The *"Baghdad Atlas"* as a validation tool for evaluated nuclear data libraries

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The Baghdad IRT-M Reactor and $(n, n'\gamma)$ data

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

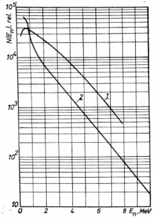


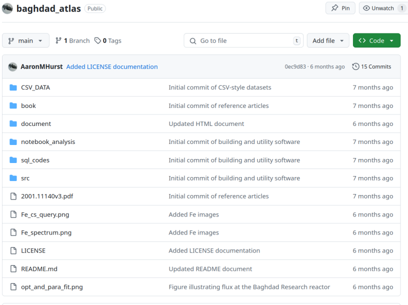
Рис. 5
Спектр нейтронов деления (*1*) и нейтронов от реактора ИРТ (*2*)

Fig. 5
Fission neutron spectrum (*1*) and the IRT reactor neutron spectrum (*2*)

- Compilation of energy-integrated inelastic neutron-scattering $(n, n'\gamma)$ data disseminated in book format.
- $\sim$ 7000 γ rays (E_γ and BR) from 105 samples: 76 natural and 29 isotopically-enriched targets.
- Ge(Li) viewing filtered fast-neutron beam line at the IRT-M Reactor: NRI, Baghdad, Iraq.
- Unique ^{56}Fe 847-keV $2_1^+ \rightarrow 0_{\rm gs}^+$ γ-ray normalization.
- Out-of-print book (*out-of-print* reactor!).
- Now Digitized database, open source dissemination.
- Project maintained on GitHub:
  github.com/AaronMHurst/baghdad_atlas
- A.M. Hurst *et al.*, NIMA **995**, 165095 (2021).

Building the project

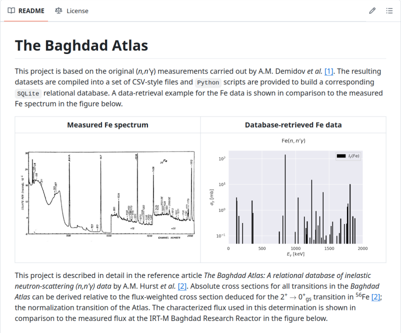
https://github.com/AaronMHurst/baghdad_atlas



baghdad_atlas Public

AaronMHurst Added LICENSE documentation 0ec9d83 · 6 months ago 15 Commits

CSV_DATA	Initial commit of CSV-style datasets	7 months ago
book	Initial commit of reference articles	7 months ago
document	Updated HTML document	6 months ago
notebook_analysis	Initial commit of building and utility software	7 months ago
sql_codes	Initial commit of building and utility software	7 months ago
src	Initial commit of building and utility software	7 months ago
2001.11140v3.pdf	Initial commit of reference articles	7 months ago
Fe_cs_query.png	Added Fe images	6 months ago
Fe_spectrum.png	Added Fe images	6 months ago
LICENSE	Added LICENSE documentation	6 months ago
README.md	Updated README document	6 months ago
opt_and_para_fit.png	Figure illustrating flux at the Baghdad Research reactor	6 months ago



The Baghdad Atlas

This project is based on the original (*n*,*n*′γ) measurements carried out by A.M. Demidov *et al.* [1]. The resulting datasets are compiled into a set of CSV-style files and `Python` scripts are provided to build a corresponding `SQLite` relational database. A data-retrieval example for the Fe data is shown in comparison to the measured Fe spectrum in the figure below.

Measured Fe spectrum	Database-retrieved Fe data

This project is described in detail in the reference article *The Baghdad Atlas: A relational database of inelastic neutron-scattering (n,n′γ) data* by A.M. Hurst *et al.* [2]. Absolute cross sections for all transitions in the *Baghdad Atlas* can be derived relative to the flux-weighted cross section deduced for the $2^+ \rightarrow 0^+_{gs}$ transition in ^{56}Fe [2]; the normalization transition of the Atlas. The characterized flux used in this determination is shown in comparison to the measured flux at the IRT-M Baghdad Research Reactor in the figure below.

- `clone` and `make` project as described in `README`.
- Build process automatically detects OS and Python version in build environment.
- Creates a SQLite database object: `atlas_baghdad_py3.db`

SQL schema and transactions

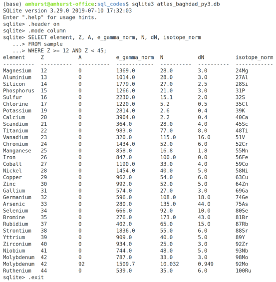
https://nucleardata.berkeley.edu/atlas/schema.html

```sql
CREATE TABLE nucleus (
    id INTEGER PRIMARY KEY,
    nuc_symb CHAR(5),          /* Chemical symbol (with mass number for enriched isotopes) of the irradiated sample */
    nuc_Z INTEGER,             /* Atomic number of irradiated sample */
    energy_gamma FLOAT,        /* Gamma-ray transition energy [keV] */
    d_energy_gamma FLOAT,      /* Uncertainty: Gamma-ray transition energy [keV] */
    intensity_gamma FLOAT,     /* Gamma-ray transition intensity [RI] */
    d_intensity_gamma FLOAT,   /* Uncertainty: Gamma-ray transition intensity [RI] */
    transition_type CHAR(2),   /* Gamma flag: f (firm); d (doublet); t (tentative); c (calibration); m (multiply placed) */
    residual CHAR(16),         /* Residual-nucleus reaction product; usually the (n,n') compound */
    residual_type CHAR(2),     /* Residual-nucleus identification flag: f (firm); t (tentative) */
    energy_ex FLOAT,           /* Excitation energy in compound nucleus [keV] */
    ex_type CHAR(2),           /* Excitation-energy flag: f (firm); t (tentative); u (unknown) */
    sample CHAR(1)             /* Sample flag: E (isotopically enriched); N (natural elemental abundance) */
);

CREATE TABLE sample (
    id INTEGER PRIMARY KEY,
    flag CHAR(1),              /* Meta-data identification flag: X */
    element TEXT,              /* Name of element/enriched isotope */
    Z INTEGER,                 /* Atomic number of element/enriched isotope */
    symbol TEXT,               /* Chemical symbol for element/enriched isotope */
    N FLOAT,                   /* Normalization factor for determination of absolute partial gamma-ray cross sections */
    dN FLOAT,                  /* Uncertainty: Cross-section normalization factor */
    e_gamma_norm FLOAT,        /* Gamma-ray transition energy used for normalization [keV] */
    A INTEGER,                 /* Atomic mass of enriched isotope (A=0 for natural elemental samples) */
    mass FLOAT,                /* Mass [g] of irradiated sample */
    exposure_time FLOAT,       /* Measurement period [h] of irradiated sample */
    enrichment FLOAT,          /* Enrichment factor [%] of principal isotope in sample (0 for natural elemental samples) */
    sample_composition TEXT,   /* Chemical composition of irradiated sample */
    isotope_norm TEXT          /* Isotope used for gamma-ray intensity normalization */
);
```

- sqlite3 engine: terminal-based front-end to SQLite libraries.
- Evaluate SQL queries interactively, e.g., normalization info.

  ```
  SELECT <variables> FROM
  <table> WHERE <conditions>;
  ```

- Batch-mode processing also (for more complicated queries).



```
(base) amhurst@amhurst-office:sql_codes$ sqlite3 atlas_baghdad_py3.db
SQLite version 3.29.0 2019-07-10 17:32:03
Enter ".help" for usage hints.
sqlite> .header on
sqlite> .mode column
sqlite> SELECT element, Z, A, e_gamma_norm, N, dN, isotope_norm
   ...> FROM sample
   ...> WHERE Z >= 12 AND Z < 45;
element     Z           A           e_gamma_norm N           dN          isotope_norm
----------  ----------  ----------  -----------  ----------  ----------  -----------
Magnesium   12          0           1369.0       28.0        3.0         24Mg
Aluminium   13          0           1014.0       28.0        3.0         27Al
Silicon     14          0           1779.0       27.0        2.5         28Si
Phosphorus  15          0           1266.0       21.0        3.0         31P
Sulfur      16          0           2230.0       15.1        2.0         32S
Chlorine    17          0           1220.0       5.2         0.5         35Cl
Potassium   19          0           2814.0       2.6         0.4         39K
Calcium     20          0           3904.0       2.2         0.4         40Ca
Scandium    21          0           364.0        28.0        4.0         45Sc
Titanium    22          0           983.0        77.0        8.0         48Ti
Vanadium    23          0           320.0        115.0       16.0        51V
Chromium    24          0           1434.0       52.0        6.0         52Cr
Manganese   25          0           858.0        16.8        1.8         55Mn
Iron        26          0           847.0        100.0       0.0         56Fe
Cobalt      27          0           1190.0       33.0        4.0         59Co
Nickel      28          0           1454.0       40.0        5.0         58Ni
Copper      29          0           962.0        54.0        6.0         63Cu
Zinc        30          0           992.0        52.0        5.0         64Zn
Gallium     31          0           574.0        27.0        3.0         69Ga
Germanium   32          0           596.0        108.0       18.0        74Ge
Arsenic     33          0           280.0        135.0       44.0        75As
Selenium    34          0           666.0        92.0        10.0        80Se
Bromine     35          0           276.0        173.0       43.0        81Br
Rubidium    37          0           402.0        65.0        15.0        87Rb
Strontium   38          0           1836.0       55.0        6.0         88Sr
Yttrium     39          0           909.0        40.0        5.0         89Y
Zirconium   40          0           934.0        25.0        3.0         92Zr
Niobium     41          0           744.0        48.0        5.0         93Nb
Molybdenum  42          0           787.0        33.0        3.0         98Mo
Molybdenum  42          92          1509.7       10.032      0.949       92Mo
Ruthenium   44          0           539.0        35.0        6.0         100Ru
sqlite> .exit
```

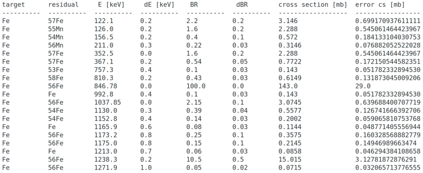
More complex SQL transactions

```sql
BEGIN TRANSACTION;

/*For Linux use the following library:*/
SELECT load_extension('../UDF/sqlite-amalgamation/libsqlitefunctions.so');

/*For Mac OS X use the following library:*/
/*SELECT load_extension('../UDF/sqlite-amalgamation/libsqlitefunctions.dylib');*/

CREATE TEMP TABLE _Variables(
        Name TEXT PRIMARY KEY,
        FeCS FLOAT,
        FeRatio FLOAT,
        d_FeCS FLOAT,
        d_FeRatio FLOAT,
        RI FLOAT
);

INSERT OR REPLACE INTO _Variables VALUES ('Constant', 143.0, 1.430, 29.0, 0.290, 100.0);
```

- For more elaborate SQL transactions it's probably better to run from a script.
- Use data from a class (table).
- Hand-typing in interpreter is long-winded and error prone.
- Examples of SQL scripts bundled with project.
- (1) Normalized ^{56}Fe partial γ-ray cross sections.
- (2) γ-ray data information contained in database.

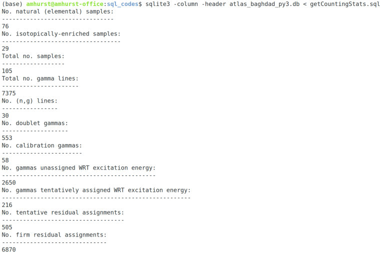
```
$ sqlite3 -column -header $DB < $SQL_SCRIPT
```

(1) Normalized Fe cross sections:



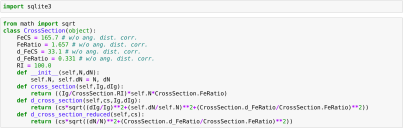
```
target      residual     E [keV]     dE [keV]    BR          dBR         cross section [mb]    error cs [mb]
----------  ----------  ----------  ----------  ----------  ----------  --------------------  ------------------
Fe          57Fe        122.1       0.2         2.2         0.2         3.146                 0.699170937611111
Fe          55Mn        126.0       0.2         1.6         0.2         2.288                 0.545061464423967
Fe          54Mn        156.5       0.2         0.4         0.1         0.572                 0.184133104030753
Fe          56Mn        211.0       0.3         0.22        0.03        0.3146                0.076882052522028
Fe          57Fe        352.5       0.0         1.6         0.2         2.288                 0.545061464423967
Fe          57Fe        367.1       0.2         0.54        0.05        0.7722                0.172150544582351
Fe          53Fe        757.3       0.4         0.1         0.03        0.143                 0.051782332894530
Fe          58Fe        810.3       0.2         0.43        0.03        0.6149                0.131873045009206
Fe          56Fe        846.78      0.0         100.0       0.0         143.0                 29.0
Fe          Fe          992.8       0.4         0.1         0.03        0.143                 0.051782332894530
Fe          56Fe        1037.85     0.0         2.15        0.1         3.0745                0.639688400707719
Fe          54Fe        1130.0      0.3         0.39        0.04        0.5577                0.126741666392706
Fe          54Fe        1152.8      0.4         0.14        0.03        0.2002                0.059065810753768
Fe          Fe          1165.9      0.6         0.08        0.03        0.1144                0.048771405556944
Fe          56Fe        1173.2      0.8         0.25        0.1         0.3575                0.160328568882779
Fe          56Fe        1175.0      0.8         0.15        0.1         0.2145                0.14946989663474
Fe          Fe          1213.0      0.7         0.06        0.03        0.0858                0.046294384108658
Fe          56Fe        1238.3      0.2         10.5        0.5         15.015                3.12781872876291
Fe          56Fe        1271.9      1.0         0.05        0.02        0.0715                0.032065713776555
```

(2) Some general database stats:



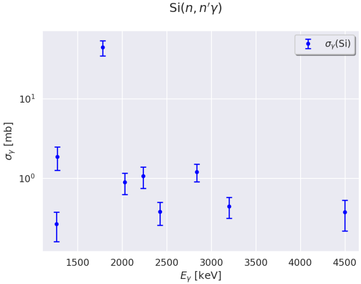
```
(base) amhurst@amhurst-office:sql_codes$ sqlite3 -column -header atlas_baghdad_py3.db < getCountingStats.sql
No. natural (elemental) samples:
--------------------------------
76
No. isotopically-enriched samples:
----------------------------------
29
Total no. samples:
------------------
105
Total no. gamma lines:
----------------------
7375
No. (n,g) lines:
----------------
30
No. doublet gammas:
-------------------
553
No. calibration gammas:
-----------------------
58
No. gammas unassigned WRT excitation energy:
--------------------------------------------
2650
No. gammas tentatively assigned WRT excitation energy:
------------------------------------------------------
216
No. tentative residual assignments:
-----------------------------------
505
No. firm residual assignments:
------------------------------
6870
```

Pythonic methods for interacting with the data



```
import sqlite3
```

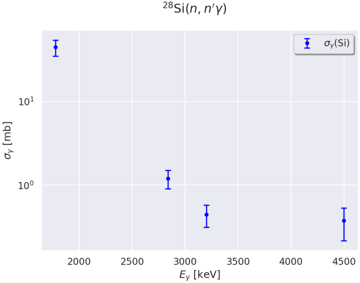
```
from math import sqrt
class CrossSection(object):
    FeCS = 165.7 # w/o ang. dist. corr.
    FeRatio = 1.657 # w/o ang. dist. corr.
    d_FeCS = 33.1 # w/o ang. dist. corr.
    d_FeRatio = 0.331 # w/o ang. dist. corr.
    RI = 100.0
    def __init__(self,N,dN):
        self.N, self.dN = N, dN
    def cross_section(self,Ig,dIg):
        return ((Ig/CrossSection.RI)*self.N*CrossSection.FeRatio)
    def d_cross_section(self,cs,Ig,dIg):
        return (cs*sqrt((dIg/Ig)**2+(self.dN/self.N)**2+(CrossSection.d_FeRatio/CrossSection.FeRatio)**2))
    def d_cross_section_reduced(self,cs):
        return (cs*sqrt((dN/N)**2+(CrossSection.d_FeRatio/CrossSection.FeRatio)**2))
```



$\mathrm{Si}(n,n'\gamma)$

- Firmly assigned γ rays only.
- γ rays from any Si isotope.

- Jupyter Notebook distributed with project: `sql_queries_atlas.ipynb`
- Implementation of Pythonic methods for handling the data.



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

- Firmly assigned γ rays only.
- γ rays from ^{28}Si only: `nucleus.residual = '28Si'`

Reactor neutrons: ^{235}U fission neutron spectrum

Different empirical relations have been proposed to describe the energy spectrum of reactor neutrons:

- **Watt:**

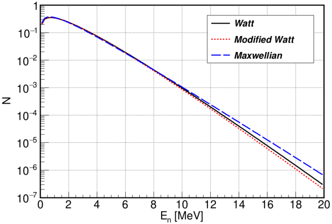
$$N(E_n) = \sqrt{\frac{2}{\pi e}}\exp(-E_n)\sinh\sqrt{(2E_n)}$$

- **Modified Watt:**

$$N(E_n) = A\exp(-bE_n)\sinh\sqrt{(cE_n)}$$

- **Maxwellian:**

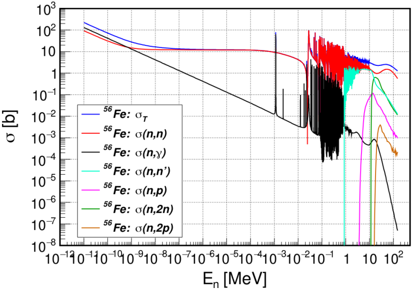
$$N(E_n) = 2\sqrt{\frac{E_n}{\pi kT^3}}\exp\left(\frac{-E_n}{kT}\right)$$

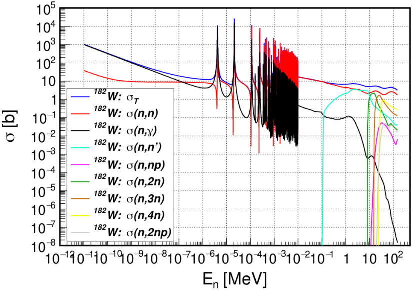


Best-fit parametrizations deduced for ^{235}U:

- Modified Watt: $A = 0.4527$, $b = 1.036$, $c = 2.29$.
- Maxwellian: $kT = 1.290$ MeV.

Neutron interactions and contributions to σ_F in ^{56}Fe and ^{182}W as function of E_n





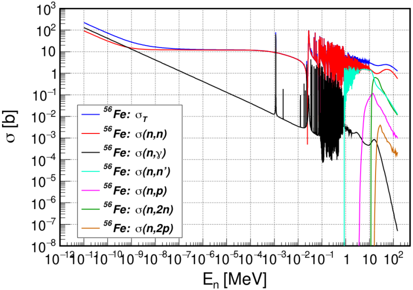
In ^{56}Fe, at $E_n = 25.3$ meV:

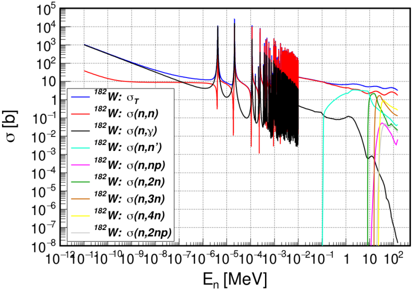
$$\sigma_F(n +^{56} \text{Fe}; E_n) = \sigma(n, \gamma).$$

In ^{182}W, at $E_n = 25.3$ meV:

$$\sigma_F(n +^{182} \text{W}; E_n) = \sigma(n, \gamma).$$

Neutron interactions and contributions to σ_F in ^{56}Fe and ^{182}W as function of E_n





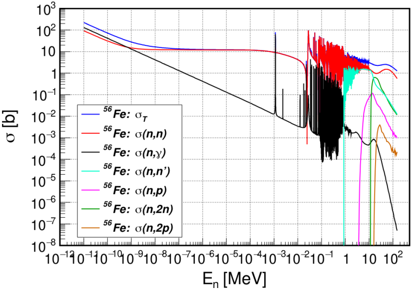
In ^{56}Fe, at $E_n = 14$ MeV:

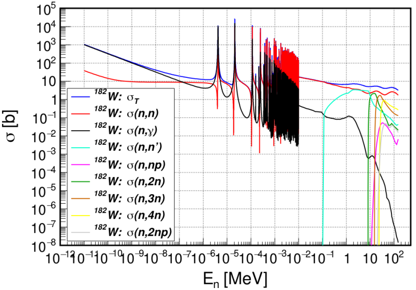
$$\sigma_F(n +^{56}\text{Fe}; E_n) = \sigma(n,\gamma) + \sigma(n,n') + \sigma(n,p) + \sigma(n,2n) + \sigma(n,2p).$$

In ^{182}W, at $E_n = 14$ MeV:

$$\begin{aligned}\sigma_F(n +^{182}\text{W}; E_n) &= \sigma(n,\gamma) + \sigma(n,n') + \sigma(n,np) + \sigma(n,2n) + \sigma(n,3n)\\ &+ \sigma(n,4n) + \sigma(n,2np).\end{aligned}$$

Neutron interactions and contributions to σ_F in ^{56}Fe and ^{182}W as function of E_n





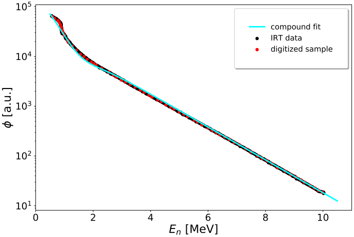
In ^{56}Fe, at $E_n = 0.86 \sim 10$ MeV:

$$\sigma_F(n + ^{56}\text{Fe}; E_n) = \sigma(n,\gamma) + \sigma(n,n') + \sigma(n,p).$$

In ^{182}W, at $E_n = 0.10 \sim 10$ MeV:

$$\sigma_F(n + ^{182}\text{W}; E_n) = \sigma(n,\gamma) + \sigma(n,n') + \sigma(n,2n).$$

Characterization the IRT-M Baghdad Reactor neutron flux



$E_n < 1.5$ MeV (Maxwellian):

$$\phi_1(E_n) = 2A_1\sqrt{\left(\frac{E_n}{\pi kT^3}\right)}\exp\left(\frac{E_n}{kT}\right).$$

$E_n \geq 1.5$ MeV (Exponential):

$$\phi_2(E_n) = A_2\exp(-\beta E_n).$$

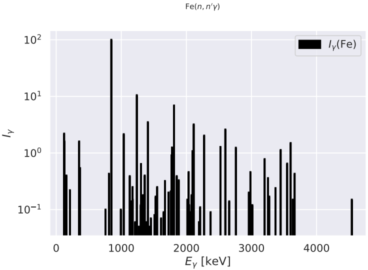
Overall fit according to parametrization of IRT-M data:

$$\phi(E_n) = \phi_1(E_n) + \left[\frac{1+\tanh[K(E_n-1.5)]}{2}\right](\phi_2(E_n) - \phi_1(E_n)).$$

$$\phi(E_n \ll 1.5\text{ MeV}) \rightarrow \phi_1(E_n);$$
$$\phi(E_n \gg 1.5\text{ MeV}) \rightarrow \phi_2(E_n).$$

Experimental Fe$(n, n'\gamma)$ γ-ray spectrum at the IRT-M

https://github.com/AaronMHurst/baghdad_atlas



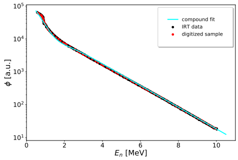
Most important γ rays in ^{56}Fe from integral fission-neutron spectrum:

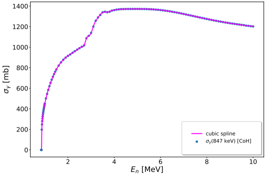
E_γ [keV]	$J_i^{\pi_i} \to J_f^{\pi_f}$	I_γ	B_A
846.8	$2_1^+ \to 0_{gs}^+$	100	1.0
1238.3	$4_1^+ \to 2_1^+$	10.5(5)	0.105(5)
1810.8	$2_2^+ \to 2_1^+$	6.9(4)	0.069(4)

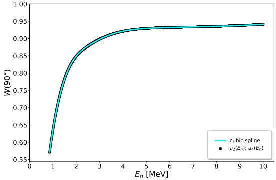
$$B_A = \frac{I_\gamma(E_\gamma)}{I_\gamma(E_\gamma = 846.8)} = \frac{I_\gamma(E_\gamma)}{100}.$$

- Well-characterized flux should reproduce measured experimental data.
- Determine flux-weighted cross section ($\langle\sigma_\gamma\rangle$) by convolving $\sigma_\gamma(E_n)$ with $\phi(E_n)$ and compare to corresponding *Baghdad Atlas* branching ratios.
- Parameterized Baghdad Reactor neutron-flux distribution yields $\langle\sigma_\gamma\rangle$ values that reproduces measured integral B_A to within $\sim 1.5\sigma$.

Determination of $\langle\sigma_\gamma(E_\gamma = 846.8\ \text{keV})\rangle$ in ^{56}Fe


Fast-reactor flux: $\phi(E_n)$

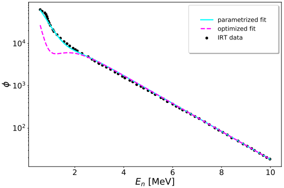

Cross section: $\sigma_\gamma(E_n)$


Angular distribution: $W_\gamma(E_n)$

$$\langle\sigma_\gamma(E_\gamma)\rangle = \frac{\int\limits_{E_n=0.862}^{E_n=10} \phi(E_n)\sigma_\gamma(E_n)W_\gamma(\theta = 90^\circ; E_n)dE_n}{\int\limits_{E_n=0}^{E_n=+\infty} \phi(E_n)dE_n}$$

- $\phi(E_n)$: Parameterized and adjusted for kT ($\phi(E_n \ll 1.5$ MeV$) \rightarrow$ Maxwellian; $\phi(E_n \gg 1.5$ MeV$) \rightarrow$ exponential).
- $\sigma_\gamma(E_n)$: γ-ray production data as function of E_n from reaction model, e.g., CoH$_3$, EMPIRE, or a nuclear data library, e.g., ENDF.
- $W_\gamma(\theta = 90^\circ; E_n)$: Experimental anisotropy-attenuation coefficients, a_2 and a_4 (not always available!).

Neutron-flux optimization: kT-adjustment to ^{56}Fe data



Reminder: the uncorrelated χ^2:

$$\chi^2 = \sum_{i=1}^{N} \frac{[y_i - f(x_i)]^2}{\sigma_i^2}.$$

Adjust kT in χ^2 minimization to find optimal flux:

$$\sum_{i=1}^{N}\sum_{j=1}^{N}[B_{A_i} - B_{kT_i}][V_{ij}^{-1}][B_{A_j} - B_{kT_j}].$$

or in matrix notation:

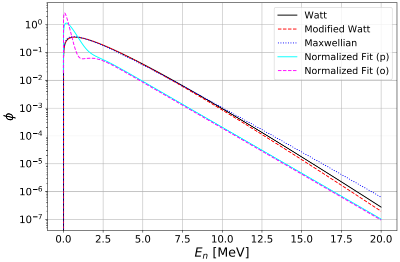
$$\chi^2 = (\boldsymbol{B_A} - \boldsymbol{B_{kT}})\boldsymbol{V}^{-1}(\widetilde{\boldsymbol{B_A}} - \widetilde{\boldsymbol{B_{kT}}}).$$

- $V \Rightarrow$ covariance matrix $\because I_\gamma$ are correlated.
- $N = 3 \Rightarrow$ number of γ rays.
- $\mathrm{ndf} = 3 - 1 = 2$.
- $\chi^2/\mathrm{ndf} \approx 0.35$ for $\mathrm{ndf} = 2$.
- Correlation coefficient in range $0 < \rho_{ij} \lesssim 0.75$ reproduces expected χ^2/ndf consistent with $kT = 0.155(30)$ MeV (cf. $kT = 1.290$ MeV for pure Maxwellian ^{235}U fission.)

Normalized fits cf. standard ^{235}U neutron-flux distributions

Flux must satisfy normalization condition:

$$\int_{0}^{+\infty} \phi^{*}(E_n)\phi(E_n)dE_n = 1$$



Expectation energies:

- 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 Flux at IRT-M $\langle E_n \rangle = 0.88$ MeV.
- Optimized Flux at IRT-M $\langle E_n \rangle = 0.63$ MeV.

kT-adjusted optimized neutron flux used to deduce flux-weighted quantities.

Optimized flux-weighted cross sections

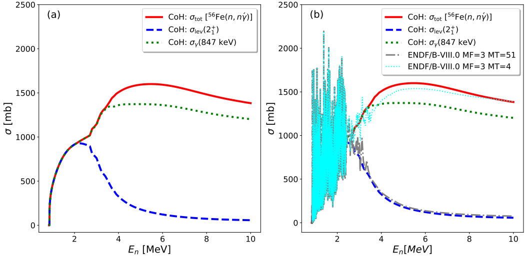
Values for $\langle\sigma_\gamma\rangle$ and $\langle\sigma_\gamma\rangle_W$ deduced according to fitted flux using compound function with optimized $kT = 0.155$ MeV:

E_γ [keV]	B_A	B_{kT}	$\langle\sigma_\gamma\rangle$ [mb]	$\langle\sigma_\gamma\rangle_W$ [mb]	$\langle\sigma_\gamma\rangle_{\mathrm{FRM}}$ [mb]	$\langle\sigma_\gamma\rangle_S$ [mb]
846.8	1.0	1.0	166(34)	143(29)	586(41)	521(106)
1238.3	0.105(5)	0.096(27)	15.9(31)	13.7(27)	58(5)	49.9(98)
1810.8	0.069(4)	0.061(18)	10.0(21)	8.7(18)	37(3)	31.7(66)

Our cross sections for ^{56}Fe are consistent with the recent FRM-II measurement* upon scaling by $\langle E_n\rangle$ at the two facilities.

*Z. Ilic *et al.*, J. Radioanal. Nucl. Chem. **325**, 641 (2020).

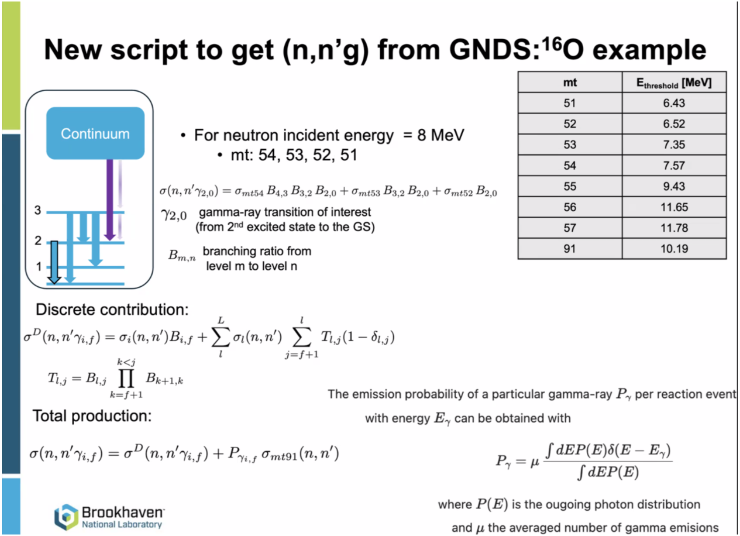
Why not take σ_γ directly from ENDF rather than a model?



	CoH	ENDF
$\langle\sigma_{\rm lev}\rangle$	113.0	101.6
$\langle\sigma_{\rm tot}\rangle$	171.8	163.6
$\frac{\langle\sigma_{\rm lev}\rangle}{\langle\sigma_{\rm tot}\rangle}$	0.658	0.621
$\langle\sigma_\gamma\rangle$	165.7	157.8

- σ_γ cannot be extracted directly from ENDF.
- Results indicate: $\frac{\langle\sigma_{\rm lev}^{\rm CoH}\rangle}{\langle\sigma_{\rm tot}^{\rm CoH}\rangle} \approx \frac{\langle\sigma_{\rm lev}^{\rm ENDF}\rangle}{\langle\sigma_{\rm tot}^{\rm ENDF}\rangle}$.
- Reasonable to expect ratios of partial γ-ray production cross section to total inelastic cross section to also be in agreement, i.e., $\langle\sigma_\gamma^{\rm ENDF}\rangle \approx \langle\sigma_{\rm tot}^{\rm ENDF}\rangle \frac{\langle\sigma_\gamma^{\rm CoH}\rangle}{\langle\sigma_{\rm tot}^{\rm CoH}\rangle}$.

Emanuel Chimanski's method for σ_γ extraction from ENDF



New script to get (n,n'g) from GNDS:^{16}O example

- For neutron incident energy = 8 MeV
  - mt: 54, 53, 52, 51

$$\sigma(n,n'\gamma_{2,0}) = \sigma_{mt54}\,B_{4,3}\,B_{3,2}\,B_{2,0} + \sigma_{mt53}\,B_{3,2}\,B_{2,0} + \sigma_{mt52}\,B_{2,0}$$

$\gamma_{2,0}$ gamma-ray transition of interest (from 2nd excited state to the GS)

$B_{m,n}$ branching ratio from level m to level n

mt	$E_{\text{threshold}}$ [MeV]
51	6.43
52	6.52
53	7.35
54	7.57
55	9.43
56	11.65
57	11.78
91	10.19

Discrete contribution:

$$\sigma^D(n,n'\gamma_{i,f}) = \sigma_i(n,n')B_{i,f} + \sum_{l}^{L}\sigma_l(n,n')\sum_{j=f+1}^{l}T_{l,j}(1-\delta_{l,j})$$

$$T_{l,j} = B_{l,j}\prod_{k=f+1}^{k<j}B_{k+1,k}$$

Total production:

$$\sigma(n,n'\gamma_{i,f}) = \sigma^D(n,n'\gamma_{i,f}) + P_{\gamma_{i,f}}\,\sigma_{mt91}(n,n')$$

The emission probability of a particular gamma-ray P_γ per reaction event with energy E_γ can be obtained with

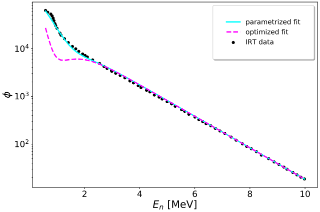
$$P_\gamma = \mu\,\frac{\int dEP(E)\delta(E-E_\gamma)}{\int dEP(E)}$$

where $P(E)$ is the ougoing photon distribution and μ the averaged number of gamma emisions

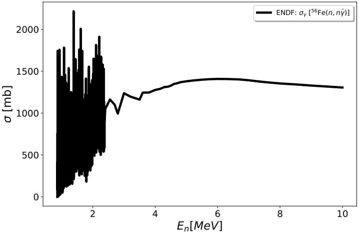
Brookhaven National Laboratory

Determination of $\langle\sigma_\gamma\rangle$ derived from ENDF for ^{56}Fe γ rays

Fast-reactor flux: $\phi(E_n)$



ENDF cross section: $\sigma_\gamma(E_n)$



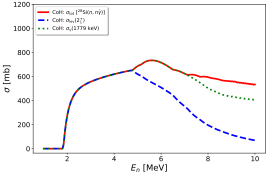
$$\langle\sigma_\gamma(E_\gamma)\rangle = \frac{\int_{E_n=0.862}^{E_n=10} \phi(E_n)\sigma_\gamma(E_n)dE_n}{\int_{E_n=0}^{E_n=+\infty} \phi(E_n)dE_n}$$

E_γ [keV]	$\langle\sigma_\gamma\rangle$ [mb] CoH	$\langle\sigma_\gamma\rangle$ [mb] ENDF
846.8	166(34)	160.3
1238.3	15.9(31)	13.5
1810.8	10.0(21)	9.4

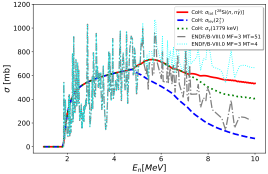
Values of $\langle\sigma_\gamma\rangle$ deduced directly from ENDF are consistent with value from well-tuned CoH$_3$ reaction-model calculation.

Flux-weighted validation for ^{28}Si$(n, n'\gamma)$: 1779 keV

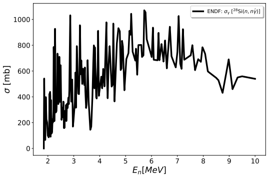
CoH$_3$



CoH$_3$ cf. ENDF



Derived σ_γ(1779) from ENDF

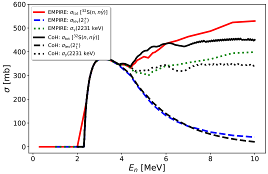


Source	$\langle\sigma_\gamma\rangle$ [mb]	$\langle\sigma_{\text{lev}}\rangle$ [mb]	$\frac{\langle\sigma_{\text{lev}}\rangle}{\langle\sigma_{\text{tot}}\rangle}$
CoH	55.69	53.45	0.957
ENDF (estimate)	48.17	46.59	0.965
ENDF (derived)	49.40	—	—
Baghdad Atlas	**47.1(94)**	—	—

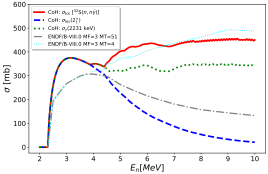
Integral measurement in agreement with 3 different validation results.

Flux-weighted validation for $^{32}S(n, n'\gamma)$: 2231 keV

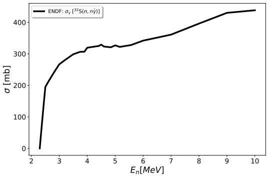
CoH$_3$ cf. EMPIRE



CoH$_3$ cf. ENDF



Derived $\sigma_\gamma(2231)$ from ENDF

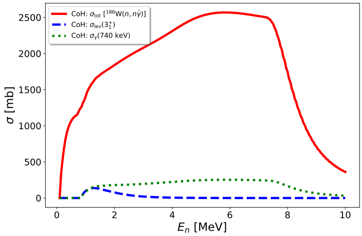


Source	$\langle\sigma_\gamma\rangle$ [mb]	$\langle\sigma_{\rm tot}\rangle$ [mb]	$\langle\sigma_{\rm lev}\rangle$ [mb]	$\frac{\langle\sigma_{\rm lev}\rangle}{\langle\sigma_{\rm tot}\rangle}$
CoH	26.57	27.91	23.95	0.858
EMPIRE	26.49	28.80	23.78	0.890
ENDF (estimate)	21.67	22.76	19.98	0.878
ENDF (derived)	21.79	—	—	—
Baghdad Atlas	**25.0(60)**	—	—	—

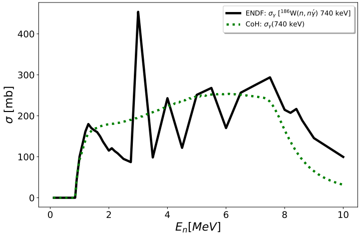
Integral measurement in agreement with 4 different validation results.

Flux-weighted validation for ^{186}W$(n, n'\gamma)$: 740 keV

CoH$_3$



CoH$_3$ cf. Derived $\sigma_\gamma(740)$ from ENDF



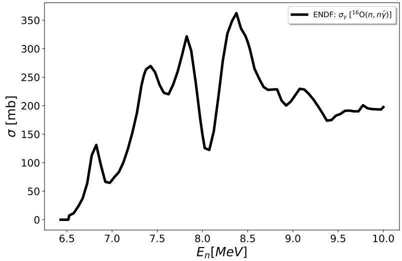
	CoH	ENDF (derived)	Baghdad Atlas
$\langle\sigma_\gamma\rangle$ [mb]	30.60	28.06	**23.9(56)**

- 740-keV γ ray resolved from doublet.
- 740-keV γ ray deexcites 862-keV level.

Integral measurement in agreement with 2 different validation results.

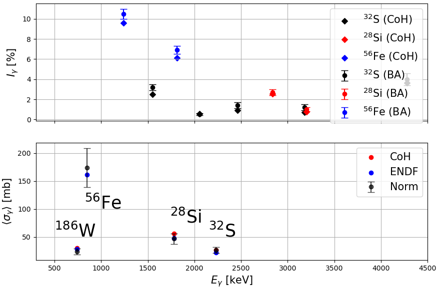
Flux-weighted validation for ^{16}O$(n, n'\gamma)$: 6129 keV

Derived $\sigma_\gamma(6129)$ from ENDF



- $\langle\sigma_\gamma\rangle = 1.09(50)$ mb (Baghdad Atlas)
- $\langle\sigma_\gamma\rangle = 0.533$ mb (ENDF)
- ^{16}O γ rays hard to measure.
- Flux at energy needed is low.
- ENDF-derived σ_γ especially needed for cases like ^{16}O which are also quite difficult to model cf. statistical Hauser-Feshbach approach.

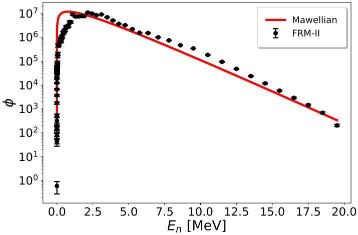
Validation using integral data for ^{28}Si, ^{32}S, ^{56}Fe, and ^{186}W

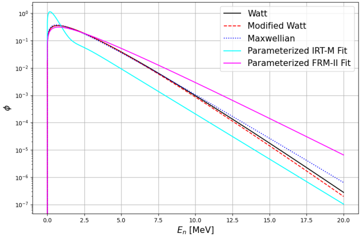


- Absolute flux-weighted quantities from CoH and ENDF reproduce known absolute integral I_γ data from the Baghdad Atlas.
- Normalization transitions and *weaker* transitions.
- Explore additional isotopes covering broader energy range.
- Gamma-Rays Induced by Neutrons (GRIN): A.M. Hurst, E.V. Chimanski, D.A. Brown, “*Validation of evaluated nuclear data for GRIN*”, LBNL-2001617 (2024).

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

Validation using FRM-II Reactor flux





Source	$\langle\sigma_\gamma\rangle_{W_\gamma}$ [mb]	$\langle\sigma_\gamma\rangle$ [mb]	$\langle\sigma_{\rm tot}\rangle$ [mb]	$\langle\sigma_{\rm lev}\rangle$ [mb]	$\frac{\langle\sigma_{\rm lev}\rangle}{\langle\sigma_{\rm tot}\rangle}$
CoH	622.5	759.4	797.3	468.8	0.59
ENDF (estimate)	590.7	720.7	756.6	461.3	0.61
ENDF (derived)	552.6	673.9	–	–	–
FRM-II	**586(41)**	**715(50)**	–	–	–

- FRM-II: $\langle E_n\rangle = 2.32$ MeV from fit cf. 2.3 MeV [Ilic 2020].
- Validation results for ^{56}Fe$(n, n'\gamma)$; $E_\gamma = 846.8$ keV $(2_1^+ \rightarrow 0_{\rm gs}^+)$.
- Additional validation datasets from FRM-II: Al, Ti, Cu, In, Ca.