

BrIcc – program to evaluate conversion coefficients
User’s manual for version 2.3b
(Updated on 16-Dec-2014)

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Abstract

The **BrIcc** program calculates the conversion electron (α_{IC}), electron–positron pair conversion coefficients (α_{π}) and the E0 electronic factors ($\Omega_{IC,\pi}(E0)$). **BrIcc** can be used in different ways. As an interactive tool it will interpolate α_{IC} , α_{π} and $\Omega_{IC,\pi}(E0)$ values for energies and atomic numbers entered on the console. As an evaluation tool the program will prepare new ENSDF records (GAMMA and GAMMA continuation) based on the content of the ENSDF file used as program input. **BrIcc** also can be used to merge the new cards into existing ENSDF data sets. The current version of **BrIcc** implements changes adopted by the 2013 NSDD meeting held in Kuwait, on the relaxation of the rounding rule of 25 for uncertainties.

Stand alone versions of the code for Windows, Linux and Mac OS can be obtained from the following web sites:

NSDD: http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/
IAEA: https://www-nds.iaea.org/public/ensdf_pgm/index.htm

Conversion coefficients can be obtained using our on-line tool at:

ANU: <http://BrIcc.anu.edu.au>

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I. VERSION HISTORY

BrIcc has been primarily developed to help ENSDF evaluators to calculate conversion coefficients using the best available theoretical data. This manual replaces the previous version [2008KiXX], published in 2005. The procedures and data tables used by **BrIcc** are now described in [2008Ki07] and this document is designed to serve as a program manual providing complementary information. The choice of the “Frozen orbital” approximation is resting on the analysis of 186 conversion coefficients [2008KiZV], which has been carried out in parallel to the development of **BrIcc**. It has adopted the same evaluation procedures and techniques as used in the ENSDF evaluations, served as a benchmark for the code. The program can be downloaded freely at the NNDC website [BrIcc-NNDC].

Conversion coefficients can be easily obtained at the **BrIcc** web interface at [BrIcc-ANU]. This interface also allows to generate chart of conversion coefficient (or ratios of conversion coefficients) v.s. transition energy, which can be useful to explore the sensitivity of ICC values to multipolarities.

A silent version of the code, **BrIccS** has also been developed to provide an easy and simple way to obtain conversion coefficients from computer programs running on various operating systems. The description of **BrIccS** is given in Sec. IX. The silent version can be obtained through the BrIcc web interface [BrIcc-ANU].

TABLE I: Timeline of the development of **BrIcc**

Version	Date	Comment
0.0	15–Nov–2003	NSDD network meeting (Vienna) adopted an action to develop <i>BrIcc</i> based on the Band–Raman (2002Ba85) tables to replace <i>HsIcc</i> .
1.0	6–Apr–2004	“ <i>No-Hole</i> ” table recalculated using RAINE.
1.1	31–Aug–2004	Benchmark testing at ANU completed.
1.2	24–Sep–2004	Benchmark testing at NNDC completed.
1.3 ^(a)	19–Nov–2004	ANU web interface created. (^a) Special version designed for world wide web.
1.3	20–Dec–2004 6–Jun–2005	Released for ENSDF evaluators for testing. NSDD network meeting (Hamilton) adopted the “ <i>Frozen Orbitals</i> ” approximation.
2.0	1–Sep–2005	“ <i>Frozen Orbitals</i> ” table recalculated using RAINE, modified program logic and error and exception handling.
2.1 ^(a)	1–Oct–2005	“ <i>Slave</i> ” version developed, new ANU web interface created. (^a) Special version designed for world wide web.
2.0	19–Dec–2005	Corrected bug in the “Merge” operation.
2.0	12–Jan–2006	Corrected bug in the “Merge” operation.
2.1 ^(a)	1–Feb–2006	User selectable data tables: “BrIccFO”, “BrIccNH”, “HsIcc”, “RpIcc”. (^a) Special version designed for world wide web.

TABLE I: Timeline of the development of **BrIcc**

Version	Date	Comment
2.2	4-Jan-2008	“BrIccFO” and “BrIccNH” data tables have been extended for $Z=5$ –110 atomic numbers and recalculated for 39 elements with new adopted mass numbers.
	31-Mar-2008	A DG CC record is generated automatically to note which one of the two user selectable ICC tables (“BrIccFO” or “BrIccNH”) was used.
2.2	9-Jul-2008	In a small number of cases the first tabulation points from RAINE output have been overlooked. For the K-shell ($Z=88, 100, 101, 102$) the V2.2 “BrIccFO” and “BrIccNH” data tables only started ~ 2 keV above the shell binding energy.
2.2	20-Jan-2009	Table for IPF, $Z=34$ returned $\Omega_K(Z=34)$ instead of $\Omega_{IPF}(Z=34)$.
	19-Oct-2009	Command line argument lengths were not treated correctly in the BrIccS program.
2.3	18-Apr-2011	All routines used in BrIcc converted to double precision to avoid over- or under-flow problems. The VAX <i>Record</i> structures have been replaced with <i>Type</i> statements. Intel Fortran Compiler is used for all supported operating systems. New features: (a) Default mixing ratio has been set to 1.0 for E2/M1 however the user can overwrite this value. For E3/M2 the default value is 1.0. For other transitions it is set 0.1. (b) Minimum CC value on the GAMMA record can be selected by the user. (c) The <i>MERGE</i> function enhanced by adding a Delete , Insert and Replace flags to the new cards in the <i>CARDS.NEW</i> file.
	13-Aug-2011	Release candidate 1 with some bug fixes in the merge option and setting minimum CC.
	9-Dec-2011	Corrected the treatment of uncertainties for mixed multipolarity cases when no mixing ratio was given.
	19-Sep-2012	Program distribution extended to Intel based Machintosh. “N+” and “NC+” shells (introduced for HsIcc) are no longer relevant (BrIcc treats all shells) and removed from the “S G” records and tabulated output.
	9-Oct-2012	If TI is given two sets of “S G” records are generated; one with the “K/T”, “L/T”, etc. ratios and the second one with the conversion coefficients.
	9-Oct-2012	Procedures to propagate large uncertainties overlapping with zero have been changed. Modified ICC value with symmetric uncertainty is adopted.
	29-Mar-2013	In some cases the record numbers of the new ENSDF cards (CARD.NEW file) were not in increasing order. This caused the MERGE routine to fail to insert all new cards into the CARDS.MRG file. The current version resolved this problem.
		New quick help was added to the program, which is accessible by the <i>BrIcc ?<CR></i> command.

TABLE I: Timeline of the development of **BrIcc**

Version	Date	Comment
2.3a	28-Jun-2013	<p>Small corrections to the program including:</p> <ul style="list-style-type: none"> – An error in the listing of the M and N sub-shells on the “S G” cards has been corrected. – In a few cases the IPC and the IPC/T values on “S G” cards were incomplete (characters missing). – Old cards with BrIcc version and default MR values will be replaced every time the program is used with an ENSDF file. Fixed an error which in certain cases left old cards in the ENSDF file. – ICC values will be calculated if the DE or DMR field contains “CA”; i.e. E or MR values were calculated. – A new routine added to test the line termination characters in the ENSDF input file. FORTRAN requires LF or CR+LF characters as line terminators. Files containing CR characters only could not be correctly read. BrIcc will not accept such files and an error message will be given on the screen. – The maximum number of records in a single ENSDF file is increased to 99999, which is much larger than the longest ENSDF mass chain. Currently the A=151 file contains 25411 records.
	7-Aug-2013	The MS Windows version dated of 28-Jun-2013 was created using MS Visual Studio 2012 and Intel Visual Fortran. Some of the C, C++ libraries are incompatible with Windows XP. The problem was rectified.
	29-Aug-2014	If total ICC was larger than 1.0E+10 the second digit of the exponent was truncated as the CC field on the G card is only 7 character long. The WriteCCdata routine was modified by reducing the significant digits to one in the mantissa.
2.3b	16-Dec-2014	The 20th NSDD meeting, held in Kuwait (27–31 January 2013) has adopted action No. 64 to relax the rounding rule of 25 for uncertainties. BrIcc has been changed to adopt the following rule: if the relative uncertainty (DICC/ICC) is bigger than 25%, the uncertainty is rounded to 2 digits. This rule applies for sub-shell ICC's and ratios of ICC values.

II. THE ENSDF FILE

The Evaluated Nuclear Structure Data File (ENSDF), is a computer-based file system designed to store nuclear structure information. It is maintained by the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory for the international Nuclear Structure and Decay Data Network.

The ENSDF file usually contains a number of data sets, each data set refers to a particular reaction or decay mode of a nucleus. Adopted level and gamma-ray properties for each nuclide are kept in a separate data set. The data sets are composed of 80-character records. The most up-to-date description of the ENSDF files is given by J.K. Tuli [2001TuZZ]. Throughout this manual we will frequently make reference to this document. Spectroscopic information is kept in predefined fields of the 80-character records. These fields are marked with bold typeface. For example the numerical value of the total conversion coefficient, stored in the **CC** field of the **GAMMA** record, is α_{tot} .

III. GAMMA TRANSITIONS RECORDS

The GAMMA and the GAMMA continuation records, designed to hold the spectroscopic information on nuclear transitions, are particularly important to the *BrIcc* program. A short description of the fields of the **G** records (see Sec. III) is given in this section. The adopted procedures, relevant to *BrIcc* are described in Sec. IV.

A. GAMMA records

Transition energy (E) and uncertainty (DE) fields: The transition energy, **E** (E_γ) and the symmetric uncertainty, **DE** (ΔE_γ) are given in keV. In a relatively small cases, asymmetric uncertainty values are given in the GAMMA continuation record using the ENSDF dictionary term, DE= with two signed, maximum two digits integer numbers. For example, E=12.4, DE=+1-2 will correspond to a transition energy of $E = 12.4_{-0.2}^{+0.1}$ keV. The asymmetric uncertainties of E_γ will be referred as ΔE_H and ΔE_L .

Photon Intensity (RI) and uncertainty (DRI): The experimental photon intensity is given in the **RI** and in the **DRI** fields. The numerical values are I_γ and ΔI_γ . Pure E0 transitions are treated differently; here **RI** is blank but the total intensity, **TI**, is given (see below).

TABLE II: Transition multipolarities and selection rules

	$\Delta\pi = +1$			$\Delta\pi = -1$	
πL	M1	M1	M3	E1	E3
$\pi' L'$	E2	E2	E4	M2	M4
$\pi'' L''$	M3	E0	M5	E3	E5

Multipolarity (M) field: can contain a maximum of 3 multipolarities, including E0,E1,E2,...E6,M1,M2,...M6 (corresponding to electric monopole, electric/magnetic dipole, etc) or D,Q,... (dipole, quadrupole, etc.). To mark assumed, doubtful, and mixed multipolarities the following characters are used [] () + and ,(comma). Some typical combinations are listed in Table VIII. In the case of mixed multipolarity the lowest two multipole orders will be used by the program *BrIcc* to calculate the conversion coefficient. $E0+M1+E2$ transitions are treated differently. The *M1* or *E2* multipolarity is considered

first and the **E0** is considered last. If any non-standard character is present in the **M** field, the multipolarity (and mixing ratio) will be omitted.

Mixing Ratio (MR) field: The multipole mixing ratio, δ is defined as the ratio of two absolute transition amplitudes [1974AIAA]:

$$\delta(\pi' L' / \pi L) = \frac{\gamma(\pi' L')}{\gamma(\pi L)} \quad (1)$$

The + or - character in the **MR** field indicates that the sign of the mixing ratio is known.

In some cases three multipolarities can mix and in a similar way to Eqn. 1 one can define:

$$\delta(\pi'' L'' / \pi' L') = \frac{\gamma(\pi'' L'')}{\gamma(\pi' L')} \quad (2)$$

Valid combination of mixed multipolarities ($0 \leq L \leq 5$) are given in Table II.

In the case of $E0+M1+E2$ transitions the **MR** field is reserved for the $\delta(E2/M1)$ mixing ratio. The $E0, E2$ mixing ratio,

$$q^2(E0/E2) = \frac{I_K(E0)}{I_K(E2)} \quad (3)$$

can be specified in the GAMMA continuation record as **MRKE0E2**. *This term is yet to be defined in the ENSDF dictionary and manual.* Conversion coefficients for mixed multipolarity transitions with E0 component (M1+E2+E0, M1+E0, E2+E0, etc.) are calculated without the monopole contribution.

Similarly, mixed transitions with three multipole components of E1-E5, M1-M5 are treated as mixed transitions with two multipole components. The correct treatment of mixed transitions with three multipole or E0 component are planned in future release of *BrIcc*.

Mixing Ratio Uncertainty (DMR) field: A single integer or two integers with + and - signs in the **DMR** field will be interpreted as symmetric or asymmetric uncertainty values, respectively. In some cases the **DMR** field contains *GE, GT, LE, LT* or *AP* strings indicating a limit on **MR** or that **MR** is an approximation. Some examples of the coding and interpretation of the **MR** and **DMR** field are given in Table VIII. The asymmetric uncertainties of δ are only indicated if **MR** has either a + or a - sign and will be referred as $\Delta\delta_H$ and $\Delta\delta_L$.

Total Conversion Coefficient (CC) and Uncertainty (DCC) fields: If the multipolarity and mixing ratio are known, the total conversion coefficient is calculated by the *BrIcc* program. Numerical value of **CC** and the symmetric uncertainty is labeled as α_{tot} and $\Delta\alpha_{tot}$. **CC** will be placed onto the new **G** record if $\alpha_{tot}/(1 + \alpha_{tot}) \geq 10^{-4}$, otherwise it will be placed on the ‘**S G**’ GAMMA continuation record. If **CC** is derived purely from theoretical conversion coefficient the **DCC** field should be left blank on the **G** record. See Sec. IV for the calculation method used.

Relative Total Intensity (TI) and uncertainty (DTI) fields: If the photon intensity, I_γ , and the total conversion coefficient, α_{tot} are known, the relative total intensity, I_{tot} is defined as

$$I_{tot} = I_\gamma * (1 + \alpha_{tot}). \quad (4)$$

For pure $E0$ transitions I_{tot} is the sum of electron conversion (I_K, I_{L1}, \dots) and pair conversion I_{IPF} intensities. Higher order effects of electromagnetic transitions are usually neglected.

If the **TI** is given, values of the $K/T, L/T, \text{etc.}$ theoretical shell to total intensity ratios, are placed in the first set of **S G** records followed by a second set of **S G** records with conversion coefficient values.

B. GAMMA continuation records

The two basic types of the GAMMA continuation records are described below.

1. ‘2 G’ GAMMA continuation records

Any character, other than 1 or S in column 6 can be used to create a GAMMA continuation record. This record is intended to store quantities, which are not defined in the **G** record. Quantities which will be read in by *BrIcc* are marked in the Table. ‘2 G’ records are created by the ENSDF evaluators.

2. ‘S G’ GAMMA continuation records

TABLE III: Default mixing ratio values used by *BrIcc* when no MR is given.

Multipolarity	MR
E2/M1 (value can be changed, see VIII B)	1.0
M2/E1, M3/E2, M3/E2, E4/M3, M4/E3, E5/M4	0.1
E3/M2	1.0

This type of record, with a character ‘S’ in column 6, is a special type of continuation record which flags the Nuclear Data Sheets production code to suppress the data contained on it for the publication. *BrIcc* generates ‘S G’ records and the data on these records are used by other programs. Conversion coefficients and uncertainties are calculated as described in Sec. IV. Electron to total intensity ratios are calculated from the conversion coefficients.

The *BrIcc* program will scan the ‘S G’ records of the input ENSDF file. A warning message will be inserted into the calculation report file if any non-standard dictionary term is found. The non-standard quantity will be placed on a new ‘S G’. See Table

VII for the list of dictionary terms expected in ‘**S G**’ records. Please note that with the exception of RadList, none of the current ENSDF utility programs extract any numerical values from the ‘**S G**’ records.

IV. CALCULATION OF CONVERSION COEFFICIENTS

Electron conversion coefficients ($\alpha_K, \alpha_{L1}, \alpha_{L2}, \dots$ etc.) and electron–positron pair conversion coefficient (α_{IPF}) are calculated by *BrIcc*. Values for pure multipolarity transitions are obtained by a cubic spline interpolation of the tabulated values (see sec **V**). Input parameters, atomic number Z , transition energy E_γ and multipolarity are obtained by the program from the **IDENTIFICATION** record: **DSID**; from the **GAMMA** record: **NUCID, E, DE, M, MR** and **DMR** fields of the **G** records. The program will verify the values obtained from the above fields and will generate warning and error messages to help resolve coding errors. As this function of the program is not designed to carry out full checking of the ENSDF file, the use of *FmtChk*, prior to use *BrIcc* is highly recommended.

If no MR is given the program will use adopted mixing ratio values listed in Table **III**. In the case of E2/M1 transitions, the default value can be changed at the console dialogue (see sec. **VIII B**).

In some of the following cases *BrIcc* will not generate new **G** or **S G** (ε_{ic} denotes the binding energy for the ic-subshell): (a) $E_\gamma + \Delta E_H < \varepsilon_{ic}$ – no calculation for that subshell but new **G** and **S G** records are generated. (b) $E_\gamma - \Delta E_L \leq \varepsilon_{ic} + 1$ keV – no calculation for that subshell and NO new **G** or **S G** records are generated. (c) $Z < 5$ or $Z > 110$ (outside of the range of the tabulations) – no calculations and NO new **G** or **S G** records are generated. (d) $E_\gamma - \Delta E_L > 6000$ keV, the energy range of the tabulations (see table **V**) – no calculation for that subshell and NO new **G** or **S G** records are generated. (e) For some subshells the energy range of the tabulations less than 6000 keV. A warning is given for the user and no calculation for that subshell but new **G** and **S G** records are generated. For mixed ($\pi L + \pi' L'$) multipolarity transitions the conversion coefficient can be obtained from the following formula:

$$\alpha = \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1 + \delta^2}, \quad (5)$$

where $\alpha(\pi L)$ and $\alpha(\pi' L')$ are the conversion coefficients for the pure multipolarities to be mixed.

The (symmetric) uncertainty of the conversion coefficient, $\Delta\alpha$, is made up of a number of contributions. In some cases $\Delta\alpha$ uncertainty is asymmetric. In this cases the larger absolute value should be adopted for the symmetric uncertainty.

While evaluating conversion coefficients for sub shells (K, L1, L2,...) and major shells (L, M,..Tot) including pure and mixed multipolarities is relatively simple. However in the case of ratios of conversion coefficients special considerations are required. For mixed

multipolarity transitions the $R_{i/j} = \alpha_i/\alpha_j$ ratio is defined as

$$\frac{\alpha_i}{\alpha_j} = \frac{\alpha_i(\pi L) + \delta^2 \alpha_i(\pi' L')}{\alpha_j(\pi L) + \delta^2 \alpha_j(\pi' L')}. \quad (6)$$

Equations 12, 14, 16 and 18 given for the $R_{i/j} = \alpha_i/\alpha_j$ ratios are only valid if α_i and α_j are uncorrelated; i.e. i and j are different sub-shells or shells.

The $R_{i/tot} = \alpha_i/\alpha_{tot}$ ratio ($i=K, L, M, \dots$), involves the same sub-shell (shell) in the nominator and the denominator therefore the $\Delta R_{i/tot}$ uncertainty is affected by covariance between α_i and α_{tot} . To overcome this problem we have adopted the following approximation:

$$R_{i/tot} = \frac{\alpha_i}{\alpha_{tot}} = \frac{1}{1 + \sum_j \alpha_j/\alpha_i}, \quad (7)$$

where $i \neq j$ and

$$\Delta R_{i/tot} \approx \frac{\sqrt{\sum_j [\Delta(\alpha_j/\alpha_i)]^2}}{\alpha_{tot}}. \quad (8)$$

The $\Delta(\alpha_j/\alpha_i)$ uncertainties can be evaluated using one of the equations of 12, 14, 16, or 18.

If there is covariance between α_i and α_j , for example $i=K$ (α_K) and $j = tot$ (α_{tot}), the uncertainties are calculated in the following way. Let us define the ratio, x as

$$x = \frac{a}{a + b}. \quad (9)$$

The uncertainty, Δx can be expressed as:

$$\Delta x = \frac{\sqrt{(\Delta a \times b)^2 + (a \times \Delta b)^2}}{(a + b)^2}. \quad (10)$$

Considering a case when nuclear transition involves the emission of gamma-rays and internal conversion *via* K-, L- and M-shells, to evaluate the I_K/I_{tot} we get $a = \alpha_K$ and $b = 1 + \alpha_L + \alpha_M$.

$\Delta\alpha_{theo}$ By comparing the electron conversion coefficients of Band et al., [2002Ba85] to experimental values, Raman et al., [2002Ra45] have concluded, that the accuracy of the theoretical α values is in the range of 0-1 %.

We have no knowledge of any information on the accuracy of the other data tables (α_{IPF} , $\Omega(E0)$) used by *BrIcc*.

Additional uncertainty may be associated to the cubic spline interpolation used in the same way for all data tables.

We adopted a relative uncertainty of 1.36% for the electron pair conversion coefficients deduced from the tables. The same uncertainty is adopted for the ratio of conversion coefficients. The $\Delta\alpha_{theo}$ symmetric uncertainty incorporates both, the accuracy of the theoretical calculations and the accuracy of the interpolation. See Table IV.

$\Delta\alpha_{\mathbf{DE.H}}$,
 $\Delta\alpha_{\mathbf{DE.L}}$

The value of the conversion coefficient, α is obtained by interpolation at the nominal transition energy, E_γ . One can define the asymmetric uncertainties, $\Delta\alpha_{DE.H}$ and $\Delta\alpha_{DE.L}$, deduced from the differences in conversion coefficients obtained for E_γ , $E_\gamma + \Delta E_H$ and $E_\gamma - \Delta E_L$ energies. In the case when either $E_\gamma + \Delta E_H$ or $E_\gamma - \Delta E_L$ is outside of the energy range of the data tables, α values are calculated at the energy limit of the tabulation.

$$\begin{aligned}\Delta\alpha_{DE.H} &= \alpha(E_\gamma + \Delta E_H) - \alpha(E_\gamma), \\ \Delta\alpha_{DE.L} &= \alpha(E_\gamma - \Delta E_L) - \alpha(E_\gamma).\end{aligned}\quad (11)$$

For the conversion coefficient ratios of mixed multiplicities we obtain:

$$\begin{aligned}\Delta\left(\frac{\alpha_i}{\alpha_j}\right)_{DE.H} &= \frac{\alpha_i}{\alpha_j}(E_\gamma + \Delta E_H) - \frac{\alpha_i}{\alpha_j}(E_\gamma), \\ \Delta\left(\frac{\alpha_i}{\alpha_j}\right)_{DE.L} &= \frac{\alpha_i}{\alpha_j}(E_\gamma - \Delta E_L) - \frac{\alpha_i}{\alpha_j}(E_\gamma),\end{aligned}\quad (12)$$

where α_i and α_j are not correlated.

If **DE** is a limit, new ‘**S G**’ record will not be generated. In some cases **E** is equal to **DE**, which will be interpreted as only a limit is known for the transition energy and no calculations will be made.

$\Delta\alpha_{\mathbf{DMR.H}}$,
 $\Delta\alpha_{\mathbf{DMR.L}}$

In the case of mixed transitions, the uncertainties in the mixing ratio, $\Delta\delta_H$ and $\Delta\delta_L$, also contribute to $\Delta\alpha$. Depending on content of **DM** and **DMR** fields, the conversion coefficient, α and the $\Delta\alpha_{DMR.H}$ and $\Delta\alpha_{DMR.L}$ uncertainties associated with **DMR**, are determined in one of the following ways.

DMR is given as symmetric or asymmetric uncertainty. The conversion coefficient, α is calculated using Eqn. 5 and the uncertainties can be obtained as:

$$\begin{aligned}\Delta\alpha_{DMR.H} &= \frac{[\alpha(\pi L) + \delta_H^2 \alpha(\pi' L')]}{1 + \delta_H^2} - \frac{[\alpha(\pi L) + \delta^2 \alpha(\pi' L')]}{1 + \delta^2}, \\ \Delta\alpha_{DMR.L} &= \frac{[\alpha(\pi L) + \delta_L^2 \alpha(\pi' L')]}{1 + \delta_L^2} - \frac{[\alpha(\pi L) + \delta^2 \alpha(\pi' L')]}{1 + \delta^2},\end{aligned}\quad (13)$$

where $\delta_H = \delta + \Delta\delta_H$ and $\delta_L = \delta - \Delta\delta_L$.

The ratio of conversion coefficient, α_i/α_j is calculated according to Eqn. 6. The uncertainties calculated as:

$$\begin{aligned}\Delta\left(\frac{\alpha_i}{\alpha_j}\right)_{DMR.H} &= \frac{[\alpha_i(\pi L) + \delta_H^2 \alpha_i(\pi' L')]}{[\alpha_j(\pi L) + \delta_H^2 \alpha_j(\pi' L')]} - \frac{[\alpha_i(\pi L) + \delta^2 \alpha_i(\pi' L')]}{[\alpha_j(\pi L) + \delta^2 \alpha_j(\pi' L')]}, \\ \Delta\left(\frac{\alpha_i}{\alpha_j}\right)_{DMR.L} &= \frac{[\alpha_i(\pi L) + \delta_L^2 \alpha_i(\pi' L')]}{[\alpha_j(\pi L) + \delta_L^2 \alpha_j(\pi' L')]} - \frac{[\alpha_i(\pi L) + \delta^2 \alpha_i(\pi' L')]}{[\alpha_j(\pi L) + \delta^2 \alpha_j(\pi' L')]}.\end{aligned}\quad (14)$$

$\Delta\alpha_{\text{DMR.H}}$,
 $\Delta\alpha_{\text{DMR.L}}$
Continued

Cases when the $\delta - \Delta\delta_L$ or $\delta + \Delta\delta_H$ overlaps with $\delta = 0.0$ requires further attention. For signed values of **MR** the program will adopt $\delta_L = 0$ if $\text{sign}(\delta)=+1$, or $\delta_H = 0$ if $\text{sign}(\delta)=-1$. For unsigned values of **DMR** the program will adopt $\delta_L = \text{Max}(\delta - \Delta\delta_L, 0)$.

DMR is a lower limit.

$$\alpha = \left[\alpha(\pi'L') + \frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1 + \delta^2} \right] \times 0.5,$$

$$\Delta\alpha_{\text{DMR.H}} = \Delta\alpha_{\text{DMR.L}} = \left| \alpha(\pi'L') - \frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1 + \delta^2} \right| \times 0.5. \quad (15)$$

In this case $\Delta\alpha_{\text{DE.H}}$ and $\Delta\alpha_{\text{DE.L}}$ are deduced from the differences in $\alpha(\pi L)$ and $\alpha(\pi'L')$, obtained for energies of E_γ , $E_\gamma + \Delta E_H$ and $E_\gamma - \Delta E_L$.

For the ratios of conversion coefficients one can obtain the following relations:

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

$$\Delta\alpha_{\text{DMR.H}} = \Delta\alpha_{\text{DMR.L}} = \left| \frac{\alpha_i(\pi'L')}{\alpha_j(\pi'L')} - \frac{\alpha_i(\pi L) + \delta^2\alpha_i(\pi'L')}{\alpha_j(\pi L) + \delta^2\alpha_j(\pi'L')} \right| \times 0.5. \quad (16)$$

DMR is an upper limit.

$$\alpha = \left[\frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1 + \delta^2} + \alpha(\pi L) \right] \times 0.5,$$

$$\Delta\alpha_{\text{DMR.H}} = \Delta\alpha_{\text{DMR.L}} = \left| \frac{\alpha(\pi L) + \delta^2\alpha(\pi'L')}{1 + \delta^2} - \alpha(\pi L) \right| \times 0.5. \quad (17)$$

In this case $\Delta\alpha_{\text{DE.H}}$ and $\Delta\alpha_{\text{DE.L}}$ are deduced from the differences in $\alpha(\pi L)$ and $\alpha(\pi'L')$, obtained for energies of E_γ , $E_\gamma + \Delta E_H$ and $E_\gamma - \Delta E_L$.

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

$$\Delta\alpha_{\text{DMR.H}} = \Delta\alpha_{\text{DMR.L}} = \left| \frac{\alpha_i(\pi L) + \delta^2\alpha_i(\pi'L')}{\alpha_j(\pi L) + \delta^2\alpha_j(\pi'L')} - \frac{\alpha_i(\pi L)}{\alpha_j(\pi L)} \right| \times 0.5. \quad (18)$$

MR is an approximate value or derived from systematics, DMR is empty, an approximate value ('AP'), derived from systematics ('SY'), or calculated ('CA'). The conversion coefficient, α is calculated using Eqn. 5 and $\Delta\alpha_{\text{DMR.H}} = \Delta\alpha_{\text{DMR.L}} = 0$. **DCC** field is set to **DMR** if it is not empty ('AP', 'SY', or 'CA').

$\Delta\alpha_{\text{DMR},H}$,
 $\Delta\alpha_{\text{DMR},L}$
Continued

No MR is given. For cases when $L \neq L'$ (for example M1+E2 or M1,E2) δ is set according to Table III and the conversion coefficient, α and the uncertainty can be obtained as:

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

$$\Delta\alpha_{\text{DMR},H} = \Delta\alpha_{\text{DMR},L} = \left| \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1 + \delta^2} - \alpha(\pi L) \right|. \quad (19)$$

For the ratios of conversion coefficients one can obtain the following relations:

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

$$\Delta\alpha_{\text{DMR},H} = \Delta\alpha_{\text{DMR},L} = \left| \frac{\alpha_i(\pi L) + \delta^2 \alpha_i(\pi' L')}{\alpha_j(\pi L) + \delta^2 \alpha_j(\pi' L')} - \frac{\alpha_i(\pi' L')}{\alpha_j(\pi' L')} \right|. \quad (20)$$

M valid, but not unique multipolarity and $L \equiv L'$ (for example M1,E1). α and $\Delta\alpha$ are calculated using the following equation:

$$\alpha = [\alpha(\pi L) + \alpha(\pi' L')] \times 0.5,$$

$$\Delta\alpha_{\text{DMR},H} = \Delta\alpha_{\text{DMR},L} = |\alpha(\pi L) - \alpha(\pi' L')| \times 0.5. \quad (21)$$

For the ratios of conversion coefficients one can obtain the following relations:

$$\frac{\alpha_i}{\alpha_j} = \frac{\alpha_i(\pi L) + \alpha_i(\pi' L')}{\alpha_j(\pi L) + \alpha_j(\pi' L')},$$

$$\Delta\alpha_{\text{DMR},H} = \Delta\alpha_{\text{DMR},L} = \left| \frac{\alpha_i(\pi L)}{\alpha_j(\pi L)} - \frac{\alpha_i(\pi' L')}{\alpha_j(\pi' L')} \right| \times 0.5. \quad (22)$$

M contains dipole (D), quadrupole (Q), octupole (O), and their combinations. No α or $\Delta\alpha$ are calculated and no new ‘G’ or ‘S G’ card will be generated.

A special case when the transition energy E is an approximate value. DE is empty, an approximate value (‘AP’), derived from systematics (‘SY’), or calculated (‘CA’). The conversion coefficient, α is calculated using Eqn. 5 and $\Delta\alpha_{\text{DMR},H} = \Delta\alpha_{\text{DMR},L} = 0$. DCC field is set to DE if is not empty (‘AP’, ‘SY’, or ‘CA’).

Combining the $\Delta\alpha_{\text{theo}}$, $\Delta\alpha_{\text{DE},H}$, $\Delta\alpha_{\text{DE},L}$, $\Delta\alpha_{\text{DMR},H}$ and $\Delta\alpha_{\text{DMR},L}$ partial values the symmetric uncertainty of the conversion coefficient is given as:

$$\Delta\alpha = \sqrt{(\Delta\alpha_{\text{theo}})^2 + (\Delta\alpha_{\text{DE}})^2 + (\Delta\alpha_{\text{DMR}})^2}, \quad (23)$$

where

$$\Delta\alpha_{\text{DE}} = \text{Max}(|\Delta\alpha_{\text{DE},H}|, |\Delta\alpha_{\text{DE},L}|), \quad (24)$$

$$\Delta\alpha_{\text{DMR}} = \text{Max}(|\Delta\alpha_{\text{DMR},H}|, |\Delta\alpha_{\text{DMR},L}|).$$

The DCC field of the new GAMMA record will be blank if the contribution of the $\Delta\alpha_{\text{DE},H}$, $\Delta\alpha_{\text{DE},L}$, $\Delta\alpha_{\text{DMR},H}$ and $\Delta\alpha_{\text{DMR},L}$ terms are insignificant compared to the $\Delta\alpha_{\text{theo}}$ term.

If the total conversion coefficient, $\alpha_{tot} \geq 10^{-4}$, then it will be inserted into the **CC** field of the **G** record. The uncertainty on the total conversion coefficient will be given (a) for mixed multipolarity transitions, or (b) if the relative uncertainty on the total conversion coefficient, $\Delta\alpha_{tot}/\alpha_{tot}$ is larger than 10^{-4} . The cut-off on α_{tot} can be changed at the terminal dialogue (see sec. 1). *BrIcc* will append further quantities onto the ‘**S G**’ record(s).

The program *BrIcc* will generate ‘**S G**’ continuation records if the conversion coefficient can be calculated. If $\alpha_{tot} < 10^{-4}$, α_{tot} and $\Delta\alpha_{tot}$ will be put on the first ‘**S G**’ continuation record. If the total intensity field, **TI** on the **G** record is empty (i.e. I_{tot} is not given) the conversion coefficient for the major shells, α_K , α_L , and α_M will be listed. Additional ‘**S G**’ continuation record(s) will be created to list the α_N , α_O , α_P , α_Q , α_R and α_{IPF} conversion coefficients individually.

If the total intensity, I_{tot} , **TI** is given, *BrIcc* will append to the first **S G** continuation record the I_K/I_{tot} , I_L/I_{tot} , I_M/I_{tot} and I_{N+}/I_{tot} intensity ratios. Additional ‘**S G**’ continuation record(s) will be generated for intensity ratios involving the N, O, P, Q, R and S shells and electron-positron pair production. (For consistency, the conversion coefficients will be also listed on separate **S G** continuation records.) For example for the K-shell we get:

$$\frac{I_K}{I_{tot}} = \frac{\alpha_K}{1 + \alpha_{tot}}. \quad (25)$$

TABLE IV: Theoretical tabulations of internal conversion coefficients and electronic factors used by *BrIcc*. The adopted accuracy of the tabulations, $\Delta\alpha_{theor}$ [2008Ki07], including the uncertainty of the interpolation, is given in percentage. The number of significant digits (D) is also listed.

Tabulations	$\Delta\alpha_{theor}$ [%]	D	Z	Shell or IPF	L	E_γ^a [keV]
Internal conversion coefficient (α_{ic})						
BrIccFO “Frozen Orbitals” approximation [2002Ba85, 2002Ra45]	1.4	4	5 – 110	All	1 – 5	$\epsilon_{ic}+1 - 6000$
BrIccNH “No-Hole” approximation [2002Ba85, 2002Ra45]	1.4	4	5 – 110	All	1 – 5	$\epsilon_{ic}+1 - 6000$
HsIcc Hager and Seltzer [1968Ha53] and Dragoun <i>et al.</i> [1971Dr11]	3.0	3	30 – 103	K, L, M, N+	1 – 4 ^b	$\epsilon_{ic}+1 - 1500^c$
RpIcc Rösel <i>et al.</i> [1978Ro22, 1978Ro21]	3.0	3	30 – 104	All	1 – 4	$\epsilon_{ic}+2 - 3000^d$
Pair conversion coefficient (α_π)						
ScPcc Schlüter and Soff [1979Sc31]	1.4	4	0 – 100 ^e	IPF	1 – 3	1100 – 8000
HoPcc Hofmann and Soff [1996Ho21]	1.4	4	50 – 100	IPF	1 – 3	1100 – 8000
Electronic factor ($\Omega(E0)$)						
HsOmg	None	3	30 – 102 ^{f,g}	K ^h ,	0	$\epsilon_{ic}+6 - \epsilon_{ic}+1500$

TABLE IV: continued

Data Table	$\Delta\alpha_{theor}$ [%]	D	Z	Shell or IPF	L	E_{γ}^a [keV]
Hager and Seltzer [1969Ha61]				L1 ⁱ , L2 ⁱ		
BeOmg	None	4	40 – 102 ^g	K	0	51 ^j – 2555
Bell <i>et al.</i> [1970Be87]			40 – 102 ^g	L1, L2	0	51 – 2555
PaOmg	None	4	8 – 40 ^g	K ^h	0	511 – 12775
Passoja and Salonen [1986PaZM]			8 – 40 ^g	IPF	0	1430.8 – 12775

^a ϵ_{ic} is the binding energy for the ic-shell.

^b K-, L- and M-shell ICC values for L=3 and 4 multiplicities have not been scaled as recommended by Németh and Veres [1990Ne01].

^c For K-shell: $\epsilon_{ic}+1 - 1500(1650)$ keV; for L-shell: $\epsilon_{ic}+1 - 1000(1550)$ keV; for M-shell: $\epsilon_{ic}+1 - 150(510)$ keV; for N+ shell: 50 – 500 keV.

^d For K-shell: $\epsilon_{ic}+2 - 3000(5000)$ keV; for L-shell: $\epsilon_{ic}+2 - 1500$ keV; for M-, N-, O-, P- and Q-shells: $\epsilon_{ic}+2 - 500(1500)$ keV.

^e Used for $Z < 50$.

^f Calculated for every fourth Z-value.

^g For even Z only.

^h Not used.

ⁱ Used for $Z < 40$.

^j For Z=40 – 58: 51.1 keV; for Z=60 – 82: 102.2 keV; for Z=84 – 96: 153.3 keV and for Z=98 – 102: 204.4 keV.

V. DATA TABLES

The data tables have been assembled from different sources and are described in detail in [2008Ki07]. The main features, including the source, ranges, adopted accuracy of the tabulation are summarized in Table IV.

Using the above tabulations (data tables) four data sets have been assembled for the various implementations of **BrIcc**. These are listed in Table V. The use of the default data set, **BrIccFO**, adopted for the ENSDF evaluations is highly recommended.

For each data table two binary computer files have been created: (a) an index file, (“*.idx”), and (b) a large data file, (“*.icc”). The structure of these files is given in Appendix V.

VI. DEVELOPMENT NOTES

The program **BrIcc** have been written in Fortran 90 and was compiled using the 32 bit Intel Fortran compiler for a number of operating systems, including Win32, Linux and Machintosh. Practically the same source code is used for all platforms. This would allow to obtain identical numerical values, however we are aware that in a small number of cases differences were noted. It was also reported, that **BrIcc**, originally compiled for 32 bit systems was successfully running on a 64 bit machines.

TABLE V: Data tables used by **BrIcc**

Data set	Coefficient	Data table	Program versions
BrIccFO (Default & Recommended)	α_{ic} α_{π} $\Omega_{ic,\pi}$	BrIccFO ScPcc, HoPcc HsOmg, BeOmg, PaOmg	<i>BrIcc, BrIccS</i>
BrIccNH	α_{ic} α_{π} $\Omega_{ic,\pi}$	BrIccNH ScPcc, HoPcc HsOmg, BeOmg, PaOmg	<i>BrIcc, BrIccS</i>
HsIcc	α_{ic}	HsIcc	<i>BrIccS</i>
RpIcc	α_{ic}	RpIcc	<i>BrIccS</i>

BrIcc – Stand alone version for ENSDF evaluations.

BrIccS – Slave version.

External libraries used to develop the code include:

NSDFLIB library: Nuclear Structure Data File Library, developed by the National Nuclear Data Center, Brookhaven National Laboratory and can be downloaded from

http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/nsdfplib/

F2KCLI library: a free implementation of the proposed Fortran F2003 command line interface, developed by Interactive Software Services Ltd. and can be downloaded from <http://www.winteracter.com/f2kcli>

VII. INSTALLATION OF BRICC

The so called stand alone version of **BrIcc** program package can be obtained from:

NSDD: http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc/

IAEA: https://www-nds.iaea.org/public/ensdf_pgm/index.htm

The distribution packages contain the following files:

BrIcc.exe – 32 bit binary executable file for Windows

bricc – 32 bit binary executable file for Linux or Machintosh

BrIccV22FO.icc – binary ICC data file; “Frozen Orbitals” approximation

BrIccV22FO.idx – binary pointer (index) file

BrIccV22NH.icc – binary ICC data file; “No-Hole” approximation

BrIccV22NH.idx – binary pointer (index) file

BrIccV23Manual.pdf – program manual (this document)

Please note, that the name of the binary executable is the same as in the previous versions, but the ICC data files and the manual has been changed. It is strongly recommended to back-up and uninstall the previous version of **BrIcc**.

A. Windows systems

The programs are compatible with all 32 bit version of the Windows operating systems. The self-extracting program archive will install the **BrIcc** program, the data files and the manual into a directory which can be selected during installation. **Note:** On 64 bits systems do not use the *C:\Program Files(X86)* folder, reserved for 64 bit applications. The installation script will create a **BrIcc** program group and will also set the “*BrIccHome*” and “*Path*” environment variables. To locate the data file the **BrIcc** program use the *BrIccHome* environment variable pointing to the directory, where the program and the data files are. In a typical installation, this directory is *C:\Program Files\BrIcc*. To enable the execution of **BrIcc** on the Command Prompt window from any working directory, the installation directory should be included into the Path variable.

To upgrade the program, please uninstall the previous version using the “*Uninstall*” link provided in the **BrIcc** program group.

To test the program first test that the *BrIccHome* environment variable has been correctly set. On a Command Prompt (DOS window) to test the environment variables type

```
SET<CR>
```

and to test the path variable type

```
PATH<CR>.
```

To launch **BrIcc** from the *Start/Programs/BrIcc* menu or on a Command Prompt type **BrIcc**<CR>. Do not forget to adjust the width of the screen to print long (120 character) lines.

B. Linux and Machintosh

The procedure to install *BrIcc* for Linux and Machintosh are identical. Create the main directory for the programs (for example */usr/local/bin/bricc*). then download the distribution package, a tarred, gzipped file onto that directory. Un-tar and un-zip all program and data files into this directory. *BrIcc* requires an environment variable *BrIccHome* to be set in order to locate the data files. Use the following bash script to set the environment variables:

```
# Script to set up BRICC using bash like shells -----  
  
# make new bin dir if not already there  
BINDIR=~ /bin;  
if [ ! -d "$BINDIR" ]; then  
    mkdir $BINDIR  
fi  
  
# add path variables to bashrc  
if [ -z "${PATH}" ]; then  
#   PATH=~ /bin; export PATH  
    echo ' ' >> ~/.bashrc
```



```

    echo 'export PATH=~/.bin' >> ~/.bashrc
else
#   PATH=/bin:$PATH; export PATH
    echo ' ' >> ~/.bashrc
    echo 'export PATH=~/.bin:$PATH' >> ~/.bashrc
fi
# End script -----

```

To test the program on the console window type *bricc* < CR >. Adjust the width of the screen to print long (120 character) lines.

VIII. RUNNING BRICC - STAND ALONE PROGRAM

BrIcc, a console application which can be used in three different ways, as described below. Typical terminal dialogues on the different operating systems are very similar, however the examples provided below are from a Win32 system. (<CR> indicates the enter key.) To obtain quick information on how to run the program use the following command on the terminal: **BrIcc ?** <CR>.

A. Interactive use

The interactive use of **BrIcc** is illustrated in Fig. 1.

B. ENSDF evaluation tool – creating new records

This mode of operation is designed to create new **G**, **G/SG** and **G/2 G** records with conversion coefficients calculated for the given nuclear transition:

BRICC <i>ENSDF-file</i> <CR>	This command will load the default BrIccFO data table and will generate new cards for gamma transitions listed in <i>ENSDF-file</i> .
BRICC <i>ENSDF-file</i> BrIccNH <CR>	As above, but using the BrIccNH data table.

Notes:

- (a) The *ENSDF* file name and other program arguments are passed as program argument. A typical terminal dialog can be seen in Fig. 2.
- (b) The input *ENSDF* file should not be modified before running the code in the MERGE mode (see sec. VIII C).
- (c) For every *ENSDF* data set a **DG** record will be created with information on the program version and the data table (BrIccFO or BrIccNH) used. The record is usually located immediately after the HISTORY record. The program also will replace this record if it is required.
- (d) Set the working directory (path) on the Command prompt (Windows) or on the Console (Linux/UNIX) to the directory where the *ENSDF* file is. This will allow one to have all input and output files in the same directory.

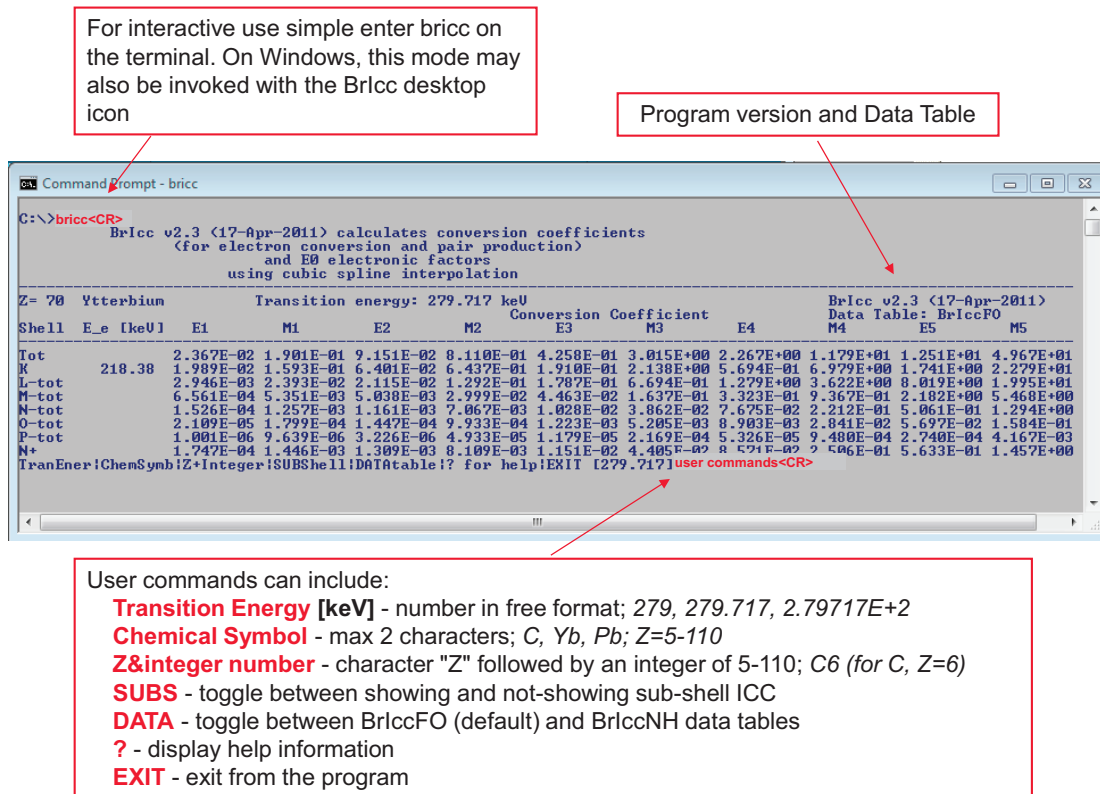


FIG. 1. Typical interactive terminal dialogue.

Output files:

- Calculation report:** Complete report of calculations. Default file: *BRICC.LST*.
- New G/SG records:** New G/2 G records generated by the program, followed by the record number in the ENSDF input file. This is used as input to the program running as a utility to MERGE records. Default file: *CARDS.NEW*. Please note the format of the file has been changed for version 2.3 and higher. The header lines starting with the hash (“#”) character contains information on the input file, the data set and the program version used. Each 80 character long ENSDF records is followed by the relevant record number and a single character indicating that the original ENSDF record will be replaced, deleted, or a new record will be inserted.
- G/SG (New/Old) comparison report:** Comparison of new and old G/2 G records. Default file: *COMPAR.LST*.

Execution control:

- List conversion coefficients for all subshells (Def. N):** The default is to only list the total conversion coefficients for the shell. Answering Yes (Y) will list all the subshell conversion coefficients in addition to the totals. Note that for higher atomic numbers this may be a very extensive list.
- Calculate conversion coefficients for all transitions (Def. N):** The default is

```

C:\Windows\system32\cmd.exe
C:\ENSDF>bricc 201Hg.ens<CR>
BrIcc v2.3 (28-Jun-2013) 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: 201Hg.ens

Output Files:
Complete calculations report, (Def: BrIcc.lst): <CR>
New G/SG records, (Def: Cards.new): <CR>
G/SG (New/Old) comparison report, (Def: Cmpar.lst): <CR>

Execution control:
List conversion coefficients for all subshells (Def. N): <CR>
Calculate conversion coefficients for all transitions (Def. N): <CR>
Lowest CC value to be put on G-card (Def. 1.00E-04): <CR>
Assumed value MR for E2/M1 transitions (Def. 1.00): <CR>

Processing started. Please wait.

Processing a new data set
1 : 201HG 201IL EC DECAY
30 : 201HG G 1.5648 10 M1+E2 0.015 6 4.7E+4 7
<W> Transition energy is within 1 keU to one of the shell binding energies.
37 : 201HG G 26.34 7 0.086 9 M1<+E2> 0.02 LT 76.1 7
<I> Uncertainties on ICC's from transition energy uncertainty is greater than 1.0%.
46 : 201HG G 5.84
50 : 201HG G 30.60 3 2.53 5 M1+E2 +0.011 4 48.5 2
54 : 201HG G 32.19 3 2.58 5 M1+E2 +0.017 4 41.9 2
62 : 201HG G 135.34 4 25.65 18 M1+E2 -0.060 10 3.45
66 : 201HG G 141.1 2 0.063 20 IE21 1.41
70 : 201HG G 165.88 7 1.55 5 M1<+E2> 0.4 LT 1.86 8
73 : 201HG G 167.43 7 100 M1+E2 0.08 +3-5 1.89 1

BrIcc finished processing 201Hg.ens
Processed:
#DataSets : 1
#AllRecords : 76
#GammaRecords : 9
#Errors : 0
#Warnings : 2
Skipped:
#DataSets : 0

C:\ENSDF>

```

FIG. 2. Terminal dialogue of the *BrIcc* evaluation tool.

to only calculate the conversion coefficients when a definite set of conversion coefficients may be obtained; see the discussion on warnings below when **BrIcc** is unable to do this and Table VIII for examples of when this will be done. To obtain a table of the E1-E5 and M1-M5 conversion coefficients for transitions with an unknown multipolarity or non-unique multipolarity answer Yes (Y). Note that for those transitions where a definite set of conversion coefficients may be obtained the output will remain unchanged from the default and new records will still be generated.

- (c) **Lowest CC value to be put on G-card (Def. 1.0E-4):** The total conversion coefficient will be inserted onto the G-card, so other programs can be used to calculate total transition intensity, intensity balance, etc (see III A). In many cases the CC value is too, therefore it is not practical to be used. The the cut-off value of the CC values shown in the ENSDF files is 1.00E-04. The user can change this value by entering a valid Fortran number, or just press enter to use the default value. NOTE: The cut-off CC value will be listed in the calculation report (BrIcc.lst).
- (d) **Assumed value MR for E2/M1 transitions (Def. 1.0):** If no MR is given BrIcc will use default values given in III. To specify different MR value for E2/M1 transitions enter a valid positive Fortran number. NOTE: The default MR value should be between 0.0 and 1.0 and it will be recorded on two G-comment records generated by *BrIcc*.

The program will process all data sets in the ENSDF file, except the IONIZED ATOM, COMMENTS and REFERENCES data sets. In the calculation report gamma-rays of a data set will be listed by increasing transition energy for each data set. (**NOTE: BrIcc** will create a binary file, *BrIcc.tmp* to store temporarily calculation reports. This file will be deleted automatically when the program terminated.)

Different type of messages are given on the console window and in the calculations report file. These messages are designed to inform the evaluator and to assist to resolve conflicts or errors in the ENSDF file.

- < I > For information only. Calculations of new ICC's are carried out and new **G** and **S G** cards are generated.
- < W > Warnings are given if the ENSDF records are correct, but some of the fields contain non-unique information or, in some cases, when calculations of the ICC values could not be carried out this is indicated in the message. For example the **M** field contains $D+Q$, or transition energy (including its uncertainty) is outside the range of **BrIcc** tables.
- < E > An error is detected either on the **G**, or **G**-continuation, or on the **IDENT**ification card. As the program progressively scans through these records, the rest of the record will not be scanned.
- < F > Reserved for indicating, that **BrIcc** encountered an internal programming error. In such a case please forward the ENSDF data set and the error message to the authors.

C. ENSDF evaluation tool – MERGEing new and old records

This program merges the new (corrected) **G**-records with the input ENSDF data set to create an updated data set.

`BRICC ENSDF-file MERGE<CR>` This command will merge; insert new records and/or replace old records in the *ENSDF-file*.

Notes: The ENSDF file name is passed as program argument. The input *ENSDF* file should not be modified before running the code in the MERGE mode.

Input file: File of new **G**-records created by **BrIcc**. Before running the merge utility, one can delete unwanted **G**-records. Default file: *CARDS.NEW*

Output files: Updated file in ENSDF format with new **G**-records inserted into the designated position. Default file: *CARDS.MRG* The ENSDF output files generated by HSICC and **BrIcc** are not identical because (a) the conversion coefficient values are different; and (b) in the latter case a number of new quantities, for example **IPC**, are on the new **S G** cards.

Terminal dialog: (see Fig. 3)

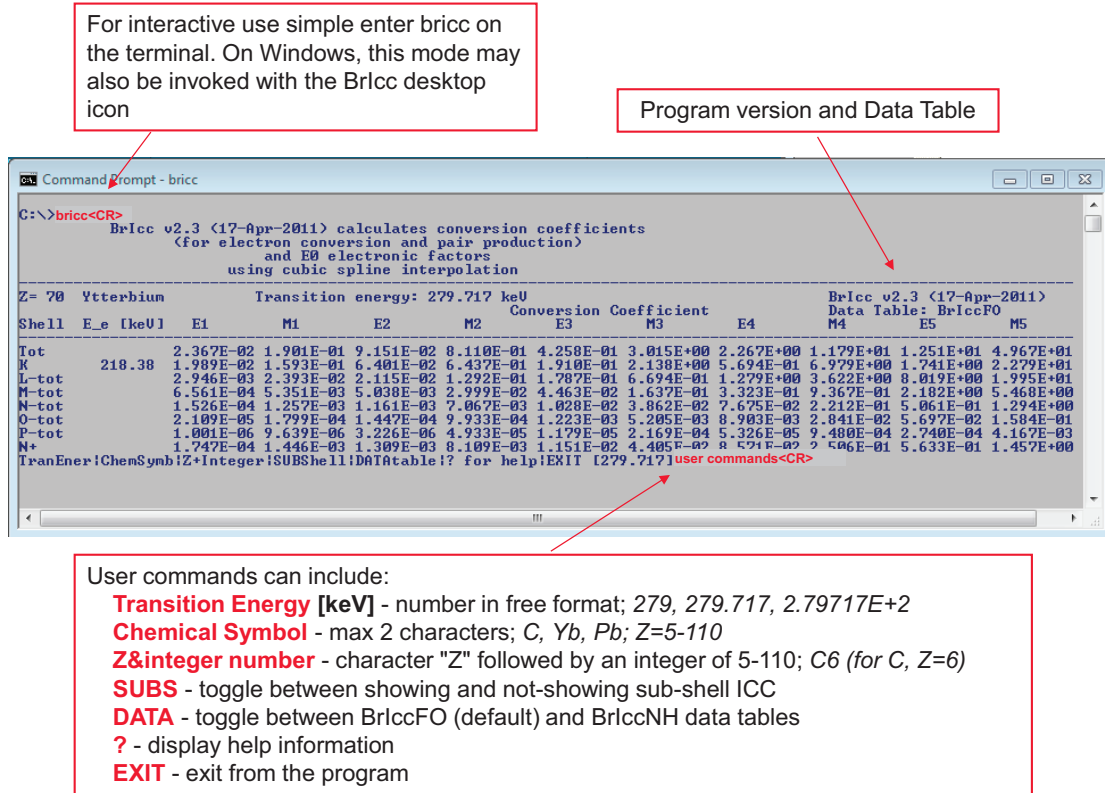


FIG. 3. *BrIcc* – ENSDF merge tool terminal dialog.

IX. RUNNING BRICCS - SLAVE PROGRAM

The slave version, *BrIccS*, a self contained executable is available to obtain conversion coefficients from applications developed using any programming language. Options with control parameters, separated by spaces, are passed at the command line. Control parameters can be integer numbers [*int*], integer or real numbers in free format [*number*], symmetric/assymmetric uncertainties given in the Nuclear Data Sheet style [*unc*], or character strings [*string*].

- Z** [*int*] Atomic number, see Table IV for valid ranges.
- g** [*number*] Transition energy in keV.
- e** [*unc*] Uncertainty in transition energy.
- L** [*string*] Pure or mixed multipolarity (max. 2) of $E0$, $E1$ – $E5$, $M1$ – $M5$. If option omitted, values for all pure multiplicities will be listed.
- d** [*number*] Mixing ratio. If omitted program will use an assumed value from Table III.
- u** [*unc*] Uncertainty in Mixing ratio.
- a** List values for all subshells.
- w** [*string*] Conversion data table to be used (see Table IV).
BrIccFO or *BrIccNH*: will also return α_π and $\Omega(E0)$ values.
HsIcc or *RpIcc*: only conversion coefficients being evaluated.
 If option omitted, the default data table of *BrIccFO* will be used.

Example 1: 1063.656(3) keV, M4+E5, $\delta=+0.020(10)$ transition in $^{207}_{82}\text{Pb}_{125}$. Format of

the command line:

```
briccs -Z 82 -g 1063.656 -e 3 -L M4+E5 -d +0.020 -u 10 -a -w BrIccFO
```

Part of the output produced by *BrIccS* is shown below:

```
<BRICC version="BrIcc v2.1 (23-Nov-2007)">
  <ELEM z="82" symb="Pb"> Lead </ELEM>
  <DATASET icc="BrIccFO"> </DATASET>
  <MULT mult1="M4" mult2="E5"> M4+E5 </MULT>
  <MR dmrh="+10" dmrl="-10"> +0.020 </MR>
  <E de="3"> 1063.656 </E>
  <MixedCC
    Shell="Tot"
    CCmult1="1.262E-01"
    CCmult2="5.773E-02"
    DCC="18">
    0.1262
  </MixedCC>
  <MixedCC
    Shell="K"
    Eic="975.65"
    CCmult1="9.462E-02"
    CCmult2="3.609E-02"
    DCC="14">
    0.0946
  </MixedCC>
  ...
</BRICC>
```

Example 2: 74 keV transition in osmium ($Z=76$). The transition energy is within 1 keV to the K-shell binding energy of 73.871 keV, therefore the α_K , the α_T and $\Omega_K(E0)$ values could not be evaluated. Format of the command line:

```
briccs -Z 76 -g 74 -a
```

Output list (partial and longer lines broken into two):

```
<BRICC version="BrIcc v2.1 (23-Nov-2007)">
  <ELEM z="76" symb="Os"> Osmium </ELEM>
  <DATASET icc="BrIccFO" omge0="Be0mg"> </DATASET>
  <E> 74 </E>
  <WARNING type="E"> Transition energy is within 1 keV to one of
    the shell binding energies. </WARNING>
  <AllCC
    Shell="K"
    Eic="0.13">
    <WARNING type="E"> EG is too close to the K-shell binding
      energy of 73.871 keV </WARNING>
  </AllCC>
  <AllCC
    Shell="L1"
```

```

    Eic="61.03">
    <MultCC Mult="E1" > 6.892E-02 </MultCC>
    <MultCC Mult="M1" > 1.634E+00 </MultCC>
    <MultCC Mult="E2" > 1.769E-01 </MultCC>
    <MultCC Mult="M2" > 3.073E+01 </MultCC>
    <MultCC Mult="E3" > 4.968E+00 </MultCC>
    <MultCC Mult="M3" > 3.604E+02 </MultCC>
    <MultCC Mult="E4" > 1.207E+02 </MultCC>
    <MultCC Mult="M4" > 3.895E+03 </MultCC>
    <MultCC Mult="E5" > 2.024E+03 </MultCC>
    <MultCC Mult="M5" > 4.146E+04 </MultCC>
  </AllCC>
  ...
  <OmgE0
    Shell="L1"
    Eic="61.03">
    1.063E+10
  </OmgE0>
  ...
</BRICC>

```

The output complies with the XML syntax and using parser routines the conversion coefficients (and uncertainties), the shell identifiers, electron kinetic energies, error or warning messages, *etc.* can be retrieved. Uncertainties are given in the Nuclear Data Sheet style. The above examples contains all *XML* entities currently defined for *BrIccS*.

-
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http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/BrIcc
- [BrIcc-ANU] The *BrIcc* web interface: <http://bricc.anu.edu.au/>

Appendix A: ENSDF GAMMA record

TABLE VI: The definition of the fields of the GAMMA record, taken from [2001TuZZ].

Field	Name	Description
1-5	NUCID	Nuclide identification
6		Blank or continuation character
7		Must be blank
8	G	Letter G is required
9		Must be blank
10-19	E	Energy of the γ -ray in keV
20-21	DE	Standard uncertainty in E
22-29	RI	Relative photon intensity
30-31	DRI	Standard uncertainty in RI
32-41	M	Multipolarity of transition
42-49	MR	Mixing ratio, δ .
50-55	DMR	Standard uncertainty in MR
56-62	CC	Total conversion coefficient
63-64	DCC	Standard uncertainty in CC
65-74	TI	Relative total transition intensity
75-76	DTI	Standard uncertainty in TI
77	C	Comment FLAG
78	COIN	Letter C denotes placement confirmed by coincidence. Symbol ? denotes questionable coincidence.
79		Blank
80	Q	The character ? denotes an uncertain placement

Appendix B: ENSDF GAMMA continuation record

TABLE VII: The definition of the fields of the GAMMA continuation record, taken from [2001TuZZ].

Field	Name	Description
1-5	NUCID	Nuclide identification
6		Any alphanumeric character other than 1. NOTE: 'S' is reserved for records not shown in the Nuclear Data Sheets
7	G	Must be blank
8		Letter G is required
9		Must be blank
10-80	DATA	Allowed quantities The general form of a data entry as described on p. 33 of [2001TuZZ] is: $\langle quant \rangle \langle op \rangle \langle value \rangle [\langle op \rangle \langle value \rangle][\langle ref \rangle]$ <p>G continuation record – any character other than 1 or S in column 6 E, DE^a, RI, DRI, M, MR^a, DMR^a, CC^a, DCC^a, TI, DTI, C, COIN, Q, BE1, BE2, ...; BE1W, BE2W, ...; BM1, BM2, ...; CE, CEK, CEL, ...; CEL1, ...; ECC^a, EKC^a, ELC^a, EL1C^a, EL2C^a, EKLC^a, EKL1C^a ...; FL, FLAG</p> <p>S G records – character 'S' in column 6 BrIcc will scan the existing 'S G' records and validate and will replace the Data entries, if they comply with the following rules:</p> <p>(a) TI not given in G record and M is known On the first S G record: CC, KC, LC, MC (electron conversion coefficients) On additional S G records: NC, OC^b, PC^b, QC^b and RC^b (electron conversion coefficients) and IPC (pair conversion coefficient^b) Obsolete data entries also verified and will be removed, including: LC+, M+, MC+, M+, NC+ and N+.</p> <p>(b) TI given in G record and M is known On the first S G record: CC (if no value is given in the G record) and K/T, L/T, M/T (intensity ratios) On additional S G records: N/T, O/T, P/T, Q/T and R/T and IP/T (internal pair to total intensity ratio^b) Obsolete data entries also verified and will be removed, including: LC/T, L+/T, MC/T, M+/T, N+/T, NC+/T, P+/T and a warning will be issued.</p> <p>Any other data entry or text will be copied onto new S G records and will be inserted as new.</p>

^a – *BrIcc* will read and interpret its numerical value.

^b – To be declared in *ENSDF* dictionary and manual.

Appendix C: Typical values of the M, MR and DMR fields of the GAMMA record

TABLE VIII: Typical values of the multipolarity (M), Mixing ratio (MR) and uncertainty (DMR) fields of the **G** record.

M	MR	DMR	Multipolarity assignment
M1			Definite M1
(M1)			Uncertain M1
[E2]			Assumed E2
M1+E2	2.5	7	M1 plus E2, definite $\delta(E2/M1) = 2.5(7)$, symmetric uncertainty
M1+E2	+0.014	+15-12	Mixed M1 plus E2, definite, $\delta(E2/M1) = +0.14^{+15}_{-12}$, asymmetric uncertainty
M1+E2	2.5	LE	M1 plus E2, definite $\delta(E2/M1) \leq 2.5$, upper limit
[M1,E2]			Assumed mixed M1 plus E2, assumed $\delta(E2/M1) = 1$ with no uncertainty
E1+M2+E3	+0.012	+6-4	Mixed E1 plus M2 plus E3, definite, $\delta(M2/E1) = +0.012^{+6}_{-4}$ (E3 multipolarity component omitted)
[E1,M2,E3]			Assumed mixed E1 plus M2 plus E3, assumed $\delta(M2/E1) = 1$ (E3 multipolarity component omitted)
E0+M1+E2	+2.7	+3-1	Mixed E0 plus M1 plus E2, definite, $\delta(E2/M1) = +2.7^{+3}_{-1}$ $q(E0/E2) = 0.24(3)$ given in the GAMMA cont. record ^a

^a To be declared in ENSDF dictionary and manual.

Appendix D: Definition of the data files

TABLE IX: Declaration of the parameter structures used in the INDEX and ICC data files. At various stages of the program development several additional programs (BldBricc, ComposeBricc, ViewBricc, etc.) have been used to create these files. The description of these programs goes beyond the scope of this manual.

Variable	Type	Length [bytes]	Dimension
INDEX FILE “*.idx”			
Elem	Record	2048	126
<i>Definition of Elem record</i>			
Atomic number	Integer	4	1
Chemical Symbol	Character	4	1
Atomic mass	Integer	4	1
Electron Shell	Record	32	41
Electron conversion: K, L1, L2, ...R2, Tot			
Pair conversion: π			
E0 electron conversion: K, L1, L2			
E0 pair conversion: π			
<i>Definition of Electron Shell record</i>			
Exist	Logical	4	1
Binding energy [keV]	Real	4	1
Tabulation	Character	8	1
Electron shell	Character	8	1
Number of energy mesh points	Integer	4	1
Record number in “*.icc” file	Integer	4	1
DATA FILE “*.icc”			
ICC data	Record	44	N ^(a)
BrIccFO:			188751
BrIccNH:			188751
HsIcc:			11616
RpIcc:			28265
<i>Definition of ICC data record</i>			
Transition energy [keV]	Real	4	1
α_{ic} electron conversion coefficient, (E1-E5,M1-M5),	Real	4	10
α_{π} pair conversion coefficient (E1-E3,M1-M3), or			
$\Omega_{ic,\pi}(E0)$ electronic factor			

^(a) Total number of energy mesh points (records)