$^{79}\text{Se}(n,\gamma)$ measurement proposal

Outline

● **Introduction**
  ○ Motivations: s-process and nuclear waste
  ○ Status of the data and evaluations
  ○ Sample
  ○ Pros & cons of experimental set-ups and EARs: combined proposal

● **Counting rate estimates and expected accuracy**
  ○ Se-79(n,g) with i-TED @ EAR1
  ○ Se-79(n,g) with C6D6 @ EAR2

● **Summary**
Motivation (I): s-process

s-process nucleosynthesis around $A = 80$

$\text{Se-79}(n,\gamma)$ + s-only $80,82\text{Kr}$ well characterized [Nature, 1988 Ott et al.]

$\text{Se-79}(n,\gamma)$: key measurement

s-process stellar site thermometer
Motivation (II): nuclear waste

In terms of long-term radiotoxicity, however, long-lived fission products like Tc-99 and I-129, together with Se-79 and Cs-135, are the main contributors in addition to the above-mentioned actinides, and dominate the potential hazard in the case of HLW not containing actinides. Figure 13.2 compares

**Handbook of advanced radioactive waste conditioning technologies**

Se-79 is one of the main contributors to the long-term radiotoxicity among fission products

**Se-79(n,γ):** relevant for nuclear waste disposal and transmutation
Status of the $^{79}\text{Se}(n,\gamma)$ data

**EXPERIMENTAL DATA**

- First measurement of this cross section at thermal, RRR and URR
- No data available in EXFOR:
- MACS via activation not possible (Se-80 stable)

**EVALUATIONS**

- **JEFF-3.3**: TALYS Calculation → Provides Resonance parameters
- **ENDF/B- VIII.0**: Systematics for the thermal point + 1/v dependence & OM for the URR

Additional calculations by A. Mengoni in Back-up

Se-$^{79}(n,\gamma)$: challenging measurement but **high impact**. No data available → High accuracy is not mandatory.
**79Se Sample**

Se-78(n,γ) @ ILL

PbSe alloy to avoid low melting point of pure Se

0.5 mm thick 6N Al casing (laser-welded)

Sample properties

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass (g)</th>
<th>natoms cm^-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Se-78</td>
<td>0.77</td>
<td>4.01E+21</td>
</tr>
<tr>
<td>Se-79</td>
<td>0.003</td>
<td>1.53E+19</td>
</tr>
<tr>
<td>Pb-208</td>
<td>2.84</td>
<td>5.51E+21</td>
</tr>
<tr>
<td>Al-27</td>
<td>1.0244</td>
<td>5.90E+21</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Activity (Bq) (Nov. 2021)</th>
<th>C. Rate C6D6 (Ethr = 250 keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Se-75</td>
<td>5.66E+06</td>
<td>2.82E+03</td>
</tr>
<tr>
<td>Ag-110m</td>
<td>2.04E+05</td>
<td>4.97E+03</td>
</tr>
<tr>
<td>Zn-65</td>
<td>2.33E+05</td>
<td>1.25E+03</td>
</tr>
<tr>
<td>Co-60</td>
<td>1.40E+06</td>
<td>2.75E+04</td>
</tr>
<tr>
<td>TOTAL</td>
<td>7.50E+06</td>
<td>3.65E+04</td>
</tr>
</tbody>
</table>
Detectors and EARs: pros & cons

Se-79(n,γ): EAR1 o EAR2?
- Small mass (3 mg Se-79 + 2.84 g Pb + 0.77 g Se-78)
- Radioactive sample
- Measurement at EAR2 seems the best idea to achieve **good statistics in the URR and thermal point and optimize capture/activity.**
- RF EAR2: uncertain to resolve resonances in the keV range (& disentangle 78Se contribution)
- Performance of C6D6 and i-TED at “new” EAR2 is still uncertain: to be commissioned
- Feasibility of (n,γ) up to hundreds of keV @ EAR1 well known
- **High accuracy measurement at EAR1 required for validation/cross check in the RRR**

Se-79(n,γ): i-TED and/or C6D6?
- **Large contribution** of neutron scattering in Pb, Se-78 and Se-79 → **Case for i-TED**
- i-TED has shown good performance @ EAR1 (commissioning 2018)
- i-TED allows to extract spectroscopic information of the Se-79(n,γ) cascade
- **C6D6 better performance at high CR** → **Better suited for EAR2**

**Combined proposal:**
i-TED (+ C6D6?) @ EAR1 & C6D6 @ EAR2

**Similar previous measurements:**
- Tm-171(n,γ) @ EAR1 and EAR2
- Cm-244/246(n,γ)
$^{79}\text{Se}(n,\gamma)$: Counting rate estimates
$^{79}\text{Se}(n,\gamma) @ \text{EAR1 with i-TED}$

**XS:** JEFF-3.3

**$(n,g)$ efficiency:** MC simulations

Empty and Lead from experimental C6D6 data.

**i-TED:** Scaled assuming than $(n,\gamma)$/background can improve a factor 5(*).

Activity counting rate via MC simulations of the sample contaminants.

**i-TED:** Energy cuts -40% of the activity

*(*) backup

Background dominated by sample activity: to be fitted and $1/v$ subtracted such as in previous measurements on highly active samples: Tm-171, TI-204, …
**$^{79}\text{Se(n,}\gamma\text{)}$ @ EAR1 i-TED: statistics**

- **MC simulation of the experiment:** Realistic counts and statistical uncertainties
- **i-TED:** reduction of activity background in 40% and the dummy in a factor $\sim$5 relative to capture (wrt to C6D6)

**STATISTICS IN EAR1 FOR MC RESAMPLING**

- PbSe sample: $2.5\times10^{18}$ protons
- Dummy: $0.5\times10^{18}$ protons

**Dummy** = Pb + Se-78 + Al + empty

**Activity** (beam-off + sample-in)

**Sample** = Dummy + Activity + Se-79
$^{79}\text{Se}(n,\gamma)$ @ EAR1 i-TED: RRR

- **Se-79 (n,g) @ EAR1:**
  - RRR (strongest resonances) of Se-79 below 1 keV with **high resolution (RF negligible)**
  - Cross-check/Validation of Se-79(n,g) @ EAR2

**PROTON REQUEST Se-79 @ EAR1**

- $3.5 \times 10^{18}$ protons
  - 2.5 Se-79 sample +
  - 0.5 dummy (Se-78 + Pb) +
  - 0.5 backgrounds/normalization
$^{79}\text{Se}(n,\gamma) @ \text{EAR2 with C6D6}$

STATISTICS IN EAR2 FOR MC RESAMPLING

PbSe sample: 1.0e18 protons

Dummy: 0.5e18 protons

\textbf{Dummy} = Pb + Se-78 + Al + empty

\textbf{Activity} (beam-off + sample-in)

Sample = \textbf{Dummy} + \textbf{Activity} + Se-79

\textbf{MC simulation of the experiment:} Realistic counts and statistical uncertainties

Activity does not dominate $\square$ Overall $(n,g)$/background better
Se(n,γ) @ EAR2 C6D6: Thermal & URR

**Thermal point:** large deviation between evaluations and other calculations
Measurement @ EAR2 required for this point

**URR:** Very relevant for the stellar capture rates (MACS)
Feasible @ EAR2 with 5-10 bpd
Statistical uncertainties in the Se-79(n,γ) yield (1 bpd)

- Integral cross section URR (useful for MACS) with statistical unc.
  < 20 % up to 100 keV

- Measurement at EAR2 provides also the thermal point: 5% unc.
  (Integral 10-100 meV))

**PROTON REQUEST Se-79 @ EAR2**

2.0 $10^{18}$ protons
- 1.0 Se-79 sample +
- 0.5 dummy (Se-78 + Pb) +
- 0.5 backgrounds/normalization
Summary

- **Motivation for Se-79(n,g):**
  - Key s-process branching point isotope: Constrain thermal conditions of massive stars
  - One of the largest contributions to the long-term radiotoxicity among FP in the nuclear waste

- **Goal of the proposal:**
  - **First measurement of this cross section** at thermal, RRR and URR
  - Get the most comprehensive knowledge of Se-79(n,g) in the 3 energy regions.

- **Se-79 sample ready and characterized @ PSI**

- **Realistic counting rate estimates of Se-79(n,g) @ EAR1 and EAR2:**
  - Realistic efficiencies from MC simulations
  - Evaluated cross sections JEFF-3.3 (TALYS for Se-79)
  - Impact of statistical uncertainties in background subtraction and RF (see Back-up for details)

- **A combined proposal would be ideal for a successful measurement of this key isotope**
  - **Se-79(n,γ) @ EAR1** with i-TED (& C6D6): RRR with high resolution and validation
    - $3.5 \times 10^{18}$ protons (2.5 sample + 0.5 dummy + 0.5 backgrounds normalization)
  - **Se-79(n,γ) @ EAR2** with C6D6: good statistics for the URR and thermal point
    - $2.0 \times 10^{18}$ protons (1.0 sample + 0.5 dummy + 0.5 backgrounds normalization)
**Summary:** proton request

<table>
<thead>
<tr>
<th>SAMPLE</th>
<th>Se-79(n,g) @ EAR1 i-TED (&amp; C6D6)</th>
<th>Se-79(n,g) @ EAR2 C6D6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Se-79 (PbSe sample)</td>
<td>2.5.10^{18} p</td>
<td>1.10^{18} p</td>
</tr>
<tr>
<td>Dummy (Se-78 + Pb + Al)</td>
<td>5.10^{17} p</td>
<td>5.10^{17} p</td>
</tr>
<tr>
<td>Au, C, Pb, Filters</td>
<td>~5.10^{17} p (*)</td>
<td>~5.10^{17} p (*)</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td>3.5.10^{18} p</td>
<td>2.5.10^{18} p</td>
</tr>
</tbody>
</table>

(*) Might be shared with other measurements

Watch **Recorded presentation** or see back-up slides for more details!
EXTRA SLIDES
LONG VERSION
Outlook

Possible sample improvement:
- Under discussion with PSI’s colleagues: Chemical purification of the PbSe sample to reduce the sample activity and make a Se Oxide sample. → Specially relevant for the measurement @ EAR1

i-TED development & characterization:
- Results of the i-TED 5.3 prototype look promising and proof the good perfomance in EAR1 (V. Babiano’s talk)
- Optimization of the position reconstruction & imaging algorithms to improve background suppression capabilities: Machine learning looks promising (J. Balibrea & J. Lerendegui’s talks)
- On-going tests @ IFIC-lab to characterize the CRT and the counting rate limit.
- Before measurement: i-TED 4 pi commissioning in EAR1 and EAR2 during target commissioning (Cesar’s talk)

Proposal timeline:
- Presentation to INTC in November
- Measurement: End 2021, early 2022 → ERC Project ends May 2022
$^{79}\text{Se}(n,\gamma)$: Counting rate estimates

COUNTING RATES: Ingredients

- Cross sections from JEFF-3.3
- Evaluated Flux EAR1/2 phase 3
- BIF: Geant4 spallation target
- $(n,\gamma)$ efficiency from MC assuming Au-197 cascade
- Ethr = 200 keV for C6D6 & i-TED (coinc.)
79Se(n,γ) @ EAR1: expected results

Theoretical estimation: After 1/v activity subtracted → Total counts vs “dummy”

**ASTROPHYSICS**: keV-to-100keV region is the most important one.

**High-resolution of EAR1 is required** here to resolve 79Se capture levels between Se-78 resonances

**Strength and level density of Se-79 may change** (BASED IN TALYS)
79\textsuperscript{Se}(n,\gamma) @ EAR1 i-TED: uncertainty

**Statistical uncertainties in the Se-79(n,\gamma) yield (1 bpd)**

- RRR; Uncertainty < 15% up to 1 keV
  
  **AIM OF EAR1**

- URR and thermal: Motivation for EAR2

**PROTON REQUEST Se-79 @ EAR1**

- 3.5 $10^{18}$ protons
- 2.5 Se-79 sample +
- 0.5 dummy (Se-78 + Pb) +
- 0.5 backgrounds/normalization
Empty and Lead experimental data with C6D6 @ EAR2

Activity counting rate calculated with MC simulations of the sample contaminants.

PHWT not applied: It may improve the capture to background ratio.

Activity background does not dominate like in EAR1
Overall (n,γ)/background better than in EAR1
$^{79}$Se($n,\gamma$) @ EAR2 C6D6: RRR

**Very good statistics in the resolved resonances of Se-79 below 1 keV**

**GOAL:**
Validation/normalization with EAR1 data

**RF @EAR2 NOT INCLUDED:**
Impact RF from target #2 (Back-up slides)
Improvement with Target #3 expected
Statistical uncertainties in the Se-79(n,γ) yield (5 bpd)

- Very small < 1% in the resonances below 200 eV
- Between 5 and 10% in the 500-2 keV range (RRR)
- URR: 20-25% up to 2-20 keV
- URR: Larger than 40% above 30 keV

AIM OF EAR2
BACK-UP SLIDES
\( ^{79}\text{Se}(n,\gamma) \)

Motivation
• Last, but not least, enhanced efforts should be directed to measurements on unstable nuclei. In addition to the activation technique, the very high neutron fluxes available at spallation neutron sources appear to be promising options for such studies. Priority should be given to the important branch points $^{79}$Se, $^{147}$Pm, $^{151}$Sm, $^{163}$Ho, $^{170}$Tm, $^{171}$Tm, $^{179}$Ta, $^{204}$Tl, and $^{205}$Pb.
$^{79}\text{Se}(n,\gamma)$
Cross section calculations
(A. Mengoni)
Thermal value: ENDF, JEFF and TALYS

A. Mengoni’s calculations:
300 sets of resonance using average parameters in TALYS:

- $\langle D_0 \rangle = 56.8$ eV
- $S_0 = 0.98 \times 10^{-4}$
- $\langle \Gamma_{\text{g}(0)} \rangle = 0.078 \pm 10\%$

JEFF-3.3 (TENDL 2019) uses $\langle \Gamma_{\text{g}(0)} \rangle = 0.100$ meV

Calculation at thermal shows remarkable differences with evaluations

- Calculation: $P(\sigma_{\text{th}} < 1\text{b}) = 80\% \ + \ P(\sigma_{\text{th}} < 10\text{b}) = 98\%$
- $\sigma_{\text{th}} = 50$ b in ENDF/B-VIII.0
- $\sigma_{\text{th}} = 11.8$ b in TENDL-2019
A. Mengoni’s calculations:
   300 sets of resonance using average parameters in TALYS:
   
   - \( <D_0> = 56.8 \text{ eV} \)
   - \( S_0 = 0.98 \times 10^{-4} \)
   - \( <\Gamma_g(0)> = 0.078 \pm 10\% \)

JEFF-3.3 (TENDL 2019) uses \( <\Gamma_g(0)> = 0.100 \text{ meV} \)

**Calculation RRR:** some realizations are compatible to JEFF-3.3 (used for the estimates). In some cases the strength of resonances is smaller

**Calculation URR:** Above 55 keV, TALYS Statistical model
$^{79}\text{Se}(n,\gamma)$ @ EAR1: i-TED imaging capabilities
Spectra normalized to integral (1140-1160 keV)

Resonance is wider in i-TED due to non-perfect trigger timing correction

NORMALIZATION TO 1.15 KeV Resonance to prove gain in (n,g) background in the keV range
i-TED Spectra: singles & add-back

(n,g) and background

Au-197(n,g)

<table>
<thead>
<tr>
<th>Counts/bin</th>
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</thead>
<tbody>
<tr>
<td>10^4</td>
</tr>
<tr>
<td>10^3</td>
</tr>
<tr>
<td>10^2</td>
</tr>
<tr>
<td>10^1</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>1</td>
</tr>
</tbody>
</table>

Deposited energy (keV)

Singles Scatterer
Singles Absorber
AddBack energy distribution

Background EAR1

<table>
<thead>
<tr>
<th>Counts/bin</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^6</td>
</tr>
<tr>
<td>10^5</td>
</tr>
<tr>
<td>10^4</td>
</tr>
<tr>
<td>10^3</td>
</tr>
<tr>
<td>10^2</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>1</td>
</tr>
</tbody>
</table>

Deposited energy (keV)

Singles Scatterer
Singles Absorber
Coincidences AddBack

Det #2
D = 50 mm
Before imaging: i-TED improves $(n,\gamma)/$background ratio in the keV range after coincidences between absorber-scatterer.

**Scatterer** alone very similar counting rate that **C6D6** but:
- Higher resolution
- Spectroscopic

See V. Babiano’s talk for more details on the i-TED prototype commissioning.
Background suppression i-TED

**i-TED CONCEPT**

- **TED**
  - n-beam
  - captured neutron
  - scattered neutron

\[ \theta = \arccos \left( 1 - m_e c^2 \left( \frac{1}{E_2} - \frac{1}{E_1 + E_2} \right) \right) \]

\[ \Delta \theta = \frac{E_1 + E_2}{\sin \theta} \left( \frac{1}{E_1^2} \left( \frac{\Delta E_1}{E_1} \right)^2 + 2 \tan^2 \theta \left( \frac{\Delta r}{r} \right)^2 \right)^{1/2} \]

- **γ-ray source**
- **Compton scattering**

**COMPTON IMAGING WITH I-TED**
Background suppression i-TED

MC : C6D6 & i-TED to capture & background

Best gain factors \((n, \gamma)/\text{bckg}\) ratio wrt to C6D6

Capture to background ratio (a.u.)

- Scatterer
- Absorber
- Coincidences
- Coincidences & t1<t2
- C6D6 @ 100 mm

Gain factor i-TED/C6D6 @ 100 mm

- i-TED @ 25 mm
- i-TED @ 50 mm
- i-TED @ 75 mm
- i-TED @ 100 mm

Values with no imaging cut

Coindicences and time resolution make a factor 2-3 in \((n, \gamma)/\text{background}\) gain

Feasible \((n, \gamma)/\text{background}\) gain: Factor 4-10 depending of the sample-i-TED distance

Optimization of the background rejection capabilities still on-going
$^{79}\text{Se}(n,\gamma) \ @ \ EAR1$: i-TED vs C6D6
### Detectors and EARs: Summary

<table>
<thead>
<tr>
<th>DETECTOR</th>
<th>EAR1</th>
<th>EAR2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>C6D6</strong></td>
<td>Higher efficiency, Worse background rejection (large neutron scattering)</td>
<td>Better Performance @ high CR More statistics Activity not an issue</td>
</tr>
<tr>
<td><strong>I-TED</strong></td>
<td>~ 5-10 x Better (n, $\gamma$)/background in the keV range. C. Rate is not an issue.</td>
<td>Performance in EAR2 is still uncertain, probably too high CR</td>
</tr>
</tbody>
</table>

**Combined proposal:**
i-TED (+ C6D6?) @ EAR1 & C6D6 @ EAR2
$^{79}$Se$(n,\gamma)$ @ EAR1: i-TED vs C6D6

Theoretical estimation: After 1/v activity subtracted → Total counts vs “dummy” sample
i-TED: improved Se-79$(n,\gamma)$/background above 100 eV
Background due to Se-78$(n,n)$ and Se-79$(n,n)$ not included and also suppressed with i-TED
Theoretical estimation: After 1/v activity subtracted → Total counts vs “dummy” sample

Reduction of the background in i-TED seems critical to observe Se-79 resonances,
Strength and level density may change (BASED IN TALYS)
\( ^{79}\text{Se}(n,\gamma) @ \text{EAR1 i-TED vs C6D6} \)

**MC simulation of the experiment:** Realistic counts and statistical uncertainties

i-TED vs C6D6: reduction of activity background in 50% and the dummy in a factor \( \sim 5 \) relative to capture

**PbSe sample:** 2.5e18 protons

**Dummy:** 0.5e18 protons

- i-TED (coinc.)
- C6D6 (or i-TED scatterer)
$^{79}\text{Se}(n,\gamma)$ @ EAR1 i-TED vs C6D6: RRR

Largest resonances of Se-79 below 200 eV clearly observed

- PbSe sample: 2.5e18 protons
- Dummy: 0.5e18 protons

i-TED (coinc.)

C6D6 (or i-TED scatterer)
Possible to measure @ EAR1 the RRR below 1 keV
URR: complementary measurement at EAR2
79Se(n,γ) @ EAR1: uncertainty

PbSe sample: 2.5e18 protons
Dummy: 0.5e18 protons

Statistical uncertainties in the Se-79(n,γ) integral yield (1 bpd)

- Below 15% up to 1 keV (both setups)
- At higher energies: Uncertainty 50-70%. Very challenging to extract any cross section
- i-TED provides better uncertainty in above 10 keV → better Se-79(n,γ)/background
$^{79}\text{Se}(n,\gamma) \ @ \ n_{\text{TOF}}$: Including RF
For a given real neutron Energy ($E_n$):

1. $L(En) = L_0 + \lambda(En) \rightarrow$ Flight path distribution
2. $TOF(En) = TOF(L(En)) \rightarrow$ TOF distribution
3. $E'(En) = E'(TOF(En)) \rightarrow$ Exp. Energy distribution
$^{79}\text{Se}(n,\gamma)$: Resolution Function

Shift resonance energy + broadening + asymmetry (low energy tail)
$^{79}\text{Se}(n,\gamma)$ @ EAR1 i-TED: Impact RF

MC simulation Experiment

PbSe sample: 2.5e18 protons
Dummy: 0.5e18 protons

Resolution function at EAR1 not sizable below 1 keV
Target #3 should not worsen the RF @ EAR1
$^{79}\text{Se}(n,\gamma) \oplus \text{EAR1 i-TED: Impact RF}$

- **PbSe sample**: 2.5e18 protons
- **Dummy**: 0.5e18 protons

Resolution function at EAR1 negligible below 1 keV

Target #3 should not worsen the RF @ EAR1
RF @ EAR2: Difficult to estimate

Exp vs SAMMY
With different RF

(See V. Alcayne’s RF talk)

RF depends on sample dimension → Standard RF overestimates → V. Alcayne ‘s Talk)

Target #3 should significantly improve the RF @ EAR2
$^{79}\text{Se}(n,\gamma) \atop \text{EAR2 C6D6: Impact RF}$

- PbSe sample: $1 \times 10^{18}$ protons
- Dummy: $0.5 \times 10^{18}$ protons

Measurement at EAR2 can observe resonances up to 1 keV even with Standard RF (overestimates → V. Alcayne ‘s Talk)

Target #3 should improve the RF @ EAR2
$^{79}\text{Se}(n,\gamma) @ \text{EAR2 C6D6: Impact RF}$

**MC simulation Experiment**

PbSe sample: 1e18 protons  
Dummy: 0.5e18 protons

**NO RF**

**WITH RF**

Challenging to analyze individual Se-79 resonances @ EAR2 above 1 keV  
Standard RF (overestimates → V. Alcayne ‘s Talk)  
Target #3 should improve the RF @ EAR2