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A Comparative Study of the COG Thermal Libraries

Edward M. Lent

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Auspices

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A Comparative Study of the COG Thermal Libraries

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This paper reports the results of a comparative study of the various libraries making up the COG thermal database.

Introduction

There are currently 15 thermal libraries in the COG database. Each library consists of several materials, each at one or more temperatures.

• **T.ENDFB3R0** (ENDF/B-III.0) - ENDF format - 10 materials
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (BeO), beryllium oxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K
- (C6H6), benzene @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (D.D2O), deuterium bound in heavy water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.CH2), hydrogen bound in polyethylene @ 296 and 350°K
- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (UO2), uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

• **T.ENDFB6R0** (ENDF/B-VI.0) – ENDF format – 8 materials
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (BeO), beryllium oxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K
- (D.D2O), deuterium bound in heavy water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.CH2), hydrogen bound in polyethylene @ 296 and 350°K
- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

• **T.ENDFB6R2** (ENDF/B-VI.2) – ENDF format – 6 materials
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (BeO), beryllium oxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K

- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

• **T.ENDFB7R0** (ENDF/B-VII.0) – ENDF format – 14 materials

- (Al), aluminum @ 20, 80, 293.6, 400, 600, and 800°K
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Be.BeO), beryllium bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K
- (C6H6), benzene @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (D.D2O), deuterium bound in heavy water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (Fe56), iron 56 @ 20, 80, 293.6, 400, 600, and 800°K
- (H.CH2), hydrogen bound in polyethylene @ 296 and 350°K
- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (O.BeO), oxygen bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (O.UO2), oxygen bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (U.UO2), uranium bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

• **T.ENDFB7R0.BNL** (ENDF/B-VII.0 Brookhaven National Laboratory) – ACE format – 14 materials

- (Al), aluminum @ 293.6°K
- (Be), beryllium metal @ 296°K
- (Be.BeO), beryllium bound in beryllium oxide @ 293.6°K
- (C), graphite @ 296°K
- (C6H6), benzene @ 296°K
- (D.D2O), deuterium bound in heavy water @ 296°K
- (Fe56), iron 56 @ 293.6°K
- (H.CH2), hydrogen bound in polyethylene @ 296°K
- (H.H2O), hydrogen bound in water @ 296°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296°K
- (O.BeO), oxygen bound in beryllium oxide @ 293.6°K
- (O.UO2), oxygen bound in uranium dioxide @ 296°K
- (U.UO2), uranium bound in uranium dioxide @ 296°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296°K

• **T.ENDFB7R0.LANL** (ENDF/B-VII.0 Los Alamos National Laboratory) – ACE format – 14 materials

- (Al), aluminum @ 20, 80, 293.6, 400, 600, and 800°K
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Be.BeO), beryllium bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K
- (C6H6), benzene @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (D.D2O), deuterium bound in heavy water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (Fe56), iron 56 @ 20, 80, 293.6, 400, 600, and 800°K
- (H.CH2), hydrogen bound in polyethylene @ 296 and 350°K
- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (O.BeO), oxygen bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (O.UO2), oxygen bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (U.UO2), uranium bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

• **T.ENDFB7R1** (ENDF/B-VII.1) – ENDF format – 15 materials

- (Al), aluminum @ 20, 80, 293.6, 400, 600, and 800°K
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Be.BeO), beryllium bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K
- (C6H6), benzene @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (D.D2O), deuterium bound in heavy water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (Fe56), iron 56 @ 20, 80, 293.6, 400, 600, and 800°K
- (H.CH2), hydrogen bound in polyethylene @ 296 and 350°K
- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (O.BeO), oxygen bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (O.UO2), oxygen bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (SiO2), silicon dioxide @ 293.6, 350, 400, 500, 800, 1000, and 1200°K
- (U.UO2), uranium bound in uranium dioxide @ 296, 400, 500, 600, 700, 800,

1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

• **T.ENDFB7R1.BNL** (ENDF/B-VII.1 Brookhaven National Laboratory) – ACE format – 14 materials
- (Al), aluminum @ 293.6°K
- (Be), beryllium metal @ 296°K
- (Be.BeO), beryllium bound in beryllium oxide @ 293.6°K
- (C), graphite @ 296°K
- (C6H6), benzene @ 296°K
- (D.D2O), deuterium bound in heavy water @ 296°K
- (Fe56), iron 56 @ 293.6°K
- (H.CH2), hydrogen bound in polyethylene @ 296°K
- (H.H2O), hydrogen bound in water @ 296°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296°K
- (O.BeO), oxygen bound in beryllium oxide @ 293.6°K
- (O.UO2), oxygen bound in uranium dioxide @ 296°K
- (U.UO2), uranium bound in uranium dioxide @ 296°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296°K

• **T.ENDFB7R1.LANL** (ENDF/B-VII.1 Los Alamos National Laboratory) – ACE format – 15 materials
- (Al), aluminum @ 20, 80, 293.6, 400, 600, and 800°K
- (Be), beryllium metal @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Be.BeO), beryllium bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (C), graphite @ 296, 400, 500, 600, 700, 800, 1000, 1200, 1600, and 2000°K
- (C6H6), benzene @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (D.D2O), deuterium bound in heavy water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (Fe56), iron 56 @ 20, 80, 293.6, 400, 600, and 800°K
- (H.CH2), hydrogen bound in polyethylene @ 296 and 350°K
- (H.H2O), hydrogen bound in water @ 296, 350, 400, 450, 500, 600, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (O.BeO), oxygen bound in beryllium oxide @ 293.6, 400, 500, 600, 800, 1000, and 1200°K
- (O.UO2), oxygen bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (SiO2), silicon dioxide @ 293.6, 350, 400, 500, 800, 1000, and 1200°K
- (U.UO2), uranium bound in uranium dioxide @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Zr.ZrH), zirconium bound in zirconium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K

- **T.IAEA2007** (IAEA-2007) – ENDF format – 7 materials
  - (C), graphite @ 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, and 3000°K
  - (D,D2O), deuterium bound in heavy water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 643.9°K
  - (H.CeH2), hydrogen bound in cerium hydride @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (H.H2O), hydrogen bound in water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.6, 800, and 1000°K
  - (H.TiH2), hydrogen bound in titanium hydride @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (H.YH2), hydrogen bound in yttrium hydride @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (H.ZrH), hydrogen bound in zirconium hydride @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K

- **T.JEF2.2** (JEF2.2) – ENDF format – 5 materials
  - (Be), beryllium metal @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (C), graphite @ 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, and 3000°K
  - (D.D2O), deuterium bound in heavy water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 673.6°K
  - (H.CH2), hydrogen bound in polyethylene @ 293.6 and 350°K
  - (H.H2O), hydrogen bound in water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 673.6°K

- **T.JEFF3.0** (JEFF3.0) – ENDF format – 5 materials
  - (Be), beryllium metal @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (C), graphite @ 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, and 3000°K
  - (D.D2O), deuterium bound in heavy water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 673.6°K
  - (H.CH2), hydrogen bound in polyethylene @ 293.6 and 350°K
  - (H.H2O), hydrogen bound in water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 673.6°K

- **T.JEFF3.1** (JEFF3.1) – ENDF format – 9 materials
  - (Be), beryllium metal @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (C), graphite @ 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, and 3000°K
  - (Ca.CaH2), calcium bound in calcium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (D.D2O), deuterium bound in heavy water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 643.9°K
  - (H.CaH2), hydrogen bound in calcium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
  - (H.CH2), hydrogen bound in polyethylene @ 293.6 and 350°K

- (H.H2O), hydrogen bound in water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Mg), magnesium @ 20, 100, 296, and 773°K

• **T.JEFF3.1.1** (JEFF3.1.1) – ACE format – 7 materials
- (Be), beryllium metal @ 293.6°K
- (BeO), beryllium oxide @ 293.6°K
- (C), graphite @ 293.6°K
- (D.D2O), deuterium bound in heavy water @ 293.6°K
- (H.CH2), hydrogen bound in polyethylene @ 293.6°K
- (H.H2O), hydrogen bound in water @ 293.6°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 293.6°K

• **T.JEFF3.1.2** (JEFF3.1.2) – ENDF format – 9 materials
- (Be), beryllium metal @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
- (C), graphite @ 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1600, 2000, and 3000°K
- (Ca.CaH2), calcium bound in calcium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (D.D2O), deuterium bound in heavy water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, and 643.9°K
- (H.CaH2), hydrogen bound in calcium hydride @ 296, 400, 500, 600, 700, 800, 1000, and 1200°K
- (H.CH2), hydrogen bound in polyethylene @ 293.6 and 350°K
- (H.H2O), hydrogen bound in water @ 293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, and 1000°K
- (H.ZrH), hydrogen bound in zirconium hydride @ 293.6, 400, 500, 600, 700, 800, 1000, and 1200°K
- (Mg), magnesium @ 20, 100, 296, and 773°K

There are two library makers used to generate COG thermal libraries from the thermal data: SABtoCOG for the ENDF formatted data, and SAB.ACEtoCOG for the ACE formatted data. SABtoCOG computes cross sections and distributions necessary to determine the scattered neutron direction and energy and stores these quantities as a COG library. The incoherent elastic cross section and distributions are derived from the Debye-Waller coefficient (MF=7 and MT=2), the coherent elastic cross section and distributions are derived from the Bragg edge-strength parameters (MF=7 and MT=2), and the inelastic cross section and distributions are derived from the $S(\alpha,\beta)$ data (MF=7 and MT=4). The ACE formatted data has been processed by NJOY [1] to produce cross sections and distributions necessary to determine the scattered neutron direction and energy. SAB.ACEtoCOG basically just stores data as a COG library, the exception being the Bragg edge-strength parameters, which are converted to the coherent elastic cross section before storing.

Results

When comparing results for various libraries we found several outcomes similar to those shown in the following figures for 293.6 °K.

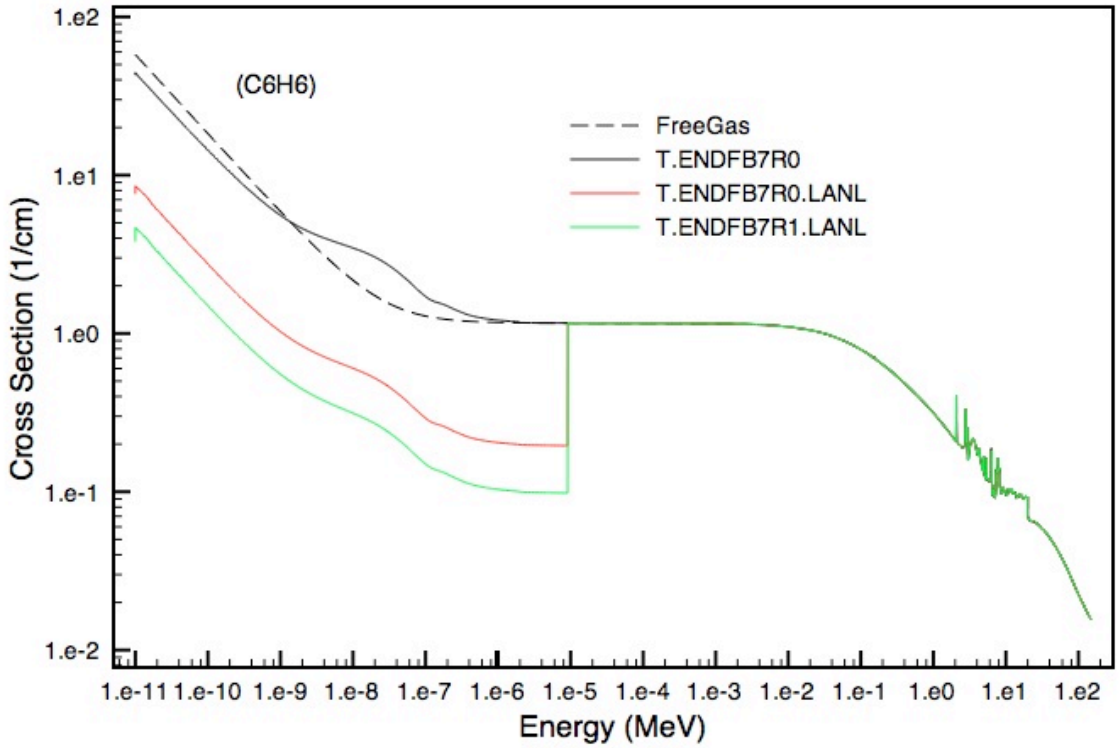

Figure 1

Figure 1 shows the results for benzene, (C6H6), obtained when comparing the output from various thermal libraries. The results for T.ENDFB7R0 show a smooth transition across the thermal boundary, T.ENDFB7R0.LANL is off by a factor of 6, and T.ENDFB7R1.LANL is off by a factor of 12.

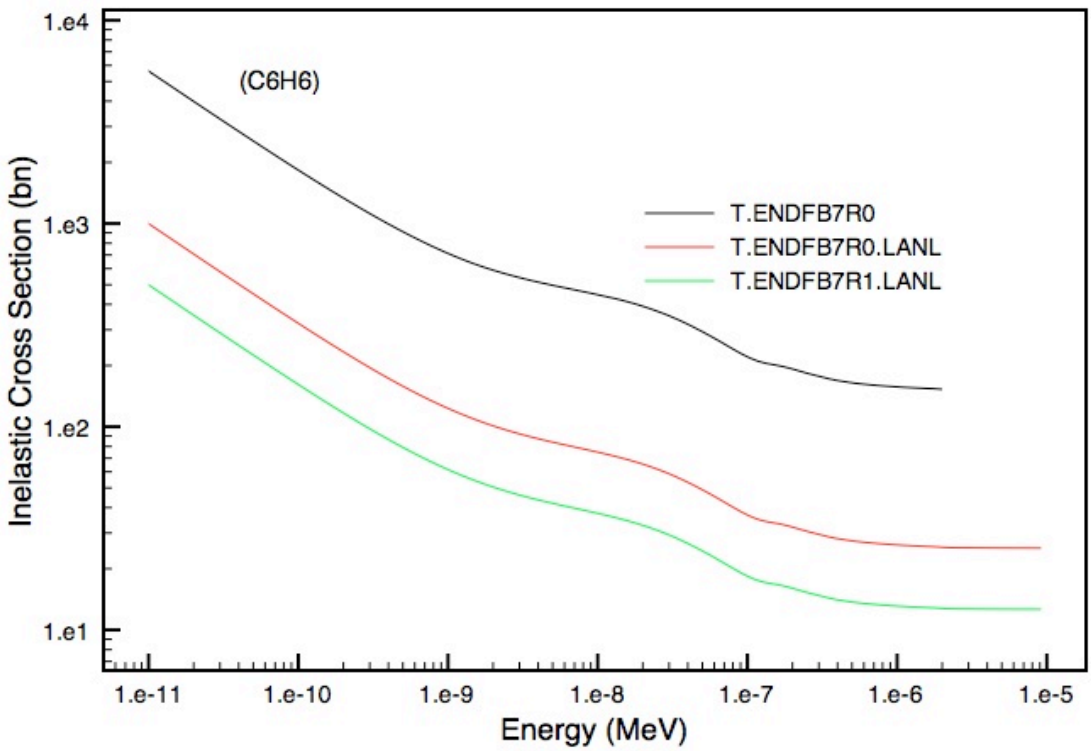

Figure 2

Figure 2 shows the corresponding thermal inelastic cross sections.

A complete study was undertaken, checking each material in each thermal library. The results are shown in the table below. The entries show the ratio of the cross section above the thermal boundary to that below.

	T.ENDFB3R0	T.ENDFB6R0	T.ENDFB6R2	T.ENDFB7R0	T.ENDFB7R0.BNL	T.ENDFB7R0.LANL	T.ENDFB7R1	T.ENDFB7R1.BNL	T.ENDFB7R1.LANL	T.IAEA2007	T.JEF2.2	T.JEFF3.0	T.JEFF3.1	T.JEFF3.1.1	T.JEFF3.1.2
Al				1	1	1	1	1	1						
Be	1	1	1	1	1	1	1	1	1		1	1	1	1	1
Be.BeO				1	2	1	1	2	1						
BeO	1	1	1											6.4	
C	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Ca.CaH2													1		1
C6H6	1			1	12	6	1	12	12						
D.D2O	0.5	0.5		0.5	1	1	0.5	1	1	0.5	0.5	0.5	0.5	1	0.5
Fe56				1	1	1	1	1	1						
H.CH2	0.5	0.5		0.5	1	1	0.5	1	1		0.5	0.5	0.5	1	0.5
H.CaH2													1		1
H.CeH2										0.5					
H.H2O	0.5	0.5	0.5	0.5	1	1	0.5	1	1	0.5	0.5	0.5	0.5	1	0.5
H.TiH2										0.5					
H.YH2										0.5					
H.ZrH	1	1	1	1	1	1	1	1	1	1			1	2	1
Mg													1		1
O.BeO				1	2	1	1	2	1						
O.UO2				1	2	1	1	2	1						
SiO2							1.6		3.3						
U.UO2				1	1	1	1	1	1						
UO2	1														
Zr.ZrH	1	1	1	1	1	1	1	1	1						

Table 1

The entries in Table 1become normalizing factors as input to SABtoCOG and SAB.ACEtoCOG to ensure the generated cross sections make a smooth transition across the thermal boundary.

What follows are sections for each thermal material. Each section consists of a plot showing the material cross section for each library containing the given material, along with some discussion of the relative validity when appropriate. Note: The thermal boundary may vary for each material and for each library for a given material, but none of the following plots show the kind of discontinuity evident in Figure 1. Each section also includes plots of the incoherent elastic or coherent elastic cross section, if applicable, along with the inelastic cross section for selected libraries.

(Al), aluminum

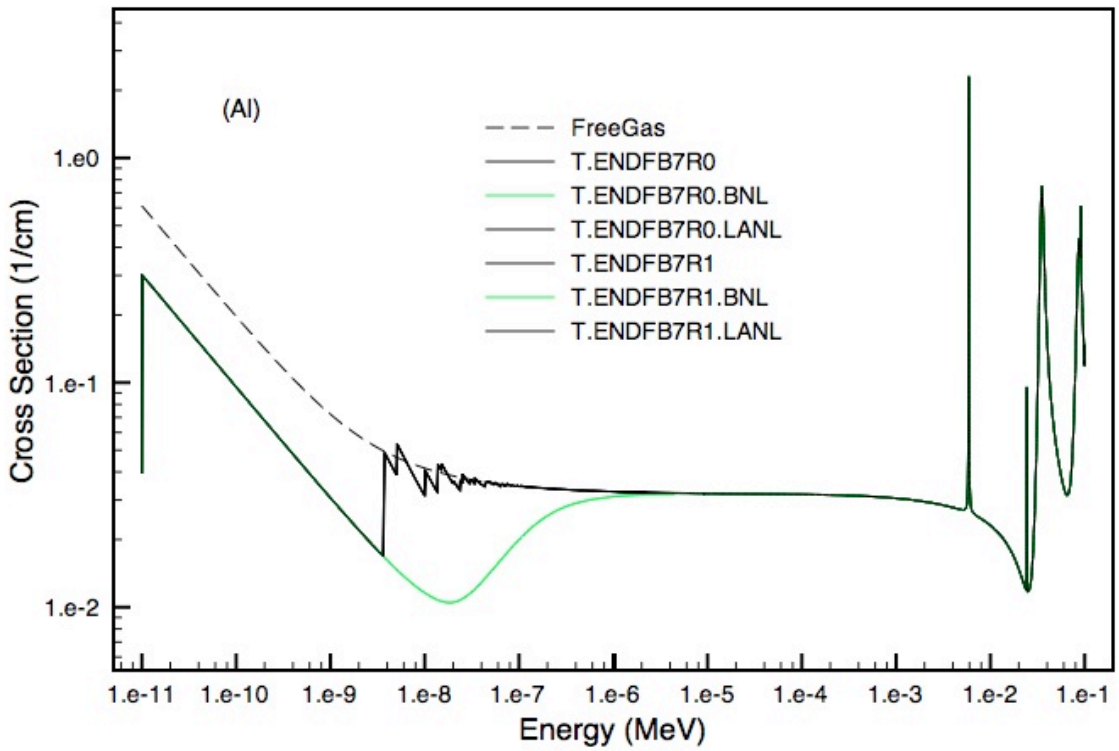

Figure 3

There is excellent agreement except for the BNL evaluations, which are missing the coherent elastic component.

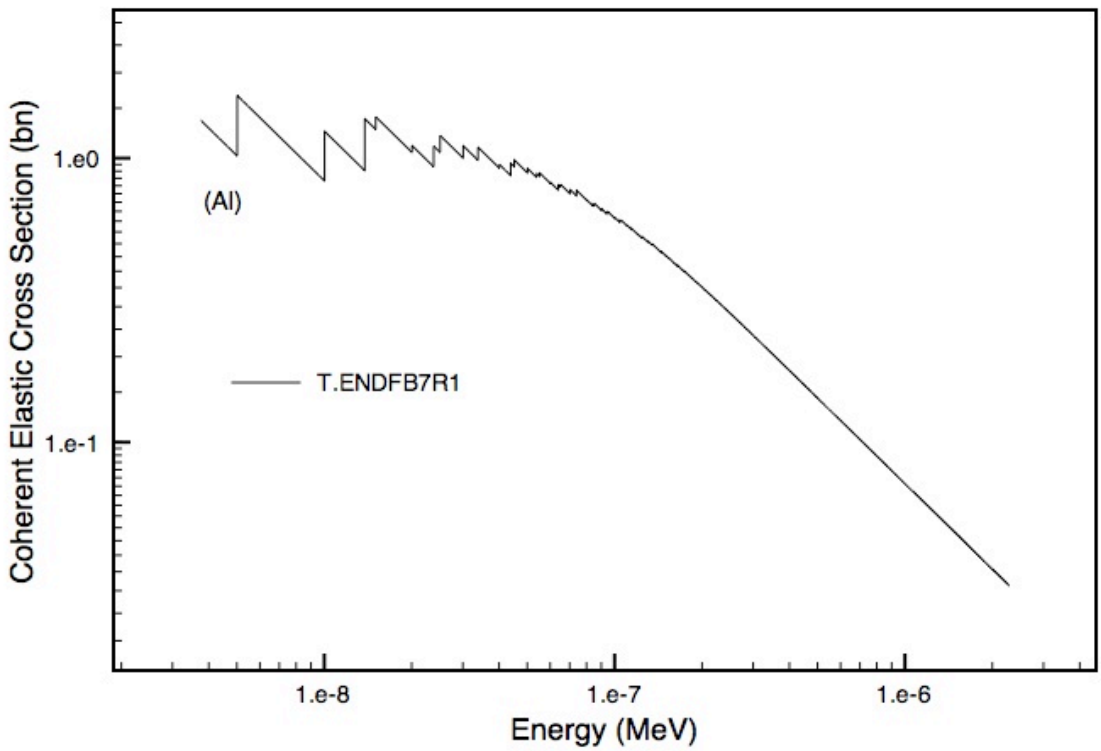

Figure 4

There is no coherent elastic component in the BNL evaluations.

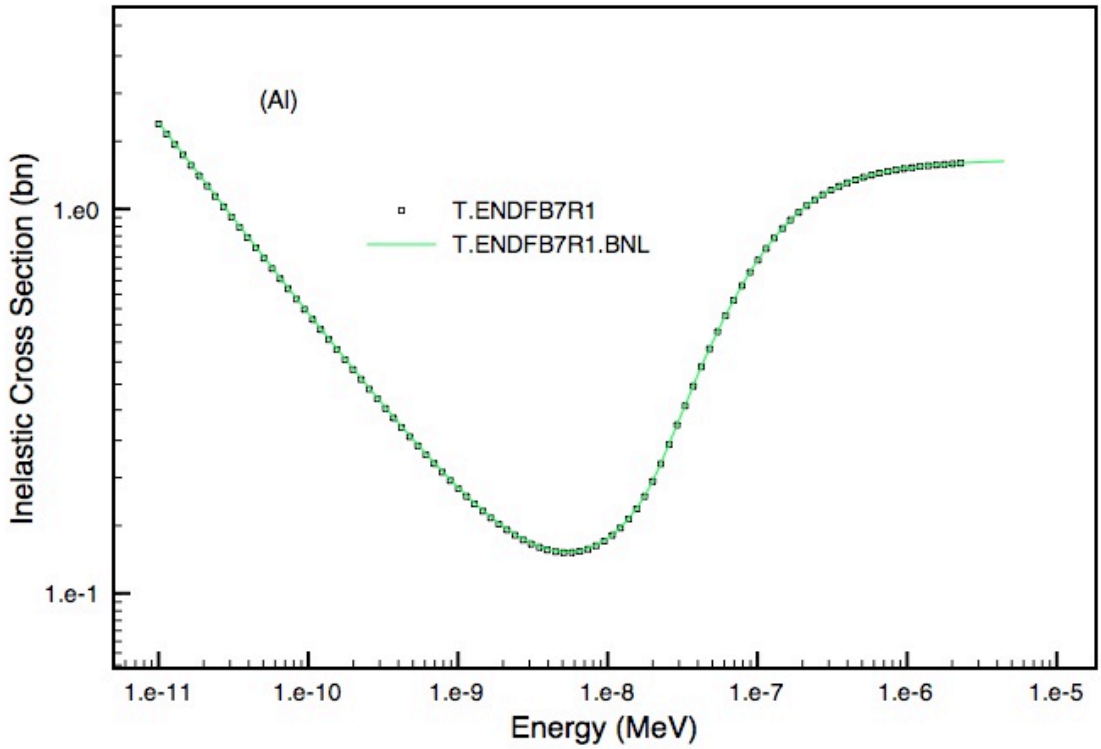

Figure 5

There is excellent agreement in the inelastic component.

(Be), beryllium metal

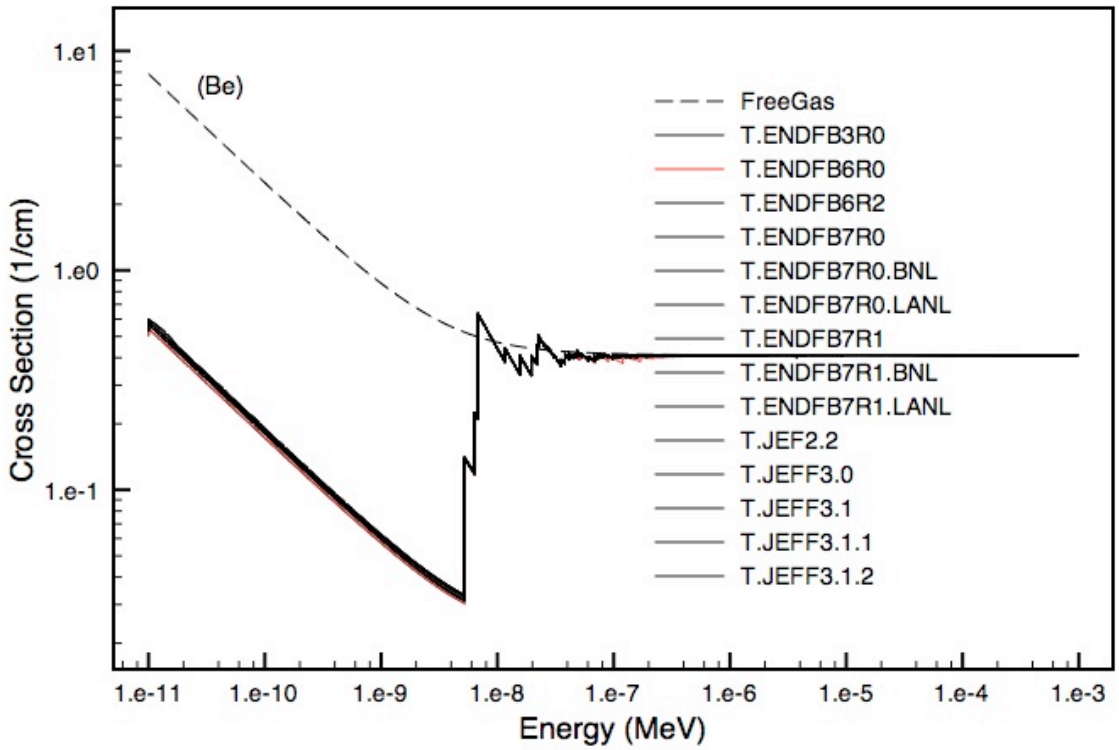

Figure 6

There is good agreement except for slight differences with T.ENDFB6R0.

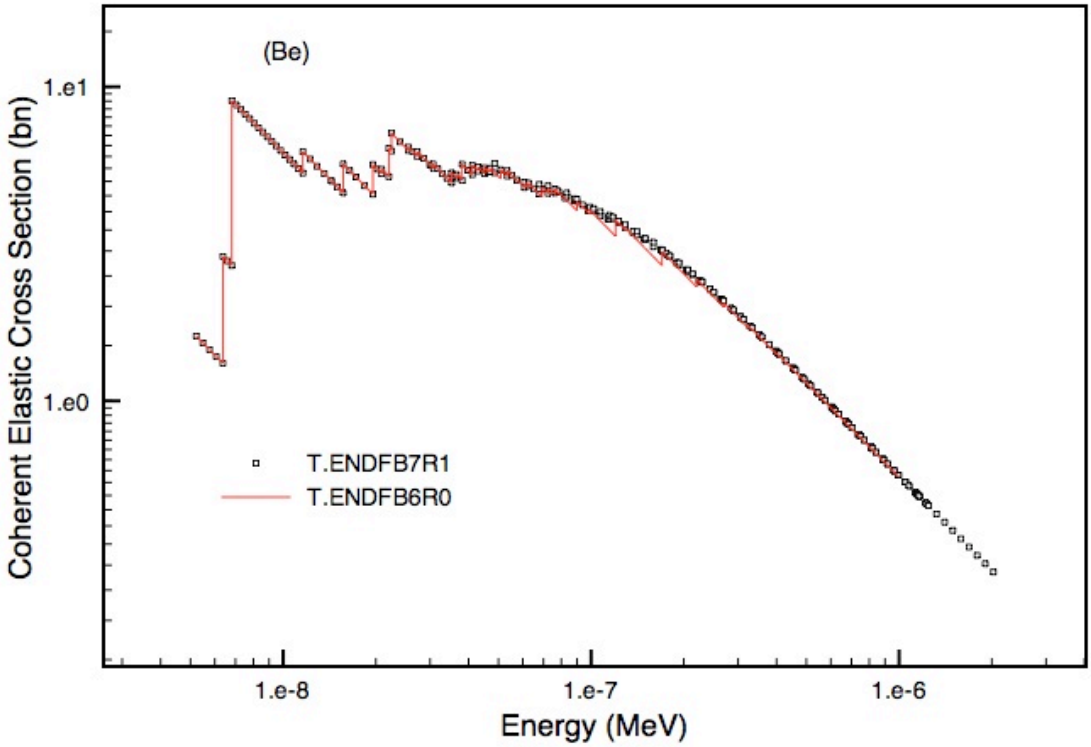

Figure 7

There is good agreement except for slight differences with T.ENDFB6R0.

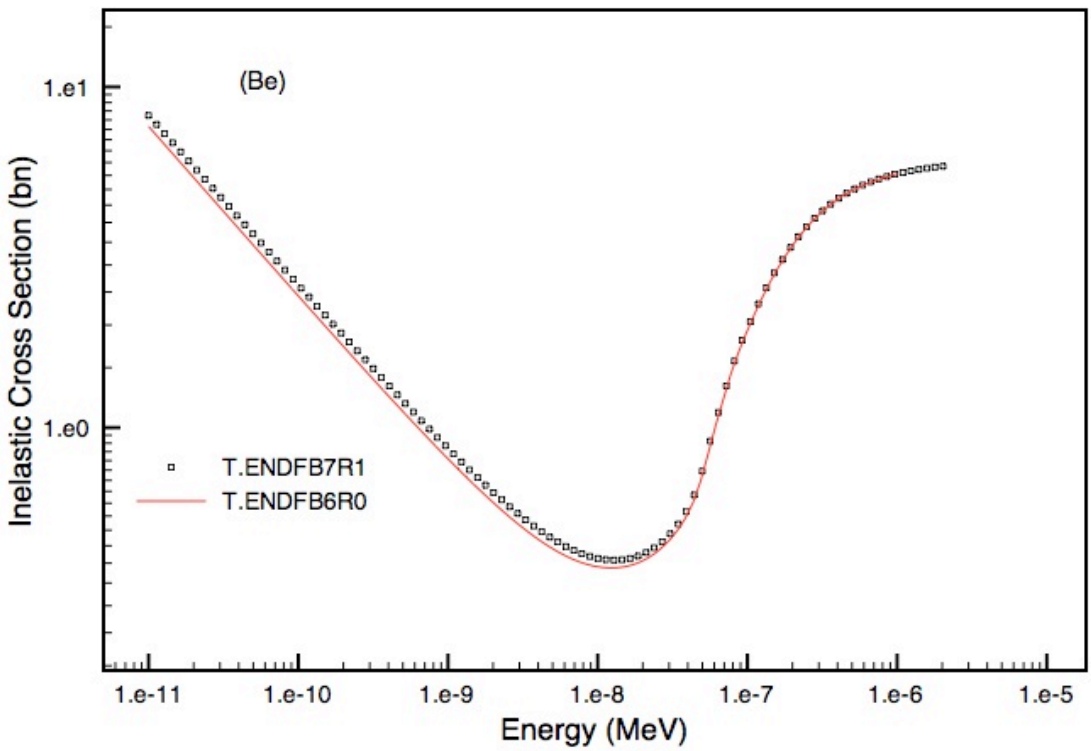

Figure 8

There is good agreement except for slight differences at energies below ~1.e-8 MeV.

(BeO), beryllium oxide

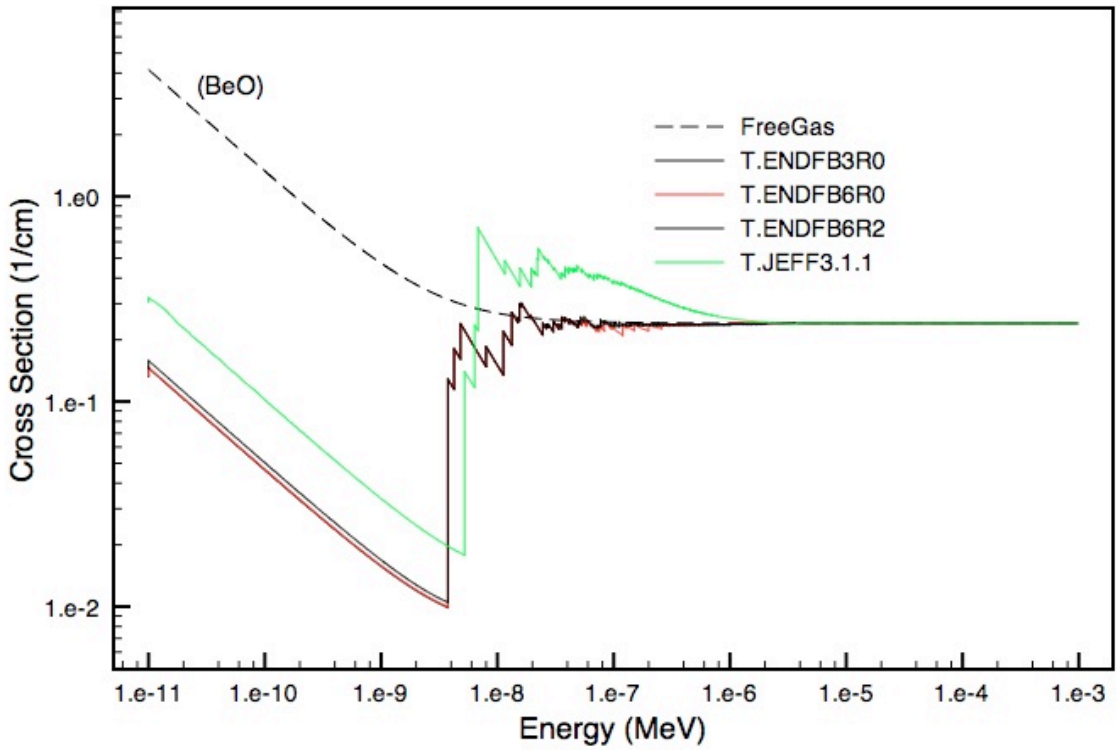

Figure 9

T.ENDFB6R0 shows some extra edge structure, while T.JEFF3.1.1 doesn't agree at all with the others.

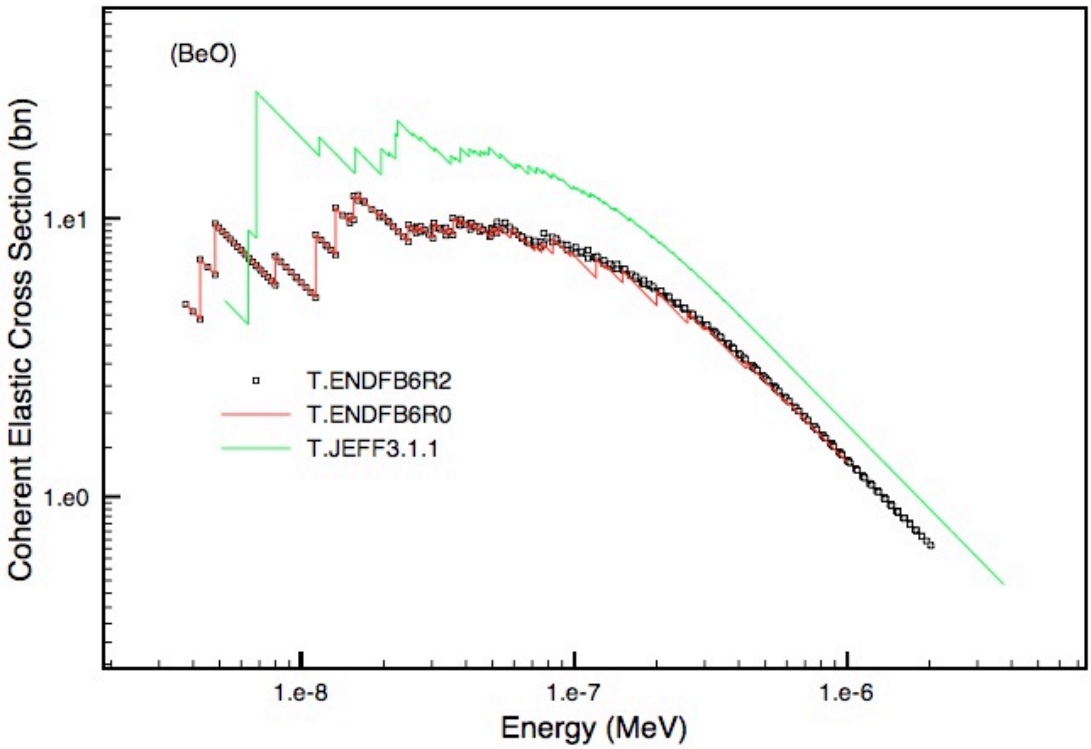

Figure 10

T.ENDFB6R0 shows some extra edge structure, while T.JEFF3.1.1 doesn't agree at all with the others.

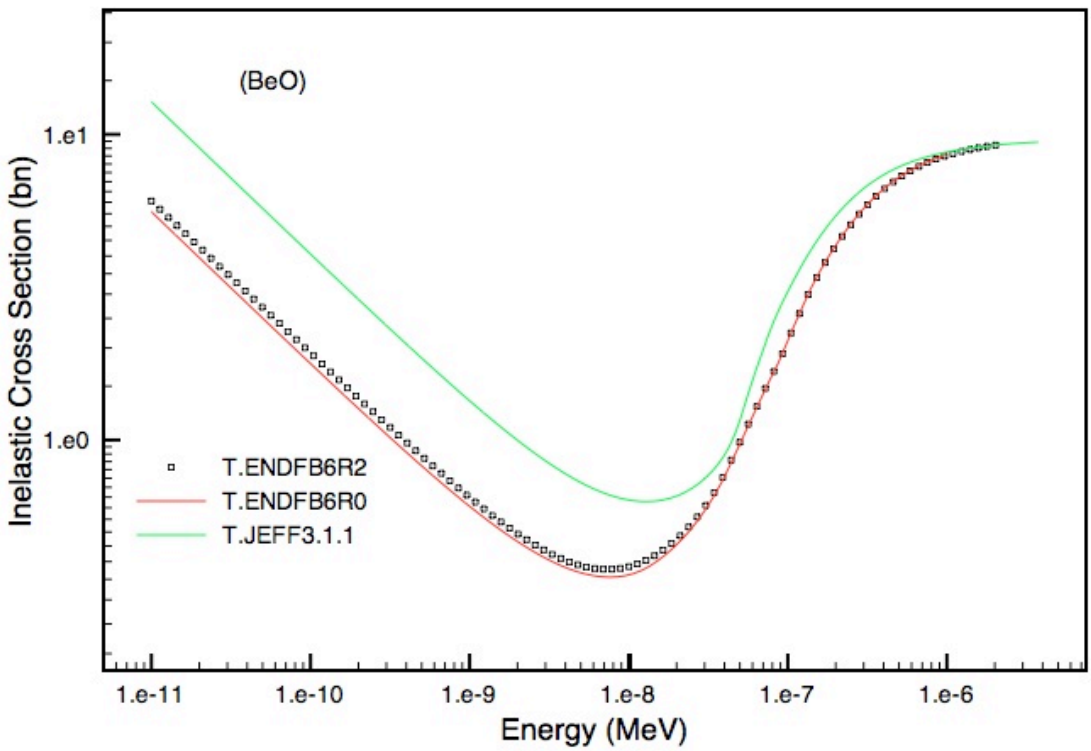

Figure 11

There are minor differences in T.ENDFB6R0 below ~1.e-8 MeV. T.JEFF3.1.1 doesn't agree at all.

(Be.BeO), beryllium bound in beryllium oxide

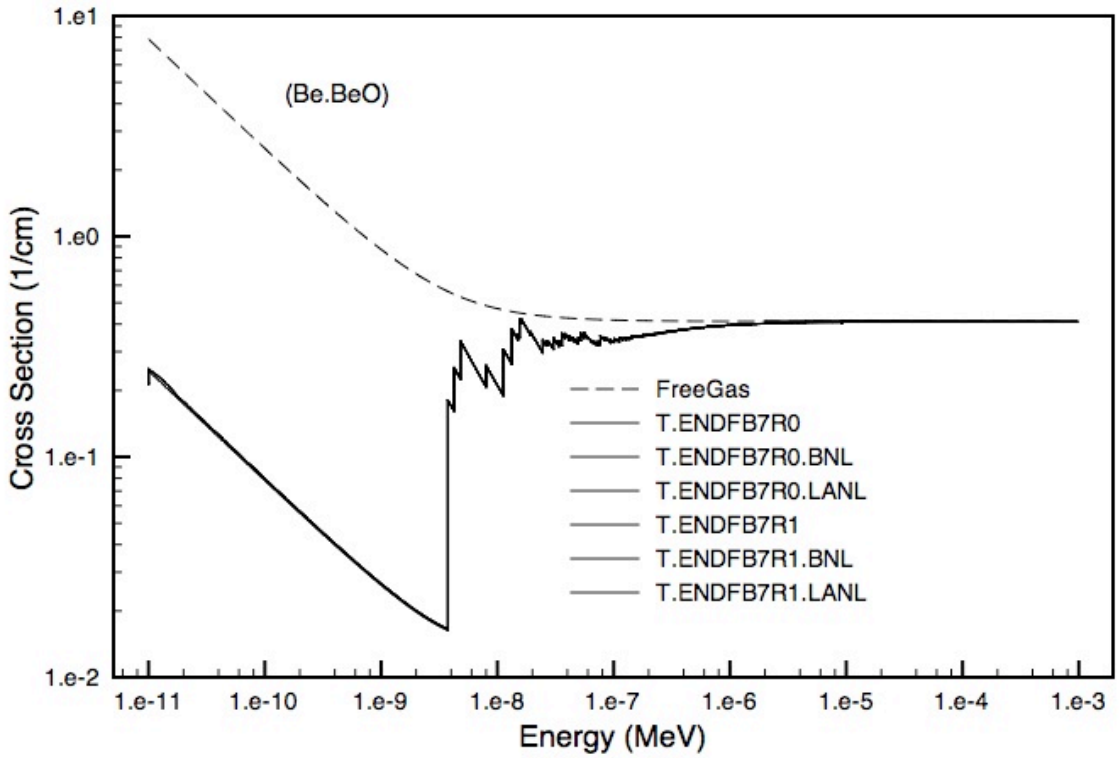

Figure 12

All show excellent agreement.

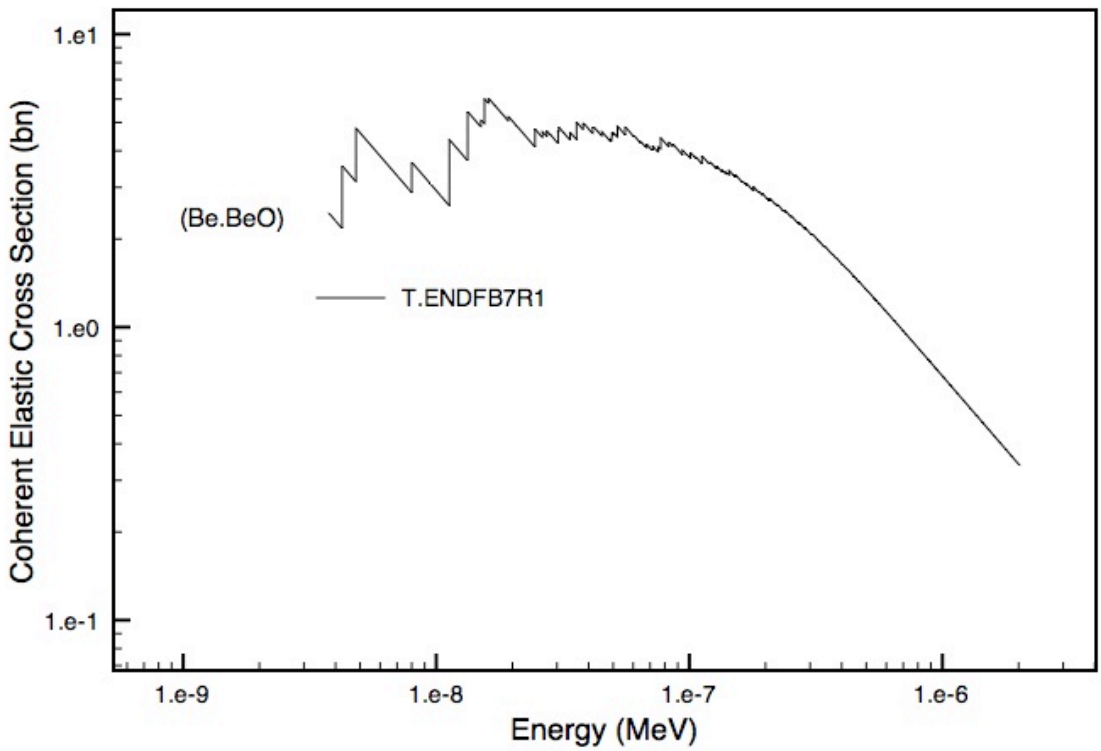

Figure 13

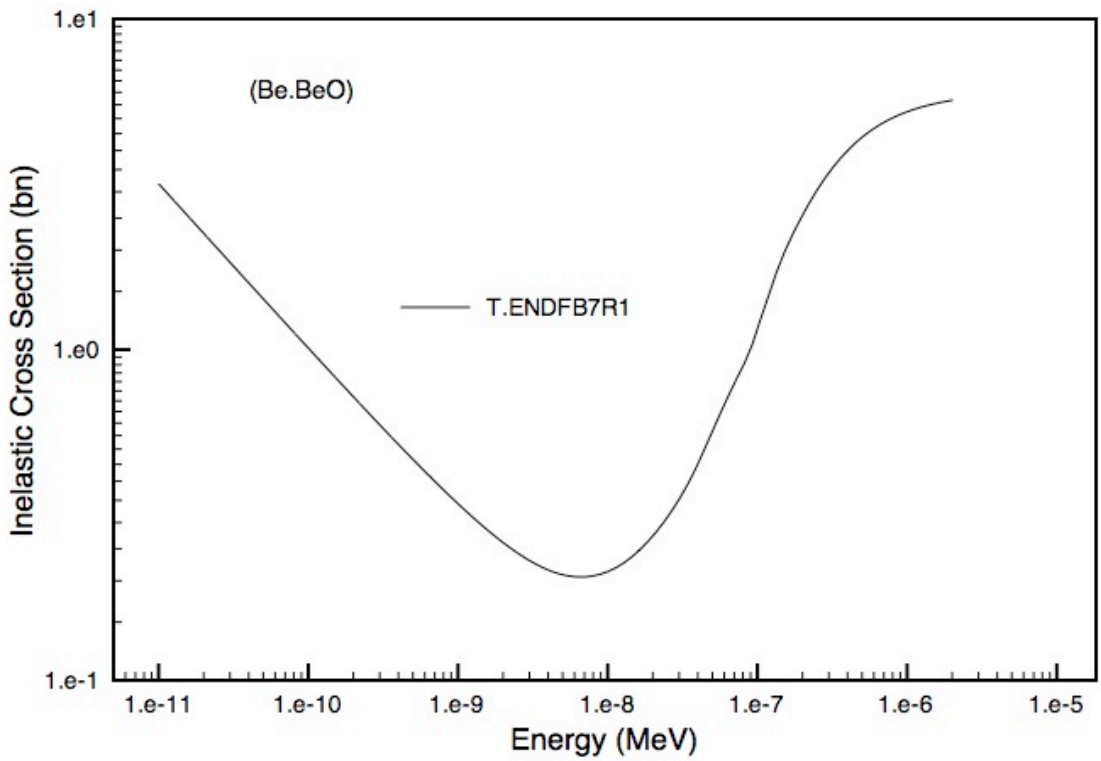

Figure 14

(C), graphite

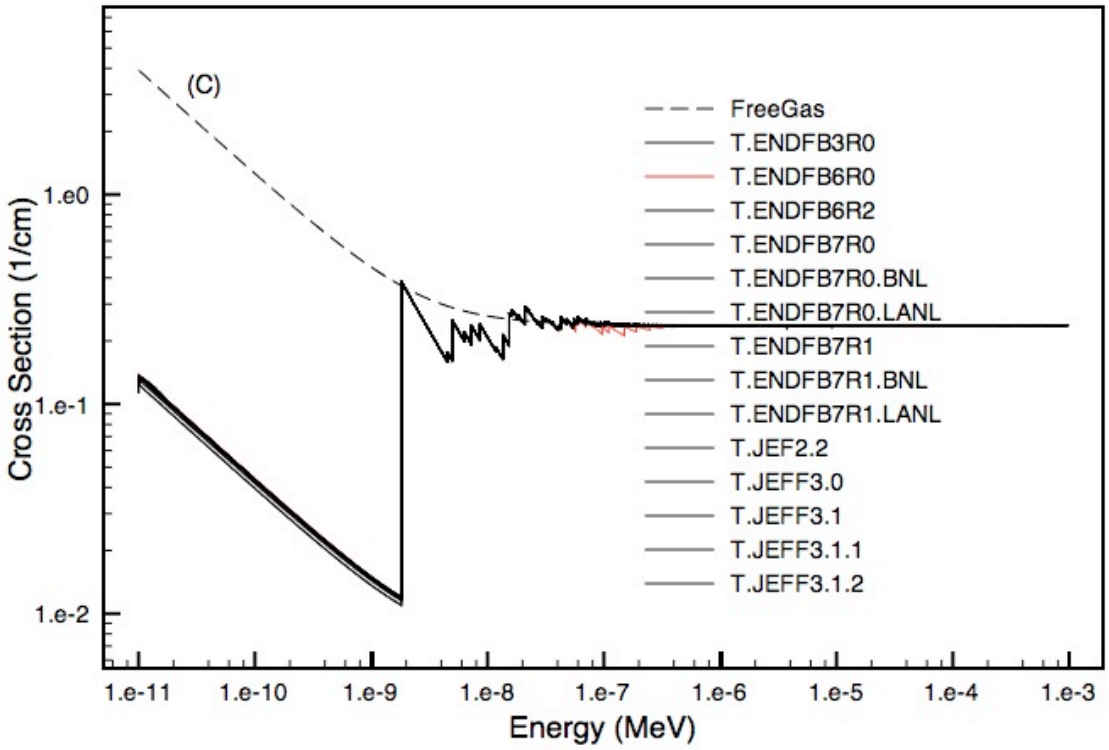

Figure 15

T.ENDFB6R0 shows some extra edge structure, the rest show excellent agreement.

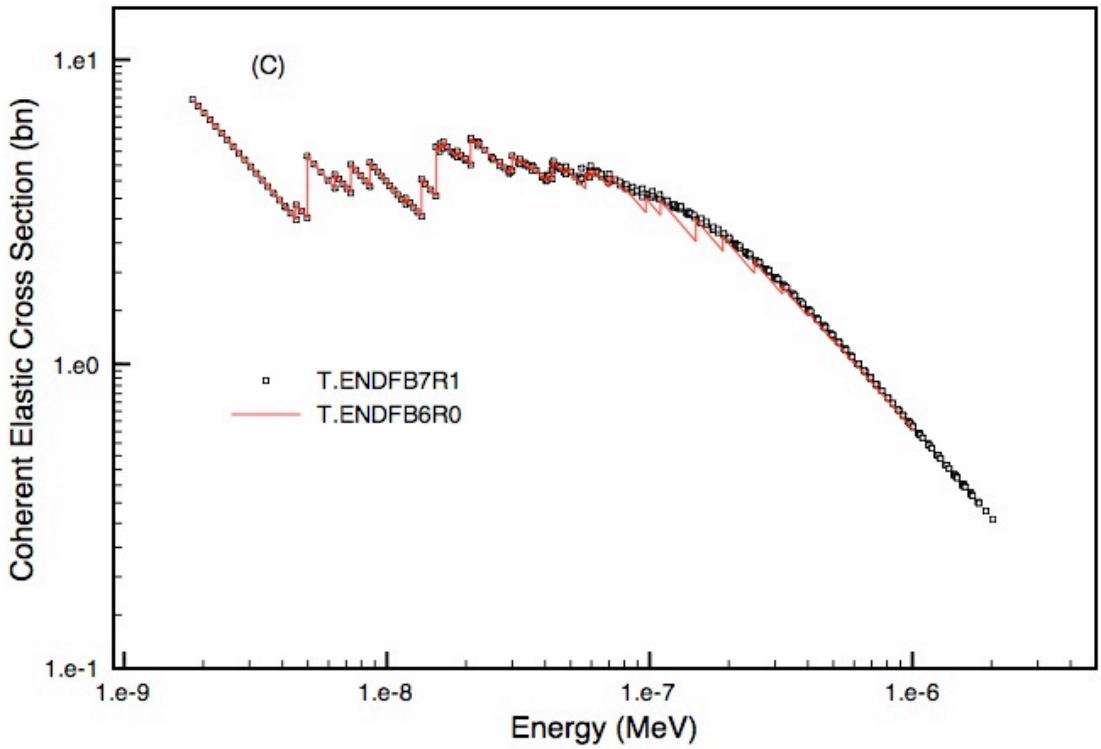

Figure 16

T.ENDFB6R0 shows some extra edge structure.

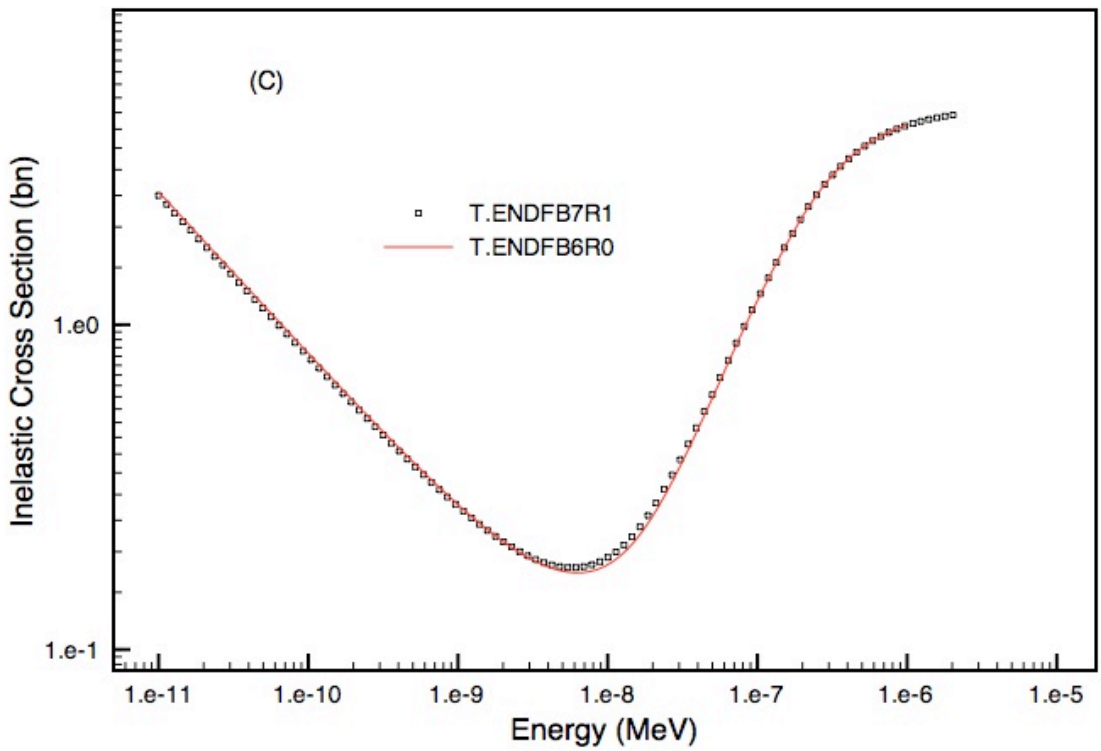

Figure 17

T.ENDFB6R0 shows some very slight differences.

(C6H6), benzene

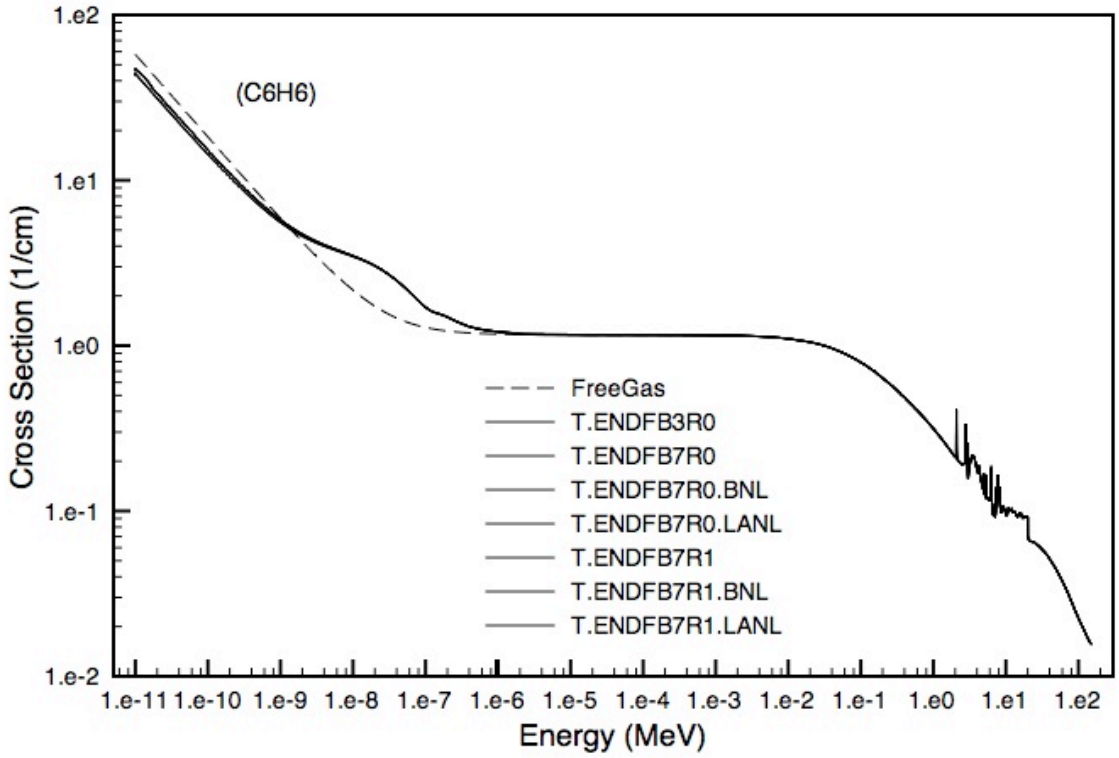

Figure 18

Good agreement – compare with Figure 1.

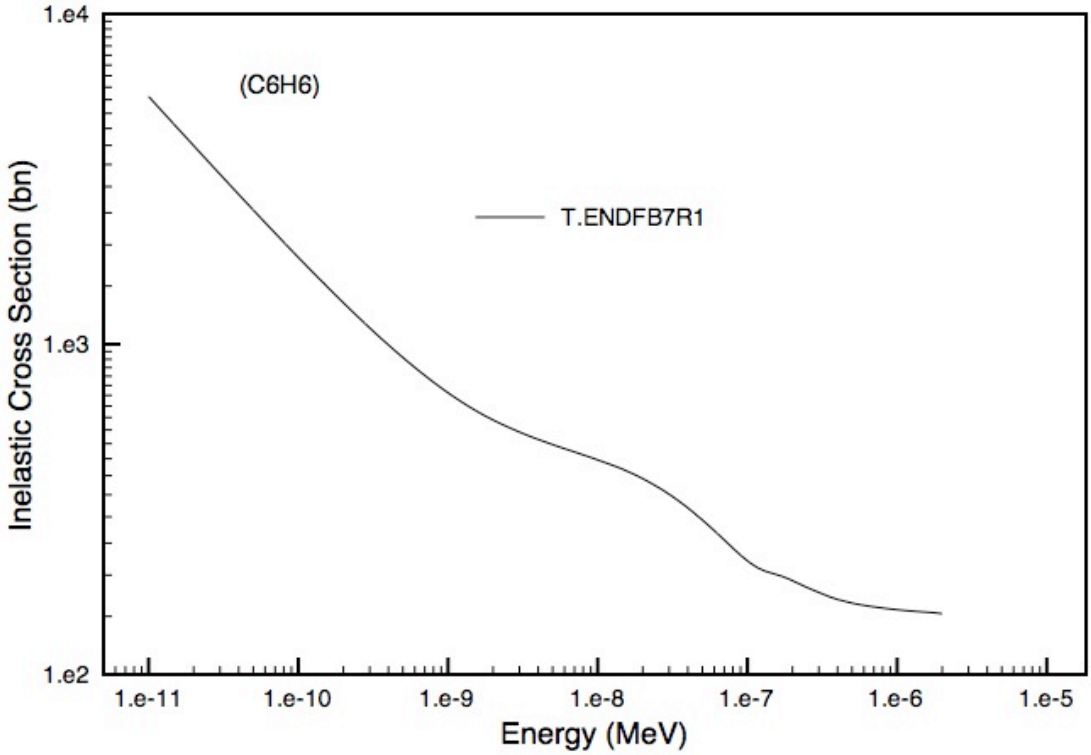
1.e4
1.e3
1.e2
Inelastic Cross Section (bn)
(C6H6)
T.ENDFB7R1
1.e-11
1.e-10
1.e-9
1.e-8
1.e-7
1.e-6
1.e-5
Energy (MeV)

Figure 19

(Ca.CaH2), calcium bound in calcium hydride

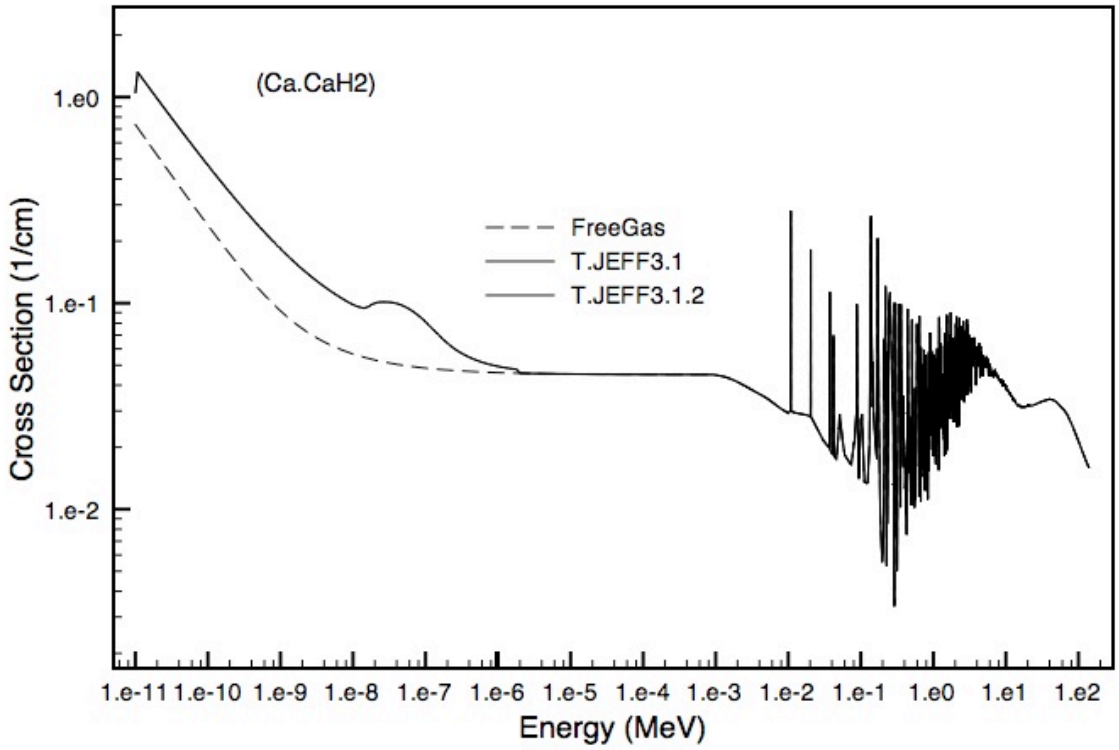

Figure 20

The results are identical.

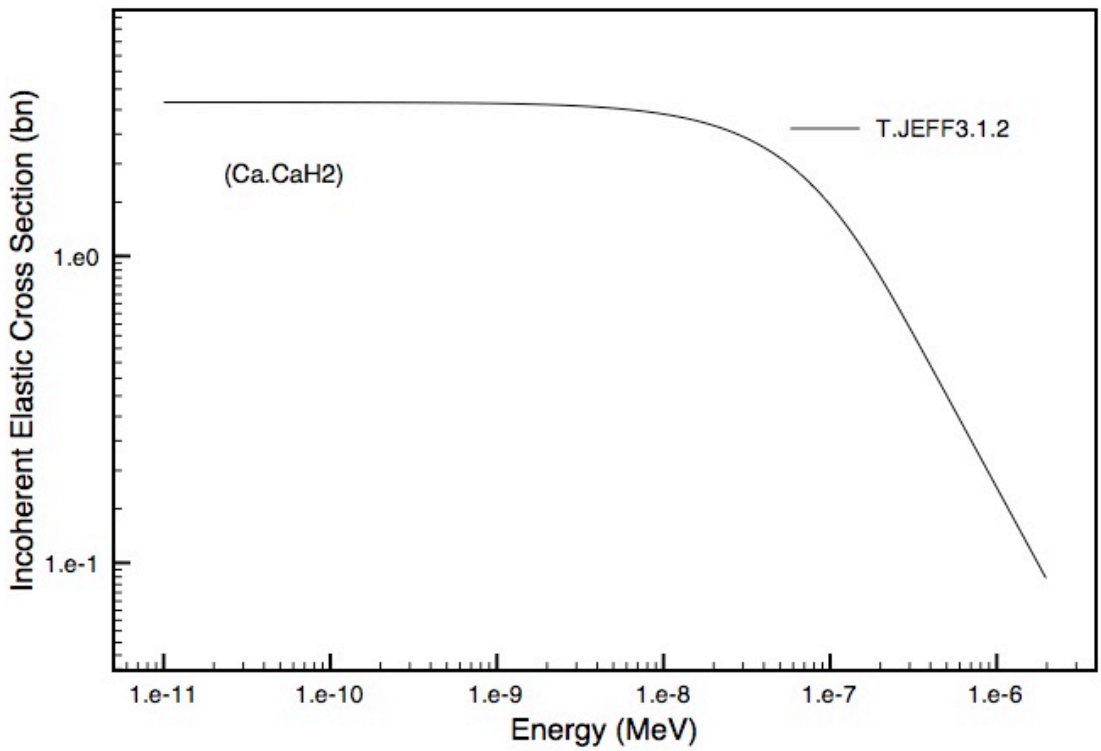

Figure 21

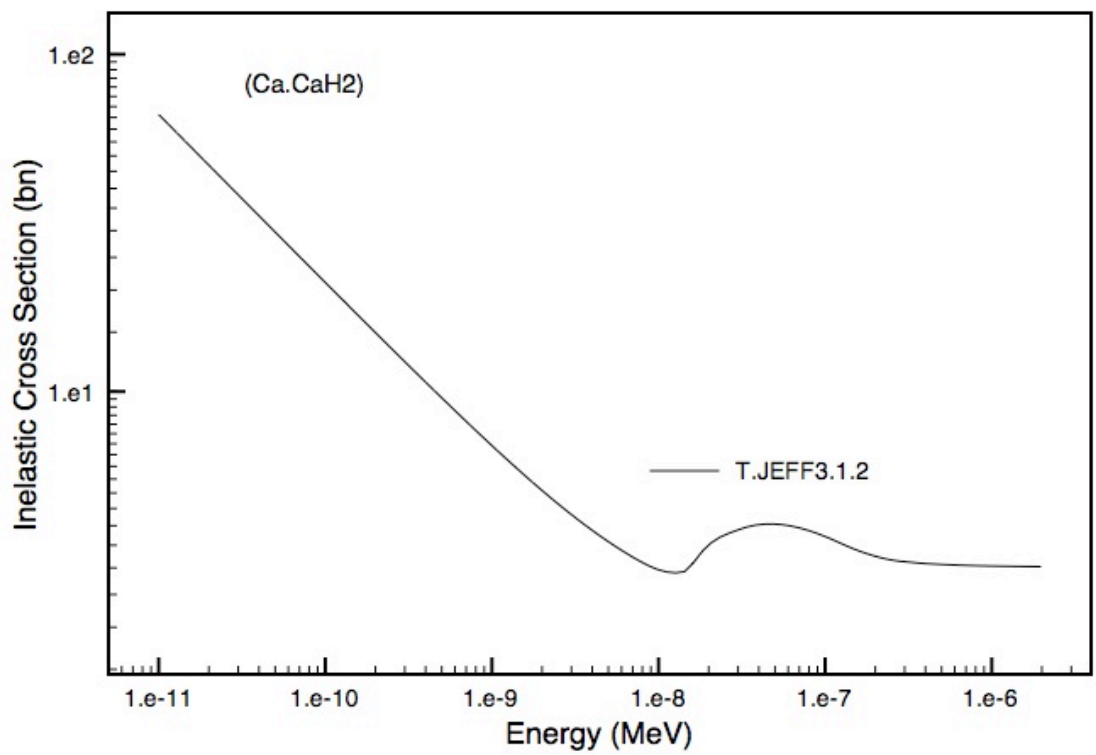

Figure 22

(D.D2O), deuterium bound in heavy water

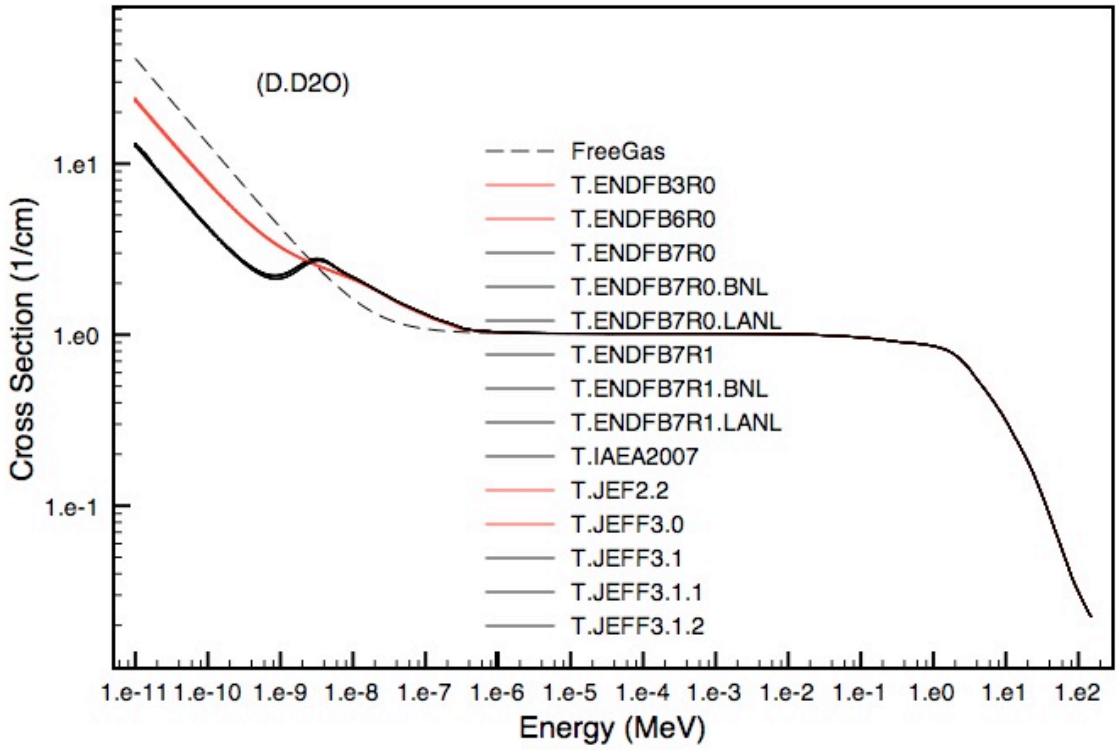

Figure 23

The early evaluations – T.ENDFB3R0, T.ENDFB6R0, T.JEF2.2, and T.JEFF3.0 – show differences. The later evaluations are in good agreement.

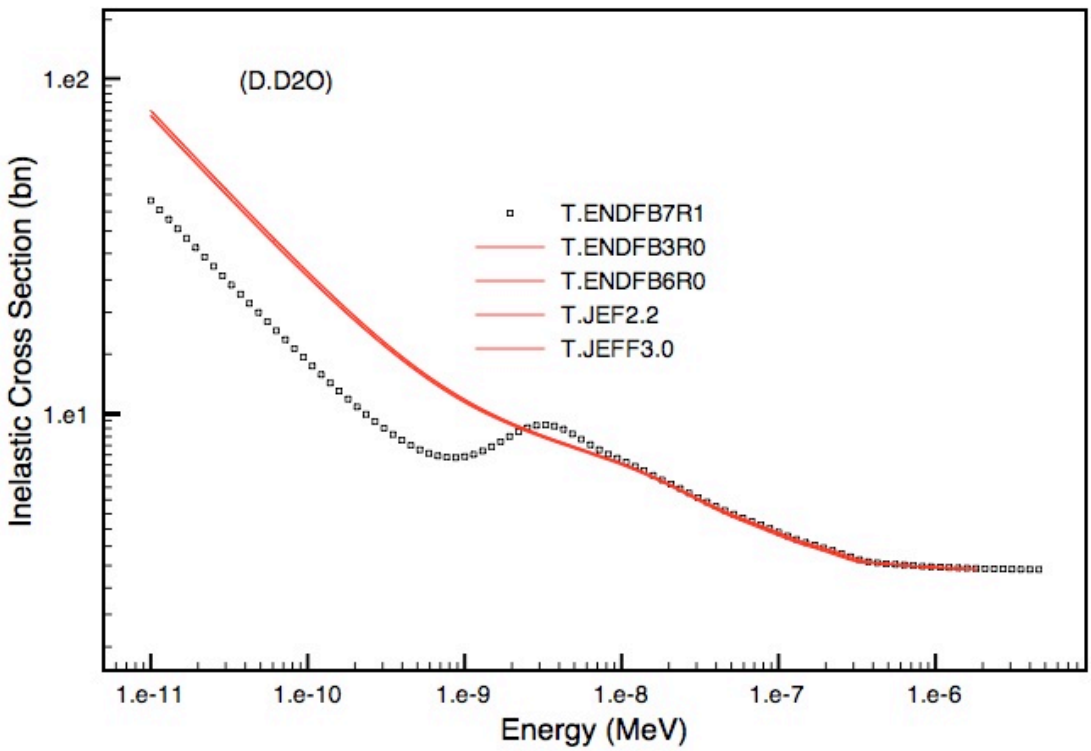

Figure 24

The early evaluations – T.ENDFB3R0, T.ENDFB6R0, T.JEF2.2, and T.JEFF3.0 – show differences.

(Fe56), iron 56

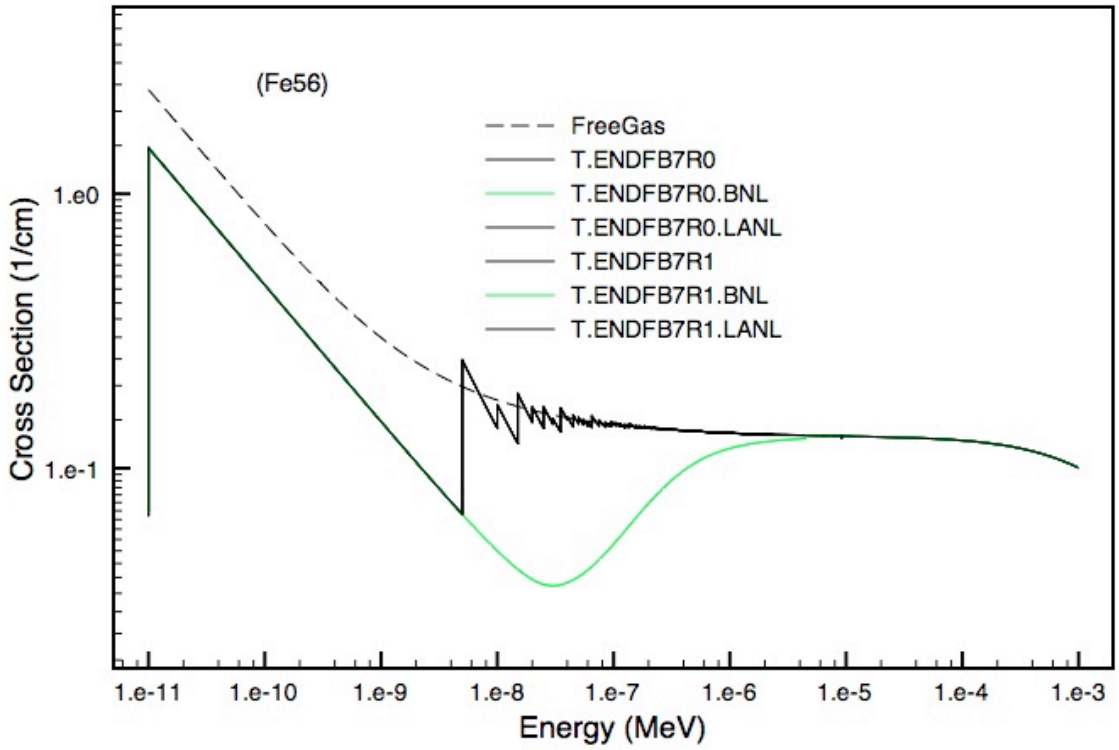

Figure 25

There is excellent agreement except for the BNL evaluations, which are missing the characteristic edge structure

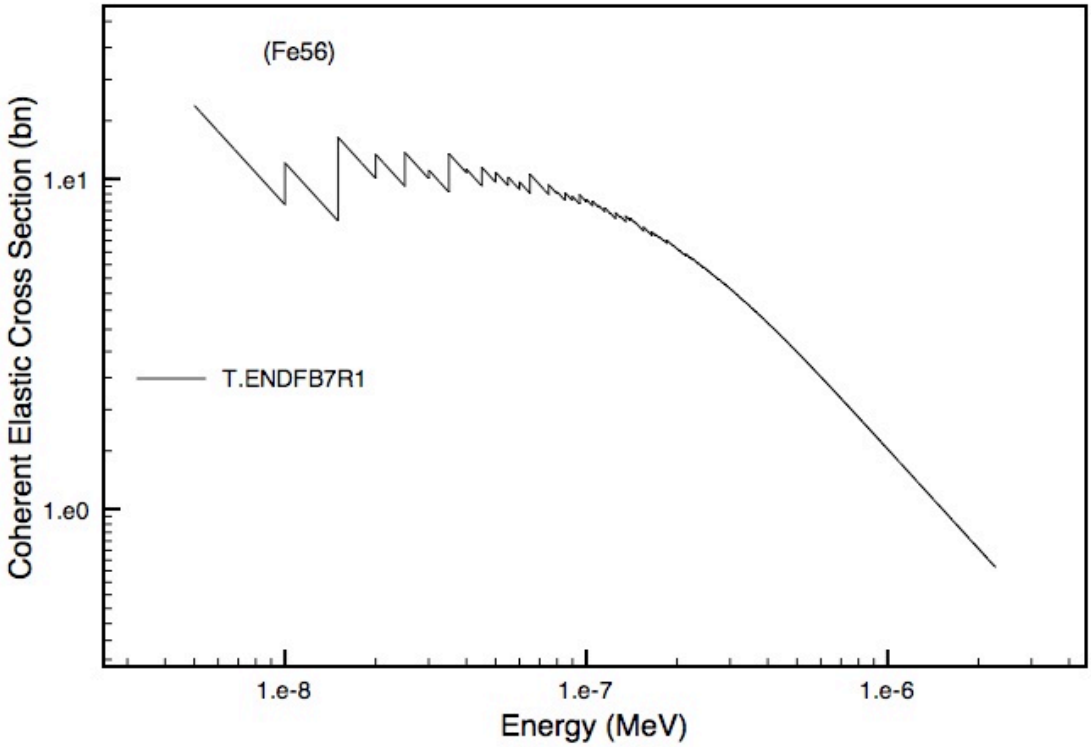

Figure 26

There is no BNL coherent elastic component.

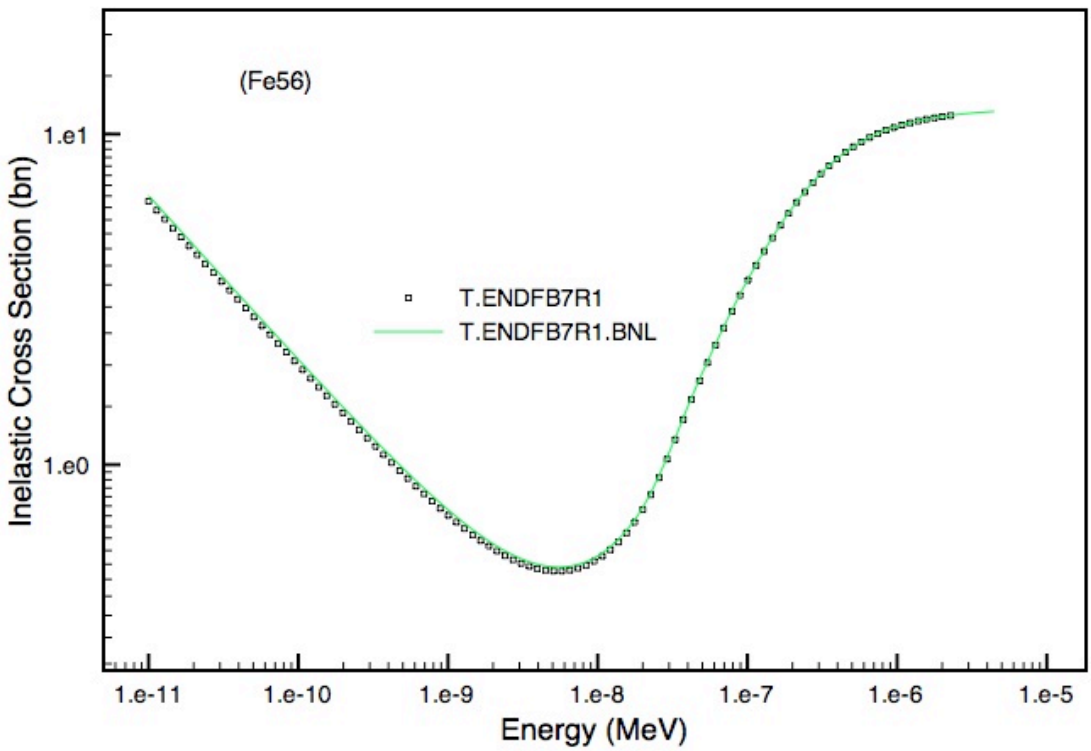

Figure 27

There is good agreement in the inelastic component.

(H.CaH2), hydrogen bound in calcium hydride

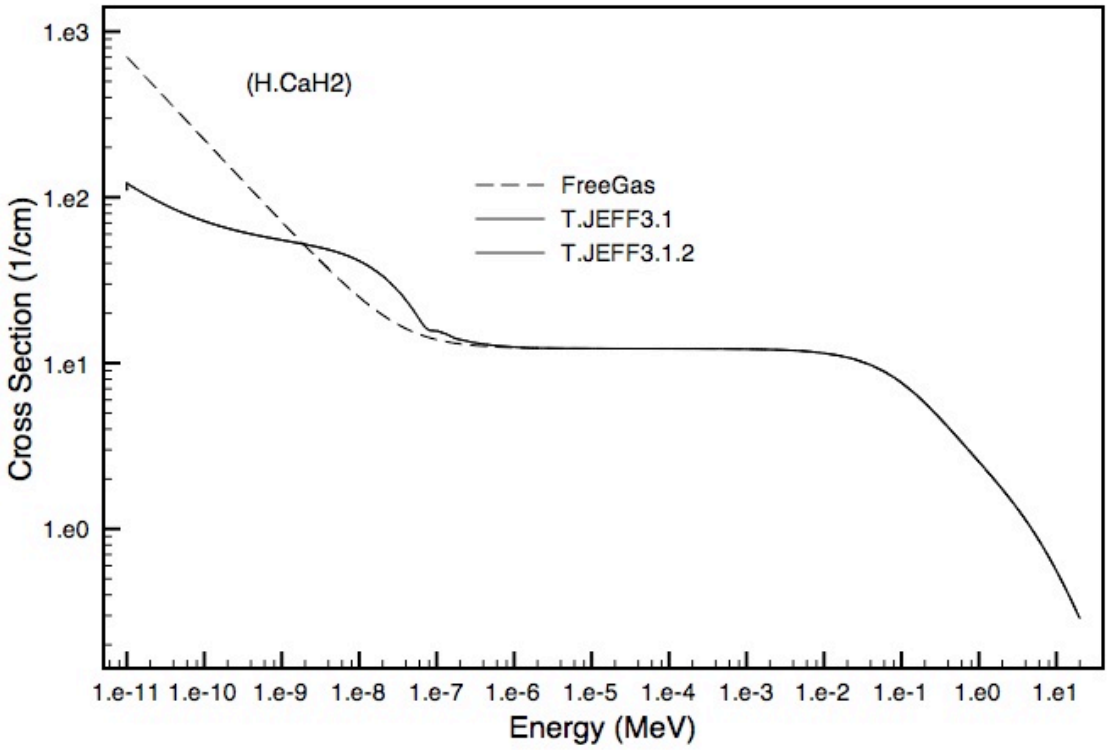

Figure 28

The results are identical.

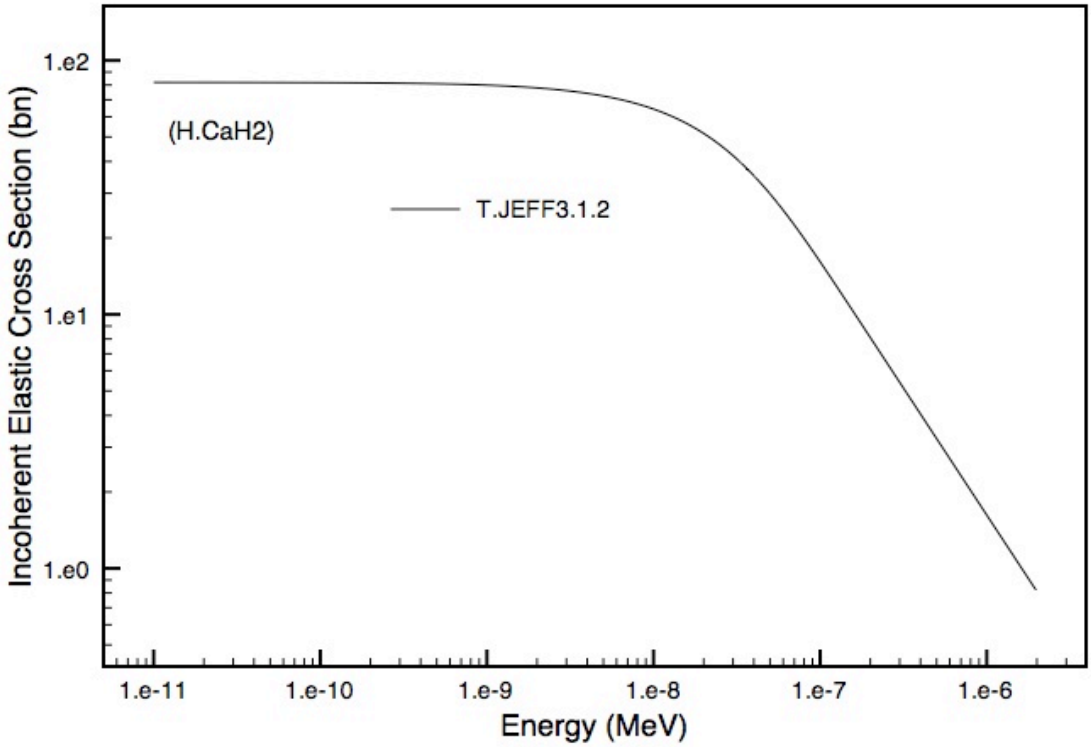

Figure 29

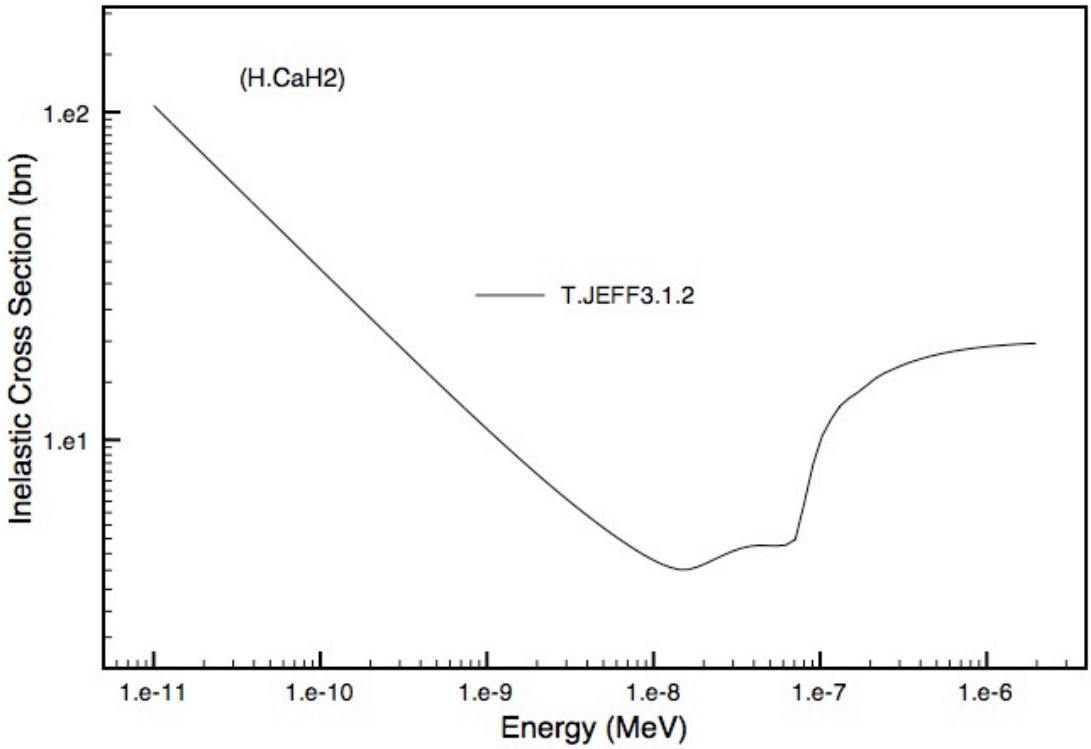

Figure 30

(H.CeH2), hydrogen bound in cerium hydride

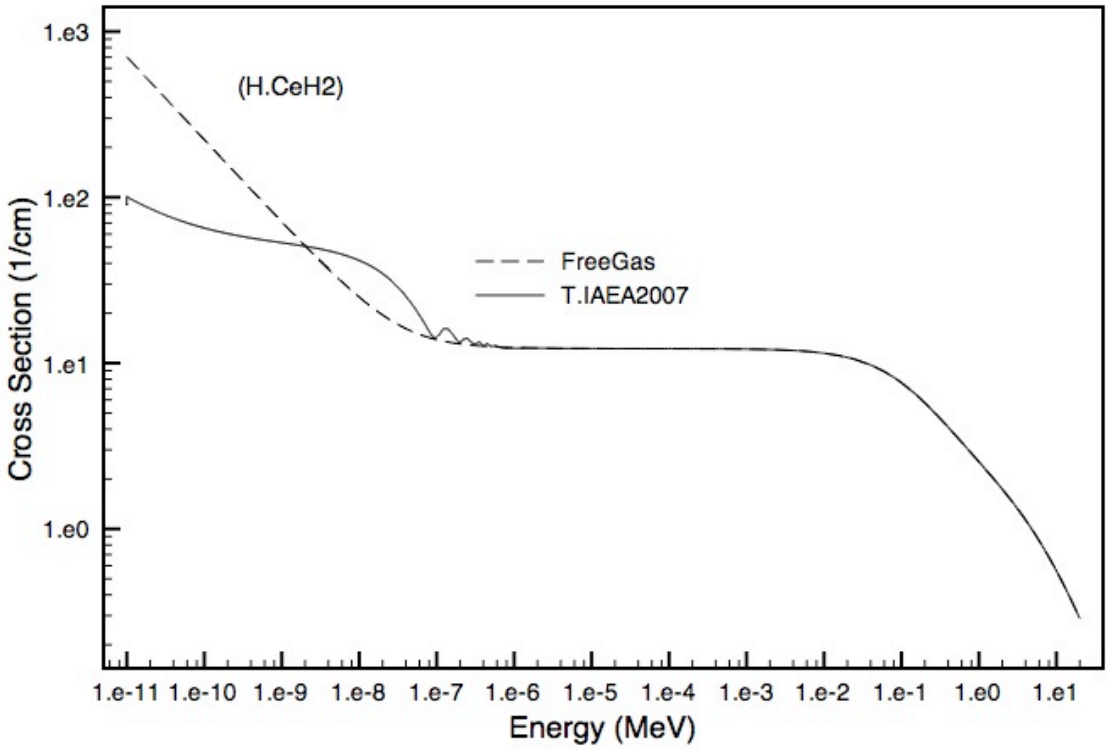

Figure 31

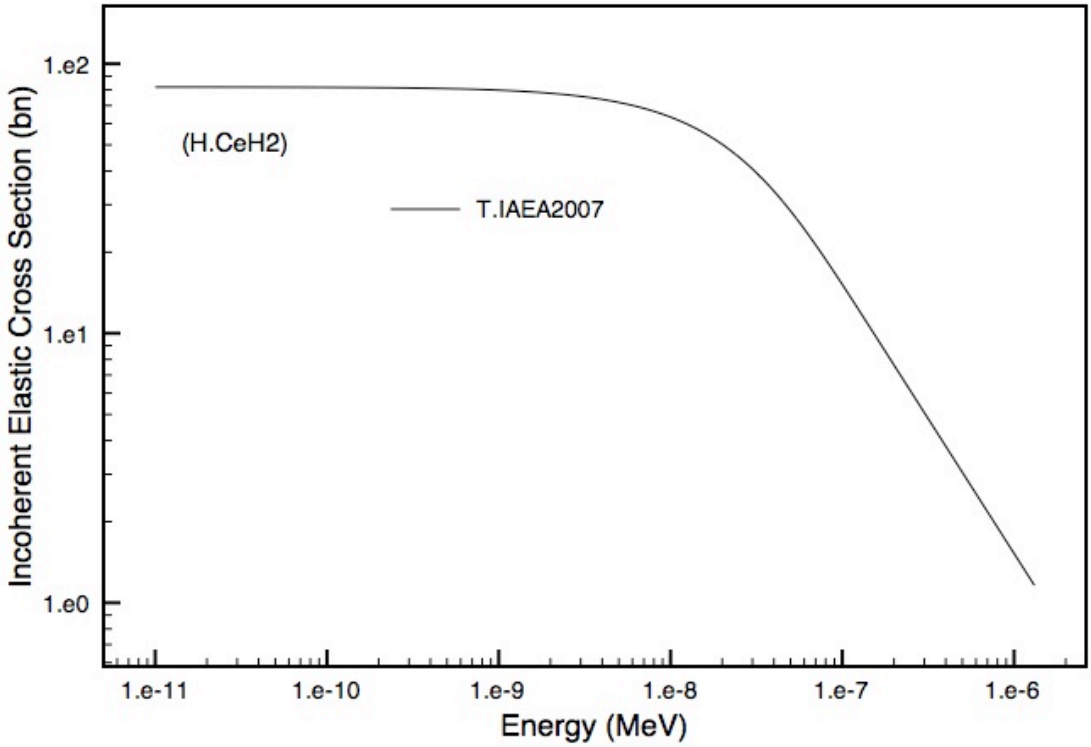

Figure 32

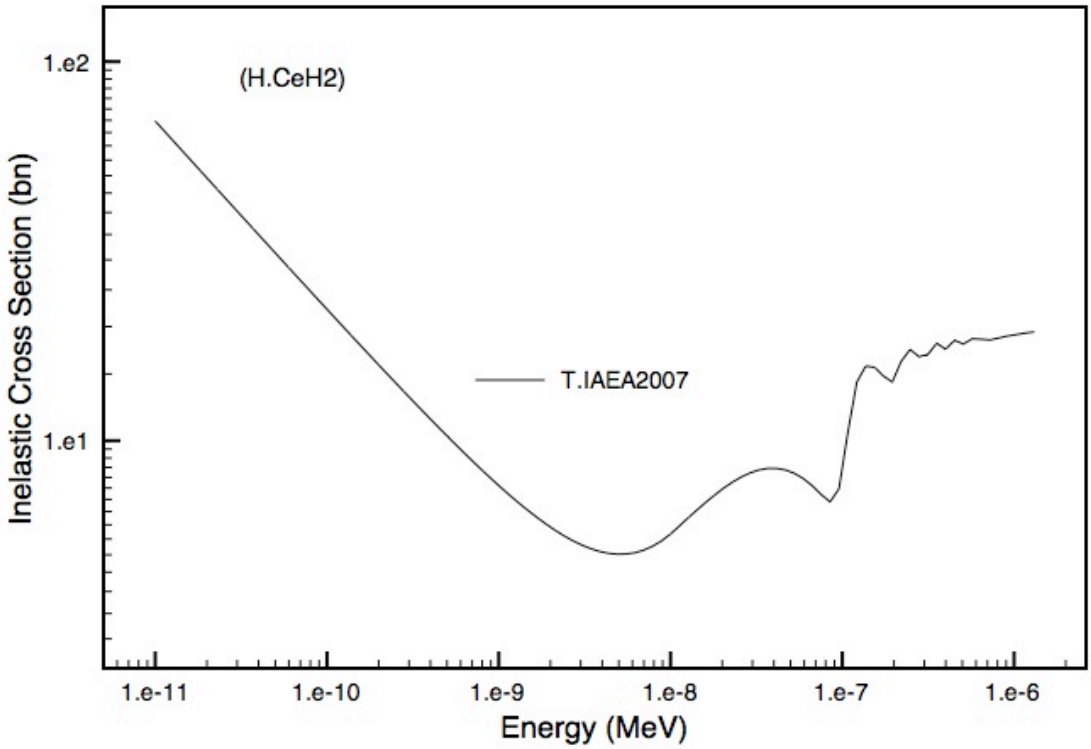

Figure 33

(H.CH2), hydrogen bound in polyethylene

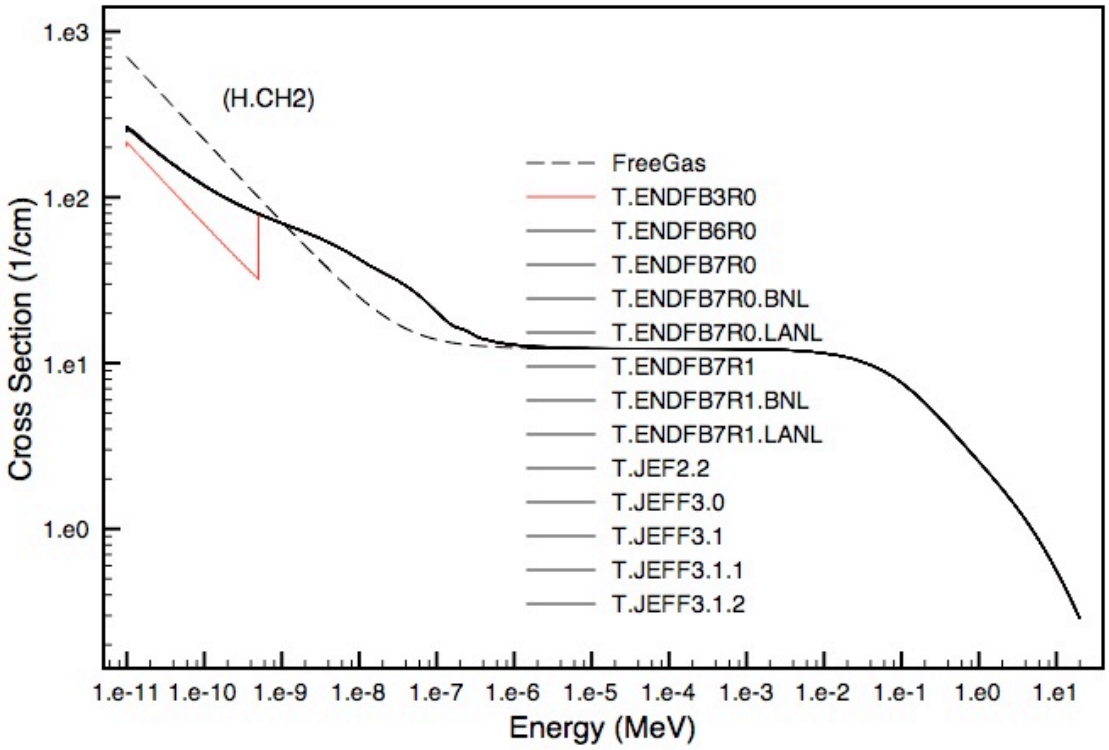

Figure 34

There is excellent agreement except for the T.ENDFB3R0 evaluation.

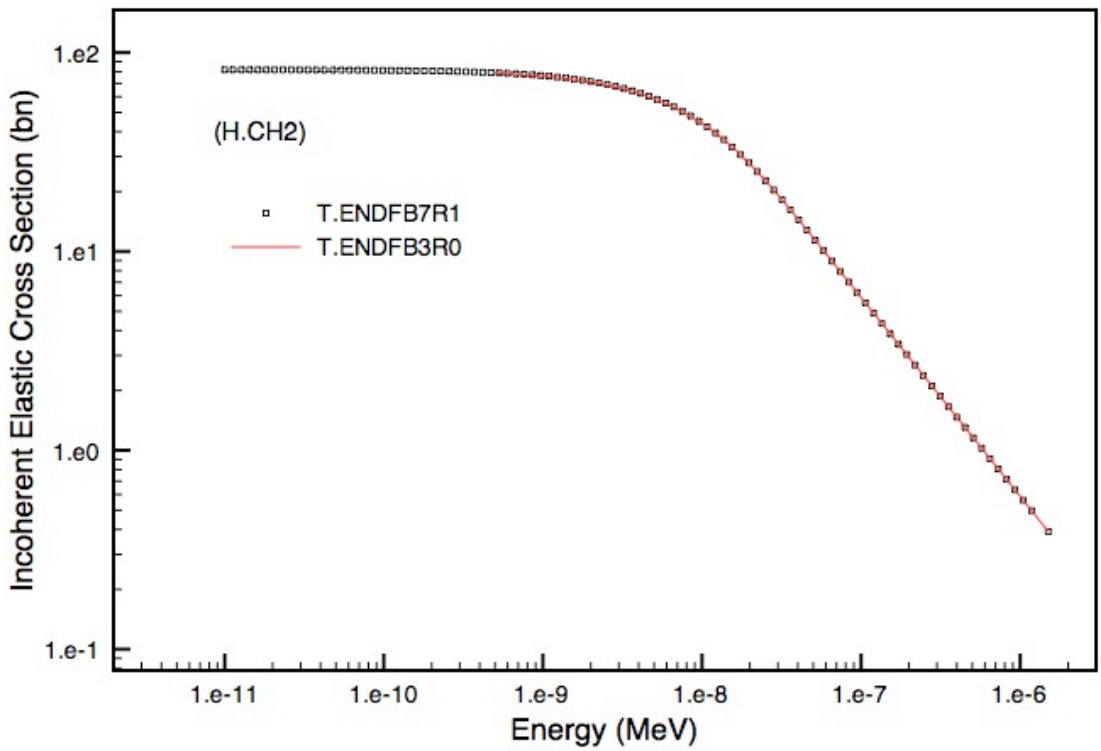

Figure 35

The T.ENDFB3R0 evaluation cuts off at 5.e-10 MeV rather than extending down to 1.e-11 MeV causing the low energy dip evident in Figure 34, otherwise there is excellent agreement.

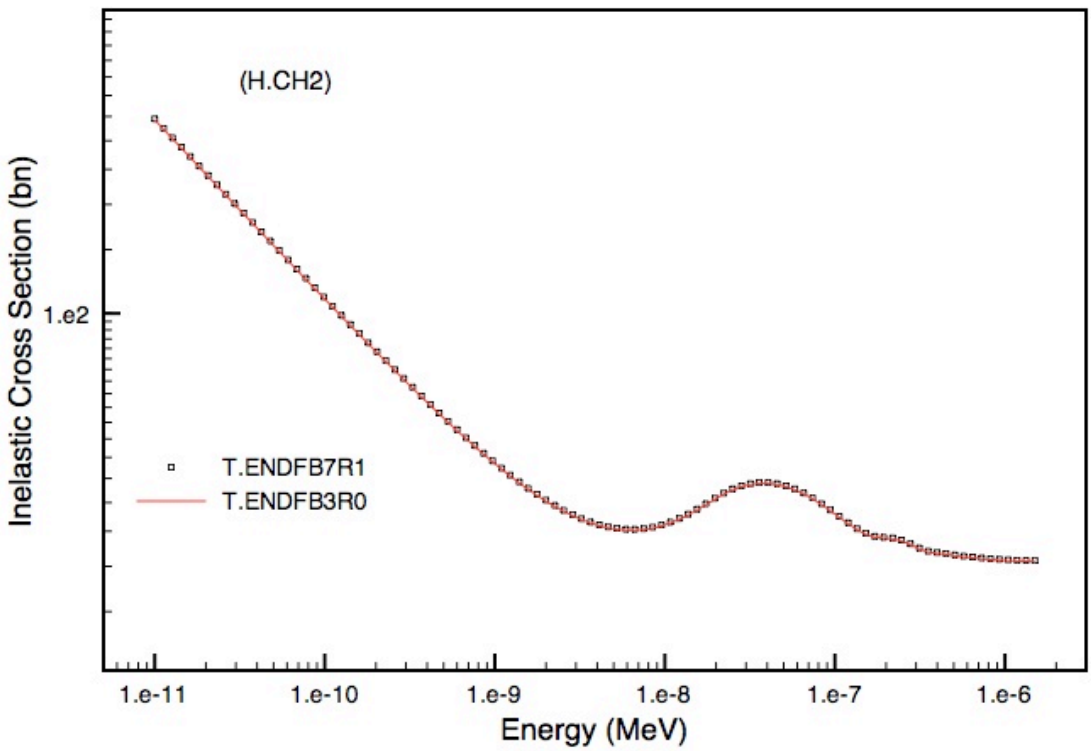

Figure 36

The inelastic cross sections show excellent agreement.

(H.H2O), hydrogen bound in water

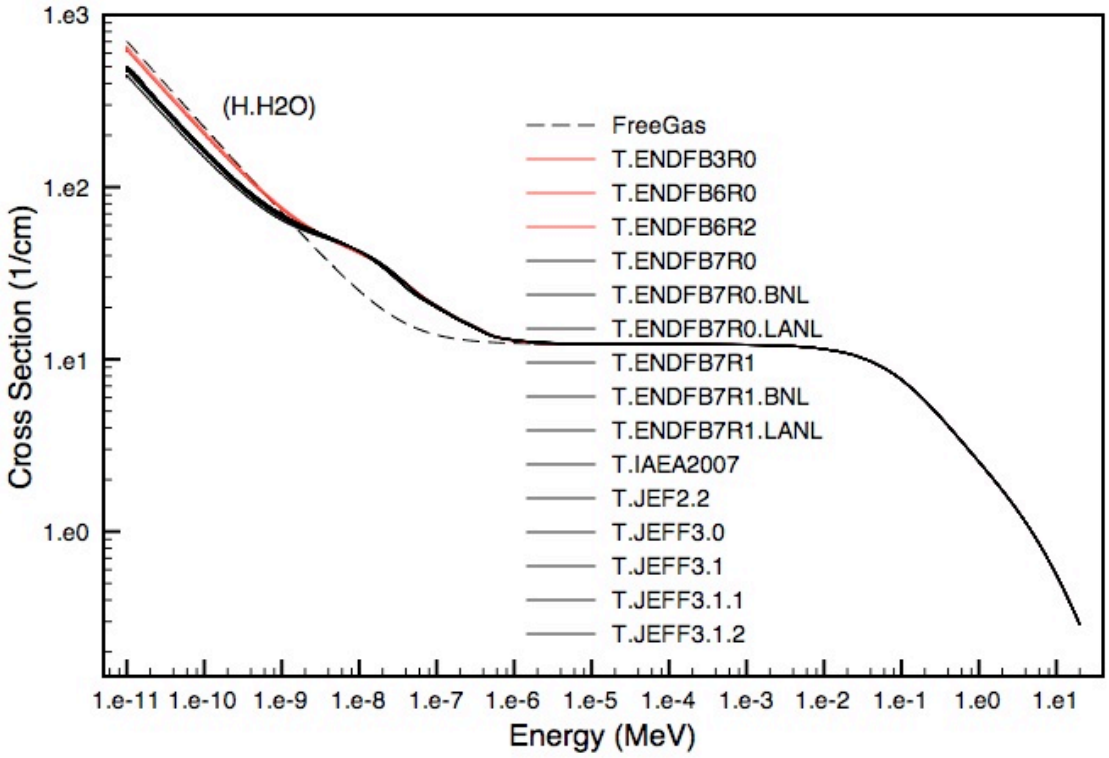

Figure 37

There is good agreement except for the T.ENDFB3R0, T.ENDFB6R0, and T.ENDFB6R2 evaluations.

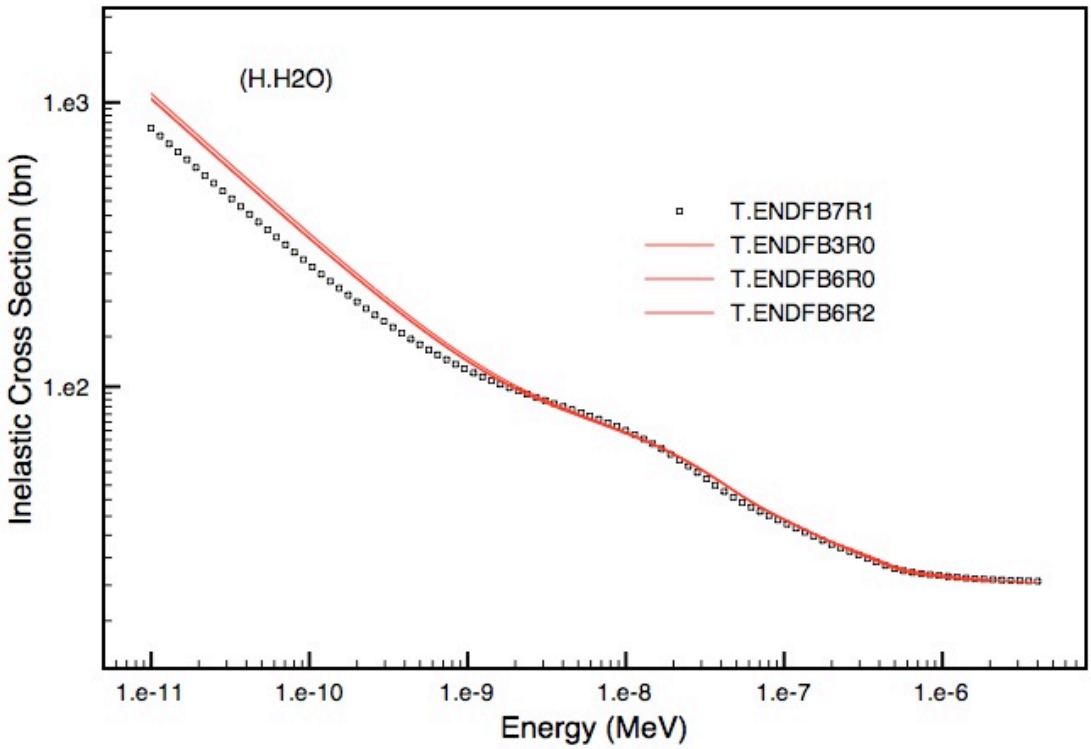

Figure 38

The T.ENDFB3R0, T.ENDFB6R0, and T.ENDFB6R2 evaluations differ from the later T.ENDFB7R1 evaluation.

(H.TiH2)

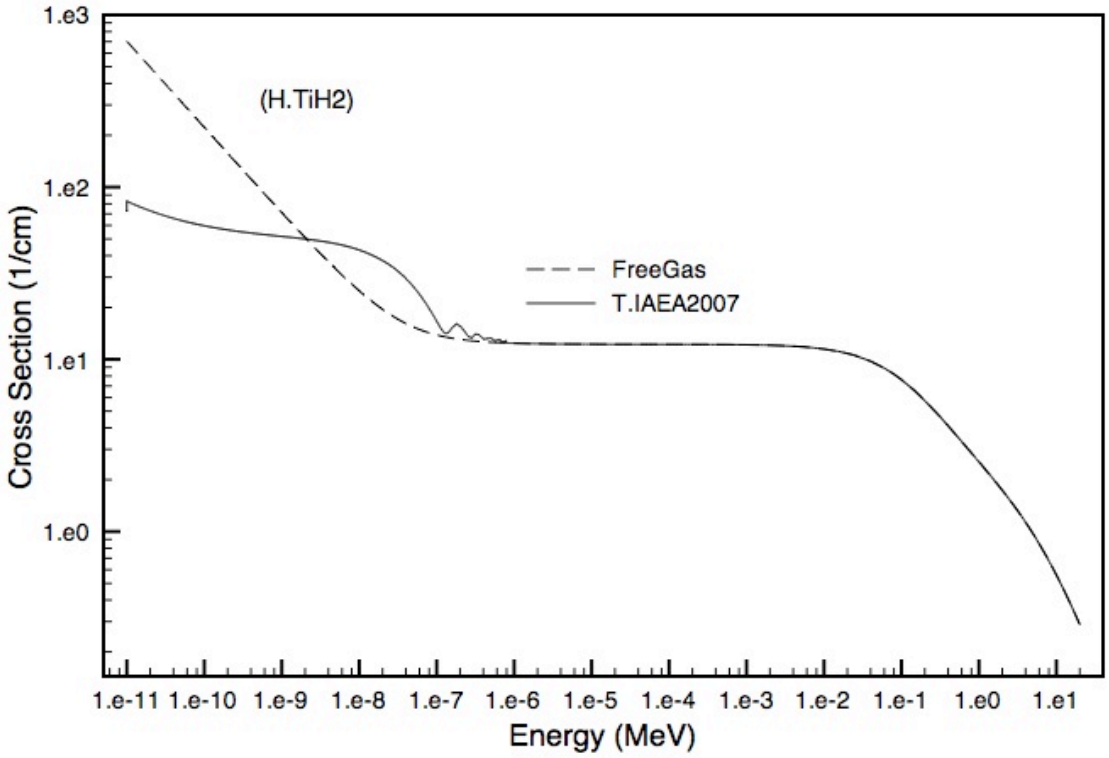

Figure 39

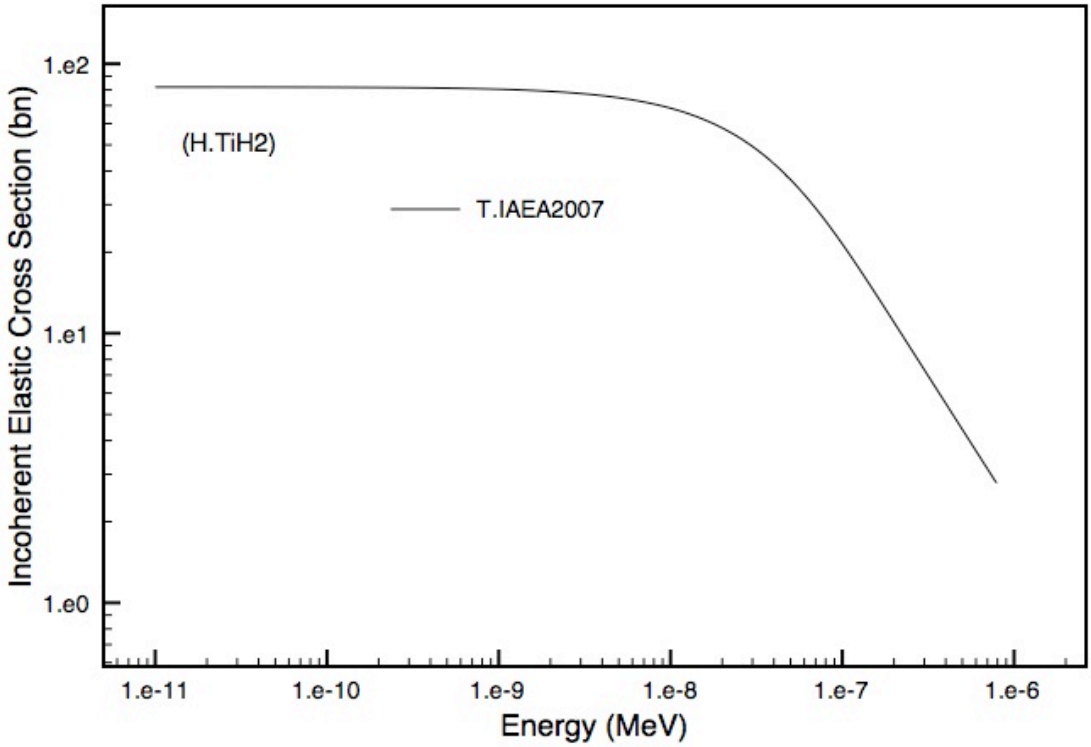

Figure 40

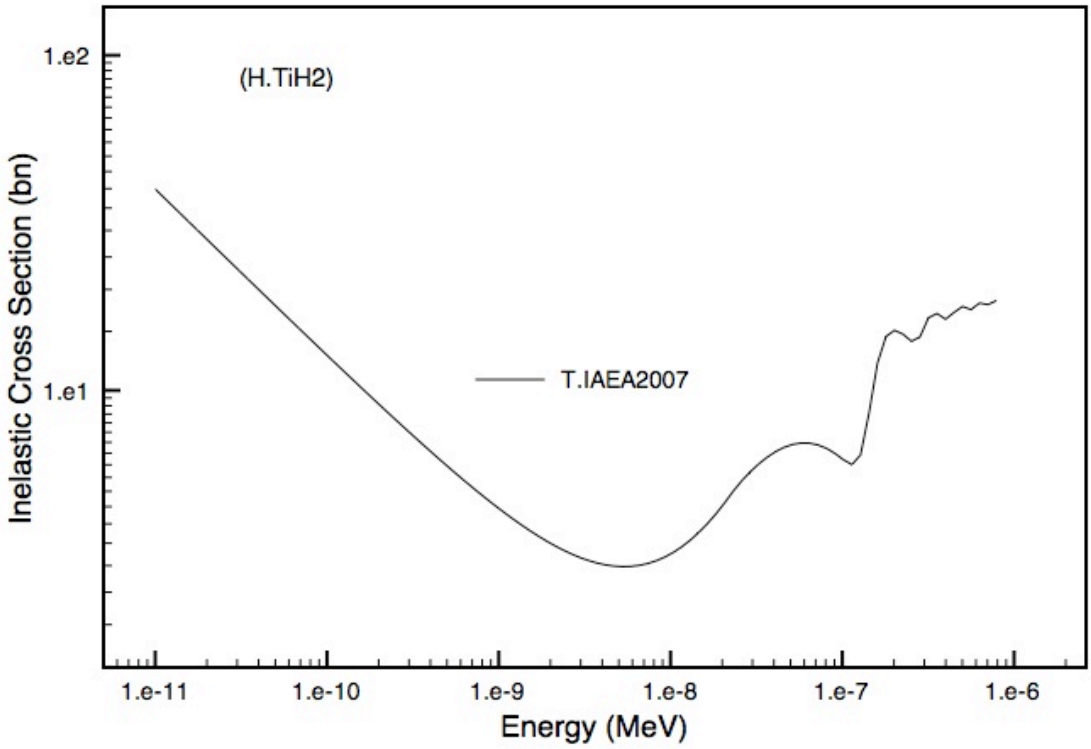

Figure 41

(H.YH2)

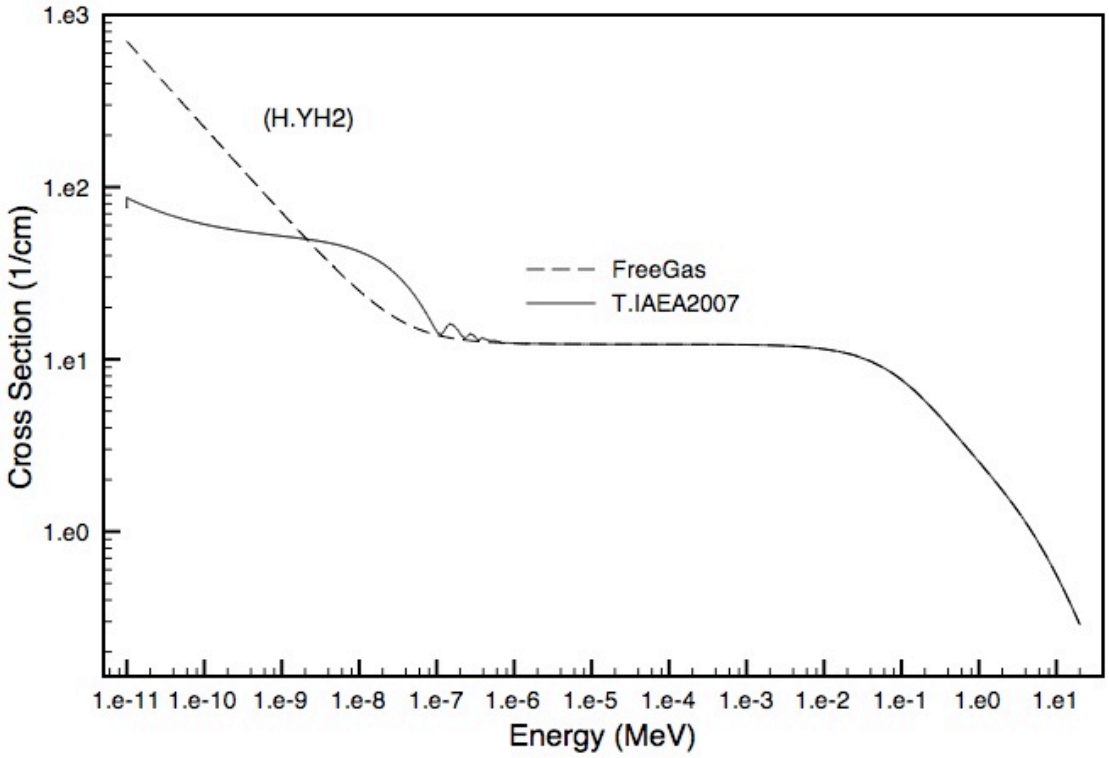

Figure 42

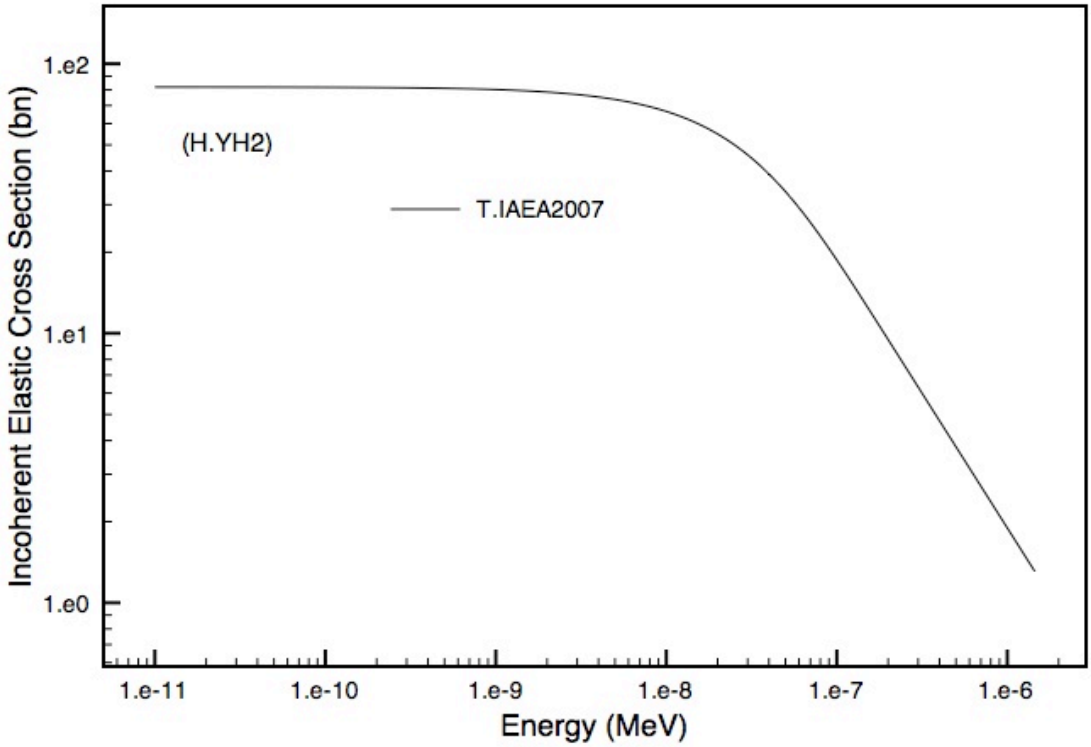

Figure 43

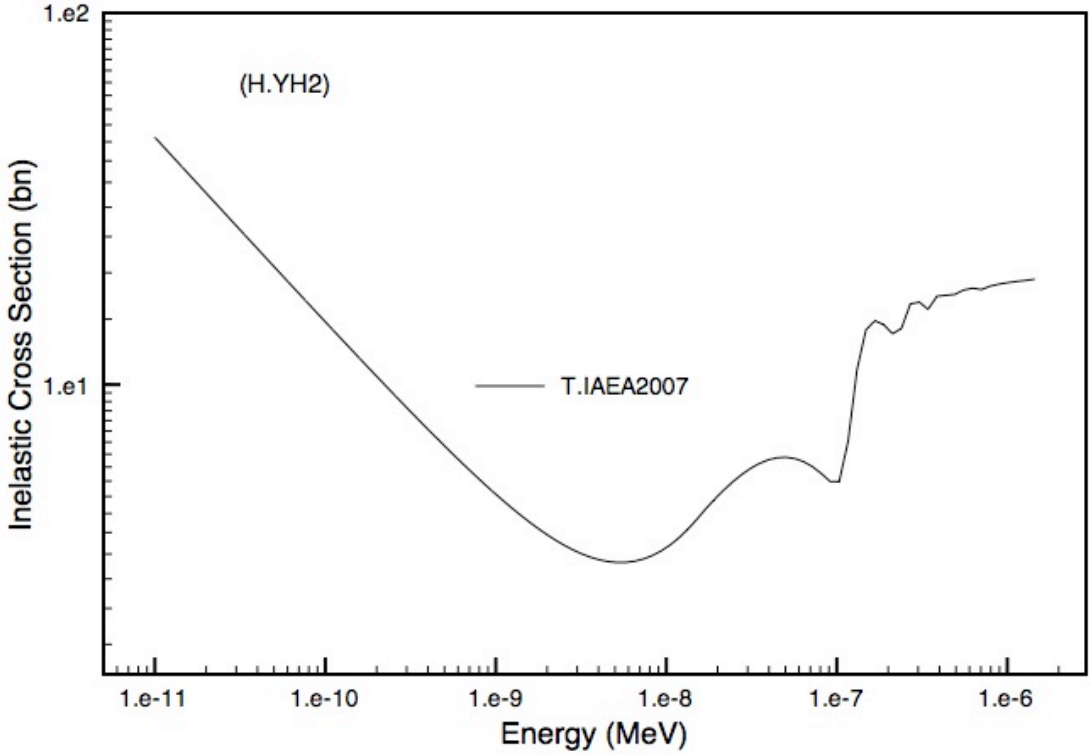

Figure 44

(H.ZrH)

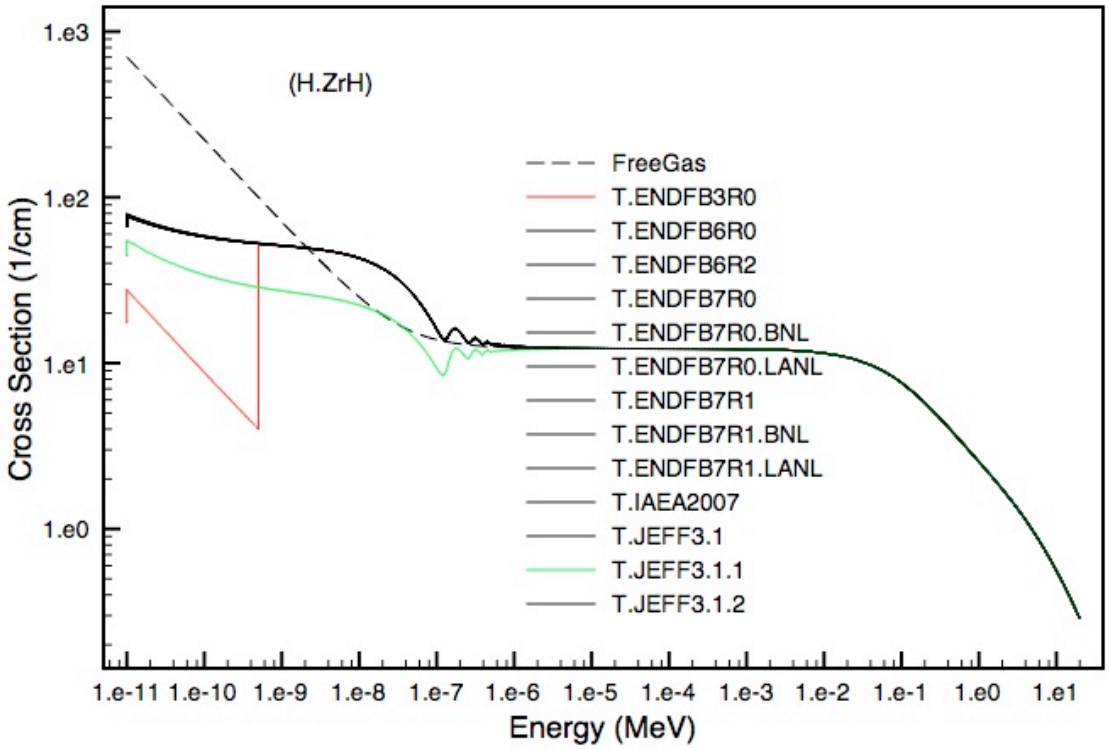

Figure 45

All agree well except for the T.ENDFB3R0 evaluation, which is low at low energies, and the T.JEFF3.1.1 evaluation, which seems definitely out of place.

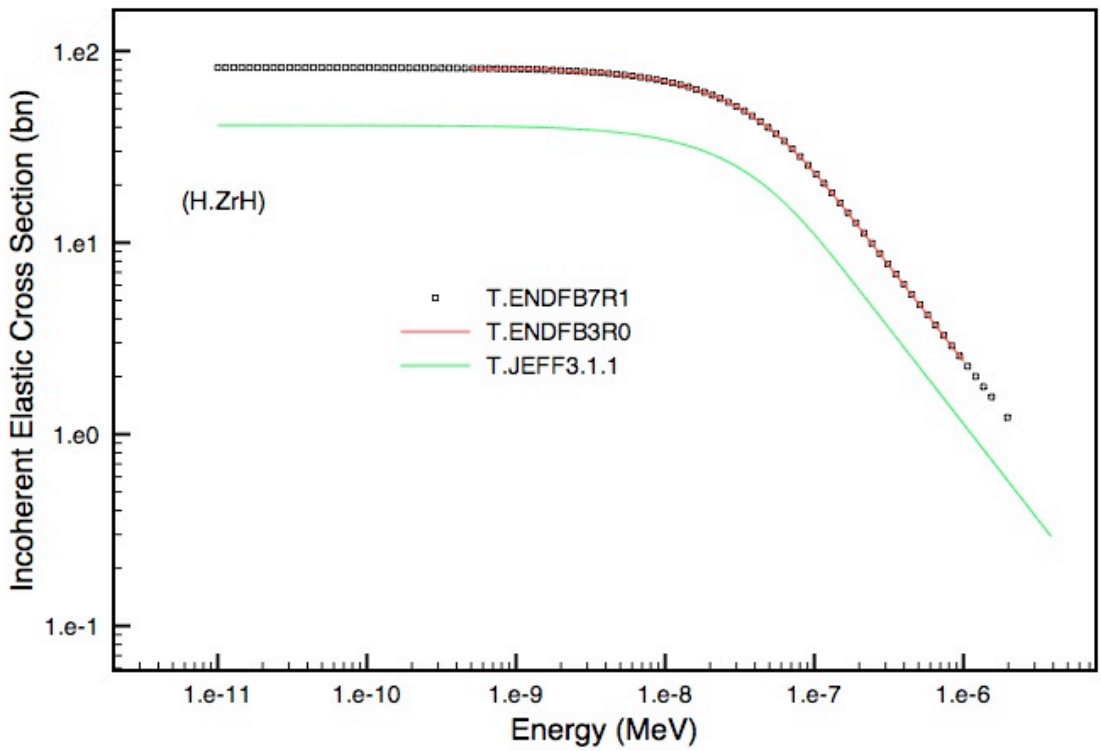

Figure 46

The T.ENDFB3R0 evaluation cuts off at 5.e-10 MeV rather than extending down to 1.e-11 MeV causing the low energy dip evident in Figure 45. The T.JEFF3.1.1 evaluation does not agree at all.

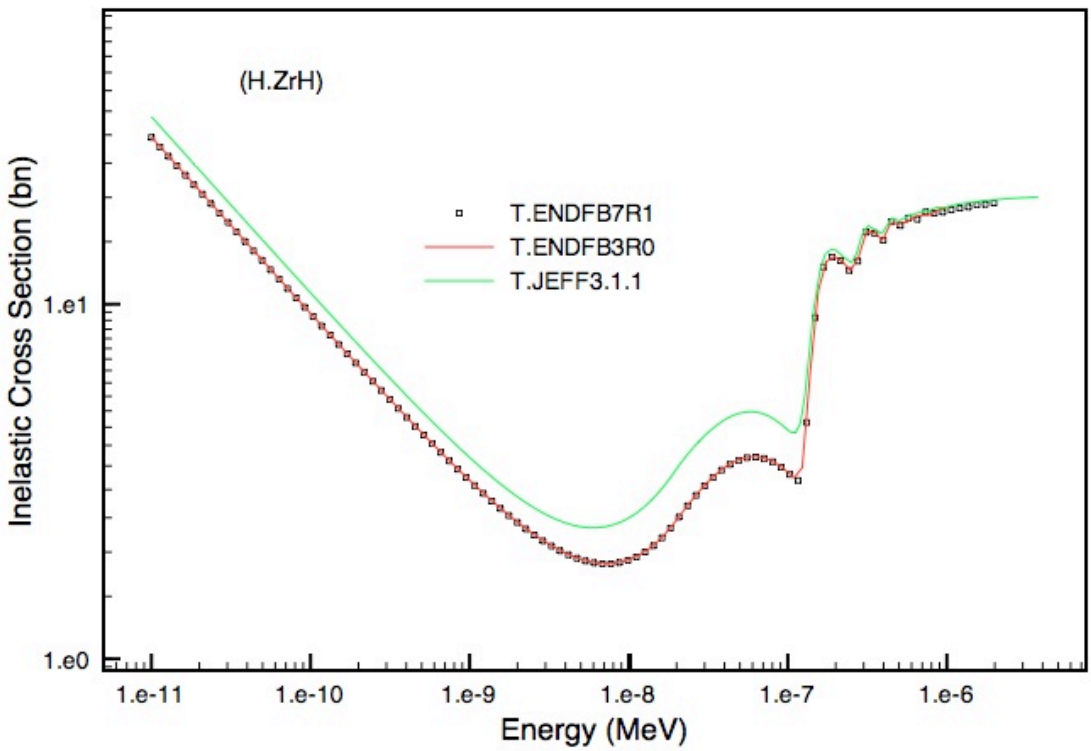

Figure 47

T.ENDFB3R0 agrees well, T.JEFF3.1.1 does not.

(Mg)

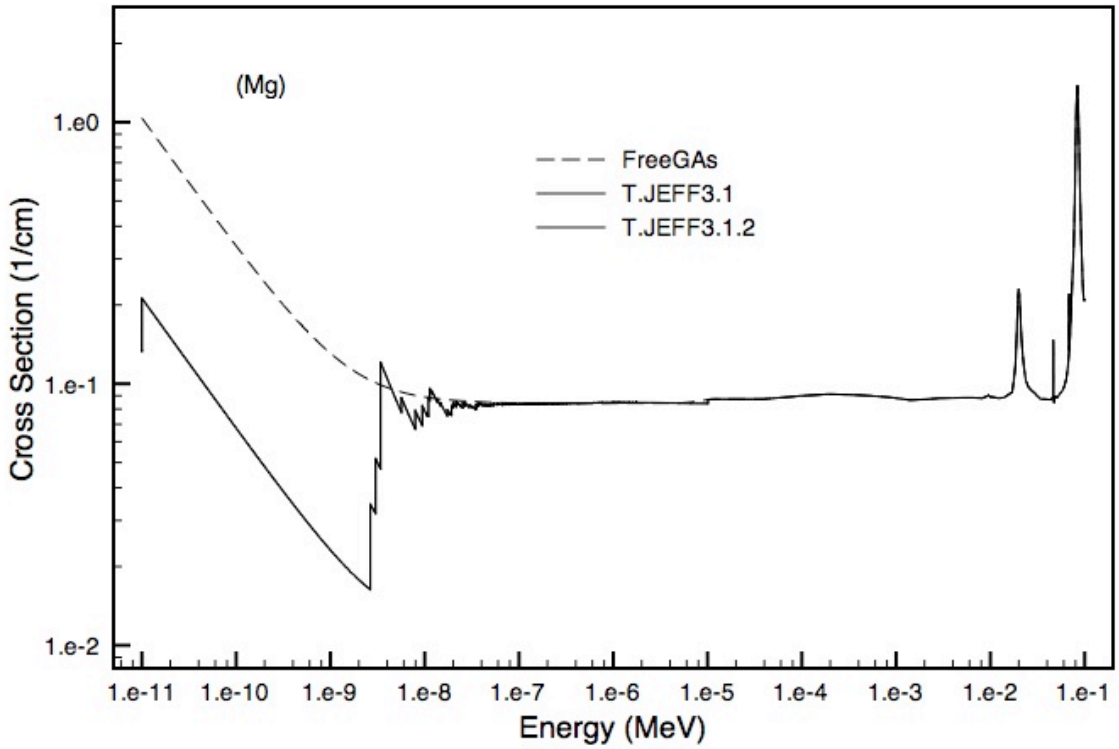

Figure 48

The results are identical.

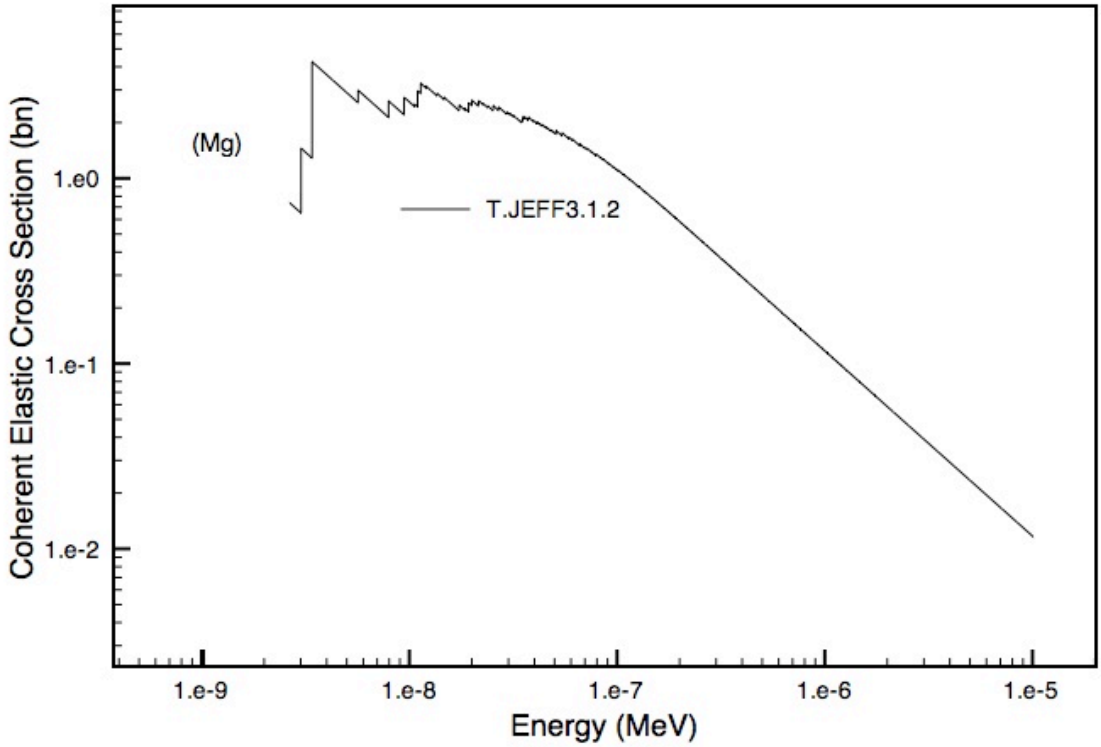

Figure 49

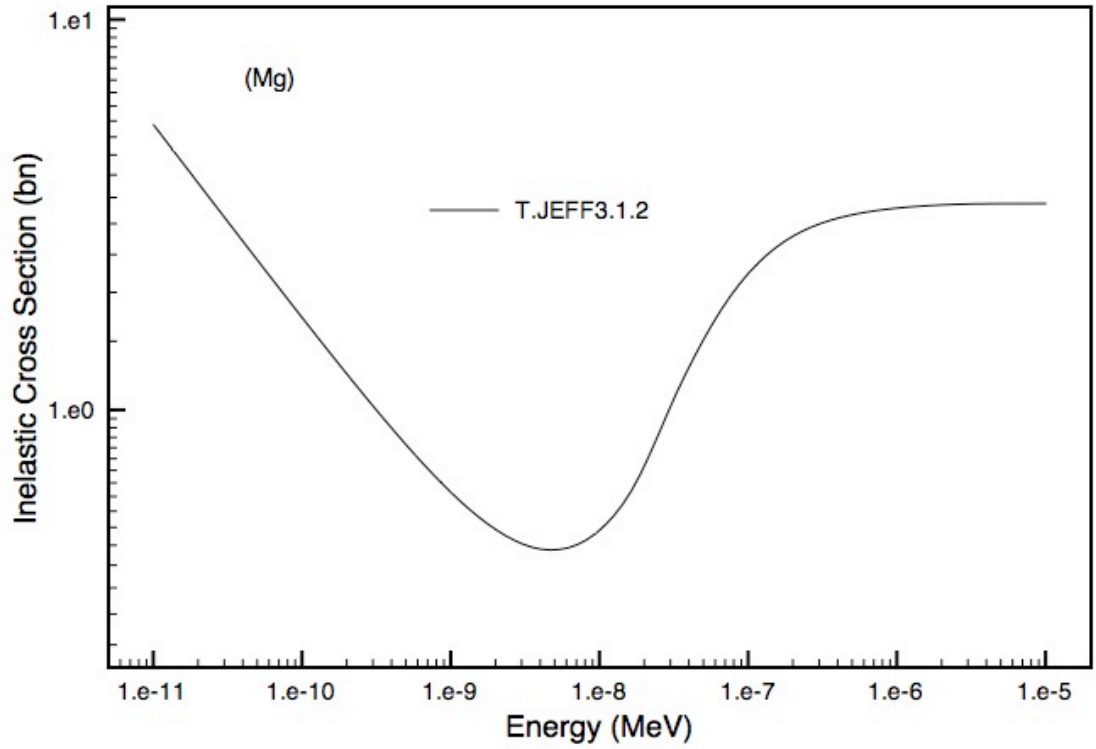

Figure 50

(O.BeO)

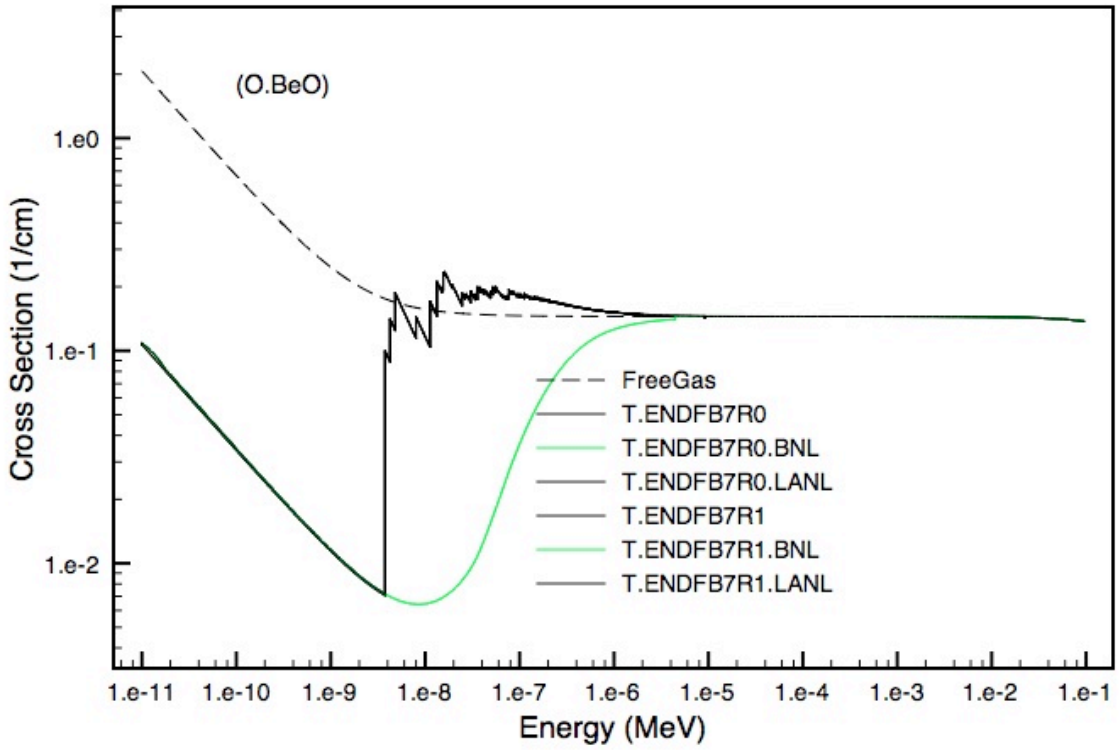

Figure 51

There is good agreement except for the BNL evaluations, which don't show the edge structure.

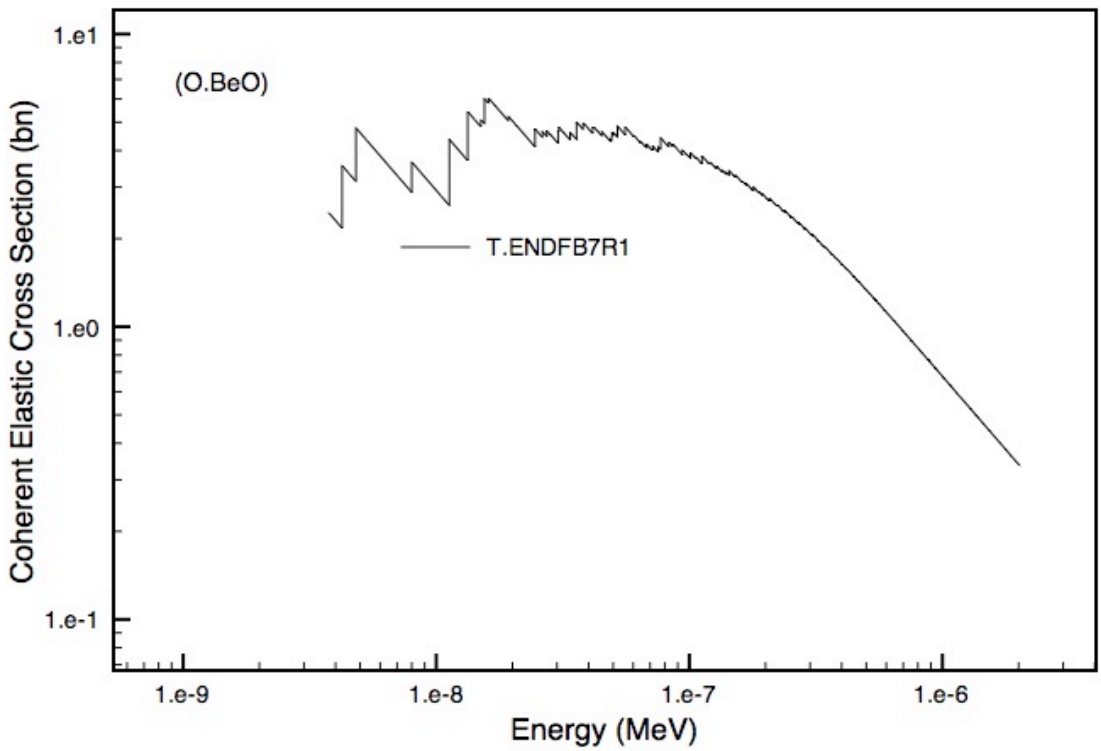

Figure 52

There is no coherent elastic component with the BNL evaluations.

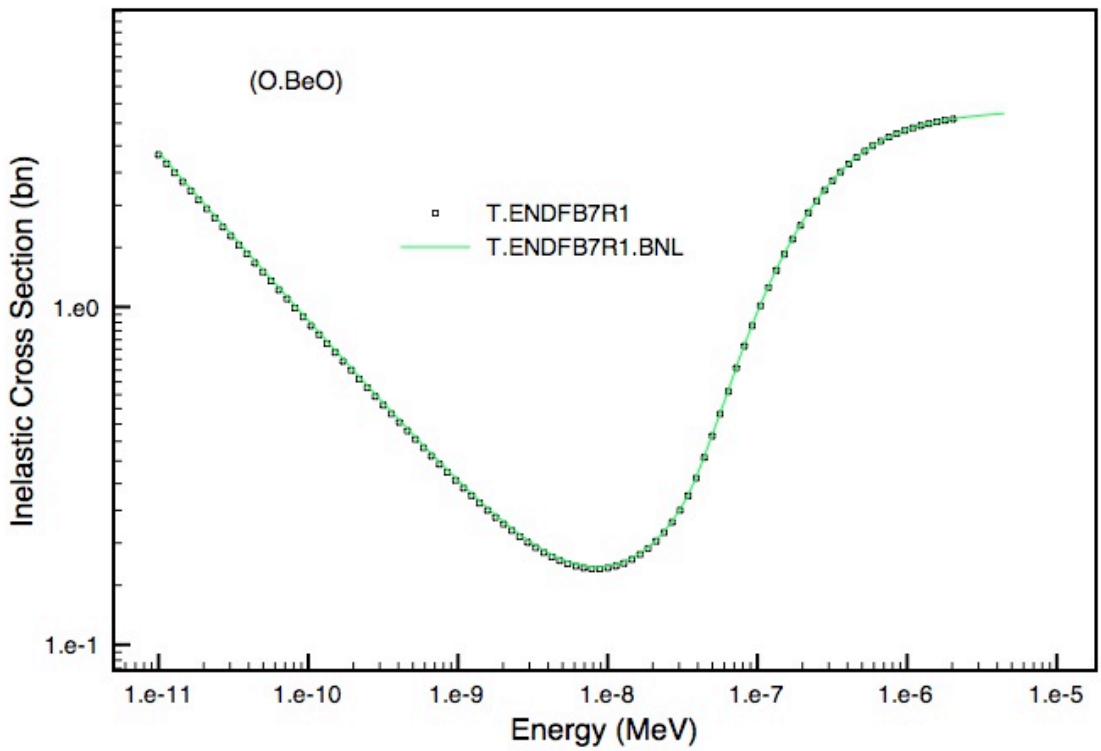

Figure 53

The inelastic components are in excellent agreement.

(O.UO2)

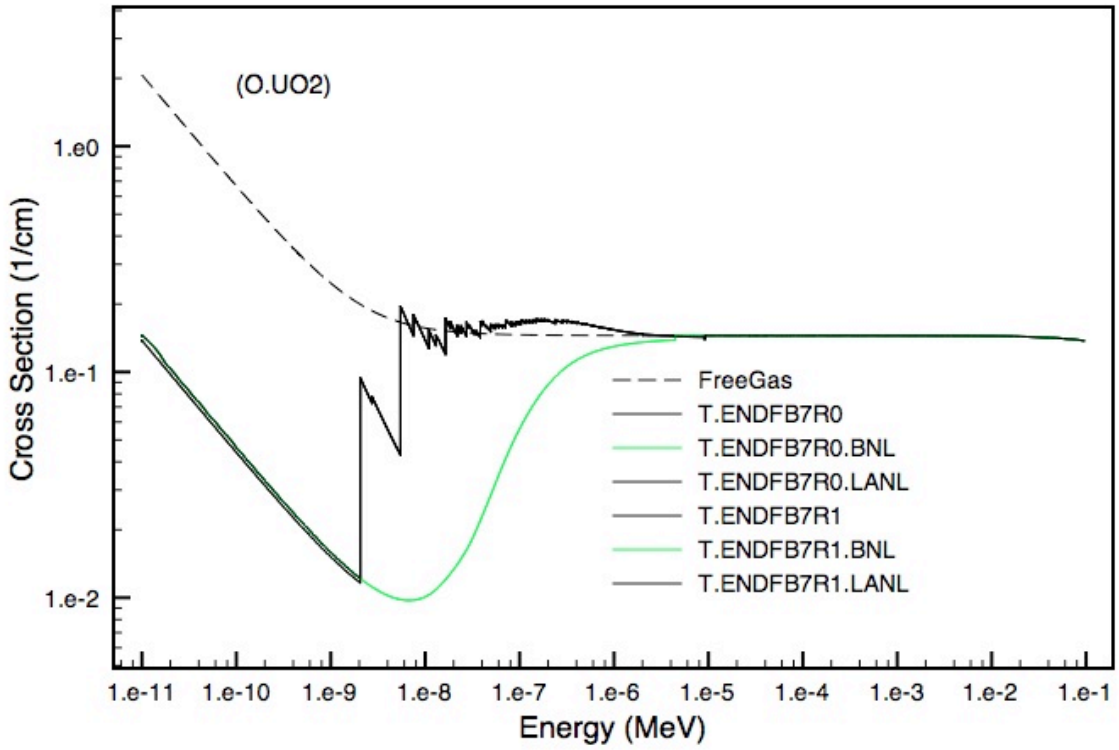

Figure 54

There is good agreement except for the BNL evaluations, which don't show the edge structure.

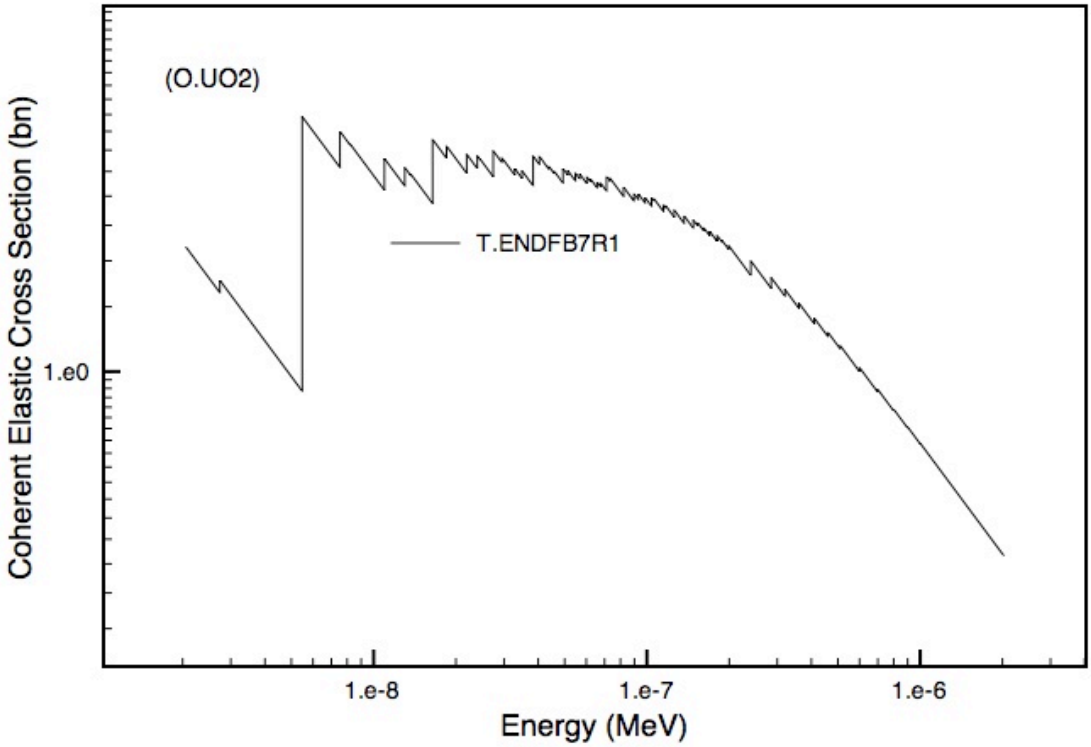

Figure 55

There is no coherent elastic component with the BNL evaluations.

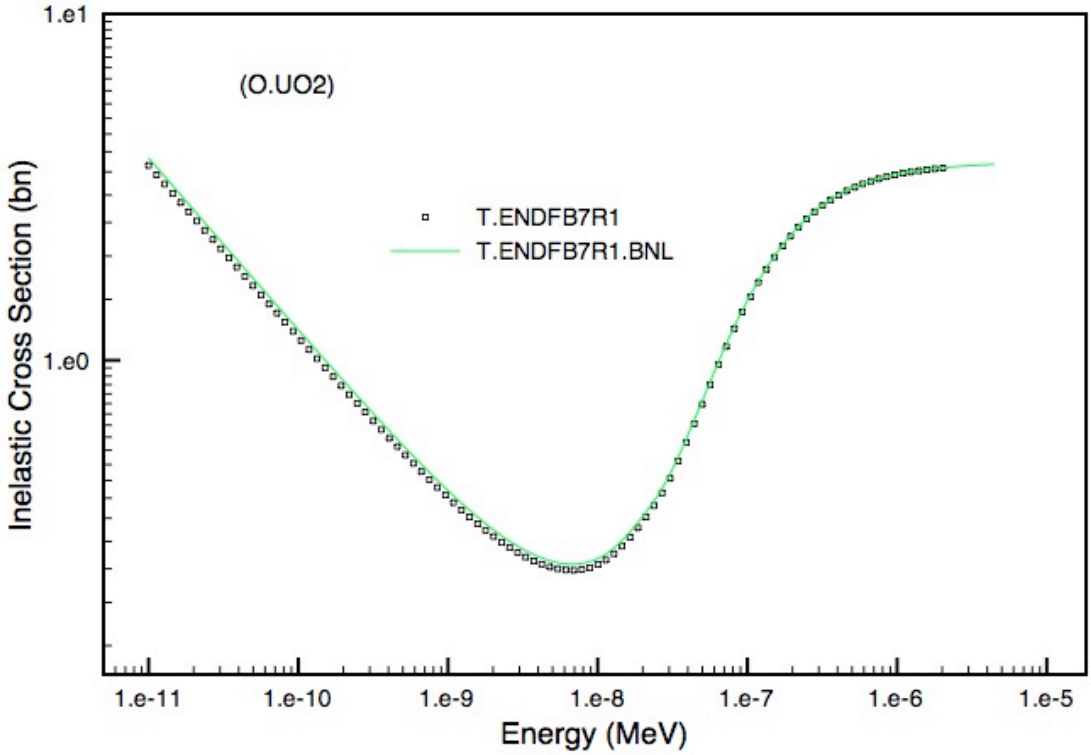

Figure 56

There is good agreement in the inelastic components.

(SiO2)

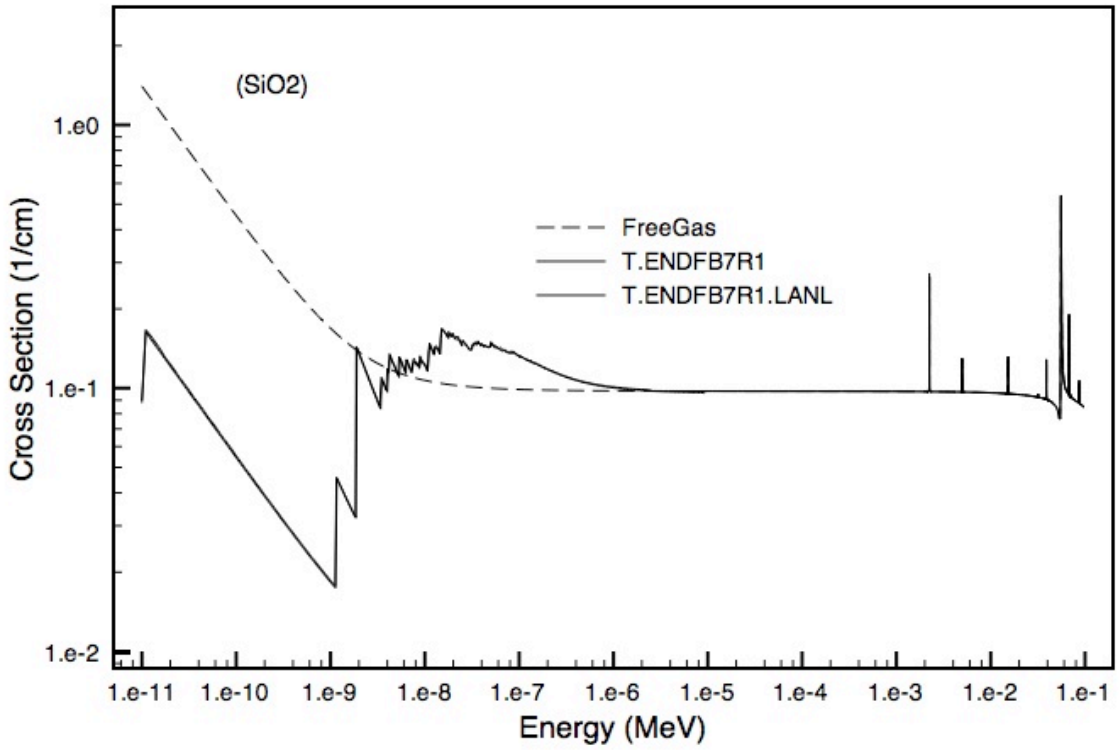

Figure 57

There is excellent agreement. The plots were truncated at 0.1 MeV to better show the thermal region.

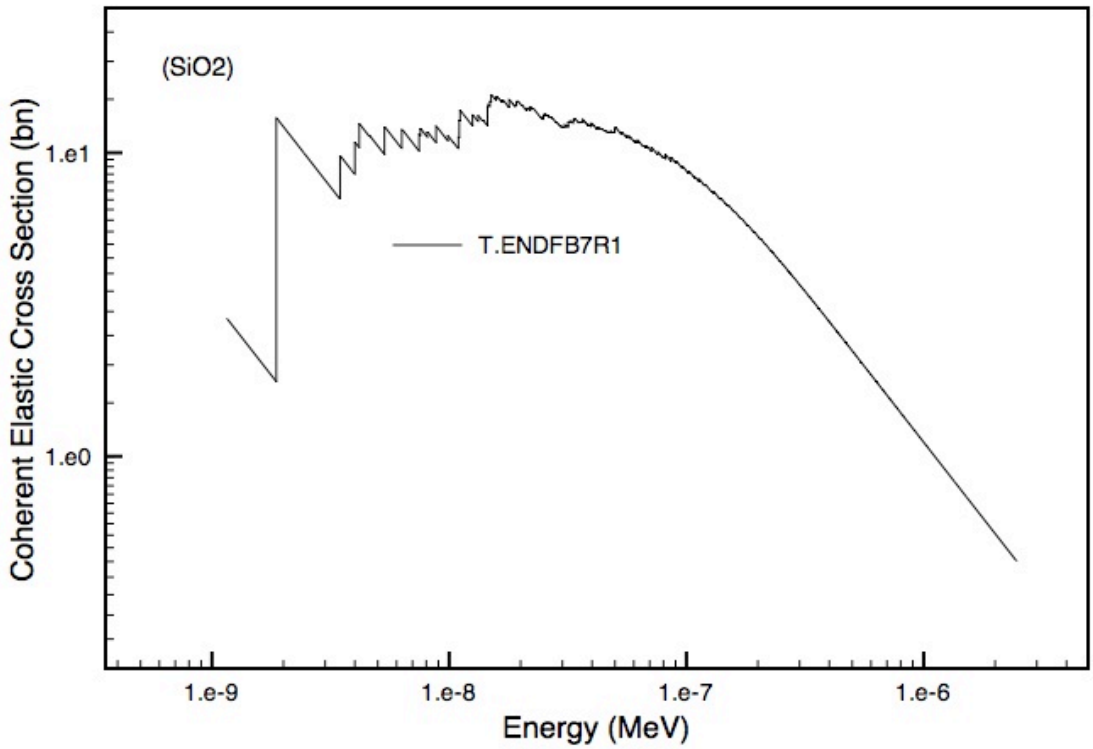

Figure 58

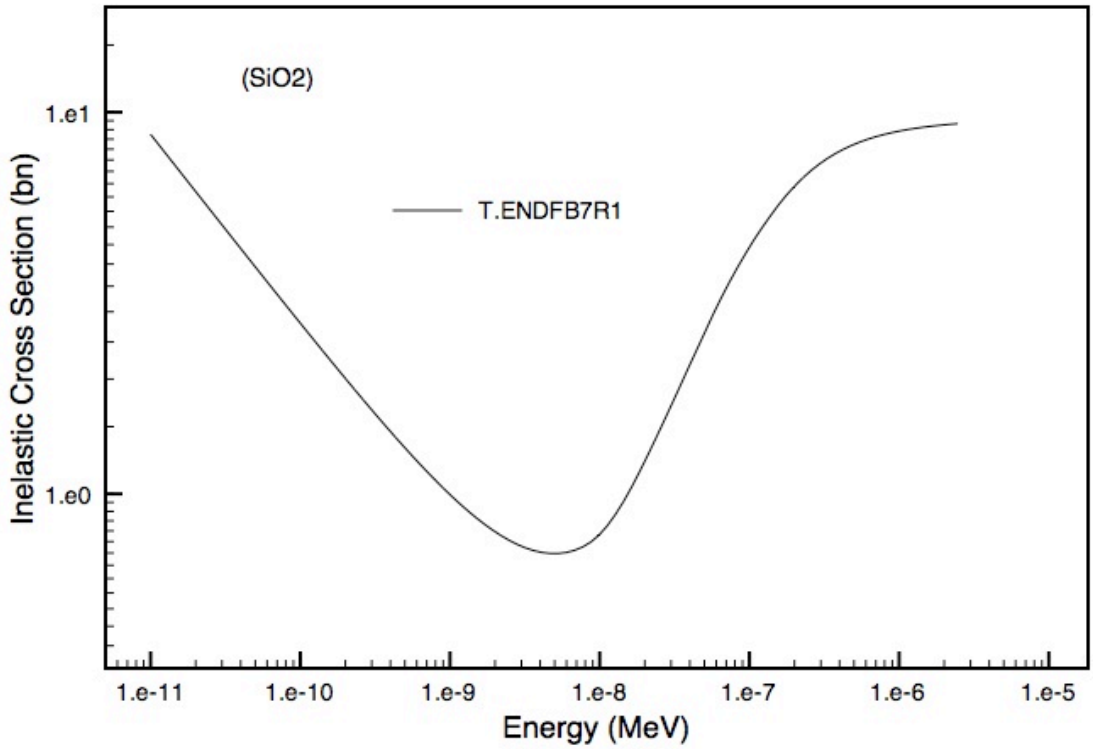

Figure 59

(U.UO2)

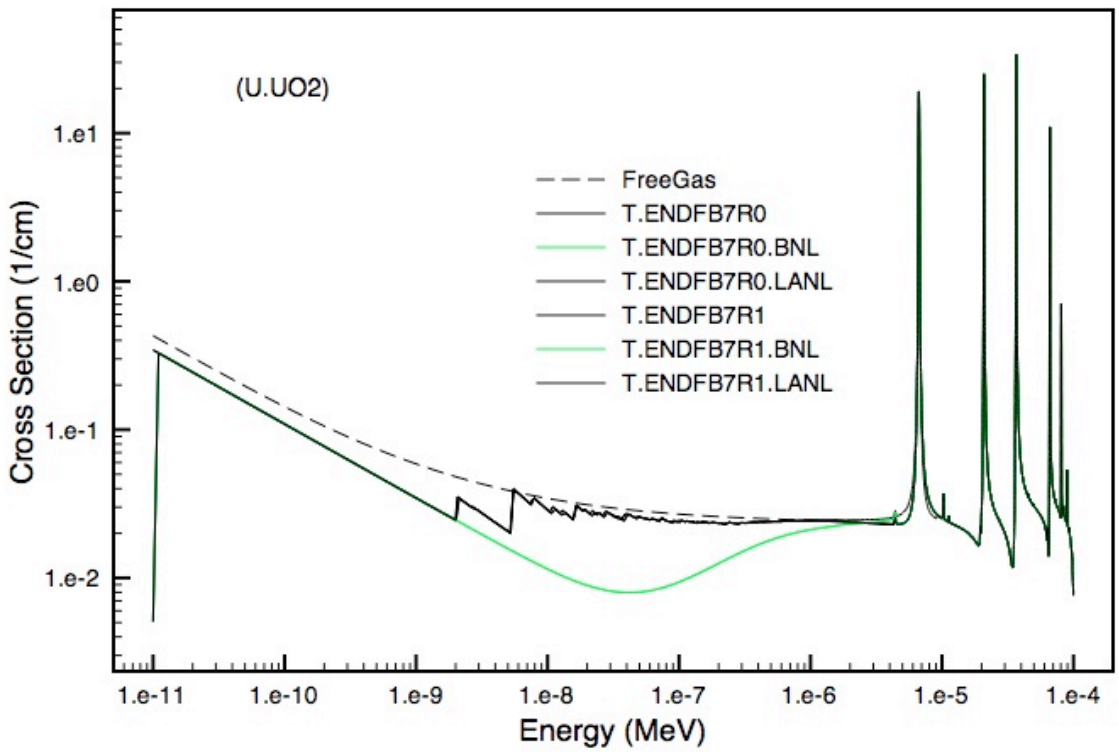

Figure 60

There is good agreement except for the BNL evaluations, which don't show the edge structure. The plots were truncated at 1.e-4 MeV to better show the thermal region.

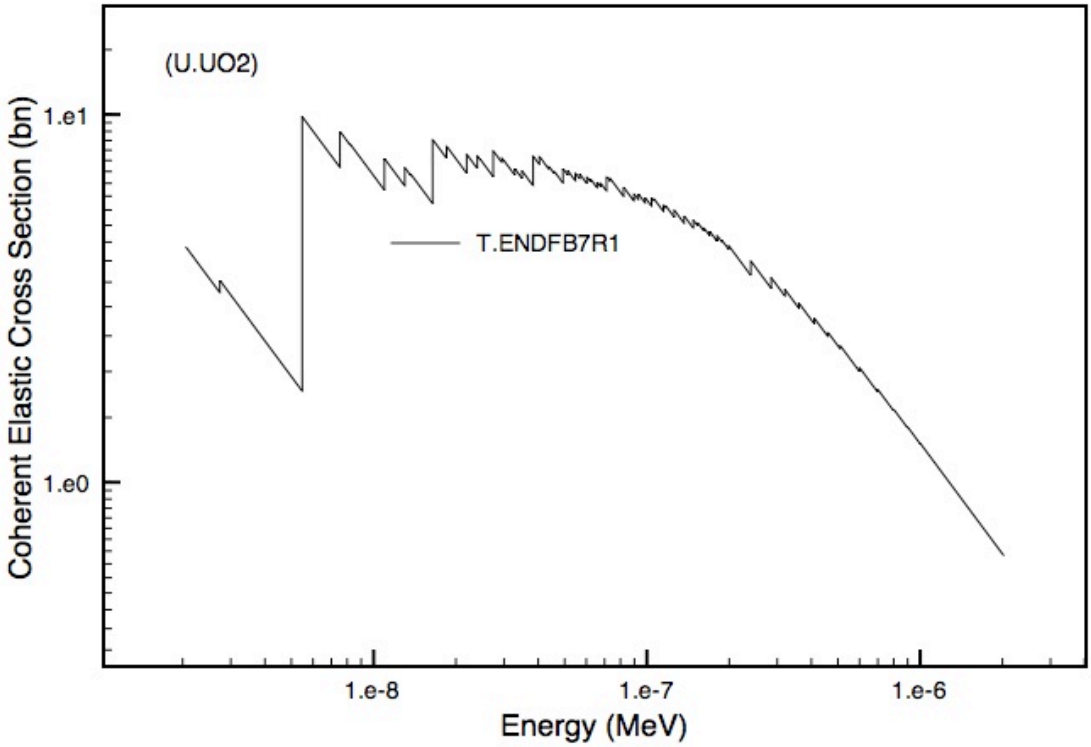

Figure 61

There is no coherent elastic component with the BNL evaluations.

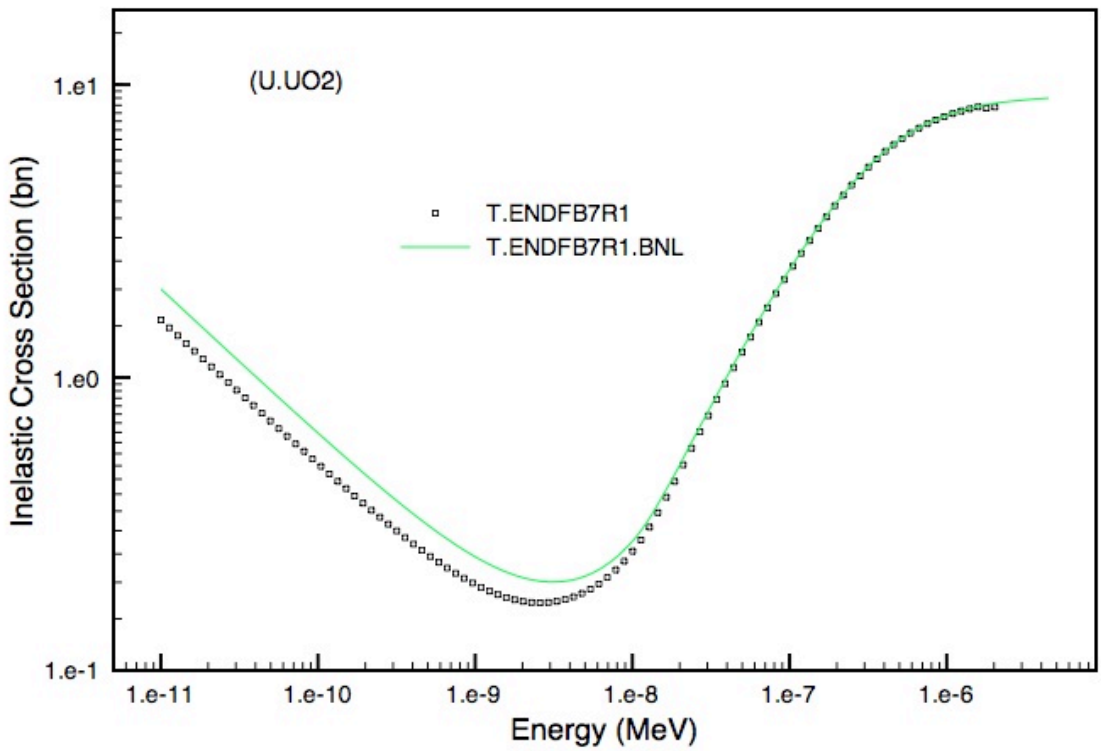

Figure 62

There are significant differences below ~1.e-8 MeV.

(UO2)

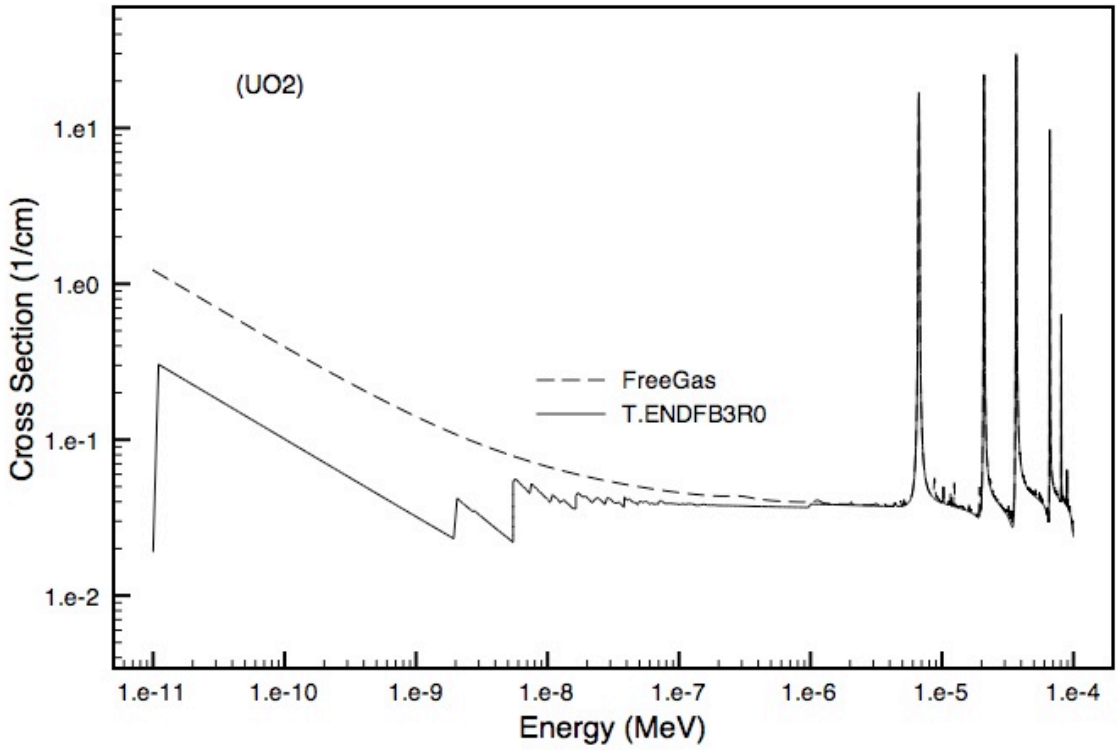

Figure 63

The plot is truncated at 1.e-4 MeV to better show the thermal region.

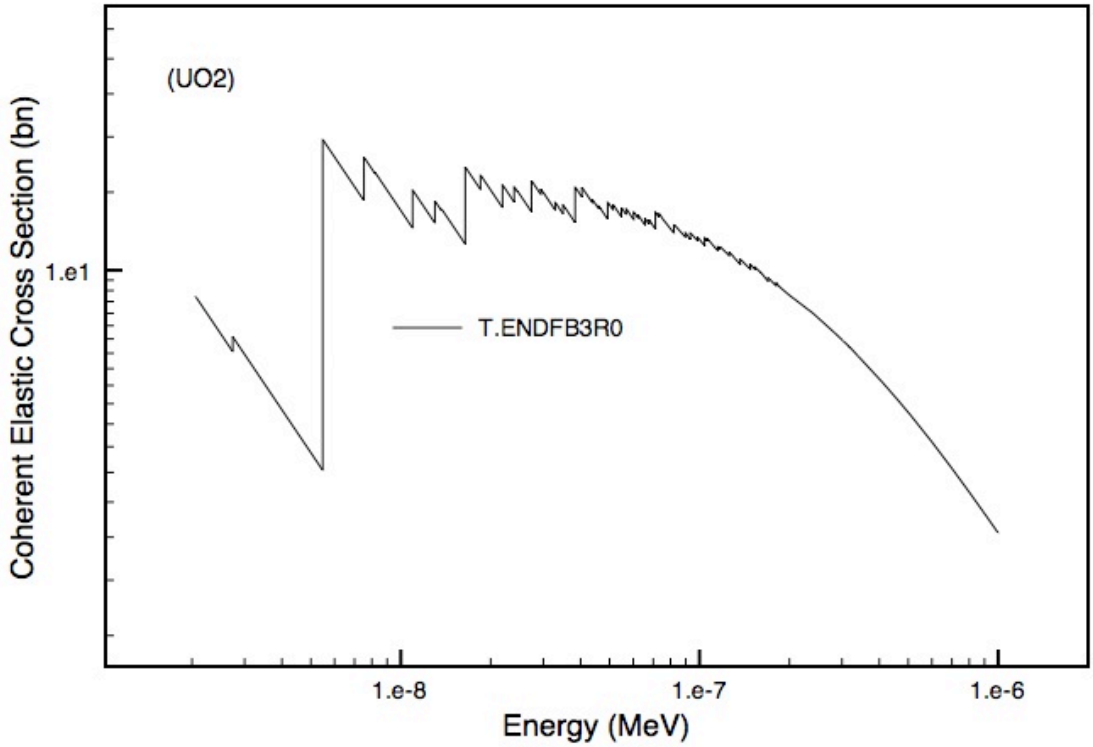

Figure 64

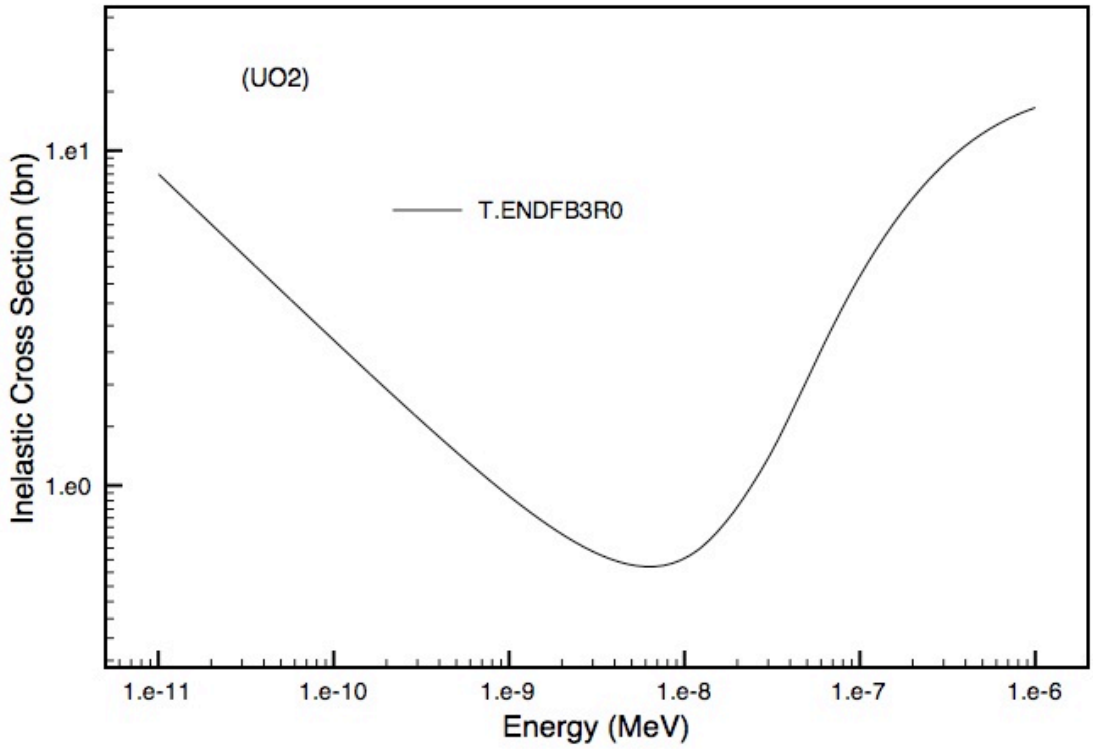

Figure 65

(Zr.ZrH)

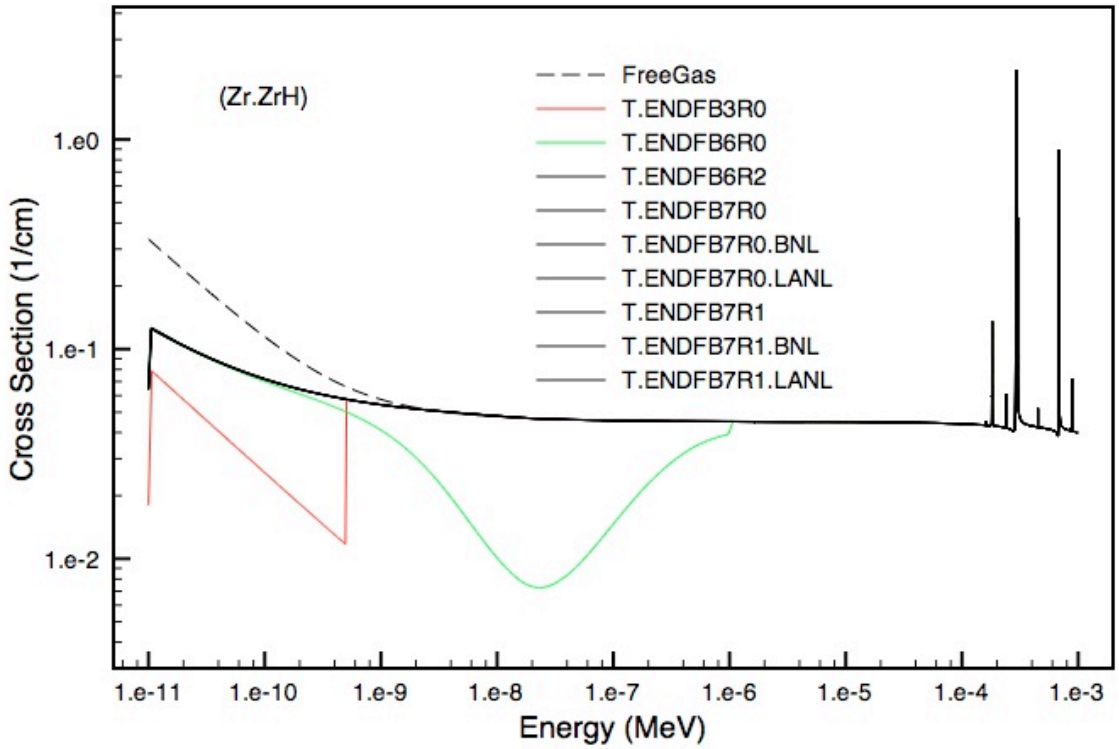

Figure 66

All agree well with the exception of T.ENDFB3R0 and T.ENDFB6R0.

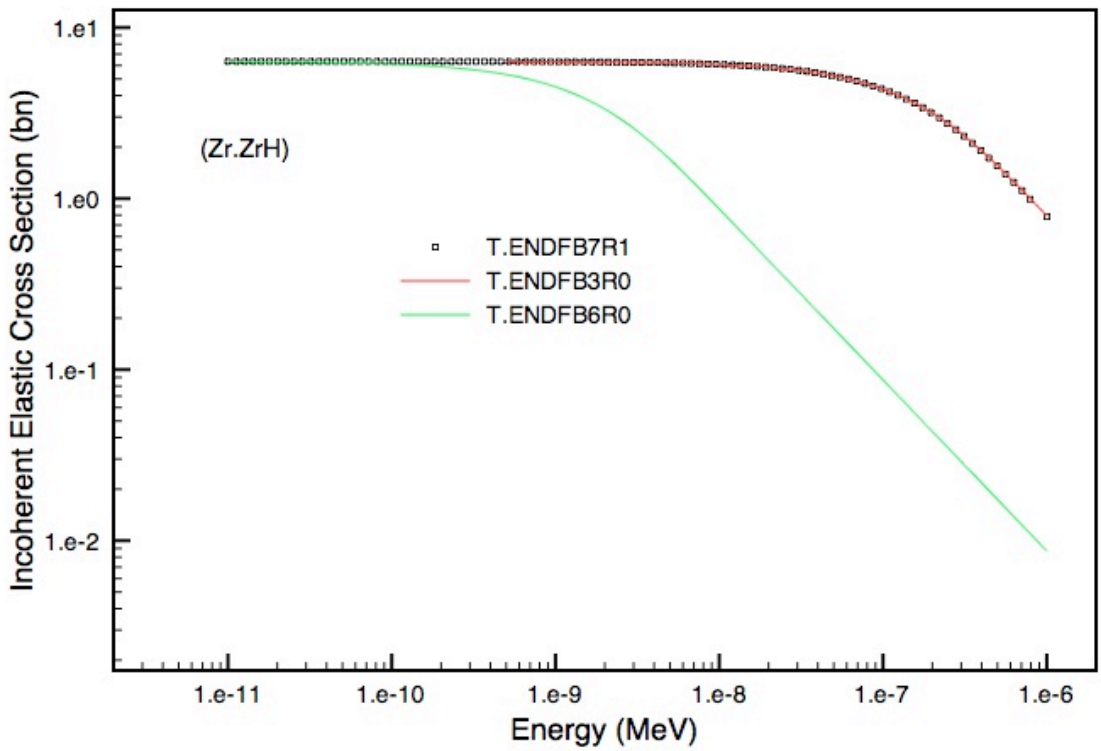

Figure 67

The T.ENDFB3R0 evaluation cuts off at 5e-10 MeV rather than extending down to 1.e-11 MeV causing the low energy dip evident in Figure 66. The T.ENDFB6R0 evaluation does not agree at all.

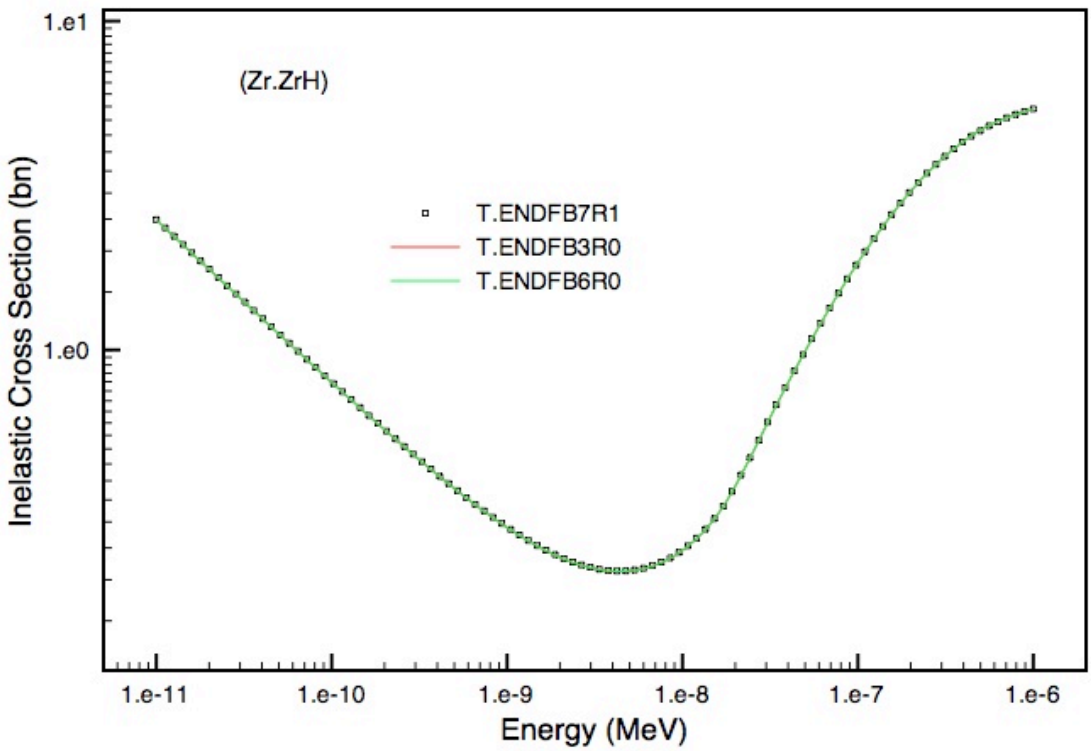

Figure 68

There is excellent agreement in the inelastic components.

Summary

1) The normalization factors needed to ensure a smooth cross section across the thermal boundary are inconsistent (see Table 1). For (H.H2O) the normalization factor is 2 for the ENDF formatted evaluations and 1 for the ACE formatted evaluations, for (C6H6) the normalization factor for the LANL evaluation for ENDF/B-VII.0 is 6 and for ENDF/B-VII.1 it is 12, and so on. The normalization factors in Table 1 were determined empirically. A more satisfying and less confusing option would be to include the normalization factors in the evaluated data.

2) The methodology of library makers SABtoCOG and NJOY/SAB.ACEtoCOG produce consistent results – see for example Figures 12, 18, and 57.

3) The BNL libraries are missing the coherent elastic component for (Al), (Fe56), (O.BeO), (O.UO2), and (U.UO2) – see Figures 3, 25, 51, 54, and 60.

4) The ENDF/B-VI.0 data shows slight differences and non-physical "saw-teeth" for (Be), (BeO), and (C) – see Figures 6-8, 9-11, and 15-17.

5) There appear to be problems with the JEFF3.1.1 data for (BeO) and (H.ZrH) – see Figures 9-11 and 45-47.

6) Other differences are due to improvements in the thermal data for (D.D2O) and (H.H2O) – see Figures 23-24 and 37-38.

References

[1] R. E. MacFarlane, D. W. Muir, "The NJOY Nuclear Data Processing System", LA-12740-M (1994).