BrIcc – Annotated Model Exercise

Extract from Presentations at the ICTP-IAEA Workshop on Nuclear Structure and Decay Data: Theory and Evaluation
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(See the BrIcc Manual, http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/BrIccManual.pdf, **for complete description)**

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Sample Terminal Dialogues:

```
C:\Documents and Settings\Burrows\My Documents\Trieste2005\Model Exercises>bricc
BrIcc v1.3 (05-Jan-2005) calculates conversion coefficients
 (for electron conversion and pair production)
           and E0 electronic factors
        using cubic spline interpolation
Index file: C:\Program Files\BrIcc\BrIcc.idx
ICC file: C:\Program Files\BrIcc\BrIcc.icc
-------------------------------------------------------
Z= 70 Ytterbium              BrIcc v1.3 (05-Jan-2005)
Transition energy: 279.717 keV
Shell  E_e                                                I C C
       [keV]       E1       M1       E2       M2       E3       M3       E4       M4       E5       M5
-------------------------------------------------------------------------------------------------------------
Tot              2.36E-02 1.90E-01 9.08E-02 8.04E-01 4.22E-01 2.98E+00 2.25E+00 1.16E+01 1.24E+01 4.90E+01
K        218.38  1.98E-02 1.59E-01 6.34E-02 6.37E-01 1.88E-01 2.10E+00 5.59E-01 6.83E+00 1.70E+00 2.22E+01
L-tot            2.95E-03 2.39E-02 2.11E-02 1.29E-01 1.78E-01 6.67E-01 1.27E+00 3.60E+00 7.97E+00 1.98E+01
M-tot            6.56E-04 5.35E-03 5.04E-03 3.00E-02 4.46E-02 1.63E-01 3.32E-01 9.35E-01 2.18E+00 5.45E+00
N-tot            1.53E-04 1.26E-03 1.16E-03 7.06E-03 1.03E-02 3.86E-02 7.67E-02 2.21E-01 5.06E-01 1.29E+00
O-tot            2.11E-05 1.80E-04 1.45E-04 9.93E-04 1.22E-03 5.20E-03 8.90E-03 2.84E-02 5.69E-02 1.58E-01
P-tot            1.00E-06 9.64E-06 3.23E-06 4.93E-05 1.18E-05 2.17E-04 5.32E-05 9.48E-04 2.74E-04 4.17E-03
TranEner / ChemSymb(2 char) / SUBShell/ EXIT [279.717] >
```

For interactive use simply enter bricc. Under Windows, this mode may also be invoked with the BrIcc desktop icon.

Paths for the index and ICC files and the program are obtained from the environment. The environment is automatically set up with the Windows installation. For Linux/UNIX, see the manual.

Enter transition energy in keV, chemical symbol (or Z followed by atomic number. Note: for Z>109, the atomic number must be used), toggle between showing and not showing the subshells (SUBS), or EXIT the program. All input is case insensitive.

```
C:\Documents and Settings\Burrows\My Documents\Trieste2005\Model Exercises>bricc hsicc-example.ens
BrIcc v1.3 (05-Jan-2005) calculates conversion coefficients
 (for electron conversion and pair production)
           and E0 electronic factors
        using cubic spline interpolation
Index file: C:\Program Files\BrIcc\BrIcc.idx
ICC file: C:\Program Files\BrIcc\BrIcc.icc
Input ENSDF file: hsicc-example.ens
Output Files
  Complete calculations report, (Def: BrIcc.lst):
  List conversion coefficients for all subshells (Def. N):
  Calculate conversion coefficients for all transitions (Def. N):
  New G/SG records, (Def: Cards.new):
  G/SG (New/Old) comparison report, (Def: Compar.lst):
      Processing a new data set
       1 :  48SC    ADOPTED LEVELS, GAMMAS
     118 :  48SC  G 130.94    4 100       M1(+E2)   0.054   LE    0.0083 2
<I> Uncertainties on ICC`s from transition energy uncertainty is greater than 2%.
     125 :  48SC  G 121.41    4 100       (M1(+E2)) -0.04   9     0.0101 21
     135 :  48SC  G 370.29    5 100       D(+Q)     -0.02   2
<W> Valid but NON-unique multipolarity. Calculation could not be performed.
     146 :  48SC  G 519.9     2 100       M1+E2
<I> Mixing ratio empty, assumed to be equal to 1.
     153 :  48SC  G 259.1     2 4.2     11D+Q
<W> Valid but NON-unique multipolarity. Calculation could not be performed.
     155 :  48SC  G 779.0     2 100.0   11E1+M2     -0.04   1
     162 :  48SC  G 489.3     3 72.5    20M1+E2
<I> Mixing ratio empty, assumed to be equal to 1.
     166 :  48SC  G 748.3     4 13.7    20D+Q
<W> Valid but NON-unique multipolarity. Calculation could not be performed.
     168 :  48SC  G 1268.3    6 11.8    20
     169 :  48SC  G 1638.8    3 100.0   20E1+M2     +0.05   3
     178 :  48SC  G 1811.8    6 31.6    14
     179 :  48SC  G 2063.9    6 100.0   14D(+Q)     -0.02   3

.
.
.
BrIcc finished processing hsicc-example.ens
 Processed:
 #DataSets     :       1
 #AllRecords   :     522
 #GammaRecords :      56
 #Errors       :       0
 #Warnings     :      25
```

As an ENSDF evaluation tool, enter bricc followed by the ENSDF file name.

BrIcc terminal dialog and defaults are very similar to those of HSICC. An additional question on listing or not listing the subshell conversion coefficients has been added.

BrIcc will list all gamma records processed in the terminal output along with any messages noted during the processing (<I> - Informational, <W> - Warning, <E> - Error, and <F> - Internal programming error).

Summary of results.

```
 Skipped:
 #DataSets     :       0

C:\Documents and Settings\Burrows\My Documents\Trieste2005\Model Exercises>bricc hsicc-example.ens merge
BrIcc v1.3 (05-Jan-2005) calculates conversion coefficients
 (for electron conversion and pair production)
           and E0 electronic factors
        using cubic spline interpolation
Index file: C:\Program Files\BrIcc\BrIcc.idx
ICC file: C:\Program Files\BrIcc\BrIcc.icc
  New G/SG cards, (Def: Cards.new):
  Output file of merged old and new cards, (Def: Cards.mrg):
```

As an ENSDF utility to merge new records into the original dataset, enter bricc followed by the ENSDF file name and "merge". Note: this replaces HSMRG.

Report File:

Only the ID record and gamma-related records of the input are included in the report.

```
        Program BrIcc v1.3 (05-Jan-2005)

Input ENSDF file: hsicc-example.ens

       1 :  48SC    ADOPTED LEVELS, GAMMAS                                          200408
       4 :  48SC CG           ALL INFORMATION IS FROM (P,NG), EXCEPT AS NOTED
       5 :  48SC cG M,MR      From |g(|q) in (p,n|g), except as noted
       6 :  48SC cG E(A)      From Ti(|m{+-},|g)
       7 :  48SC cG M(B),MR(D)$From |g(|q) and linear polarization in (p,n|g)
     118 :  48SC  G 130.94    4 100       M1(+E2)   0.054   LE    0.0083 2
     119 :  48SCS G KC=0.00740 13$LC=0.000669 13
     120 :  48SC cG M,MR      from |a(exp) in (p,n|g)

.
.
.
==============================================================================
 BrIcc Z= 21 Egamma= 130.94 4 keV          Multipolarity= M1(+E2)
                                           M1(+E2)    Mixing ratio = 0.054 LE
 <I> Uncertainties on ICC`s from transition energy uncertainty is greater than 2%.
                                        M1+E2 Mixed Icc
 Shell    M1        E2                  Icc      dIcc       dIccDMRL   dIccDMRH   dIccDEL    dIccDEH
         --------- ---------           --------- --------- ---------- ---------- ---------- ----------
 K       7.193E-03 9.680E-02           7.323E-03 2.277E-04  1.303E-04  1.303E-04  1.158E-04  1.157E-04

 L-tot   6.465E-04 8.860E-03           6.585E-04 2.077E-05  1.194E-05  1.194E-05  1.075E-05  1.073E-05
 K/L     1.113E+01 1.093E+01           1.112E+01 4.926E-01
```

BrIcc checks for instances where the uncertainty associated with $\Delta I\gamma$ may contribute to the $\Delta\alpha$ and includes this in the results.

```
 M-tot   8.004E-05 1.088E-03          8.151E-05 2.557E-06  1.466E-06  1.466E-06  1.317E-06  1.315E-06
 L/M     8.077E+00 8.142E+00          8.079E+00 3.594E-01

 N-tot   4.420E-06 5.700E-05          4.496E-06 1.360E-07  7.644E-08  7.644E-08  6.755E-08  6.753E-08
 L/N     1.463E+02 1.554E+02          1.465E+02 6.401E+00

 Tot     7.924E-03 1.068E-01          8.067E-03 2.511E-04  1.437E-04  1.437E-04  1.279E-04  1.278E-04

  Compare OLD/NEW cards
     118 :  48SC  G 130.94    4 100       M1(+E2)   0.054   LE    0.0083 2                   <Old Card>
     118 :  48SCS G KC=0.00740 13$LC=0.000669 13                                             <Old Card>
     118 :  48SC  G 130.94    4 100       M1(+E2)   0.054   LE    0.0081 3                   <New Card>
     118 :  48SCS G KC=0.00732 23$LC=0.00066 2$                                              <New Card>
.
.
.
==========================================================================================================
 BrIcc Z= 21 Egamma= 1638.8 3 keV          Multipolarity= E1+M2                          10-APR-05
                                           E1+M2      Mixing ratio = +0.05 3
                                         E1+M2 Mixed Icc
 Shell    E1        M2                    Icc      dIcc       dIccDMRL   dIccDMRH
         --------- ---------             --------- --------- ---------- ----------
 K       1.783E-05 5.191E-05            1.791E-05 3.817E-07 -7.138E-08  1.318E-07

 L-tot   1.555E-06 4.550E-06            1.562E-06 3.333E-08 -6.272E-09  1.158E-08
 K/L     1.147E+01 1.141E+01            1.146E+01 3.457E-01

 M-tot   1.927E-07 5.643E-07            1.936E-07 4.130E-09 -7.781E-10  1.436E-09
 L/M     8.070E+00 8.063E+00            8.070E+00 2.435E-01

 N-tot   1.084E-08 3.176E-08            1.089E-08 2.323E-10 -4.380E-11  8.086E-11
 L/N     1.435E+02 1.433E+02            1.435E+02 4.329E+00

 IPF     3.731E-04 4.692E-05            3.723E-04 7.555E-06  6.829E-07 -1.261E-06

 Tot     3.927E-04 1.040E-04            3.919E-04 7.921E-06  6.045E-07 -1.116E-06

  Compare OLD/NEW cards
     169 :  48SC  G 1638.8    3 100.0   20E1+M2     +0.05   3                                 <Old Card>
     169 :  48SC  G 1638.8    3 100.0   20E1+M2     +0.05   3     0.000391                    <New Card>
     169 :  48SCS G NC+=0.00037 1$                                                            <New Card>
     169 :  48SCS G IPC=0.00037 1$                                                            <New Card>
```

Comparisons of old and new records are summarized in Compare.lst.

BrIcc will also calculate the internal electron-positron pair formation coefficient.

To maintain downward compatibility, K, L, M, and NC+ are placed on one “S G” record. The components of NC+ are enumerated on a subsequent “S G” record.

Brief Comparison of HSICC and BrIcc:

	HSICC	BrIcc 2.0
Sources	R.S. Hager & E.C. Seltzer. Nucl. Data **A4**, 1 (1968). O. Dragoun, *et al*. Nucl. Data Tables **A9**, 119 (1971).	I.M. Band, *et al*. At. Data Nucl. Data Tables **81**, 1 (2002)[1] T. Kibédi, *et al*. AIP Conference Proceedings **769** (1), 268-271 (2005)
Shells	K through M5 & N+O+…	K through Q1 and internal electron-positron pair formation
Multipolarity	E1-E4 and M1-M4	*E0*[2], E1-E5, and M1-M5
Energy Range (keV)	ε_i+1 to 1500	ε_i+1 to 6000
ΔE_γ	Attempts to warn	Included in $\Delta\alpha$
Elements	Z=30-103	Z=10-95
Theory	Hole included	"Frozen orbitals" hole approximation

[1] The original table used the "No Hole" approximation and spanned an energy range from ε_{L1}+1 keV to 2 MeV. The current table is based on the "Frozen orbitals" hole approximation, has an expanded energy range, additional points for accurate interpolation, handles E0 transitions and internal electron-positron pair formation. See the BrIcc Manual (http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/BrIccManual.pdf) for details.
[2] Requires new ENSDF formats before full implementation.