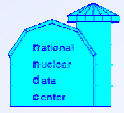
Implementation of Band-Raman Internal Conversion Coefficients (BRICC)

Presentation for the USNDP 2003 Meeting
November 6-7, 2003

Thomas W. Burrows

Brookhaven Science Associates
U.S. Department of Energy



BROOKHAVEN
NATIONAL LABORATORY

BRICC - 1

- Completed
  - PERL script to convert table to BRICCSEQ.DAT. Similar format to ICCSEQ.DAT
    - Upper limit of 2000 keV instead of 1500 keV
    - Extended to include E5 and M5 transitions
    - More shells, subshells, and total ICC
    - Includes electron binding energies
  - Comparison of BRICCSEQ.DAT and ICCSEQ.DAT
    - ICCSEQ.DAT includes Z=3 and 6 – Not used by HSICC
    - ICCSEQ.DAT extends to 6000 keV for $Z \leq 30$ – Not used by HSICC
    - Except for K, L1, and N+ shells, ICCSEQ.DAT generally extends to lower energies – Discussed this with Raman.

BRICC – 2

Comparison of E_γ Thresholds for Thorium

Z=90	BRICC		HSICC
	E_γ(ICC)	BE	E_γ(ICC)
L1	21.00	20.480	21.47
L2	21.00	19.700	20.69
L3	21.00	16.300	17.30
M1	21.00	5.185	6.18
M2	21.00	4.833	5.83
M3	21.00	4.049	5.05
M4	21.00	3.494	4.49
M5	21.00	3.335	4.33
N1-N7	21.00	0.338-1.330	50.00

BRICC – 3

Low-energy γ's with α's for Th Isotopes in NuDat

Nuclide	E_γ	Mult.	α_{total}
^{227}Th	9.3 *1*	(E2)	334000.0
^{227}Th	15.2 *2*	[M1+E2]	≈12000.0
^{228}Th	18.4	[E1]	6.6

BRICC - 4

- BLDBRT.FOR — Constructs direct access index and table files. Similar to BLDHST.FOR
  - Index also includes electron binding energies
  - Table includes E5 and M5 transitions, more shells and subshells, and total ICC
- SEQBRT. FOR — Recreates BRICCSEQ.DAT from direct access files.
- Subprogram package to calculate population fraction for valence electron subshells.
  - ≈ 89 out of 117 Z's have one or more unfilled subshells
  - May allow calculations for bound-state β^- decay??
- Subroutine to fill the arrays for internal conversion coefficients.

BRICC - 5

- In progress or to be done
  - Cubic spline fitting and other calculational subroutines
    - For some subshells, ICC does not vary smoothly as a function of the energy ("bumps"). Also occurs in the Rösel tables (Raman).
  - Report file
    - Length of report may increase significantly
      - Only echo the ID record to the report file
    - Width of report will exceed 132 characters
      - Convert to HTML formatted file
  - Output file (CARDS.NEW) — Need to maintain downward compatibility
    - One "S G" with KC, LC, MC, NC+
    - Second "S G" record with NC, OC, PC, QC, and RC

BRICC - 6

- Communication with Tibor Kibedi
  - Extend to include calculation of internal pair formation coefficients
  - Finer grid at lower energies to make the interpolation more reliable (“bumps”?)
  - Extend to higher energies using older data

BRICC - 7

- Other considerations
  - $T_{1/2}$ dependencies on BE2↑'s as noted by C. Reich
  - I_γ-normalizations dependent on α_{tot}
  - Normalizations of I_{ce}
  - Intensity balancing
  - Explanatory material for users
    - Before cutoff date A, Hager & Seltzer and Dragoun *et al*. used except as noted.
    - Since cutoff date A, Band *et al.* used except as noted.
  - Built-in assumption of 3% uncertainty due to theory in some codes