EGAF modernization

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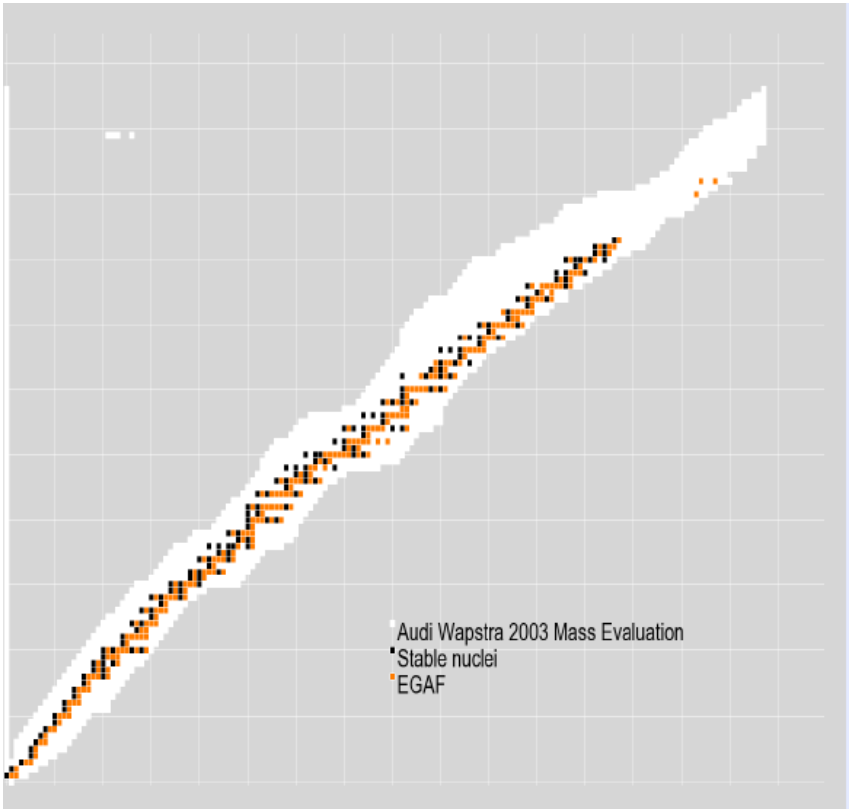
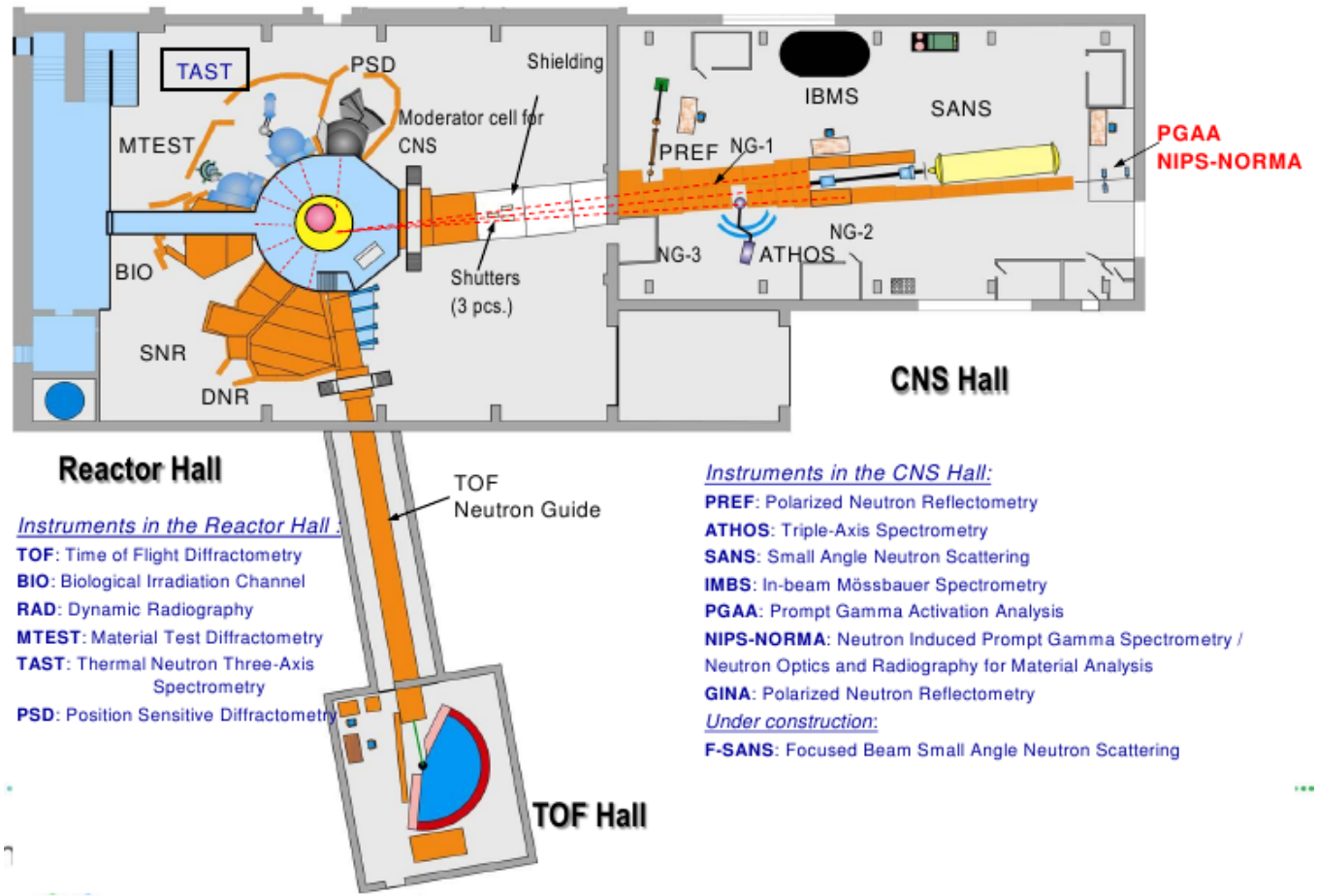
Evaluated Gamma-ray Activation File (EGAF)



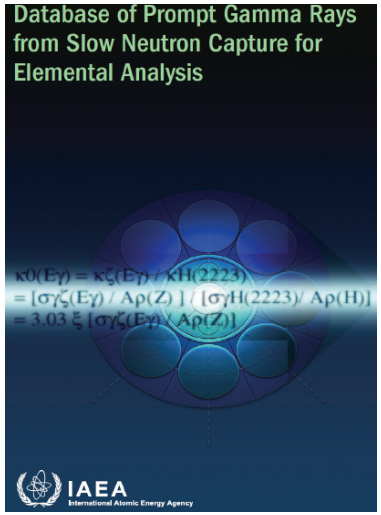
- IAEA CRP initiative led by **Rick Firestone** (LBNL/UCB) and researchers from the Budapest Research Reactor (BRR).
- Partial thermal neutron-capture γ-ray cross-section data measured at BRR.
- Natural targets $Z = 1 - 82, 90, 92$ except for $Z = 2, 61$ (245 data sets).
- $\sim 32,000$ prompt and $\sim 3,000$ decay γ-ray lines.

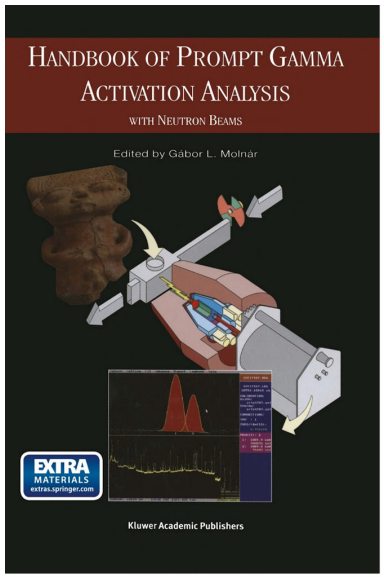
Prompt gamma activation analysis @ Budapest Research Reactor



All (n, γ) measurements performed in a consistent manner using the same experimental configuration

Where to get the EGAF database

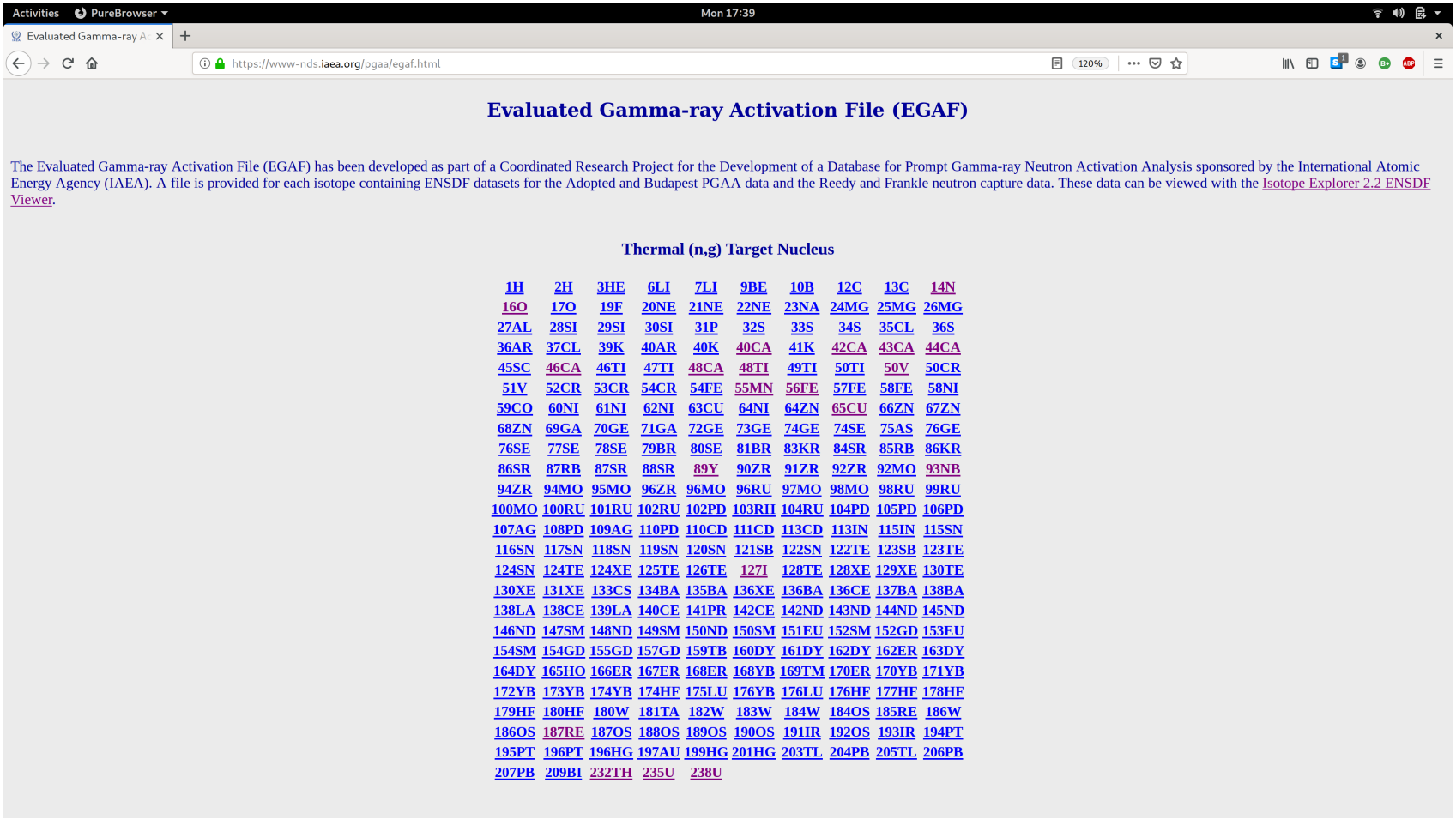




- *Database of Prompt Gamma Rays from Slow Neutron Capture for Elemental Analysis* (IAEA, Vienna, 2007).
- *Handbook of PGAA with Neutron Beams*, Ed. G. L. Molnár (Kluwer Academic, Dordrecht, the Netherlands, 2004).
- Peer-reviewed publications.
- EGAF contains many useful observables: E_γ, S_n, σ_γ, σ_0, J^π, δ_γ.

EGAF disseminated through the IAEA

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 Budapest PGAA data and the Reedy and Frankle neutron capture data. These data can be viewed with the Isotope Explorer 2.2 ENSDF Viewer.

Thermal (n,g) Target Nucleus

1H	2H	3HE	6LI	7LI	9BE	10B	12C	13C	14N
16O	17O	19F	20NE	21NE	22NE	23NA	24MG	25MG	26MG
27AL	28SI	29SI	30SI	31P	32S	33S	34S	35CL	36S
36AR	37CL	39K	40AR	40K	40CA	41K	42CA	43CA	44CA
45SC	46CA	46TI	47TI	48CA	48TI	49TI	50TI	50V	50CR
51V	52CR	53CR	54CR	54FE	55MN	56FE	57FE	58FE	58NI
59CO	60NI	61NI	62NI	63CU	64NI	64ZN	65CU	66ZN	67ZN
68ZN	69GA	70GE	71GA	72GE	73GE	74GE	74SE	75AS	76GE
76SE	77SE	78SE	79BR	80SE	81BR	83KR	84SR	85RB	86KR
86SR	87RB	87SR	88SR	89Y	90ZR	91ZR	92ZR	92MO	93NB
94ZR	94MO	95MO	96ZR	96MO	96RU	97MO	98MO	98RU	99RU
100MO	100RU	101RU	102RU	102PD	103RH	104RU	104PD	105PD	106PD
107AG	108PD	109AG	110PD	110CD	111CD	113CD	113IN	115IN	115SN
116SN	117SN	118SN	119SN	120SN	121SB	122SN	122TE	123SB	123TE
124SN	124TE	124XE	125TE	126TE	127I	128TE	128XE	129XE	130TE
130XE	131XE	133CS	134BA	135BA	136XE	136BA	136CE	137BA	138BA
138LA	138CE	139LA	140CE	141PR	142CE	142ND	143ND	144ND	145ND
146ND	147SM	148ND	149SM	150ND	150SM	151EU	152SM	152GD	153EU
154SM	154GD	155GD	157GD	159TB	160DY	161DY	162DY	162ER	163DY
164DY	165HO	166ER	167ER	168ER	168YB	169TM	170ER	170YB	171YB
172YB	173YB	174YB	174HF	175LU	176YB	176LU	176HF	177HF	178HF
179HF	180HF	180W	181TA	182W	183W	184W	184OS	185RE	186W
186OS	187RE	187OS	188OS	189OS	190OS	191IR	192OS	193IR	194PT
195PT	196PT	196HG	197AU	199HG	201HG	203TL	204PB	205TL	206PB
207PB	209BI	232TH	235U	238U					

ENSDF-formatted EGAF data sets

$$^{28}\mathrm{Si}(n,\gamma)^{29}\mathrm{Si}$$

```
29SI    28SI(N,G) E=THERMAL: {~EGAF}
29SI c  Evaluated Gamma-ray Activation File (EGAF).
29SI2c  Evaluated by R.B. Firestone (LBNL), December 2003.
29SI c  BR$|s{-0}=0.177 5 (1981MuZQ)
29SI cG RI$Elemental |s(|g) assuming %Abundance=92.2297  7
29SI  N  1.084249  8
29SI PN                                                              C
29SI2PN Thermal cross section in barns.
29SI cN NR$Isotopic |s(|g)=NR*RI.
29SI2cN Divide by |s{-0} for intensity per neutron capture.
29SI  L       0.0   1/2+             STABLE
29SI  L  1273.379 17 3/2+             290 FS    10
29SI  G  1273.349 17  0.0289 6
```

- All γ-ray information needed is provided in EGAF:
  - `NR`, `RI`, and abundance.
  - Adopted σ_0.

- Lots of applications source thermal-capture data.
- Different applications/users may want different subsets of data.
- γ-ray energies and *intensities* certainly...
- I_γ: Partial elemental or isotopic cross sections; populations per neutron capture; relative intensities.
- Associated decay-scheme properties, e.g., initial and final levels (floats and/or indices); identification of *primary* and *secondary* γ rays...
- Difficult to capture all this information in ENSDF.
- ENSDF is inconvenient to work with for the uninitiated and requires a parser.

New JSON and RIPL format for EGAF

- New JSON format overcomes space-limited *cryptic* ENSDF format.
- Include more complete information in an intuitive manner.
- For example, separation energies:

```
"energyNeutronSeparationAME2020": 8473.6025,
"energyNeutronSeparationEGAF": 8473.537,
"energyProtonSeparationAME2020": 12333.3331,
```

- Developed software package pyEGAF for interacting with and manipulating the EGAF JSON data sets.
- Reaction and statistical-model codes (e.g., DICEBOX, CoH, TALYS) often require (n, γ) data in RIPL format.
- JSON and RIPL data sets generated for corresponding EGAF files (245 total).

```
29Si    29    14    14    46    13     8     8.473603    12.333333
 1    0.000000    0.5   1   -1.00E+00   0 0                      1/2+  0
 2    1.273379    1.5   1    2.90E-13   1 0                      3/2+  0
                                                1      1.273   1.000E+00   1.000E+00   0.000E+00
 3    2.028060    2.5   1    3.06E-13   2 0                      5/2+  0
                                                2      0.755   6.367E-02   6.367E-02   0.000E+00
                                                1      2.028   9.363E-01   9.363E-01   0.000E+00
```

pyEGAF

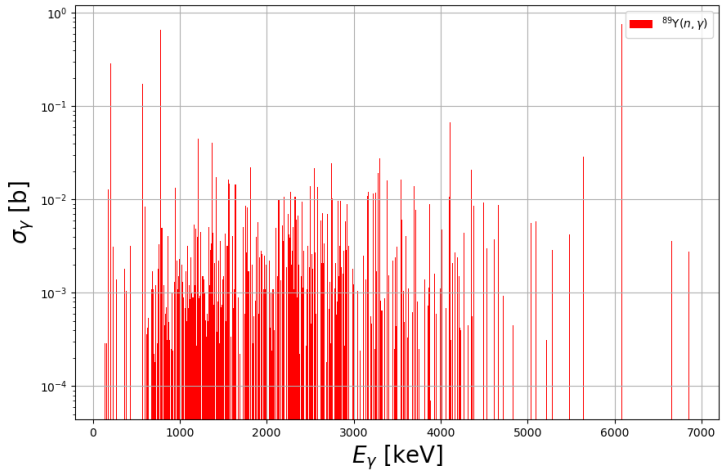
```
$ ipython
In [1]: import pyEGAF as egaf
In [2]: e = egaf.EGAF()
In [3]: data = e.load_egaf()
```

```
|  get_residual_levels(self, list, *args)
|      Returns decay scheme of levels as a list for a defined residual
|      nucleus.  The list elements correspond to:
|
|      level index, level energy, d_energy, number of gammas,
|      number of spins, spin, parity, spin flag, parity flag.
|
|      In cases where number of spins > 1, the spin and parity of the
|      first permutation is listed.  The spin and parity flags indicate
|      tentative and firm assignments.  For example, to get the decay scheme
|      for 28Si(n,g)29Si:
|
|      get_residual_levels(my_egaf_json_file_list, "Si29")
|      get_residual_levels(my_egaf_json_file_list, 14, 29)
|
```

```
In [4]: e.get_residual_levels(data, "Si29")
[[0, 0.0, 0.0, 0, 1, 0.5, 1, 'J_FIRM', 'PI_FIRM'],
 [1, 1273.379, 0.017, 1, 1, 1.5, 1, 'J_FIRM', 'PI_FIRM'],
 [2, 2028.06, 0.06, 2, 1, 2.5, 1, 'J_FIRM', 'PI_FIRM'],
 [3, 2425.876, 0.023, 3, 1, 1.5, 1, 'J_FIRM', 'PI_FIRM'],
 [4, 3066.95, 0.03, 2, 1, 2.5, 1, 'J_FIRM', 'PI_FIRM'],
 [5, 4840.23, 0.08, 2, 1, 0.5, 1, 'J_FIRM', 'PI_FIRM'],
 [6, 4934.339, 0.024, 5, 1, 1.5, -1, 'J_FIRM', 'PI_FIRM'],
 [7, 6380.554, 0.021, 5, 1, 0.5, -1, 'J_FIRM', 'PI_FIRM'],
 [8, 6712.9, 0.4, 1, 1, None, 0, 'J_TENTATIVE', 'PI_TENTATIVE'],
 [9, 6908.48, 0.05, 5, 1, None, 0, 'J_TENTATIVE', 'PI_TENTATIVE'],
 [10, 7057.94, 0.07, 4, 1, 0.5, 1, 'J_FIRM', 'PI_FIRM'],
 [11, 7523.13, 0.12, 2, 1, None, 0, 'J_TENTATIVE', 'PI_TENTATIVE'],
 [12, 7996.4, 0.16, 1, 1, None, 0, 'J_TENTATIVE', 'PI_TENTATIVE'],
 [13, 8473.537, 0.023, 13, 1, 0.5, 1, 'J_FIRM', 'PI_FIRM']]
```

pyEGAF: Gammas

```
gamma_spectrum(self, list, *args, **kwargs)
    Returns a gamma-ray spectrum together with associated decay-scheme
    properties for a defined residual-nucleus input as a numpy array:

    initial level index, final level index, initial level energy,
    final level energy, gamma energy, d_gamma_energy, <intensity>,
    <d_intensity>, conversion coefficient, d_conversion_coefficient

    The <intensity> is set according to choice of input keyword argument
    passed to the function:

    intensity='elemental' # elemental partial gamma-ray cross sections
    intensity='isotopic' # isotopic partial gamma-ray cross sections
    intensity='population' # population per neutron capture

    For example, for 89Y(n,g)90Y:

    gamma_spectrum(my_egaf_json_file_list, "Y90", intensity='isotopic')
    gamma_spectrum(my_egaf_json_file_list, 39, 90, intensity='isotopic')
```




```
In [4]: e.gamma_spectrum(data, "Y90", intensity="isotopic")

array([[1.000000e+00, 0.000000e+00, 2.025090e+02, ..., 7.000000e-03,
        0.000000e+00, 0.000000e+00],
       [2.000000e+00, 1.000000e+00, 6.820000e+02, ..., 0.000000e+00,
        0.000000e+00, 0.000000e+00],
       [3.000000e+00, 1.000000e+00, 7.766170e+02, ..., 7.000000e-03,
        0.000000e+00, 0.000000e+00],
       ...,
       [6.000000e+01, 3.000000e+00, 6.857008e+03, ..., 4.000000e-02,
        0.000000e+00, 0.000000e+00],
       [6.000000e+01, 1.000000e+00, 6.857008e+03, ..., 1.900000e-04,
        0.000000e+00, 0.000000e+00],
       [6.000000e+01, 0.000000e+00, 6.857008e+03, ..., 1.500000e-04,
        0.000000e+00, 0.000000e+00]])
```

pyEGAF: Isomers and J^{π}

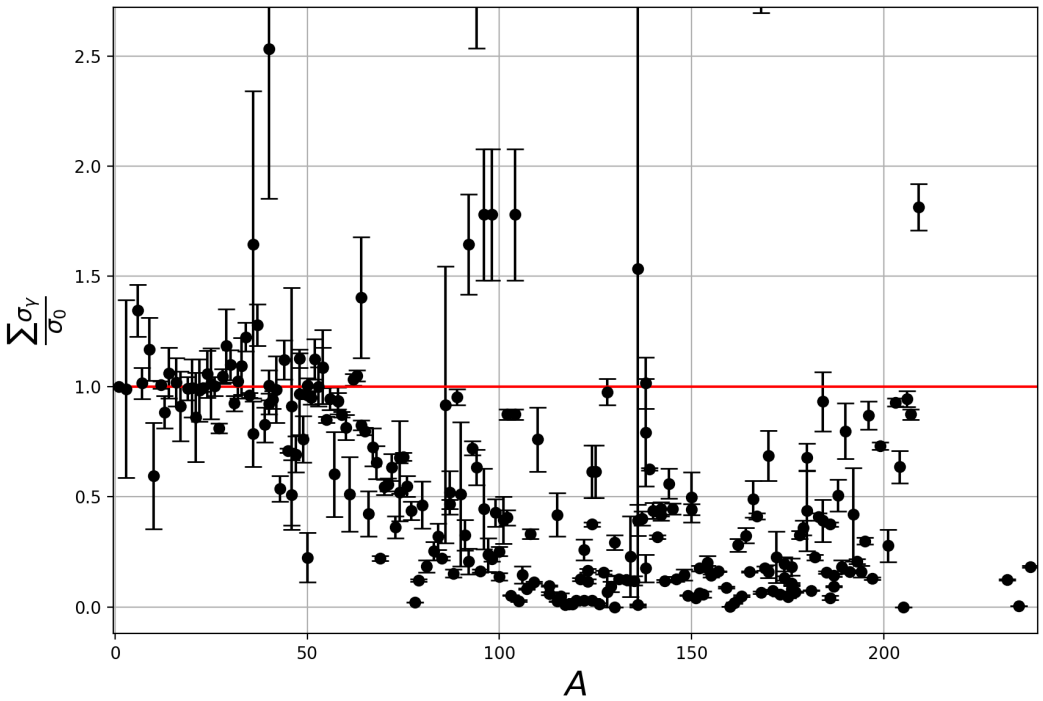
```
find_isomers(self, list, *args, **kwargs)
    Finds all isomers in a decay scheme and returns a list:

    level index, level_energy, d_energy, halflife, d_halflife, unit

    Halflives are returned in their "best" units (i.e., those given in
    the original ENSDF-formatted EGAF file) or in seconds according
    to input keyword argument.  For example, for 23Na(n,g)24Na:

    find_isomers(my_egaf_json_file_list, "Na24", units='best')
    find_isomers(my_egaf_json_file_list, "Na24", units='seconds')
    find_isomers(my_egaf_json_file_list, 11, 24, units='best')
    find_isomers(my_egaf_json_file_list, 11, 24, units='seconds')

find_multiple_jpi(self, list, *args)
    Finds all levels and spins in residual-nucleus decay scheme with
    multiple JPi permutations.  The corresponding list is returned as:

    level index, level energy, d_energy, number of spins, spin index,
    spin, parity

    For the 140La decay scheme:
    find_multiple_jpi(my_egaf_json_file_list, "La140")
    find_multiple_jpi(my_egaf_json_file_list, 57, 140)

find_unique_jpi(self, list, *args)
    Finds all levels and spins in residual-nucleus decay scheme with
    unique JPi assignments.  The corresponding list is returned as:

    level index, level energy, d_energy, spin index, spin, parity

    Only levels with both firm spins and parities are returned.  For the
    17O(n,g)18O decay scheme:
    find_unique_jpi(my_egaf_json_file_list, "O18")
    find_unique_jpi(my_egaf_json_file_list, 8, 18)
```

Analysis using pyEGAF methods

- Total (n, γ) absorption cross section given by:

$$\sigma_0 = \sum_{k=1}^{P} \sigma_{\gamma_k}^{\text{primary}} = \sum_{i=1}^{N} \sigma_{\gamma_{i0}}^{\text{expt}}(1 + \alpha_{i0}) + \sum_{j=1}^{M} \sigma_{\gamma_{j0}}^{\text{sim}}.$$

- Find sum of primary γ-ray cross sections for given residual and compare to corresponding adopted total cross section.
- $\sum_{k=1}^{P} \sigma_{\gamma_k}^{\text{primary, EGAF}} / \sigma_0^{\text{adopted}}$ provides a measure of *"completeness"*.



Outlook

- All 245 EGAF data sets have been translated into representative JSON and RIPL formats.
- S_n and S_p taken from AME2020.
- Adopted σ_0 taken from Atlas of Neutron Resonances [Mughabghab]; mainly earlier but some current values.
- Suite of Python modules have been developed to interact with JSON schema (pyEGAF).
- *Side note: Python package also developed to interact with γ/γ, γ/X-ray coincidence database: All primary- and continuation-record ENSDF decay data; coincidence energies and intensities.*
- Deploy packages in the near future.