## **Brlcc Program Package**

#### Presentation for the USNDP 2004 Meeting November 3-5, 2004

T. Kibédi (ANU), <u>T.W. Burrows</u> (BNL), M.B. Trzhaskovskaya (PNPI), & C.W. Nestor, Jr (ORNL).





# **Bricc Program Package**

- Data Base
- Additions to Original Band-Raman Table
- Testing
- Programs
- Implementation





#### Brlcc Program Package Data Base

Internal Conversion Coefficients

- 2002Ba85 Original Band-Raman Table (Z≥96)
- 2004KiAA Additions for BrIcc (Z=10 95)
- 2002Ba85 and 2004KiAA merged in a consistent manner
- Conversion Coefficients for Electron-Positron Pairs
  - 1979Sc31 (Z<50)
  - 1996Ho21 (Z≥50)
- Electronic Factors for E0 Transitions
  - 1969Ha61 (Z=30 38)
  - 1970Be87 (Z=40 102)
  - 1986PaZM (Z=8 40)





# Brlcc Program Package Additions to Original Band-Raman Table

- Large changes (≈10<sup>3</sup>) between adjacent points
  - Additional points added
- "Resonance"-like regions (s<sub>1/2</sub> shells, E2 E5)
  - Additional points added
  - Interesting systematics?
- Lower limit changed from  $\varepsilon_{L1}$ +1 to  $\varepsilon_{ic}$ +1
  - Encountered threshold non-regularities (s<sub>1/2</sub> shells, E4 E5)
     Additional points added
  - Interesting systematics?
- Extended energy range to 6 MeV (Z=10 95)
  - Wild fluctuations Program modified to increase mesh





#### Brlcc Program Package "Resonance"-like Regions









# Brlcc Program Package Testing (CC's)

- Extracted all IT decay datasets (1773 transitions) and one B- or EC decay dataset per Z (17637 transitions)
- Looked into cases where CC(ENSDF)/CC(Brlcc) deviated from 1.0 by >10%
  - If probable ENSDF problem, removed from comparison
  - If BrIcc problem, removed from comparison and fixed the program
  - Others left in
- Average difference  $\approx 2\%$





#### Brlcc Program Package ENSDF to Brlcc Comparison (CC's)







# Brlcc Program Package Testing (KC, LC, MC, & NC+)

More limited testing done for KC, LC, MC, and NC+

- IT decay datasets
- Known problems (including round off) excluded
- Missing or incorrect "S G" records in ENSDF (≈10%)

Shell	Order	Average	#γ′s
КС	All	1.024±0.025	631
LC	All	$1.011 \pm 0.024$	631
MC	All	1.009±0.036	481
NC+	L=1	1.079±0.022	83
	L=2	1.092±0.027	165
	L=3	1.118±0.043	63
	L=4	1.170 ±0.052	24





## Brlcc Program Package Additional Testing?

- Observations from Murray Martin (Z=94, E=52-223 keV):
  - Bricc E2 values are about 3% lower than HSICC as expected
  - Brlcc M1 values are about 7% lower than HSICC
    - K, L1, M1, and CC 7%
    - L2 and M2 4.5%
    - L3 and M3 unchanged





## Brlcc Program Package Programs

- Windows 95/98/2000/NT/ME/XP, Compaq Tru64 Unix, and Linux
- BldBrlcc Builds direct access files from ASCII files
  - Replaces BLDHST
- Brlcc
  - Terminal input (bricc)
    - Chemical symbol or Z,  $E_{\gamma}$ , enable/disable list of subshells
  - ENSDF evaluation tool (bricc <ensdf file>)
    - Replaces HSICC
  - ENSDF merge tool (bricc <ensdf file> merge)
    - Replaces HSMRG





# Brlcc Program Package Brlcc Terminal Dialogue

```
C:\BrIcc>bricc ba1978bo18.ens<cr>
BrIcc v1.2 (22-Sep-2004) calculates conversion coefficients
 (for electron conversion and pair production)
          and EO electronic factors
       using cubic spline interpolation
Index file: c:\BrIcc\BrIcc.idx
ICC file: c:\BrIcc\BrIcc.icc
Input ENSDF file: ba1978bo18.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 : 172YB
               172LU EC DECAY (6.70 D)
  104 : 172YB G 155.87 7 0.032 7 M1(+E2) 0.7
                                                       LT
                                                             0.90
  107 : 172YBS G KC=0.72 8$LC=0.139 18$MC=0.032 5$NCC+=0.0085 12
                                                 ******
          WARNING - Non-standard data will be over-written
  109 : 172YB G 174.671 190.180 8
  112 : 172YB G 348.83 220.015 11
  113 : 172YB G 596.75 150.102
                                    23
  114 : 172YB G 604.65 190.050
                                    23
  115 : 172YB G 990.75 150.12
                                    6 D,E2
   . . .
   . . .
  1251 : 172YB G 770.4
                           2 0.012 2
  1257 : 172YB G 588.3
                           2 0.0093 19
  1259 : 172YB G 2197.3
                           2 0.006 3
  1265 : 172YB G 1932.0
                           2 0.0019 5
  1267 : 172YB G 2211.4
                           2 0.0034 6
 BrIcc finished processing ba1978bo18.ens
 Processed:
 #DataSets
               1
 #AllRecords : 1269
  #GammaRecords :
                  286
  #Warnings
               ÷.
                    2
  Skipped:
 #DataSets
               :
```

6





#### Brlcc Program Package Brlcc "2 G" Record Comparison

1	:	170YB		170LU EC	DECAY		1990	ABZT,1972CA21	,1970DZ1102NDS	200211			
Compa	are	OLD/NE	W	cards									
105	:	170YB	G	223.40	1545.0	15M1		0	. 360		<01d	Card>	
105	:	170YBS	G	KC=0.301	9\$LC=0.0454	14\$MC=0.0	101	3\$NC+=0.00298	9		<01d	Card>	
105	:	170YB	G	223.40	1545.0	15M1		0	. 350		<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	
105	:	170YBS	G	KC=0.293	6\$LC=0.0444	9\$MC=0.00	993	20\$NC+=0.00268	8\$		<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	
105	:	170YBS	G	NC=0.0023	33 5\$OC=0.00	033 1\$					<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	
								•					
								•					
Compa	are	OLD/NE	W	cards									
546	:	170YB	G	1753.9	3 100	5 M1 (+E2+E	EO)			G ?	<01d	Card 1	Kept>
								•					
								•					
Compa	are	OLD/NE	W	cards									
694	:	170YB	G	2191.15	153.55E+3	10E1				С	<01d	Card>	
694	:	170YBS	G	CC=0.0003	39\$KC=0.0003	4\$EKC=0.00	0039	2			<01d	Card>	
694	:	170YB	G	2191.15	153.55E+3	10E1		0	.00109	С	<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	
694	:	170YBS	G	KC=0.0003	34 1\$						<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	
694	:	170YBS	G	IPC=0.000	D69 1\$						<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	
694	:	170YBS	G	EKC=0.000	039 2						<new< td=""><td>Card&gt;</td><td></td></new<>	Card>	





### Brlcc Program Package Implementation

#### Program Remarks

- Treatment of uncertainties
- Extend below Z=10?
- "No hole" versus "hole"
- ENSDF dictionary and manual additions
- Implementation in ENSDF and Nuclear Data Sheets





## Brlcc Program Package Treatment of Uncertainties

$\Delta lpha_{ ext{theory}}$	2%	1% assumed for theory and 1% for interpolation. Increase in "resonance" regions?	
$\Delta \alpha_{\delta}$	Maximum of $ \alpha(\delta) - \alpha(\delta - \Delta \delta) $ and $ \alpha(\delta) - \alpha(\delta + \Delta \delta) $		
$\Delta lpha_{ m E\gamma}$	Maximum of $ \alpha(E_{\gamma})-\alpha(E_{\gamma}-\Delta E_{\gamma}) $ and		
	$ \alpha(E_{\gamma})-\alpha(E_{\gamma}+\Delta E_{\gamma}) $		
$\Delta \alpha_{\text{total}}$	$\sqrt{\Delta \alpha}$	$(\Delta \alpha_{\delta})^2 + (\Delta \alpha_{\delta})^2 + (\Delta \alpha_{E\gamma})^2$	
$\Delta(\alpha/(1+\alpha_{total}))$ somewhat overestimated at present			





## Brlcc Program Package Extend below Z=10?

- Possible
- One experimental datum found ENSDF
- May require validation





## Brlcc Program Package "No hole" versus "hole"

- Current internal conversion coefficients table is based on calculations without taking into account the effect of the hole.
- About three weeks to calculate table taking into account the effect of the hole
  - May need to check mesh near threshold non-regularities
- Easy to rebuild direct access files
  - About one minute on a fairly modern PC
- Should have little effect on ENSDF evaluation tool
- Do the hole calculations need validation?





# Brlcc Program Package ENSDF Dictionary & Manual Additions

Needed by Brlcc				
MRKE0/E2	$q^{2}(E0/E2)=I_{K}(E0)/I_{K}(E2)$ <i>E0,E2</i> mixing ratio			
ENSDAT, FTMCHK, NDS publication codes, Web codes				
Produced by Brlcc				
NC,,RC	Additional shell conversion coefficients and ratios			
N/T ,,R/T				
IPC,IP/T	Internal electron-positron pair formation coefficient			
	and ratio			
ENSDAT, FTMCHK, NDS publication codes, RadList, Web codes				
May also need definition for E0 electronic factors				





## Brlcc Program Package Implementation in ENSDF & NDS

- Can not automatically update ENSDF due to dependencies on α in other quantities (*e.g.*, T<sub>1/2</sub>'s, normalizations, *etc.*)
- Set implementation date All evaluations received after this date to use BrIcc
  - Give evaluators enough time to convert
  - Evaluations using BrIcc received before this date should note this use in the Comments dataset
- General policies need to be updated
  - Need archiving of old policies for conversion coefficients Web site?
  - Refer to this archive in new policies?



