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**Joint ICTP-IAEA Workshop on Nuclear Structure and Decay Data:
Theory and Evaluation**

28 April - 9 May, 2008

Description and use of Brlcc.

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ANU

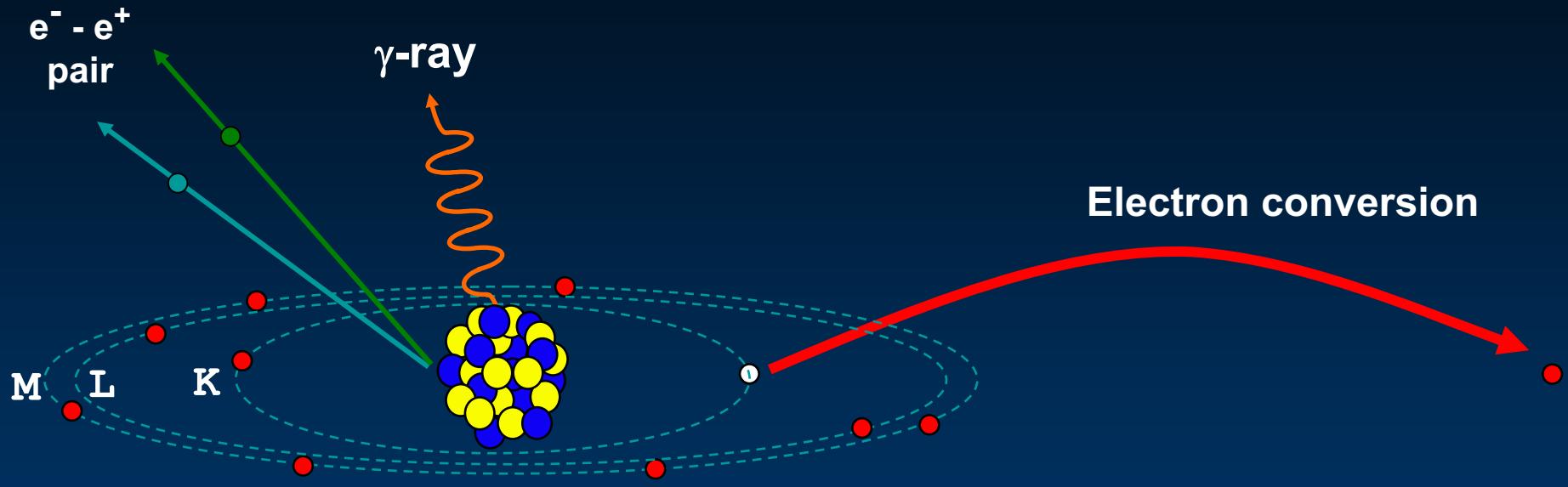
THE AUSTRALIAN NATIONAL UNIVERSITY

Description and use of BrIcc

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Basic concept



Transition probability

$$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M + \dots + \lambda_\pi$$

Conversion Coefficient

$$\alpha_{ce,\pi} = \lambda_{ce,\pi} / \lambda_\gamma$$

Electron conversion

Selection rules (πL)

$$|L - j_i| \leq j_f \leq L + j_i$$

$$\pi = (-1)^L \text{ for } EL$$

$$\pi = (-1)^{L+1} \text{ for } ML$$

Evaluating theoretical conversion coefficients

$$\alpha_{i,\pi} \sim E_\gamma \pm \delta E_\gamma$$

Z – atomic number

electron shell or

electron-positron pair

πL - transition multipolarity

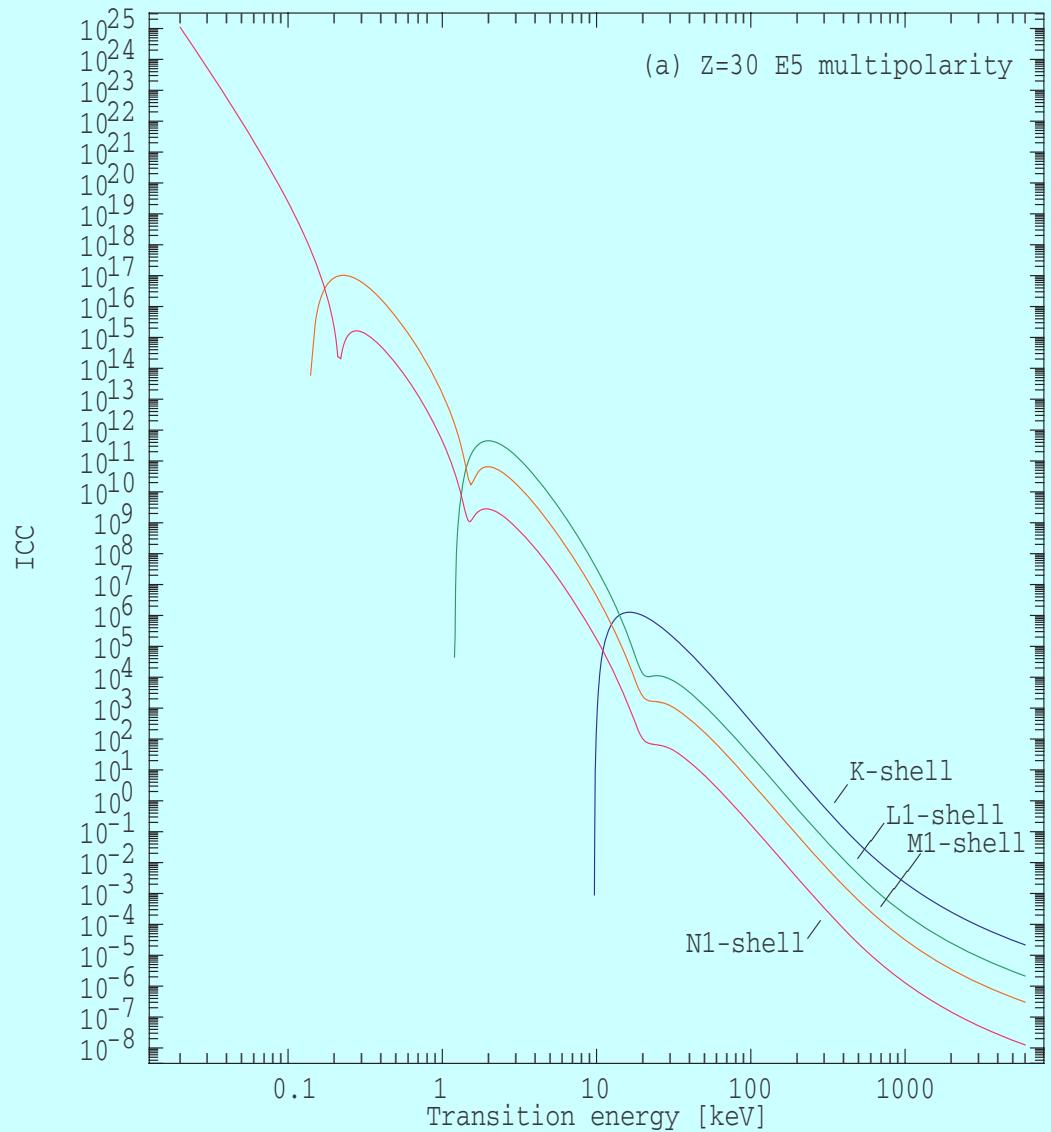
Mixed multipolarity

$$\alpha_i = \frac{\alpha_i(\pi L) + \delta^2 \alpha_i(\pi' L')}{1 + \delta^2}$$

Mixing ratio with uncertainty or limit

$$\delta(\pi' L' / \pi L) = \frac{\gamma(\pi' L')}{\gamma(\pi L)}$$

where $L' = L+1$



Brlcc vs. Hslcc

- Hslcc – Hager-Seltzer (1969Ha61) tabulations used up to 2005
 - Accuracy ~3%
 - Not all shells covered, limited energy and Z range
- Brlcc based on Band-Raman ICC model (2002Ba85)
 - Increased accuracy to ~1%
 - Improved atomic model to treat atomic vacancies created in the conversion process
 - Wider energy range (from 1 keV above binding energy)
 - Wider Z-range (5-110)
 - Calculated for all atomic shells
 - Adopted for ENSDF (2005)

Brlcc v2.2 – data tables

- α_i – electron conversion coefficients – “Frozen orbitals” atomic model
 - ▶ Z=5-110
 - ▶ All atomic shells
 - ▶ 1 keV – 6000 keV
 - ▶ E1-E5 and M1-M5 multipolarities
- α_π – pair conversion coefficients
 - ▶ Z=0-100
 - ▶ 1100 keV – 8000 keV (energy threshold 1022 keV)
 - ▶ E1-E3 and M1-M3 multipolarities
- $\Omega_{i,\pi}(E0)$ – electronic factors
 - ▶ K, L1, L2 shells and π
 - ▶ Z=8 – 100 (incomplete!)

Brlcc – Interactive use

Command Prompt - bricc version

```
C:\Tibor\ENSDF\Trieste2008>|bricc<CR>
Brlcc v2.2 (18-Apr-2008) calculates conversion coefficients
(for electron conversion and pair production)
and E0 electronic factors
using cubic spline interpolation

Z= 70 Ytterbium          Transition energy: 279.717 keU
                                                Conversion Coefficient
Shell   E_e [keU]     E1      M1      E2      M2      E3      M3      E4      M4      E5      M5
Tot           2.367E-02 1.901E-01 9.151E-02 8.110E-01 4.258E-01 3.015E+00 2.267E+00 1.179E+01 1.251E+01 4.967E+01
K            218.38   1.989E-02 1.593E-01 6.401E-02 6.437E-01 1.910E-01 2.138E+00 5.694E-01 6.979E+00 1.741E+00 2.279E+01
L-tot        2.946E-03 2.393E-02 2.115E-02 1.292E-01 1.787E-01 6.694E-01 1.279E+00 3.622E+00 8.019E+00 1.995E+01
M-tot        6.561E-04 5.351E-03 5.038E-03 2.999E-02 4.463E-02 1.637E-01 3.323E-01 9.367E-01 2.182E+00 5.468E+00
N-tot        1.526E-04 1.257E-03 1.161E-03 7.067E-03 1.028E-02 3.862E-02 7.675E-02 2.212E-01 5.061E-01 1.294E+00
O-tot        2.109E-05 1.799E-04 1.447E-04 9.933E-04 1.223E-03 5.205E-03 8.903E-03 2.841E-02 5.697E-02 1.584E-01
P-tot        1.001E-06 9.639E-06 3.226E-06 4.933E-05 1.179E-05 2.169E-04 5.326E-05 9.480E-04 2.740E-04 4.167E-03
N+          1.747E-04 1.446E-03 1.309E-03 8.109E-03 1.151E-02 4.405E-02 8.571E-02 2.506E-01 5.633E-01 1.457E+00
TranEner!ChemSymb!Z+Integer!SUBShell!DATATable!?: for help!EXIT [279.717] >
```

Input parameter can be:

- **Transition Energy [keV]:** 123; 123.0, 1.23E2
- **Chemical Symbol [max 2 char]:** Os
- **Z+integer [5-110]:** Z76 selects Os
- **SUBS:** toggles between to show/NOT to show sub shell ICCs
- **DATA table:** toggles between “Frozen Orbitals” (BrIccFO) and “No Hole” (BrIccNH) approximations
- **?:** displays information on how to use BrIcc

Brlcc – using as an evaluation tool

Decay Data Set

172YB 172TM B- DECAY (63.6 H)

1974RE07, 1967OT03, 1968WI2295NDS

199509

GAMMA record

	1	2	3	4	5	6	7	8
172YB	G	90.605	25	0.40	3 E2+M1	-1.64	2	4.7
<i>DSID</i>	<i>Energy</i>	<i>Unc</i>		<i>Multipol</i>	<i>MixRat</i>	<i>Unc</i>	<i>CC</i>	<i>UNC</i>

↓ *input*

$$\alpha_i \sim f(E_{TranEner}; Z; Mult; Atomic\ shell)$$

Brlcc – using as an evaluation tool

Decay Data Set

172YB 172TM B- DECAY (63.6 H) 1974RE07, 1967OT03, 1968WI2295NDS 199509

172YB DG CC\$ FROM BrIcc v2.2 (18-Apr-2008) 2008KIAA, "Frozen orbitals" appr.

GAMMA record

	1	2	3	4	5	6	7	8
172YB	G 90.605	25 0.40	3 E2+M1	-1.64 2	4.65			C
<i>DSID</i>	<i>Energy</i>	<i>Unc</i>	<i>Multipol</i>	<i>MixRat</i>	<i>CC</i>	<i>DCC</i>		

Curved arrows indicate data flow from the GAMMA record fields to the input parameters of the formula:

- An orange arrow labeled "input" points from the *DSID*, *Energy*, and *Unc* fields to the *input* parameter.
- A green arrow labeled "Put CC if $CC \geq 0.01$ " points from the *CC* field to the *input* parameter.
- A green arrow labeled "Put DCC if $DCC/CC \geq 1.4\%$ " points from the *DCC* field to the *input* parameter.
- A green arrow labeled "Put CC if $CC < 0.01$ " points from the *CC* field to the *input* parameter.

$$\alpha_i \sim f(E_{TranEner}; Z; Mult; Atomic\ shell)$$

172YBS G KC=1.92 3\$LC=2.09 4\$MC=0.511 8\$NC+=0.1304 20
 172YBS G NC=0.1167 18\$OC=0.01359 20\$PC=0.0001017 17

Brlcc – using as an evaluation tool

Command Prompt

```
C:\Tibor\ENSDF\A172\172Yb>brlcc ba1974re07.ens<CR>
BrIcc v2.2 (18-Apr-2008) calculates conversion coefficients
  (for electron conversion and pair production)
  and E0 electronic factors
  using cubic spline interpolation
  Theoretical Dirac-Fock conversion coefficients based on
  the so-called "Frozen Orbital" approximation

Input & Data Files:
  Input ENSDF file: ba1974re07.ens ← Input file

Output Files:
  Complete calculations report, (Def: BrIcc.lst): ← Calculations report file
  New G/SG records, (Def: Cards.new): ← New ENSDF records
  G/SG (New/Old) comparison report, (Def: Compar.lst): ← New/Old comparison report file

Execution control:
  List conversion coefficients for all subshells (Def. N): ← List sub-shell ICC's
  Calculate conversion coefficients for all transitions (Def. N): ← List ICC's for all transitions;
                                                               i.e. no multipolarity given

Processing started. Please wait.

  Processing a new data set
    1 : 172YB   172TM B- DECAY (63.6 H)
    71 : 172YB   G 78.750   7 109   8 E2           8.18
    79 : 172YB   G 181.520   9 45.9   24E2         0.369
    83 : 172YB   G 279.40   7 0.08   2 E2         0.0912
    89 : 172YB   G 964.11   6 5.7    3 [E2]        0.00400
    96 : 172YB   G 857.54   4 2.29   13
    97 : 172YB   G 1039.06   7 2.30   12
    99 : 172YB   G 1117.93   150.86  12
   103 : 172YB   G 1076.15   3 13.2   7 D
<W> Valid but NON-unique multipolarity. Calculation could not be performed.
   107 : 172YB   G 1154.91   8 2.73   16
```

} Transitions being processed

} Warnings, Errors or Information

Brlcc – using as an evaluation tool

```
Command Prompt
<W> Valid but NON-unique multipolarity. Calculation could not be performed.
 236 : 172YB G 528.26   4 2.10    12M1(+E2) +0.01   3   0.0355
 238 : 172YB G 1440.26  130.27    3
 239 : 172YB G 1621.73  111.20    8
Brlcc finished processing ba1974re07.ens
Processed:
#DataSets      :      1
#AllRecords    :    240
#GammaRecords  :      48
#Errors        :      0
#Warnings      :     17
Skipped:
#DataSets      :      0
C:\Tibor\ENSDF\A172\172Yb>_
```

}

Summary

Look for Errors and or Warnings

Brlcc – using as an evaluation tool

Brlcc verifies G, G-cont cards. Some examples:

150GD G 650.33 0 .3 (E2)

<E> Invalid uncertainty on transition energy.

181RE G 148.4 2 0.8 3M1 0.13 LT 1.724 17

<E> Invalid mixing ratio.

Use FMTCHK before running Brlcc!

For some Elements and Atomic shells Brlcc energy range is limited:

<W> ICC could not be calculated for EG+DEGH above 398.000 keV

Extra user information

146SM G 2644.43 5 0.108 3E1+(M2)

<I> Mixing ratio empty, assumed to be equal to 1.

246CM G 42.9 2 2 AP E2

<I> Uncertainties on ICC's from transition energy uncertainty is greater than 1.0%.

Brlcc – MERGE: combining new and old records

172YB DG CC\$ FROM BrIcc v2.2 (18-Apr-2008) 2008KiaA, "Frozen Orbitals" appr.		4
172YB G 78.750 7 109 8 E2	8.25	71
172YBS G KC=1.543 22\$LC=5.12 8\$MC=1.265 18\$NC+=0.321 5		71
172YBS G NC=0.288 4\$OC=0.0328 5\$PC=7.37E-5 11		71
172YB G 181.520 9 45.9 24E2	0.372	79
172YBS G KC=0.217 3\$LC=0.1189 17\$MC=0.0289 4\$NC+=0.00742 11		79
172YBS G NC=0.00662 10\$OC=0.000791 11\$PC=9.92E-6 14		79
172YB G 279.40 7 0.08 2 E2	0.0918	83
172YBS G KC=0.0642 9\$LC=0.0212 3\$MC=0.00506 8\$NC+=0.001314 19		83
172YBS G NC=0.001166 17\$OC=0.0001453 21\$PC=3.23E-6 5		83
172YB G 964.11 6 5.7 3 [E2]		89
172YBS G CC=0.00400 6\$KC=0.00332 5\$LC=0.000528 8\$MC=0.0001189 17\$NC+=3.18E-5 5		89
172YBS G NC=2.78E-5 4\$OC=3.88E-6 6\$PC=1.87E-7 3		89
172YB G 90.605 250.40 3 M1+E2 -1.64 2 4.65		130
172YBS G KC=1.92 3\$LC=2.09 4\$MC=0.511 8\$NC+=0.1304 20		130
172YBS G NC=0.1167 18\$OC=0.01359 20\$PC=0.0001017 17		130
172YBS G KC=0.0223 4\$LC=0.00331 5\$MC=0.000738 11\$NC+=0.000196 3		141
172YBS G NC=0.0001716 25\$OC=2.37E-5 4\$PC=1.117E-6 16		141
172YBS G KC=0.10 5\$LC=0.0193 17\$MC=0.0044 3\$NC+=0.00118 9		144
172YBS G NC=0.00103 7\$OC=0.000139 19\$PC=6.E-6 3		144
172YBS G KC=0.06 3\$LC=0.0114 19\$MC=0.0026 4\$NC+=0.00069 11		147
172YBS G NC=0.00061 9\$OC=8.3E-5 17\$PC=3.6E-6 18		147
172YB G 423.04 6 0.26 2 [E2] 0.0276		150
172YBS G KC=0.0212 3\$LC=0.00497 7\$MC=0.001158 17\$NC+=0.000305 5		150
172YBS G NC=0.000268 4\$OC=3.50E-5 5\$PC=1.144E-6 16		150
172YB G 321.70 110.06 1 [E1] 0.01680		161
172YBS G KC=0.01414 20\$LC=0.00207 3\$MC=0.000462 7\$NC+=0.0001232 18		161
172YBS G NC=0.0001075 15\$OC=1.493E-5 21\$PC=7.21E-7 11		161
172YB G 358.86 6 0.16 2 [E2] 0.0437		164
172YBS G KC=0.0325 5\$LC=0.00861 12\$MC=0.00202 3\$NC+=0.000530 8		164
172YBS G NC=0.000468 7\$OC=6.00E-5 9\$PC=1.713E-6 24		164
172YBS G KC=0.1496 22\$LC=0.0225 4\$MC=0.00502 7\$NC+=0.001357 20		176
172YBS G NC=0.001179 17\$OC=0.0001689 24\$PC=9.05E-6 13		176
172YBS G KC=0.0505 7\$LC=0.00749 11\$MC=0.001672 24\$NC+=0.000452 7		179
172YBS G NC=0.000393 6\$OC=5.63E-5 8\$PC=3.03E-6 5		179

Cards.new file:

Delete records if not wanted to be added

ENSDF file:

Index of G-records

Do not delete records before running BrIcc MERGE!

Brlcc – MERGE: combining new and old records

```
Command Prompt - X
C:\Tibor\ENSDF\A172\172Yb>bricc ba1974re07.ens merge<CR>
    BrIcc v2.2 (18-Apr-2008) calculates conversion coefficients
        (for electron conversion and pair production)
            and E0 electronic factors
            using cubic spline interpolation
    MERGE: inserting/replacing G_S record
    New G/SG cards, <Def: Cards.new>: ← New ENSDF records
    Output file of merged old and new cards, <Def: Cards.mrg>: ← Output ENSDF file
Merge operation completed!
C:\Tibor\ENSDF\A172\172Yb>
```

Brlcc – if something goes wrong

➤ Check installation

BrIccHome *environment variable points where files are*
bricc.exe

briccFO.idx & briccFO.icc
briccNH.idx & briccNH.icc

➤ Consult with BrIcc manual

➤ Please report any errors or problems encountered promptly to **Tibor Kibédi** (Tibor.Kibedi@anu.edu.au) with a CC to **Thomas W. Burrows** (burrows@bnl.gov).