Description and Use of Brlcc
(Band-Raman Internal Conversion Coefficients) and HSICC
(Hager-Seltzer Internal Conversion Coefficients)

Presentation for the ICTP-IAEA Workshop on Nuclear Structure and Decay Data: Theory and Evaluation

20 February - 4 March 2006

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Description and Use of Brlcc/HSICC
Brlcc *versus* HSICC

	Brlcc v.2.0	Brlcc v.1.3	HSICC
Source	2005KIZT	2002Ba85, 2005KIZW	1968Ha52, 1971Dr11
Shells	K - R, IPFC		K, L, M, N+
Multipolarities	*E0*, E1-E5, M1-M5		E1-E4, M1-M4
E_γ (keV)	ε_i+1 - 6000		ε_i+1 - 1500
ΔE_γ	Accounted for		N/A
Elements	Z=10-95	Z=10-126	Z=30-103
Theory	*Frozen-orbitals*	No hole	Hole included

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Description and Use of BrIcc
BrIcc *Description*

BrIcc calculates the internal conversion electron and internal electron-positron pair formation coefficients and E0 electronic form factors by spline (cubic) interpolation of tabulated values from several sources.

BrIcc can be used in different ways: as an interactive tool to interpolate conversion coefficients and E0 electronic form factors and as an ENSDF evaluation tool. As an evaluation tool, the program will prepare new ENSDF records (GAMMA and GAMMA continuation) and may also be used to merge the new records into existing ENSDF data sets.

Interactive access is available *via* the Web.

Description and Use of BrIcc
BrIcc *Overview and HINTS*

- For Linux, MS Windows, and UNIX , only BrIcc is required
  - The binary files BrIccFO.idx and BrIccFO.icc are included with the distribution
- Current estimated uncertainty on calculations is 1.4% consisting of:
  - Average (α(exp.)-α(theo.)/α(theo.): -1.01% *21*
  - Average (α(int.)-α(theo.)/α(theo.): +0.0% *3*
- BrIcc using the "frozen-orbitals" approximation was adopted at the 2005 NSDD meeting in McMaster as the replacement for HSICC
  - At present, calculations for ≥96 cannot be performed
    - Use BrIcc v.1.3
    - Use HSICC

Description and Use of BrIcc
BrIcc *Overview and HINTS – 2*

- As an Evaluation tool:
  - If $\alpha_{tot} \leq 0.0001$, it is put on the continuation record instead of the CC field of the gamma record.
  - If the total transition intensity is given, the ratios of the partial conversion intensities to the total transition intensity are output instead of the partial conversion coefficients.

Description and Use of BrIcc
Input/Output (Interactive Use)

- Program execution: bricc
  - It will invoke the program with default values of Z=70 (Ytterbium) and Eγ=279.717 keV.
- Terminal dialog: The program uses 117-character lines to report conversion coefficients. A list of interpolated conversion coefficients for all major and sub-shells, for internal electron-positron pair creation, and E0 electronic form factors.
- Parameter input:
  - Chemical symbol: Maximum of 2 characters.
  - Atomic number: Character Z followed by an integer, between 1 and 126 will be interpreted as an atomic number.
  - Transition energy: A positive number in free format, in keV.
  - SUBShell: Will enable or disable the list of subshell ratios.
  - EXIT: Terminates the program execution.

Description and Use of Brlcc
Input/Output (Evaluation tool)

- Input files:
  - ENSDF formatted file.
  - Index to the coefficients and form factors. BrlccFO.idx.
  - Table of the coefficients and form factors. BrlccFO.icc.
- Program execution: bricc *ENSDF-file*
  - The ENSDF file name is passed as command-line argument.
  - NOTE: The input *ENSDF-file* data should not be modified before running the code in the MERGE mode.
- Output files:
  - Brlcc.lst – Calculation report
  - Cards.new – New G/"S G" records
  - Compar.lst – Comparison of old and new records

Description and Use of Brlcc
Input/Output (Evaluation tool) – 2

- Terminal dialog:
  - Output Files:
    - Complete calculations report, (Def: Brlcc.lst):
    - New G/SG records, (Def: Cards.new):
    - G/SG (New/Old) comparison report, (Def: Compar.lst):
  - Execution control:
    - List conversion coefficients for all subshells (Def. N):
      - Enter "Y" or "y" to list all subshells. Note: this can result in large tables for higher Z's.
    - Calculate conversion coefficients for all transitions (Def. N):
      - Enter "Y" or "y" to calculate for all transitions. Otherwise, calculations will be performed only for those transitions with multipolarities and mixing ratios given.

Description and Use of Brlcc
Input/Output (Utility to merge records)

- Program execution: bricc *ENSDF-file* merge
  - NOTE: The input *ENSDF-file* data should not be modified before running the code in the MERGE mode.
- Terminal dialogue:
  - New G/SG cards, (Def: Cards.new):
  - Output file of merged old and new cards, (Def: Cards.mrg):
- Note: The Cards.new files generated by HSICC and Brlcc are not compatible.

Description and Use of HSICC
HSICC *Description*

The HSICC program package consists of the programs HSICC (calculates internal conversion coefficients), HSMRG (merges new gamma records created by HSICC with the original input data), BLDSHST (builds direct access files of the internal conversion coefficient table), and SEQHST (recreates a sequential file of the internal conversion table from the direct access file).

HSICC calculates the internal conversion coefficients by spline (cubic) interpolation of tabulated values from Hager and Seltzer for the K, L, and M shells and from Dragoun *et al.* for the N+O+….

Interactive access is available *via* the Web.

Description and Use of HSICC
HSICC *Overview and Hints*

- For Linux and MS Windows, only HSICC and HSMRG are required.
  - The direct access files ICCNDX.DAT and ICCTBL.DAT are included in the ZIP or self-extracting ZIP files.
- If E_γ is near the threshold for conversion, new records may not created.
  - Missing contributions from some subshells.
  - Contribution due to the uncertainty in E_γ.
- Old continuation records may be overwritten.
  - Mixing data from HSICC with other information on the same record.
  - Using "S G" for a continuation record.
- No calculations for E5, M5, and higher or for E0.

Description and Use of HSICC
Overview and Hints - 2

- L=3,4 components are multiplied by 0.975±0.010 and 0.975±0.005, respectively.
  - See Nemeth and Veres [Nucl. Instr. Meth. **A286**, 601 (1990)].
- If $\alpha_{tot} \leq 0.0001$, it is put on the continuation record instead of the CC field of the gamma record.
- If the total transition intensity is given, the ratios of the partial conversion intensities to the total transition intensity are output instead of the partial conversion coefficients.

Description and Use of HSICC
Input/Output (HSICC)

- Input files:
  - ENSDF formatted file. Sample file is data.tst.
  - Index to the internal conversion coefficients. ICCNDX.DAT included for LINUX and MS Windows.
  - Table of the internal conversion coefficients. ICCTBL.DAT included for LINUX and MS Windows.
- Output files:
  - Report file. Sample file is HSCALC.LST
  - File of new records for input to HSMRG. Sample file is CARDS.NEW.
  - Comparison of old to new records. Sample file is COMPAR.LST.

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Description and Use of HSICC
Input/Output (HSICC) - 2

- Terminal dialog:
  - INPUT FILES –
    - DATA DECK (DEF: data.tst):
    - ICC INDEX (DEF: ICCNDX.DAT):
    - ICC TABLE (DEF: ICCTBL.DAT):
  - OUTPUT FILES –
    - COMPLETE H.S. CALCULATIONS REPORT (DEF: hscalc.lst):
    - NEW G/SG CARD DECK (DEF: cards.new):
    - G/2G (NEW/OLD) COMPARISON REPORT (DEF: compar.lst):
    - CALC CONV. COEFS. ONLY IF MULTIPOL. KNOWN (Y OR CR):
      - Y to calculate only if multipolarity is known. Carriage return (Enter) for all.

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Description and Use of HSICC
Input/Output (HSMRG)

- Input files:
  - Input data file (ENSDF format). This **must** be the same input file used by HSICC. Sample input file: DATA.TST.
  - Correction file of gamma records created by HSICC. Sample input file: CARDS.NEW. Note: the CARDS.NEW files generated by Brlcc and HSICC are not compatible.
- Output file: Updated file in the ENSDF format. Sample output file: CARDS.MRG.

Description and Use of FMTCHK (Format and Syntax Checking)

Presentation for the ICTP-IAEA Workshop on Nuclear Structure and Decay Data: Theory and Evaluation

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Thomas W. Burrows

Description and Use of FMTCHK *Description*

FMTCHK analyzes the format of an ENSDF formatted file to verify that it conforms to "EVALUATED NUCLEAR STRUCTURE DATA FILE. A Manual for Preparation of Data Sets" by J.K. Tuli, Brookhaven National Laboratory Report BNL-NCS-51655-01/02-Rev (February 2001) and subsequent memos.

Documentation consists of README-FMTCHK.TXT("Printer friendly") and README-FMTCHK.HTML.

Description and Use of FMTCHK
Overview

- Should be run every time the ENSDF formatted file has been manually changed before executing any of the other programs and before submittal of the evaluation.
- Four types of messages
  - Fatal errors ("<F>") — All fatal errors should be corrected.
    - INVALID NUCID - Either the mass or chemical symbol has not been given for the NUCID or the chemical symbol is incorrect.
  - Errors ("<E>") — If possible, all errors should be corrected.
    - MISSING MULT - A mixing ratio has been given but there is no multipolarity.
  - Warnings ("<W>") — Should be checked to see if there are problems that may need correction.
    - MISSING MR - A mixed multipolarity has been found in the MULT field of the GAMMA record but no mixing ratio has been given.

Description and Use of FMTCHK
Overview - 2

  - Informational ("<I>") — These messages give assumptions or changes in checking or note when various internal storage limits are exceeded.
    - Assuming x=# - Value of nonnumeric energy assumed by the program for checking level order and gamma final levels.
- Some error or warning messages are given because of the possible effects on other programs.
  - Mixing ratio is given but no associated mixed multipolarity.
  - No "FL=" given and no final levels with a certain limit or more than one possible final level based on E_{level}-E_{γ}.

Description and Use of FMTCHK
Overview - 3

- For level energies of the form X, Y, Z, *etc.* or E+X, E+Y, E+Z, *etc.*, an arbitrary energy is assigned to the first occurrence of the character based on the energy of the previous level energy. This is reported as an informational message in the report file and is used to see if the levels are in the proper energy order.

Description and Use of FMTCHK
Input/Output

- Input file (ENSDF format): Sample is DATA.TST.
- Output file: Report file. Sample is FMTCHK.RPT.
- Terminal dialog:
  - INPUT file to be checked: data.tst
  - OUTPUT file for report: fmtchk.rpt
  - Errors only or full report (E, F):
  - Check continuation cards (Y, N):
    - Not checking continuation records may cause erroneous error messages.
  - Report only fatal errors (N, Y):
    - If yes, the following prompt will be suppressed and error and warning messages will be suppressed.
    - Totals of error and warning messages will still be noted in the terminal output.
  - Suppress warning messages (N, Y):
    - If yes, total warnings will still be noted in the terminal output.
  - Suppress XREF/DSID check (N, Y):

Description and Use of FMTCHK
Input/Output - 2

- Sample terminal output:

```
205TL    205HG B- DECAY              1971HI01                    78NDS    197803
                        3 warning(s) reported
```

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Description and Use of GTOL (Gamma to Level)

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Description and Use of GTOL
Description

In GTOL, gamma-ray energies are used to derive a set of least-squares adjusted level energies. The net feeding at each level is calculated from the input gamma intensities and conversion coefficients or total transition intensities and compared to the feedings given on the β-, ε/β^+, or α records. Unplaced or questionable gammas or gammas whose final level is ambiguous or unknown are ignored. The program parses the DSID of each data set and, if there is no indication of possible gamma records within the data set, skips it. In addition, the program will not calculate the intensity balancing for adopted datasets or datasets whose production normalization record indicates branching ratios.

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Description and Use of GTOL
Description - 2

Documentation is available in:

- B.J. Barton and J.K. Tuli. PHYSICS ANALYSIS PROGRAMS FOR NUCLEAR STRUCTURE EVALUATION. Brookhaven National Laboratory Informal Report BNL-NCS-23375/R (1977).

- L.P. Ekström and P. Andersson. FORTRAN 77 VERSIONS OF STRING HANDLING SUBPROGRAMS AND THE PROGRAMS GTOL AND MEDLIST. Nuclear Physics Report LUNFD/(NFFR-3049)/1-27 (Lund University, Lund Sweden. 1983).

Description and Use of GTOL
Overview and Hints

- If the level energies are of the form X, Y, Z, *etc.* or E+X, E+Y, *etc.*, the least-squares fit is done separately for each group of states and merged back into the final results.
  - Energy assigned for the first member of a group similar to FMTCHK
  - Used to sort the levels in the energy comparison but not used when creating the new output file.
- If connecting information is too sparse, the matrix created may not be able to be inverted.
  - Check the report file for levels that do not deexcite and fix these levels.

Description and Use of GTOL
Overview and Hints - 2

- Uncertainly placed γ's are ignored in the least-squares fit and the intensity balance calculations.
  - Estimate of the excitation energies of levels only connected by such transitions:
    - Remove the "?" in column 80 of the relevant gamma records
    - Add "F" or "G" in the energy fields of any connected level records which also are fed or deexcited by other γ's.
  - Estimate of the effect on the intensity balance:
    - Remove all "?" in column 80 of the gamma records.
    - Compare the original results to these to obtain an estimate
- Level records with SP, SN, or SA in the energy field and their associated gammas are ignored.

Description and Use of GTOL
Overview and Hints - 3

- If the resultant intensity balance seems non-physical (*i.e.*, the probability function overlaps 0.0), an estimate of the upper limit (90% confidence) for the two methods described by Louis Lyons in Statistics for Nuclear and Particle Physicists (Cambridge University Press) will be provided.
  1. Over the positive part of the distribution
  2. Over the whole distribution

  If method 1 is used, add comment for I_{β}, $I_{\varepsilon+\beta+}$, or I_{α}

Description and Use of GTOL
Input/Output

- Input file: An ENSDF formatted file with the following optional information:
  - An option record with 'OPTION' in col. 1-6 may precede any data set and contain any of the following options in free format.

Option	Meaning
NOREC	No recoil correction, *i.e.* recoil correction has already been applied to E_γ.
RECOIL	Perform recoil correction (Default)

Description and Use of GTOL
Input/Output - 2

Option	Meaning
MARKED	Process only data sets preceded by a card with '*GTOL' in col. 1-5
ALL	Process all data sets (default)

Description and Use of GTOL
Input/Output - 3

DEG=	For the current data set, override default assumption of 1 keV where no uncertainty on the gamma energy is given. Following the equal sign may be either a number or a number followed by a percent sign. A number alone indicates the uncertainty on EG in keV while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.

Description and Use of GTOL
Input/Output - 4

DRI=	For the current data set, assume a default uncertainty for the relative photon intensity (RI) when none given. A number alone indicates the uncertainty on RI in the current relative units while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.
DTI=	Same description as for DRI= but applied to the total intensity (TI).

Note that a blank option card resets the defaults.

Description and Use of GTOL
Input/Output - 5

- A level energy can be held fixed by adding the "F" or "G" separated from the energy somewhere in the field (columns 10-21). If the output option to create a new file containing the adjusted level energies is chosen, the "F" or "G" will be removed and a level documentation record will be added (LEVEL ENERGY HELD FIXED IN LEAST-SQUARES ADJUSTMENT) in the new ENSDF file generated.
  - "F" - ΔE(level) ignored
  - "G" - ΔE(level) included in calculations
- If DRI or DTI are specified on an OPTION record, the assumed uncertainty may be overridden for an individual intensity, by adding an "E" separated from the intensity in either the RI or TI fields.

Description and Use of GTOL
Input/Output - 6

- If DEG, DRI, or DTI are specified on an OPTION record and a new file is created, FOOTNOTE COMMENTS will be generated and inserted as necessary.
- Sample input file: DATA.TST

■ Output files:

- Report file. The report file will contain a summary of the data input and actions taken by the program (*e.g.*, unplaced or questionable gammas ignored) and the following optional outputs for each data set:
  - Comparison of input to calculated level energies
  - Comparison of input to calculated transition energies with χ^2's
  - Comparison of input gamma energies to those calculated based on the adjusted level energies.
  - Comparison of calculated net feedings to each level with values input on β^- (B), β^+/ε (E), or α (A) records.

Description and Use of GTOL
Input/Output - 7

- Comparison of the original ENSDF file to the created ENSDF file.
  - Level energies kept or changed
  - "FL=" fields on gamma continuation records kept or changed.
- Sample report file: DATA.TST
- Sample ENSDF file generated: GTOL.NEW

Description and Use of GTOL
Input/Output - 8

- Terminal dialog:
  - INPUT FILE (DEF: gtol.inp):
  - REPORT FILE (DEF: gtol.rpt):
  - Do you wish to create a new file with level energies replaced by GTOL results(N/Y)? Y
    - If No, the following prompt will be suppressed
  - Enter OUTPUT ENSDF FILE NAME (DEF: gtol.out):
  - Do you wish to suppress gamma energy comparison(N/Y)?
    - If you are interested in adding or modifying feedings in the dataset, you may wish to suppress this comparison.
  - Do you wish to suppress intensity comparison(N/Y)?
  - Assumed DCC theory (Hsicc-3%, Bricc-1.4%, Other-?)
    - Default is HSICC. If other is specified, there will be prompt for the uncertainty in percent to assume.

Description and Use of GTOL
Input/Output - 8

- Sample terminal output:

```
GTOL started, wait patiently!

CURRENT DATA SET: 205TL    205HG B- DECAY
END OF FILE
```

Description and Use of LOGFT

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Description and Use of LOGFT
Description

LOGFT calculates log *ft* for beta decay. It also calculates the partial capture fractions for electron capture, the electron capture to positron ratio for positron decay, and the average beta energies. It will do special calculations for first and second forbidden unique; all other categories are treated as allowed.

Interactive access available *via* the Web.

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Description and Use of LOGFT
Overview and Hints

- New records will not be created if there are non-numeric parent or level energies, Q-values, or non-numeric uncertainties for these values.
  - Modify the dataset by replacing the non-numeric values with estimates.
    - If the Q-value is a systematic value from Audi and Wapstra, replace "SY" with the estimated uncertainty.
    - If the parent level is "X" and X<18, use X=9±9.
  - Rerun LOGFT on the modified dataset.
    - Return the modified values to the original uncertainties.
    - Dependent on the effect of the estimated uncertainties, either use the appropriate non-numeric uncertainties on the calculated quantities or add footnotes or comments noting the assumptions made in the calculation.

Description and Use of LOGFT
Overview and Hints - 2

- If Lyons' method 1 has been used to estimate I_{β^-} or $I_{\varepsilon+\beta^+}$, LOGFT should also be run using the original values in addition to the estimate.
  - Compare results to see the effect of the estimate.
  - Add appropriate documentation. For example, a comment on $I_{\varepsilon+\beta^+}$ might be "estimated upper limit (90% confidence limit) from -40 *90*".
- At present only allowed and first and second forbidden unique transitions are handled. All others are calculated by assuming an allowed shape.
  - Comment record added noting this assumption.
  - Coding has been added to handle higher-order unique but needs extensive testing before release.

Description and Use of LOGFT
Overview and Hints - 3

- Radial wave function data used in calculating electron-capture fractions are assumed to be exact.
  - Results in an underestimate of the uncertainties when electron capture is significant.
  - Plans to replace these data with equivalent data from Schőnfeld *et al.*

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Description and Use of LOGFT
Input/Output

- Input files:
  - ENSDF formatted file. Sample file is DATA.TST.
  - Radial wave function data. Data file included is LOGFT.DAT.
- Output files:
  - Report file. Sample output is LOGFT.RPT.
  - New ENSDF formatted file with appropriate values for β^- and ε/β^+ cards updated. Sample output is LOGFT.NEW.
- Terminal dialog:
  - INPUT DATA SET FILE (data.tst):
  - OUTPUT REPORT FILE (logft.rpt):
  - DATA TABLE (logft.dat):
  - OUTPUT DATA SET FILE (logft.new):

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Description and Use of LOGFT
Input/Output - 2

- Sample terminal output:

```
Processing=====>205TL    205HG B- DECAY
```