Uncertainty quantification of depletion calculations for specific isotopes using ORIGEN2

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Outline

Introduction

- Determing composition of irradiated fuel importance
  - Flux calculations
  - Reprocessing
  - Irradiation history verification
- Usually determined with a type of Bateman solver
- Uncertainties rarely reported
  - Flux Shape
  - Fission yield
  - **Cross Sections**
  - Half-lives

Current Problem

- Use of depletion code ORIGEN2
  - Solves with exponential method
  - Requires libraries
    - Decay information
    - Fission yield data
    - Single group cross sections
- PWR system with 3 wt% enriched uranium
- Varied σ_γ and σ_f for: ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu
  - Originally, σ_γ and γ for the FP were considered

Quantities of Interest

^{133}Cs	^{136}Ba	^{153}Eu
^{134}Cs	^{138}Ba	^{154}Eu
^{135}Cs	^{149}Sm	^{239}Pu
^{137}Cs	^{150}Sm	^{242}Pu
^{148}Nd	^{106}Rh	^{125}Sb

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ORIGEN2 Model

- Model irradiates 1 metric ton of US PWR fuel for a single cycle (15,000 MWd/Mt)
- Constant power assumption (37.5 W/g)
- Does not include oxygen
- Verified with ^{137}Cs content

$$\frac{552.8 \text{ g } {}^{137}\text{Cs}}{Mt} \cdot \frac{6.022E23 \text{ atoms}}{137 \text{ g } {}^{137}\text{Cs}} \cdot \frac{\text{Fission}}{0.06 \text{ atoms}} \cdot \frac{200 \text{ MeV}}{\text{Fission}} \cdot \frac{1.602E{-19} \text{ MJ}}{1 \text{ MeV}} \cdot \frac{1 \text{ day}}{86400 \text{ s}} = 15,018 \ \frac{\text{MWd}}{Mt}$$

ORIGEN2 Model

```
  RDA   Irradiation of 1 MT of PWR fuel
  RDA   Fuel enrichment is 3.0 w/o U-235
  RDA
  LPU 922350 922380 942390 942400 942410 -1
  LIB   1   1 2 3  601 -602 603  9  8 0 1 38
  PHO       101 102 103  10
  INP   1   1  -1  -1   1   1
  BUP
  IRP 100.0 37.5 1 2 4 2 BURNUP=3,750 MWD/MT
  IRP 200.0 37.5 2 3 4 0 BURNUP=7,500 MWD/MT
  IRP 300.0 37.5 3 4 4 0 BURNUP=11,250 MWD/MT
  IRP 400.0 37.5 4 5 4 0 BURNUP=15,000 MWD/MT
  DEC 500.0      5 6 4 0 DECAY FOR 100.0 DAYS
  DEC 4150.0     6 7 4 0 DECAY FOR 10 YEARS
  DEC 73500.0    7 8 4 0 DECAY FOR 200.0 YEARS
  BUP
  OPTL 24*8
  OPTA 4*8 5 19*8
  OPTF 4*8 5 19*8
  OUT     8   1  -1   0
  END
2 922340 270. 922350 30000. 922380 969730. 0 0.0
```

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How the manual says it is* ...

- TAPE9.inp (8th input on LIB card)
- TAPE8.inp (9th input on LIB card)
  - Sorry for the confusion
- LPU card
  - Short for Lost Plutonium*
- Programed both, neither worked
  - The first lied to my face
  - The second complained about: "An endfile record was detected in a READ statement (unit= 8)"
  - Didn't find out about the lying until last night

LIB	NUCLID	(n,γ)	(n,2n)	(n,3n)	(n,f)	(n,γ^*)	(n,2n*)	YYN

* Its not Really

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Cross-section calculations

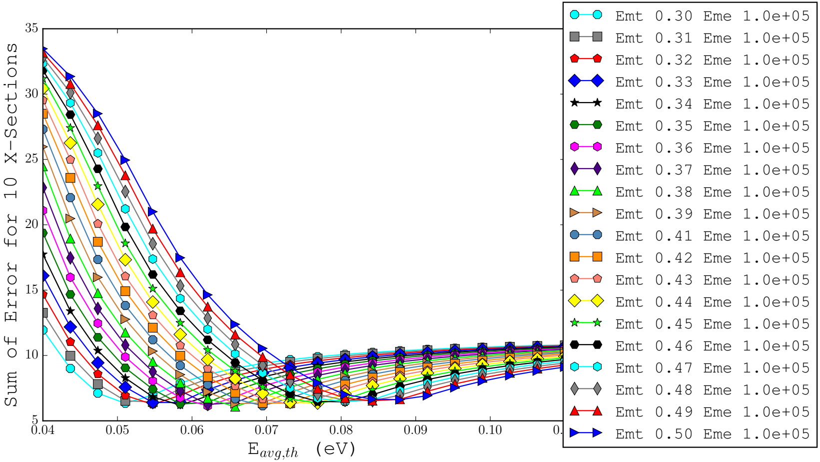
$$\sigma = \frac{\int \sigma(E)\phi(E)dE}{\int \phi(E)dE}$$

$$\begin{aligned}
\phi(E) =& C_1 \cdot \frac{E}{E_0^2} \cdot exp\left(-\frac{E}{E_0}\right) && E < E_{max,th} \\
=& \frac{C_2}{E} && E_{max,th} < E < E_{max,epi} \\
=& C_3 \cdot \frac{\sqrt{\frac{E}{E_f}}}{E_f} \cdot exp\left(-\frac{E}{E_f}\right) && E > E_{max,epi}
\end{aligned}$$

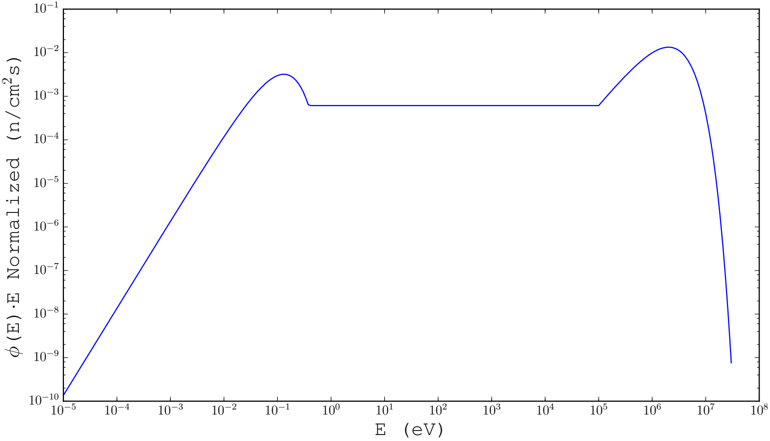
$$\begin{aligned}
C_1 =& \frac{E_0^2}{E_{max,th}^2} e^{E_{max,th}/E_0} \\
C_2 =& 1 \\
C_3 =& \frac{E_f}{E_{max,epi}} \cdot e^{\frac{E_{max,epi}}{E_f}} \frac{1}{\sqrt{\frac{E_{max,epi}}{E_f}}}
\end{aligned}$$

$E_{max,th} = 0.50$ eV, $E_{max,epi} = 1E5$ eV, $\theta_{th} = 0.09$ eV (764 K), $\theta_{fis} = 1.35E6$ eV

Difference Minimization



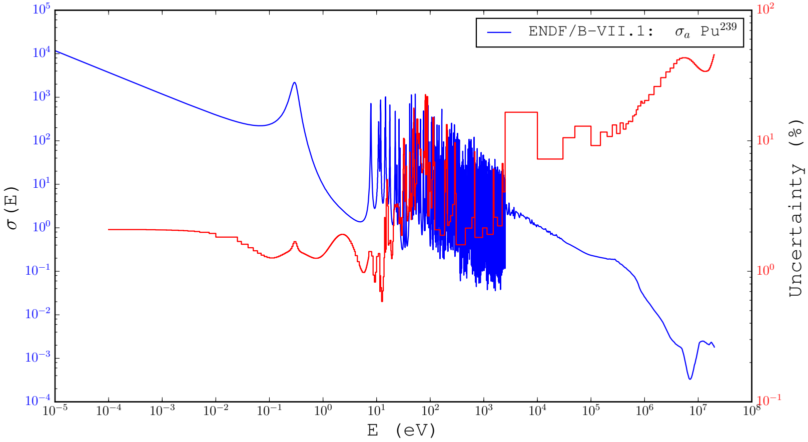
Flux Distribution

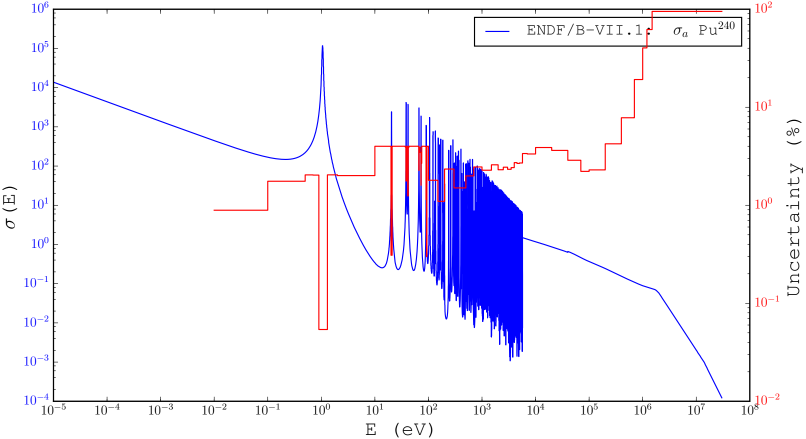


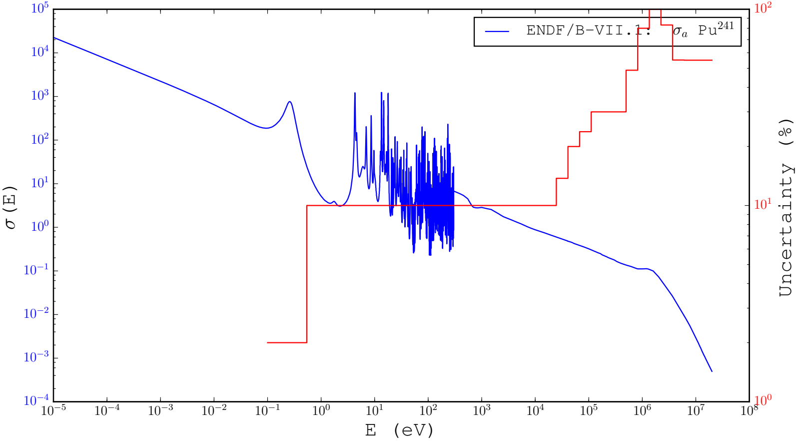
Flux Spectra used for weighting x-sections and yields

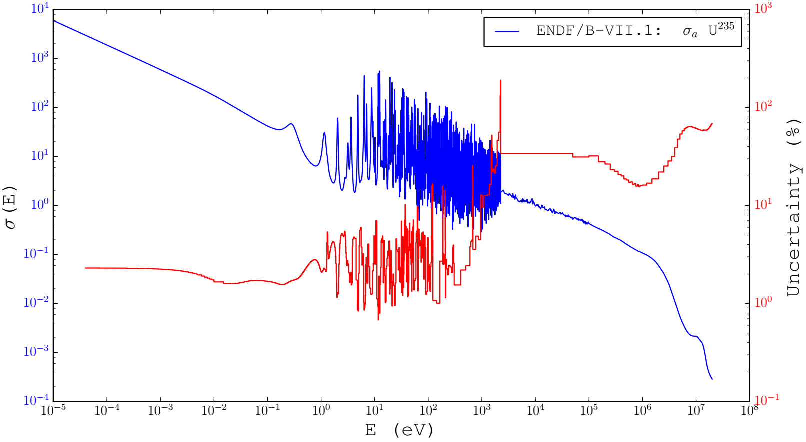
One Group Cross Section Comparison

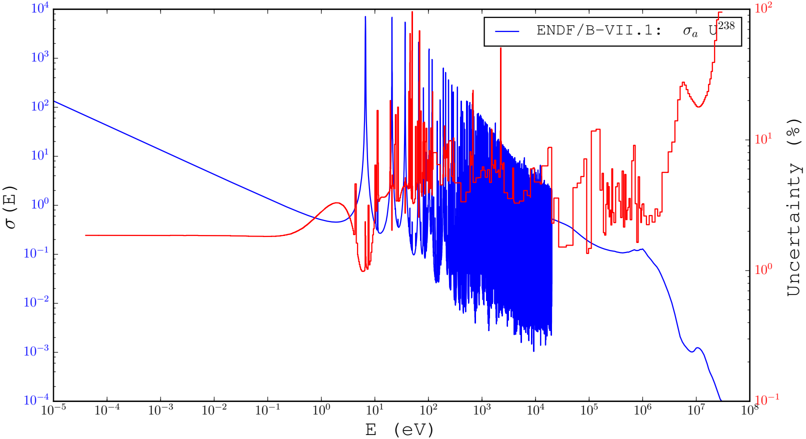
$\text{Isotope}^{\text{Rxn}}$	ENDF VII	ORIGEN2	Ratio
$^{239}\text{Pu}^{\gamma}$	6.544e+01	6.909E+01	1.06
$^{240}\text{Pu}^{\gamma}$	1.521e+02	2.228E+02	1.46
$^{241}\text{Pu}^{\gamma}$	4.518e+01	4.202E+01	0.93
$^{235}\text{U}^{\gamma}$	9.387e+00	1.068E+01	1.14
$^{238}\text{U}^{\gamma}$	4.098e+00	8.872E-01	0.22
$^{239}\text{Pu}^{\text{f}}$	1.179e+02	1.211E+02	1.03
$^{240}\text{Pu}^{\text{f}}$	9.609e-01	5.787E-01	0.60
$^{241}\text{Pu}^{\text{f}}$	1.253e+02	1.259E+02	1.01
$^{235}\text{U}^{\text{f}}$	4.621e+01	4.752E+01	1.03
$^{238}\text{U}^{\text{f}}$	2.091e-01	9.281E-02	0.44


ENDF/B-VII.1: σ_a Pu^{239}
σ(E)
Uncertainty (%)
E (eV)
10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5}
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
10^{-1} 10^{0} 10^{1} 10^{2}

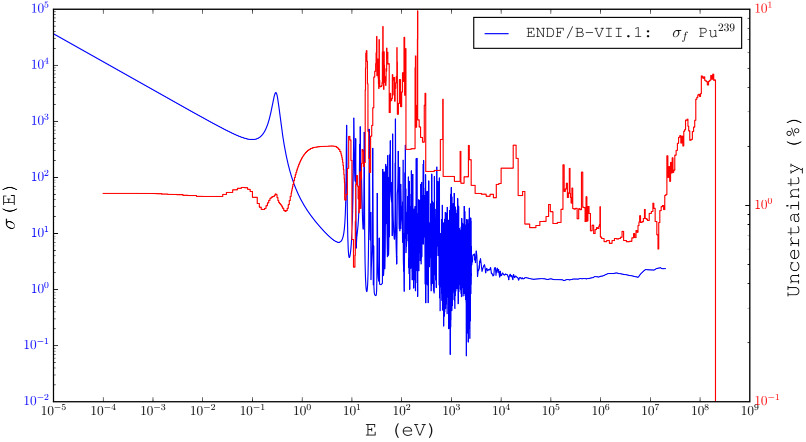

ENDF/B-VII.1: σ_a Pu^{240}
σ(E)
E (eV)
Uncertainty (%)
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
10^{6} 10^{5} 10^{4} 10^{3} 10^{2} 10^{1} 10^{0} 10^{-1} 10^{-2} 10^{-3} 10^{-4}
10^{2} 10^{1} 10^{0} 10^{-1} 10^{-2}

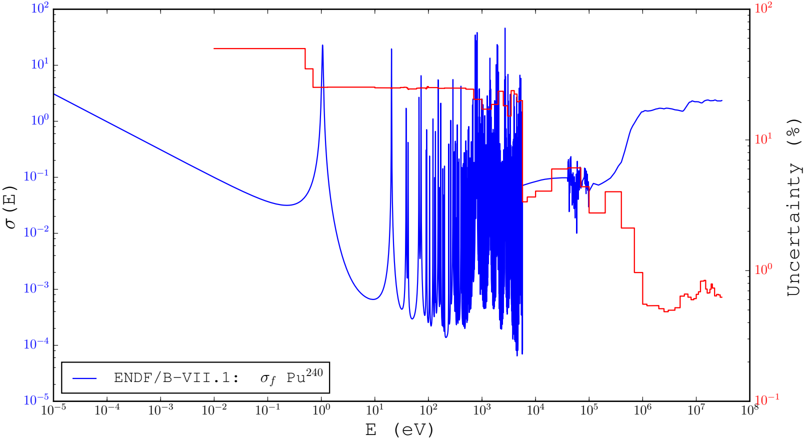

ENDF/B-VII.1: σ_a Pu^{241}
σ(E)
E (eV)
Uncertainty (%)
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
10^{5} 10^{4} 10^{3} 10^{2} 10^{1} 10^{0} 10^{-1} 10^{-2} 10^{-3} 10^{-4}
10^{2} 10^{1} 10^{0}


ENDF/B-VII.1: σ_a U^{235}
σ (E)
Uncertainty (%)
E (eV)
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{5}
10^{6}
10^{7}
10^{8}

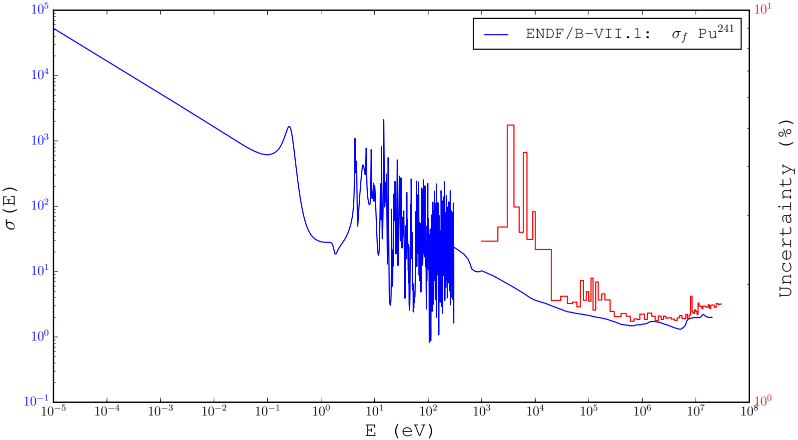


ENDF/B-VII.1: σ_a U^{238}
σ(E)
E (eV)
Uncertainty (%)
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{5}
10^{6}
10^{7}
10^{8}


ENDF/B-VII.1: σ_f Pu^{239}
σ(E)
Uncertainty (%)
E (eV)
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8} 10^{9}
10^{1}
10^{0}
10^{-1}



ENDF/B-VII.1: σ_f Pu^{240}
σ(E)
E (eV)
Uncertainty (%)
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
10^{-1} 10^{0} 10^{1} 10^{2}



ENDF/B-VII.1: σ_f Pu^{241}
σ(E)
E (eV)
Uncertainty (%)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
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10^{6}
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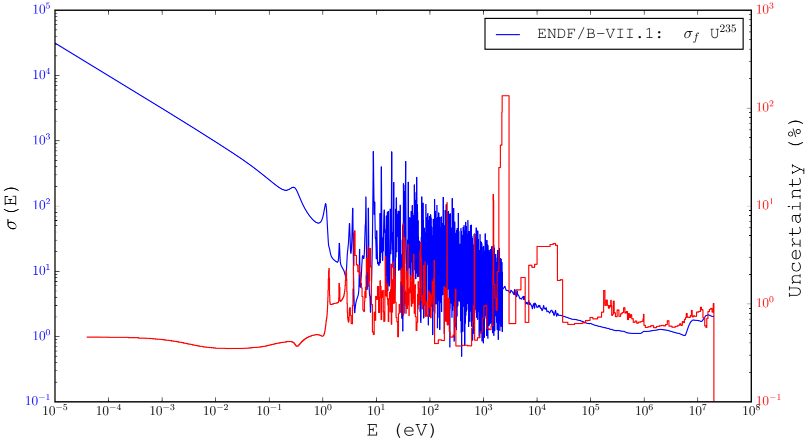
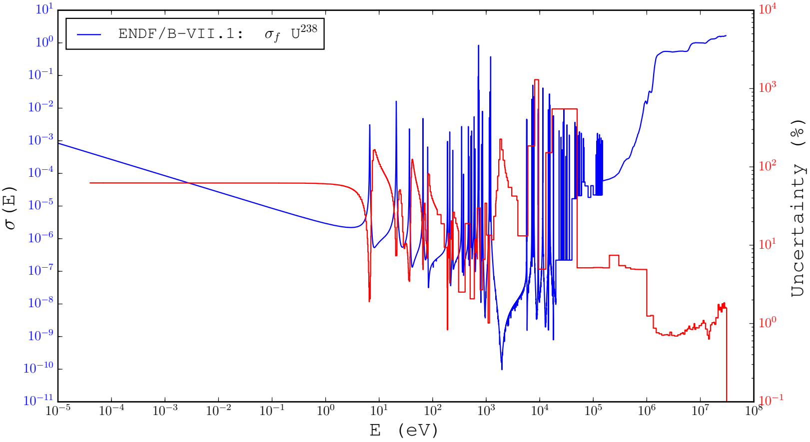
10^{8}
10^{0}
10^{1}


ENDF/B-VII.1: σ_f U^{235}
$\sigma(E)$
Uncertainty (%)
E (eV)
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5}
10^{-1} 10^{0} 10^{1} 10^{2} 10^{3}


ENDF/B-VII.1: σ_f U^{238}
σ(E)
E (eV)
Uncertainty (%)
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
10^{1} 10^{0} 10^{-1} 10^{-2} 10^{-3} 10^{-4} 10^{-5} 10^{-6} 10^{-7} 10^{-8} 10^{-9} 10^{-10} 10^{-11}
10^{4} 10^{3} 10^{2} 10^{1} 10^{0} 10^{-1}

Isotope$^{\mathrm{Rxn}}$	σ with 1STD Error
$^{239}\mathrm{Pu}^{\gamma}$	69.09 ± 8.15
$^{240}\mathrm{Pu}^{\gamma}$	222.8 ± 50.9
$^{241}\mathrm{Pu}^{\gamma}$	42.02 ± 10.92
$^{235}\mathrm{U}^{\gamma}$	10.68 ± 3.23
$^{238}\mathrm{U}^{\gamma}$	0.887 ± 0.175
$^{239}\mathrm{Pu}^{\mathrm{f}}$	121.1 ± 1.2
$^{240}\mathrm{Pu}^{\mathrm{f}}$	0.579 ± 0.003

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Results

Irradiation

Dissolution of the spent fuel pellet

Glovebox

Experiments

Conclusions