Berkeley Nuclear Database Projects

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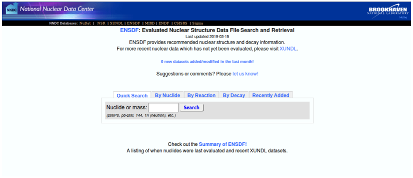
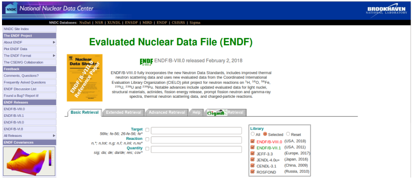
ENSDF and potential applications

Structure (ENSDF) and Reactions (ENDF)

Libraries hosted at the National Nuclear Data Center (NNDC)





- Evaluated Nuclear Structure Data File (ENSDF)
- E_L, J^π, E_γ, δ_γ, $\alpha\ldots$
- Basic science
- String

- Evaluated Nuclear Data File (ENDF)
- σ from (n, x) reactions
- Applications
- Numerical

Migration of data into nuclear databases

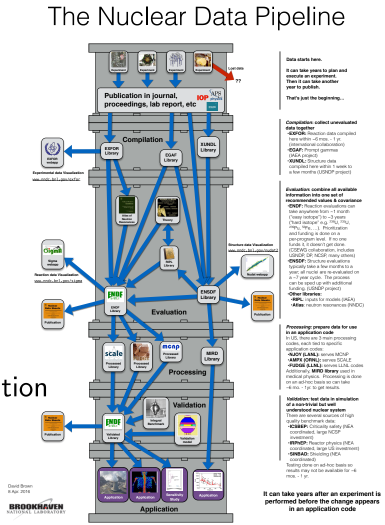
Publish data

Compile data

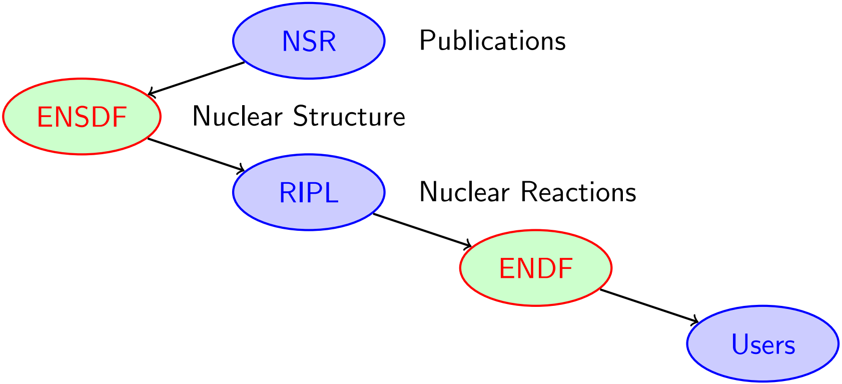
Evaluate data

Processing/validation

Application



Nuclear data library development

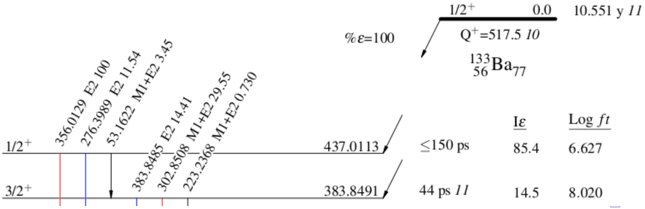


NSR: Nuclear Science References
RIPL: Reference Input Parameter Library

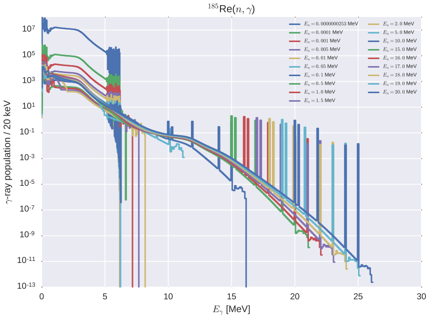
ENSDF data types

- *Standard records*, e.g., the Level `L` record (E, J^{π}, $T_{1/2}\ldots$); the Gamma `G` record (E_{γ}, I_{γ}, $\alpha\ldots$).
- *Continuation records*, e.g., `L`: particle-decay modes (α, β^{-}, etc.); `G`: reduced transition probabilities ($B(M1)$, $B(E2)$, etc.).

```
133CS  L 437.0113   91/2+              150 PS    LE
133CS cL T$from 1964Va25, 1970Va34
133CS  E                         85.4   5  6.627 18
133CSS E CK=0.671 5$CL=0.251 4$CM+=0.0777 11
133CS cE           |eK(exp)=0.65 {I3} (1992Sa28)
133CS cE           |eL(exp)/|eK(exp)=0.371 {I7} (1967Sc10)
133CS  G 53.1622   6 3.45     5M1+E2     0.08    +2-3  5.66   10
133CS3 G EKC=5.0 10$ EL1C=0.51 7$ EL2C=0.069 15$
```



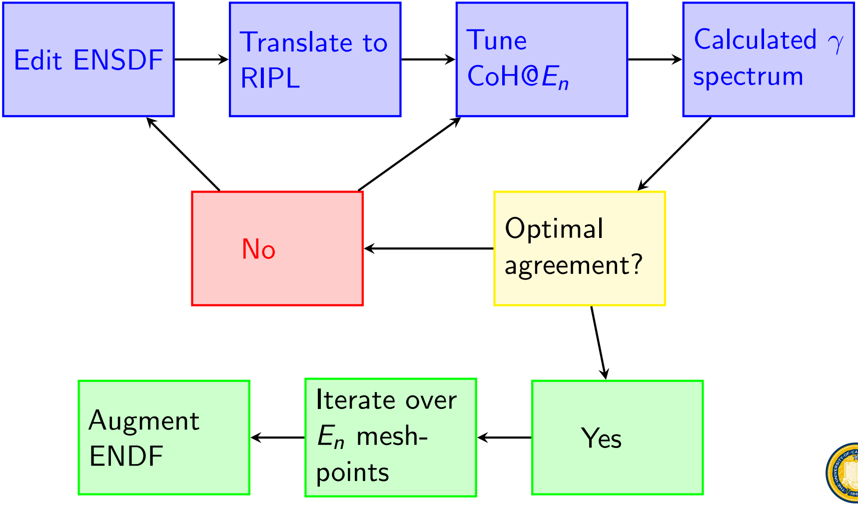
ENSDF-to-RIPL translator for reaction calculations



Application: Calculate (n,γ) γ-ray spectrum as function of increasing E_n. Requires **structure** data and reaction-model parametrizations.

- Reaction calculations often use RIPL-formatted data sets.
- Reaction codes: `CoH`, `EMPIRE`, `TALYS`.
- RIPL may be out of date (RIPL-3 2009).
- Structure data sets often prepared in ENSDF format.

Application processing methodology



ENSDF-to-RIPL: Representative translation for ^{243}Pu

^{242}Pu(n,γ) data set

ENSDF

```
243PU    242Pu(N,G) E=THERMAL
243PU  Q 580        3  5033.9 26 6.95E+320 4757.0   2.8     2012WA38
243PU cQ $S(2n)=11344 {I3}; S(2p)=13019 syst {i298} (2012Wa38)
243PU  L   0.0        7/2+             4.956 H    3
243PU2 L %B-=100
243PU  L 58.28        8 9/2+
243PU cG 58.3        10 0.0031  4  [M1]                    27.2  4
243PU2cG Must be there, Based on intensity balance
243PU3cG to close to Am241d so not observed
243PU  G 58.3        10 0.0059 22  [M1]                    27.2  4
243PU cG Based on DICEBOX Expectation
243PU  L 124.65      10 11/2+
243PU  G 66.37       71 0.0003125  [M1]                    18.61
243PU2cG 66 Dicebox increased
---  243Pu_Adopt.ens    Top (14,80)    (Fundamental)----------------------------
243PU  G 1042.37      8 0.0074  3  [M1]                    0.041
243PU  L 1437.60     20 31/2+
243PU cG 347.5
243PU  L 1444         3
243PU  L 1465         3
243PU  L 1491.82     20  1/2-,3/2-
243PU  L 1516.39     10  (3/2-)
243PU  G 838.45      10 0.0065  6  [E1]                    0.0055
243PU  L 1627.6         33/2+
243PU  L 1.7E+3       3                46 NS      13
243PU2 L %SF=100
243PU  L 5036.33      7 1/2+
243PU  G 3519.08     11 0.0052  4  [E1]                    0.002
243PU  G 3544.50     18 0.0041  4
```

RIPL

```
243Pu  243   94   73   91   31    7    5.033900    6.950000
  1   0.000000   3.5  1   1.78E+04  0 0                    7/2+  1 =    100.0000 %B-
  2   0.058280   4.5  1   0.00E+00  1 0                    9/2+  0
                                         1      0.058  3.546E-02  1.000E+00  2.720E+01
  3   0.124650   5.5  1   0.00E+00  2 0                   11/2+  0
                                         2      0.066  2.424E-02  4.753E-01  1.861E+01
                                         1      0.125  7.819E-02  5.247E-01  5.710E+00
  4   0.207100   6.5  1   0.00E+00  0 0                   13/2+  0
  5   0.287560   2.5  1   0.00E+00  2 0                    5/2+  0
                                         2      0.229  5.761E-03  8.757E-03  5.200E-01
                                         1      0.288  4.236E-01  9.912E-01  1.340E+00
  6   0.299000   7.5  1   0.00E+00  0 0                   15/2+  0
  7   0.333430   3.5  1   0.00E+00  3 0                    7/2+  0
                                         5      0.046  1.138E-02  6.401E-01  5.526E+01
                                         2      0.275  1.413E-01  3.554E-01  1.515E+00
                                         1      0.333  2.395E-03  4.524E-03  8.890E-01
  8   0.383640   0.5  1   3.30E-07  1 0                  (1/2+)  0
-UU-:----F1  z094_ripl.dat   Top (16,87)    (Fundamental)-------------------------------
 67   1.444000  -1.0  0   0.00E+00  0 0                          0
 68   1.465000  -1.0  0   0.00E+00  0 0                          0
 69   1.491820   0.5 -1   0.00E+00  0 1               1/2-,3/2-  0
 70   1.516390   1.5 -1   0.00E+00  1 0                  (3/2-)  0
                                        25      0.838  9.945E-01  1.000E+00  5.500E-03
 71   1.627600  16.5  1   0.00E+00  0 0                   33/2+  0
 72   1.700000  -1.0  0   4.60E-08  0 0                          1 =    100.0000 %SF
 73   5.036330   0.5  1   0.00E+00 16 0                    1/2+  0
                                        70      3.519  7.517E-02  7.532E-02  2.000E-03
                                        69      3.545  5.927E-02  5.927E-02  0.000E+00
                                        66      3.599  3.180E-02  3.180E-02  0.000E+00
                                        64      3.615  1.287E-01  1.287E-01  0.000E+00
                                        62      3.649  8.384E-02  8.384E-02  0.000E+00
                                        57      3.735  6.216E-02  6.216E-02  0.000E+00
                                        49      3.860  2.024E-02  2.024E-02  0.000E+00
                                        47      3.907  5.204E-02  5.204E-02  0.000E+00
                                        40      4.087  4.192E-02  4.192E-02  0.000E+00
                                        37      4.131  6.794E-02  6.794E-02  0.000E+00
```

ENSDF-to-XML: ^{133}Cs gamma (G) record

^{133}Ba ϵ-decay data set

```
    <level id="Cs133_e2" index="2">
      <energy value="160.6121" unit="keV">
        <uncertainty value="0.0009" pdf="normal"/>
      </energy>
---  ENSDF_133Cs.xml    31% (168,84)    (XML)------------------------------------
    <level id="Cs133_e3" index="3">
      <energy value="383.8491" unit="keV">
        <uncertainty value="0.0008" pdf="normal"/>
      </energy>
---  ENSDF_133Cs.xml    49% (258,84)    (XML)------------------------------------
      <decay mode="gamma">
        <gammaEnergy value="223.2368" unit="keV">
          <uncertainty value="0.0013" pdf="normal"/>
        </gammaEnergy>
        <branchingRatio value="0.730">
          <uncertainty value="0.005" pdf="normal"/>
        </branchingRatio>
        <multipolarity value="M1+E2"/>
        <mixingRatio value="0.114" sign="-">
          <uncertainty value="0.014" pdf="normal"/>
---  ENSDF_133Cs.xml    58% (303,84)    (XML)------------------------------------
        <finalLevel>
          <flevel id="Cs133_2" index="2"/>
          <fenergy value="160.6121" unit="keV"/>
        </finalLevel>
---  ENSDF_133Cs.xml    63% (317,84)    (XML)------------------------------------
133CS  G 223.2368  13 0.730   5M1+E2     -0.114  14     0.0975
```

- Interpreted numeric ENSDF data useful
- XML output can be verbose
- No longer space limited
- Numerical accuracy and LSD no longer an issue
- Level indexing: include final levels associated with γ decay

ENSDF-to-XML: ^{133}Cs $T_{1/2}$ (T) and δ_γ (MR) quantities

https://escholarship.org/uc/item/23v3f35g

```
<parent id="Ba133" A="133">
  <level>
    <energy value="0.0" unit="keV">
      <uncertainty value="0.0" pdf="NA"/>
    </energy>
    <spin string="1/2" value="0.5" unit="hbar"/>
    <parity value="+"/>
    <halflife value="10.551" unit="y">
      <uncertainty value="0.011" pdf="normal"/>
    </halflife>
    <lifetime value="15.222" unit="y">
      <uncertainty value="0.016" pdf="normal"/>
    </lifetime>
    <Q-value value="517.5" unit="keV" transition="G.S. to G.S.">
--  ENSDF_133Cs.xml     4% (38,0)      (XML)-----------------------------------
        </branchingRatio>
        <multipolarity value="M1+E2"/>
        <mixingRatio value="0.08" sign="None">
          <uncertainty upperBound="+0.02" lowerBound="-0.03" pdf="asymmetric">
            <symmetrizationMethods>
              <method1 value="0.075000">
                <uncertainty value="0.025000" pdf="normal"/>
              </method1>
              <method2 value="0.072021">
                <uncertainty value="0.025226" pdf="normal"/>
              </method2>
            </symmetrizationMethods>
          </uncertainty>
        </mixingRatio>
--  ENSDF_133Cs.xml    83% (429,0)     (XML)-----------------------------------
```

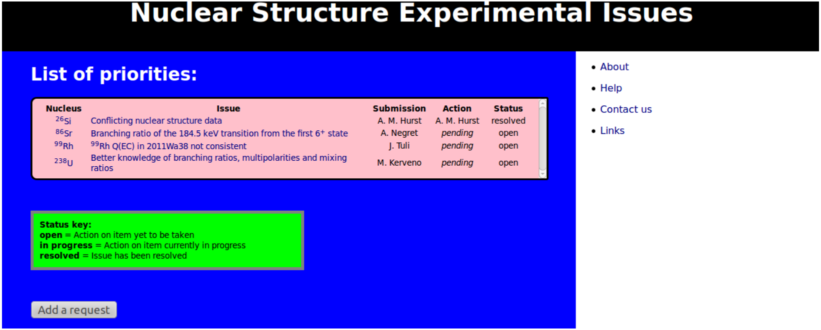
- Allows for inclusion of derived quantities
- Derive τ from parsed $T_{1/2}$ field
- Symmetrization methods for handling asymmetric uncertainties

Implicit ENSDF $\Rightarrow$ **Explicit** XML

Nuclear Structure Experimental Issues Website

http://nucleardata.berkeley.edu/hpnsrl

"Create website of high-priority nuclear structure and decay-data measurements for information and guidance."



Nuclear Structure Experimental Issues

List of priorities:

Nucleus	Issue	Submission	Action	Status
^{26}Si	Conflicting nuclear structure data	A. M. Hurst	A. M. Hurst	resolved
^{86}Sr	Branching ratio of the 184.5 keV transition from the first 6^+ state	A. Negret	*pending*	open
^{99}Rh	^{99}Rh Q(EC) in 2011Wa38 not consistent	J. Tuli	*pending*	open
^{238}U	Better knowledge of branching ratios, multipolarities and mixing ratios	M. Kerveno	*pending*	open

Status key:
open = Action on item yet to be taken
in progress = Action on item currently in progress
resolved = Issue has been resolved

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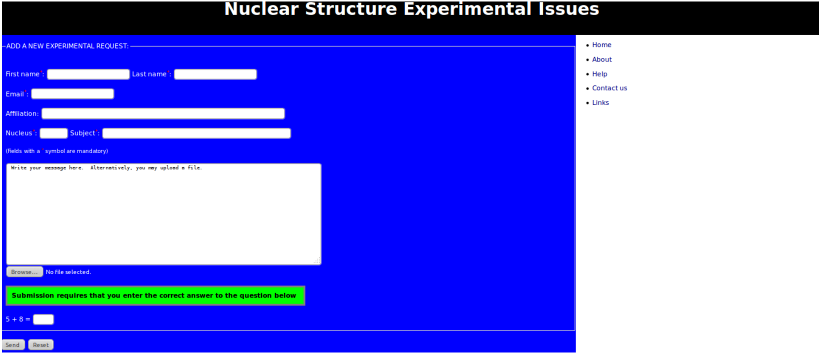
New request page

http://nucleardata.berkeley.edu/hpnsrl



Raised experimental issues

http://nucleardata.berkeley.edu/hpnsrl

EXPERIMENTAL REQUEST:

Name: Alexandru Negret
Affiliation: IFIN-HH
Email: alnegret@tandem.nipne.ro
Nucleus: ^{86}Sr **Subject:** Branching ratio of the 184.5 keV transition from the first 6^+ state

REQUEST MOTIVATION:

Contradicting information exist in recent literature regarding the branching ratio of the 184.5-keV gamma transition decaying from the first 6+ level (E=2857 keV):
2017Du08 - 23.7(14)%
2016Li25 - 8.1(10)%
2014Li25 - 3.2(2)%

In the latest ENSDF evaluation (2015), the value is 5.7(25)%. A gamma-gamma coincidence measurement may clarify the issue.

Responsible Individual (RI): *Pending assignment* **Email:**

RI COMMENTS:

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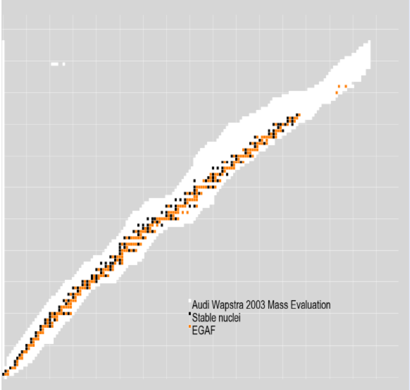
- ^{86}Sr: Discrepant branching ratios for the 184.5-keV γ ray.
- 23.7(14)%; 8.1(10)%; 3.2(2)%; ENSDF $\Rightarrow$ 5.7(25)%.
- γ-γ coincidence measurement may help.

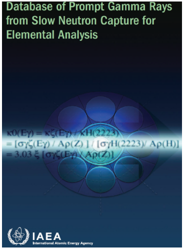
EGAF

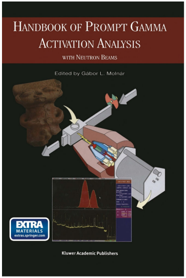
The EGAF project



- Evaluated Gamma-ray Activation File (EGAF)
- IAEA initiative led by Rick Firestone (LBNL) and researchers from the Budapest Reactor
- Thermal-capture cross-section data
- Isotopes close to stability
- Natural targets $Z = 1 - 82, 90, 92$ except for $Z = 2, 61$
- $\sim 32,000$ prompt and $\sim 3,000$ decay γ-ray lines

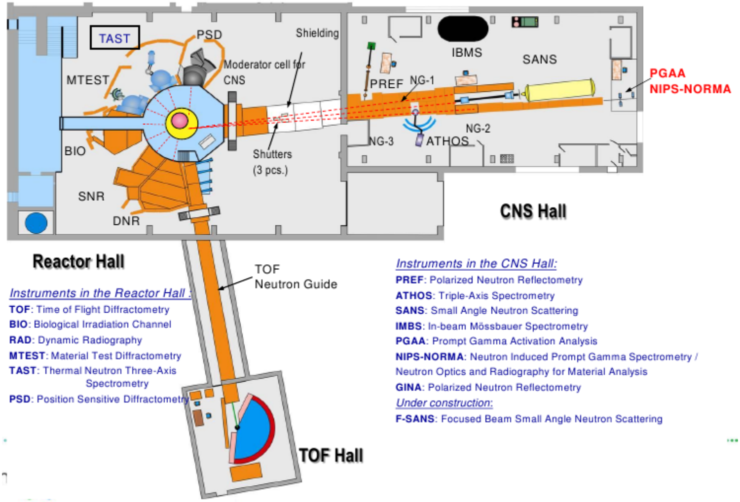
The EGAF database





- *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).
- http://www-nds.iaea.org/pgaa/egaf.html
- EGAF 2007 - present: Prompt γ-ray analysis and statistical modeling enriched isotopes.
- Peer-reviewed publications.
- E_γ, S_n, σ_γ, σ_0, Γ_0, J^π, δ_γ.

PGAA @ Budapest Reactor: Experimental Facility



Nondestructive assay (NDA) of materials

- Enable NDA: Guide Evaluated Nuclear Data File (ENDF) library development using high-resolution HPGe-quality γ-ray line data from EGAF.
- Improved capture-γ and inelastic-γ data needed for high-priority isotopes for accurate simulation of interrogation systems.

- Interrogation system: Evaluating munitions for presence of explosives, chemicals or nerve agents.
- SF, DD, DT neutron sources.
- Characteristic γ rays (primaries).

(Gus Caffrey, Ed Seabury, INL)

"NA-22" Priority List

Z	Element	Z	Element	Z	Element
1	H	26	Fe	74	W
3	Li	28	Ni	75	Re
4	Be	29	Cu	77	Ir
5	B	31	Ga	78	Pt
6	C	39	Y	79	Au
7	N	40	Zr	82	Pb
8	O	41	Nb	84	Po
12	Mg	42	Mo	88	Ra
13	Al	46	Pd	90	Th
14	Si	57	La	92	U
22	Ti	63	Eu	93	Np
23	V	64	Gd	94	Pu
24	Cr	73	Ta	95	Am

"NA-22" Priority List

Z	Element	Z	Element	Z	Element
1	H	26	Fe	74	W
3	Li	28	Ni	75	Re
4	Be	29	Cu	77	Ir
5	B	31	Ga	78	Pt
6	C	39	Y	79	Au
7	N	40	Zr	82	Pb
8	O	41	Nb	84	Po
12	Mg	42	Mo	88	Ra
13	Al	46	Pd	90	Th
14	Si	57	La	92	U
22	Ti	63	Eu	93	Np
23	V	64	Gd	94	Pu
24	Cr	73	Ta	95	Am

(n,γ) analysis published

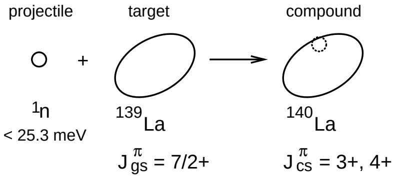
Thermal neutron capture: $^{139}\mathrm{La}(n,\gamma)$

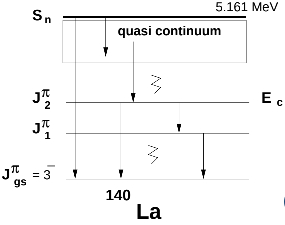
- $T = 293$ K $\Rightarrow E_n = 25.3$ meV
- s-wave capture ($l = 0$): compound @ $E \approx S_n$
- Capture-state spin (J_{CS}) is related to G.S. spin (J_{gs}) of target:

$$\boldsymbol{J_{CS}} = \boldsymbol{J_{gs}} + \boldsymbol{l} + \boldsymbol{s}$$

$$\pi_{CS} = \pi_{gs}(-1)^l$$

- Beneath threshold for particle evaporation
- Deexcitation via γ emission
- Bohr's extreme statistical model





EGAF case study: $^{139}\text{La}(n,\gamma)$

APPLICATIONS

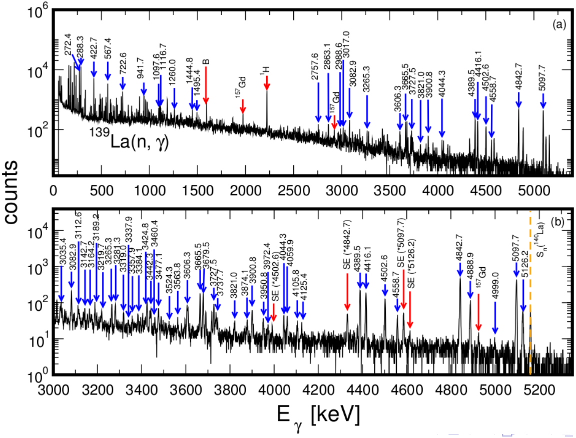
- ^{139}La is abundant fission product with significant cumulative yield from thermal- and fast-n fission of ^{233,235}U and fast-n fission of ^{239}Pu.
- Neutron-capture cross sections for ^{139}La provide useful ingredient for nuclear-reactor fuel-related applications.

BASIC SCIENCE

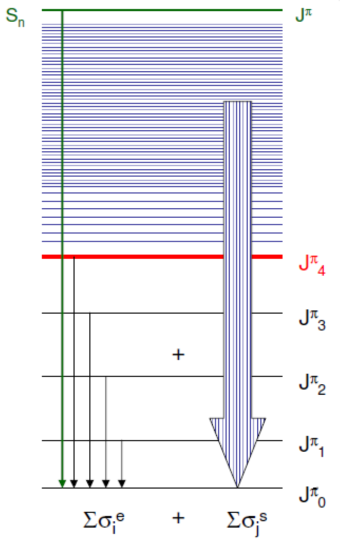
- $^{139}\text{La}(n,\gamma)$ reaction to probe statistical properties of nuclei near $N = 82$ shell closure.
- Assess decay-scheme nuclear structure information for the compound nucleus ^{140}La.

Prompt γ-ray energy spectra: $^{139}\mathrm{La}(n, \gamma)$

- La_2O_3: $T_{IRR} = 2.7$ h; $\phi \approx 2.3 \times 10^6$ n/cm^2/s (thermal).
- extract partial γ-ray cross sections $\sigma_\gamma(E_\gamma)$

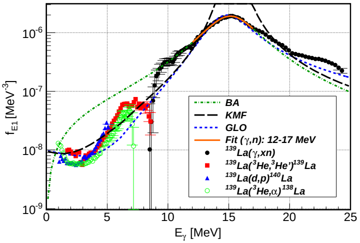


Simulation of the γ-decay cascade



- Monte Carlo approach
- Generate (n, γ) decay scheme simulations originating at S_n
- All levels and γ rays below E_c are taken from experiment
- All levels and γ rays above E_c are randomly generated
- Primary γ rays from experiment when known
- Adopted photon strength function (PSF) and level density (LD) models to calculate simulated level-feedings and compare to experimental data

Model assessment

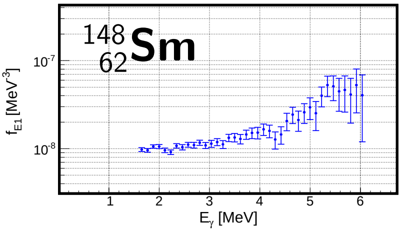


- PSF constrained by high-energy (γ, n) data (Giant Dipole Electric Resonance).
- **BA**: Brink-Axel
  GLO: Generalized Lorentzian
  KMF: Kadmenski-Markushev-Furman
- BA, GLO describe (γ, n) data rather well.
- GLO, KMF describe low-energy Oslo-type data rather well.

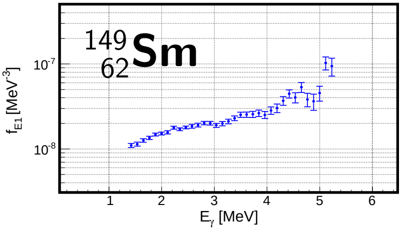
- Assess PSF systematics approaching $N = 82$ shell closure.
- PSF for ^{140}La ($N = 83$) is best described using models that "flatten out" as $E_\gamma \to 0$.

PSF in nuclei near $N = 82$

Siem *et al.*, Phys. Rev C **65**, 044318 (2002)



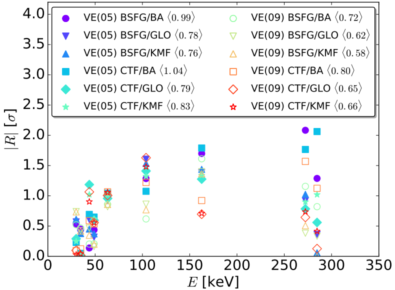
- ^{148}Sm ($N = 86$; $\beta_2 = 0.16$)
- $E_\gamma \to 0$: $f_{E1}(E_\gamma) \to\sim$ const
- cf. $^{138-140}$La ($N = 81 - 83$; $|\beta_2| \leq 0.045$), ^{144}Nd ($N = 84$; $\beta_2 = 0$)



- ^{149}Sm ($N = 87$; $\beta_2 = 0.18$)
- $E_\gamma \to 0$: $f_{E1}(E_\gamma)$ differs from ^{148}Sm
- Addition of 1 particle $\Rightarrow$ pronounced change in PSF

PSF informs nuclear shape?

Simulated level populations in ^{140}La

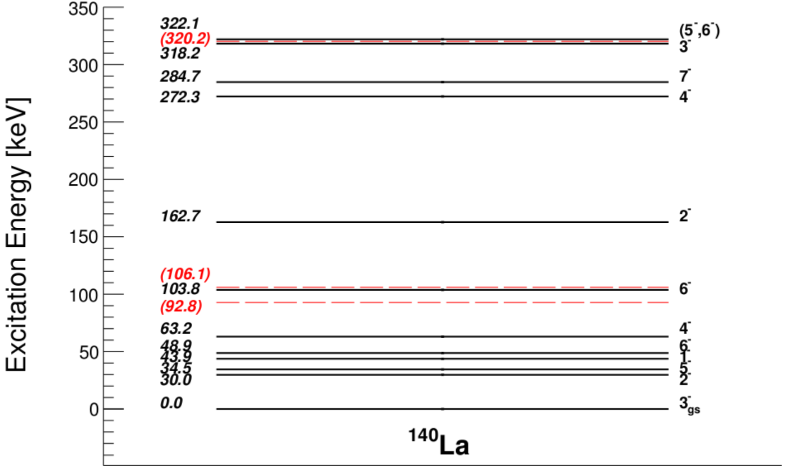


- Fair treatment requires assessment of PSF + Nuclear Level Density (NLD) model combinations.
- Residuals indicate all levels below E_{crit} adequately reproduced by all PSF + NLD model combinations.
- Only model combinations with $|R| > 2\sigma$ invoke BA PSF.
- Adopted width $\Gamma_0 = 50(2)$ meV: Combinations invoking KMF and GLO (+ nuclear level density) generate $\langle \Gamma_0 \rangle$ within 2-σ.
- All PSF+NLD combinations yield statistically-consistent ground-state feeding (P_0).

Average total radiative-capture cross section $\sigma_0 = 9.36(74)$ b

Low-lying levels in ^{140}La (compound nucleus)

Partial decay scheme from ENSDF for $E_L < 350$ keV



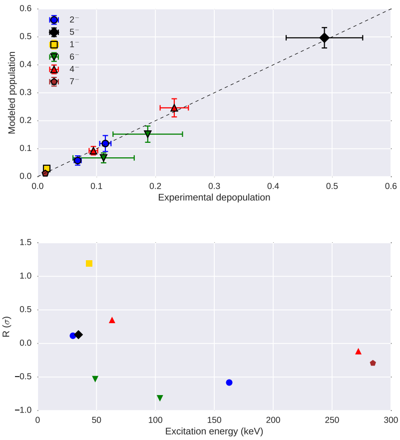
Interpretation of ^{140}La low-lying levels

- Below excitation energy $E_L \lesssim 600$ keV in ^{140}La: single-particle states.
- Orbitals near Fermi surface: $\pi(1g_{7/2})$ and $\pi(2d_{5/2})$ quasiprotons coupling with $\nu(2f_{7/2})$ quasineutrons [and to a lesser extent $\nu(3p_{3/2})$]:

$$|\pi(1g_{7/2}) \otimes \nu(2f_{7/2}); J^{\pi} = 0^-, 1^-, 2^-, 3^-, 4^-, 5^-, 6^-, 7^-\rangle,$$
$$|\pi(2d_{5/2}) \otimes \nu(2f_{7/2}); J^{\pi} = 1^-, 2^-, 3^-, 4^-, 5^-, 6^-\rangle.$$

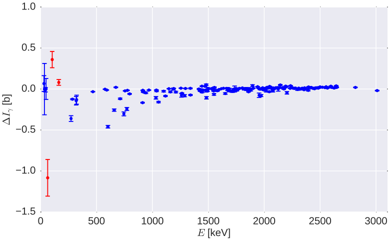
- 14 levels expected based on above configurations with mixed and pure state vectors.
- Can we interpret known decay scheme based on above multiplet of states?

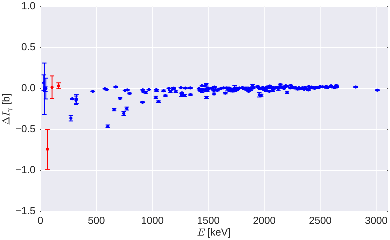
^{139}La(n,γ): Statistical-model analysis using ENSDF data



- Measured σ_γ taken from ^{139}La(n,γ) and are consistent with I_γ (branching ratios) from the Evaluated Nuclear Structure Data File (ENSDF).
- Internal conversion (α), mixing ratios (δ_γ) and spin-parity (J^π) data taken from ENSDF.
- Compare calculated population of levels to experimental data.
- Residuals show good agreement implying well-characterized decay scheme for $E_c = 285$ keV?

^{139}La(n,γ): γ-ray intensity balance for ^{140}La



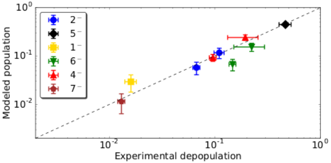


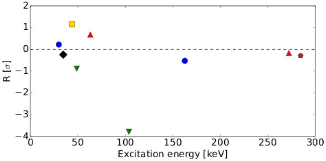
- γ-ray intensity balance for *all* levels decay scheme:

$$\Delta I_\gamma = \sum_{i=1}^{M} I_{\gamma_i}(\mathrm{in}) - \sum_{j=1}^{N} I_{\gamma_j}(\mathrm{out})$$

- Condition: $\sum_{j=1}^{N} I_{\gamma_j}(\mathrm{out}) \geq \sum_{i=1}^{M} I_{\gamma_i}(\mathrm{in})$
- Upper plot: ENSDF data for α and δ_γ
- Lower plot: α and δ_γ optimized according to measured I_γ from ^{139}La(n,γ)

Statistical-model analysis using optimized γ-decay data

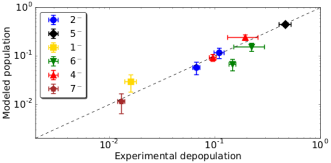


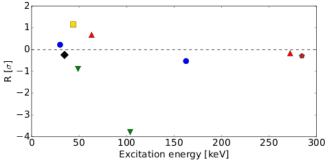


ENSDF:

$J^{\pi}(E_L = 103.8) = 6^{-}$

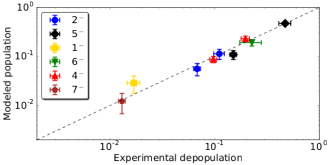
Statistical-model analysis using optimized γ-decay data

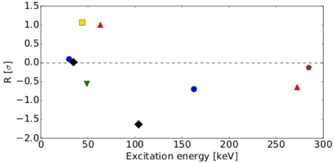




ENSDF:

$$J^{\pi}(E_L = 103.8) = 6^{-}$$





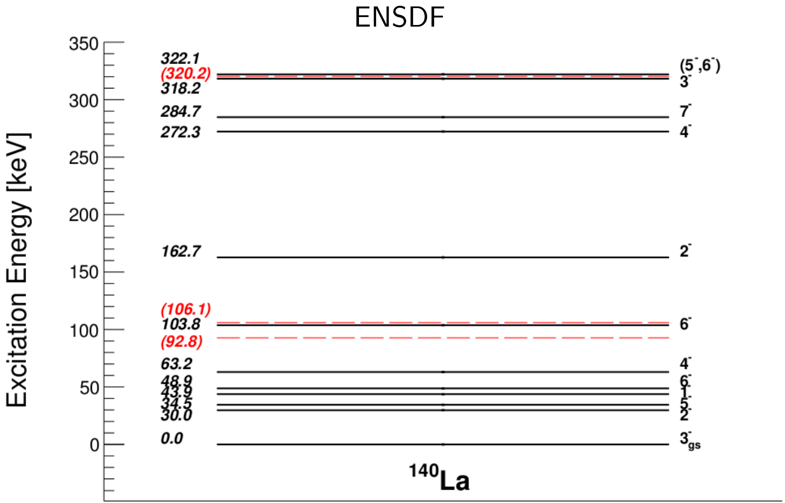
^{139}La(n,γ):

$$J^{\pi}(E_L = 103.8) = \mathbf{5}^{-}$$

Changes to ^{140}La decay scheme

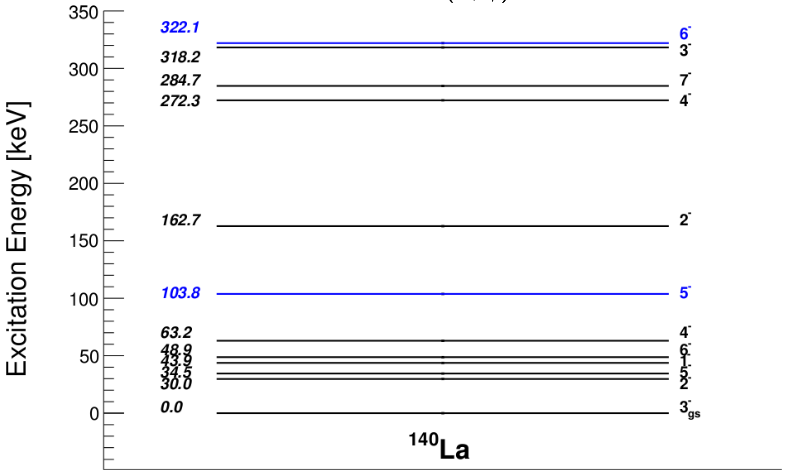
- New $J^{\pi} = 5^{-}$ for $E_L = 103.8$ keV [previously $J^{\pi} = 6^{-}$] from statistical-model analysis.
- New $J^{\pi} = 6^{-}$ for $E_L = 322.1$ keV [previously $J^{\pi} = (5^{-}, 6^{-})$] from expected multiplet of states.
- 322.1-keV $J^{\pi} = 6^{-}$ level $\Rightarrow$ pure $\pi(2d_{5/2}) \otimes \nu(2f_{7/2})$ configuration.
- α and δ_{γ} optimized according to ΔI_{γ} balance for low-lying γ-ray transitions.
- No evidence for tentative ENSDF-reported levels at (92.8), (106.1), and (320.2) keV.
- Physical Review C **99**, 024310 (2019).

Properties of the ^{140}La low-lying levels

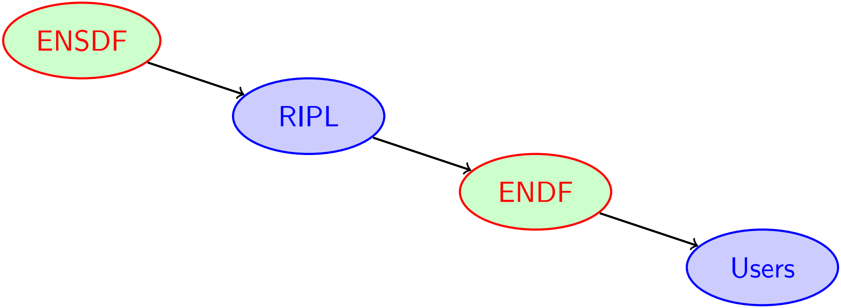


Properties of the ^{140}La low-lying levels

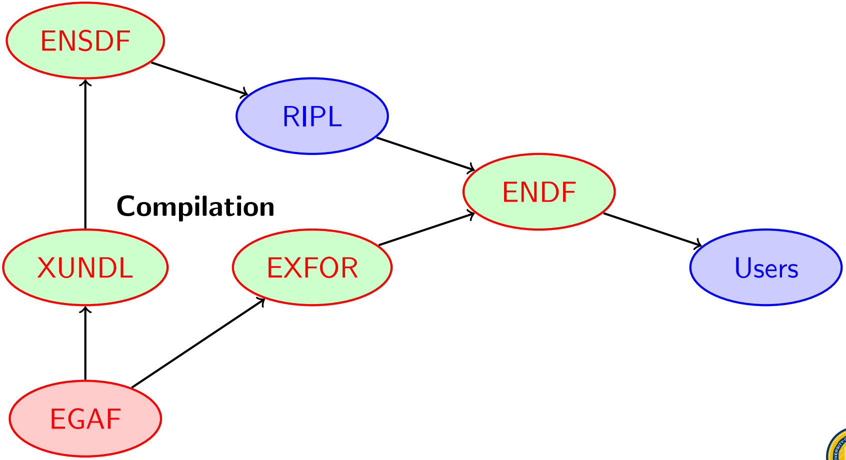
EGAF: $^{139}\mathrm{La}(n,\gamma)$



Augmentation of the nuclear data libraries



Augmentation of the nuclear data libraries



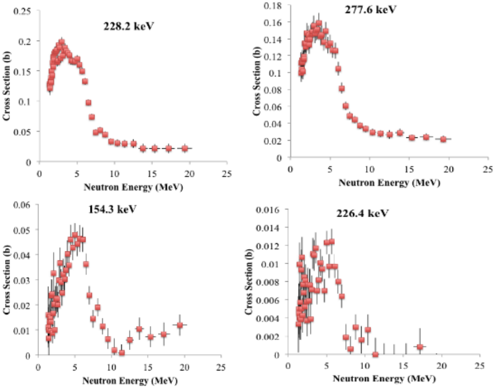
The Baghdad Atlas

Inelastic $(n, n'\gamma)$ reactions

- Radiative-capture (n, γ) reactions provide diagnostic for NDA applications
- But is it the most useful γ-ray signature?
- $\sigma_{(n,\gamma)}(E_n = \text{thermal})$ is high; $\sigma_{(n,\gamma)}(E_n > \text{thermal})$ is small
- Can we learn anything from high-energy neutrons?
- Other reaction channels are open
- (n, n') is primary energy-loss mechanism for fast neutrons in heavy nuclei $\Rightarrow$ look for $(n, n'\gamma)$ signatures in NDA

Improved $(n, n'\gamma)$ data needed for accurate simulations of interrogation systems [NDNCA Workshop, LBNL (2015)]

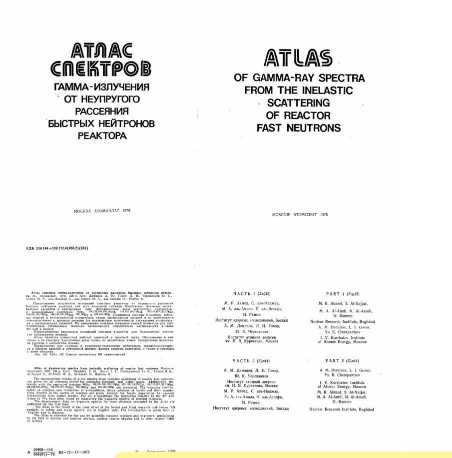
Current status



^{239}Pu$(n, n'\gamma)$ yeilds measured at LANL, but focus was ^{239}Pu$(n, 2n)$: L. A. Bernstein *et al.*, PRC **65**, 021601 (R) (2002); (EXFOR 2015)

- Available data are *scattered* amongst published literature
- LANL, GELINA, Ohio, Kentucky (structure)
- **G**amma **E**nergy **N**eutron **E**nergy **S**pectrometer for **I**nelastic **S**cattering (GENESIS) @ 88" Cyclotron LBNL

"The Baghdad Atlas": Fast neutron γ-ray data from (n, n')


АТЛАС СПЕКТРОВ
ГАММА-ИЗЛУЧЕНИЯ ОТ НЕУПРУГОГО РАССЕЯНИЯ БЫСТРЫХ НЕЙТРОНОВ РЕАКТОРА

МОСКВА АТОМИЗДАТ 1978

ATLAS
OF GAMMA-RAY SPECTRA FROM THE INELASTIC SCATTERING OF REACTOR FAST NEUTRONS

MOSCOW ATOMIZDAT 1978

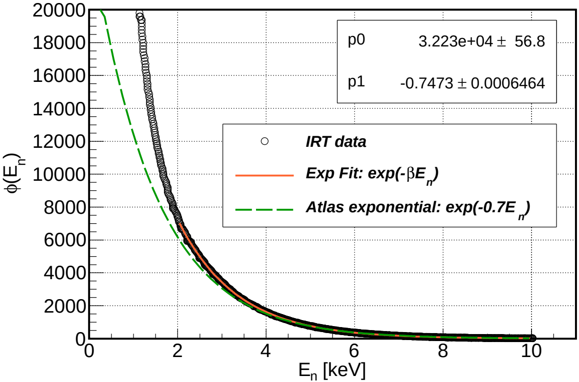
- Compilation of energy-integrated inelastic neutron-scattering $(n, n'\gamma)$ data disseminated in book format
- ~ 7000 γ rays (E_γ and BR) from 105 samples: 76 natural and 29 isotopically-enriched targets
- Set of consistent measurements performed under identical conditions
- Ge(Li) viewing filtered fast-neutron beam line at the IRT-5000 Reactor: NRI, Baghdad, Iraq

Trkov (IAEA) $\Rightarrow$ Firestone (LBNL) $\Rightarrow$ Sleaford (LLNL)

The IRT-5000 Reactor

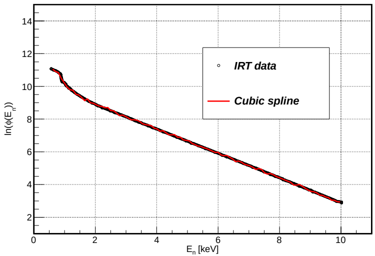
No longer accepting beam-time proposals

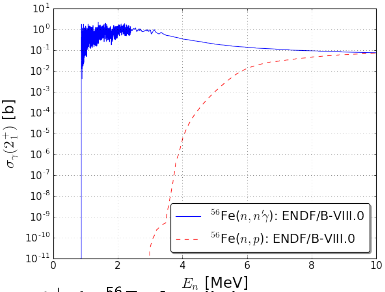
The IRT-5000 Reactor flux



$$\phi(E_n) \propto \exp(\beta E_n); \quad \forall E_n \gtrsim 1.5 \text{ MeV}$$

The Baghdad Atlas: $(n, n'\gamma)$ data

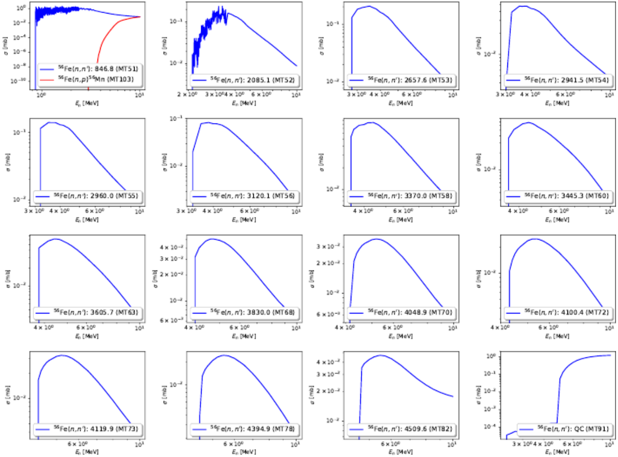




- Extract $\sigma_\gamma(E_\gamma)$ relative to 847-keV $2^+_1 \to 0^+_{\rm gs}$ in ^{56}Fe for all data sets.
- Convolve IRT-500 spectrum ^{56}Fe$(n, n'\gamma_{847})$ from ENDF-B/VIII.0:

$$\langle \sigma_\gamma \rangle = \frac{\int_{E_n=0}^{E_n=10} \phi(E_n)\sigma_\gamma(E_n)dE_n}{\int_{E_n=0}^{E_n=10} \phi(E_n)dE_n} \equiv \frac{\sum_{k=0}^{N} \phi(E_n)\sigma_\gamma(E_n)\Delta E_n}{\sum_{k=0}^{N} \phi(E_n)\Delta E_n}.$$

Direct and indirect feeding of the ^{56}Fe 2_1^+ state



Flux-weighted $\langle \sigma_\gamma \rangle = 979(13)$ mb

Development of relational database I

http://nucleardata.berkeley.edu

- Serves applications community (nonproliferation, NDA)
- Nuclear data evaluation: benchmarking reaction models in fast-fission neutron-energy range
- Limited use $\Rightarrow$ data *was* only available in printed form
- Data now compiled into a set of CSV-style ASCII tables
- Developed suite of Python scripts and C modules to build SQLite relational database
- Downloadable software platform hosted at:
  National Nuclear Data Center (NNDC)
  http://www.nndc.bnl.gov/lbnlatl.html
  Nuclear Science and Security Consortium (NSSC)
  http://nssc.berkeley.edu/research/nuclear-data/atlas/

Development of relational database II

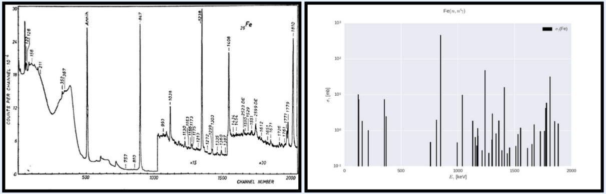
http://nucleardata.berkeley.edu

Motivation Introduction Installation Schema Data access Cross sections Download

Atlas of Gamma-Ray Spectra from the Inelastic Scattering of Reactor Fast Neutrons

[A.M. Demidov *et al.*, Nuclear Research Institute, Baghdad, Iraq (Moscow, Atomizdat 1978)]

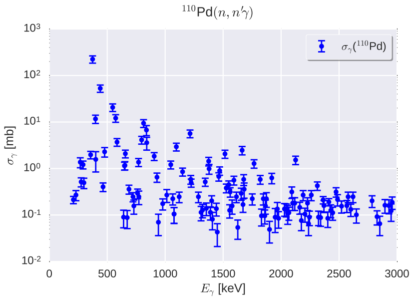
Measured ^{nat}Fe(n,$n'\gamma$) spectrum cf. γ-ray energy spectrum retrieved from SQL database query

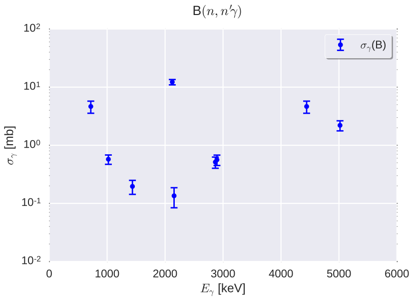


Aaron Hurst <amhurst@berkeley.edu>

Department of Nuclear Engineering, University of California, Berkeley

Jupyter Notebook: Automating cross-section calculations





Enriched ^{110}Pd

- `Z = int(46)`
- `A = int(110)`
- `Chem_symb=str(‘‘110Pd’’)`

Natural B

- `Z = int(5)`
- `A = int(0)`
- `Chem_symb = str(‘‘B’’)`

A short demonstration

Acknowledgments

- **UC Berkeley** – J. C. Batchelder, L. A. Bernstein, R. B. Firestone, A. M. Hurst, J. Vujic
- **LBNL** – M. S. Basunia, L. A. Bernstein

Tarball contents

- Approach: Distribute database to expert user community in as general a form as possible
- Source code to build database locally
- Source CSV-style data sets for all 105 samples
- SQL scripts and Jupyter Notebook provided to exemplify methods for retrieving and interacting with the data
- HTML documentation installation instruction and help pages (offline viewing)
- A PDF of the original book by A. M. Demidov *et al.*
- Total package size: $\sim$ 22 Mb

Installing the Baghdad Atlas

- Linux or Mac OS X only (not Windows)
- Requirements: SQLite3 database engine, The GNU C compiler gcc, Python libraries
- Jupyter Notebook requires Python 2.7 or 3
- More info: nucleardata.berkeley.edu/into.html
- A `Makefile` is provided to automatically detect OS and Python version
- Download in `$HOME` and build:

```
cd ~/BaghdadAtlas/src
make # build C extension-functions library
make run # build the SQLite database
make install # install the library and database
```

- To cleanup any of the C, Python, SQLite artifacts, Notebook objects, or remove database: `make help`
- More info: nucleardata.berkeley.edu/install.html

Terminal-based access

- sqlite3 engine: terminal-based front-end to SQLite libraries
- Evaluate SQL queries interactively (or use batch/shell)

```
amhurst@amhurst-office:sql_codes$ sqlite3 atlas_baghdad_py3.db
SQLite version 3.13.0 2016-05-18 10:57:30
Enter ".help" for usage hints.
sqlite> .header on
sqlite> .mode column
sqlite> SELECT symbol, sample_composition, mass, exposure_time
...> FROM sample
...> WHERE Z >= 30 AND Z <=40;
symbol      sample_composition  mass        exposure_time
----------  ------------------  ----------  -------------
Zn          Zn                  31.5        6.0
Ga          Ga                  15.5        23.0
Ge          Ge                  4.7         44.0
As          As                  22.1        21.0
Se          Se                  24.0        12.9
Br          BrInGlass           32.0        12.0
Rb          Rb2CO3              15.5        23.0
Sr          SrCO3               12.1        9.0
Y           Y_NO3_3_6H2O        28.9        22.0
Zr          ZrO2                42.0        16.1
sqlite>
sqlite>.exit
amhurst@amhurst-office:sql_codes$
```

SQL scripting methods

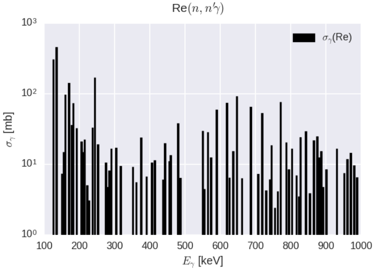
target	sample	compound	E [keV]	dE [keV]	BR	dBR	cross section [mb]	error cs [mb]
Pd	E	110Pd	356.9	0.2	0.88	0.04	1.97471562992	0.361782109365736
Pd	E	110Pd	373.8	0.08	100.0	0.0	224.3995034	39.8261771881664
Pd	E	110Pd	398.8	0.2	5.2	0.5	11.6687741768	2.35536807678854
Pd	E	110Pd	401.0	0.7	0.7	0.3	1.5707965238	0.728640054634137
Pd	E	110Pd	439.76	0.08	23.6	0.3	52.9582828024	9.42305577970604
Pd	E	110Pd	463.9	0.4	0.18	0.02	0.40391910612	0.084576879268378
Pd	E	110Pd	477.5	0.3	1.02	0.15	2.28887493468	0.527559892343483
Pd	E	110Pd	547.04	0.1	9.2	0.5	20.6447543128	3.83194927683448
Pd	E	110Pd	572.89	0.1	5.4	0.3	12.1175731836	2.25351613122552
Pd	E	110Pd	584.48	0.1	1.65	0.1	3.7025918061	0.694390021635276
Pd	E	110Pd	641.0	1.1	0.04	0.015	0.08975980136	0.037239367444231
Pd	E	110Pd	648.51	0.16	0.51	0.04	1.14443746734	0.222062867920516
Pd	E	110Pd	653.1	0.2	0.52	0.05	1.16687741768	0.235536807678854
Pd	E	110Pd	656.42	0.15	0.93	0.06	2.08691538162	0.394096114934713
Pd	E	110Pd	672.4	1.1	0.039	0.015	0.087515806326	0.037070744596919
Pd	E	110Pd	687.7	0.3	0.16	0.02	0.35903920544	0.077940258672717
Pd	E	110Pd	722.5	0.4	0.11	0.015	0.24683945374	0.055246729283649
Pd	E	110Pd	729.9	1.0	0.07	0.02	0.15707965238	0.052833762272471
Pd	E	110Pd	762.2	0.4	0.13	0.02	0.29171935442	0.068518287363096
Pd	E	110Pd	770.3	0.2	0.61	0.05	1.36883697074	0.267597594929364
Pd	E	110Pd	773.0	0.8	0.11	0.03	0.24683945374	0.080319193550216
Pd	E	110Pd	796.83	0.1	1.84	0.12	4.12895086256	0.780711003345544
Pd	E	110Pd	813.52	0.1	4.2	0.3	9.4247791428	1.80308614799129
Pd	E	110Pd	838.5	0.3	3.0	0.5	6.731985102	1.63902116479168
Pd	E	110Pd	840.9	0.7	1.6	0.4	3.5903920544	1.10078609988999
Pd	E	110Pd	905.2	0.2	0.82	0.06	1.84007592788	0.353240503496184
Pd	E	110Pd	929.2	0.3	0.29	0.04	0.65075855986	0.146274153749854
Pd	E	110Pd	941.5	1.2	0.031	0.014	0.069563846054	0.033754810642283
Pd	E	110Pd	978.8	0.5	0.078	0.016	0.175031612652	0.047477253384699

- Useful for complicated queries
- Several SQL scripts provided
- Schema defined in HTML documentation

- Manipulate data in `sample` (normalization) and `nucleus` (γ-ray properties) relational tables
- Convert enriched ^{110}Pd intensities to partial $\sigma_\gamma(n, n'\gamma)$ i.e. calculate relative to $\langle\sigma_\gamma(n, n'\gamma)\rangle$ for $2_1^+ \rightarrow 0_{\rm gs}^+$ in ^{56}Fe
- Condition on γ-ray energies: $300 \leq E_\gamma \leq 1000$ keV
- Display selected variables

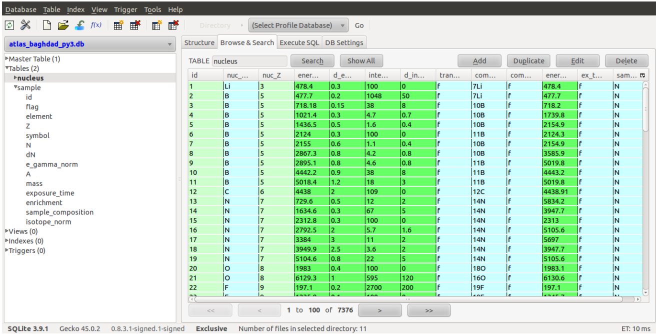
Interaction using the Jupyter Notebook

```
In [7]: f, ax = plt.subplots(figsize=(9,6))

        conn = sqlite3.connect('atlas_baghdad_py3.db')
        curs = conn.cursor()
        sql_cmd = "SELECT energy_gamma, ((nucleus.intensity_gamma/100.0) * sample.N * (468.0/100.0)) \
            AS cross_section FROM nucleus, sample \
            WHERE nuc_Z = 75 \
            AND nucleus.nuc_Z = sample.Z \
            AND nucleus.energy_gamma < 1000.0;"
        curs.execute(sql_cmd)
        db_info = array(curs.fetchall())
        ax.bar(db_info[:,0],db_info[:,1],label=r"$\sigma_{\gamma}$(Re)",color='black',linewidth=3)

        conn.close()
        ax.legend(loc=1)
        ax.set_yscale('log')
        ax.set_xlabel(r'$E_{\gamma}$ [keV]')
        ax.set_ylabel(r'$\sigma_{\gamma}$ [mb]')
        f.suptitle(r"Re$(n,n'\gamma)$")

        plt.show()
        f.savefig("Re_cs_query.pdf",dpi=f.dpi)
        f.savefig("Re_cs_query.png",dpi=f.dpi)
```



- Execute Python code in Jupyter Notebook
- To run sample Notebook provided requires a few additional Python libraries: `numpy`, `sqlite3`, `matplotlib`, `seaborn`
- SQL query: Convert natural rhenium intensities to cross sections for all lines with $E_\gamma < 1000$ keV and plot the results
- Inline visualization
- Share workflow with colleagues

Using GUI to access data



- SQLite Manager add-on for Firefox browser
- Connect to database to browse and view data
- Manipulate data and execute SQL code through GUI