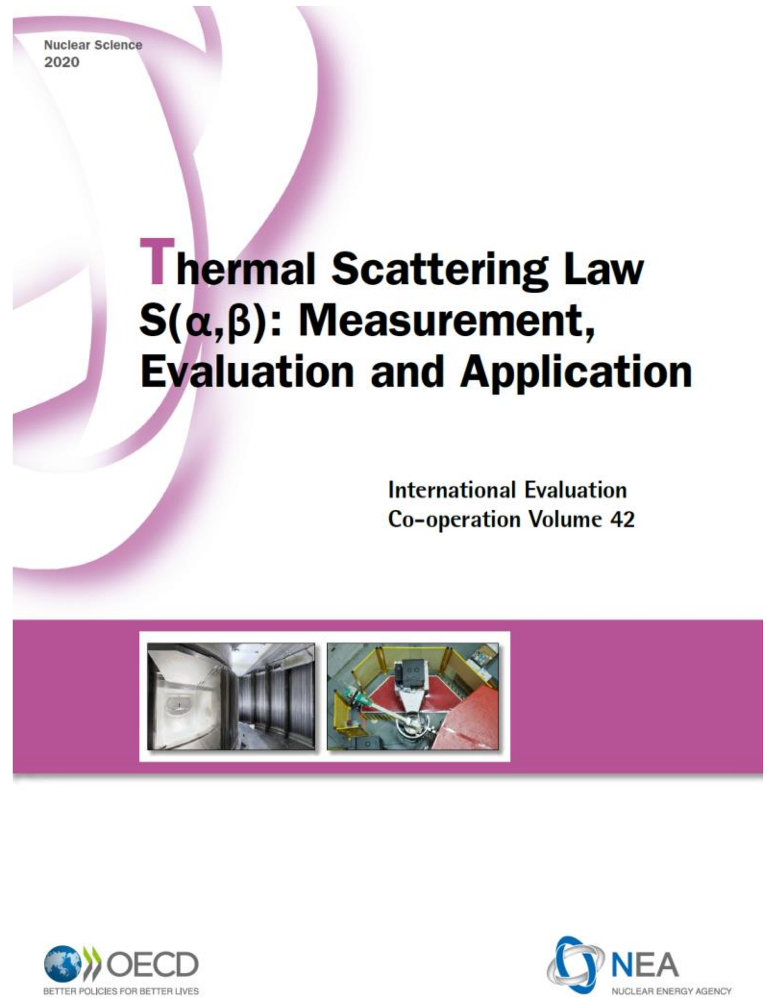
$$S_{total}(\alpha,\beta) = \left(S_{diff.}(\alpha,\beta) * S_{cont.}(\alpha,\beta)\right)$$



NEA
Nuclear Energy Agency

WPEC Subgroup 42

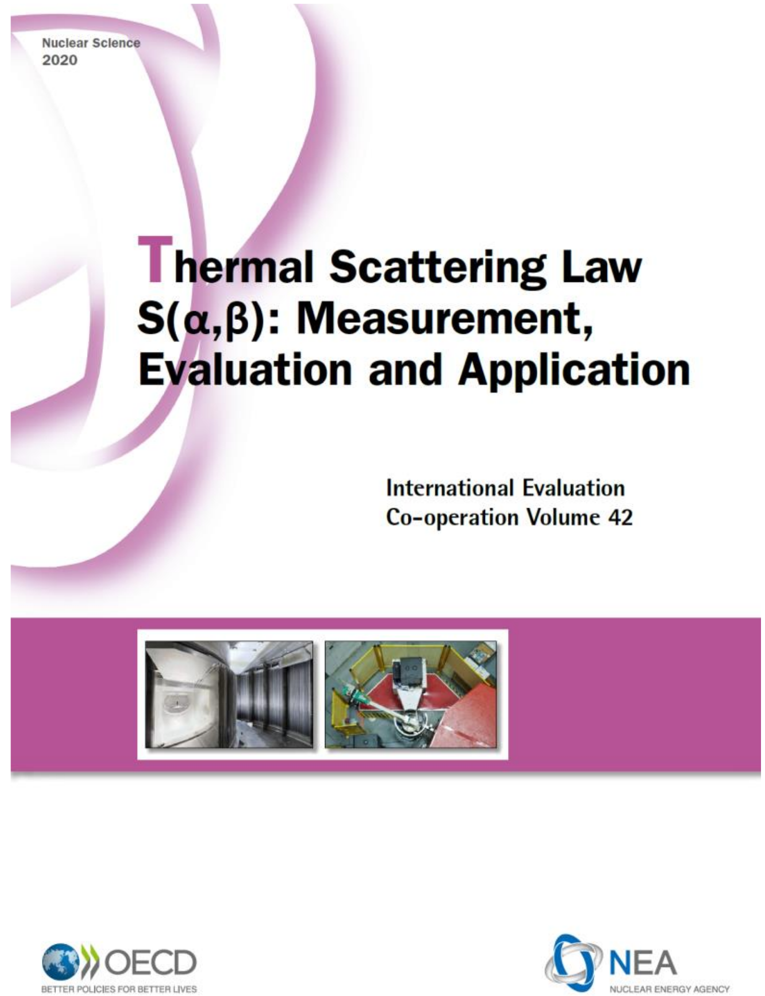
- Kick-off in May 2015 during WPEC meeting
- Operated during 2016 – 2018
- Final report developed during 2018 – 2019 and issued 2020



NEA
Nuclear Energy Agency

WPEC Subgroup 42

Table of contents



SG42 TSL Evaluations

⇒ **Largest historical contribution of TSL evaluations**
⇒ **More than 50% are first-of-a-kind evaluations**

Table 4.1. **New and updated TSL libraries in the ENDF/B-VIII.0 and JEFF-3.3 releases contributed by NCSU, CAB, CNL and BAPL**

Material	Evaluation basis	Institution	Library
Beryllium metal	DFT/LD	NCSU	ENDF/B-VIII.0
Beryllium oxide (beryllium)	DFT/LD	NCSU	ENDF/B-VIII.0
Beryllium oxide (oxygen)	DFT/LD	NCSU	ENDF/B-VIII.0
Polymethyl methacrylate (Lucite)	MD	NCSU	ENDF/B-VIII.0
Polyethylene (hydrogen)	MD	NCSU	ENDF/B-VIII.0
Crystalline graphite	MD	NCSU	ENDF/B-VIII.0
Reactor graphite (10% porosity)	MD	NCSU	ENDF/B-VIII.0
Reactor graphite (30% porosity)	MD	NCSU	ENDF/B-VIII.0
Silicon carbide (silicon)	DFT/LD	NCSU	ENDF/B-VIII.0
Silicon carbide (carbon)	DFT/LD	NCSU	ENDF/B-VIII.0
Silicon dioxide (alpha phase)	DFT/LD	NCSU	ENDF/B-VIII.0
Silicon dioxide (beta phase)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium dioxide (oxygen)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium dioxide (uranium)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium nitride (nitrogen)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium nitride (uranium)	DFT/LD	NCSU	ENDF/B-VIII.0
Light water ice I_h (hydrogen)	DFT/LD	BAPL	ENDF/B-VIII.0
Light water ice I_h (oxygen)	DFT/LD	BAPL	ENDF/B-VIII.0
Yttrium hydride (hydrogen)	DFT/LD	BAPL	ENDF/B-VIII.0
Yttrium hydride (yttrium)	DFT/LD	BAPL	ENDF/B-VIII.0
Light water (hydrogen)	Exp. data/MD	CAB, CNL	ENDF/B-VIII.0
Heavy water (deuterium)	Exp. data/MD	CAB, CNL	ENDF/B-VIII.0, JEFF-3.3
Heavy water (oxygen)	Exp. data/MD	CAB, CNL	ENDF/B-VIII.0, JEFF-3.3
Sapphire (aluminium)	Exp. data/Debye model	CAB	JEFF-3.3
Sapphire (oxygen)	Exp. data/Debye model	CAB	JEFF-3.3
Ortho-deuterium	Exp. data	CAB	JEFF-3.3
Para-deuterium	Exp. data	CAB	JEFF-3.3
Light water ice I_h (hydrogen)	Exp. data	CAB	JEFF-3.3
Mesitylene Ph. II (hydrogen)	Exp. data	CAB	JEFF-3.3
Ortho-hydrogen	Exp. data	CAB	JEFF-3.3
Para-hydrogen	Exp. data	CAB	JEFF-3.3
Toluene Ph. II (hydrogen)	Exp. data	CAB	JEFF-3.3
Silicon	Exp. data/Debye model	CAB	JEFF-3.3

Notes: NCSU – North Carolina State University; CAB – Centro Atómico Bariloche; CNL – Canadian Nuclear Laboratories; BAPL – Bettis Atomic Power Laboratory; DFT – density functional theory; LD – Lattice dynamics; MD – Molecular dynamics; ENDF – Evaluated Nuclear Data File; JEFF – Joint Evaluated Fission and Fusion File.

JEFF-3.3 Thermal Scattering Law (TSL) sublibrary

The **JEFF-3.3 thermal neutron scattering sublibrary** contains 20 evaluations for 16 materials. Notably, the evaluation for heavy water is updated and now has components for deuterium and oxygen bound in heavy water. Nine new materials (sapphire- Al_2O_3, silicon, mesitylene, toluene, ortho- and para- hydrogen, ortho- and para-deuterium, and light water ice) have been included in this release. The remaining evaluations are carried forward from JEFF-3.2.

The origin of the new or updated JEFF-3.3 TSL evaluations is summarized below.

Thermal scattering libraries included in JEFF 3.3.

SG42 recommendations

- **Support the development of open source tools for thermal scattering data evaluation and processing**
- **Strengthen the collaboration with the neutron science and advanced neutron source communities**
- **Support the data collection effort in the relevant databases**
- **Identify benchmark experiments that most appropriate for supporting the TSL evaluation process**
- **Converge on a modern format for TSL data in consultation with the GNDS effort**
- **Study the accuracy requirements for TSL evaluations, data processing and utilization**

Consequently, during the last session of SG42, the participants unanimously recommended the start of a follow-up subgroup to continue the coordination of the international effort in TSL development and evaluation. This recommendation was also supported by entire WPEC body in the meeting held on May 20, 2018.

OECD/NEA WPEC Subgroup 48
Kickoff May 13, 2020

NEA
Nuclear Energy Agency

Advances in Thermal Scattering Law Analysis

Continued growth in the area of thermal neutron scattering data motivates the formation of a new subgroup within the WPEC nuclear data collaboration

- ⇒ **Motivate the TSL evaluation effort in support of various nuclear science and engineering applications**
  - ⇒ **Advanced reactors (e.g., various molten salts)**
  - ⇒ **Criticality safety (e.g., various U and Pu based fuels)**
  - ⇒ **Neutron science (e.g., cryogenic moderators)**

- ⇒ **Review the development of advanced TSL evaluation methods and tools with consideration of modern simulation approaches**

- ⇒ **Address issues related to data validation, covariance generation, and data formats, …**

- ⇒ **Act as the focal point with other WPEC subgroups (SG44, SG45, GNDS, etc.)**

OECD/NEA WPEC Subgroup 48
Kickoff May 13, 2020

NEA
Nuclear Energy Agency

Advances in Thermal Scattering Law Analysis

<u>**Time-Schedule and Deliverables**</u>

During the 3-year period, discussion of new and upcoming TSL evaluations, that are being considered for release into the databases (ENDF, JEFF, etc.), will continue. Coordination with other WPEC subgroups will be ongoing.

In addition, the following deliverables will be pursued

- ⇒ **2020-2021: Review and documentation of advances in TSL evaluation methods and tools. Consideration will be given to emerging modern nuclear science and technology analysis modalities.**
- ⇒ **2021-2022: Review and documentation of TSL data validation, uncertainties, and formats.**
- ⇒ **2022-2023: Summary and formulation of the SG findings, conclusions and recommendations.**

In Memoriam

Margarete Mattes (1940-2020)

The sad news reached us that Margarete Mattes, physicist, retired from IKE Stuttgart, Germany, passed away on 2. April 2020.

Margarete has participated for almost 30 years in the JEFF meetings and has contributed a substantial amount of work to improving and to validating this Joint Evaluated Fission-Fusion file.

It started in 1983, when she and her team contributed the first thermal scattering law data for JEF. Originally JEF had been conceived and developed for the needs of joint European fast reactor projects, in particular because the ENDF/B-V data were not available outside the USA.

She had insisted from the start that producing evaluated nuclear data files exclusively for fast reactor applications was shortsighted and that such data must cover comprehensively the needs of nuclear applications. Later, she and her team contributed additionally to thermal scattering law data also data required for studies in low temperature media, another important area of nuclear research. Not only, she also provided modifications to the processing codes so that scattering law data could be processed over the full temperature range, from cryogenic to epithermal temperatures. Another substantial part of her contributions covers the validation of JEFF data using experimental integral data benchmarks and full size reactor configurations. She produced data libraries needed for deterministic, Monte Carlo and hybrid methods. She has contributed a large number of presentations and documents at JEFF meeting. Her name appears in more than 300 such documents. She is the author of the second official JEFF Report. In Germany she was considered as one of the best experts of her times in nuclear data.

Margarete was known for her professional competence, high quality work, for her kindness, friendliness and availability for cooperation.

NJOY User Group
Meeting 1989
Data Bank Saclay

May she rest in peace.

Enrico Sartori

Questions
&
Discussion