

Nuclear data needed to develop new nuclear systems, role of n\_TOF facilities to measure resonance cross-sections and nuclear data needs of thorium fuel cycle

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**World context:**

**Preliminary research for the Energy Amplifier concept proposed by Carlo Rubbia and others in the world use existing nuclear data developed for thermal, fast and fusion reactors and those generated towards fundamental physics understanding of the nucleus and applications such as in astrophysics.**

**•The quality assurance in design and safety studies in nuclear energy in the next few decades and centuries require new and improved nuclear data with high accuracy and energy resolution that is possible only with the facilities such as the CERN n\_TOF.**

**•Carefully planned measurements with facilities such as n\_TOF are essential as the existing strength of the state-of-the-art nuclear databases in use for various applications is highly commendable but inadequate to meet the nuclear data needs of new reactor concepts as different neutron energy spectra and materials and compositions are involved.**

**India recognizes the need for reliable nuclear data for all evaluations for several hundreds of isotopes/elements in all stages of the nuclear fuel cycle.**

**BARC has signed LOI with CERN on n\_TOF collaboration for 2006-2011.**

**The Indian participation in the n\_TOF programmes stands to benefit not only in her ADSS studies for thorium utilization but also because there is a considerable overlap between the Advanced Heavy Water Reactor (AHWR) and Compact High Temperature Reactor (CHTR) Indian programmes with respect to thorium as a fuel and the on-going international efforts to develop innovative, inherently safe, proliferation-resistant and long-life-cores, with features using thorium such as in INPRO and Generation IV**

The role of n\_TOF measurements to meet the demands on accurate nuclear data in the extended resolved resonance region that affect plant safety related feedback coefficients such as Doppler and coolant void reactivity effects as a function of burn-up for advanced systems are high.

The experimental validation efforts in critical facilities can never exactly verify the simulated states of higher burn-up.

Improved nuclear data are therefore essential for fission products and minor actinides in developing advanced reactor systems, such as actinide burner systems and to reduce the number of costly integral experiments.

As a remark, the existing data of U-Pu cycle also needs improvement for long burnup cores.

**Reliable design and operator's manual for each stage of the nuclear fuel cycle based upon accurate knowledge of nuclear data will help in safe use of nuclear energy by providing proper guidance on safety precautions and behaviour under all system conditions.**

**For multiple recycled fuel, the quality of nuclear data of higher isotopes of plutonium, minor actinides (isotopes of Am and Cm) and fission products need to be brought on par to that of main fissile and fertile nuclei. The demands on accurate nuclear data in the resonance region that affect plant safety related feedback coefficients such as Doppler and coolant void reactivity effects as a function of burnup for advanced systems are high.**

# **BETTER NUCLEAR DATA**

## **For safe operation of existing reactors: A practical example**

Recently, an incident involving power rise took place in KAPS, Unit 1. Nat- UO<sub>2</sub>, D<sub>2</sub>O, PHWR 220 MWe unit. A recent public release dated April 22, 2004 by the Atomic Energy Regulatory Board provides the details of this incident.

**[www.aerb.gov.in/prsrel/prsrel.asp](http://www.aerb.gov.in/prsrel/prsrel.asp)**

**On March 10, 2004, KAPS-1 experienced an incident involving incapacitation of reactor regulating system, leading to an unintended rise in reactor power from 73%FP to near 100%FP, with trip occurring on Steam Generator DELTA T High Level 2 on INES Scale.**



The slow rise overpower transient could not be explained by the Design manual.

Now we find that the fuel temperature coefficient (FTC) calculated by the new 69-group “iaea.lib” library gives significantly different results at higher burn-ups and explains as a preliminary observation the unexpected power rise that occurred in the KAPS-1 unit.

The FTC is due to the combined effect of Doppler effect and fuel re-thermalization effect.

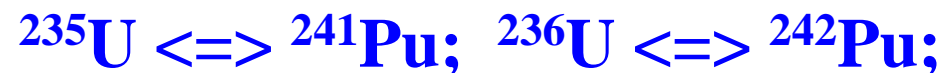
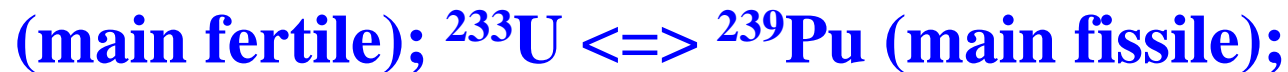
In a Pressurized Heavy Water Reactor, the precise cross-over point in burnup where the FTC becomes positive depends on many parameters such as the temperature range and 19 versus 37 rod cluster.

The 27 group wims1981 library has a cross over point, for FTC at about 12000MWD/Te burnup; at about 9400MWD with the same but 69-group library, at about 6000MWD for a 19 rod cluster with the new “iaea.lib” library and at about 4500MWD for 37 rod cluster of PHWR with the “iaea.lib” library.

Actually the cross over point of the FTC is not just the issue but how negative it should be to overcome the xenon kill feedback that is positive whenever power transient occurs. We have also observed that the calculated coolant void reactivity using the new “iaea.lib” library is lower than the earlier results obtained using the 1971 library. The KAPS-1 overpower transient could be explained only with the use of new WLUP libraries.

The status of nuclear data of the major and minor isotopes in the thorium fuel cycle needs to be brought at least to the present level of quality that exists for the isotopes in U-Pu Cycle.

The rough equivalence of the isotopes



**GENERIC ISSUES**

**IN BASIC DATA**

## Measuring nuclear data accurately is challenging and involves **CUTTING EDGE TECHNOLOGY**

$$\text{Reaction Rate response} = \int \Sigma(E) \phi(E) dE$$

The cross section at energy  $E_0$ ,  $\sigma(E_0)$ , is then obtained as the response quantity:

$$\sigma(E_0) = \frac{1}{N} \int \Sigma(E) \delta(E - E_0) dE$$

In order to determine the cross section at a given energy, we need to obtain the response function using mono-energetic neutron source. We then require mono-energetic neutron source of sufficient intensity, pure samples of sufficient number of atoms and efficient detector systems. The analyses part is also quite complex due to thickness of the sample, neutron beam profile, energy and detector resolutions, spatial non-homogeneities in the target sample and several corrections, such as, due to temperature and impurities.

- As a general rule, the generation of new nuclear data by the international community should continue to be encouraged as

- more intense neutron sources,**
- purier elemental/isotopic target samples,**
- more efficient detectors and better electronics**

evolve.

- Required scientific activities also are extensive follow up of experimental data generation with a comprehensive compilation, critical evaluation, production of new ENDF/B formatted libraries extending to higher energies, and quality assured nuclear data processing activities to provide the designers/users/ of innovative systems with “ready to plug-in” processed data, that are integrally validated, for use in applications.

$$\eta = v \sigma_f / \sigma_a$$

Achievable “Best” accuracy with state-of-art

$$v \quad 0.5\%$$

$$\sigma_f \quad 2-3\%$$

$$\sigma_a \quad 2-6\%$$

Depends on energy region

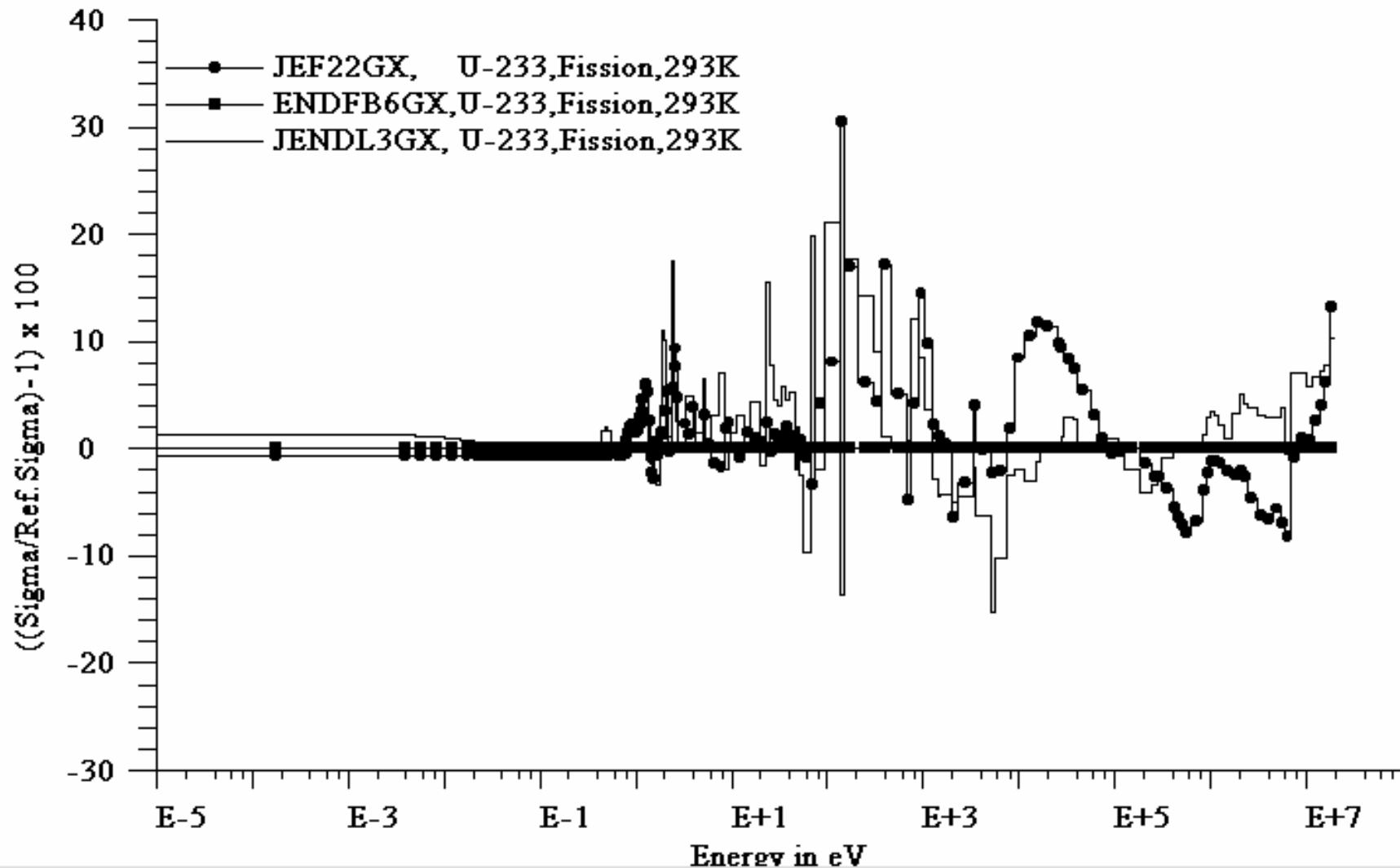
For 1mk (0.001) in K-infinity we require less than

0.1% This is the “desirable” accuracy!!!

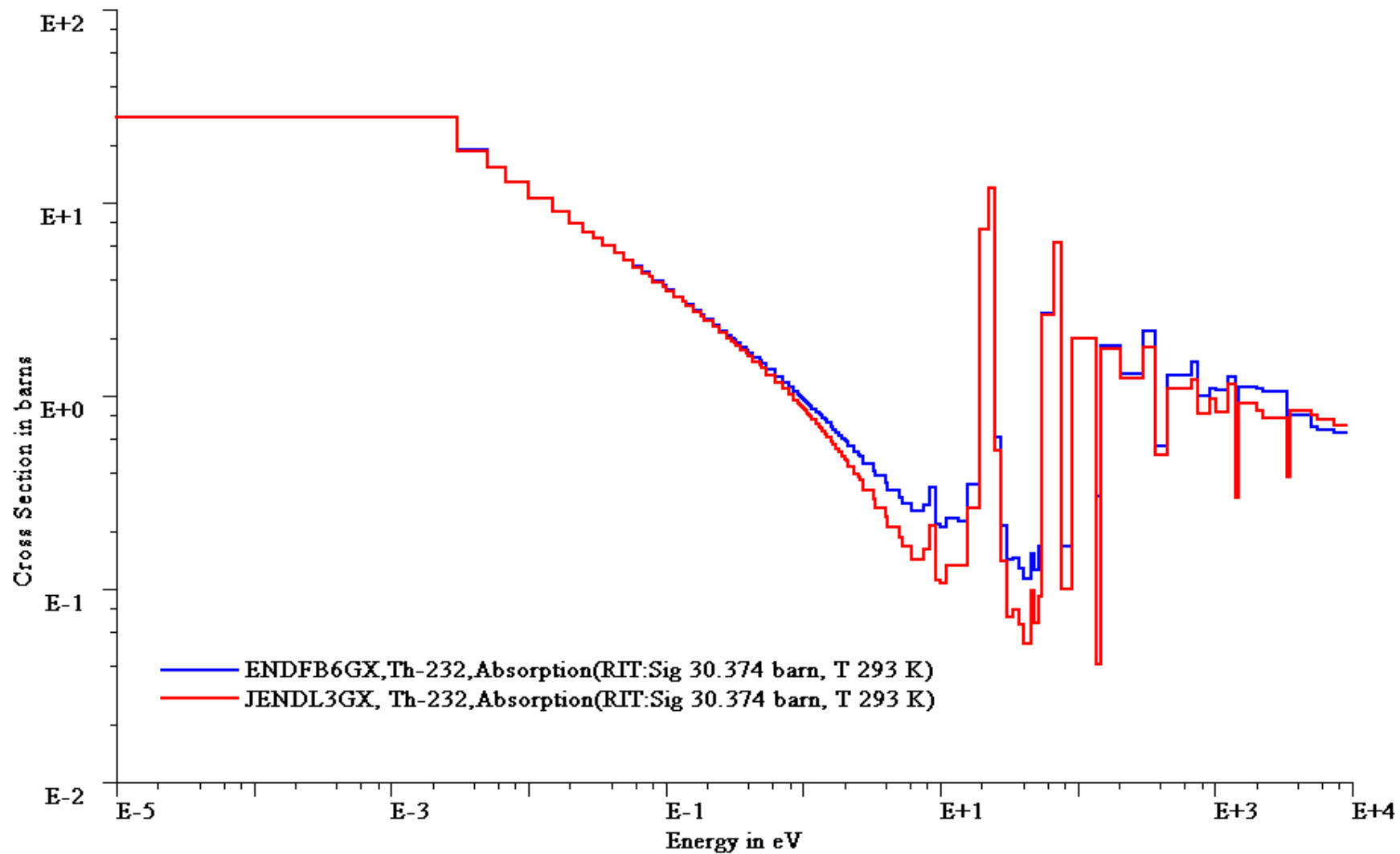
Achievable accuracy : State of art.



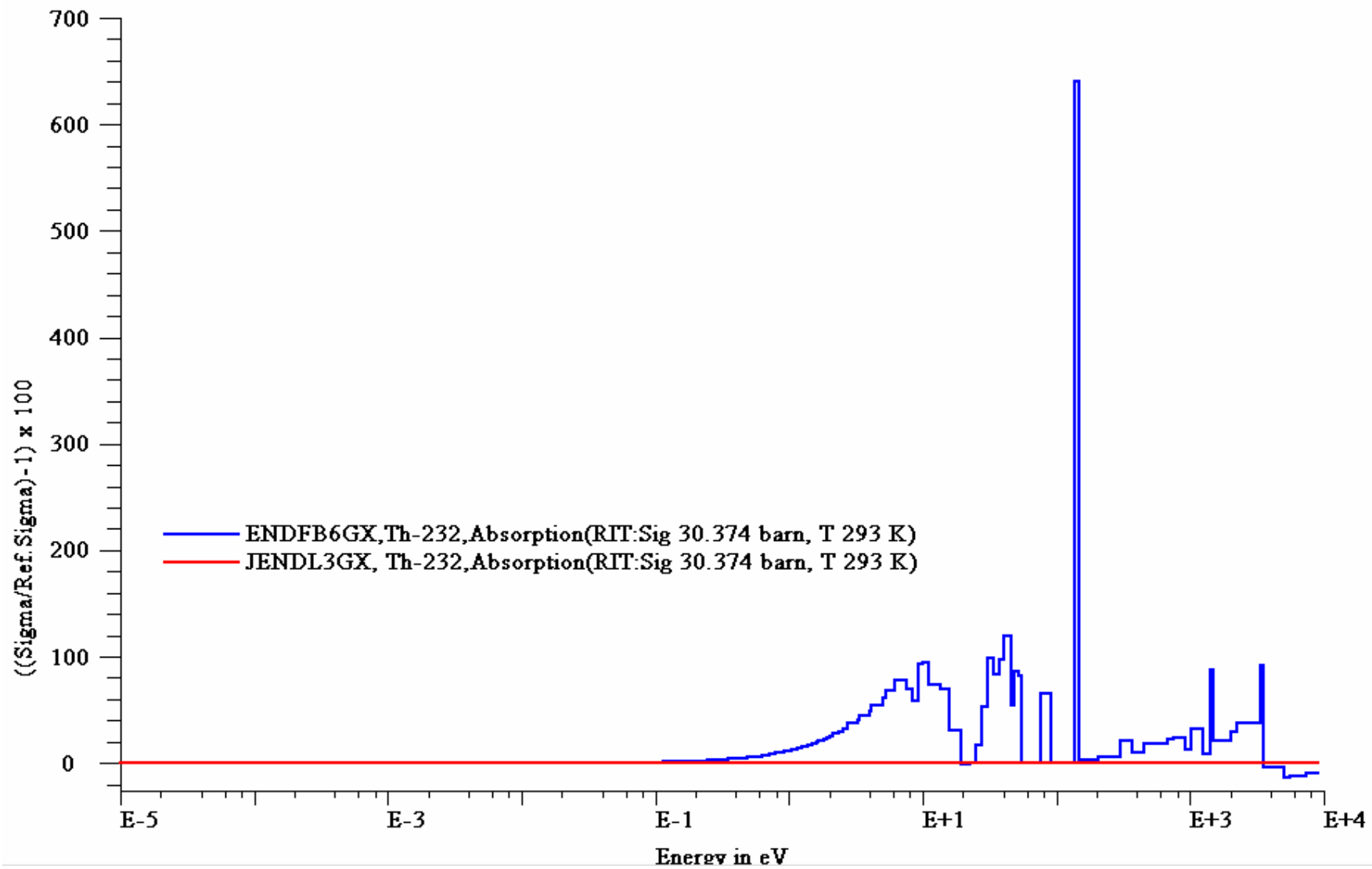
**EXAMPLES OF  
DISCREPANCIES  
THORIUM FUEL  
CYCLE**



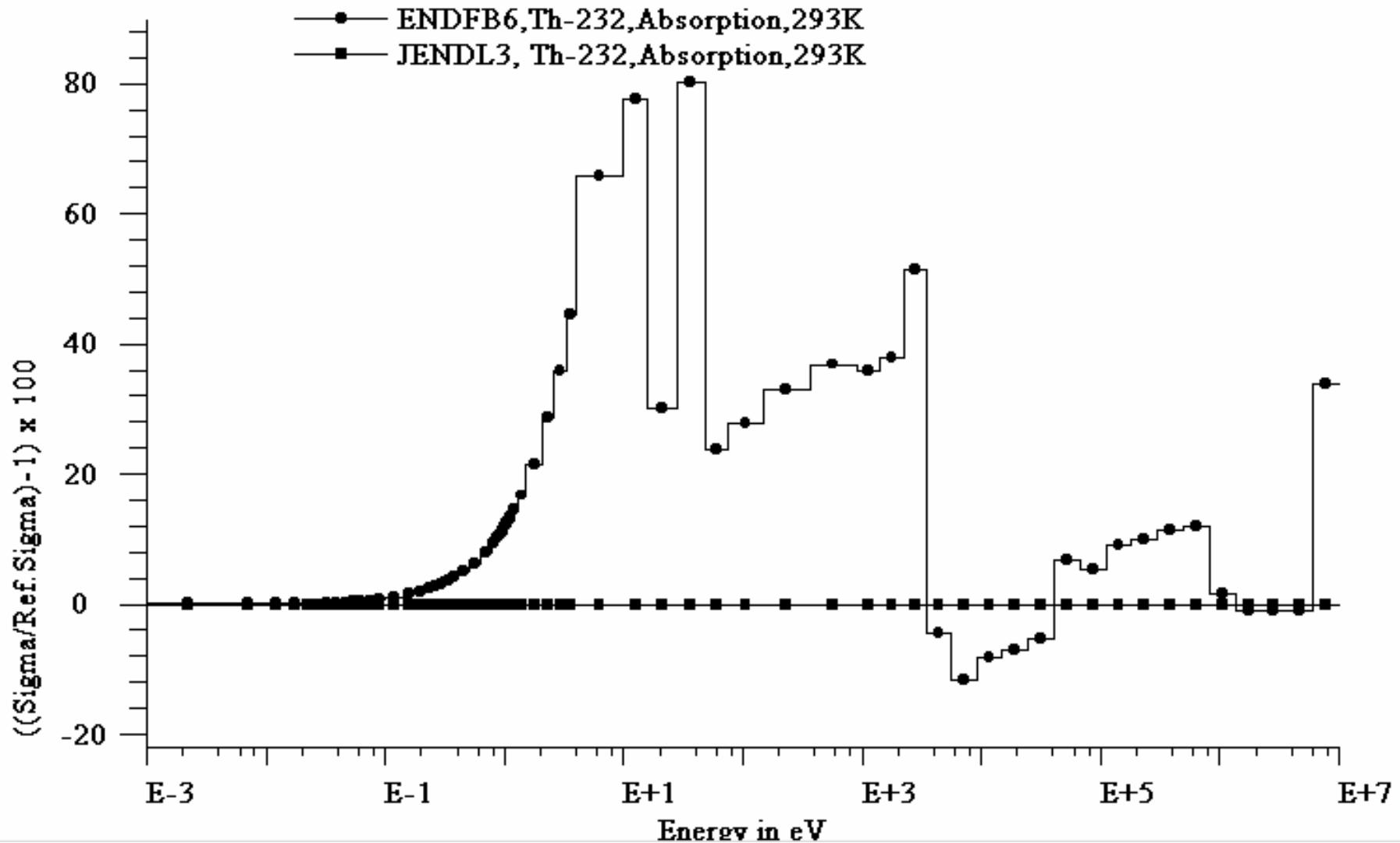
**Comparison of fission cross sections of  $^{233}\text{U}$  in 172 groups. The large discrepancies seen are far beyond the target of 1% accuracy. Example of the need for n\_TOF to reduce discrepancies in resonance region**



**Large discrepancies in the resonance shielded cross sections. Next slide shows the ratio for clarity.**



**An accuracy of 1% is desirable**



**Comparison of WIMS-D absorption cross sections of  $^{232}\text{Th}$  in 69 groups. The large discrepancies seen in self-shielded cross sections are far beyond the target of 1 % accuracy.**

# Comparison of fission cross sections of $^{233}\text{U}$ derived from JENDL-3.2 and ENDF/B-VI (Rev. 5) Files

## DESCRIPTION

## DISCREPANCY

Zero Kelvin

−89.60 to 1495%

296 K

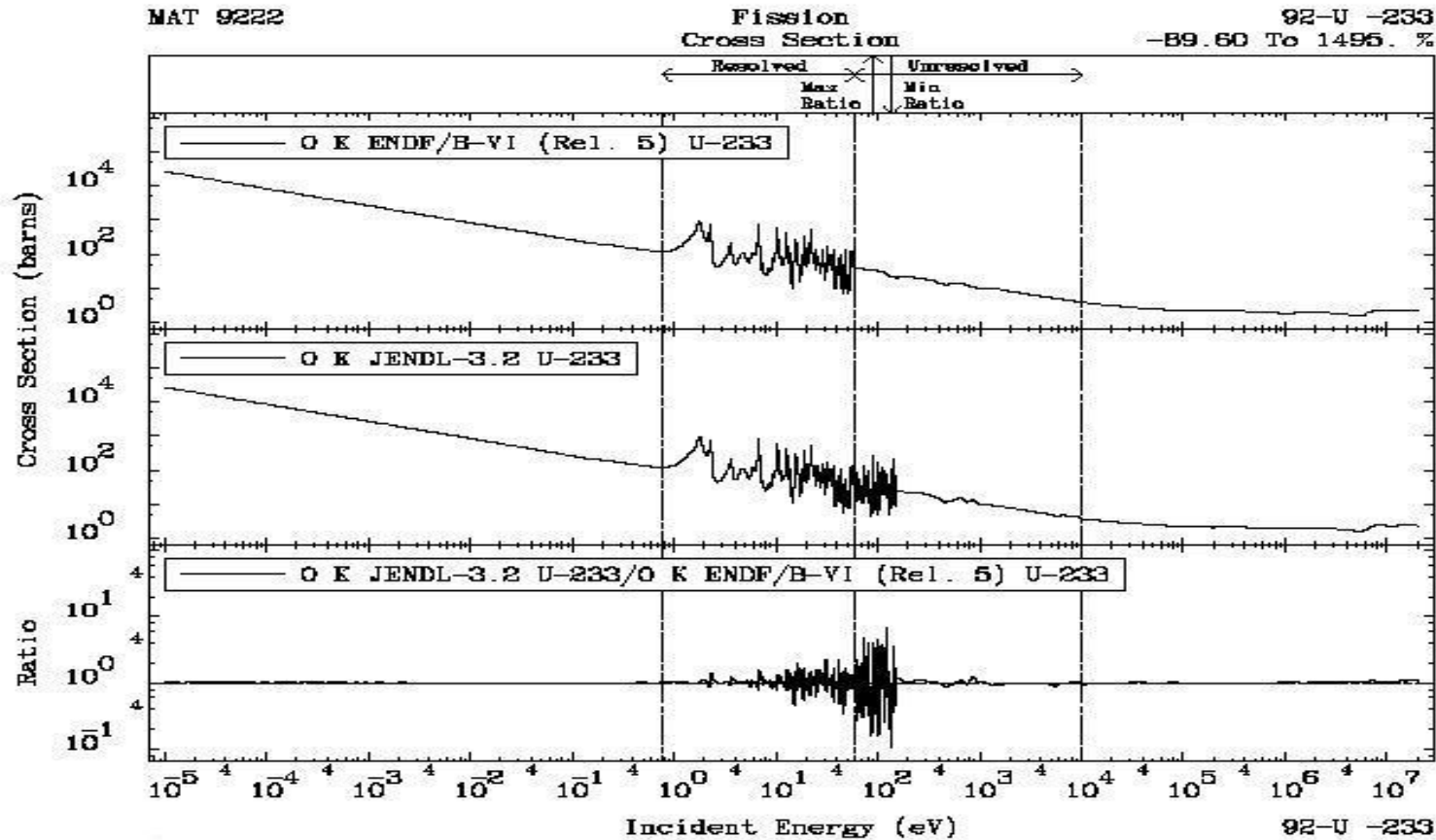
−88.44 to 597.9%

175 groups

−63.34 to 97.35%.

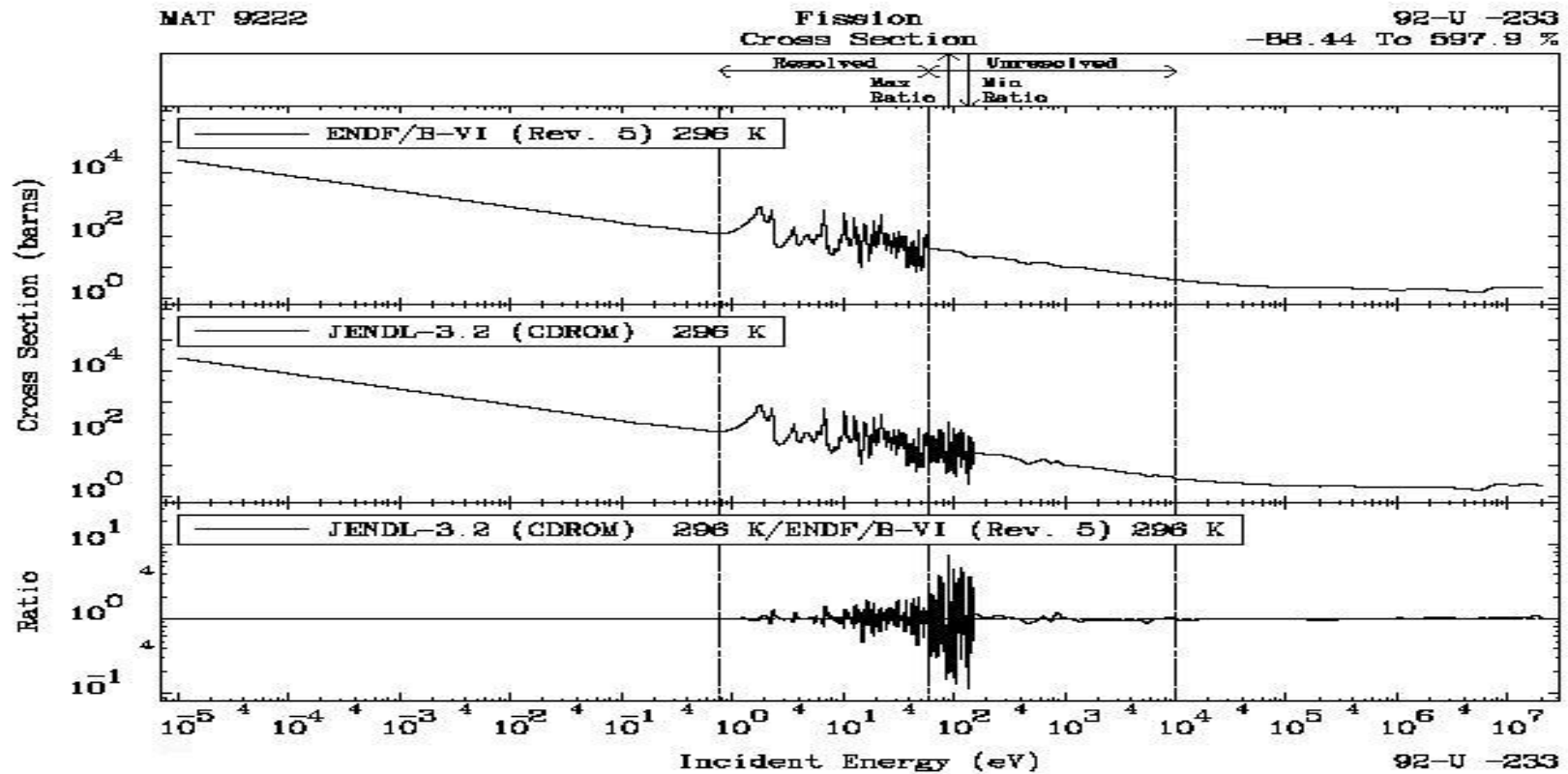
69 Groups

−4.735 to 8.470%.



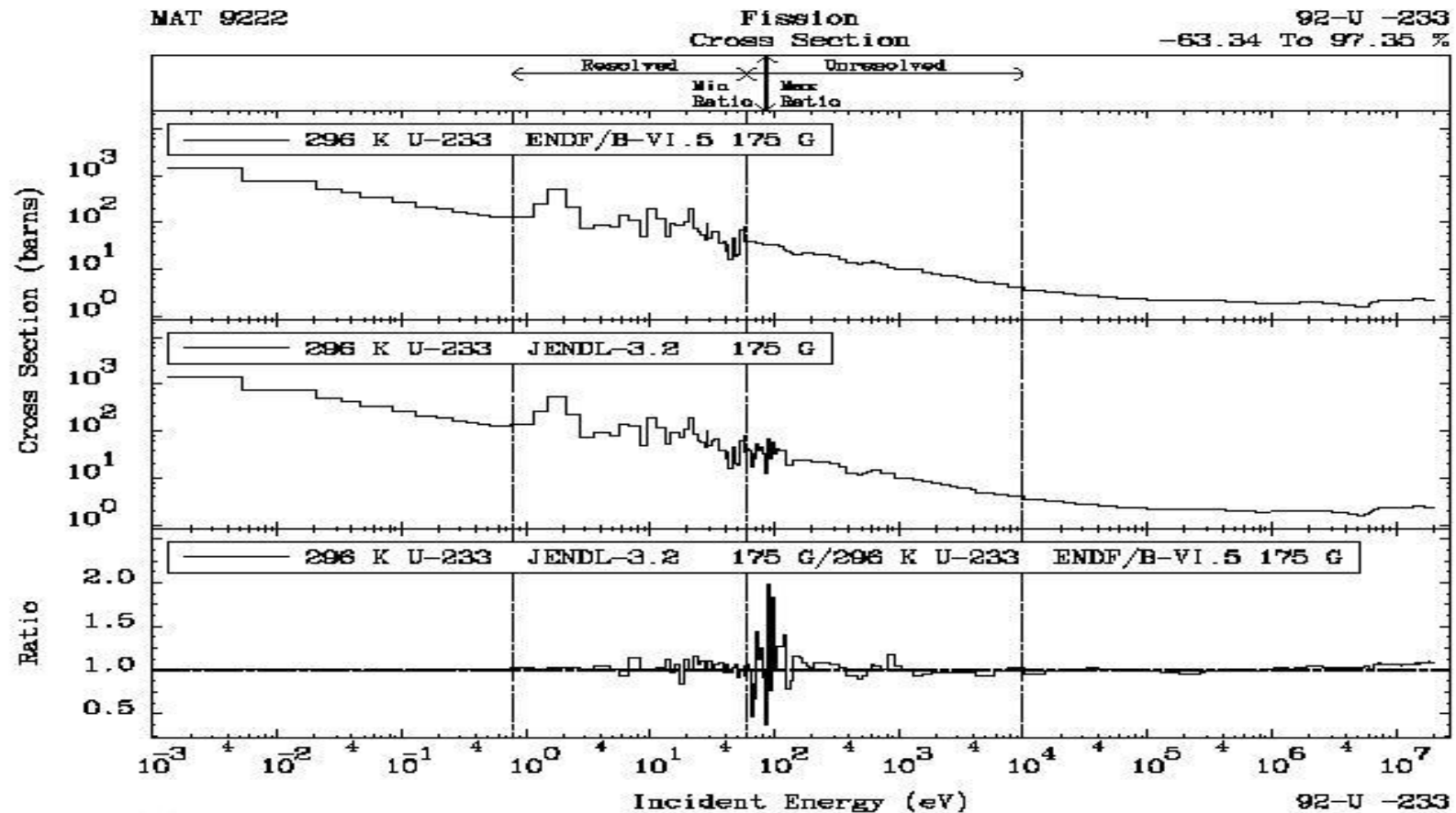
Resonance-reconstructed point fission cross-sections of  $^{233}\text{U}$  at zero $^{\circ}$  K. Derived from JENDL-3.2 and ENDF/B-VI (Rev. 5) using the LINEAR/RECENT/COMPLIT codes of the PREPRO system.

A reconstruction tolerance of 0.1 was used in LINEAR and in RECENT. Zoomed portions of this plot are therefore presented in Figs. 6 to 11 of the text.

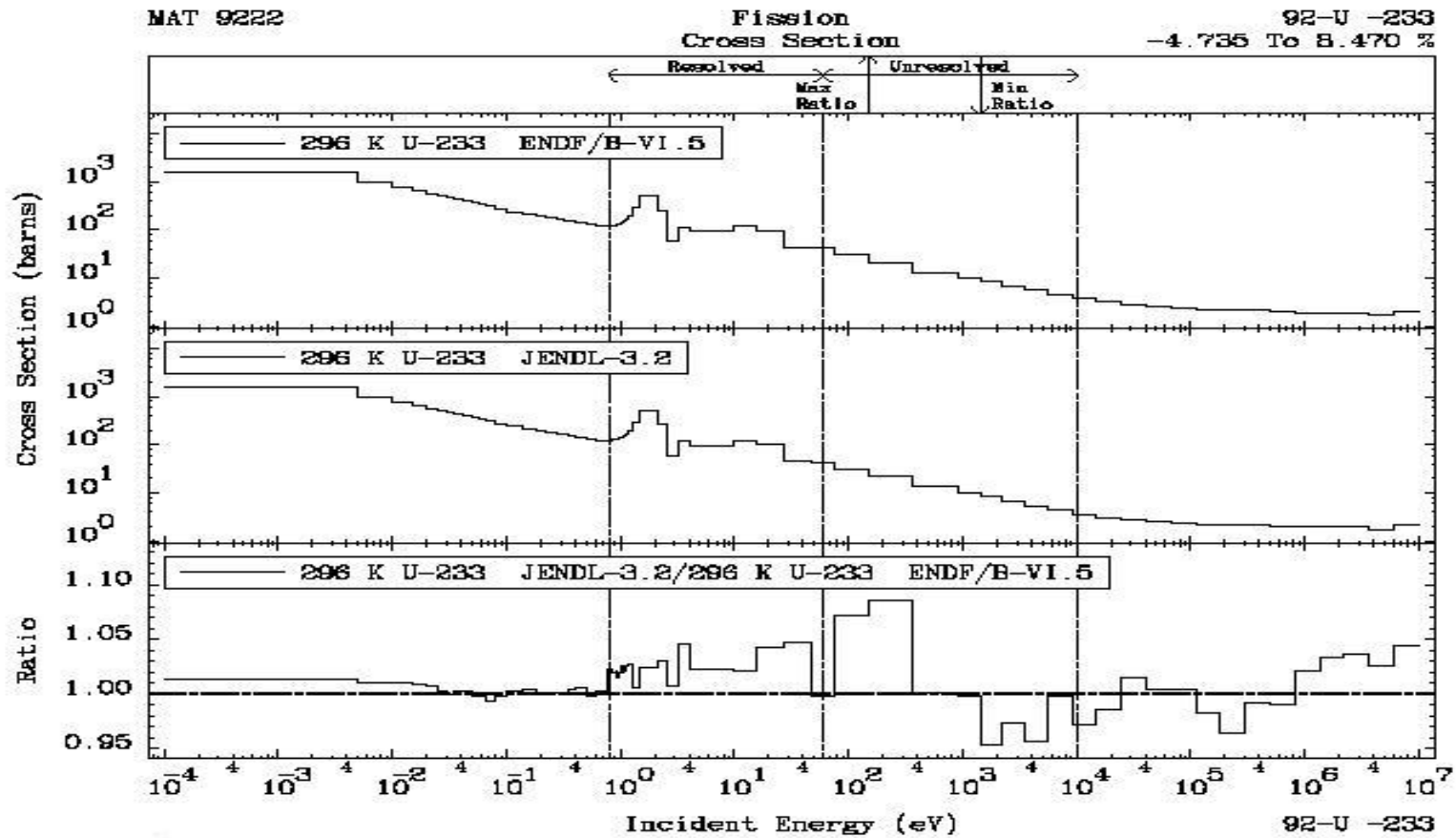


Point fission cross sections of  $^{233}\text{U}$  at  $296^\circ$  Kelvin. Obtained by Doppler broadening the line shapes of Fig. 1 using the SIGMA1 code. Note that, as compared to Fig. 1, the effect of Doppler broadening results in reducing the values of fission cross section at the resonance peaks and increasing the values at the wings of the resonances. The spread of discrepancy between the two data files JENDL-3.2 and ENDF/B-VI.5 for the fission cross section of  $^{233}\text{U}$  is reduced to  $-88.44$  to  $597.9\%$  as compared to the value of  $89.6$  to  $1494\%$  seen in Fig. 1.





The “point” fission cross sections at 296° K were multi-grouped using the GROUPIE code of the PREPRO system into 175 values in the TART175 group energy structure. Note that as result of some cancellation of discrepancies that are seen in the positive and negative sides in Fig. 2, the discrepancies in the 175 broad groups are now –63.34 to 97.35%.

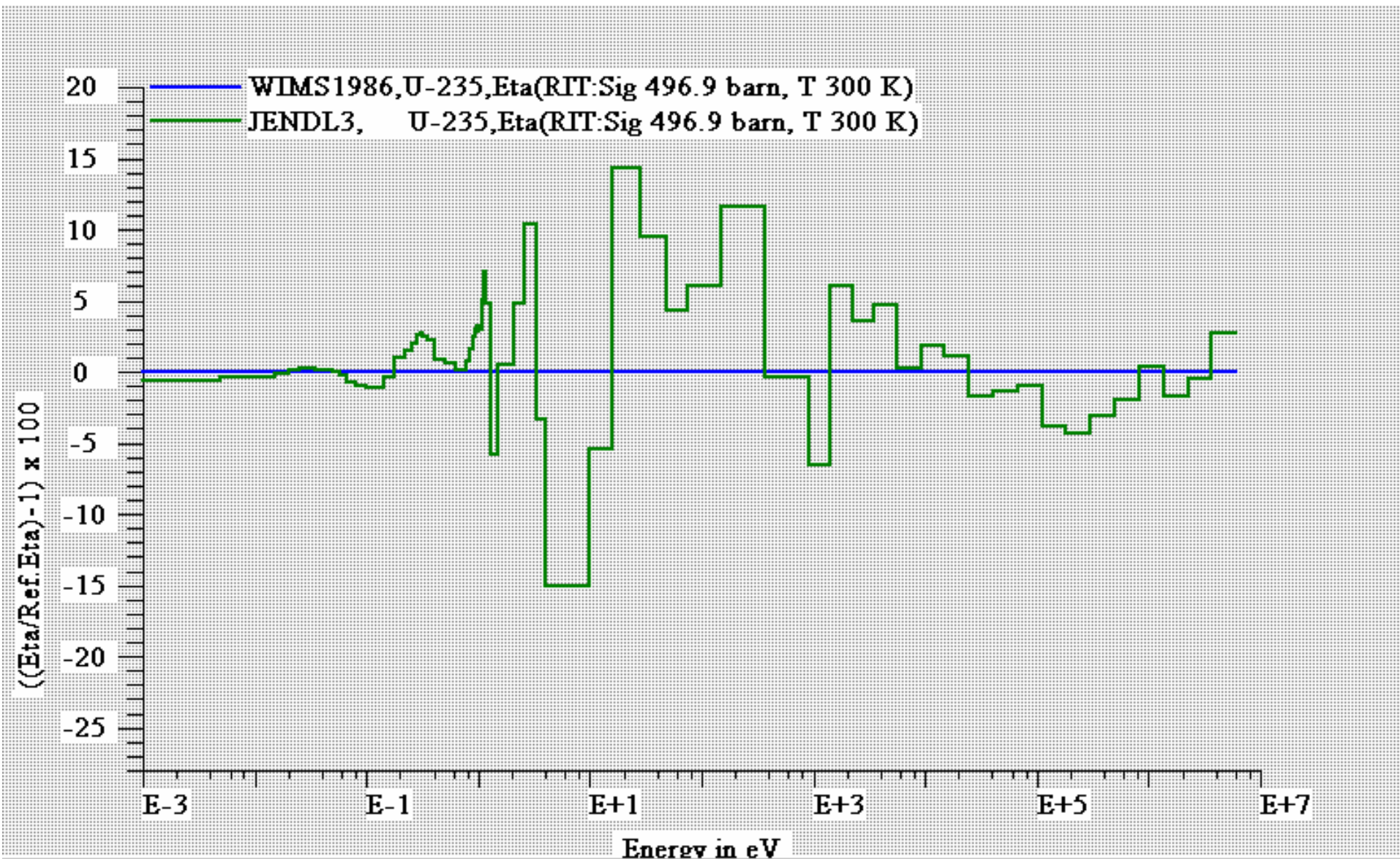


The “point” fission cross sections at 296° K were multi-grouped using the GROUPIE code of the PREPRO system into 69 values in the WIMS69 group energy structure. Note that as result of significant “within-group” cancellation of discrepancies that are seen in the positive and negative sides in Fig. 2, the discrepancies in the 69 broad groups are now in the range  $-4.735$  to  $8.470\%$ . Note the good agreement at thermal energies.

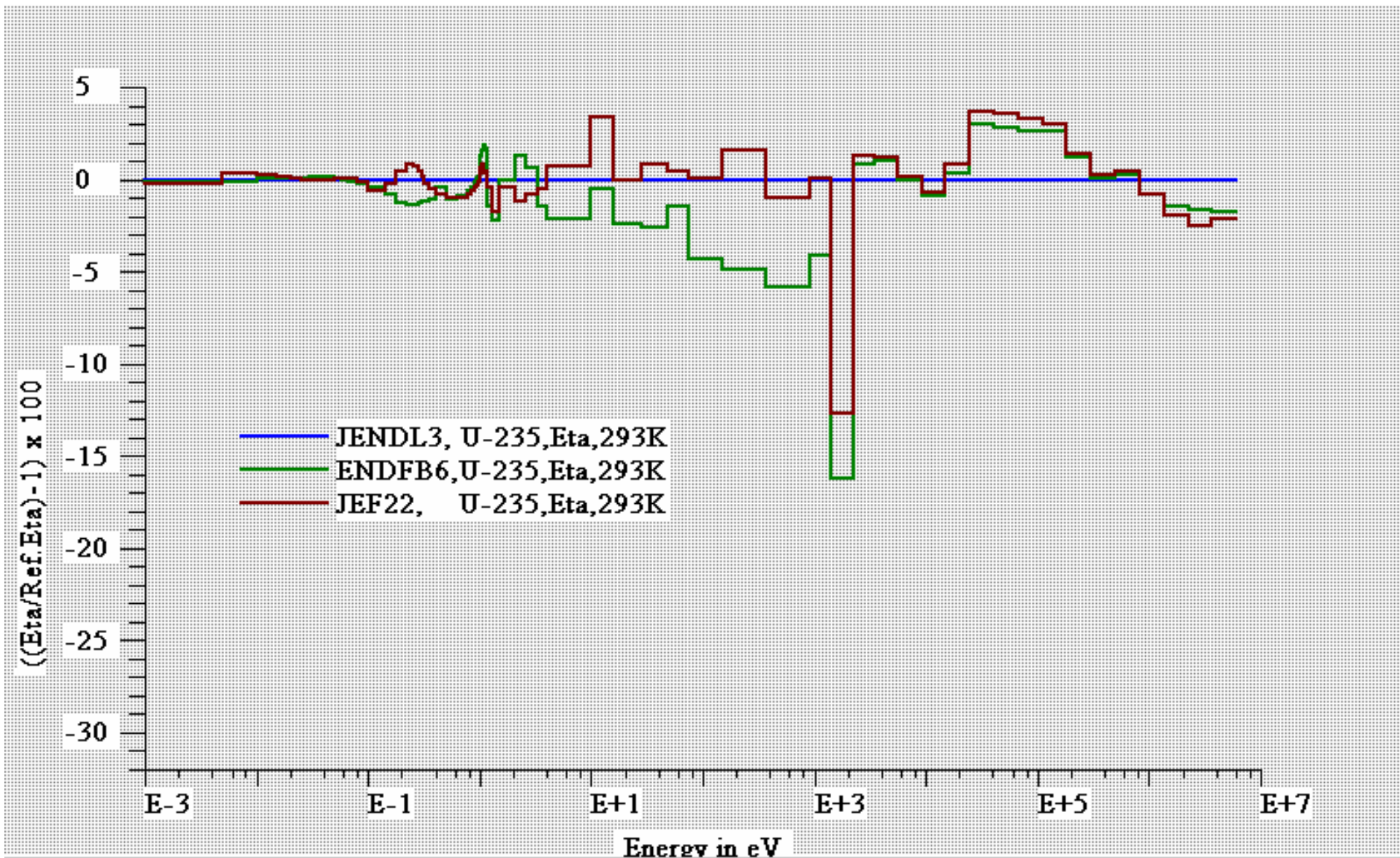
# ENERGY RANGES OF RESOLVED AND UNRESOLVED RESONANCE REGIONS.

Isotope	Upper limit of the resolved resonance range		Upper limit of the unresolved resonance range	
	ENDF/B-VI (Rev.5)	JENDL-3.2	ENDF/B-VI (Rev.5)	JENDL-3.2
$^{230}\text{Th}$	251eV	564.26eV	No parameters given	No parameters given
$^{232}\text{Th}$	4keV	3.5keV	50keV	50keV
$^{232}\text{U}$	53eV	200eV	1keV	No parameters given
$^{233}\text{U}$	60eV (> 600eV in – ENDF/B-VII) ND2004, ORNL	150eV	10keV	30keV
$^{234}\text{U}$	1.5keV	1.5keV	100keV	50keV
$^{231}\text{Pa}$	14.3eV	115eV	1keV	40keV
$^{233}\text{Pa}$	38.5eV	16.5eV	10keV	40keV

**An example of old and new  
data inter-comparison for U-  
235 eta**



**How has eta values of U-235 changed in the last 3 to 4 decades ?**



**How much discrepant is eta of U-235 among recent data evaluated data files?**



- The interesting results of large discrepancies obtained by the author in the calculated criticality properties of minor actinides, such as,  $^{241}\text{Am}$ ,  $^{243}\text{Am}$ ,  $^{231}\text{Pa}$ ,  $^{232}\text{U}$  and  $^{233}\text{Pa}$  shed light on the inadequacy of nuclear data of these minor actinides in the fast energy region.
- The minor actinides nuclear data are crucial also in international formulation of radioactive transport regulations. All these requirements demonstrate the immediate need for the research carried out in n\_TOF experiments.
- The new measurements of nuclear data such as those planned at CERN n\_TOF help to reduce the existing uncertainties in simulations studies of existing and advanced systems.

## An Example: Comparison of calculated $k_{\infty}$ , the infinite medium multiplication factor of $^{243}\text{Am}$ and critical mass

Data file used	$k_{\infty}$	Critical radius /mass	Remarks
ENDF/B-V	Not available	(14.0203) 157kg	MCNP4A Ref. 5
JENDL-3.2	1.44929± .00113	17.20/291kg	Present calculations
JEF-2.2	1.59128± .00116	15.45/210kg	Present calculations
ENDF/B-VI.6	1.68713± .00117	13.61/144kg	Present calculations
ENDF/B-IV	1.926	22.89cm / 596.24kg	Density used =11.87g/cc Refs. 6-9
	Not available	(31.71405cm) / 1824kg	SCALE4.3 code system Density=13.6g/cc. Ref. 5, Ref. 10
	1.11338± .00087	36cm / 2668.66kg	Present calculations
ANS STANDARD	Not available	(13.9cm) / 153kg	
ANS STANDARD	Not available	(9.823255cm)/ 54kg	



**RESOLUTION OF EXISTING  
DISCREPANCIES CAN BE  
RESOLVED ONLY BY NEW  
AND MORE ACCURATE  
BASIC NUCLEAR DATA  
EXPERIMENTS**

- **Nuclear power is an inevitable option for India**
- **National policy is to implement a closed fuel cycle programme involving multiple fuels.**
- **As multiple fuel cycles (e.g., U-Pu, Th-U), with the option of closing the fuel cycle are envisaged, the nuclear data requirements that are needed to develop the new systems with high burnup are demanding and include all the range of actinides and fission products for multiple fuels.**
- **There is considerable overlap between the Indian programme with respect to thorium as a fuel and the on-going international efforts to develop innovative, inherently safe, proliferation-resistant and long-life-cores, with features using thorium as in INPRO and Generation IV systems**

## **Indian Context:**

**Indian nuclear data activities generically encompass the user oriented approach starting from the basic evaluated nuclear data files distributed by the IAEA.**

**India is actively participating  
in the  
IAEA Co-ordinated Research  
Project on  
“Evaluated Data for the  
Thorium-Uranium fuel cycle”  
2003-2006**

# CREATION OF EXPERIMENTAL INDIAN BENCHMARKS

India has formally joined USDOE/NEADB Efforts since 2005 on creation of experimental benchmarks for international distribution. The two immediate tasks on hand this year are the following:

- 1. KAMINI (233U fueled) experimental criticality benchmark: Published in the International Criticality Safety Benchmark Evaluation Project of the US-DOE/NEA-DB: International quality description of the benchmark.**
- 2. Thorium Irradiation experiments and burnup measurements in PHWRs. A benchmark is under preparation.**

- The currently envisaged main new components, included in the Indian road map for Advanced Nuclear Power Systems, comprise the following:
  - Advanced Heavy Water Reactor (and other thorium fuelled reactor systems)
  - Advanced fuel cycle (front end and back end) facilities
  - Compact High Temperature Reactor
  - Accelerator Driven Systems
  - **A number of slides on the above Indian activities will also be shown subject to interest and availability of time to illustrate the use of improved nuclear data.**