ENSDF-translation efforts at LBNL

Aaron M. Hurst
AMHurst@lbl.gov

Isotopes Project
Lawrence Berkeley National Laboratory

21st Technical Meeting of the Nuclear Structure and Decay Data Network
International Atomic Energy Agency

April 20-24, 2015

Overview

- Python translator: ENSDF-2-RIPL
- Python translator: ENSDF-2-XML
- ENSDF utility codes (PABS): Renormalized particle-decay branches and uncertainties
- SQL Database: Atlas of $(n, n'\gamma)$ data from inelastic scattering of fast reactor neutrons (Baghdad Atlas)

ENSDF-2-RIPL translator

- Motivation: preparing (n, γ) data sets in RIPL format for reaction calculations for NA-22 (nonproliferation) applications
- Historically (n, γ) data sets from the EGAF project were prepared in ENSDF format (still maintained)
- Translator coded in Python
- ENSDF single-card records needed for translation to RIPL format:
  `L` – energy level card (including continuation-`L` records)
  `G` – γ-ray transition card
  `Q` – Q-value card
- RIPL decay schemes now include primary γ rays
- Range of particle-decay modes extended to include: ``%B-A''

ENSDF-2-RIPL representative input: ^{243}Pu 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
```

ENSDF-2-RIPL represenative output: ^{243}Pu 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
```

Parsing issues: continuation-L records

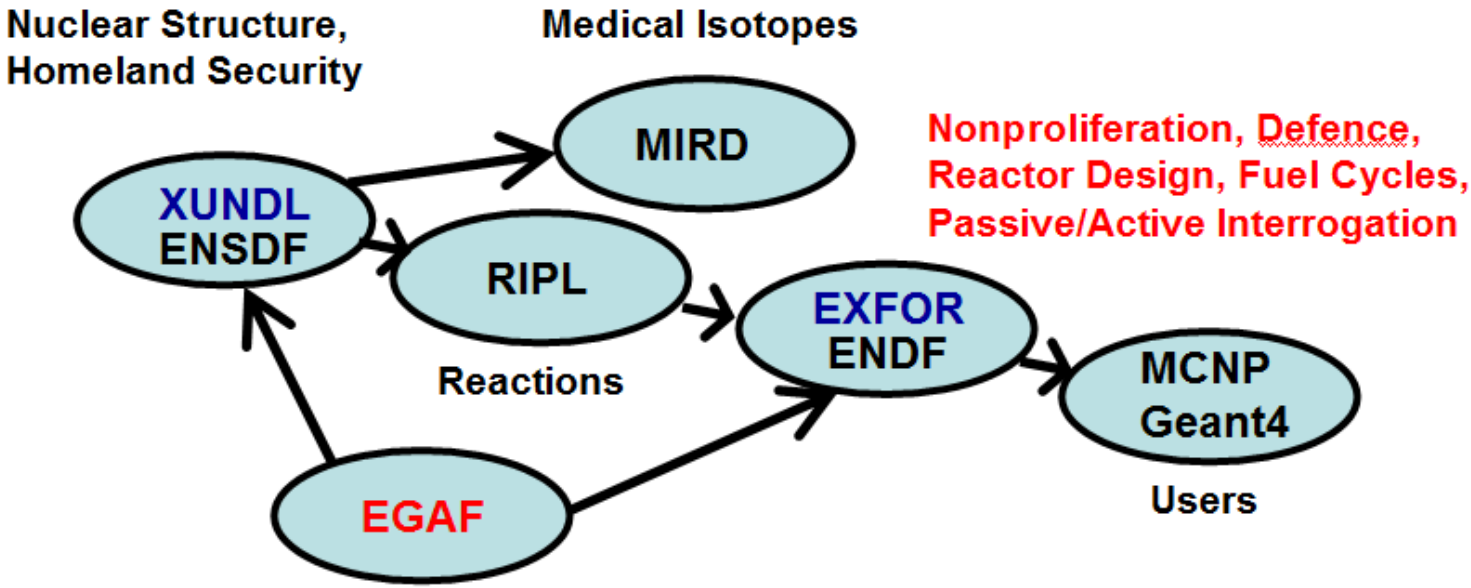
- Effective parsing and interpretation is best served by systematic data entry
- Too much *democracy* in data storage may lead to difficulties in accurately interpreting the correct data
- Fields in continuation ENSDF records are not as rigourously defined (cf. standard single-card records)
- Multiple representations of the same data

```
93RU  L 734.40    10 (1/2-)           10.8 S    3                          M1
93RU2 L %IT=22.0 23$%EC+%B+=78.0 23$ %ECP=0.027 5 (1983Ay01)

93RU  L 734.40    10 (1/2-)           10.8 S    3                          M1
93RU2 L $%IT=22.0 23$%EC+%B+=78.0 23$ %ECP=0.027 5 (1983Ay01)

93RU  L 734.40    10 (1/2-)           10.8 S    3                          M1
93RU2 L %IT=22.0  $%EC+%B+=78.0   $ %ECP=0.027
```

- A systematic representation would make writing parsing applications easier

Nuclear data library development: ENSDF-2-XML translator?

- Many nuclear data libraries serving many applications
- Effort @LLNL to develop Generalized Nuclear Data (GND) format: XML-translated RIPL and ENDF data part of GND
- Inherent synergy between RIPL and ENSDF: Define common nomenclature for variables in RIPL and ENSDF (e.g. E, J^{π}, E_{γ}, etc.)
- Python translator to facilitate ENSDF-2-XML developed @LBNL
- Interpreted numeric ENSDF data (simple CSV) benefit many analyses



ENSDF mixed-record format

- The Identification Record
- The History Record
- The Q-Value Record
- The Cross-Reference Record
- The Comment Record
- The Parent Record
- The Normalization Record
- The Production Normalization Record
- The Level Record
- The Beta (β^-) Record
- The EC (or EC + β^+) Record
- The Alpha Record
- The (Delayed-) Particle Record
- The Gamma Record
- The Reference Record
- *The End Record*

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ENSDF-2-XML translator: A snippet of ^{133}Cs decay scheme

```
<level id="Cs133_e4" index="4">
  <energy value="437.0113" uncertainty="0.0009" unit="keV"/>
  <spin valueString="1/2" valueNumber="0.5" unit="hbar"/>
  <parity value="+"/>
  <halflife value="150" uncertainty="150" unit="ps"/>
  <lifetime value="216" uncertainty="216" unit="ps"/>
  <decay mode="electron capture (or EC + beta^+)">
    <ecEnergy value="None" uncertainty="None" unit="keV"/>
    <betaIntensity value="None" uncertainty="None"/>
    <ecIntensity value="85.4" uncertainty="0.5"/>
    <logft value="6.627" uncertainty="0.018"/>
    <ecBetaTotalIntensity value="None" uncertainty="None"/>
    <coincidence record=" "/>
    <forbiddenness record="allowed"/>
    <placement record="certain"/>
  </decay>
  <decay mode="gamma">
    <energy value="53.1622" uncertainty="0.0006" unit="keV"/>
    <branchingRatio value="3.45" uncertainty="0.05"/>
    <multipolarity value="M1+E2"/>
    <icc value="5.66" uncertainty="0.10"/>
    <mixingRatio value="0.08" upperLimit="+0.02" lowerLimit="-0.03">
      <symMixingRatioMeth1 value="0.075000" uncertainty="0.025000"/>
      <symMixingRatioMeth2 value="0.072021" uncertainty="0.025226"/>
    </mixingRatio>
    <totalIntensity value="22.977" uncertainty="0.47949348275"/>
    <finalLevel>
      <flevel id="Cs133_3" index="3"/>
      <fenergy value="383.8491" unit="keV"/>
    </finalLevel>
  </decay>
  <decay mode="gamma">
    <energy value="276.3989" uncertainty="0.0012" unit="keV"/>
    <branchingRatio value="11.54" uncertainty="0.07"/>
    <multipolarity value="E2"/>
    <icc value="0.0566" uncertainty="0.0000"/>
```

- XML output can be verbose!
- LSD no longer an issue
- Could include derived quantities, e.g. $T_{1/2}$ & τ
- More options for handling asymmetric uncertainties [G. Audi: NUBASE2012]
- Include daughter levels as properties of the γ decay

Information **implicit** in ENSDF $\Rightarrow$ **Explicitly** defined in XML

Spins in ENSDF, RIPL, XML

Representations of the same level in different formats:
$E = 1114.2(2); J^{\pi} = (5/2^{-}, 7/2^{-})$

(1) ENSDF

```
187W    L 1114.2     2   (5/2-,7/2-)
```

(2) XML

```
<level id="W187_e64" index="64">
  <energy value="1114.2" uncertainty="0.2" unit="keV"/>
  <spin valueString="(5/2,7/2)" unit="hbar">
    <altSpin_0 value="5/2" unit="hbar"/>
    <altSpin_1 value="7/2" unit="hbar"/>
  </spin>
  <parity value="-"/>
  <halflife value="None" uncertainty="None" unit="None"/>
  <lifetime value="None" uncertainty="None" unit="None"/>
</level>
```

(3) RIPL

```
 65    1.114200    2.5 -1    0.00E+00   0 1                (5/2-,7/2-)   0
```

- RIPL generally interprets first spin in tentative list: `(5/2-,7/2-)` ⇒ `2.5  -1`
- Preferred J as a systematic comment for RIPL translator? e.g. `JRIPL=7/2-`

ENSDF-2-XML: Outlook

- Stage I: Standard one-card records are systematic (facilitates translation)
- Once XML schema for RIPL is decided upon (LLNL) $\Rightarrow$ finalize translation of standard records and agree upon common nomenclature for variables where appropriate
- Changes are coming!
  Attribute $\Rightarrow$ Subelement (with additional attributes)
  `uncertainty = "..."` $\Rightarrow$
  `<uncertainty value = "..." type = "normal"/>`
- Stage II: Continuation records, somewhat systematic but tricky to handle
- Stage III: How to extract real data from the comments?

Particle-emission probabilities and their uncertainties: PABS

Emission-probability of i^{th} particle group p_I and its corresponding uncertainty dp_I:

$$p_I(\%) = \frac{BI_i}{\sum I_k},$$

$$\frac{dp_I(\%)}{p_I(\%)} = \sqrt{\left(\left(\frac{dI_i}{I_i}\right)^2\left(1 - \frac{2I_i}{\sum I_k}\right) + \frac{\sum dI_k^2}{(\sum I_k)^2} + \left(\frac{dB}{B}\right)^2\right)}$$

$I_i \Rightarrow$ Relative intensity of i^{th} particle group

$B \Rightarrow$ Percentage particle branching

E. Browne, NIM **A249**, 461 (1986); E. Browne, NIM **A265**, 541 (1988)

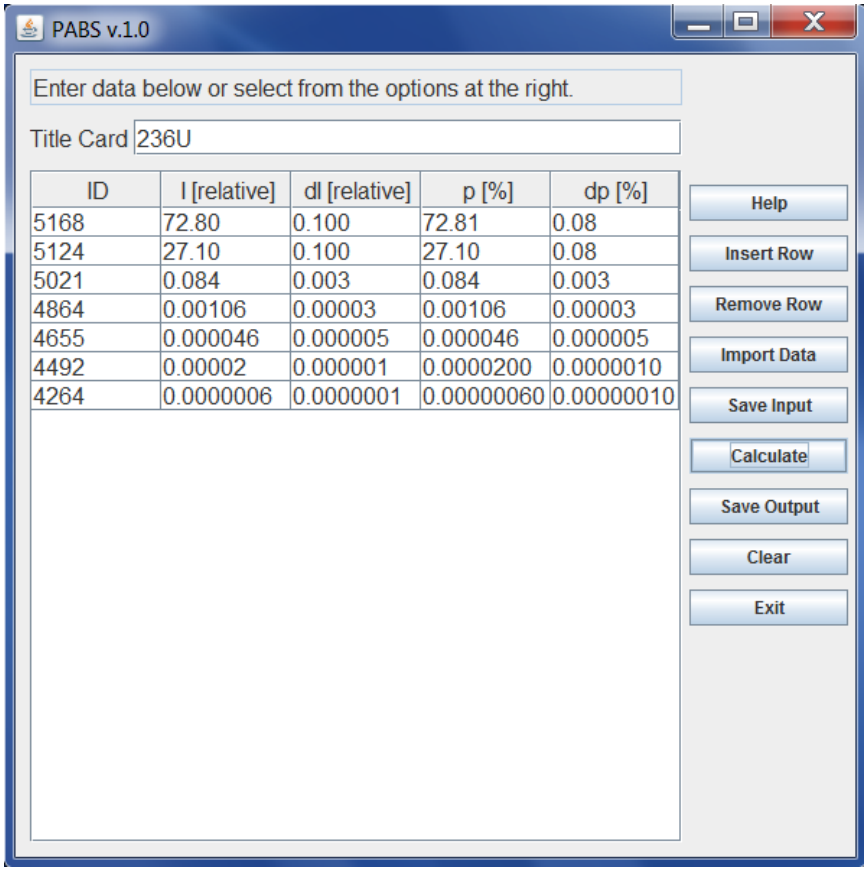
Calculate p_I and dp_I using analysis code PABS

PABS: $^{240}\mathrm{Pu} \rightarrow {}^{236}\mathrm{U} + \alpha$ ($B = 100\%$)

Source ENSDF data set: 236U.ENS

```
236U   L 0            0+
236U   A 5168.17   15 72.8   1  1.00                                        A
236U  cA IA        73.51 {I36} (1977Ba69); 72.8 {I1} (1984Ah06).
236U   L 45.244    2  2+               0.234 NS  6
236U  cL T         from 1960Be25, 1970ToZZ
236U   A 5123.68   23 27.1   1  1.40                                        A
236U  cA IA        26.39 {I21} (1977Ba69); 27.1 {I1} (1984Ah06).
236U   G 45.244    2  0.0447 9 E2                    589
236U S G LC=429 6$MC=118.6 17$NC+=40.7 6
236U S G NC=32.1 5$OC=7.36 11$PC=1.191 17$QC=0.00285 4
236U  cG E         From 1981He16. Others: 45.242 {I6} (1972Sc01); 45.232 {I5}
236U 2cG (1976GuZY); (1958Sa21,1959Tr37,1971GuZY).
236U  cG RI        Weighted average of 0.0453 {I9} (1976GuZY), 0.0435 {I9}
236U 2cG (1981He16), 0.0461 {I14} (1976Um01, 1986LoZT).
236U 3cG L2:L3=1.05 {I5}; M2:M3=1.40 {I5} (1958Sa21)
236U 4cG L2:L3=1.15; M2:M3=1.10 (E2 theory)
236U   L 149.478    7 4+               0.142 NS  10
236U  cL T         (1970ToZZ)
236U   A 5021.23   15 0.084  3  95.9
236U  cA IA        0.096 {I5} (1977Ba69, 1972Sc01); 0.090 {I5} (1984Ah06).
236U   G 104.234   6  0.00714 9E2                   10.99
236U S G LC=8.00 12$MC=2.22 4$NC+=0.764 11
236U S G NC=0.603 9$OC=0.1385 20$PC=0.0227 4$QC=9.41E-5 14
236U  cG E         From 1981He16. Others: 104.233 {I10} (1971GuZY); 104.233 {I5}
236U 3cG (1972Sc01); 104.244 {I5} (1976GuZY).
236U  cG RI$Weighted average of 0.00698 {I14} (1976GuZY, 1986LoZT), and
236U 2cG 0.00718 {I7} (1981He16).
236U   L 309.786    7 6+
236U   A 4863.60   150.00106 3  648.
---  236U.ENS       28% (62,80)    (Fundamental)--------------------------------
```

PABS: a comparison between two analysis codes



- GUI-based code written in Java
- Particle-decay data entered manually
- D. S. Caron, LBNL-2623E (2009)

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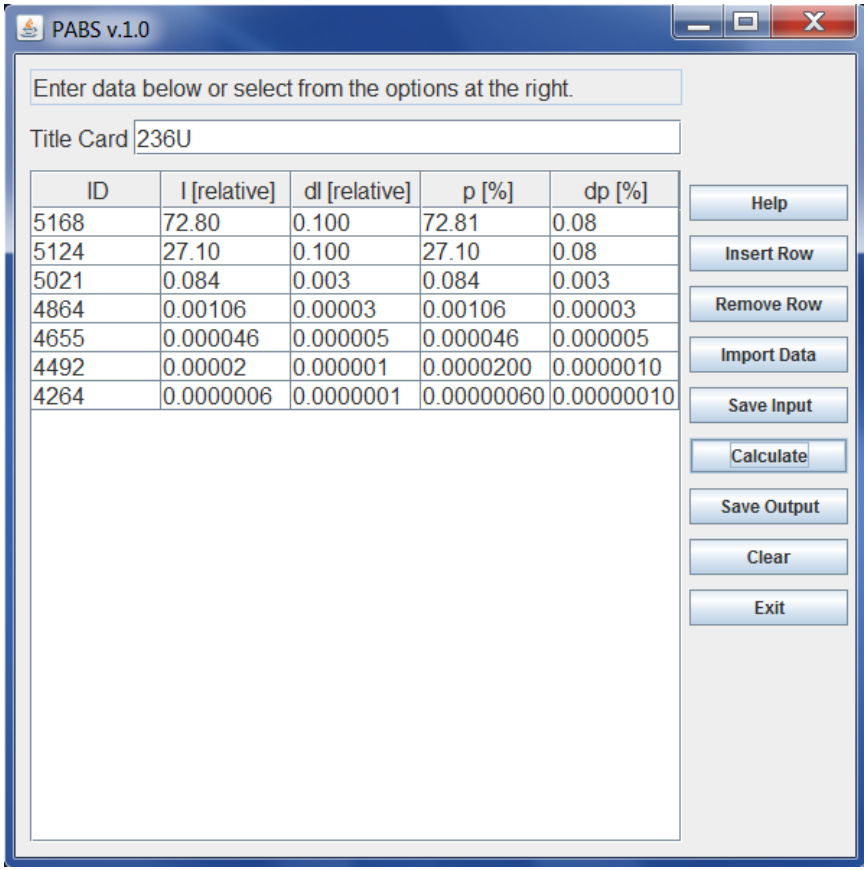

- GUI-based code written in Java
- Particle-decay data entered manually
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```
amhurst@amhurst-office:alpha_decay$ python pabs_i.py
ENSDF file to be read?
236U.ENS
5168.17 0.15    72.8000000      0.1000000       72.8108295      0.0777640
5123.68 0.23    27.1000000      0.1000000       27.1040313      0.0777876
5021.23 0.15    0.0840000       0.0030000       0.0840125       0.0030003
4863.60 0.15    0.0010600       0.0000300       0.0010602       0.0000300
4654.69 0.16    0.0000460       0.0000050       0.0000460       0.0000050
4492.07 0.17    0.0000200       0.0000010       0.0000200       0.0000010
4264.38 0.21    0.0000006       0.0000001       0.0000006       0.0000001
amhurst@amhurst-office:alpha_decay$
```

- Coded in Python (pyPABSi)
- Reads ENSDF file directly
- *No manual data entry required*
- Results consistent with earlier Java code PABS

PABS II: Particle-emission probabilities from γ decay

Emission-probability to l^{th} level p_l and its corresponding uncertainty dp_l:

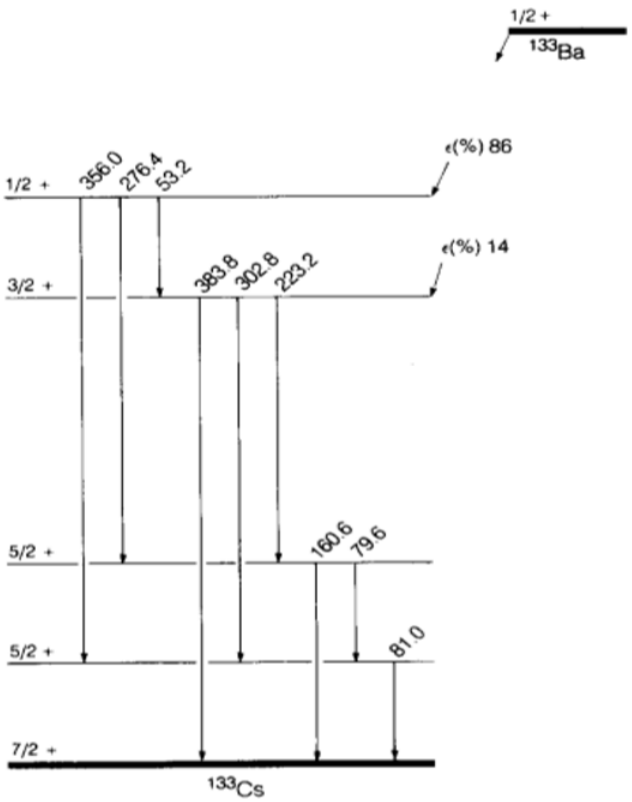
$$p_l(\%) = BG\frac{\sum T_{lf} - \sum T_{il}}{\sum T_{jg}},$$

$$dp_l^2 = \left(\frac{BG}{\sum T_{jg}}\right)^2 \left[\sum dT_{il}^2 + \sum dT_{lf}^2(1-\delta_{fg}) + \left(1-\frac{p_l}{BG}\right)^2 \sum dT_{lg}^2 \right.$$
$$\left. \left(\frac{p_l}{BG}\right)^2 \sum dT_{jg}^2(1-\delta_{jl})\right] + p_l^2\left(\frac{dG}{G}\right)^2 + p_l^2\left(\frac{dB}{B}\right)^2$$

$T \Rightarrow$ conversion-corrected γ-ray intensity
$B \Rightarrow$ Percentage particle-emission of parent nucleus
$G \Rightarrow$ Fraction of particle decay which does not populate g.s. in daughter
(i.e. $G = 1$ for population of excited states exclusively)

E. Browne, NIM **A265**, 541 (1988)

PABS II: $^{133}Ba + \epsilon \rightarrow {}^{133}Cs$



E. Browne / Uncertainties of particle emission probabilities 547

Table 2
γ-rays from ^{133}Ba electron capture decay

γ-ray energy [keV]	Photon intensity (I_γ, relative)	Transition intensity [a] $T = I_\gamma(1+\alpha)$
53.161	2.179 ± 0.022	15.25 ± 0.67
79.62	2.62 ± 0.06	7.07 ± 0.19
80.997	34.06 ± 0.27	89.6 ± 2.2
160.61	0.645 ± 0.008	0.836 ± 0.011
223.23	0.450 ± 0.004	0.494 ± 0.004
276.398	7.164 ± 0.022	7.57 ± 0.03
302.853	18.33 ± 0.06	19.13 ± 0.07
356.017	62.05 ± 0.19	63.6 ± 0.2
383.851	8.94 ± 0.03	9.12 ± 0.03

[a] Conversion coefficients (α) are theoretical values from ref. [4], with 3% uncertainty assumed for pure multipolarities.

- $\epsilon_{384}(\%) = 14 \pm 0.67$
- $\epsilon_{437}(\%) = 86 \pm 0.67$
- E. Browne, NIM **A265**, 541 (1988)

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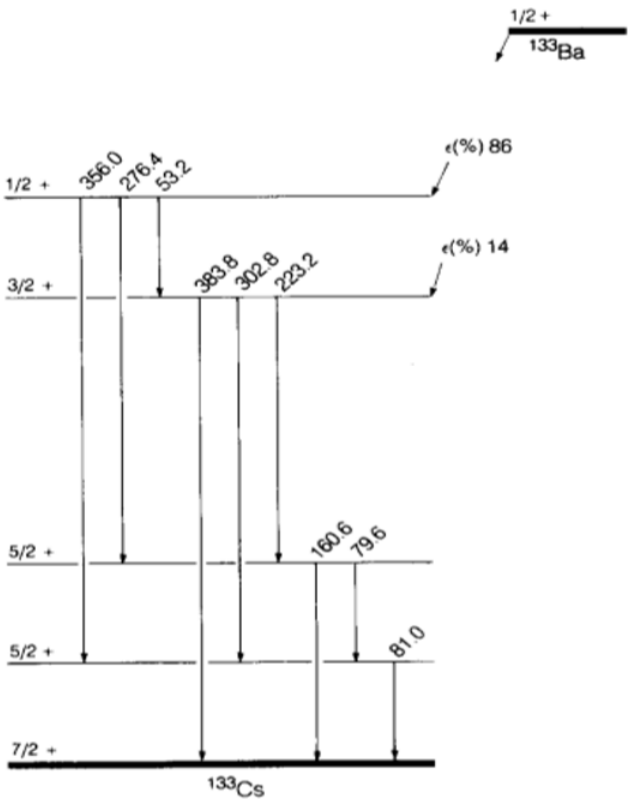

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pyPABSii:

```
amhurst@amhurst-office:indirect_feeding$ python pabs_ii.py
ENSDF file to be read?
133CS.ENS

sum g.s. feeding: 99.5560
sum PNF->PF feeding: 99.9140

Level index 3: p = 13.5056 % dp = +/- 0.67437306 %
Level index 4: p = 86.4944 % dp = +/- 0.67437306 %
amhurst@amhurst-office:indirect_feeding$
```

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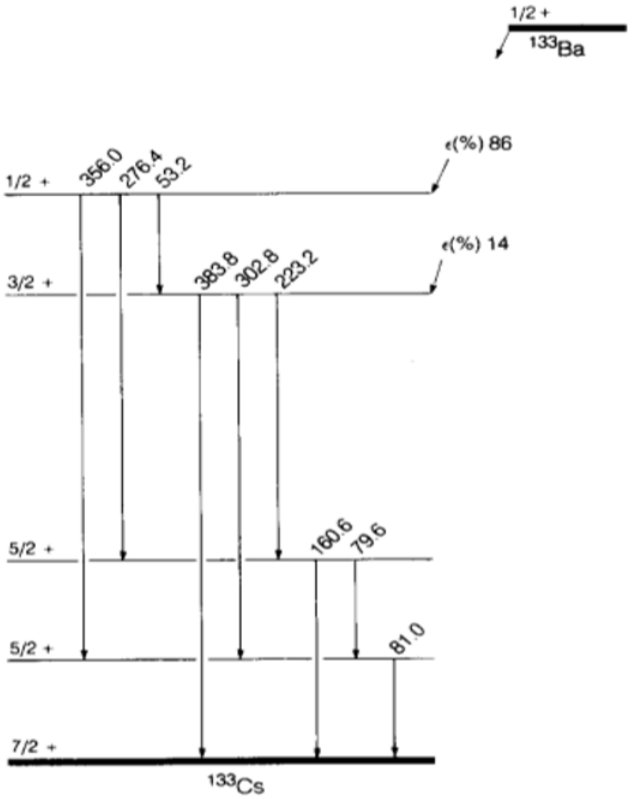

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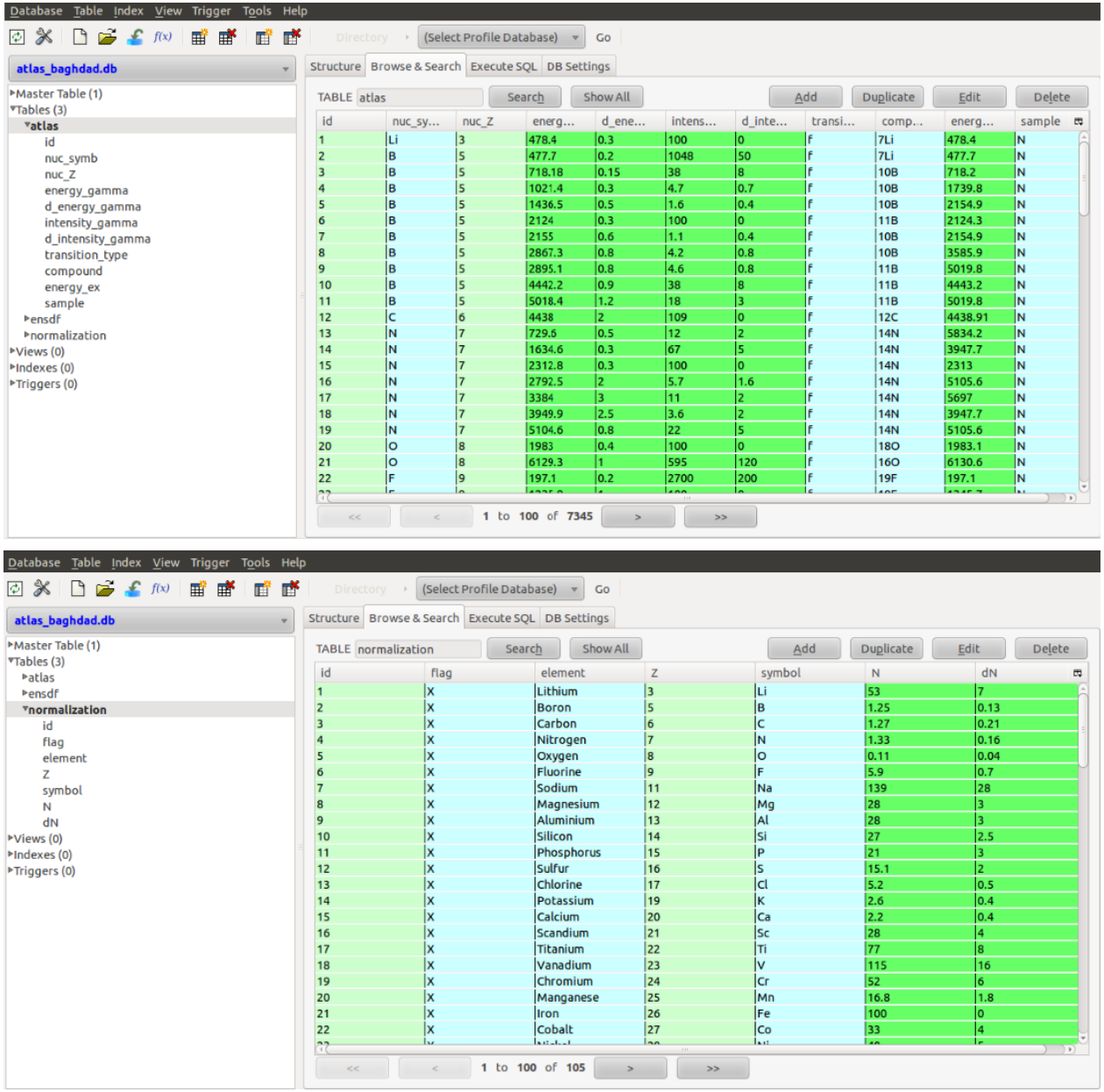
E [keV]	ϵ(GTOL) [%]	ϵ(PABS II) [%]
384	14.5 ± 0.4	14.502 ± 0.247
437	85.4 ± 0.5	85.498 ± 0.247

SQL Schema for $(n, n'\gamma)$ data from Baghdad Atlas

```
CREATE TABLE atlas (id INTEGER PRIMARY KEY,
        nuc_symb CHAR(2), /* target elemental symbol */
        nuc_Z INTEGER, /* atomic number */
        energy_gamma FLOAT, /* gamma-ray energy */
        d_energy_gamma FLOAT, /* uncertainty: gamma-ray energy */
        intensity_gamma FLOAT, /* gamma-ray intensity */
        d_intensity_gamma FLOAT, /* uncertainty gamma-ray intensity */
        transition_type CHAR(1), /* transition flag */
        compound CHAR(16), /* excited compound nucleus */
        energy_ex FLOAT, /* excitation energy */
        sample CHAR(1) /* flag: natural (N) or enriched (E) target */ );
CREATE TABLE ensdf (id INTEGER PRIMARY KEY,
        nucleus VARCHAR(8), /* nucleus ID */
        symbol VARCHAR(2), /* elemental symbol */
        A INTEGER, /* atomic mass */
        Z INTEGER, /* atomic number */
        energy_level FLOAT, /* excitation energy */
        d_energy_level FLOAT, /* uncertainty: excitation energy */
        energy_level_id INTEGER, /* parent energy level ID */
        spin_parity TEXT, /* spin-parity of parent level */
        gamma_energy FLOAT, /* deexcitation gamma-ray energy */
        d_gamma_energy FLOAT, /* uncertainty: deexcitation gamma-ray energy */
        BR FLOAT, /* gamma-ray branching ratio */
        dBR FLOAT /* uncertainty: gamma-ray branching ratio */ );
CREATE TABLE normalization (id INTEGER PRIMARY KEY,
        flag CHAR(1), /* header flag */
        element TEXT, /* Name of elemental/isotopic sample */
        Z INTEGER, /* atomic number */
        symbol TEXT, /* target elemental symbol */
        N FLOAT, /* cross-section normalization factor */
        dN FLOAT /* uncertainty: cross-section normalization factor */ );
```

- A **S**tructured **Q**uery **L**anguage format spectroscopic $(n, n'\gamma)$ data
- Data retrieval using 3 relational tables in current construct: `atlas`; `ensdf`; `normalization`

Visualization of data in SQL



- 105 data sets:
  76 natural;
  29 enriched
- Over 7000 γ lines in database
- `TABLE atlas`
  completely populated for all samples
  (E_γ, I_γ, E_{ex})
- `TABLE normalization`
  completely populated for all samples
  ($N \Rightarrow \sigma_\gamma$)

Querying the database

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	0.944019648	0.172460592992611
Pd	E	110Pd	373.8	0.08	100.0	0.0	107.27496	18.9814874907528
Pd	E	110Pd	398.8	0.2	5.2	0.5	5.57829792	1.12336132006618
Pd	E	110Pd	401.0	0.7	0.7	0.3	0.75092472	0.348174955859454
Pd	E	110Pd	439.76	0.08	23.6	0.3	25.31689056	4.49117641358686
Pd	E	110Pd	463.9	0.4	0.18	0.02	0.193094928	0.040344498162347
Pd	E	110Pd	477.5	0.3	1.02	0.15	1.094204592	0.251750073340714
Pd	E	110Pd	547.04	0.1	9.2	0.5	9.86929632	1.82681433414117
Pd	E	110Pd	572.89	0.1	5.4	0.3	5.79284784	1.07433557076616
Pd	E	110Pd	584.48	0.1	1.65	0.1	1.77003684	0.331057002919737
Pd	E	110Pd	641.0	1.1	0.04	0.015	0.042909984	0.017792572389775
Pd	E	110Pd	648.51	0.16	0.51	0.04	0.547102296	0.105889509617127
Pd	E	110Pd	653.1	0.2	0.52	0.05	0.557829792	0.112336132006618
Pd	E	110Pd	656.42	0.15	0.93	0.06	0.997657128	0.18789605156465
Pd	E	110Pd	672.4	1.1	0.039	0.015	0.0418372344	0.017712404890167
Pd	E	110Pd	687.7	0.3	0.16	0.02	0.171639936	0.037184360451213
Pd	E	110Pd	722.5	0.4	0.11	0.015	0.118002456	0.026360715904069
Pd	E	110Pd	729.9	1.0	0.07	0.02	0.075092472	0.025236127807713
Pd	E	110Pd	762.2	0.4	0.13	0.02	0.139457448	0.032698904990246
Pd	E	110Pd	770.3	0.2	0.61	0.05	0.654377256	0.127607310508747
Pd	E	110Pd	773.0	0.8	0.11	0.03	0.118002456	0.038362374058153
Pd	E	110Pd	796.83	0.1	1.84	0.12	1.973859264	0.372227763547894
Pd	E	110Pd	813.52	0.1	4.2	0.3	4.50554832	0.859729566441032
Pd	E	110Pd	838.5	0.3	3.0	0.5	3.2182488	0.782281986690531
Pd	E	110Pd	840.9	0.7	1.6	0.4	1.71639936	0.525702074118599
Pd	E	110Pd	905.2	0.2	0.82	0.06	0.879654672	0.168431622615454
Pd	E	110Pd	941.5	1.2	0.031	0.014	0.0332552376	0.016130086887437
Pd	E	110Pd	978.8	0.5	0.078	0.016	0.0836744688	0.022667317671123

- Query `atlas` and `normalization` relational tables
- Retrieve $\sigma_\gamma(n, n'\gamma)$ in enriched (`E`) ^{110}Pd (`compound`)
- $\sigma_\gamma(n, n'\gamma)$ relative to $2_1^+ \rightarrow 0_{gs}^+$ in ^{56}Fe ($\sigma_\gamma(846.78 - \mathrm{keV}) = 468$ mb)
- $300 \leq E_\gamma(\mathrm{keV}) \leq 1000$

Acknowledgments

M. S. Basunia[1], L. A. Bernstein[1,2,3], E. Browne[4], R. B. Firestone[1,3], A. M. Hurst[1], B. W. Sleaford[2]

(1) Lawrence Berkeley National Laboratory
(2) Lawrence Livermore National Laboratory
(3) University of California, Berkeley
(4) Brookhaven National Laboratory