BrIccMixing – ENSDF evaluation tool to determine Mixing Ratio (MR) and Normalization Factor (R) from conversion electron data
User's manual for version 2.3d – 22-May–2019

T. Kibédi*
Department of Nuclear Physics, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia

Abstract

The **BrIccMixing** program can be used to determine the multipole mixing ratio (MR) and an optional normalization factor from conversion electron data. The current version also allow to include experimental MR data deduced from gamma-ray angular distribution or correlation measurements, however the fitting procedure only allows symmetric uncertainties on the input data.

BrIccMixing can be downloaded for Windows, Linux and Mac OS from the following web site at the IAEA: https://www-nds.iaea.org/public/ensdf_pgm/index.htm

*Electronic address: Tibor.Kibedi@anu.edu.au

I. INTRODUCTION

The program *BrIccMixing* can be used to determine the absolute value of the Mixing Ratio (MR) and Normalization Factor (R) from conversion electron data. The basic relation between conversion coefficients (α_i) and mixed transition multipolarity can be expressed as

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

where δ is the multipole mixing ratio, defined as: $\delta(\pi`L`/\pi L) = \gamma(\pi`L`)/\gamma(\pi L)$. Here $\gamma(\pi`L`)$ and $\gamma(\pi L)$ are the absolute transition amplitudes involving photon emission, $\alpha_i(\pi`L`)$ and $\alpha_i(\pi L)$ are the conversion coefficients of the $\pi`L`$ and πL multipole components. The current version of the program accepts only $L \geq 1$ multipolarities and the valid combinations are listed in the Table I.

TABLE I: Transition multipolarities and selection rules

	$\Delta\pi = +1$			$\Delta\pi = -1$		
πL	M1	M3	M5	E1	E3	E5
$\pi' L'$	E2	E4	E6	M2	M4	M6

The current version of the program allows to include experiment MR values together with the conversion electron data. Such MR values could be obtained from gamma-ray angular correlation or distribution measurements. Often these values have asymmetric uncertainties, or are only known as limits. The *BrIccMixing* program will only accept experimental input values with symmetric uncertainties. In some cases asymmetric uncertainties can be symmetrized, using procedures described for example by Audi *et al.* [2012Au07].

The program uses two procedures to determine the best parameter values and uncertainties:

(a) Chi-squared fit, based on the CFIT [1980Ry04] program; and

(b) Searching the $\chi^2(ICC_{Theor}(MR), ICC_{Exp})$ hypersurface.

Using method (a) the fitted MR value will always have a symmetric uncertainty. On the other hand, method (b) has the facility to deduce MR values with symmetric, asymmetric uncertainties or establish limits. In many ways, method (b) could be considered as a more robust approach.

Theoretical conversion coefficients are determined using BrIcc [2008Ki07] routines and numerical tables calculated with the "Frozen Orbital" (BrIccFO) approximation. The second procedure is similar to the method used by the DELTA program [1983Ekstrom], however our solution takes into account the uncertainty on the theoretical ICC values attributed to the energy uncertainty and the accuracy of the calculations. This could be particularly important for low energy nuclear transitions, where the theoretical ICC values have a strong energy dependence.

II. SPECIFYING EXPERIMENTAL CONVERSION ELECTRON DATA

Each data entry contains 5 parameters given in a single line separated by arbitrary number of spaces (no TAB's are allowed):

NsrKey Maximum 20 character long string identifying the data source, for example the NSR key number of the publication.

Shell Maximum 20 character long string identifying the atomic shells (K, L, L1, L12, etc.) or ratios of shells (K/L, K/L1, etc.). The program will accept all atomic shells (K, L, M, N, O, P, Q) and the corresponding subs-shells (L1, L2, L3). Summed sub-shell values can be also specified. For example L1+L2 can be given as L12. To specify a mixing ratio put **MR** into the Shell field. NOTE: Do not use sign for the MR value.

IccVal Numerical value of the conversion coefficient, CE intensity or their ratio. For mixing ratio data put the **MR** value in the IccVal field. Valid FORTRAN numbers are accepted: 125, 125.3, 1.253E+2.

Unc Uncertainty of the numerical value in Nuclear Data Sheet style

Type Type of data, single character of **A**, **R** or **N**. For Mixing Ratio (**MR**) data always uses **A**!

The three types of experimental conversion electron data acceptable for the program:

A–type **Absolute** values of experimental conversion coefficients: α_K, α_L, α_{L1}, ... α_{R2}, α_{Total}, ... etc. *Example:* `1962Wo09 K 0.180 12 A`; or `1974Ga01 MR 0.118 6 A`

R–type Ratios of conversion electron intensities or ratios of conversion coefficients: α_K/α_K, α_{L1}/α_{L2}, α_{L1}/α_{L3}, ... etc. *Example:* `1961Br09 L1/L2 6.76 23 R`

N–type Un–normalized conversion electron intensities. Program will deduce the same normalization factor for a given data set. *Example:* `1977Se10 K 0.043 3 N`

Each data set of the input file can contain up to 100 data entries. The header information of a data set contains the following 3 header lines:

Data set title Up to 132 character long description of the data set, for example the GAMMA record: `180HF G 500.697 13 15.2 3M2+E3 -5.5 2`

Transition Nuclide (5 characters), Transition energy in keV and uncertainty. Each parameter separated by a space character. For example: `180HF 500.697 13`

Multipolarity Mixed multipolarity and initial mixing ratio. For example: `M2+E3 1.5`

Data sets are separated with a line containing `*NEW`. The number of data sets in an input file is not limited. Any line starting with the hash character (#) will be skipped. These facility can be also used to insert user comments into the input file.

A sample input file, *briccmixing.in* is distributed with the program. It contains a number of data sets combining various type of input data.

III. TERMINAL DIALOGUE AND GRAPHICAL OUTPUT

The *BrIccMixing* program is designed to run from a terminal console. At this stage only 32–bit versions are distributed for Windows, Linux and Mac OS operating systems.

The graphical output of the program will be displayed using the GNUPLOT software, freely available at http://www.gnuplot.info/. Please make sure, that a recent version of GNUPLOT has been installed and the installation directory has been included into the *Path* environment variable. This will allow *BrIccMixing* to invoke GNUPLOT.

As first step, prepare the input file with the experimental data. Running *BrIccMixing* it will process each data set and will display the χ^2/ν plot. Detailed calculation report is generated into an ASCII file with the default file name of *briccmixing.lst*. Part of the terminal dialogue using the data on the 140.511(1) keV E1(+M2) transition in ^{99}Tc is shown below. The 6 experimental values taken from 3 measurements includes conversion coefficients (type "A"), ratio of the L1, L2 and L2 conversion electron intensities (type "R") and mixing ratio (MR) data (type "A").

```
c:\ENSDF>briccmixing 99tc_briccmixing.in :
  * * * * * * * * * * * * * BrIccMixing v2.3d (22-May-2019) * * * * * * * * * * * * *
 The program calculates the mixing ratio and normalization factor from CE data
 by T. Kibedi (ANU; Tibor.Kibedi@anu.edu.au)
 Based on
 CFIT - [1980Ry04] M. Rysavy, O. Dragoun, Comp. Phys. Commun. 19 (1980) 93
 BrIcc v2.3d (03-Apr-2019) - [2008Ki07] T. Kibedi, T.W. Burrows,
        M.B. Trzhaskovskaya, P.M. Davidson, C.W. Nestor Jr.,
        Nucl. Instr. and Meth. A v589 (2008) 202
 NOTE:  The plotting program GNUPLOT (http://www.gnuplot.info) is required
 ================================================================================
 Index file: C:\Program Files\BrIcc\BrIccFOV22.idx
 ICC file:   C:\Program Files\BrIcc\BrIccFOV22.icc
 ================================================================================
 Transition:  99Tc   140.511(1) keV
 Multipolarity: M1+E2
 Initial Mixing Ratio (MR): 0.13
                 Initial R: 1.0

 Icc data:
  NSRkey      Shell         Icc(Unc)              Type
  1969Ag04    L1/L2         12(4)                 R
  1969Ag04    L1/L3         18(7)                 R
  1969Ag04    L2/L3         1.7(7)                R
  1969Vu03    T             0.122(5)              A
  1973Le29    T             0.118(3)              A
  1974Ga01    MR            0.118(6)              A
```

```
 1981Ge05    K             0.097(3)              A
 1981Ge05    T             0.119(3)              A

Chi-squared FIT ---------------------------------------------------------------
   Iter      Delta        Chi**2/N
    0        1.498D-02    5.736D+01
    1        1.940D-02    5.664D+01
    2        2.303D-02    5.625D+01
    3        2.578D-02    5.606D+01
    4        2.778D-02    5.596D+01
    5        2.920D-02    5.591D+01
Prescribed precision reached in   5 iterations
Mixing ratio (MR) from Chi2 fitting = 0.2(3); reduced Chi2=  5.59E+01

Parabolic search of the Chi-squared hypersurface ------------------------------
MixingRatio = 0.123(+15-16); reduced Chi2=  1.95E+00

                          Experiment        Fit
  NSRkey      Shell       Icc(Unc)          Icc(Unc)          Type
1969Ag04    L1/L2        12(4)             15.8(4)           R
1969Ag04    L1/L3        18(7)             31.0(7)           R
1969Ag04    L2/L3        1.7(7)            1.96(4)           R
1969Vu03    T            0.122(5)          0.1130(16)        A
1973Le29    T            0.118(3)          0.1130(16)        A
1974Ga01    MR           0.118(6)          0.1233            A
1981Ge05    K            0.097(3)          0.0985(14)        A
1981Ge05    T            0.119(3)          0.1130(16)        A
Hit return to continue
```

For each data set the program will generate a GNUPLOT script and the data file with the input experimental values as well as the χ^2–hypersurface plot. The gnuplot script and data file names are automatically generated from the input file name. For example for the *briccmixing.in* sample input file they will be called as *briccmixing_1.plt*, *briccmixing_1.dat*, *briccmixing_2.plt*, *briccmixing_2.dat*, etc. Typical graphical output using the above data on the 140.511(1) keV transition in ^{99}Tc is shown in Fig. 1.

IV. INSTALLATION NOTES

The program assumes that *BrIcc version 2.3* and *GnuPlot* have been installed on your system. It is assumed that the installation directory for *BrIcc* and the "/gnuplot/bin" directory for *GnuPlot* have been added to the search path. For further details consult with the documentation of *BrIcc* and *Gnuplot* programs.

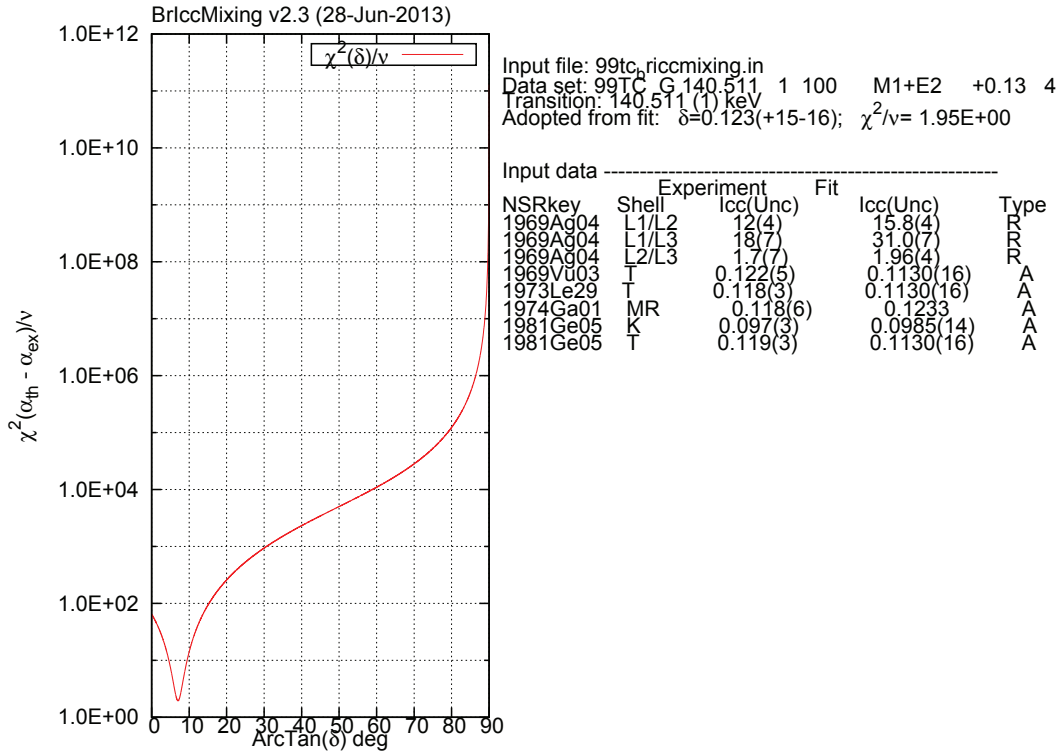

FIG. 1: Graphical output for the 140.511(1) keV transition in ^{99m}Tc.

The *BrIccMixing* program should be installed into the *BrIcc* installation directory. The current distribution contains the following files: *BrIccMixing.exe* (executable), *BrIccMixing.in* (sample input file) and *BrIccMixing.pdf* (program manual).

Windows The program is distributed as a self contained installation script, *BrIccMixingV23setup.exe*.

Linux and Mac OS The program distributed as a tarred, gzipped file.

V. TROUBLESHOOTING

If the program crashes or works incorrectly please e-mail the problem to the following account bricc@anu.edu.au. Please include a screen dump of the console window, the operating system used together with the input file.

[1980Ry04] M. Ryŝavỳ and O. Dragoun, Comput. Phys. Commun. **19** (1980) 93.

[1983Ekstrom] L.P. Ekstrom, *"DELTA - a computer program to analyze gamma-gamma correlations from unaligned states"*, Nuclear Physics LUNFD6/(NFFR-3048) 1-27 (Lund University. 1983).

[2008Ki07] T. Kibédi, T.W. Burrows, M.B. Trzhaskovskaya, P.M. Davidson, C.W. Nestor, Jr., Nucl. Instr. and Meth. **A 589** (2008) 202.

[2012Au07] G. Audi, F.G. Kondev, M. Wang, B. Pfeiffer, X. Sun, J. Blachot, M. MacCormick, Chi. Phys. **C 36** (2012) 1157.