From cutting-edge pointwise cross-section to groupwise reaction rate: a primer

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Elemental periodic table

Periodic Table of the Elements

Atomic Number
Symbol
Name
Atomic Mass

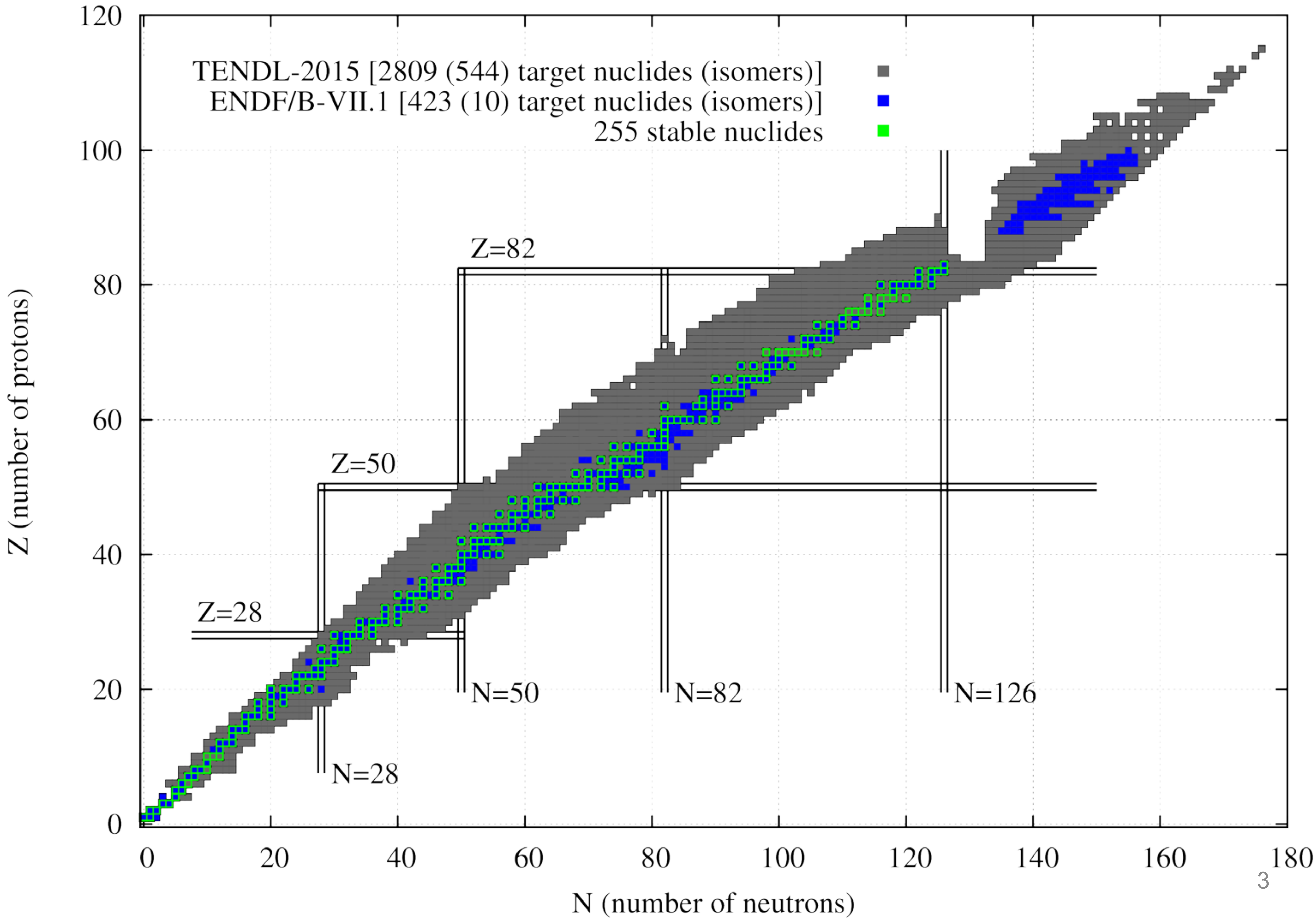
1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.972	35 Br Bromine 79.904	36 Kr Krypton 84.798
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294
55 Cs Cesium 132.905	56 Ba Barium 137.328	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide Series	57 La Lanthanum 138.905	58 Ce Cerium 140.116	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.242	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.500	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

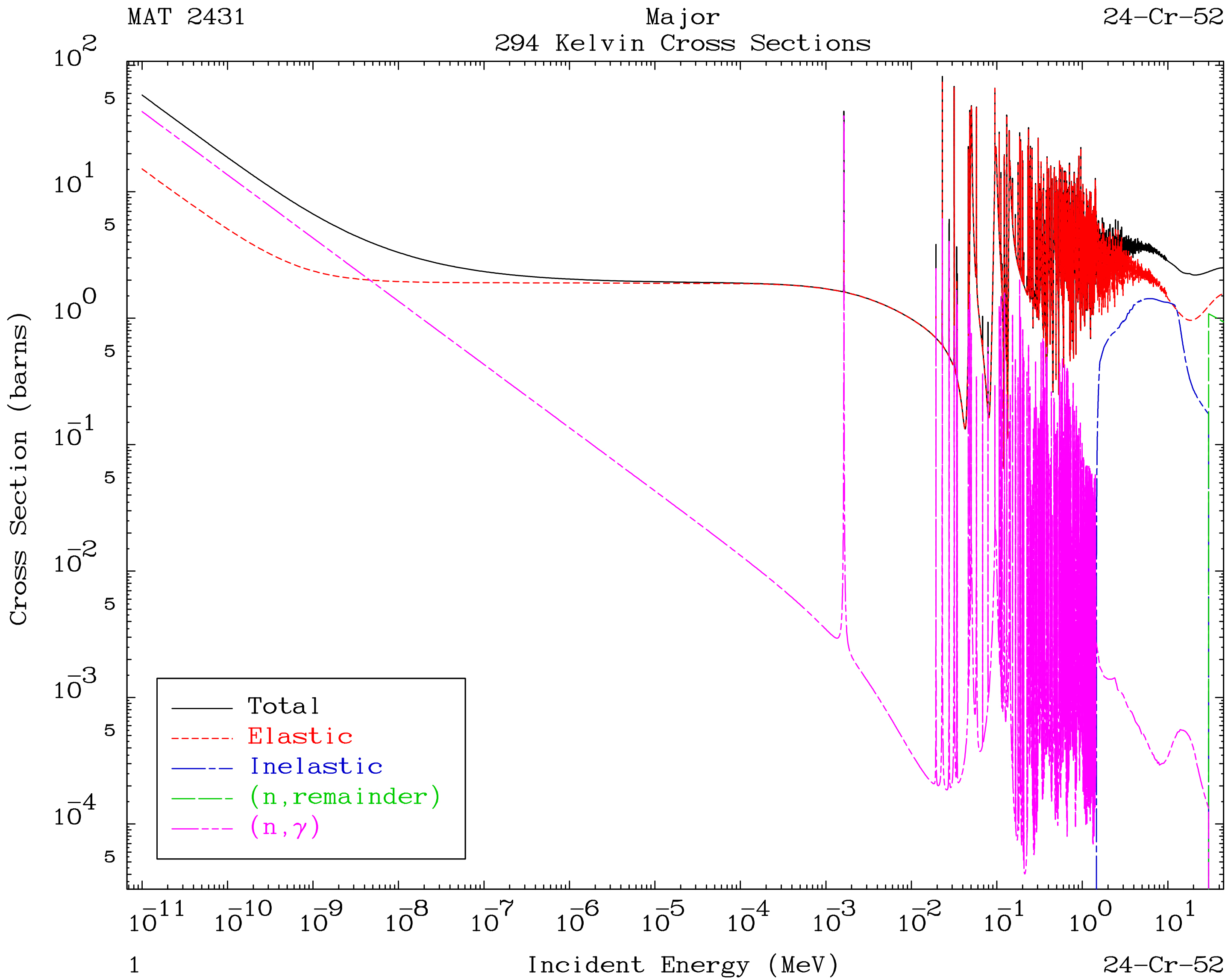
Alkali Metal | Alkaline Earth | Transition Metal | Basic Metal | Semimetal | Nonmetal | Halogen | Noble Gas | Lanthanide | Actinide

Dawn Shaughnessy

Isotopic targets



TENDL-2015 pendf, 200 MeV



90 reaction types

(n, remainder) =mf3-mt5*mf6 above 30 MeV

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Processing steps: three codes

ENDF file

- **NJOY12-064**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - purr
    - acer
    - groupr

ACE file

cross-check

- **PREPRO-2015**
  - **linear**
  - **recent**
  - **sigma1**
  - **sixpack**
  - **activate**
  - **merger**
  - **dictin**
  - **groupie**

Processed ENDF file

cross-check

- **CALENDF-2010**
  - calendf
  - regroutp
  - lecritp
  - ....

PT file

Single script for an entire library

Extract and reduce library data

- Condense run extracts from decay files:
  - decay constant λ
  - decay constant uncertainty Δλ
- Collapse constructs flux spectrum weighted averages:

➢ Library input
- cross-section vs energy
- covariances vs energy
- flux spectrum vs energy

$$W_i = \frac{\phi_i}{\sum_{i=1}^{i=1102} \Phi_i}$$

$$\overline{XS} = \sum_{i=1}^{1102} w_i \sigma_i$$

➢ Data used in code
- collapsed cross-section $\overline{XS}$
- collapsed uncertainty Δ

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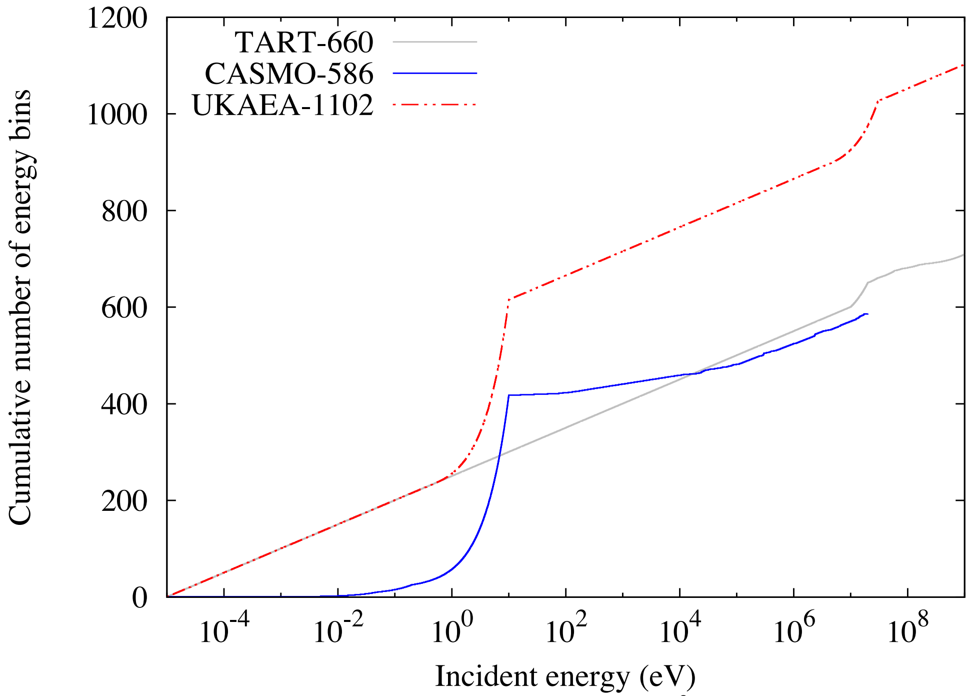
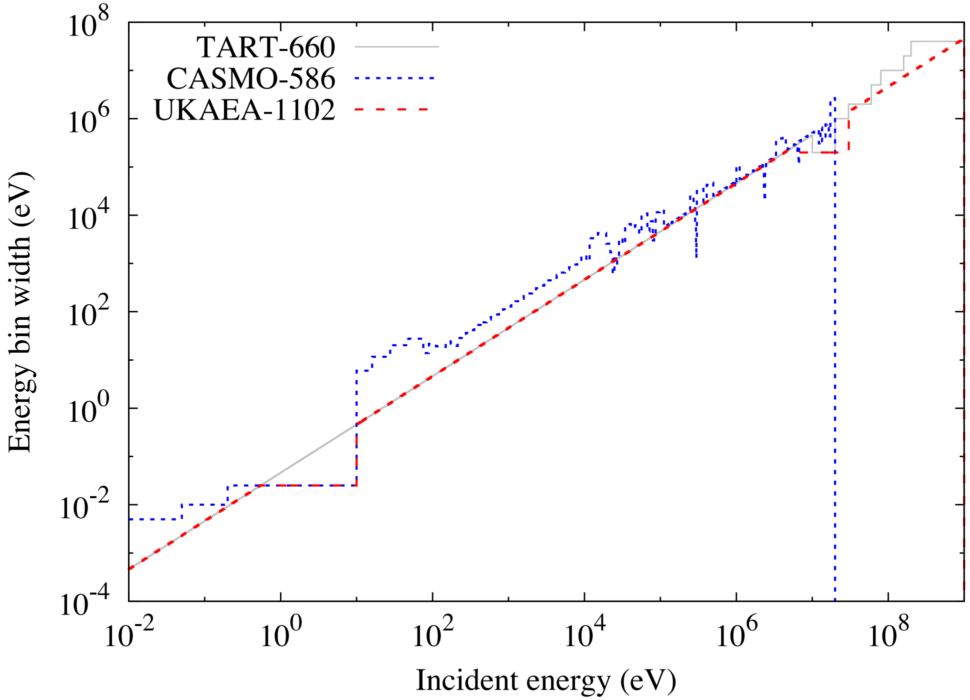
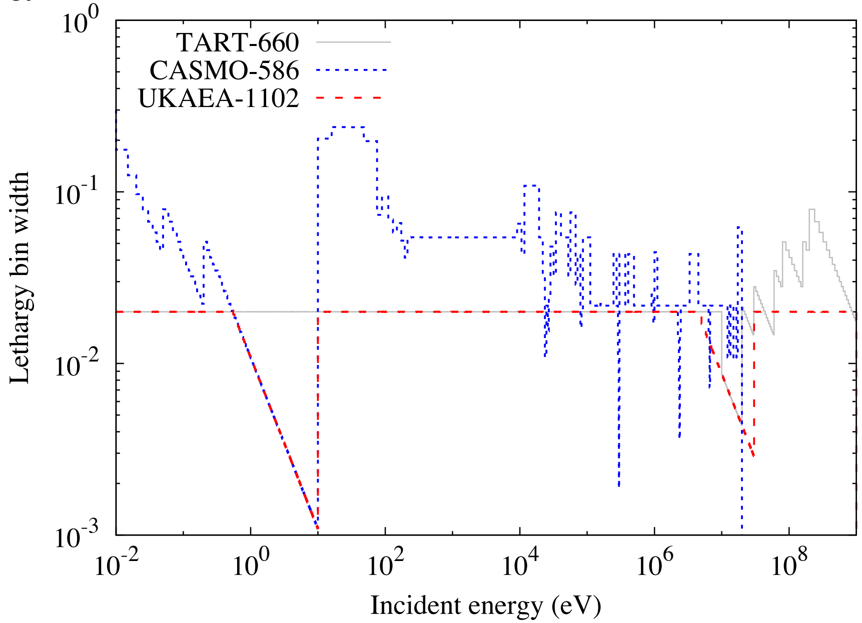
Group structures







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Group structures

- For all 2809 TENDL target nuclides
- 1102 energy groups for all applications alike

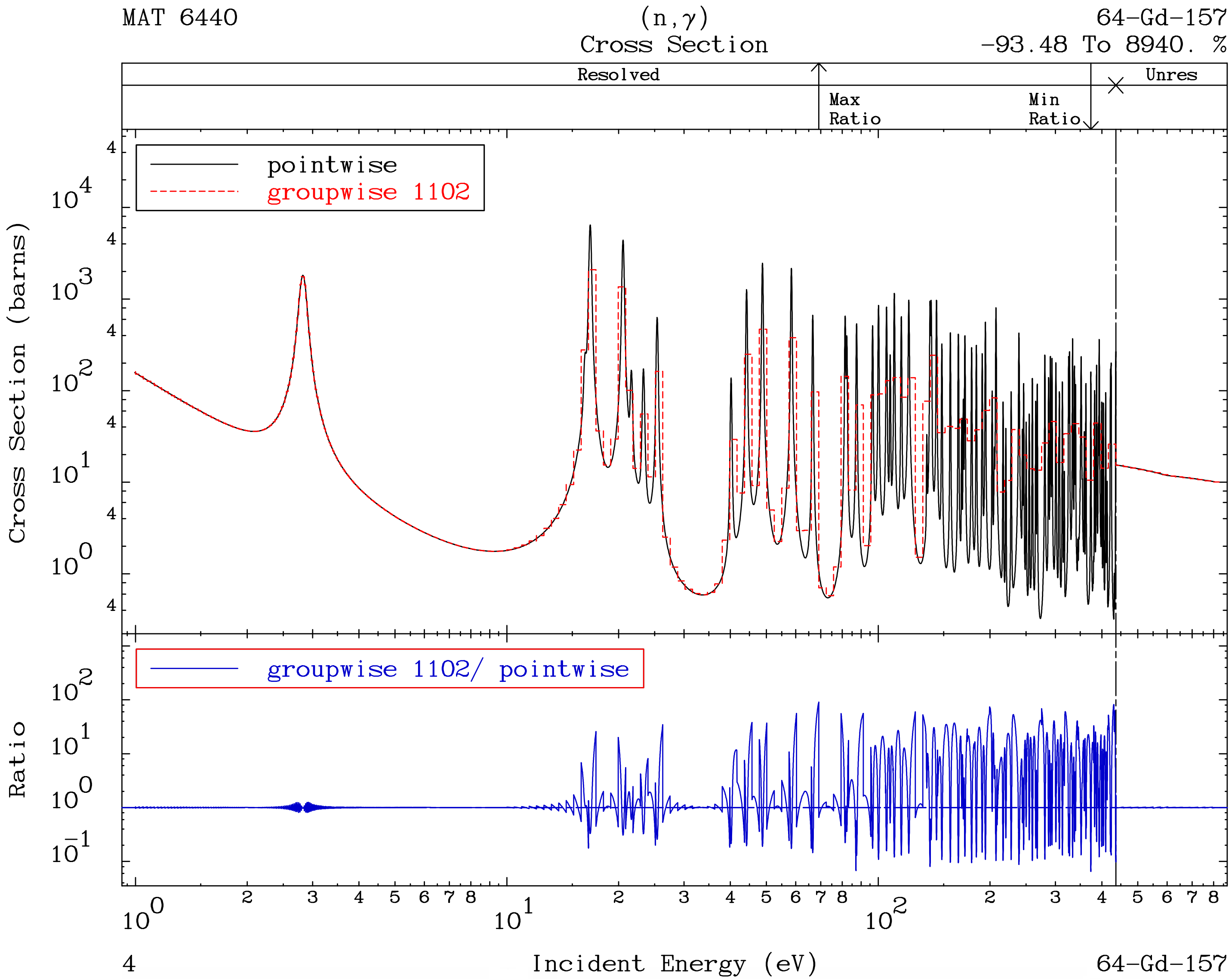
Thermal	Resonance fine	Resonance shielded	Fast Fusion	Fast	High Energy
50 equal U per decade	Equal energy 0.025 eV	50 equal U per decade	Equal energy 200 KeV	50 equal U per decade	Equal lethargy
237 gprs	378 gprs	285 gprs	125 gprs	27 gprs	50 gprs

1e-5 eV — 0.55 eV — 10 eV — 5 MeV — 30 MeV — 100 MeV — 1 GeV

615 groups — 1025 groups

- 378 fine groups in the resonance range
- Resonance shielded data available in the RRR (0.1 eV) up to the end of the URR for all nuclides IDs
- Fast fine structure for accurate threshold XS reaction rate

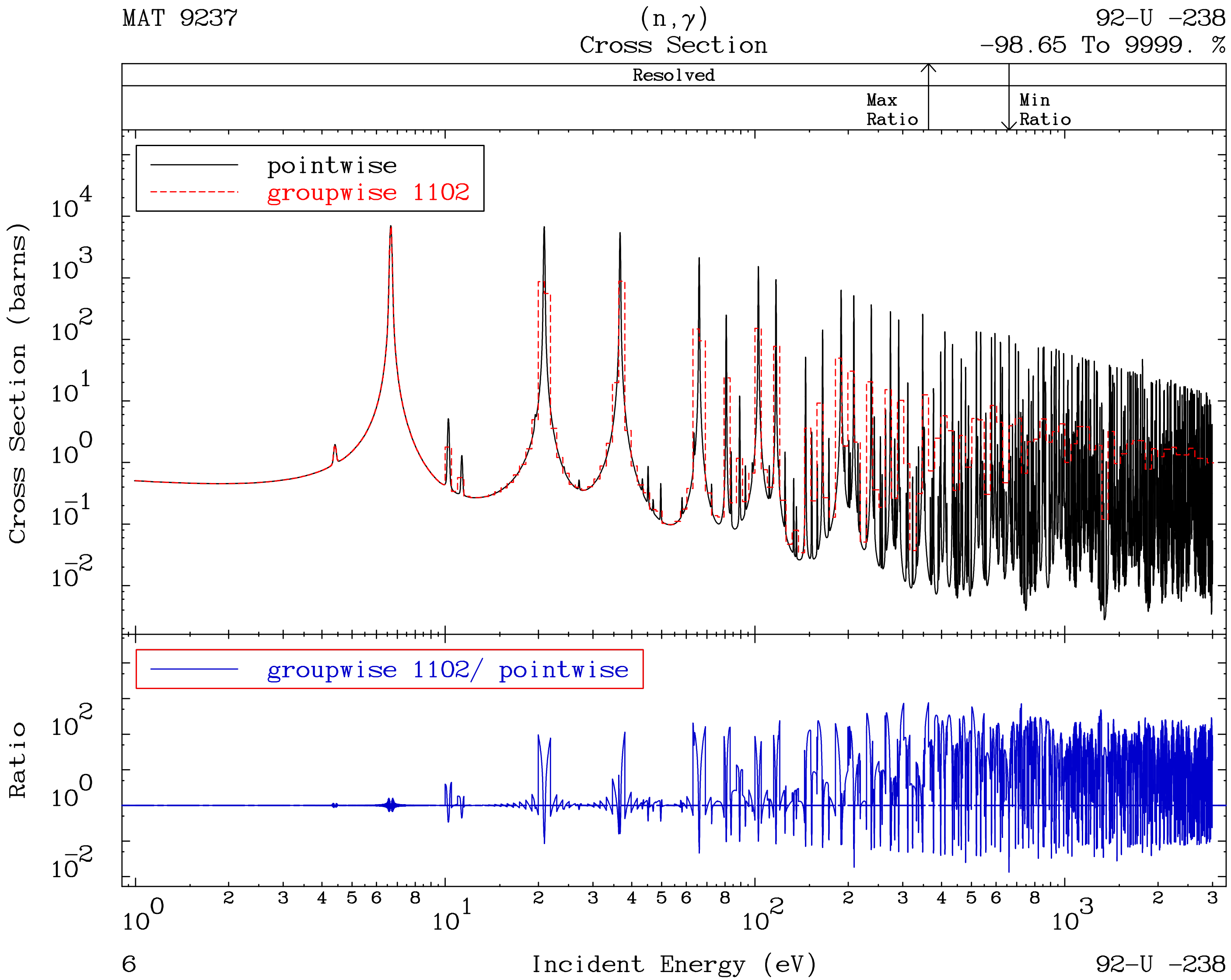
Group structure: 1102



Fine group to 10 eV

Resonance shielded to end of URR

Group structure: 1102



Fine group to 10 eV

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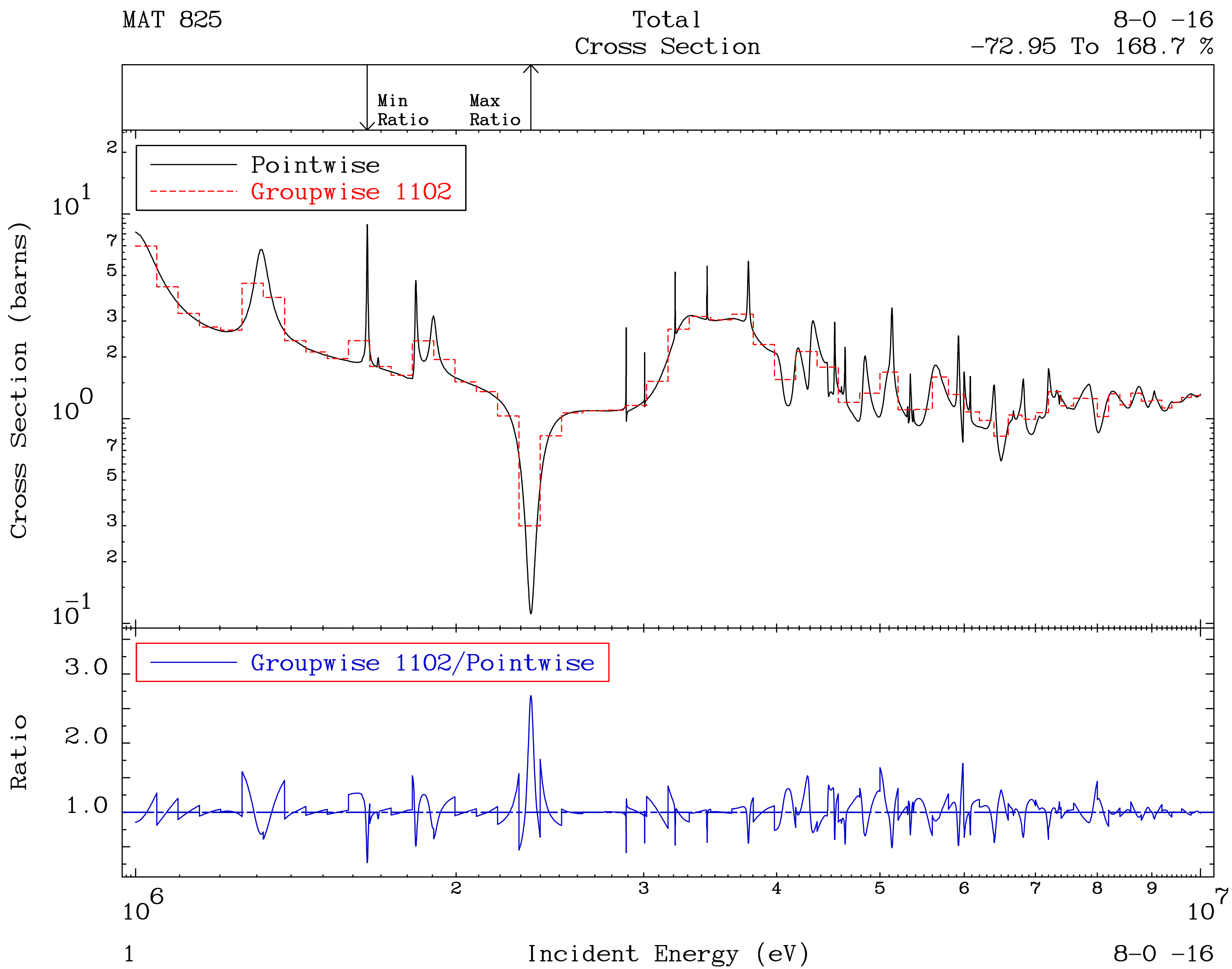
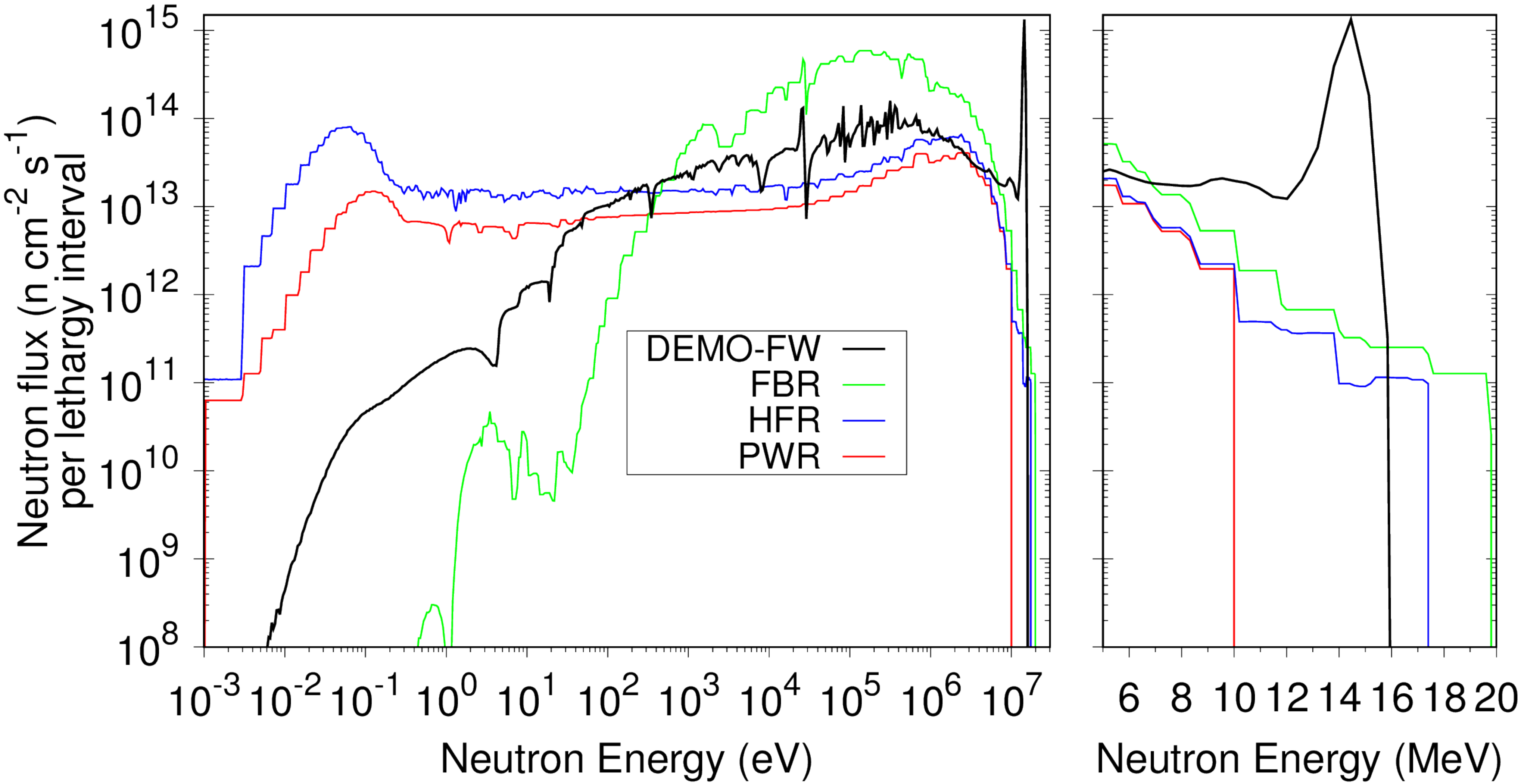


Peak and trough are well described

Typical neutron spectra

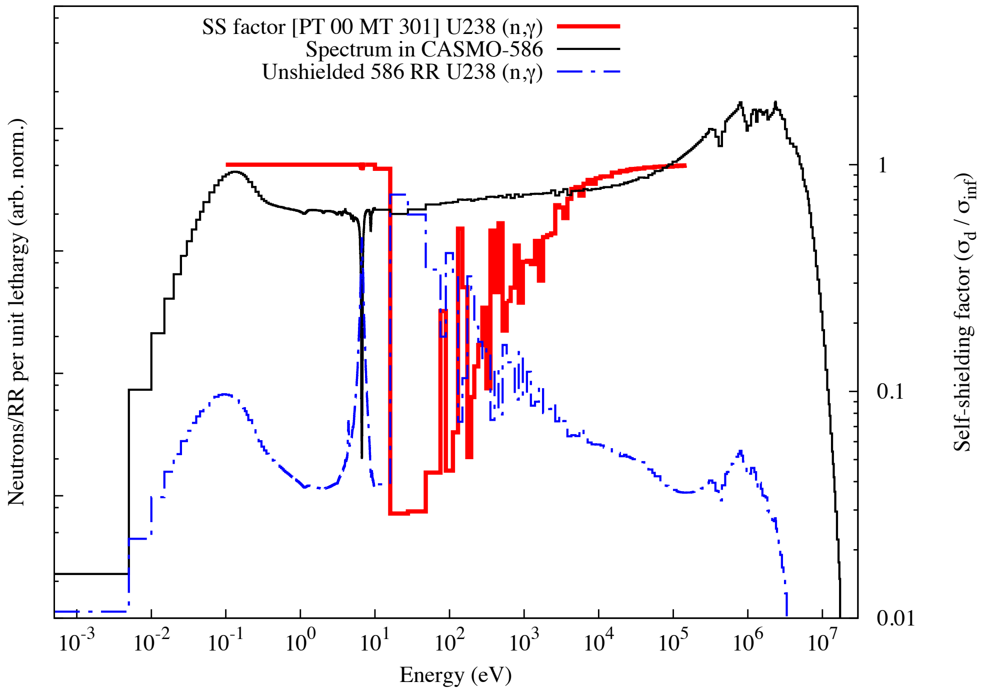


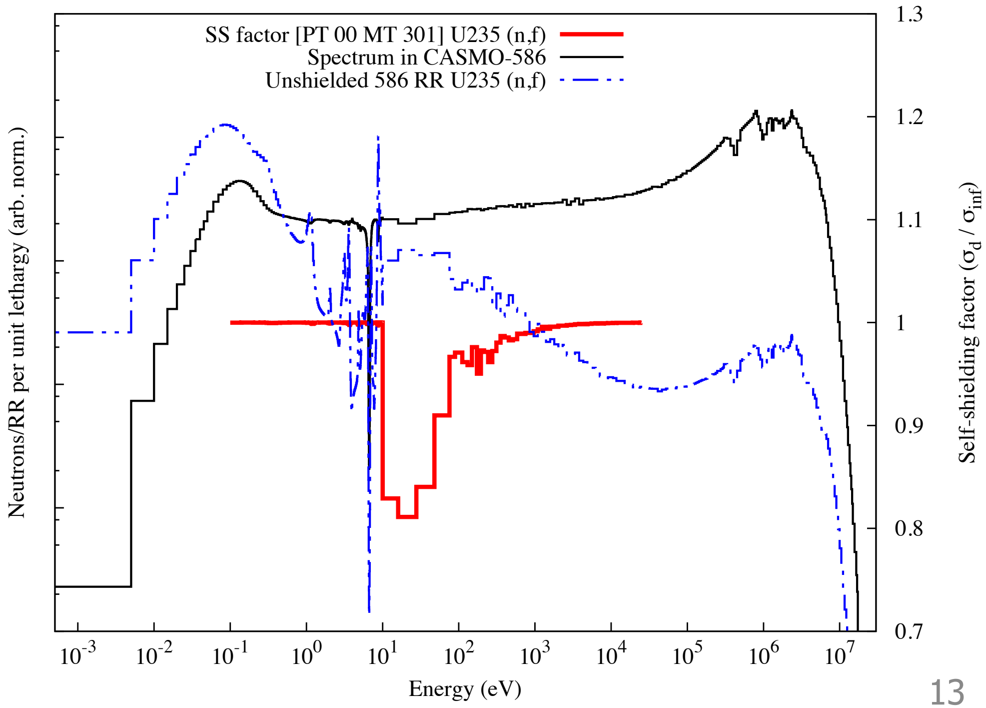
- Fusion demo first wall, Fast breeder (Phenix),High flux reactor Petten, light water reactor (Paluel)
- Importance of the tails: below 10^{-2} eV and above 10 MeV

LWR assembly simulations

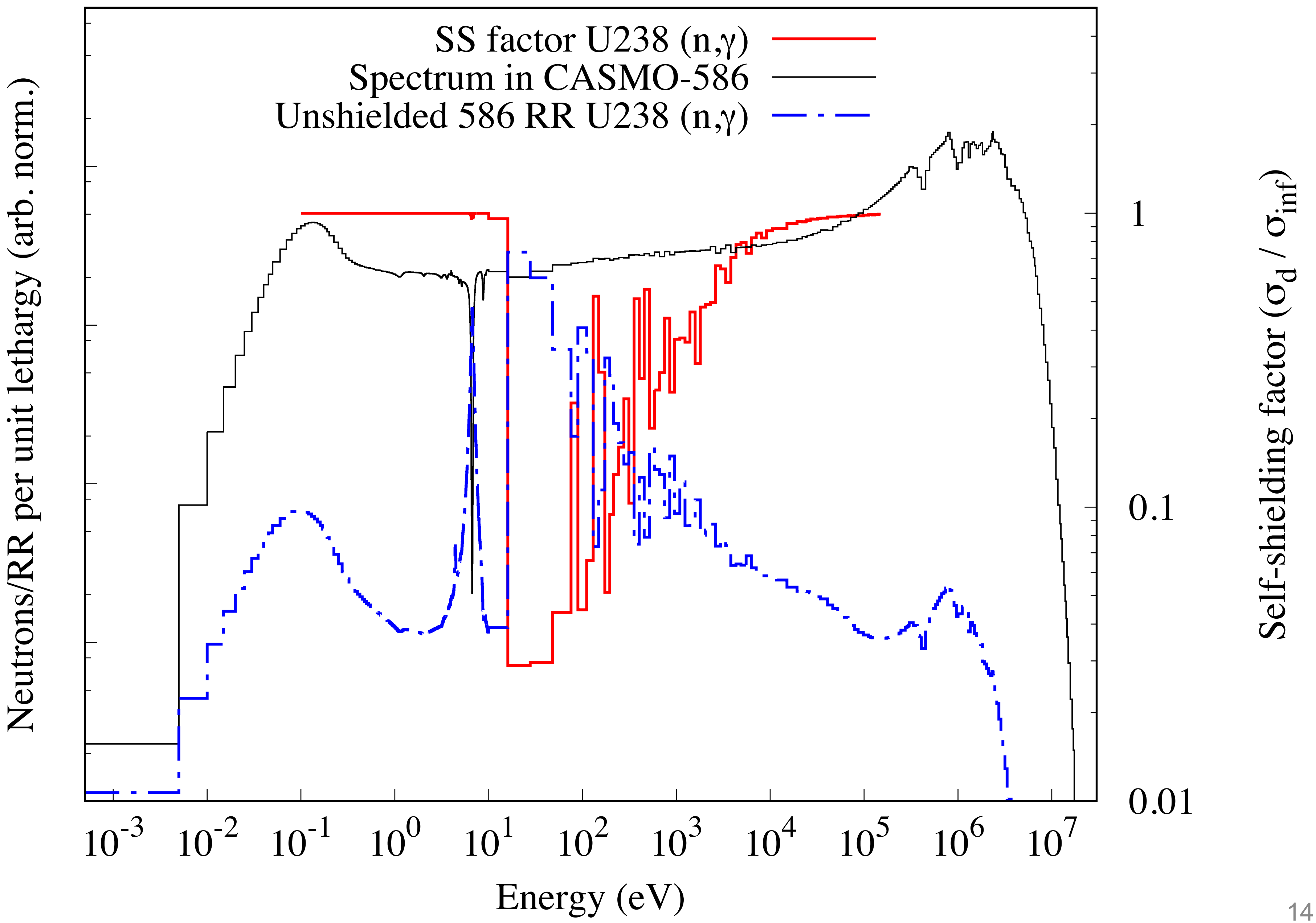
- 586 gprs CASMO data for ENDF/B-VII.1, with CALENDF PTs for self-shielding. Applied to major actinides, but can in principle apply to any nuclide
- **Left**: U8 capture RR and SSFs **Right**: U5 fission RR+SSFs

Note: CASMO 586 treatment of <10 eV requires no SSFs! No so for >10 eV, where significant SS occurs and must be accounted for.

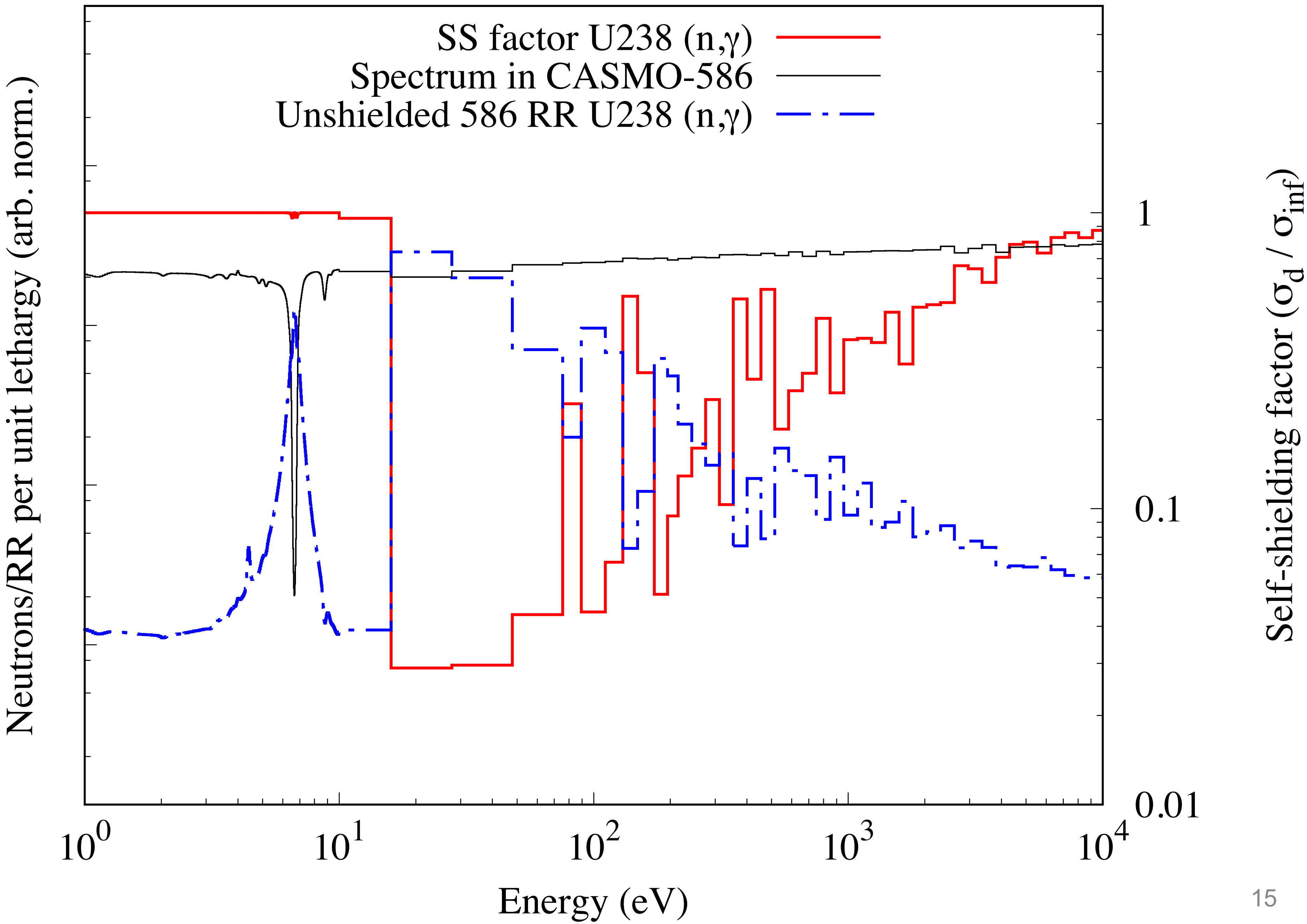


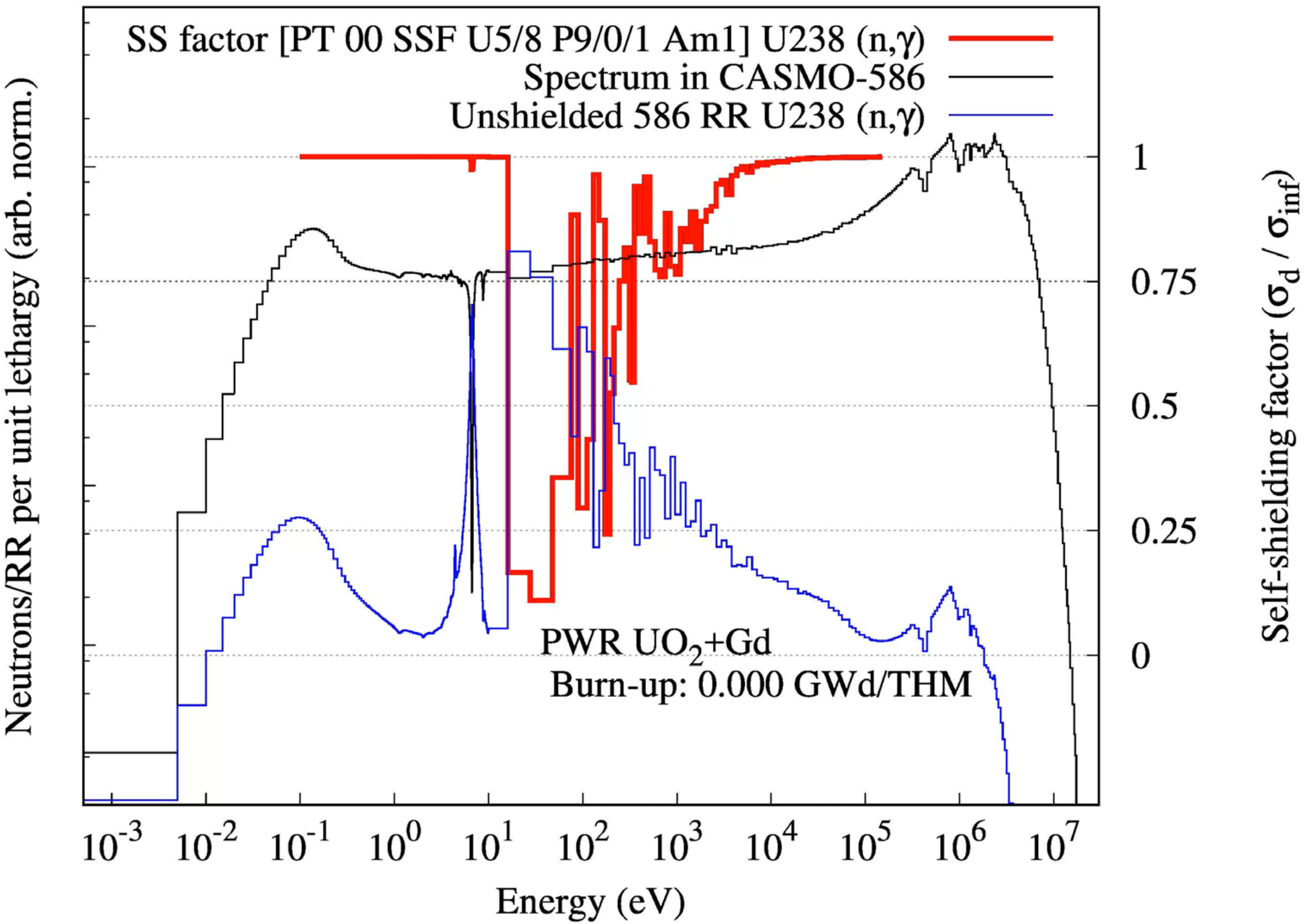


U^{238} reaction rate

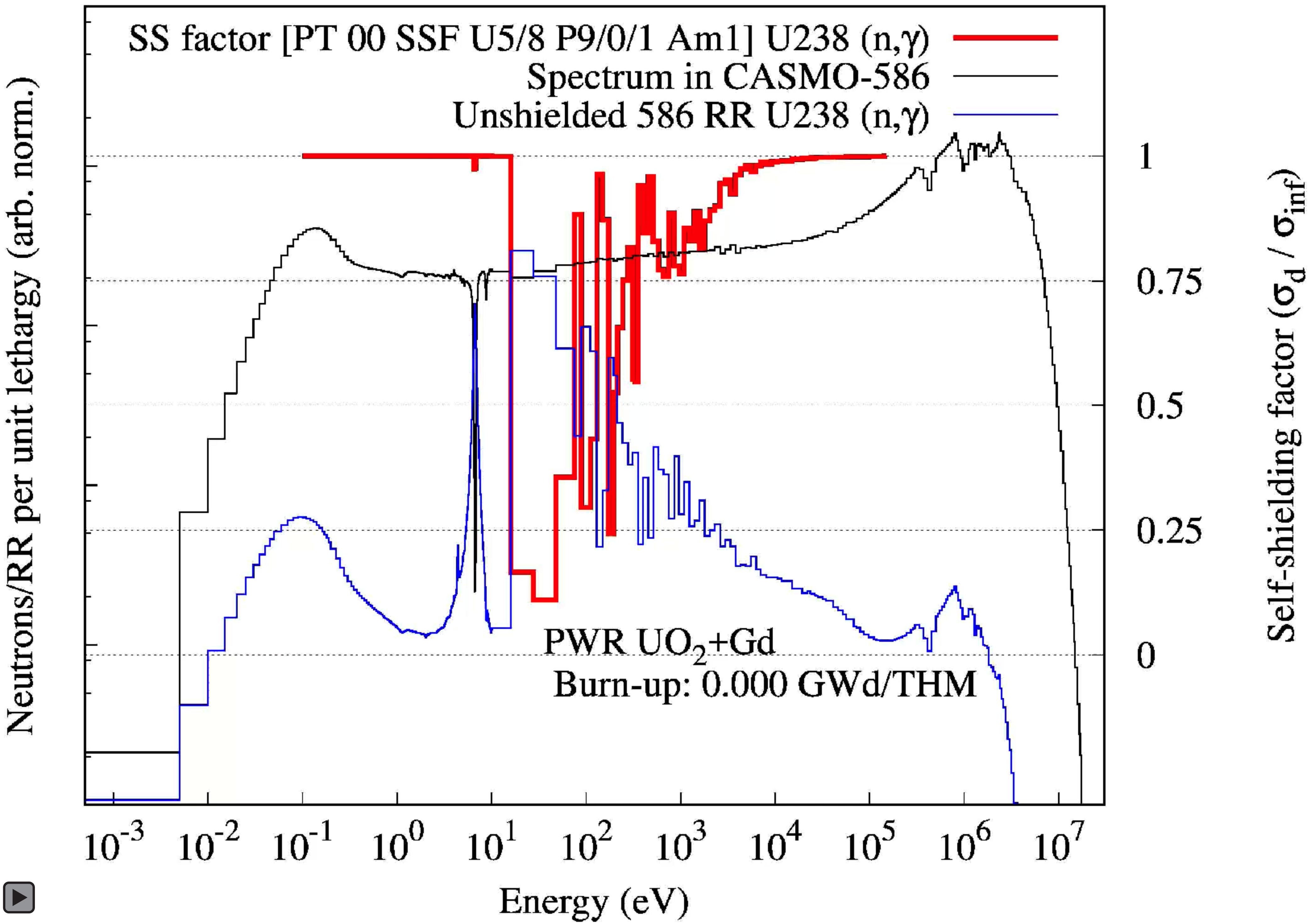


U^{238} reaction rate





SS factor [PT 00 SSF U5/8 P9/0/1 Am1] U238 (n,γ)
Spectrum in CASMO-586
Unshielded 586 RR U238 (n,γ)
PWR UO2+Gd
Burn-up: 0.000 GWd/THM
Neutrons/RR per unit lethargy (arb. norm.)
Self-shielding factor (σd / σinf)
Energy (eV)
1
0.75
0.5
0.25
0
10-3
10-2
10-1
100
101
102
103
104
105
106
107



SS factor [PT 00 SSF U5/8 P9/0/1 Am1] U238 (n,γ)
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Unshielded 586 RR U238 (n,γ)
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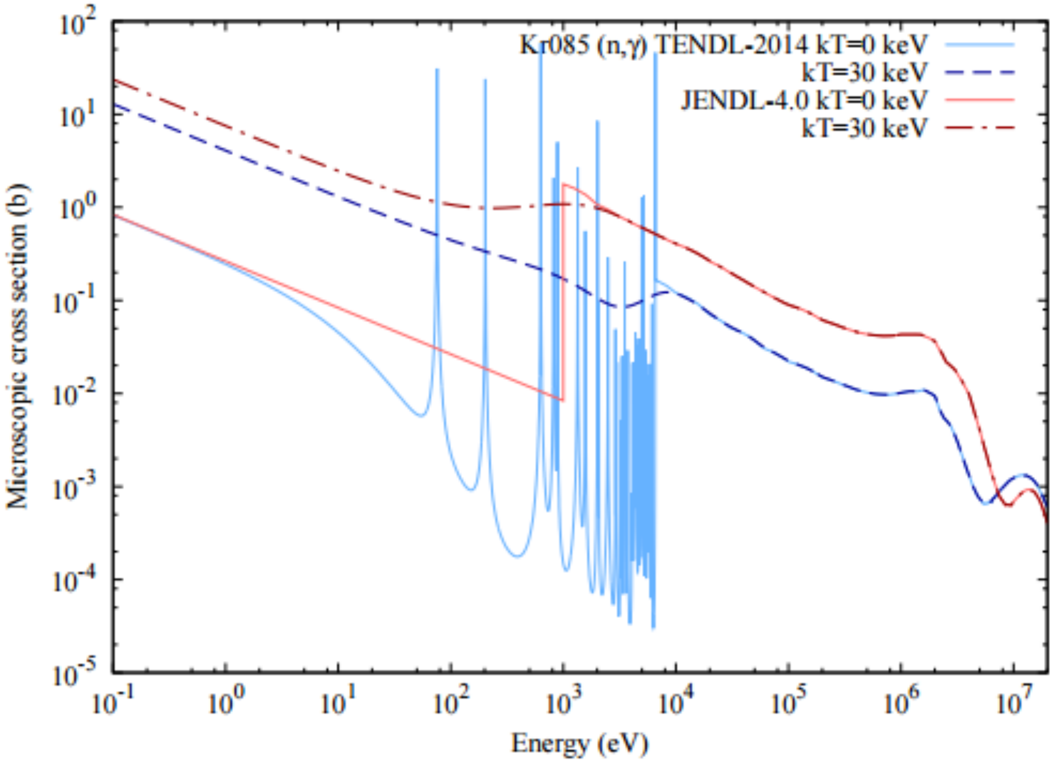
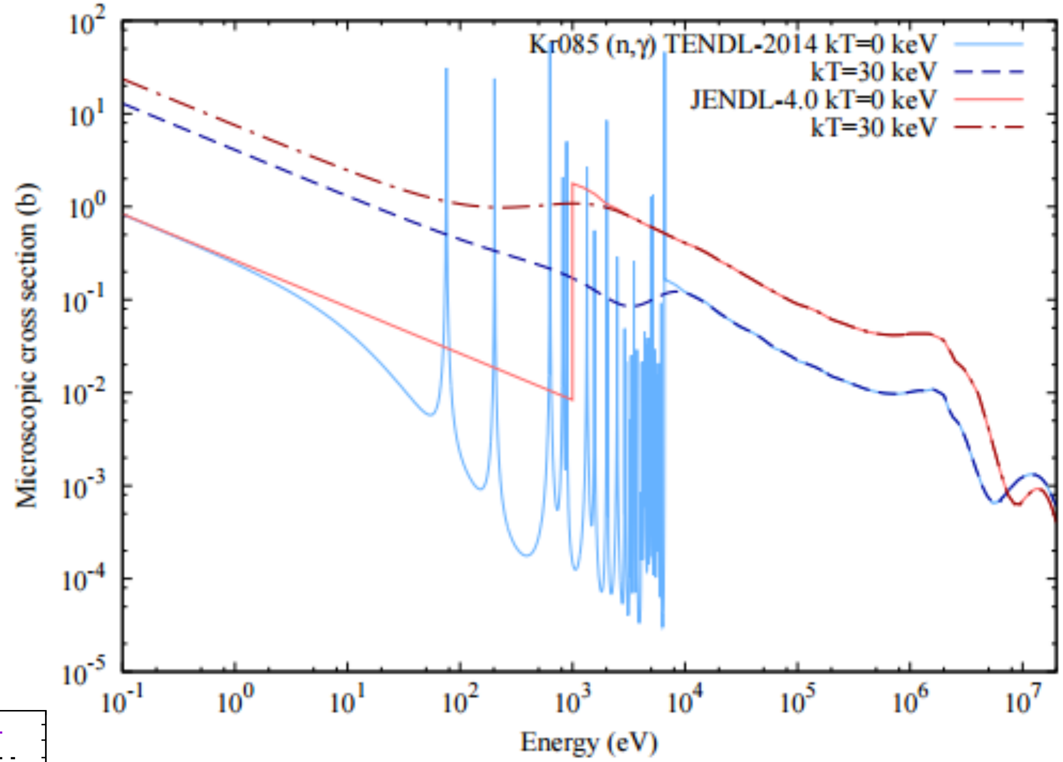
Burn-up: 0.000 GWd/THM
Neutrons/RR per unit lethargy (arb. norm.)
Self-shielding factor (σd / σinf)
Energy (eV)
10-3
10-2
10-1
100
101
102
103
104
105
106
107
1
0.75
0.5
0.25
0

Capture reactions

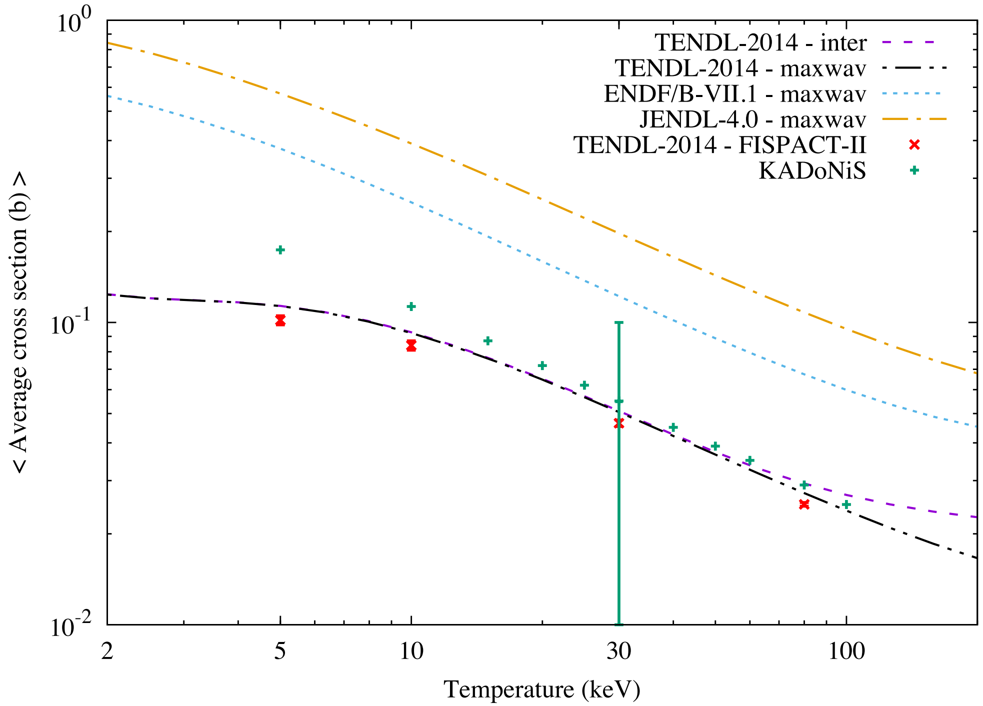
- Neutron capture and other reactions are exothermic, allowing the reaction at any incident energy
- These reactions possess resonance structure which often determines reaction rate (aside from thermal spectra systems)
- Either the resonances have been measured, we statistically resolve them or (in non-TENDL) we get unphysical straight lines…



Astrophysics reaction rates



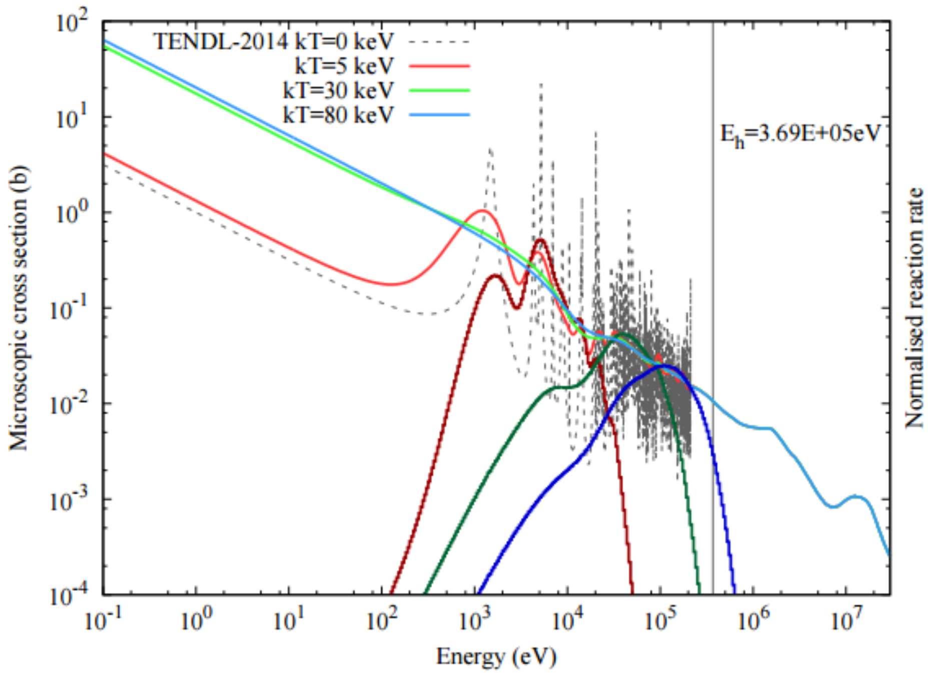
0k and kT=30 KeV
broadened cross-sections



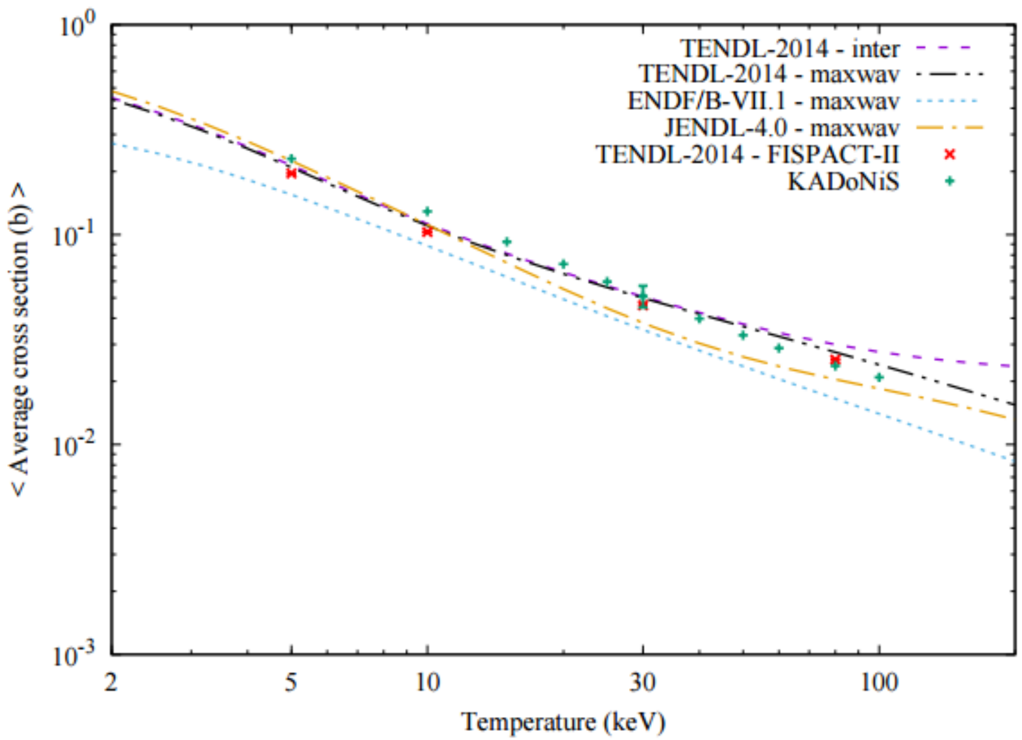
Temperature-dependent averaged cross-sections
Astrophysical 5-80 KeV
FISPACT-II forms: 1102 groups

Nuclear data & KADoNiS

- The KADoNiS database includes some 357 nuclides over 11 Maxwellian-averaged temperatures for RR comparison



Broadened cross-sections



Temperature-dependent averaged cross-sections

HFR Petten Irradiation scenario

- W irradiated under EXTREMAT-II in 2008 & 2009
- Target of 282 days of irradiation (10 cycles), but in fact only irradiated in 8 cycles & in two different positions:

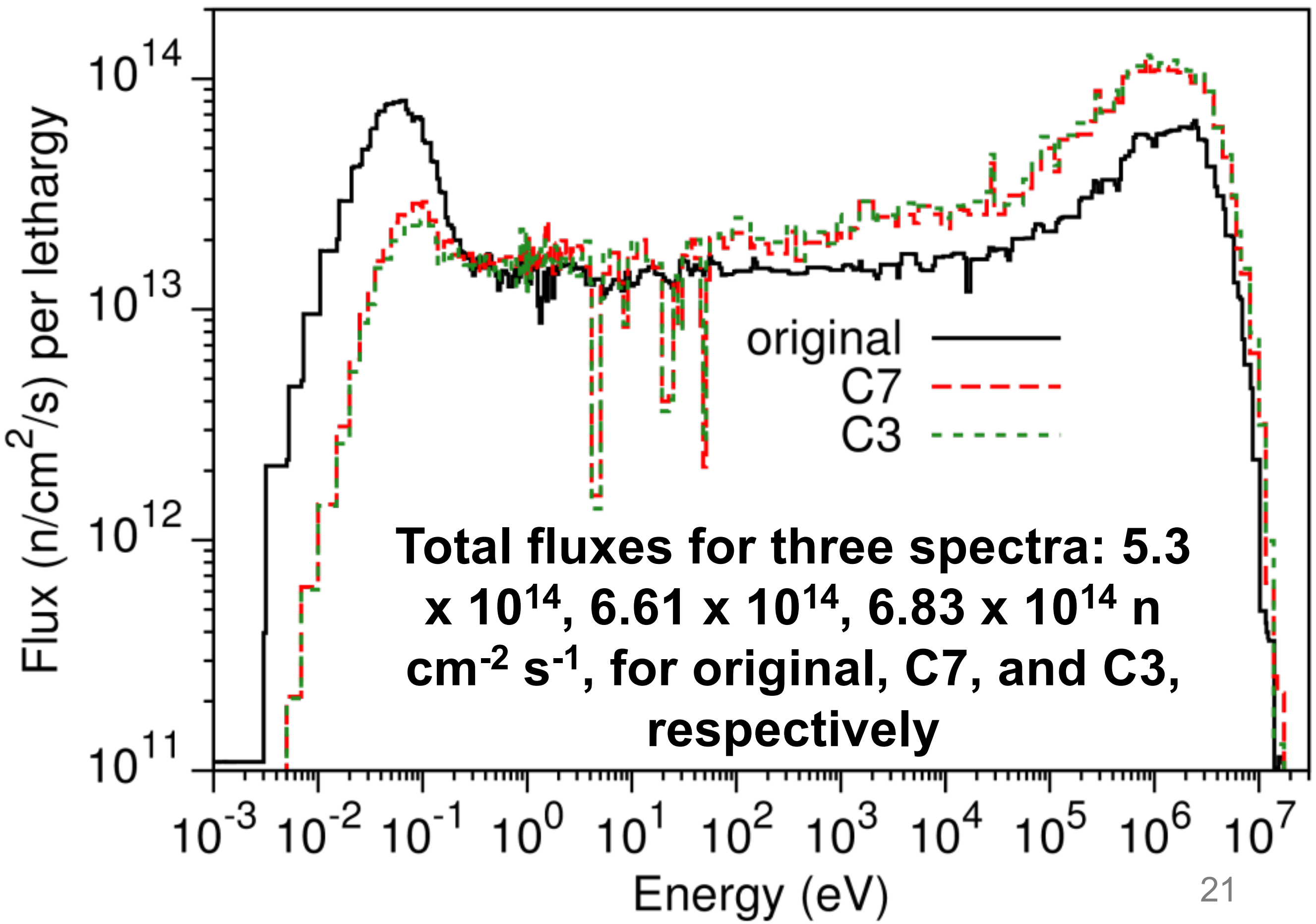
Position	Cycle	EFPD	Start date	End date
C7	08-May	30.72	22-May-08	22-Jun-08
	08-Jun	29.71	28-Jun-08	28-Jul-08
C3	09-Jan	27.69	12-Feb-09	12-Mar-09
	09-Feb	24.99	01-Apr-09	26-Apr-09
	09-Mar	30.77	29-Apr-09	30-May-09
	09-Apr	24.71	02-Jun-09	27-Jun-09
	09-May	17.61	30-Jun-09	18-Jul-09
	09-Jun	22.06	17-Aug-09	08-Sep-09
Total		**208.26**		

- EFPD – effective full power days

Neutron spectrum

- Samples were positioned next to another experiment with very strong thermal neutron absorption properties
  - W exposed to a lower than normal (for HFR) fraction of thermal neutrons creating reduced transmutation

- **New spectra calculated for the approximate axial position of EXTREMAT-II, averaged over radial extent of experiment and over around 4 cm of height**



FISPACT-II input coding details

- To correctly account for self-shielding in all isotopes of W
  - During collapse:

```
PROBTABLE 1 1
SSFCHOOSE 1 0 W
SSFMASS 1.0 1
W 100.0
GETXS 1 709
```

- Other option (`SSFFUEL`) allows explicit specifications of isotopes to self-shield

Important Reactions

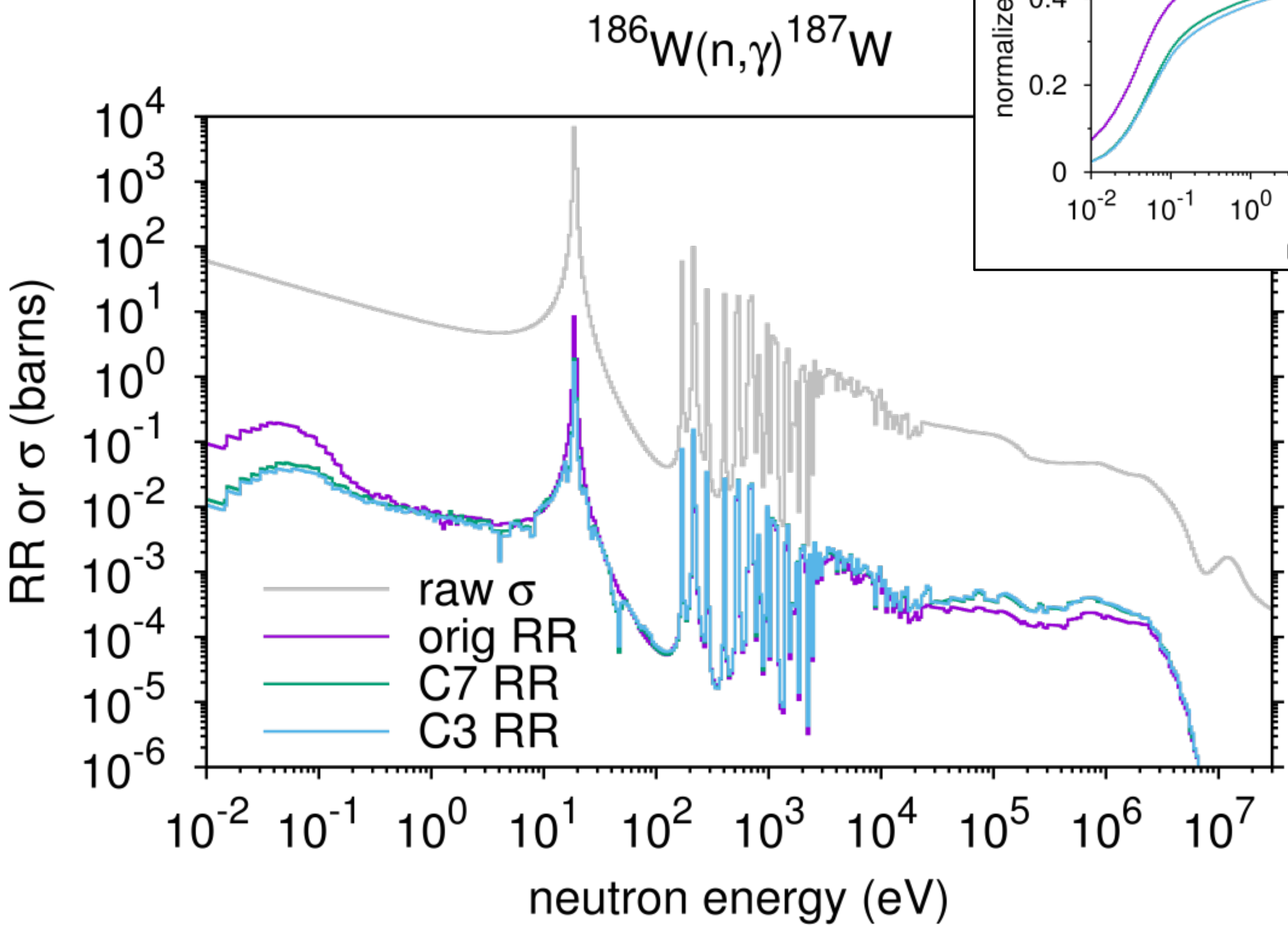
- Main Re isotopes produced during irradiation are ^{185}Re and ^{187}Re
  - Produced via (n,γ) reactions on ^{184}W and ^{186}W, followed by β-decay of ^{185}W ($T_{1/2}$=75 days) and ^{187}W (24 hours), respectively.
- Raw total collapsed reaction rate (RR) for these (n,γ) reactions and self-shielding (SS) corrected values:

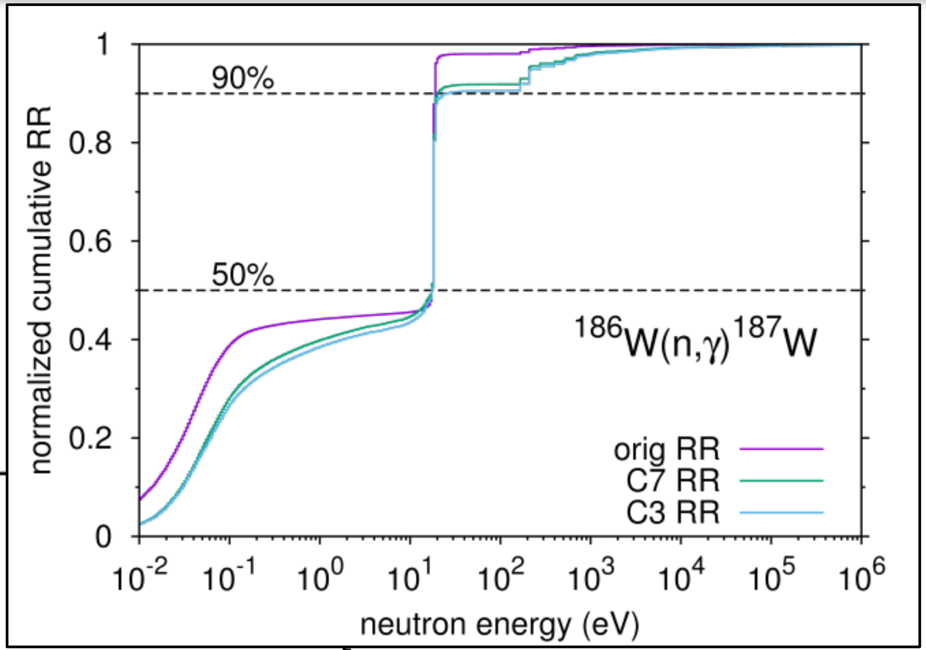
Reaction	Original spectrum		C7		C3	
	Raw RR	SS RR	Raw RR	SS RR	Raw RR	SS RR
^{186}W(n,γ)^{187}W	22.5 (0.01)	17.2	6.21 (0.09) (-72%)	4.67	5.54 (0.1) (-75%)	4.13
^{184}W(n,γ)^{185}W	0.92 (0.71)	0.60	0.63 (1.8) (-32%)	0.29	0.64 (1.8) (-30%)	0.29

(all RR in barns, black bracket values are +/- errors, green bracket values are % reduction in RR relative to original spectrum)

Collapsed reaction rates

- Almost 50% of RR comes from thermal neutrons below 10 eV

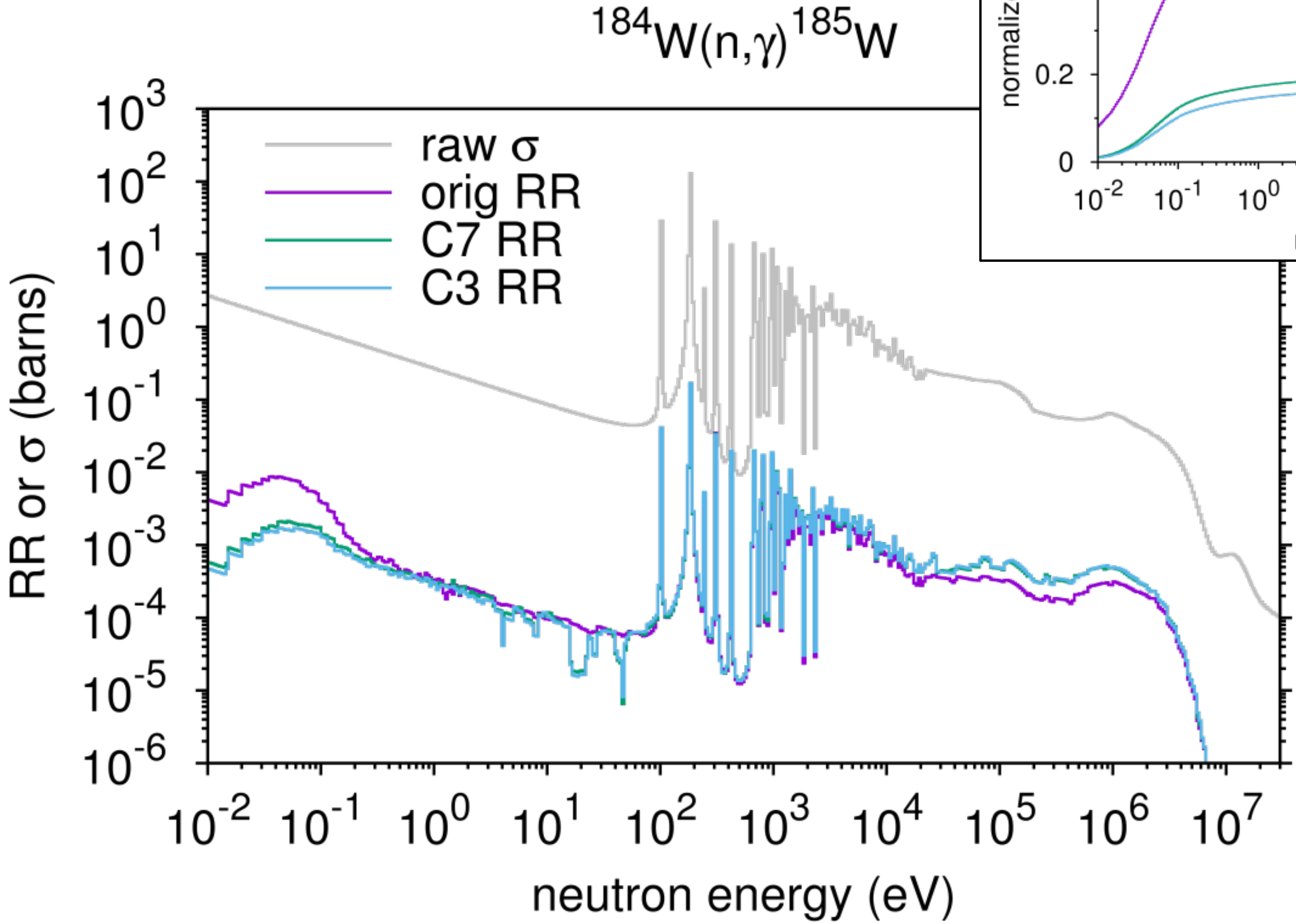


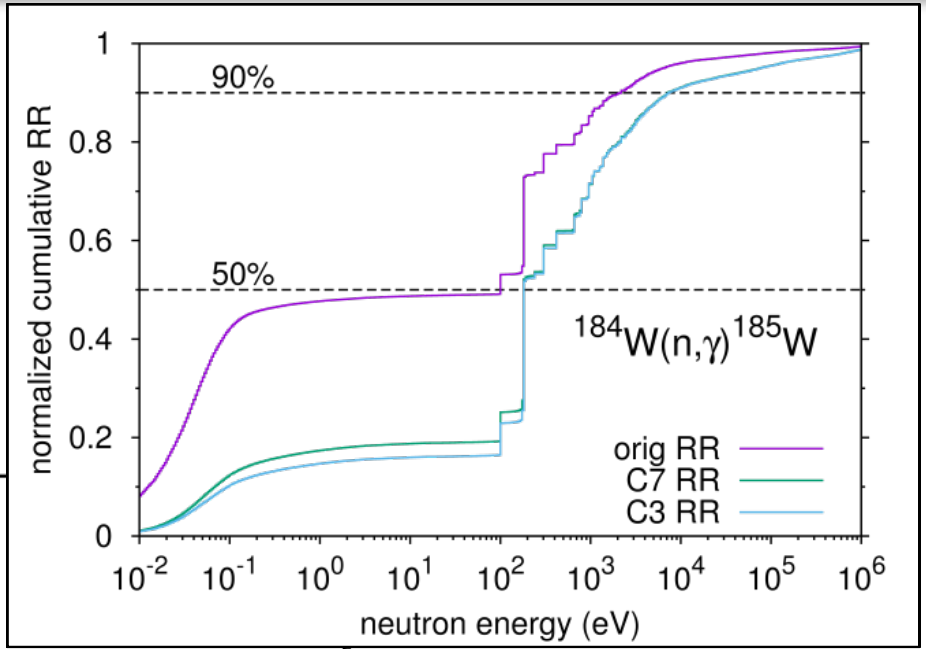


(RR and σ in a fine group structure with 660 bins below 30 MeV)

Collapsed reaction rates

- For new spectra, only 20% of RR comes from thermal neutrons below 100 eV





(RR and σ in a fine group structure with 660 bins below 30 MeV)

Simulation of irradiation

- Inventory simulation with FISPACT-II of pure tungsten with fully detailed irradiation schedule (including gaps and change in position) and new spectra
  - TENDL 2014 nuclear libraries in 660 energy groups
  - Self-shielding correction of reaction cross sections included ($\longrightarrow$ 2% Re predicted without SSF correction)

- Results after 208.26 effective full power days:
  - 1.4 atomic % Re (and 0.1% Os)
    - good agreement with 1.2-1.4% values from measurements
    - And much better than ~4% prediction based on usual HFR neutron spectrum
  - Leading to 1.6 effective DPA in the tungsten (using E_d = 55 eV)

Summary

- In order to provide accurate RR simulations for all and not only the one aspects of reactor physics it is important to keep in mind that although certain parameters are correlated their often missing correlation matrices are energy dependent:
  - Operational K_{eff} could be predicted to the pcm in a LWR without any knowledge of the flux above 10 MeV or below 10^{-2} eV, however the calculation of any reaction rate outside this energy region is doubtful
  - Unfortunately many other aspects of reactor physics such as inventory, material sciences rely on a reliable knowledge of the particle spectra in those tails and in other energy ranges that do not impact the K_{eff}
  - Most integral information relates to effective cross section, what about the uncertainty in the calculation of the SSF's?
  - Cross section, neutron flux, SSF are three quantities that make the reaction rates
  - Beware of the hidden uncertainty derived from data forms processing and interpretations