

# Berkeley Nuclear Database Projects

Aaron M. Hurst

[amhurst@berkeley.edu](mailto:amhurst@berkeley.edu)

25th Technical Meeting of the International Network of Nuclear Structure and  
Decay Data Evaluators,  
IAEA Headquarters, Vienna, Austria

April 15 – 19, 2024



# Table of Contents

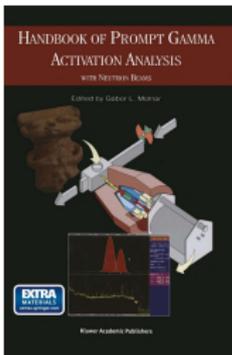
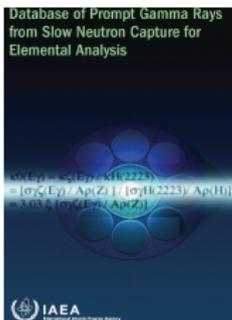
<https://nucleardata.berkeley.edu/databases/>

- 1 Reactions
  - pyEGAF
  - APGAA
  - Baghdad Atlas
  
- 2 Structure and Decay
  - BEApR
  - paceENSDF



# EGAF disseminated in printed form and through the IAEA

<https://www-nds.iaea.org/pgaa/egaf.html>



Activities - Firefox

Mon 11:30

https://www-nds.iaea.org/pgaa/egaf.html

### Evaluated Gamma-ray Activation File (EGAF)

The Evaluated Gamma-ray Activation File (EGAF) has been developed as part of a Coordinated Research Project for the Development of a Database for Prompt Gamma-ray Neutron Activation Analysis sponsored by the International Atomic Energy Agency (IAEA). A file is provided for each isotope containing ENSDF datasets for the Adopted and Bagdadi PGAA data and the Resdy and Fianble neutron capture data. These data can be viewed with the [language:ExpJest 2.2.ENSDF Viewer](#).

**Thermal (n,g) Target Nucleus**

1H	2H	3He	6Li	7Li	8Be	10B	12C	13C	14N
16O	17O	18O	20Ne	21Ne	22Ne	23Na	24Mg	25Mg	26Mg
27Al	28Si	29Si	30Si	31P	32S	33S	34S	35Cl	36S
36Ar	37Cl	38K	39K	40K	40Ca	41K	42Ca	43Ca	44Ca
45Sc	46Ca	48Ti	47Ti	48Ca	49Ti	50Ti	51V	50Cr	52Cr
51V	52Cr	53Cr	54Cr	54Fe	55Mn	56Fe	57Fe	58Fe	59Ni
59Co	60Ni	61Ni	62Ni	63Cu	64Ni	64Zn	65Zn	66Zn	67Zn
68Zn	69Ga	70Ga	71Ga	72Ge	73Ge	74Ge	75Se	76Se	77Se
78Se	79Br	80Br	81Br	82Br	83Br	84Br	85Br	86Br	87Br
89Kr	90Rb	91Rb	92Rb	93Rb	94Rb	95Rb	96Rb	97Rb	98Rb
99Zr	100Zr	101Zr	102Zr	103Zr	104Zr	105Zr	106Zr	107Zr	108Zr
109Mo	108Ru	109Ru	110Ru	111Ru	112Ru	113Ru	114Ru	115Pd	116Pd
117Ag	118Pd	119Pd	120Pd	121Pd	122Pd	123Pd	124Pd	125Pd	126Pd
128Sn	129Sn	130Sn	131Sn	132Sn	133Sn	134Sn	135Sn	136Sn	137Sn
138Xe	139Xe	140Xe	141Xe	142Xe	143Xe	144Xe	145Xe	146Xe	147Xe
148Ba	149Ba	150Ba	151Ba	152Ba	153Ba	154Ba	155Ba	156Ba	157Ba
158Dy	159Dy	160Dy	161Dy	162Dy	163Dy	164Dy	165Dy	166Dy	167Dy
168Er	169Er	170Er	171Er	172Er	173Er	174Er	175Er	176Er	177Er
179Ho	180Ho	181Ho	182Ho	183Ho	184Ho	185Ho	186Ho	187Ho	188Ho
189Tm	190Tm	191Tm	192Tm	193Tm	194Tm	195Tm	196Tm	197Tm	198Tm
199Pt	200Pt	201Pt	202Pt	203Pt	204Pt	205Pt	206Pt	207Pt	208Pt
209Bi	210Bi	211Bi	212Bi	213Bi	214Bi	215Bi	216Bi	217Bi	218Bi
219Po	220Po	221Po	222Po	223Po	224Po	225Po	226Po	227Po	228Po
232Th									

Source ENSDF-formatted datasets @ IAEA



# Open-source Python library pyEGAF on GitHub

[https://github.com/AaronMHurst/python\\_egaf](https://github.com/AaronMHurst/python_egaf)

- Translated all 245 ENSDF-formatted EGAF datasets to a new JSON format.
- Generated RIPL-format EGAF for reaction calculations.
- Developed suite of Python modules enabling interaction, analysis, and visualization of the EGAF ( $n, \gamma$ ) data.
- Docstrings provided for all methods.
- JSON schema keys documented extensively in README.
- 224 unit tests (multiple virtual Python3 environments).
- Installation, testing scripts, and Jupyter Notebooks provided.
- ENSDF, RIPL, and JSON files bundled with software.
- Over 800 downloads.

The screenshot shows the GitHub repository page for `python_egaf`. The repository is owned by `AaronMHurst` and is a Python package for accessing, manipulating, and analyzing data from the Evaluated Gamma-ray Activation File (EGAF) datasets. The README content is visible, including the title "pyEGAF: An open-source Python library for the Evaluated Gamma-ray Activation File" and the authors "A.M. Hurst<sup>1</sup>, R.R. Firestone<sup>2</sup>, E.V. Chirraoui<sup>3</sup>". The article is published in the journal "Nuclear Inst. and Methods in Physics Research, A" by Elsevier. The article title is "pyEGAF: An open-source Python library for the Evaluated Gamma-ray Activation File". The abstract states: "The Evaluated Gamma-ray Activation File (EGAF) is one of the most comprehensive resources for atomic nuclear-capture data. This database contains data from prompt gamma activation analysis measurements carried out in a consistent manner using the same conventional nomenclature of the Baghdad Research Reactor for 245 isotopes. Although these valuable datasets have been freely available for many years, use of the datasets in the standard and simple Evaluated Nuclear Structure Data File (ENSDF) format is severely impeded for dissemination, making it difficult for users unfamiliar with the format to access and utilize the data contained therein. Furthermore, the ENSDF format does not readily lend itself to modern computational techniques and a parser is required to traverse the complex nested record format. To help overcome these challenges, we have developed a standard, accessible, and user-friendly Python-based interface to the EGAF data. This interface is implemented in Python, pyEGAF, that is designed to interact with the JSON data structure for prompt gamma-ray activation analysis, manipulation, and analysis of the nuclear-capture  $n, \gamma$  data in EGAF. The same format, together with the pyEGAF library, greatly enhances access to the wider applications community where JSON data may be useful or required."

`git clone https://github.com/AaronMHurst/python_egaf.git`



# pyEGAF on the Python Package Index (PyPI) repository

<https://pypi.org/project/pyEGAF/>

The screenshot shows the PyPI project page for pyEGAF 1.0.0. At the top, there is a search bar and navigation links for Help, Sponsors, Log in, and Register. The main header displays the package name 'pyEGAF 1.0.0' and a 'Latest version' button. Below this, a code block shows the installation command: `pip install pyEGAF`. A release date of 'Released: Sep 7, 2023' is also visible. A descriptive paragraph states: 'Allows for interaction, manipulation, and analysis of thermal-neutron capture gamma-ray data from the EGAF library.' The page is divided into sections: 'Navigation' with links for Project description (selected), Release history, and Download files; 'Project links' with a link to the Homepage; and 'Statistics' showing GitHub statistics (Stars: 1, Forks: 0, Open issues: 0, Open PRs: 0). The 'Project description' section contains a detailed paragraph about the project's purpose and data source, followed by a nuclear chart plot.

**Navigation**

- Project description
- Release history
- Download files

**Project links**

- Homepage

**Statistics**

GitHub statistics:

- Stars: 1
- Forks: 0
- Open issues: 0
- Open PRs: 0

**Project description**

This project is a Python package enabling interaction, manipulation, and analysis of thermal-neutron capture gamma-ray data from the Evaluated Gamma-ray Activation File (EGAF) library [\[PR2007\]](#), [\[REV2004\]](#). The EGAF library is a database of  $\gamma$ -ray energies and their corresponding partial  $\gamma$ -ray cross sections from thermal-neutron capture measurements carried out with a guided neutron beam at the Budapest Research Reactor for 245 isotopes encompassing measurements of natural elemental samples for targets from  $Z = 1, 83, 90$ , and  $92$ , except for Tc ( $Z = 43$ ) and Pm ( $Z = 61$ ). The database comprises a total of 8172 primary  $\gamma$  rays and 29655 secondary  $\gamma$  rays (a total of 37777  $\gamma$  rays) associated with 12664 levels. The  $(n, \gamma)$  targets and corresponding residual compound nuclides relevant to the EGAF project are summarized in the schematic of the nuclear chart shown in the figure below.

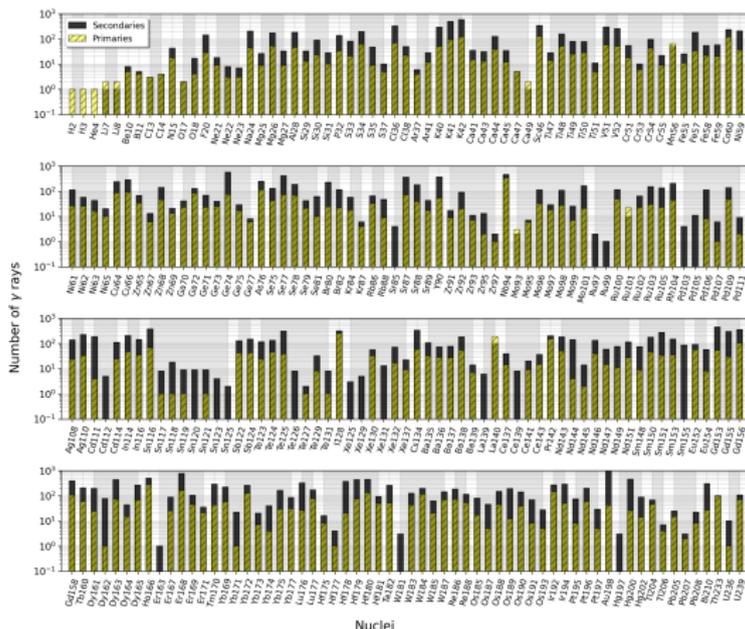
The nuclear chart plot shows the number of neutrons (N) on the y-axis (ranging from 0 to 80) versus the number of protons (Z) on the x-axis. Red dots represent EGAF (n,  $\gamma$ ) targets, and blue dots represent EGAF (n,  $\gamma$ ) residuals. The plot shows a clear linear trend of data points along the diagonal, indicating a strong correlation between the number of protons and neutrons in the targets and residuals.

- `pip install pyegaf`
- pyEGAF 1.0.0: Production/stable development release.
- FreeBSD License.



# What data is in EGAF?

And what else do we need?



- Courtesy: *E.V. Chimanski, BNL*
- 8,172 primary  $\gamma$  rays.
- 29,605 secondary  $\gamma$  rays.
- 12,564 levels.
- Cross sections:  $\sigma_\gamma$ ,  $\sigma_0$
- Associated nuclear structure properties, e.g.,  $J^\pi$ ,  $I_\gamma \dots$
- $\alpha$ ,  $\delta_\gamma$ ,  $\lambda L$  for improved RIPL and ENDF libraries.



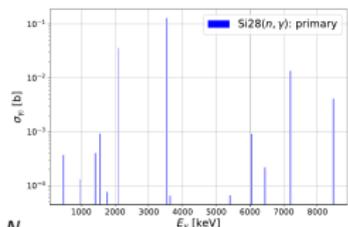
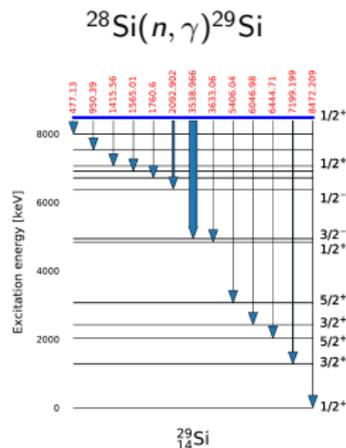
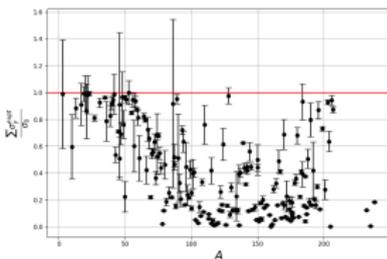
# Assess completeness of capture- $\gamma$ data using pyEGAF



- The cross section for fusion in entrance channel (a) is given by the sum of cross sections for decay to all final channels ( $b_i$ ):

$$\sigma_F(a) = \sum_{b_i}^N \sigma_{a \rightarrow b_i}^C \quad \therefore \quad \sigma_0 = \sum_{i=1}^N \sigma_{\gamma_i}^{\text{primary}}$$

- Compare  $\sum_{i=1}^N \sigma_{\gamma_i}^{\text{primary}}$  from pyEGAF to  $\sigma_0$ .

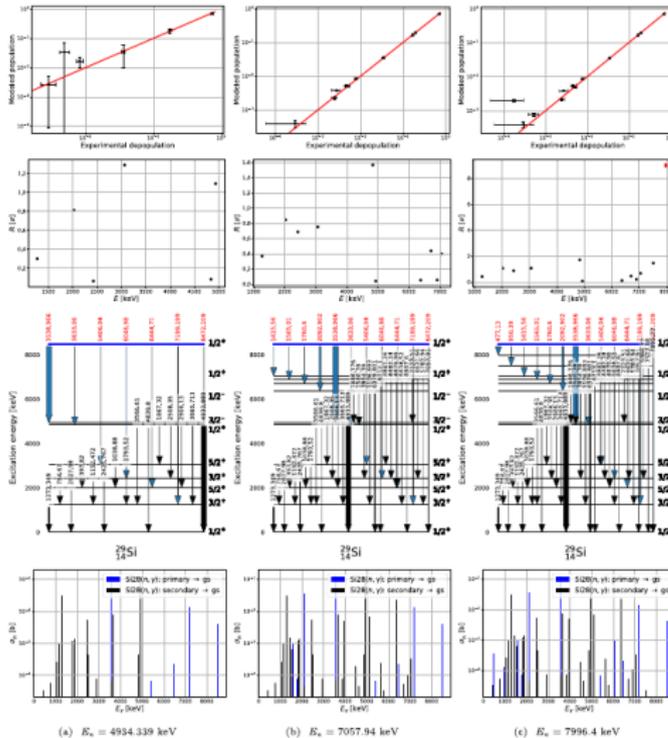


$$\sum_{i=1}^N \sigma_{\gamma_i}^{\text{primary}} = 0.185(2) \text{ b [pyEGAF]}$$

$$\sigma_0 = 0.177(5) \text{ b [Adopted]}$$



# Modeling the $(n, \gamma)$ reaction using pyEGAF methods



- Statistical-model analysis of  $(n, \gamma)$  reaction, e.g.,  $^{28}\text{Si}(n, \gamma)$ .
- Compare modeled population of levels to experimental data.
- Establish critical energy  $E_C$ .



# CapGam cf. pyEGAF : : capgam

## CapGam

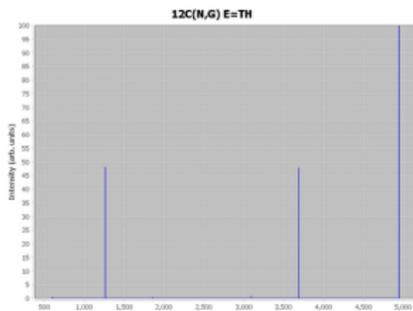
12C(N,G) E=TH  
Target: <sup>12</sup>C  
Product: <sup>13</sup>C

Last modified: 06/01/2023

[PDF](#)

Strongest Transition:  
E( $\gamma$ ) = 4945.301  $\pm$  0.003  
I( $\gamma$ ) = 67.47  $\pm$  0.92

Thermal Neutron Capture Cross Section (2000MuZX):  
0.00353 b  $\pm$  0.00007 b



Type	E( $\gamma$ ) (keV)	$\Delta E(\gamma)$ (keV)	I( $\gamma$ )/I( $\gamma$ ) <sub>max</sub> × 100	$\Delta(I(\gamma)/I(\gamma))_{max}$
Secondary	595.013	0.014	0.3527	0.6156
Primary	1261.764	0.012	47.9621	0.9225
Primary	1856.716	0.012	0.2371	0.6152
Secondary	3089.049	0.020	0.6373	0.6309
Secondary	3683.921	0.023	47.6300	1.6482
Primary	4945.301	0.003	100.0000	1.5233

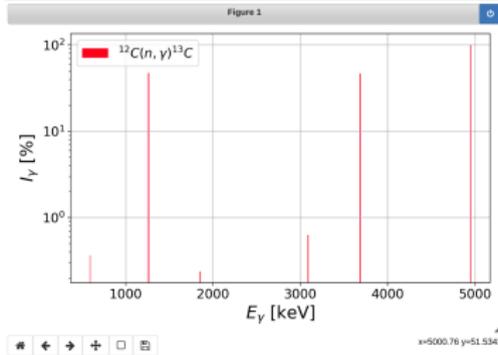
## pyEGAF

```
In [4]: # Define compound nucleus as a string, e.g., 12C(n,g)13C:
compound_nucleus = 'C13'

In [5]: # Extract capture-gamma data for defined compound nucleus and write results to CSV file in pwd
df=c.capgam(edata, "(0)", format(compound_nucleus))
df.to_csv("cappga_style_00.csv", format(compound_nucleus), index=False)
print(df.to_string(index=False))

Target nucleus: C12
Residual (compound nucleus): C13
C12(n,g)C13
Total radiative thermal neutron-capture cross section = 0.00387 b  $\pm$  3e-05
Reference: 2018MuZT
Maximum  $\Sigma$  = 0.0026389710000000004 b at E = 4945.301 keV; RI = 100.
Type      E      dE      RI      dRI
secondary 595.015 0.009  0.363985 0.015226
primary   1261.765 0.009  47.509579 1.149512
primary   1856.717 0.009  0.237548 0.015326
secondary 3089.057 0.009  0.632184 0.030652
secondary 3683.920 0.009  46.743295 1.149509
primary   4945.301 0.003  100.000000 1.915939

In [6]: # Plot gamma-ray intensities from DataFrame
plot_df_data(df['E'], df['RI'], "(0)".format(compound_nucleus))
```



# CapGam cf. pyEGAF : : capgam

## CapGam

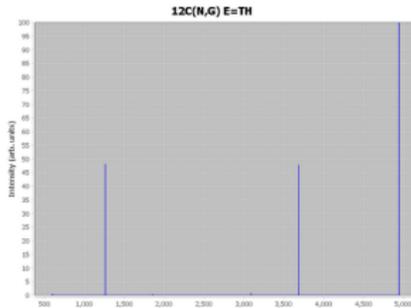
**<sup>12</sup>C(N,G) E=TH**  
Target: <sup>12</sup>C  
Product: <sup>13</sup>C

Last modified: 06/01/2023

[PDF](#)

Strongest Transition:  
E(γ) = 4945.301 ± 0.003  
I(γ) = 67.47 ± 0.92

Thermal Neutron Capture Cross Section (2000MuZX):  
0.00353 b ± 0.00007 b



[Download as .csv](#)

Type	E(γ) (keV)	ΔE(γ) (keV)	I(γ)/I(γ)max × 100	Δ(I(γ)/I(γ)max)
Secondary	595.013	0.014	0.3557	0.0156
Primary	1261.764	0.012	47.9621	0.9225
Primary	1856.716	0.012	0.2371	0.0152
Secondary	3089.049	0.020	0.6373	0.0309
Secondary	3683.921	0.023	47.6300	1.0482
Primary	4945.301	0.003	100.0000	1.9237

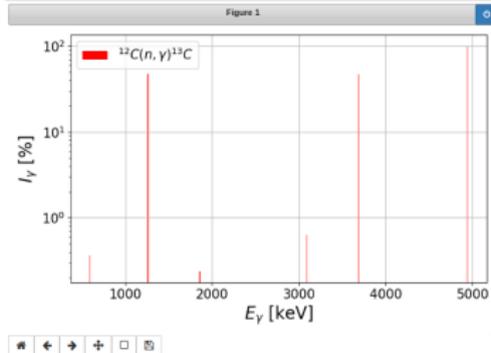
## pyEGAF: 'more'

```
In [4]: # Define compound nucleus as a string
        compound_nucleus = '13C'

In [5]: # Extract capture-gamma data for defined compound nucleus and write results to CSV file in pdf
        df = capgam(edata, '{0}'.format(compound_nucleus), 'more')
        df.to_csv('capgam_style {0}.csv'.format(compound_nucleus), index=False)
        print(df.to_string(index=False))

Target nucleus: 13C
Residual (compound nucleus): 13C
C12(n,g)13C
Total radiative thermal neutron-capture cross section = 0.00387 b ± 3e-05
Reference: 2018MuZy
Maximum E = 0.0026389710000000004 b at E = 4945.301 keV; RI = 100.
Reference: 2018MuZy
Type  I  f      E(I)      E(f)      E  dE  RI      dRI
secondary 2  1  3684.400  3089.451  595.015  0.009  0.363985  0.015326
primary  3  2  4946.311  3684.400  1261.765  0.009  47.505979  1.149512
primary  3  1  4946.311  3089.451  1856.717  0.009  0.237548  0.015326
secondary 1  0  3089.451  0.000  3089.057  0.009  0.632184  0.030652
secondary 2  0  3684.400  0.000  3683.920  0.009  46.743295  1.149509
primary  3  0  4946.311  0.000  4945.301  0.003  100.000000  1.91939

In [6]: # Plot gamma-ray intensities from DataFrame
        plot_of_data(df['E', 'df', 'RI'], '{0}'.format(compound_nucleus))
```



pyEGAF also displays associated level information.



# Attenuation in Prompt Gamma Activation Analysis

[https://github.com/AaronMHurst/attenuation\\_integration](https://github.com/AaronMHurst/attenuation_integration)

- C++ implementation for calculating attenuation integrated over sample thickness ( $t$ ):

$$\frac{I_\gamma}{I_0} = \int_{x=0}^{x=t} dx \exp\left(-\rho \left(\frac{\mu_\gamma}{\rho}\right) E_\gamma x \cos\theta\right)$$

- Build project out-of-source with CMake.
- Finds unique solution for effective  $t$  corresponding to observed attenuation.
- Project bundled with mass-attenuation coefficients for 100 elements (H ( $Z = 1$ ) to Fm ( $Z = 100$ )) taken from XMuDat.
- Interpolated energies from 1 keV to 20 MeV.
- Program can also be used to calculate simple attenuation for elemental (e.g., Re, La...) or stoichiometric compound (e.g.,  $\text{ReCl}_3$ ,  $\text{LaCl}_3 \cdot 7\text{H}_2\text{O}$ ...) samples.



Determination of the effective sample thickness via radiative capture  
A.M. Hurst<sup>a,\*</sup>, N.C. Summers<sup>b</sup>, L. Szentmihályi<sup>c</sup>, R.B. Firestone<sup>d</sup>, M.S. Basunia<sup>e</sup>, J.E. Escher<sup>f</sup>, R.W. Staiford<sup>g</sup>

<sup>a</sup>Lamont-Doherty Earth Observatory, Palisades, NY 10964, USA  
<sup>b</sup>Lamont-Doherty Earth Observatory, Palisades, NY 10964, USA  
<sup>c</sup>Center for Energy Research, Hungarian Academy of Sciences, H-1525 Budapest, Hungary

#### ARTICLE INFO

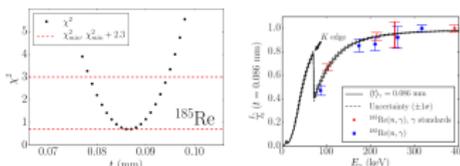
Article history:  
Received 26 June 2015  
Received in revised form 10 August 2015  
Accepted 9 September 2015

Keywords:  
Prompt Gamma Activation Analysis (PGAA)  
High-resolution  
Neutron activation  
Radiative capture  
Gamma-ray production cross-sections

#### ABSTRACT

A procedure for determining the effective thickness of non-uniformly shaped samples via radiative capture is described. In this technique, partial  $\gamma$ -ray production cross sections of a compound nucleus produced in a neutron capture reaction are measured using Prompt Gamma Activation Analysis and compared to their corresponding standardized absolute values. For the low-energy transitions, the measured cross sections are lower than their standard values due to significant photoelectric absorption of the  $\gamma$  rays within the bulk sample volume itself. Using standard theoretical techniques, the amount of  $\gamma$ -ray self-absorption and neutron self-shielding can then be calculated by iteratively varying the sample thickness until the observed cross sections converge with the known standards. The correct attenuation, then, provides a measure of the effective sample thickness illuminated by the neutron beam. This procedure is illustrated through radiative neutron capture using powdered metal samples comprising enriched  $^{185}\text{Re}$  and  $^{187}\text{Re}$  from which their respective equivalent effective thicknesses are deduced to be 0.073(1) mm and 0.040(3) mm, respectively.

© 2015 Elsevier B.V. All rights reserved.



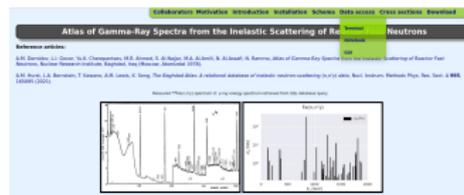
[D.A. Matters *et al.* PRC **93**, 054319 (2016)]



# The "Baghdad Atlas": Fast-reactor ( $n, n'\gamma$ ) database

<https://nucleardata.berkeley.edu/atlas/>

- Energy-integrated ( $n, n'\gamma$ ) data disseminated in book format.
- $\sim 7000$   $\gamma$  rays ( $E_\gamma$ ,  $I_\gamma$ ,  $E_L$ ) from 105 samples: 76 natural and 29 enriched.
- Ge(Li) viewing filtered fast-neutron beam line at the IRT-M Reactor, NRI, Baghdad, Iraq.
- Unique  $^{56}\text{Fe}$  847-keV  $2_1^+ \rightarrow 0_{gs}^+$   $\gamma$ -ray normalization.
- Digitized database, open source dissemination.
- Downloadable SQLite platform built with Makefile.
- Enhanced mathematical functionality provided by shared-object library compiled from C module during build.
- Interact with data using SQL scripts or Jupyter Notebook.
- *Future: Deploy to GitHub and develop PyPI project.*



The Baghdad Atlas: A relational database of inelastic neutron-scattering ( $n, n'\gamma$ ) data

A.M. Hurst<sup>a,\*</sup>, L.A. Bernstein<sup>a,b</sup>, T. Kawano<sup>c</sup>, A.M. Lewis<sup>d</sup>, K. Song<sup>e</sup>

<sup>a</sup>Department of Nuclear Engineering, University of California, Berkeley, CA 94720, USA

<sup>b</sup>Lamont-Doherty Earth Observatory, Palisades, NY 10961, USA

<sup>c</sup>Research Institute for Nuclear Energy and Material Sciences, Oarai, Ibaraki, 311-1201, Japan

<sup>d</sup>Florida Nuclear Laboratory, University of Florida, Gaines, FL 32611, USA

<sup>e</sup>Florida Nuclear Laboratory, University of Florida, Gaines, FL 32611, USA

\*Corresponding author. E-mail: hurst@nuc.berkeley.edu

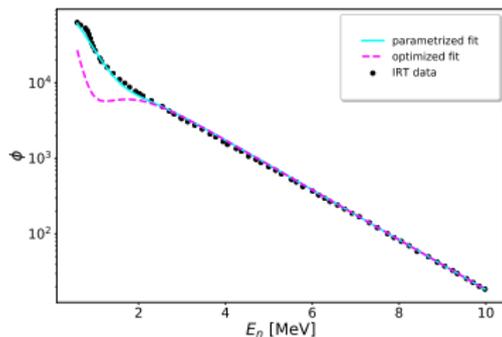
**ARTICLE INFO**

**ABSTRACT**

A relational database has been developed based on the original  $(n, n'\gamma)$  work carried out by A. M. Dendin et al. at the Nuclear Research Institute in Baghdad, Iraq (Dendin et al., 1970) for 181 independent measurements comprising 76 elemental samples of natural composition and 29 isotopically-enriched samples. The information from the Atlas includes: entry energies and relative intensities; available and listed data corresponding to the initial reaction and state data associated with the target nuclei; the values for the correction of the flux-weighted  $(n, n'\gamma)$  cross sections for a given transition relative to a defined value; the optimized angular distribution corrected for multiple scattering; the weighted partial  $\sigma_{tot}$  cross section for the production of the  $h\nu$ ;  $2 \leq E_\gamma \leq 20$  eV transitions in  $^{56}\text{Fe}$ , determined to be  $\sigma_{tot} = 14025$  mb, as used for this program. However, different values for the adopted cross section can be readily implemented to accommodate user preferences based on revised interpretations of this quantity. The Atlas  $(n, n'\gamma)$  data has been compiled from a series of CD-ROMs and a set of Python scripts have been developed to build and search the database locally. The database can then be accessed directly through the SQLite engine, or using alternative methods such as the Jupyter Notebook Python browser interface. Several examples exploring different interaction mechanisms are distributed with the complete software package.



## Flux at the Baghdad Research Reactor



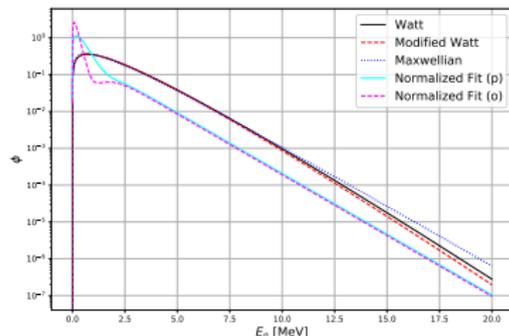
Flux described by compound function:

$$\phi(E_n) = \text{Maxwellian}(E_n \ll 1.5) + \text{Exponential}(E_n \gg 1.5).$$

- Adjust  $kT$  in  $\chi^2$  minimization using  $^{56}\text{Fe}$  data to optimize flux:

$$\chi^2 = (B_{Fe} - B_{kT})V^{-1}(\widetilde{B_{Fe}} - \widetilde{B_{kT}}).$$

- $^{56}\text{Fe}$  data well reproduced for the three strongest transitions:  $E_\gamma = 846.8, 1238.3, 1810.8$  keV.



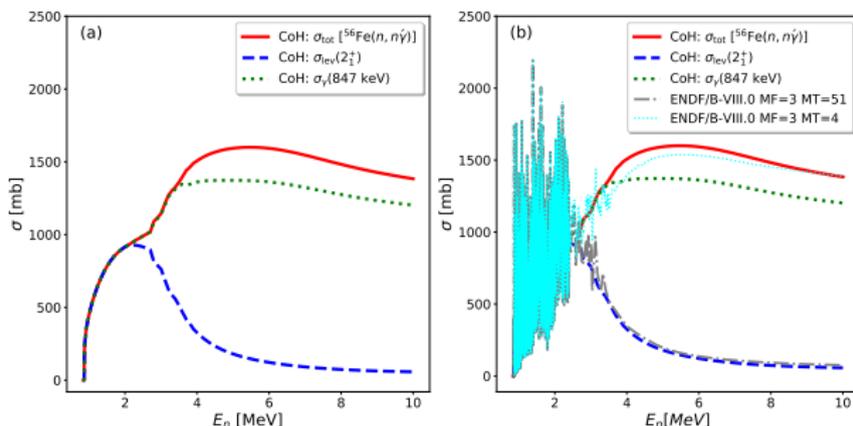
Flux satisfies normalization condition:

$$\int_{-\infty}^{+\infty} \phi^*(E_n)\phi(E_n)dE_n = 1$$

- Watt  $\langle E_n \rangle = 2.00$  MeV.
- Modified Watt  $\langle E_n \rangle = 1.98$  MeV.
- Maxwellian  $\langle E_n \rangle = 1.94$  MeV.
- Parameterized IRT-M  $\langle E_n \rangle = 0.88$  MeV.
- Optimized IRT-M  $\langle E_n \rangle = 0.63$  MeV.



# Convolution of flux with $^{56}\text{Fe}(n, n'\gamma)$ reaction calculations and data libraries



- Deduce flux-weighted averages for all graphed quantities for  $^{56}\text{Fe}$ .

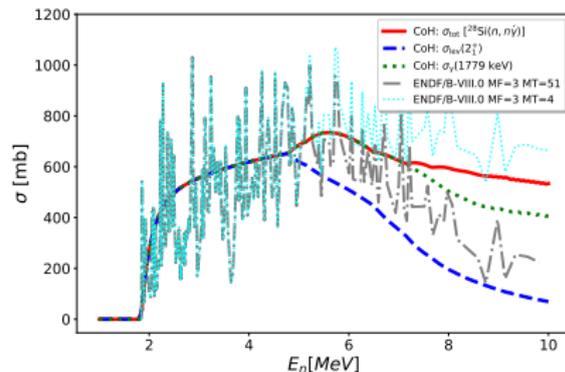
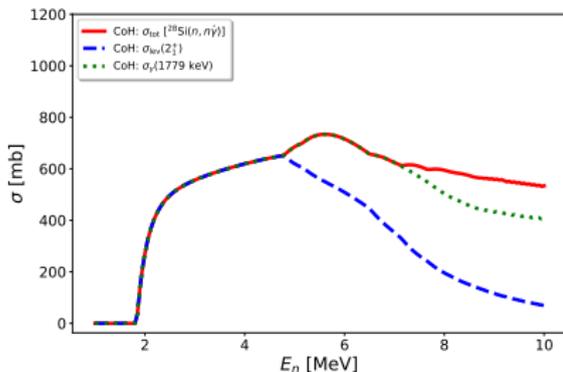
- Results indicate:  $\frac{\langle \sigma_{\text{CoH}}^{\text{lev}} \rangle}{\langle \sigma_{\text{CoH}}^{\text{tot}} \rangle} \approx \frac{\langle \sigma_{\text{lev}}^{\text{ENDF}} \rangle}{\langle \sigma_{\text{tot}}^{\text{ENDF}} \rangle}$ .

- Find  $\langle \sigma_{\gamma}^{\text{ENDF}} \rangle \approx \langle \sigma_{\text{tot}}^{\text{ENDF}} \rangle \frac{\langle \sigma_{\gamma}^{\text{CoH}} \rangle}{\langle \sigma_{\text{CoH}}^{\text{tot}} \rangle}$ .

- CoH calculation and ENDF are consistent for  $^{56}\text{Fe}(n, n'\gamma)$ .



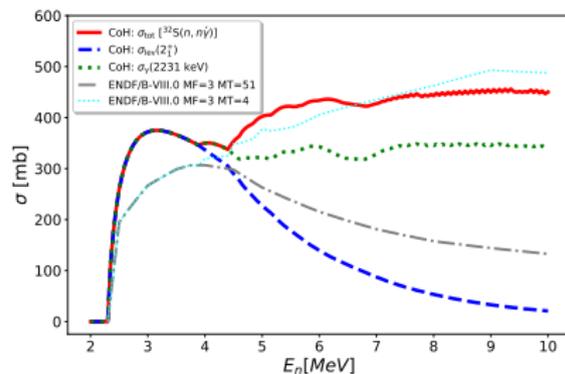
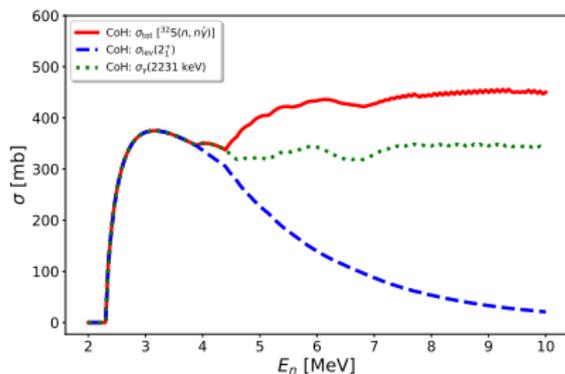
# Validation using the flux: $^{28}\text{Si}(n, n'\gamma)$ ; $E_\gamma = 1779$ keV



Source	$\langle \sigma_\gamma \rangle$ [mb]	$\langle \sigma_{\text{tot}} \rangle$ [mb]	$\langle \sigma_{\text{lev}} \rangle$ [mb]	$\frac{\langle \sigma_{\text{lev}} \rangle}{\langle \sigma_{\text{tot}} \rangle}$
CoH	55.69	55.84	53.45	0.957
ENDF	48.17	48.30	46.59	0.965
Baghdad Atlas	<b>47.1(94)</b>	—	—	—



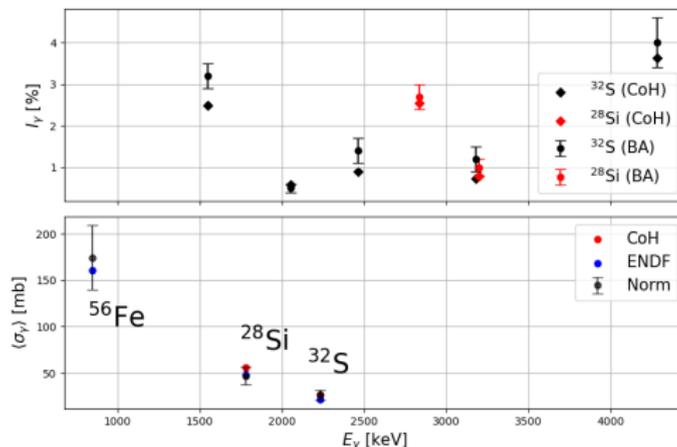
# Validation using the flux: $^{32}\text{S}(n, n'\gamma); E_\gamma = 2231 \text{ keV}$



Source	$\langle \sigma_\gamma \rangle$ [mb]	$\langle \sigma_{\text{tot}} \rangle$ [mb]	$\langle \sigma_{\text{lev}} \rangle$ [mb]	$\frac{\langle \sigma_{\text{lev}} \rangle}{\langle \sigma_{\text{tot}} \rangle}$
CoH	26.57	27.91	23.95	0.858
ENDF	21.67	22.76	19.98	0.878
Baghdad Atlas	<b>26.3(53)</b>	—	—	—



# Reproduction of known data in $^{56}\text{Fe}$ , $^{32}\text{S}$ , and $^{28}\text{Si}$ using the flux



- Absolute flux-weighted quantities from CoH and ENDF reproduce known absolute  $I_\gamma$  data in the Baghdad Atlas.
- Explore additional isotopes covering broader energy range.

Neutron flux at the Baghdad Research IRT-M Reactor is *well characterized* in region  $0.862 \leq E_n \leq 5.0$  MeV.



# BEApR: BErkeley Alpha and proton Radioactivity

<https://nucleardata.berkeley.edu/research/betap.html>



- Led by J.C. Batchelder.
- Work in progress: Downloadable PDFs  
 $-4 \leq T_Z \leq +19$ .
- Arranged by  $T_Z$  and  $Z/A$ .
- JSON format developed.
- Python project development underway.
- Built up from *many* source datasets, e.g.,

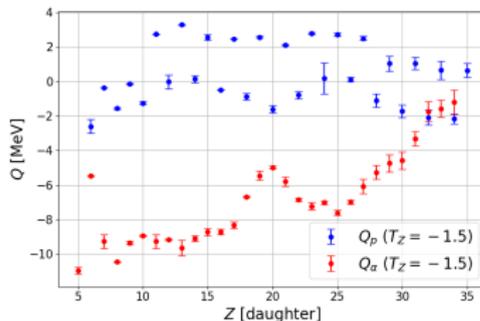
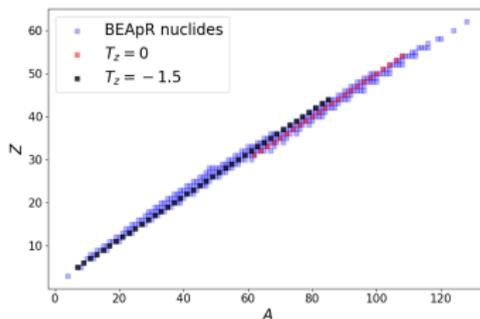
```

"electronCapture": {
  "isEnergeticallyPossible": true,
  "energySystematics": {
    "fromSystematics": false,
    "keyLabel": "2022Wu18",
    "digitalObjectIdentifier": "http://dx.doi.org/10.3888/1874-1137/ab00df"
  }
}

```

<sup>39</sup>Ca  $\epsilon$  decay

[2021Wa16]: M. Wang, W.J. Huang, F.G. Kondev, G. Audi, S. Naimi, "The AME 2020 atomic mass evaluation", Chin. Phys. C 45, 030003 (2021).

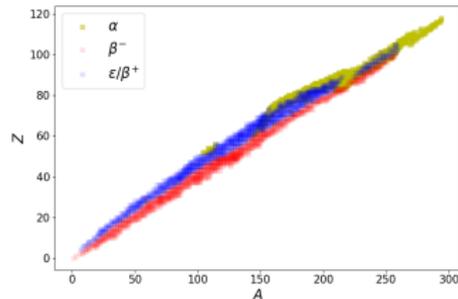


# Open-source Python library paceENSDF on GitHub

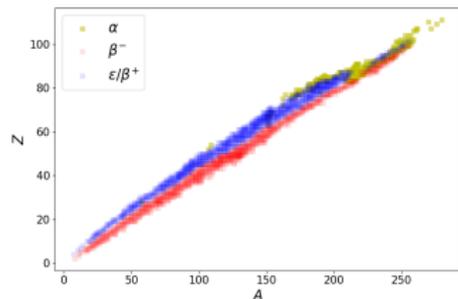
[https://github.com/AaronMHurst/pace\\_ensdf](https://github.com/AaronMHurst/pace_ensdf)

- *Python Archive of Coincident Emissions from ENSDF.*
- Translated 3254 ENSDF-decay datasets to JSON format.
- Converted each ENSDF-decay dataset into RIPL format.
- Generated 2394 JSON-formatted coincidence datasets, i.e., only those containing  $\gamma$  rays.
- Developed suite of Python modules enabling interaction, analysis, and visualization of the **ENSDF-decay** data and derived **coincidence**  $\gamma - \gamma$  and  $\gamma - X$ -ray data.
- Docstrings provided for all methods.
- JSON schema keys documented extensively in README.
- 283 unit tests (multiple virtual Python3 environments).
- Installation, testing scripts, and Jupyter Notebooks.
- JSON and RIPL files bundled with software.
- Over 2500 downloads.

ENSDF decay (all)



ENSDF decay (with  $\gamma$  data)



`git clone https://github.com/AaronMHurst/pace_ensdf.git`



## paceENSDF on the Python Package Index (PyPI) repository

<https://pypi.org/project/paceENSDF>


## Navigation

Project description

Release history

Download files

## Project links

Homepage

## Statistics

GitHub statistics:

Stars: 1

Forks: 0

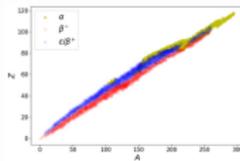
Open Issues: 0

Open PPRs: 0

View statistics for this project via  
Libraries.io or by using our public  
dashboard on Google BigQuery.

## Project description

The `paceENSDF` (Python Archive of Coincident Emissions from ENSDF) project [1] is a Python package enabling access, manipulation, analysis, and visualization of the radioactive decay data from the Evaluated Nuclear Structure Data File (ENSDF) library [2]. A total of 2264 data sets encompassing 1034,  $\beta^-$  (1244), and 419 (1279) have been extracted from the ENSDF archive [3], parsed and translated into a representative JavaScript Object Notation (JSON) format (described below). The JSON-formatted data sets constitute a total of 92,264 description  $\gamma$ -rays associated with 41,818 levels. Additionally, we also provide a reference equal-structure library (ESDF) [4] HTML-translated format of the corresponding decay-scheme data. These data sets are bundled together with the analysis toolkit. A schematic illustrating the portion of the nuclear chart of relevance to the aforementioned decay data from ENSDF is shown in the figure below.


 **pip install paceENSDF**
 **FreeBSD License**
EPJ Web of Conferences **284**, 18002 (2023)  
ND2022<https://doi.org/10.1051/epjconf/202328418002>A decay database of coincident  $\gamma$ - $\gamma$  and  $\gamma$ -X-ray branching ratios for in-field spectroscopy applicationsA.M. Hurst<sup>1,\*</sup>, B.D. Pierson<sup>2</sup>, R.C. Archambault<sup>2</sup>, L.A. Bernstein<sup>1,2</sup>, and S.M. Tannous<sup>3</sup><sup>1</sup>Department of Nuclear Engineering, University of California, Berkeley, California, 94720, USA<sup>2</sup>Pacific Northwest National Laboratory, Richland, Washington, 99352, USA<sup>3</sup>Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

**Abstract.** Current fieldable spectroscopy techniques often use single detector systems heavily impacted by interferences from intense background radiation fields. These effects result in low-confidence measurements that can lead to misinterpretation of the collected spectrum. To help improve interpretation of the fission products and short-lived radionuclides produced in a composite sample, a coincidence  $\gamma$ -database is being developed in support of a robust portable  $\gamma$  and X-ray coincidence detection system concurrently under development at the Pacific Northwest National Laboratory for in-field deployment. Hitherto, no database exists containing coincident  $\gamma$ - $\gamma$  and  $\gamma$ -X-ray branching-ratio information on an absolute scale that will greatly enhance isotopic identification for in-field applications. As part of this project, software has been developed to parse all radioactive-decay data sets from the Evaluated Nuclear Structure Data File (ENSDF) archive to enable translation into a more useful JavaScript Object Notation (JSON) format that more readily supports query-based data manipulation. The coincident database described in this work is the first of its kind and contains coincidence  $\gamma$ - $\gamma$  and  $\gamma$ -X-ray transitions and their corresponding uncertainties, together with auxiliary metadata associated with each decay data set. The new JSON format provides a convenient and portable means of data storage that can be imported into analysis frameworks with relatively low overhead allowing for meaningful comparison with measured data.

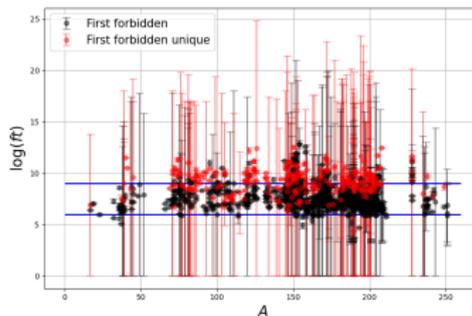
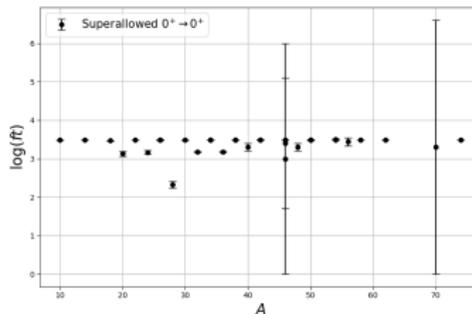


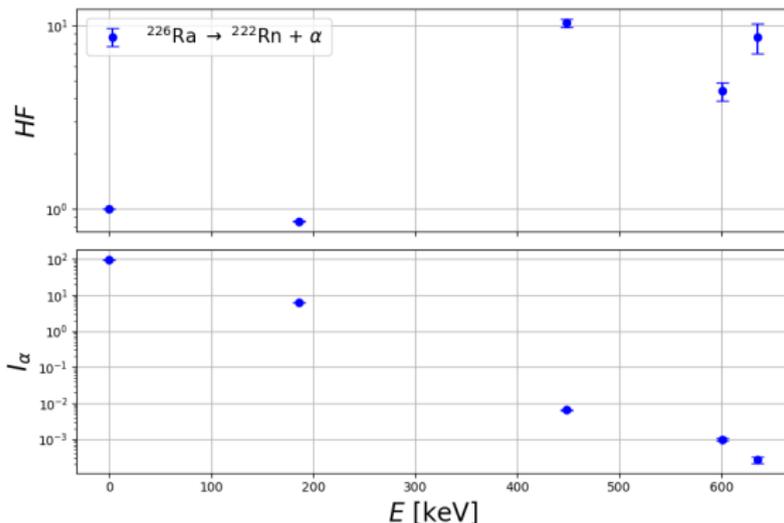
# Querying the ENSDF data

Superallowed transitions in  $\epsilon/\beta^+$  and first-forbidden transitions in  $\beta^-$  decay

Transition	$\log(ft)$	$l$
SA	3.5	0
A	4 – 7.5	0
1 <sup>st</sup> F	6 – 9	1
2 <sup>nd</sup> F	10 – 13	2
3 <sup>rd</sup> F	14 – 20	3
4 <sup>th</sup> F	$\approx 23$	4

- Angular momentum selection rules for **firm**  $J^\pi$  assignments.
- Examine trends and anomalies.



Hindrance factors in  $\alpha$  decay

- Low-lying levels populated in  $\alpha$  decay of  $^{226}\text{Ra} \rightarrow ^{222}\text{Rn}$ .
- Variance and correlation between  $I_\alpha$  and hindrance factors.
- Negative correlation.

$$V = \begin{pmatrix} 14.91 & -80.80 \\ -80.80 & 1368.72 \end{pmatrix}$$

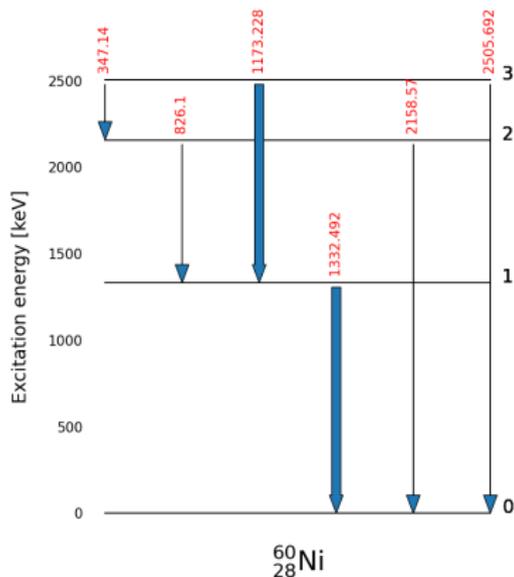
$$C = \begin{pmatrix} 1 & -0.57 \\ -0.57 & 1 \end{pmatrix}$$



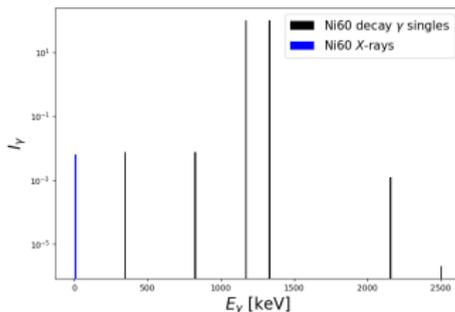
# Delayed $\gamma$ -ray emission from radioactive compounds

Example:  $^{59}\text{Co}(n,\gamma)^{60}\text{Co} \rightarrow ^{60}\text{Ni} + \beta^- [T_{1/2} = 1925.28(14) \text{ d}]$

Delayed  $\gamma$  rays observed in  $^{60}\text{Ni}$  some time after  $n$ -interrogation of  $^{59}\text{Co}$ : Activation signatures from paceENSDF (*Python Archive of Coincident Emissions from ENSDF*).



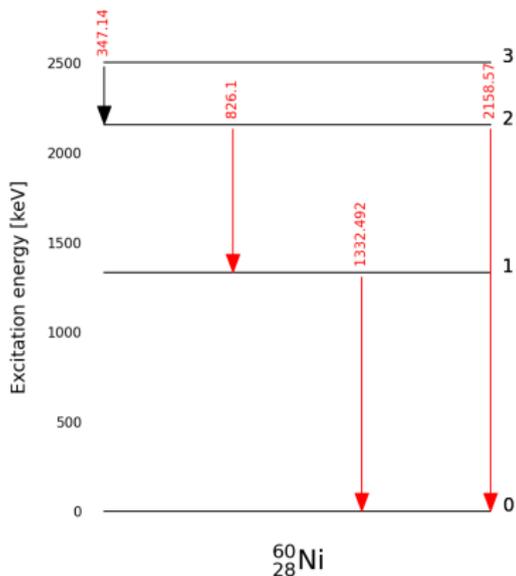
Total projection



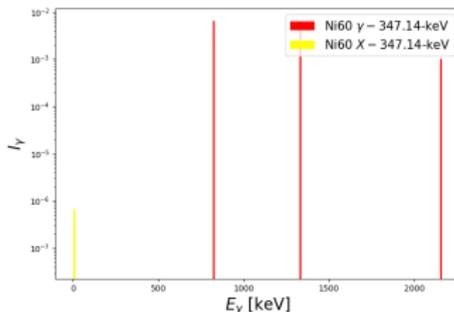
# Delayed $\gamma$ -ray emission from radioactive compounds

Example:  $^{59}\text{Co}(n,\gamma)^{60}\text{Co} \rightarrow ^{60}\text{Ni} + \beta^- [T_{1/2} = 1925.28(14) \text{ d}]$

Delayed  $\gamma$  rays observed in  $^{60}\text{Ni}$  some time after  $n$ -interrogation of  $^{59}\text{Co}$ : Activation signatures from paceNSDF (*Python Archive of Coincident Emissions from ENSDF*).



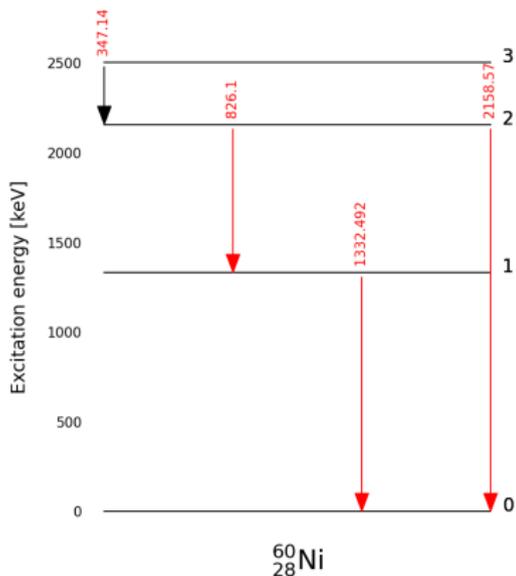
Gate on 3  $\rightarrow$  2 transition (347 keV)



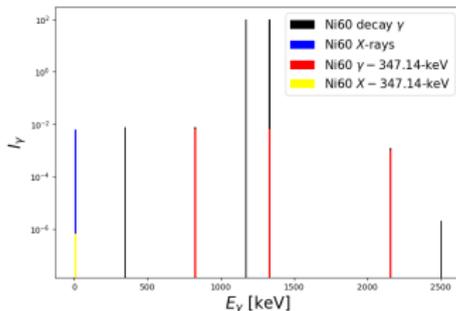
# Delayed $\gamma$ -ray emission from radioactive compounds

Example:  $^{59}\text{Co}(n,\gamma)^{60}\text{Co} \rightarrow ^{60}\text{Ni} + \beta^- [T_{1/2} = 1925.28(14) \text{ d}]$

Delayed  $\gamma$  rays observed in  $^{60}\text{Ni}$  some time after  $n$ -interrogation of  $^{59}\text{Co}$ : Activation signatures from paceENSDF (*Python Archive of Coincident Emissions from ENSDF*).



“Before” and “after”



# Parallel paths in $\gamma$ -ray cascades

```
>>> help(e.show_cascades)
```

```
In [3]: # Show the cascade gamma-ray sequence between the 3->2 and 1->0 transitions in 60Ni following  
# 60Co beta-minus decay (G.S.)  
e.show_cascades(cdata,"BM","Co60",0,3,2,1,0)
```

```
Cascade sequence between coincidence gammas: g(347.14 keV)-g(1332.492 keV):  
g(3 [2505.748 keV] -> 2 [2158.612 keV]) - g(1 [1332.508 keV] -> 0 [0.0 keV])
```

Path number 1:

```
Transition sequence: 3 -> 2: g(347.14 keV) [2505.748 keV -> 2158.612 keV]  
Transition sequence: 2 -> 1: g(826.1 keV) [2158.612 keV -> 1332.508 keV]  
Transition sequence: 1 -> 0: g(1332.492 keV) [1332.508 keV -> 0.0 keV]
```

```
Out[3]: [(3, 2), (2, 1), (1, 0)]
```

```
In [4]: # Show the cascade gamma-ray sequence between the 9->6 and 1->0 transitions in 147Pm following  
# 147Nd beta-minus decay (G.S.)  
e.show_cascades(cdata,"BM","Nd147",0,9,6,1,0)
```

```
Cascade sequence between coincidence gammas: g(53.1 keV)-g(91.105 keV):  
g(9 [685.899 keV] -> 6 [632.85 keV]) - g(1 [91.1051 keV] -> 0 [0.0 keV])
```

Path number 1:

```
Transition sequence: 9 -> 6: g(53.1 keV) [685.899 keV -> 632.85 keV]  
Transition sequence: 6 -> 3: g(222.27 keV) [632.85 keV -> 410.515 keV]  
Transition sequence: 3 -> 1: g(319.41 keV) [410.515 keV -> 91.1051 keV]  
Transition sequence: 1 -> 0: g(91.105 keV) [91.1051 keV -> 0.0 keV]
```

Path number 2:

```
Transition sequence: 9 -> 6: g(53.1 keV) [685.899 keV -> 632.85 keV]  
Transition sequence: 6 -> 1: g(541.79 keV) [632.85 keV -> 91.1051 keV]  
Transition sequence: 1 -> 0: g(91.105 keV) [91.1051 keV -> 0.0 keV]
```

```
Out[4]: [(9, 6), (6, 3), (3, 1), (1, 0)], [(9, 6), (6, 1), (1, 0)]
```

Allows for  $\gamma$ -ray cascade reconstruction and re-calculation of coincidence intensities if required.



Forensics applications: Search for  $\gamma - \gamma$  and  $\gamma - X$ -ray pairs $\gamma - X$ -ray search

In [33]: # Find all isotopes containing a gamma-X-ray coincidence pair with a 52-keV X ray and 688-keV gamma, # respectively, assuming the default tolerance=0.5 keV  
e.find\_xray\_coinc(cdata, 52, 688)

Out[33]:

Parent	Decay Index	Ex. Energy	Daughter	Decay Mode	Xray Label	Photon 1	Photon 2
0 Dy195	0	0.0	Tb165	electronCaptureBetaPlusDecay	Kbeta2	51.688	688.4
1 Th104	0	0.0	Dy164	betaMinusDecay	Kbeta1	52.113	695.46
2 Th164	0	0.0	Dy164	betaMinusDecay	Kbeta2	51.947	686.46
3 Lu164	0	0.0	Yb164	electronCaptureBetaPlusDecay	Kalpha1	52.389	667.83
4 Th170	0	0.0	Dy170	betaMinusDecay	Kbeta1	52.113	687.72
5 Th170	0	0.0	Dy170	betaMinusDecay	Kbeta2	51.947	667.72
6 Lu170	0	0.0	Yb170	electronCaptureBetaPlusDecay	Kalpha1	52.389	686.0
7 Hf163	0	0.0	Lu163	electronCaptureBetaPlusDecay	Kalpha2	52.443	686.25
8 Lu169	0	0.0	Yb169	electronCaptureBetaPlusDecay	Kalpha1	52.389	667.93
9 Hf157	0	0.0	Dy157	electronCaptureBetaPlusDecay	Kbeta1	52.113	686.1
10 Hf157	0	0.0	Dy157	electronCaptureBetaPlusDecay	Kbeta2	51.947	688.1

In [35]: # Tune the tolerance to narrow the search window to +/- 0.15 keV  
e.find\_xray\_coinc(cdata, 52, 688, 0.15)

Out[35]:

Parent	Decay Index	Ex. Energy	Daughter	Decay Mode	Xray Label	Photon 1	Photon 2
0 Hf157	0	0.0	Dy157	electronCaptureBetaPlusDecay	Kbeta1	52.113	686.1
1 Hf157	0	0.0	Dy157	electronCaptureBetaPlusDecay	Kbeta2	51.947	688.1

 $\gamma - \gamma$  search

In [37]: # Find all isotopes containing a coincidence pair of gamma rays  
# at 106 keV and 392 keV (default tolerance=0.5 keV)  
e.find\_gamma\_coinc(cdata, 106, 392)

Out[37]:

Parent	Decay Index	Ex. Energy	Daughter	Decay Mode	Gamma 1	Gamma 2
0 Cm243	0	0.0	Pu239	alphaDecay	106.47	392.4
1 Np239	0	0.0	Pu239	betaMinusDecay	106.47	392.4

In [38]: # Tune the tolerance to expand the search window to +/- 2.0 keV  
e.find\_gamma\_coinc(cdata, 106, 392, 2.0)

Out[38]:

Parent	Decay Index	Ex. Energy	Daughter	Decay Mode	Gamma 1	Gamma 2
0 La135	0	0.0	Ba135	electronCaptureBetaPlusDecay	107.32	392.08
1 Fr227	0	0.0	Ra227	betaMinusDecay	107.306	391.57
2 Cm243	0	0.0	Pu239	alphaDecay	106.47	392.4
3 Nd133	0	0.0	Pv133	electronCaptureBetaPlusDecay	105.1	393.3
4 Kr90	0	0.0	Rb90	betaMinusDecay	106.05	392.6
5 Kr90	0	0.0	Rb90	betaMinusDecay	106.92	392.6
6 Tl196	0	0.0	Hg196	electronCaptureBetaPlusDecay	107.0	392.2
7 Np239	0	0.0	Pu239	betaMinusDecay	106.47	392.4
8 Mo104	0	0.0	Tc104	betaMinusDecay	105.2	393.1
9 Cs145	0	0.0	Ba145	betaMinusDecay	105.94	391.15

Search methods for single  $\gamma$  rays and  $X$  rays also implemented in addition to  $\gamma - \gamma$  and  $\gamma - X$ -ray pairs.



# Acknowledgments

Brookhaven National Laboratory  
Lawrence Berkeley National Laboratory  
Los Alamos National Laboratory  
Pacific Northwest National Laboratory  
University of California, Berkeley

This material is based upon work supported by the Department of Energy National Nuclear Security Administration through the Nuclear Science and Security Consortium under Award Number DE-NA0003996.

