# DDEP external calculation codes

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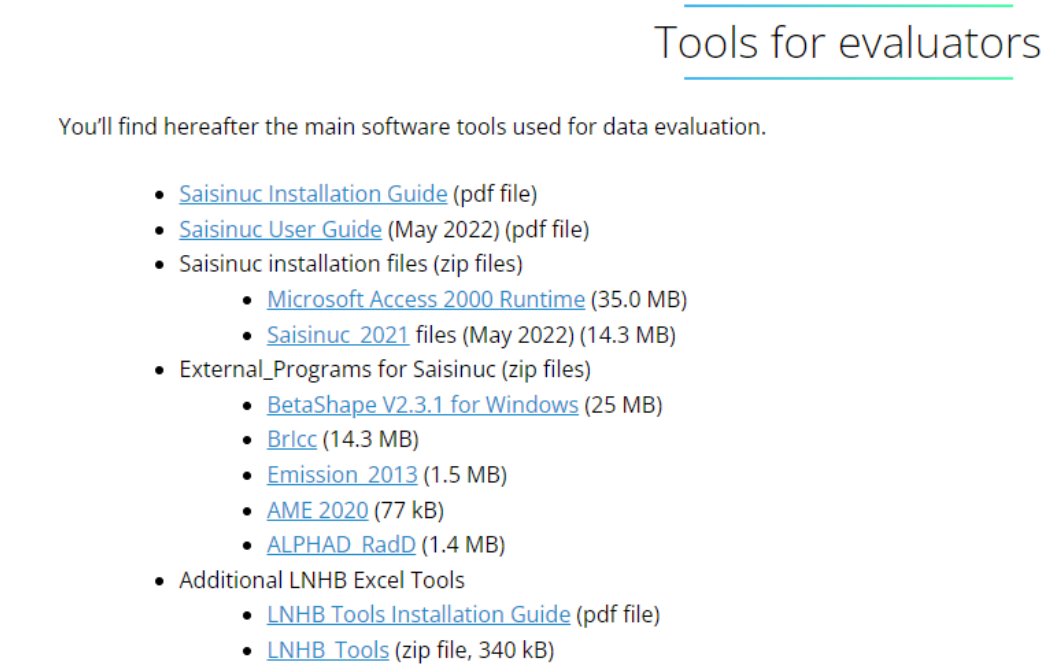
# Usage of calculation codes in DDEP

Recommended data in DDEP can be deduced from three different methods:

- Analysing experimental results
  - Require usage of an averaging tool
- Using an evaluated database
  - Such as Q-value or X-ray energies
- Using theoretical / phenomenological calculation codes
  - BetaShape (Beta transitions)
  - BrIcc (conversion coefficients)
  - Emission (X-ray and Auger intensities)
  - ALPHAD RadD (Hindrance Factors)



Tools for evaluators

You'll find hereafter the main software tools used for data evaluation.

- Saisinuc Installation Guide (pdf file)
- Saisinuc User Guide (May 2022) (pdf file)
- Saisinuc installation files (zip files)
  - Microsoft Access 2000 Runtime (35.0 MB)
  - Saisinuc_2021 files (May 2022) (14.3 MB)
- External_Programs for Saisinuc (zip files)
  - BetaShape V2.3.1 for Windows (25 MB)
  - BrIcc (14.3 MB)
  - Emission_2013 (1.5 MB)
  - AME 2020 (77 kB)
  - ALPHAD_RadD (1.4 MB)
- Additional LNHB Excel Tools
  - LNHB Tools Installation Guide (pdf file)
  - LNHB_Tools (zip file, 340 kB)

**Available from the LNHB website**
**http://www.lnhb.fr/home/nuclear-data/tools-for-evaluators/**

# BetaShape code: overview

Calculation code used for $\beta^-$ / $\beta^+$ / EC decays

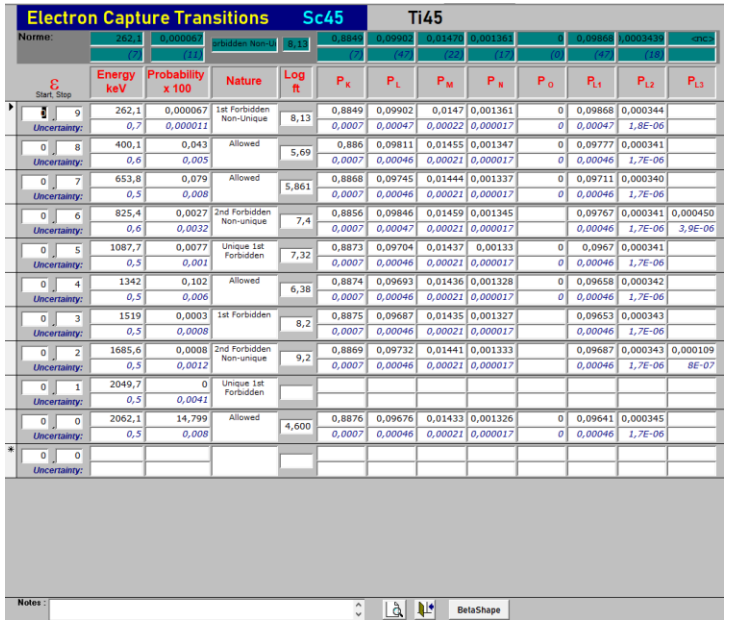
- Developed at LNHB by Xavier Mougeot and continuously updated
- Based on Xavier's theoretical developments on beta spectrum calculations
  - Also include experimental shape factors database
- Provides for each transition
  - $\beta^-$ / $\beta^+$: maximum energy, mean energy, log ft and nature of the transition
  - EC: energy of the transition, log ft, capture coefficients ($P_K$, $P_L$, $P_M$, …) and nature of the transition
  - $\beta^+$ / EC: balance of the transition
- Propagation and processing of experimental uncertainties

**More details available in Xavier's presentation**

# BetaShape code: usage

```
45SC    45TI EC DECAY (3.083 H)
45SC C  References:1941Al02, 1950Re**, 1950Te**, 1952Ru23, 1959Po64, 1965Gf01,
45SC2C  1966Po04, 1968El11, 1971Zu01, 1986Bo06, 1996Sc06, 2000Sc47, 2008Bu01,
45SC3C  2008Ki07, 2015Ku16, 2021Wa16
45SC T  Auger electrons and X ray energies and emission intensities:
45SC T       {U Energy (keV)}   {U Intensity}  {U Line}
45SC T
45SC T        4.0862             0.778   21     XKA2
45SC T        4.0906             1.53    4      XKA1
45SC T
45SC T        4.4604          ]  0.305   10     XKB1
45SC T        4.4866          ]                 XKB5II
45SC T
45SC T
45SC T        0.3487                            XLL
45SC T        0.4006-                           XLA
45SC T        0.3534                            XLC
45SC T        0.40501-0.4992                    XLB
45SC T        0.40973-0.40973                   XLG
45SC T
45SC T        3.451-3.649     ]                 KLL AUGER
45SC T        3.925-4.084     ]  10.74    7     KLX AUGER
45SC T        4.385-4.48      ]                 KXY AUGER
45SC T        0.2946-0.4931       1.456    7     L AUGER
45TI  P 0.0          7/2-              3.083 H   8              2062.1    5
45SC  N 1.0          1.0       1         1.0
45SC  L 0            7/2-              STABLE
45SC  E                                                        99.755    12
45SC2 E EAV=438.06   22$CK=0.13168  10$CL=0.01435   7$CM=0.002126 31
45SC3 E CN=1.967E-4 25
45SC  L 12.40      5 3/2+              318 MS    7
45SC  E                                                        0.0000    41 1U
45SC2 E EAV=461.95   22$CK=0.1316    1$CL=0.01441   7$CM=0.002135 31
45SC3 E CN=1.975E-4 25
45SC  G 12.40      5 0.000026 9(M2)                  423     9
45SC2 G KC=362       8$LC=53.5     12$MC=6.63      15$NC=0.298     7
45SC  L 376.50     123/2-              43.3 PS   23
45SC  E                                                        0.0010    12 2
45SC2 E EAV=302.04   22$CK=0.7099    6$CL=0.07790   37$CM=0.01153  17
45SC3 E CN=0.001067 14
```

- Command line executable, no graphical interface
- Input
  - Format: ENSDF 80 columns
  - Requires: Parent and daughter nucleus, levels energies and spin parities, total transition intensities
- Output
  - Format: ENSDF 80 columns, CSV file
  - Report file (.rpt) contains all information and hypothesis used for the calculations
- Code implemented in Saisinuc



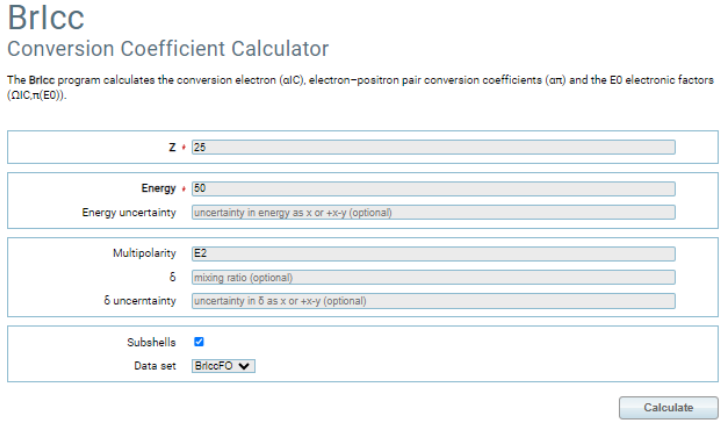
# BrIcc code: overview

Calculation code used to estimate the internal conversion coefficients for a gamma transition

- Developed at ANU by Tibor Kibédi
- Based on Tibor's work on conversion coefficients
- Provides for each gamma transition
  - Total conversion coefficient: $\alpha_T$
  - Each shell conversion coefficients: $\alpha_K$, $\alpha_L$, $\alpha_M \ldots$
  - Each sub-shell conversion coefficients: $\alpha_{L_1}$, $\alpha_{L_3}$, $\alpha_{L_3} \ldots$
  - Pair production coefficient: $\alpha_\pi$
- Propagation and processing of experimental uncertainties

# BrIcc code: usage

- Command line executable and online application
- Input
  - Format: ENSDF 80 columns, manual input
  - Requires: Z of considered nucleus, energy of gamma transition and Multipolarity (mixing ratio if necessary)
- Output
  - Format: ENSDF 80 columns, text file
- Code implemented in Saisinuc




BrIccS v2.3 (9-Dec-2011)
Z=25 (Mn, Manganese)
γ-energy: 50 keV
Data Sets: BrIccFO

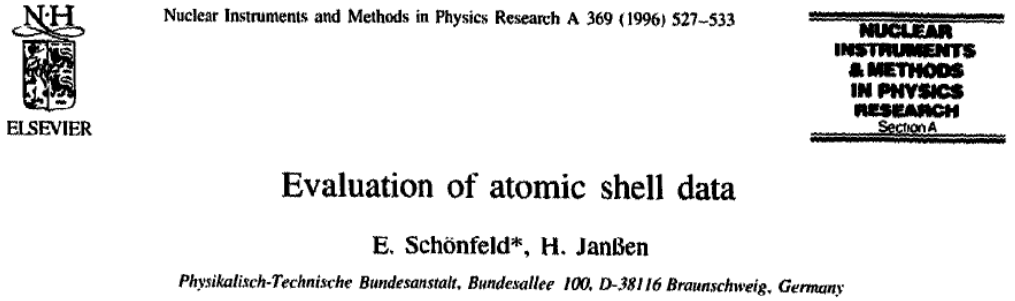
| Shell | E(ce) | E2 |
|---|---|---|
| Tot | | 6.47 (9) |
| K | 43.46 | 5.67 (8) |
| L1 | 49.23 | 0.469 (7) |
| L2 | 49.35 | 0.0863 (12) |
| L3 | 49.36 | 0.1431 (20) |
| L-tot | 49.27 | 0.698 (10) |
| K/L | | 8.13 (16) |
| M1 | 49.92 | 0.0629 (9) |
| M2 | 49.95 | 0.01117 (16) |
| M3 | 49.95 | 0.0181 (3) |
| M4 | 50.00 | 1.628E-5 (23) |
| M5 | 50.00 | 2.19E-5 (3) |
| M-tot | 49.93 | 0.0923 (13) |
| L/M | | 7.57 (15) |
| N1 | 50.00 | 0.00306 (5) |
| N-tot | 50.00 | 0.00306 (5) |
| L/N | | 228 (5) |

*https://bricc.anu.edu.au/*

# Emission code: overview

Calculation code used to estimate the X-rays and Auger electron intensities

- Developed at PTB by E. Schönfeld around 2006
- Not updated since 2011
- Based on Schönfeld's work on atomic data
  - Include fluorescence yields evaluation from 1995
- Provides
  - X-ray intensities for K and L shells (and L subshells)
  - Auger intensities for KLL, KLY, KXY and L shell



# Emission code: usage

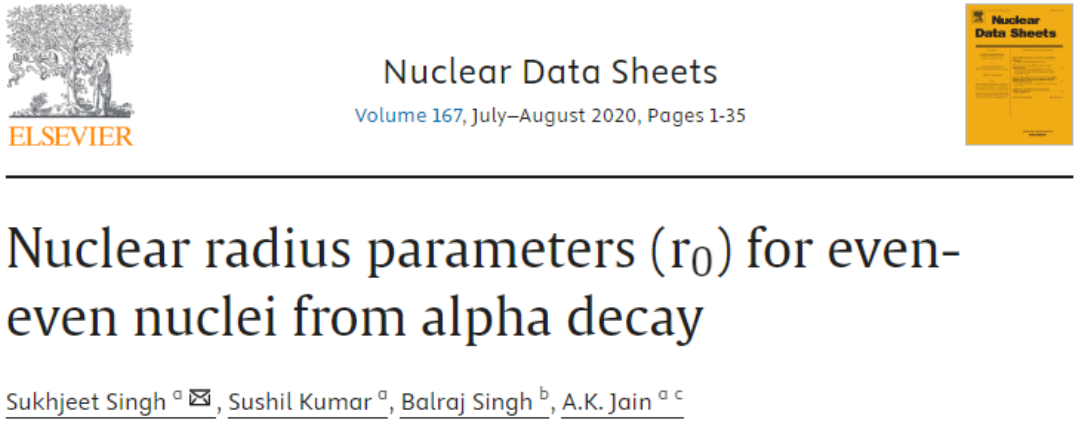
```
; Cs137.102
; EMISSION.EXE

; Radionuclide  -- Cs-137 ---> Ba-137
  Cs-137
  56
  END

; Electron Capture Transitions
; pEC     pK      pL1      pL2      pL3
; Pec(u)     Pk(u)     PL1(u)     PL2(u)     PL3(u)
0(0)     0(0)     0(0)     0(0)     0(0)
  END

; Gamma Transitions
; E     pGamma     AlphaK     AlphaL1     AlphaL2     AlphaL3
;Energie     Pg     Ak     al1     al2     al3
283,46     0,0006(1)     0,0461(7)     0,00531(8)     0,001129(16)     0,000817(12)
661,6553     85,01(20)     0,0915(13)     0,01311(19)     0,00185(3)     0,001521(22)
378,2     0,0000106(9)     0,463(7)     0,0591(9)     0,198(3)     0,0870(13)
  END
```

- Command line executable
- Input
  - Format: text file
  - Requires: Z of the daughter nucleus, conversion coefficients, electron capture coefficients
- Output
  - Format: text file
  - Output file quite detailed including all the fluorescence yields used for the calculation
- Code implemented in Saisinuc

# ALPHAD-RadD code: overview

Calculation code used to estimate the hindrance factor of α-transitions

- Developed in 2020 at Akal University by S. Singh and S. Kumar under B. Singh guidance
- Based on Preston's spin-independent formulation (1947)
  - Update on the calculation of the nuclear radius
- Provide for alpha transition
  - Radius estimation
  - Hindrance factor



# ALPHAD-RadD code: usage

- Command line executable
- Input
  - Format: ENSDF file
  - Requires: Parent and daughter nucleus, energy spin and parities of level involved
- Output
  - Format: ENSDF file + report file
- Code implemented in Saisinuc

# LNHB tools: overview

Series of macros and functions in Excel

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1952XXU0 | 12 | 3 | | 3,7036E-05 | 0,0242982 | | | 12 | 3 |
| 19575XU2 | 11,2 | 0,1 | | 0,0333321 | 0,00331336 | | | 11,2 | 0,1 |
| 1983XXU4 | 11,18 | 0,02 | MIN | 0,83330247 | 0,08383406 | | | 11,18 | 0,02 |
| 1990XXU4 | 11,25 | 0,05 | | 0,1333284 | 0,47952014 | | | 11,25 | 0,05 |
| | | | CONSISTENT | Chi2 : | 0,59096577 | Chi2 crit.: | 3,78591257 | Nb Inp. Val.: | 4 |
| | | | UWM : | 11,4075 | uc(UWM) : | 0,19804776 | | Nb. iter.: | 1 |
| | | | WM : | 11,19003 | uc(WM)int. : | 0,01825708 | uc(WM)ext. | 0,014035 | |
| | | | LWM : | 11,19003 | uc(LWM) : | 0,01825708 | Min. Inp. Un | 0,02 | 11,18 |
| | | | LWM : | 11,19 | uc(LWM) : | 0,018 | (rounded val | 11,190 (18) | |
| | | | LWM has use | | | | | | |

- Developed by Christophe Dulieu at LNHB
- Based on DDEP introduction table and GUM recommendations
- Provide simple and practical way to
  - Calculate unweighted mean, weighted mean and LWM
  - Round a value based on the associated uncertainty
  - Symmetrise a non Gaussian uncertainty
  - …