Evaluating conversion coefficients using BrIcc

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Outline

- EM processes
- History of measuring and calculating ICC`s
- BrIcc – conversion electron calculations
- E0 electronic factors
- Electron positron pair conversion
- Some comments on obtaining, using and deducing ICC
- BrIcc/BrIccS/BrccG/BrIccMixing/BrIccEmis

ANU HIAS

NEC 14UD tandem electrostatic accelerator (1975)

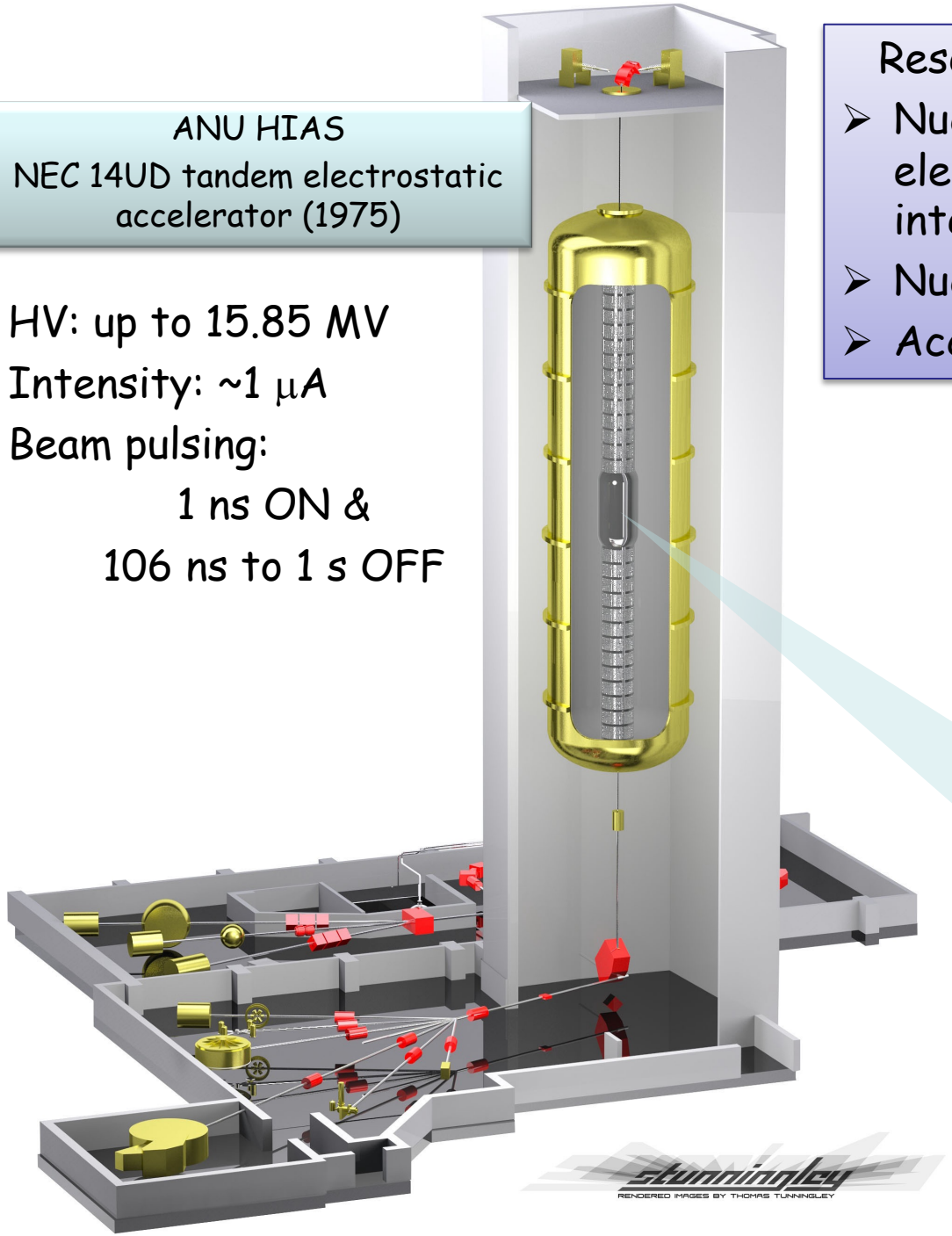
HV: up to 15.85 MV

Intensity: ~1 μA

Beam pulsing:

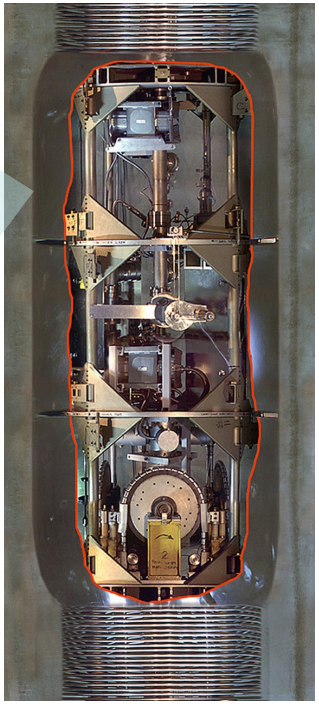
1 ns ON &

106 ns to 1 s OFF

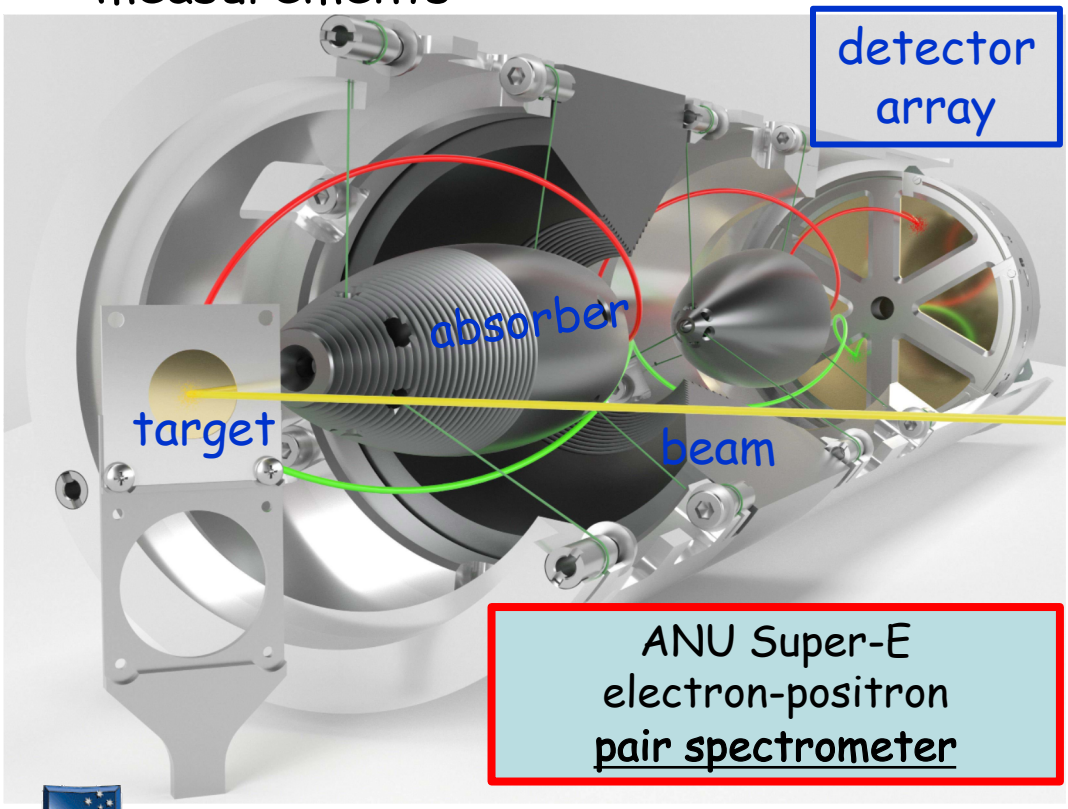


Research areas

- Nuclear Structure (γ-ray, conversion electron spectroscopy, hyperfine interactions)
- Nuclear Reaction Dynamics
- Accelerator Mass Spectrometry



- **Super-E**: 2.1 tesla solenoid to transport up to 15 MeV β-rays
- Operational since 1991; CE and electron-positron pair measurements
- 2 loops absorber system: complete suppression of γ- and X-rays
- Si(Li) array in sum-coincidences: FWHM < 10 keV energy resolution at 7.65 MeV
- Well defined electron transport: high accuracy in intensity measurements



Recent highlights

- **Carbon production in the universe**
  PRL 125 (2020) 182701
  PRC 102 (2020) 024320
- Searching for E0 in ^{24}Mg, ^{40}Ca, ^{50,52}Cr, ^{54,56}Fe, ^{58,60,62}Ni
  PLB 779 (2018) 396
  PRC 99 (2019) 024306
  EPJ Web of Conf. 232 (2020) 04004

Electromagnetic Decay Processes

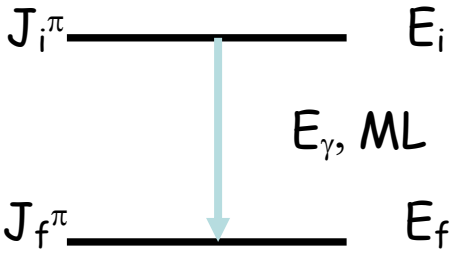
EM decay: energy and momentum carried away

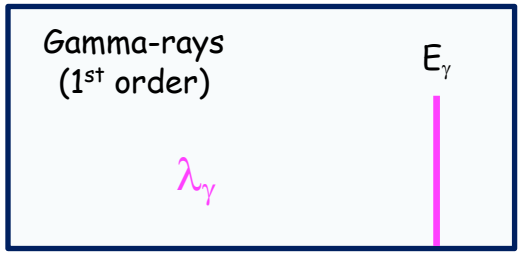
Selection *rules* (πL)

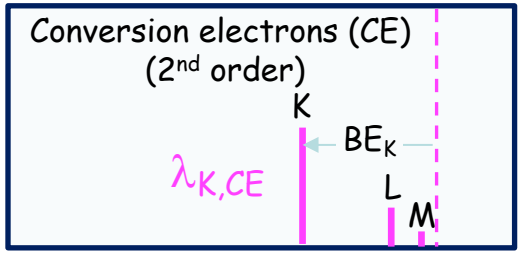
$|L-j_i| \lesssim j_f \lesssim L+j_i$

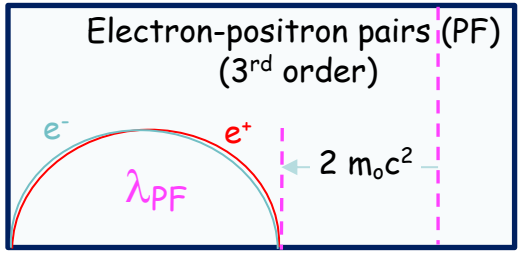
$\pi = (-1)^L$ for EL

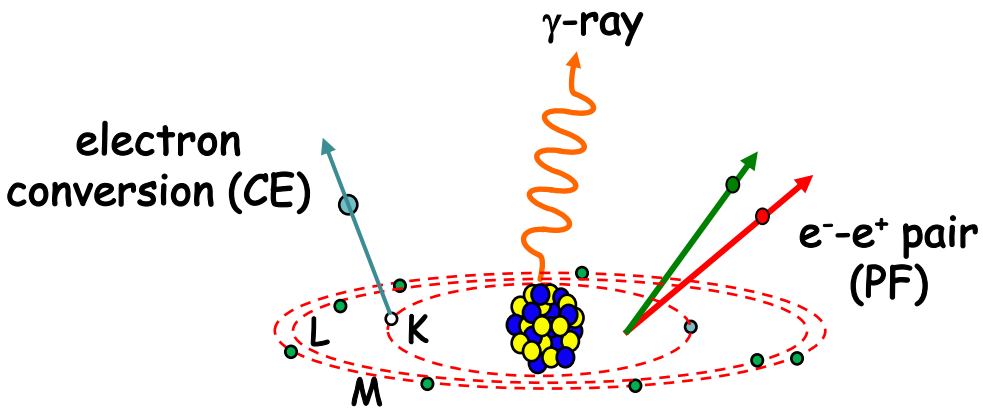
$\pi = (-1)^{L+1}$ for ML











Transition probability

$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M \ldots\ldots + \lambda_{PF}$

Conversion coefficient

$\alpha_{CE,PF} = \lambda_{CE,PF} / \lambda_\gamma$

$\lambda_{CE,PF} = \lambda_\gamma \times \alpha_{CE,PF}$

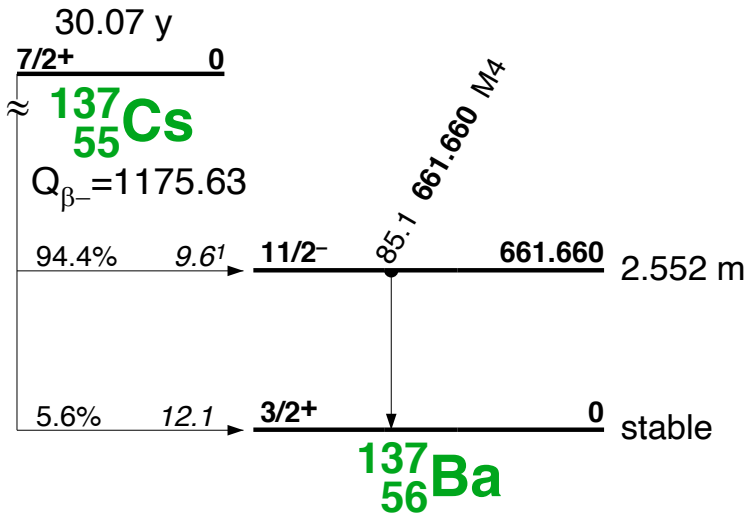
Energetics

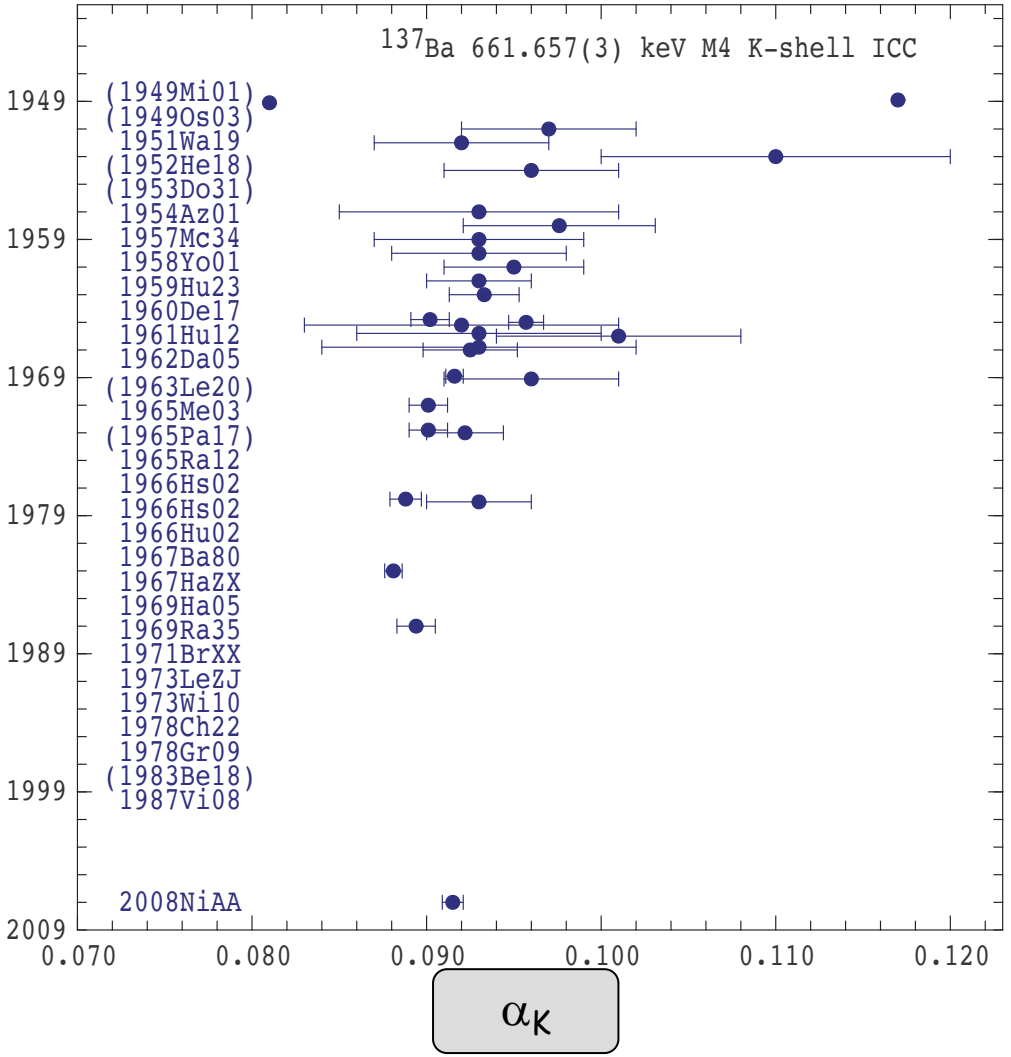
Gamma $E_\gamma = E_i - E_f + T_r$

CE $E_{CE,i} = E_i - E_f - E_{BE,i} + T_r$

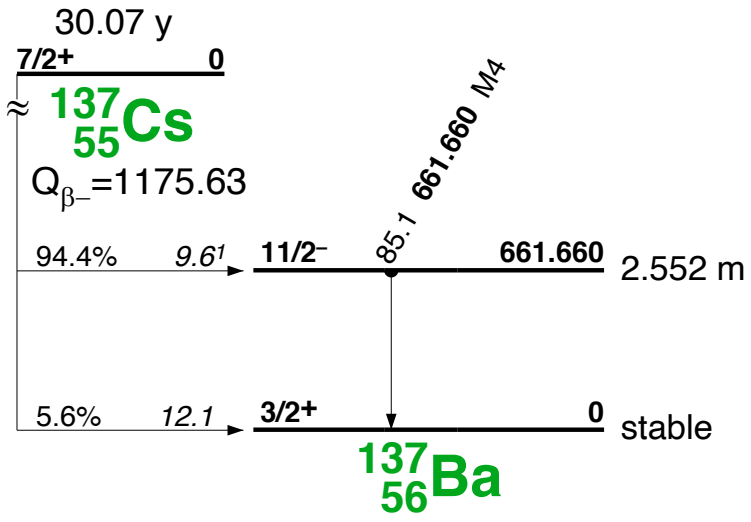
PF $E^+ + E^- = E_i - E_f - 2m_oc^2 + T_r$

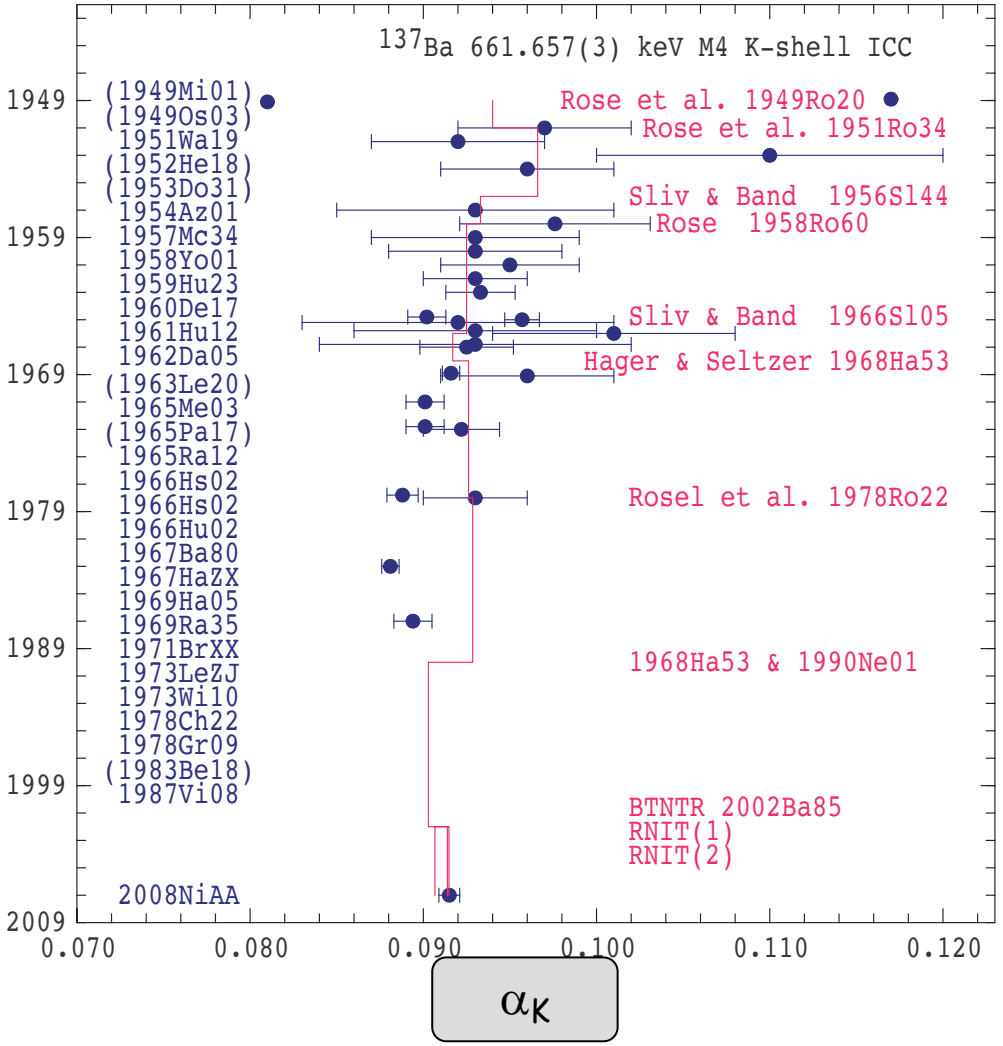
Experiments over 60 years





Calculations over 60 years





BrIcc - Calculations of conversion coefficients

I.M. Band, et al., ADNDT **81** (2002) 1. (RAINE code)

S. Raman, et al., PRC **66 (2002)** 044312 (overview of the theoretical calculations)

Physical model

- Calculations up to the first nonvanishing order of the perturbation theory

Atomic field model

- One-electron approximation
- Free neutral atom
- Screening of the nuclear field by the atomic electrons
- Spherically symmetric atomic potential
- Relativistic electron wave functions
- Experimental electron binding energies

Nuclear model

- Finite nuclear size
- Spherically symmetric nucleus; most abundant isotope

BrIcc - Calculations of conversion coefficients

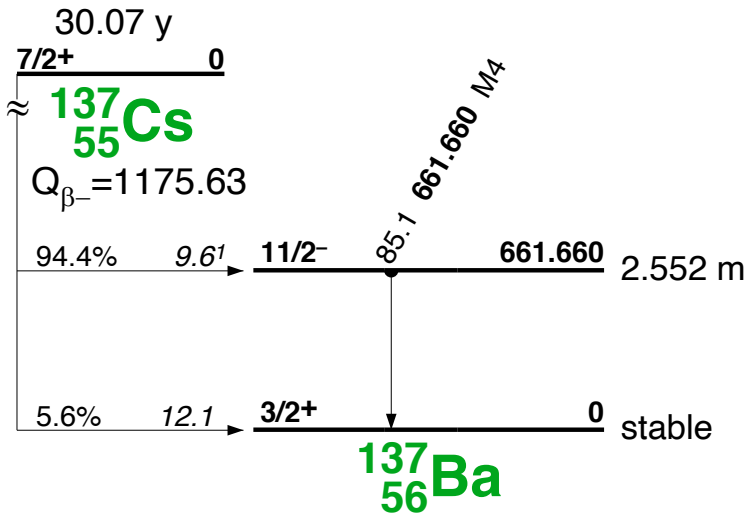
I.M. Band, et al., ADNDT **81** (2002) 1. (RAINE code)

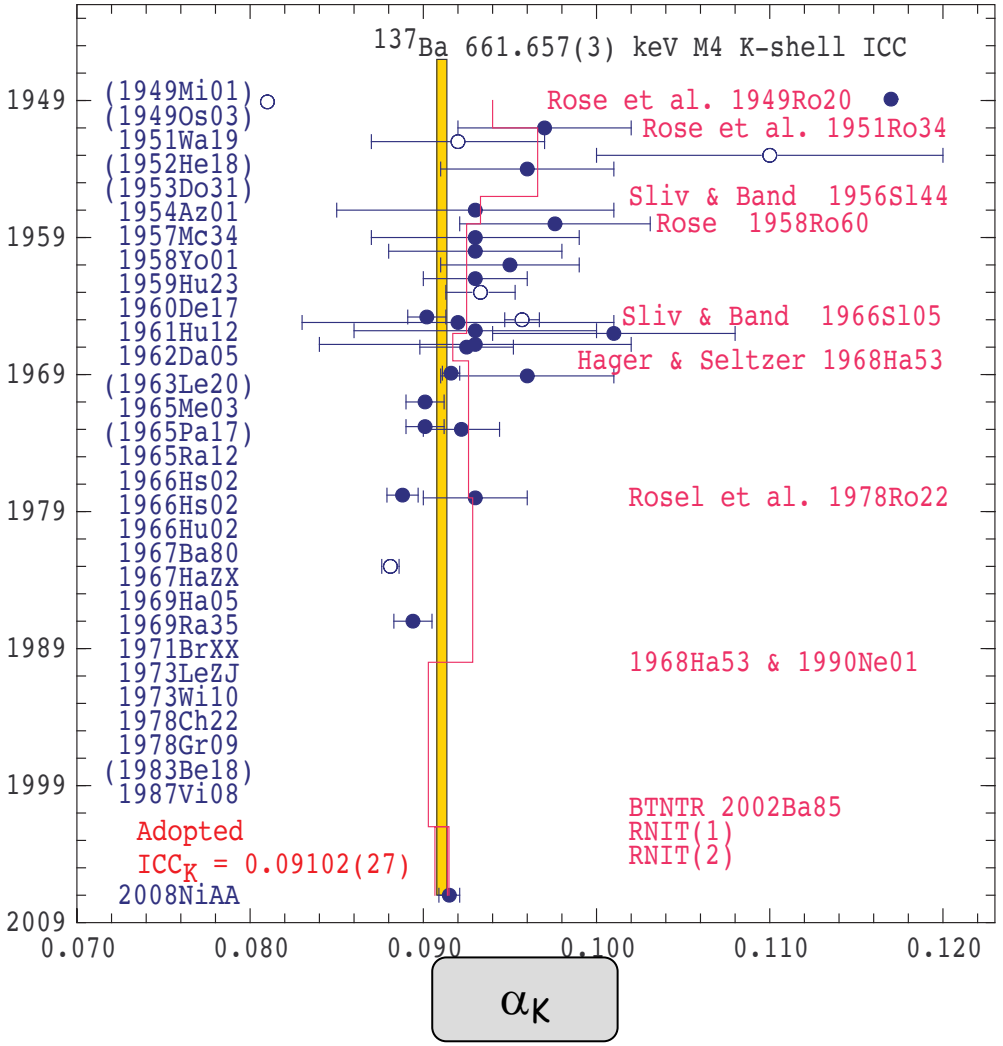
S. Raman, et al., PRC **66 (2002)** 044312 (overview of the theoretical calculations)

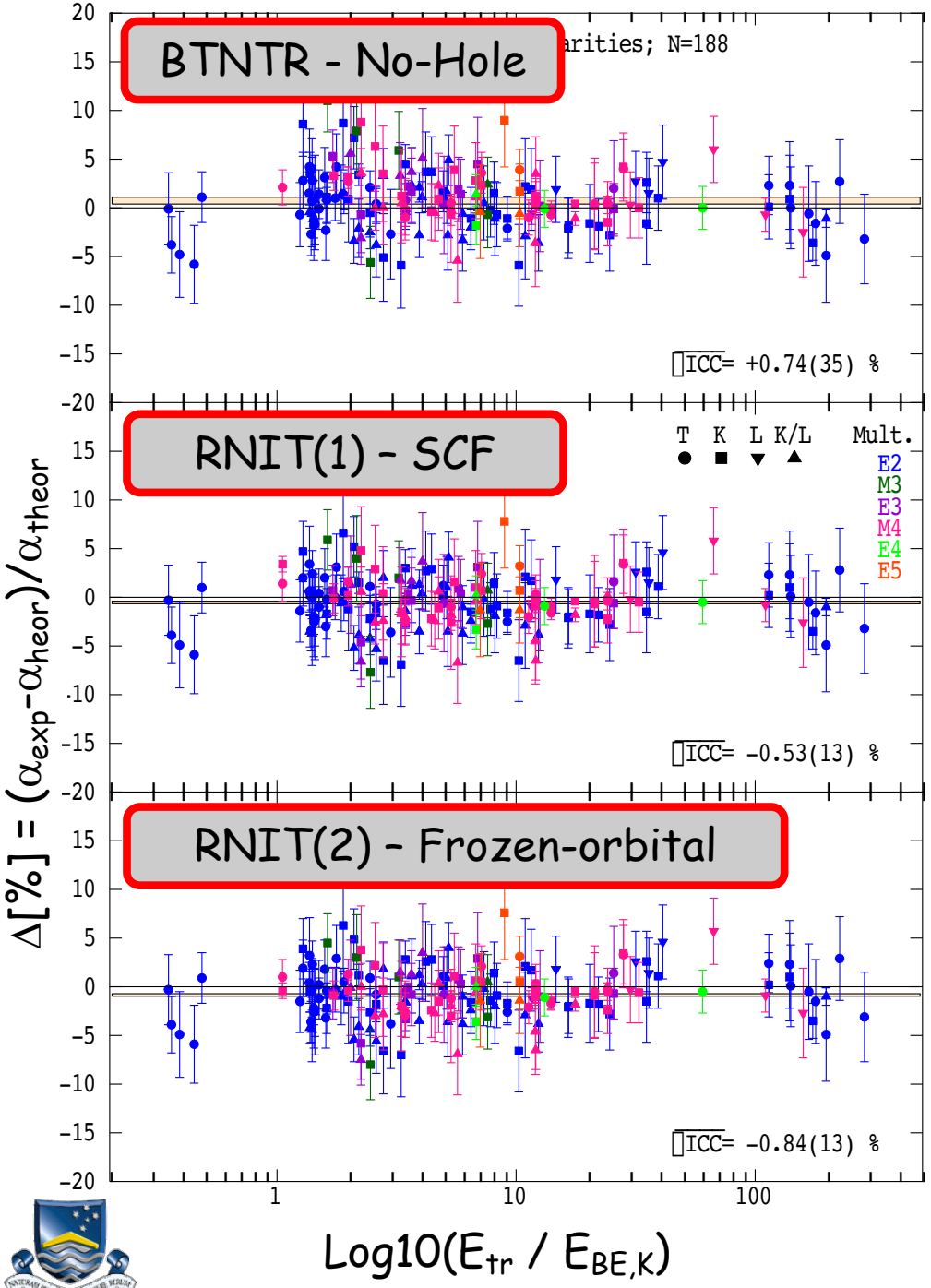
Higher order effect – ignored in most models

- Atomic many body correlations: factor ~2 for $E_{kin}(ce) < 1$ keV
- Partially filled valence shell: non-spherical atomic field
- Binding energy uncertainty: <0.5% for $E_{kin}(ce) > 10$ keV
- Chemical effects: <<1%
- Intranuclear conversion - Penetration effect

How good the ICC`s are now?







How good the ICC`s are now?

- Measure of goodness:

  $\Delta[\%] = (\alpha_{exp}-\alpha_{theor})/\alpha_{theor}$

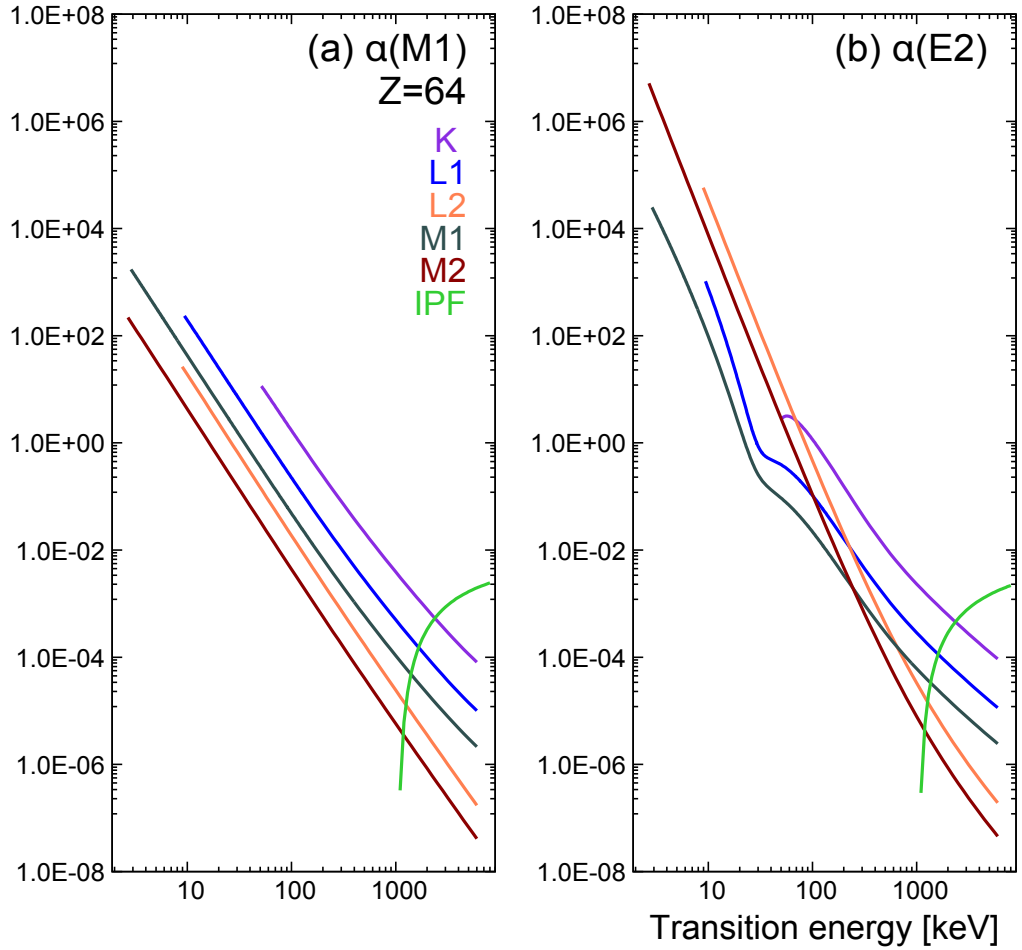
- 188 transitions ($\Delta\alpha/\alpha$ < 10%)
- E2, M3, E3, M4, E4, E5 mult.
- Z=20 to Z=95
- Largest difference at $E_{tr}/E_{BE,K} = 1$
- Inclusion of hole

  Initial / Final WF not orthogonal

- BrIcc: Frozen-Orbital approx.
  - Hole remains unfilled
  - Initial WF: neutral atom SCF
  - Final WF: constructed from bound WF of a neutral atom (not SCF of an ion)

Theoretical electron conversion coefficients

http://bricc.anu.edu.au



α_i Conversion coefficients:

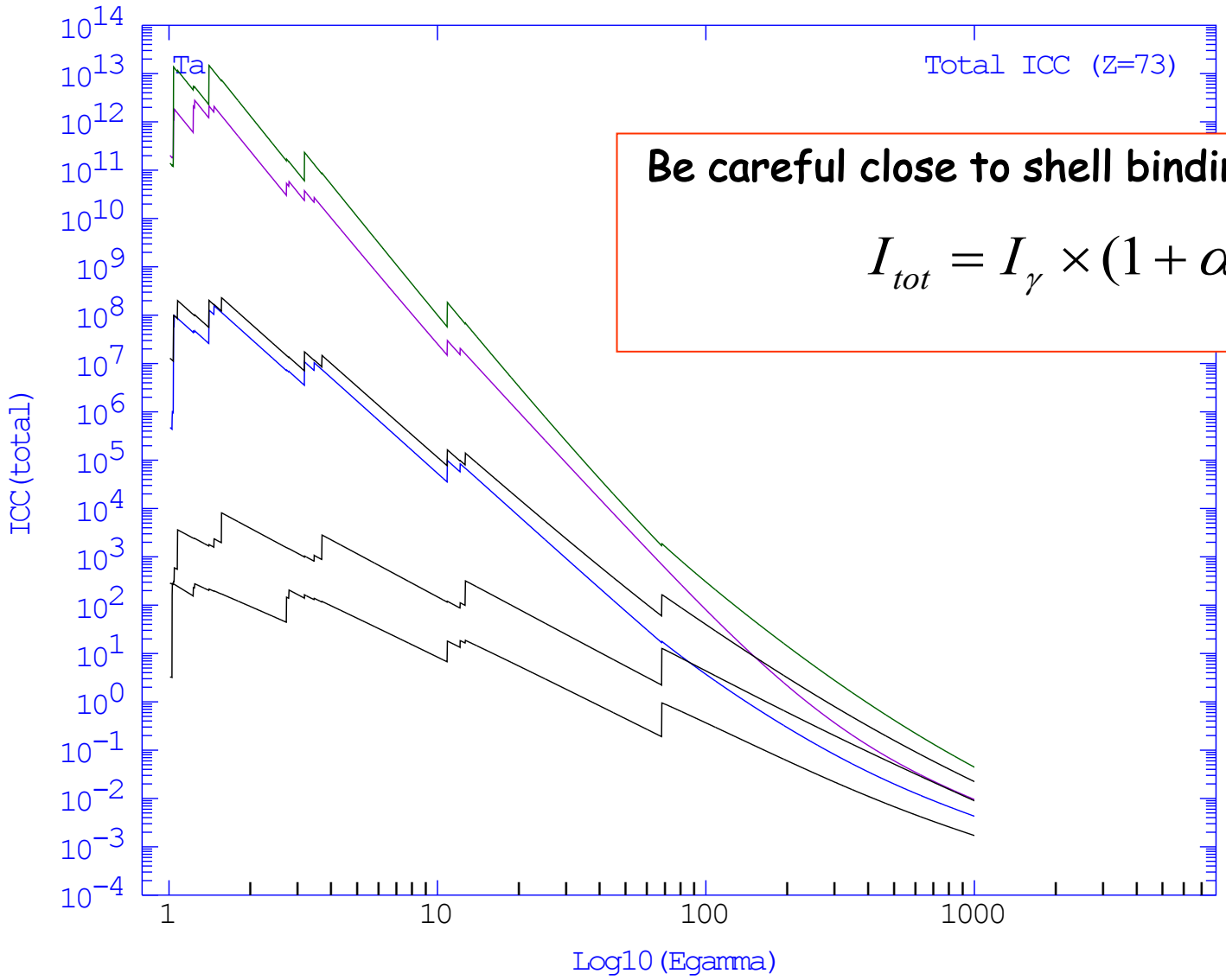
TK, et al., NIM **A589** (2008) 202

Z=5:110

TK, et al., ADNDT, 98 (2012) 313

Z=111:126

- ❑ K-Q2 atomic shells
- ❑ 1-6000 keV transition energy
- ❑ Starting 1 keV above shell BE
- ❑ E1-E5 & M1-M5 mult.
- ❑ Decreases by energy
- ❑ Increases by L
- ❑ Decreases by atomic shell
- ❑ Increases by Z



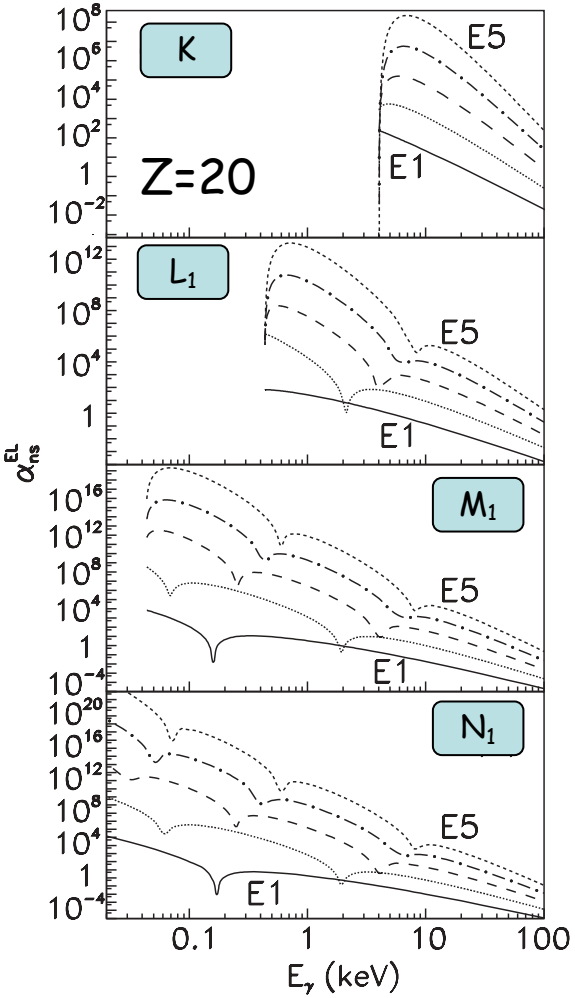
Be careful close to shell binding energies

$$I_{tot} = I_{\gamma} \times (1 + \alpha^{tot})$$

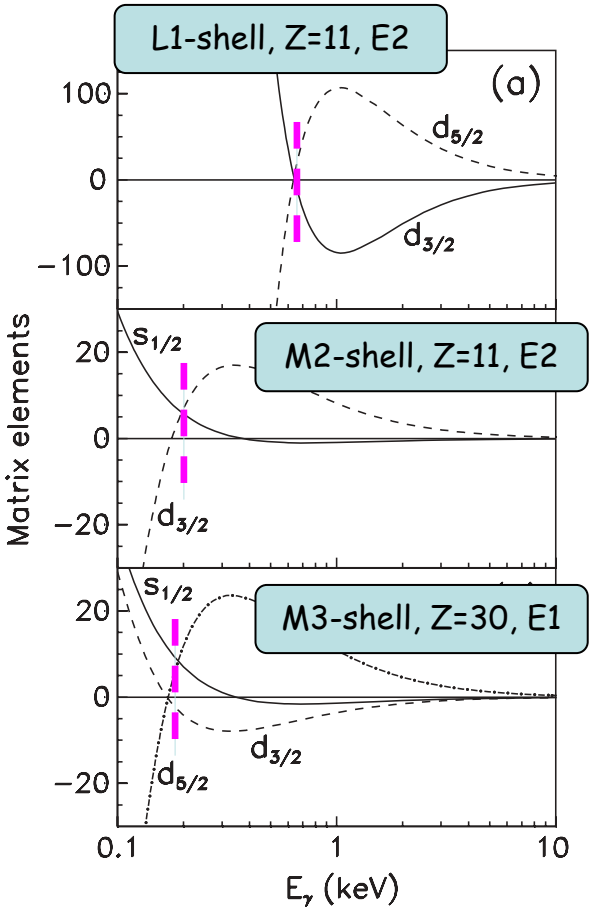
Resonances in E1-E5 conversion coefficients at low energy

- Observed in all elements
- Only for electric transitions

M.B. Trzhaskovskaya, et al. PRC **81** (2010) 024326

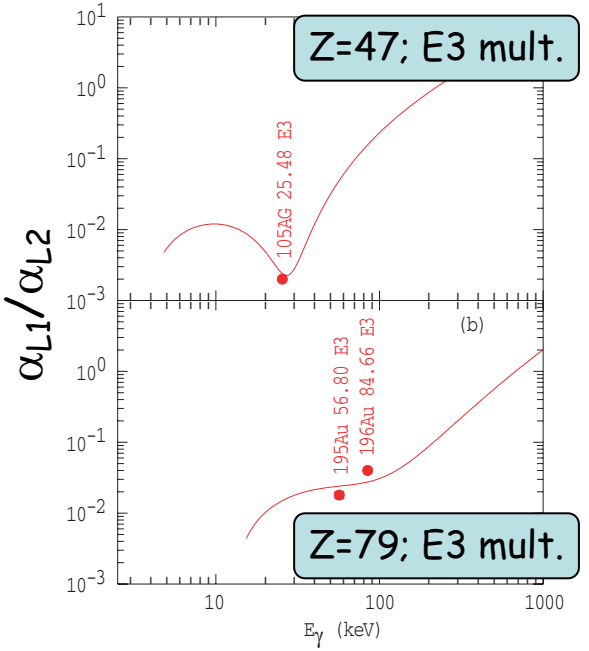


Partial conversion matrix elements vanishing at certain energies



Is it real?

Using BrIcc found 13 ICC in resonant energy regions



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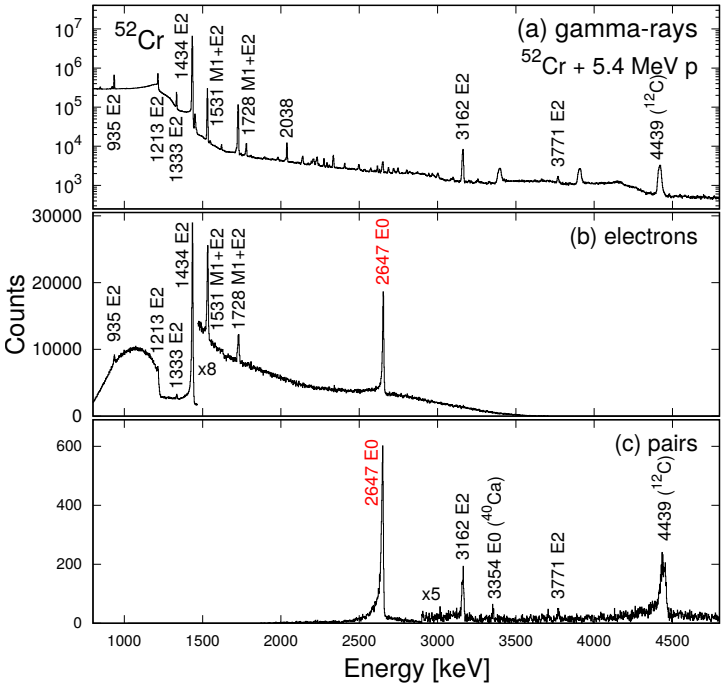
E0 - electric monopole transitions



J.T.H. Dowie, et al., EPJ Web of Conf. **232**, 04004 (2020)

Selection rule for E0:

$$j_i = j_f;\ \Delta\pi = 0$$

E0 conversion coefficient NOT DEFINED

$$\alpha(E0) = \lambda_{CE,PF}(E0) / \lambda_\gamma(E0)$$

E0 transition rate

$$\lambda_{CE,PF}(E0) = \rho^2(E0)\ \Omega_{CE,PF}(E0)$$

$\rho(E0)$ – monopole strength parameter, contains all nuclear structure information

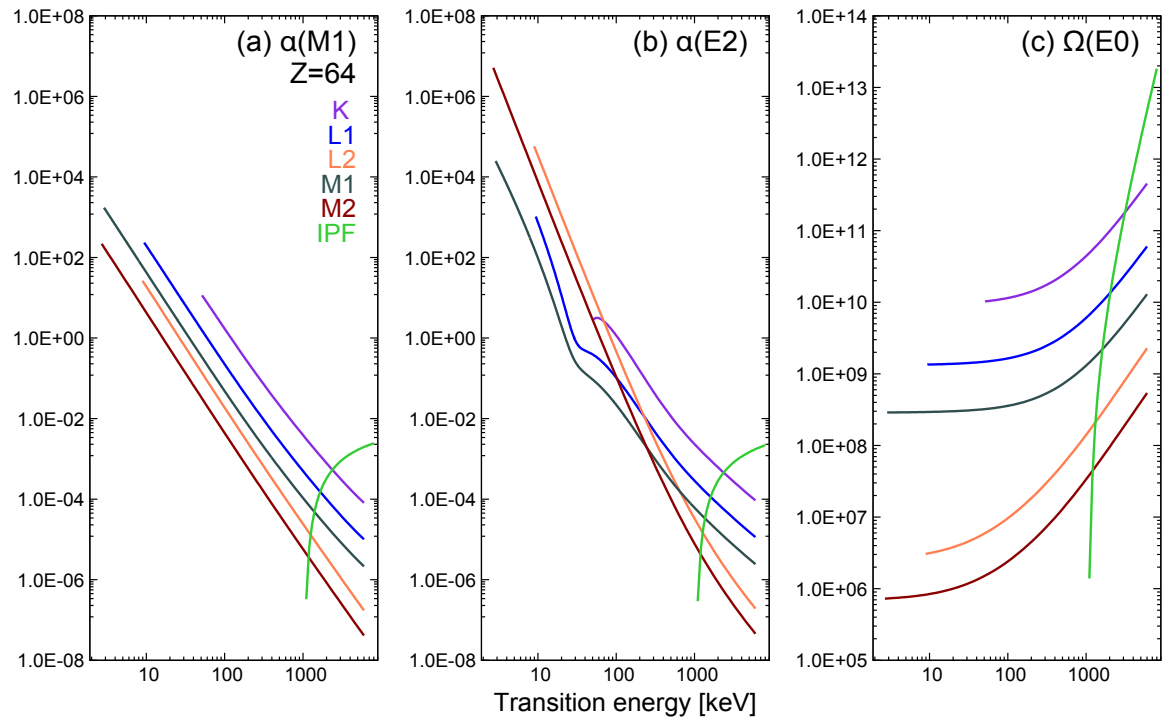
$\Omega_{CE,PF}(E0)$ – theoretical E0 electronic factor

E0 reduced transition rate

$$B(E0) = \rho^2(E0)\ e^2R_o^4$$

CE, IPF or double (M1 & E1) photon emission
No single photon emission is allowed!

Conversion coefficients & E0 electronic factors



α_i Conversion coefficients:

TK, et al., NIM **A589** (2008) 202

Z=5:110

TK, et al., ADNDT, 98 (2012) 313

Z=111:126

Ω_i(E0) electronic factors

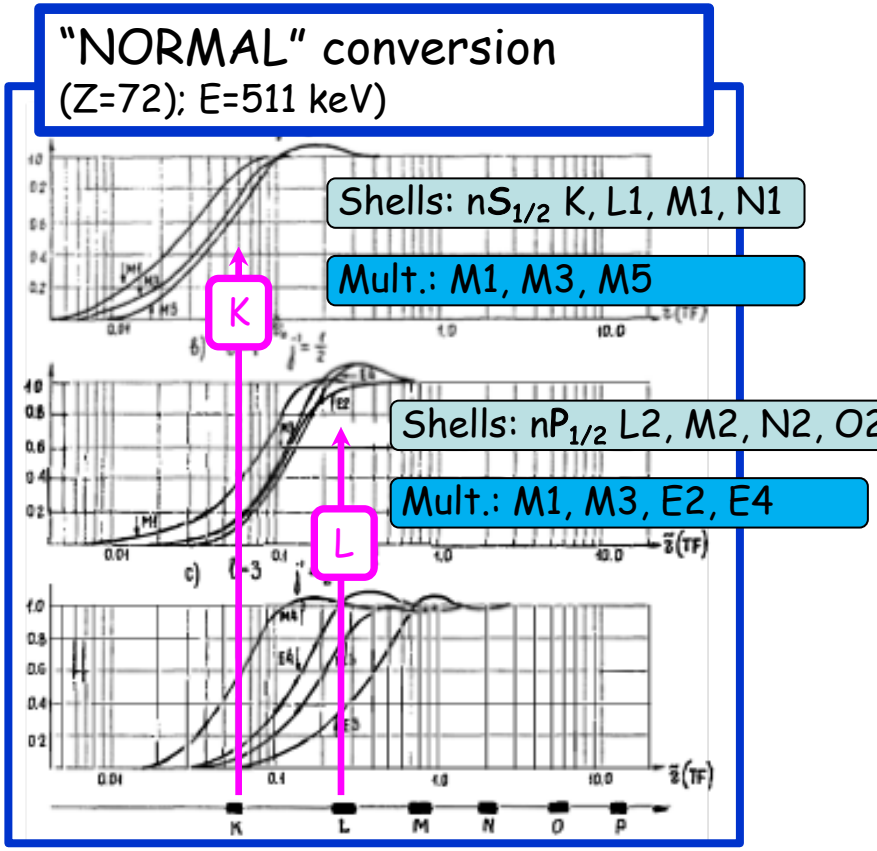
J.T.H. Dowie, et al., ADNDT, 131 (2020) 101283

Z=4:126

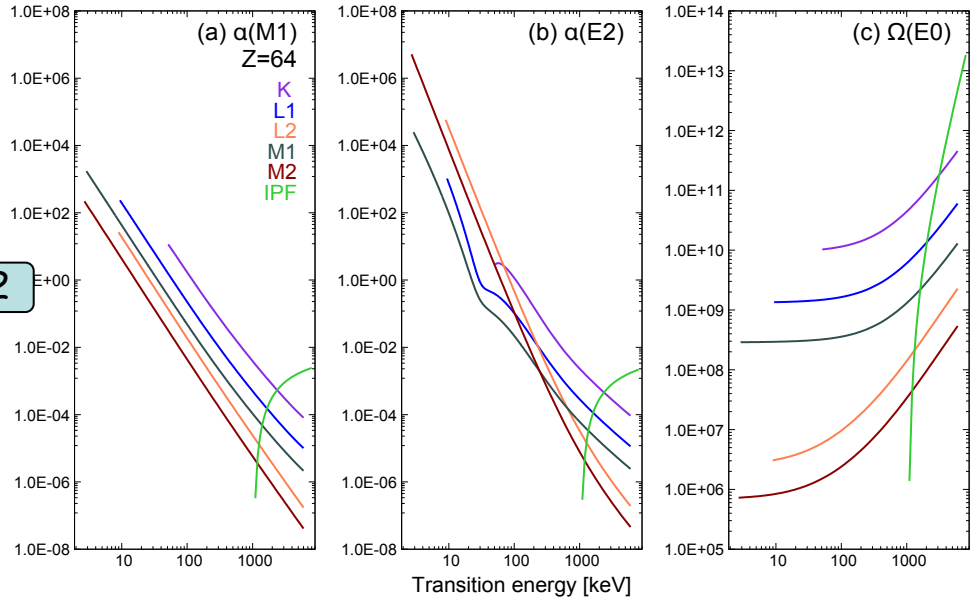
- E0 conversion on $nS_{1/2}$ and $nP_{1/2}$ shells only
- Energy dependence
  - α(M1,E2): ⬇ up 14+ orders of magnitude
  - Ω(E0): ⬆ 2-3 orders of magnitude
  - Opposite for pair conversion
- Atomic shells (K, L, M):

  Always decreasing

"Normal" vs E0 conversion



I.M. Band, et al., NP A156 (1970) 170



Different nuclear matrix elements & formation regions

Atomic structure

Transition rates:

"Normal" conversion $\Gamma_{i,CE} = \Gamma_\gamma \times \alpha_i$

Formation: extra-nuclear

E0 conversion $\Gamma_{i,CE} = \rho^2 \times \Omega_i$

Formation: intra-nuclear

Nuclear structure

Penetration effect

- E1 and M1 transitions could be hindered. Atomic WF overlap with could be larger
- ^{203}Tl: E_γ=279.1955(12) keV; M1+E2; δ=+1.17(5)
  α_K(exp) =0.1642(11) *from 7 measurements*
  α_K(Hslcc)=0.216
  α_K(Brlcc)=0.209
- "Static effects" are taken into account approximately, but consistently (SC model, Sliv)
- Hindered transitions: correction for "dynamic effects" (Pauli)

measured

a_{1i}, a_{2i}, a_{3i}, a_{4i}, a_{5i}, b_{1i}, b_{2i}: depend on ***electronic*** parameters (from theoretical calculations)

$$\alpha_i(ML) = \alpha_i^{\circ}(ML)\left(1 + b_{1i}\,\lambda + b_{2i}\,\lambda\right)$$

$$\alpha_i(EL) = \alpha_i^{\circ}(EL)\left(1 + a_{1i}\,\eta + a_{2i}\,\eta^2 + a_{3i}\,\eta\xi + a_{4i}\,\xi + a_{5i}\,\xi^2\right)$$

theoretical

λ, η, ξ: depend on ***nuclear*** parameters (from fit to the experimental data)

Electron-positron pair conversion

EM decay: energy and momentum carried away

Selection rules *(πL, $L>0$)*

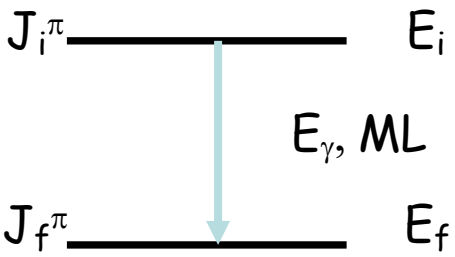
$|L-j_i| \leq j_f \leq L+j_i$

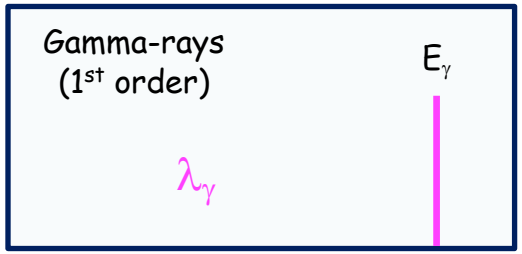
$\pi = (-1)^L$ for EL

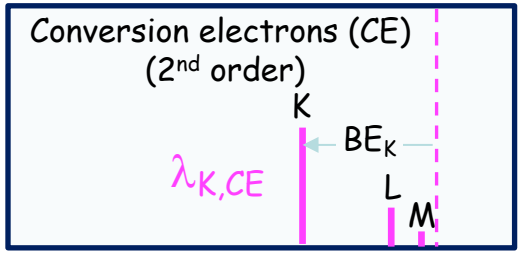
$\pi = (-1)^{L+1}$ for ML

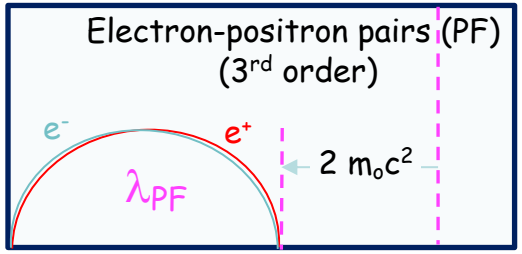
Selection rules *(E0)*

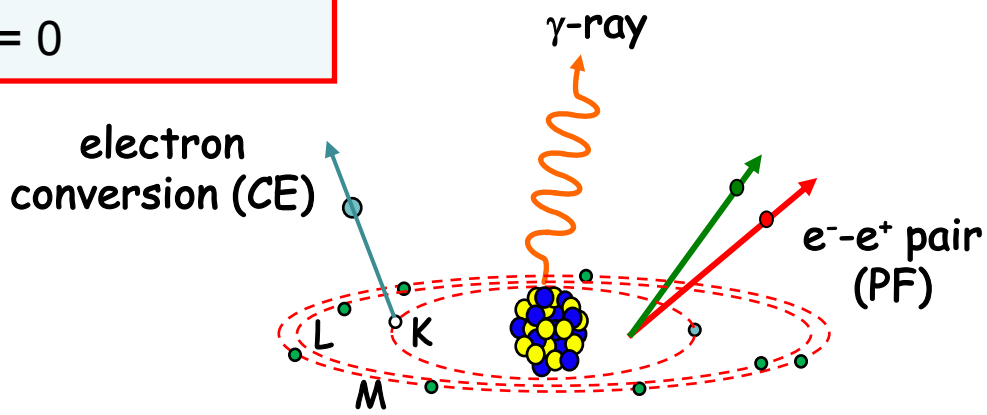
$j_i = j_f$; $\Delta\pi = 0$











Transition probability

$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M \ldots\ldots + \lambda_{PF}$

Conversion coefficient

$\alpha_{CE,PF} = \lambda_{CE,PF} / \lambda_\gamma$

$\lambda_{CE,PF} = \lambda_\gamma \times \alpha_{CE,PF}$

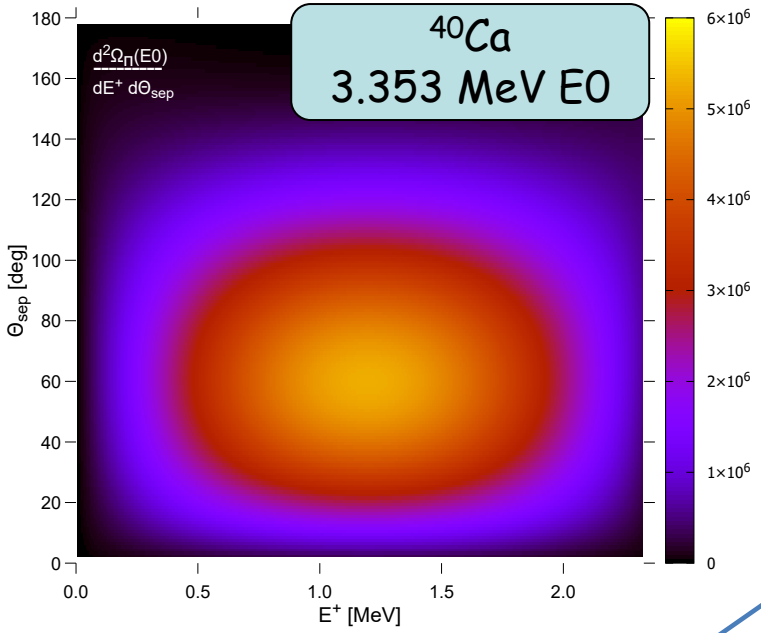
Energetics

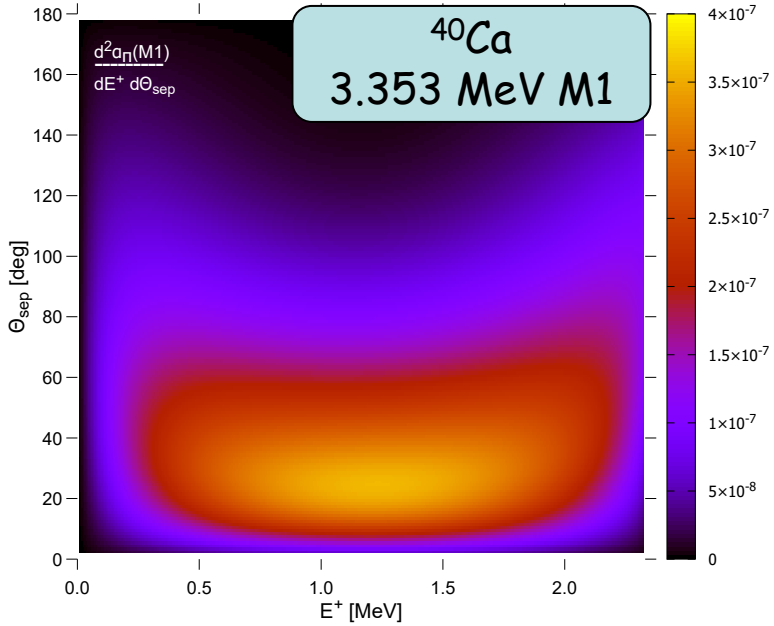
Gamma $E_\gamma = E_i - E_f + T_r$

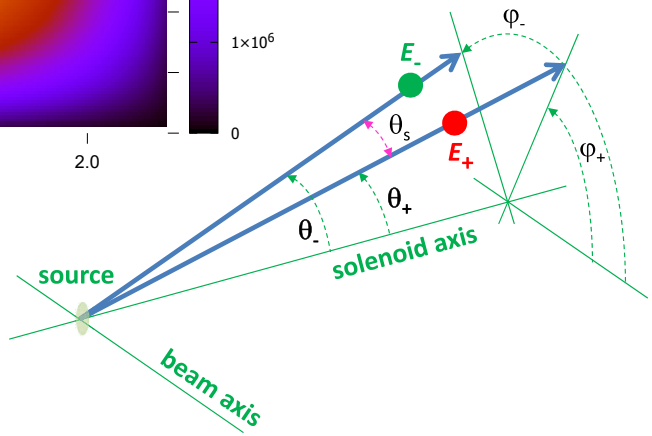
CE $E_{CE,i} = E_i - E_f - E_{BE,i} + T_r$

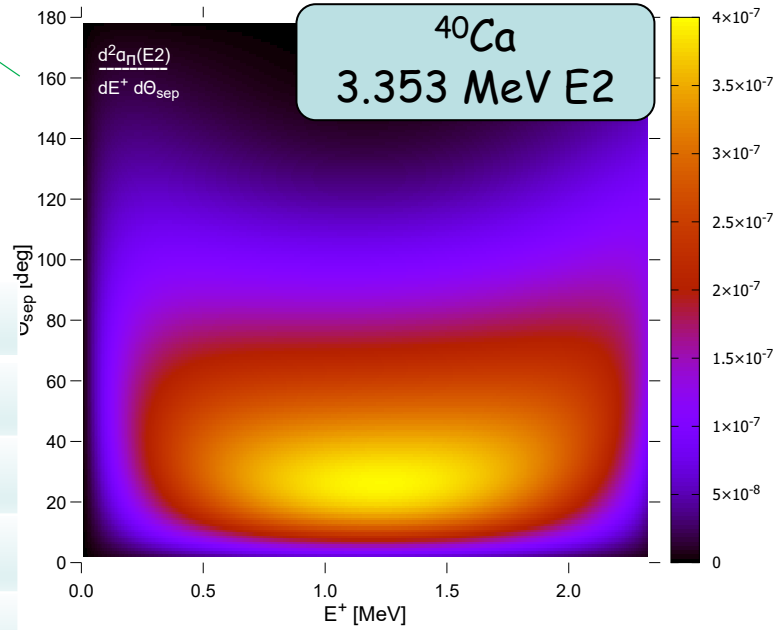
PF $E^+ + E^- = E_i - E_f - 2m_oc^2 + T_r$

Electron-positron pair conversion





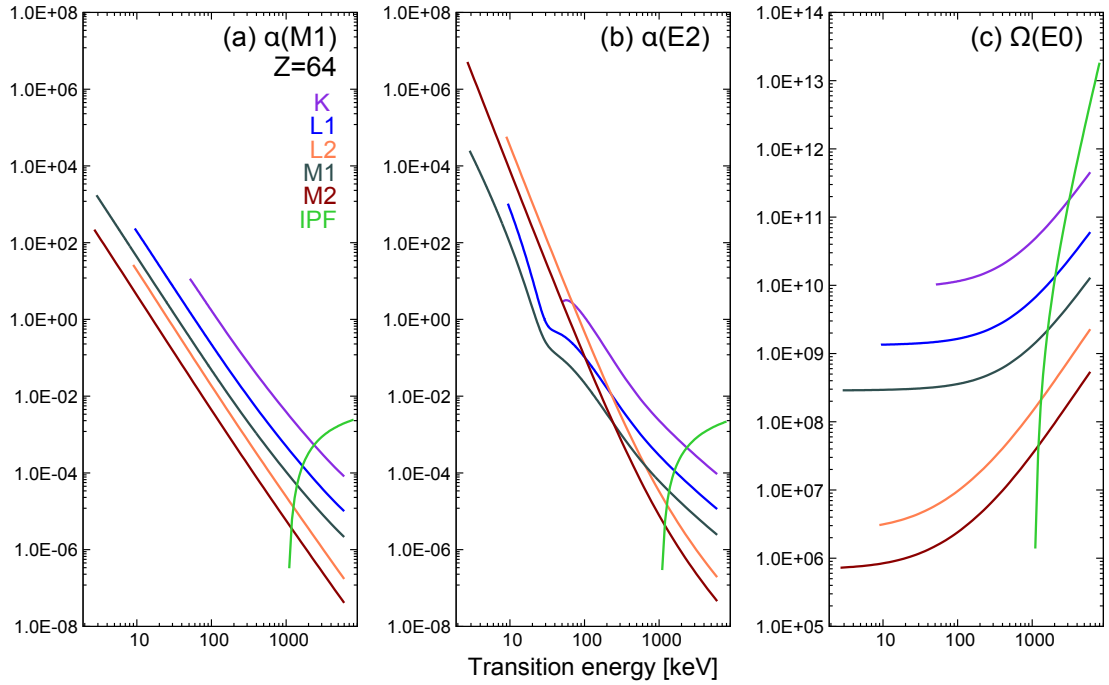




3.353 MeV in ^{40}Ca (Z=20)

	M1	E2	E0
K	7.9E-6	8.2E-6	8.5E+7
L	6.7E-7	7.0E-7	7.2E+6
IPF	8.1E-4	9.3E-4	1.2E+10
IPF/K	103	113	141

BrIcc data tables



α_i Conversion coefficients (CE)

TK, et al., NIM **A589** (2008) 202

Z=5:110

TK, et al., ADNDT **98** (2012) 313

Z=111:126

α_π Conversion coefficients (pairs)

P. Schlüter, G. Soff, ADNDT **24** (1979) 509

Z=0:50

C.R. Hofmann, G. Soff, ADNDT 63 (1996) 189

Z=51:100

Ω_i(E0) electronic factors (CE) *

J.T.H. Dowie, et al., ADNDT **131** (2020) 101283

Z=5:126

Ω_π(E0) electronic factors (pairs) *

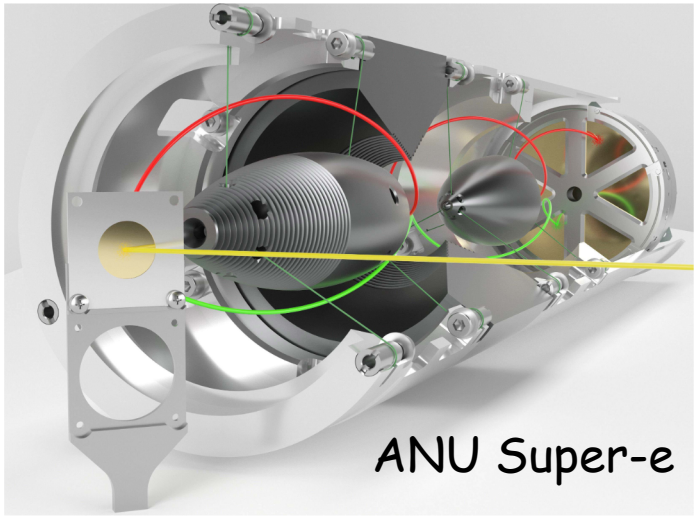
J.T.H. Dowie, et al., ADNDT, **131** (2020) 101283

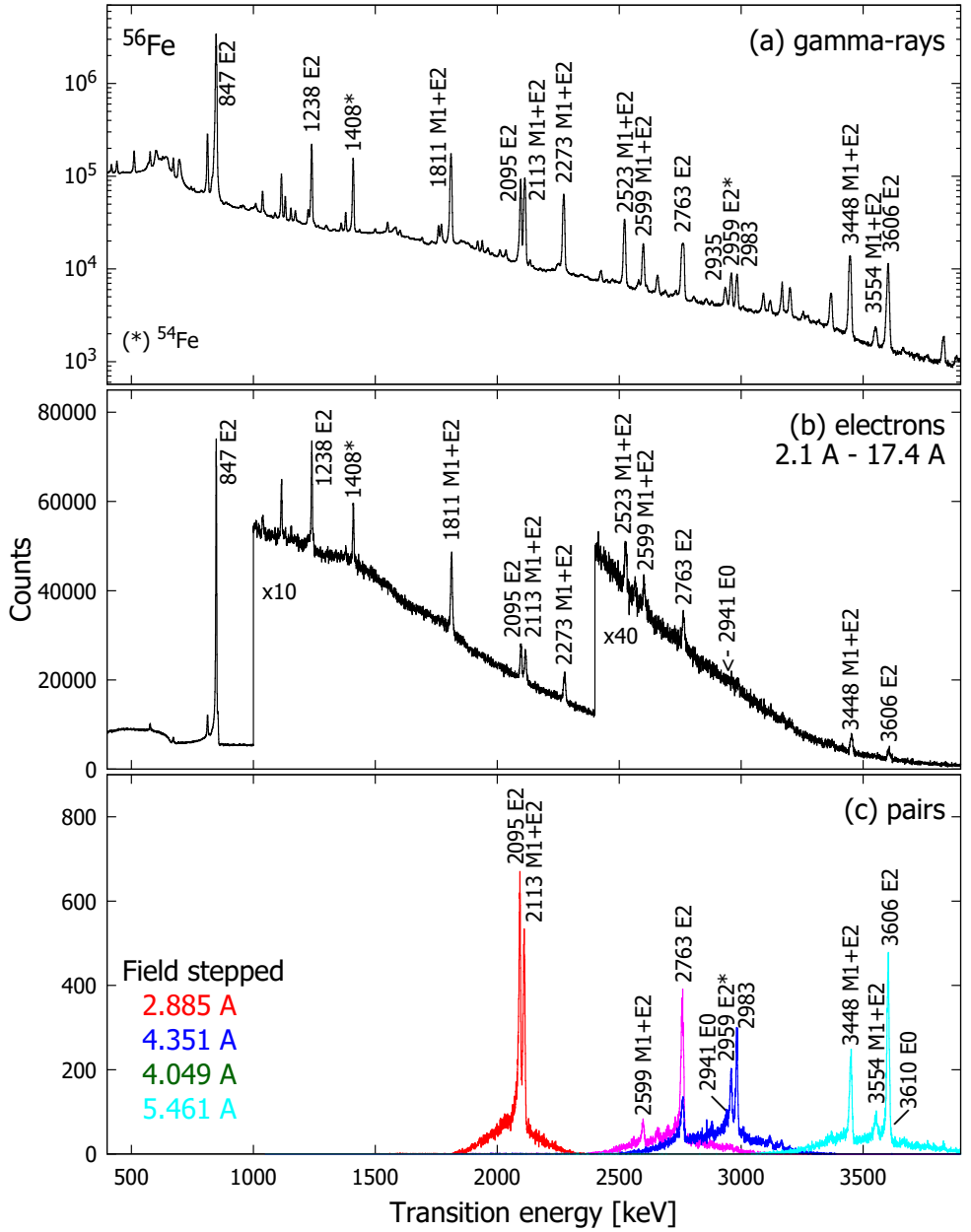
Z=4:100

* Will be available through BrIcc (early 2022)

Combining γ-, CE & pair spectroscopy

^{56}Fe(p,p') @ 6.7 MeV
1.5 mg/cm^2 nat Fe
1 μA beam





T. Kibédi, ANU

Mixed transitions

EM decay: energy and ang. momentum carried away

Selection *rules* (πL)

$|L-j_i| \lesssim j_f \lesssim L+j_i$

$\pi = (-1)^L$ for EL

$\pi = (-1)^{L+1}$ for ML

Example: 2^+ to 1^+ transition, $\Delta J=-1$; $\Delta\pi = +$

- M1 ($\Delta J=-1,0,+1$)
- E2 ($\Delta J=-2,-1,0,+1,+2$)
- mixed M1+E2 ($\Delta J=-1,0,+1$)

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

γ-ray transition probability:

$$\lambda_\gamma(\pi' L'/\pi L) = \lambda_\gamma(\pi` L`) + \lambda_\gamma(\pi, L)$$

Mixing ratio (MR) $\delta^2(\pi' L'/\pi L) = \dfrac{\lambda_\gamma(\pi' L')}{\lambda_\gamma(\pi L)}$

Mixing of 3 multipolarities:

^{184}W 536.674(15) keV

E1+M2+E3

δ(M2/E1)=+0.070(6)

δ(E3/M2)=-0.025(4)

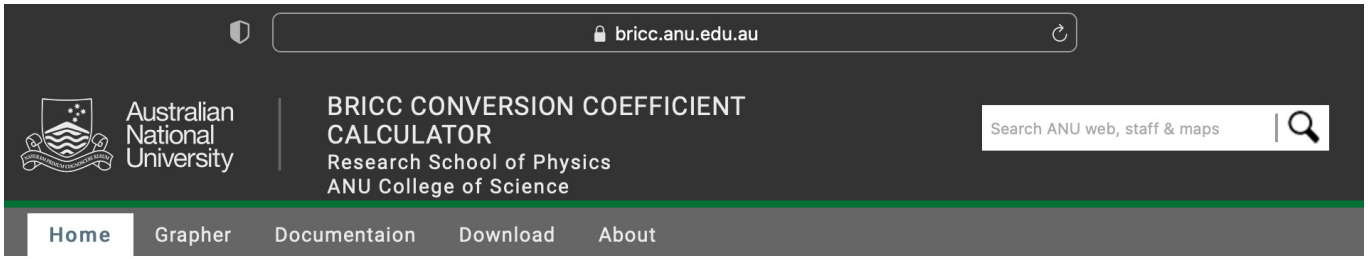
λ=-2.1(2)

Conversion coefficient for CE and IPF

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

Obtaining conversion coefficients

https://bricc.anu.edu.au



BrIcc

Conversion Coefficient Calculator

The **BrIcc** program calculates the conversion electron (αIC), electron−p
(ΩIC,π(E0)).

Z * er

Energy * 1447.820

Energy uncertainty 25

Multipolarity M1+E2

δ +0.5

δ uncerntainty 3

Subshells

Data set BrIccFO

Calculate

- ❑ Chemical symbol or Z
- ❑ Transition energy [keV]
- ❑ Energy uncertainty
- ❑ Multipolarity
- ❑ Mixing ratio
- ❑ Mixing ratio uncertainty
- ❑ Calculate Subshell ICC`s
- ❑ Data set BrIccFO, BrIccNH, RpIcc or HsIcc

All input parameters verified
Minimum input: Chemical symbol/Z & Eγ

Obtaining conversion coefficients factors

BrIccS v2.3 (9-Dec-2011)

Z=68 (Er, Erbium)

γ-energy: 1447.820 *(+25 -25)* keV

Mixing Ratio δ: +0.5 *(+3 -3)*

Data Sets: BrIccFO HoPcc

Conversion coefficient for CE and IPF

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

Warning

- ICC could not be calculated for EG+DEGH above 398.000 keV
- ICC could not be calculated for EG+DEGH above 398.000 keV

Oscillations in the ICC calculations

Shell	E(ce)	M1	E2	Mixed ICC
Tot		2.603E-03	1.673E-03	0.00242 (18)
K	1390.33	2.152E-03	1.367E-03	0.00200 (16)
L-tot	1438.11	3.001E-04	1.955E-04	0.000279 (21)
K/L		7.170E+00	6.994E+00	7.1 (8)
M-tot	1445.62	6.606E-05	4.314E-05	6.1E-5 (5)
L/M		4.544E+00	4.531E+00	4.5 (5)
N6	1447.81			
N7	1447.82			
N-tot	1447.38	1.541E-05	1.003E-05	1.43E-5 (11)
L/N		1.948E+01	1.948E+01	19.5 (20)
O-tot	1447.76	2.243E-06	1.442E-06	2.08E-6 (16)
L/O		1.338E+02	1.355E+02	134 (14)
P-tot	1447.81	1.276E-07	7.790E-08	1.18E-7 (10)
L/P		2.353E+03	2.509E+03	2.4E3 (3)
IPF		6.738E-05	5.557E-05	6.50E-5 (25)
Tot(CE)		2.536E-03	1.617E-03	0.00235 (16)

Contribution to uncertainties

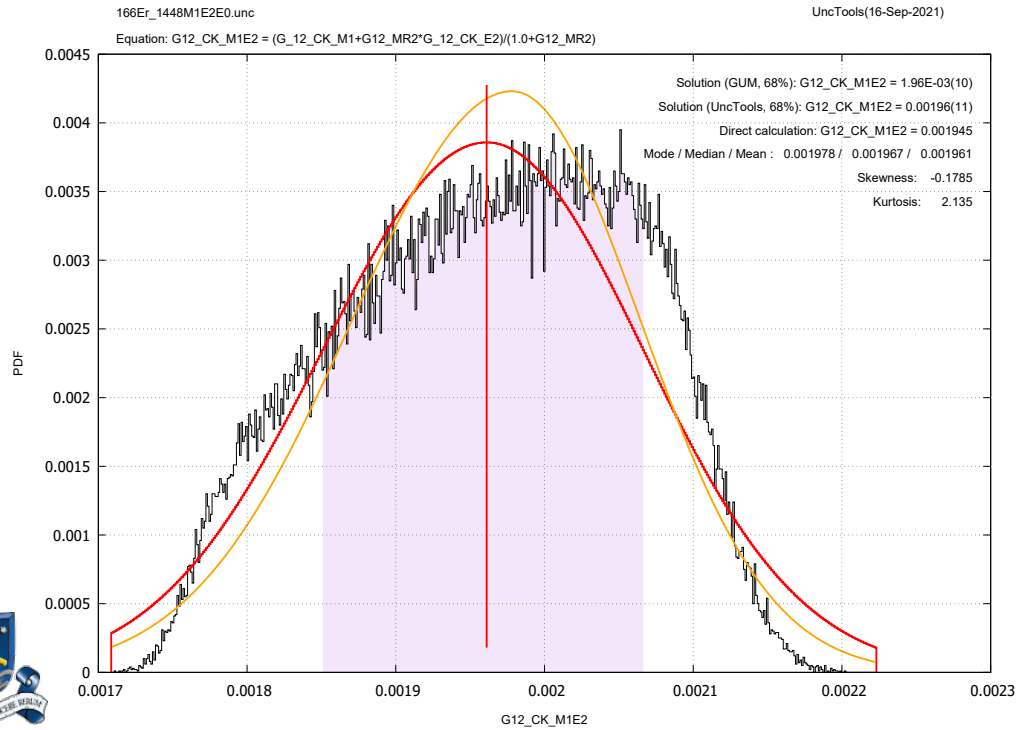
- Transition energy (dependence on transition energy
- Multipole mixing ratios
- Model constrains, tabulation/interpolation
  - 1.4% of the ICC; 5% of the Ω(E0)

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

<u>ENSDF: Use the Gaussian method for uncertainty propagation</u>

- Based on partial derivatives; only valid for small relative uncertainties!

<u>New Monte Carlo based uncertainty propagation</u>



^{166}Er 1447.820 M1+E2 δ=+0.5(3)

Gaussian method: α_K=0.00200(16)

MC α_K=0.00196(11)

Obtaining conversion coefficients

BrIcc – desktop application
from IAEA: https://www-nds.iaea.org/public/ensdf_pgm/

```
-------------------------------------------------------------------------------------------------------------------
Z= 68  Erbium            Transition energy: 1447.820 keV                                  BrIcc v2.3e (17-Jun-2020)
                                                  Conversion Coefficient                  Data Table: BrIccFO
Shell  E_e [keV]   E1        M1        E2        M2        E3        M3        E4        M4        E5        M5
-------------------------------------------------------------------------------------------------------------------
Tot              8.681E-04 2.603E-03 1.673E-03 5.932E-03 3.201E-03 1.077E-02 5.797E-03 1.842E-02 1.019E-02 3.075E-02
K       1390.33  6.049E-04 2.152E-03 1.367E-03 4.973E-03 2.636E-03 8.950E-03 4.692E-03 1.509E-02 8.006E-03 2.471E-02
L-tot            8.038E-05 3.001E-04 1.955E-04 7.305E-04 4.226E-04 1.411E-03 8.584E-04 2.589E-03 1.690E-03 4.676E-03
M-tot            1.757E-05 6.606E-05 4.314E-05 1.619E-04 9.455E-05 3.157E-04 1.950E-04 5.860E-04 3.899E-04 1.072E-03
N-tot            4.088E-06 1.541E-05 1.003E-05 3.779E-05 2.198E-05 7.371E-05 4.531E-05 1.369E-04 9.055E-05 2.505E-04
O-tot            5.923E-07 2.243E-06 1.442E-06 5.486E-06 3.122E-06 1.064E-05 6.349E-06 1.959E-05 1.252E-05 3.548E-05
P-tot            3.333E-08 1.276E-07 7.790E-08 3.070E-07 1.576E-07 5.797E-07 2.966E-07 1.029E-06 5.377E-07 1.781E-06
IPF              1.605E-04 6.738E-05 5.557E-05 2.308E-05 2.252E-05 8.729E-06
TranEner|ChemSymb|Z+Integer|SUBShell|DATAtable|? for help|EXIT [1447.820] >
```

Designed to work with ENSDF files

- Step#1: evaluate ICC`s for all transitions

  BrIcc 166Ho_beta.ens

  Output files: calculation report, new *GAMMA* records

- Step#2: insert new records into ENSDF file

  BrIcc 166Ho_beta.ens merge

Obtaining conversion coefficients

BrIccS – slave application to be called from other codes

from ANU: https://bricc.anu.edu.au/download.php

User input on the command line

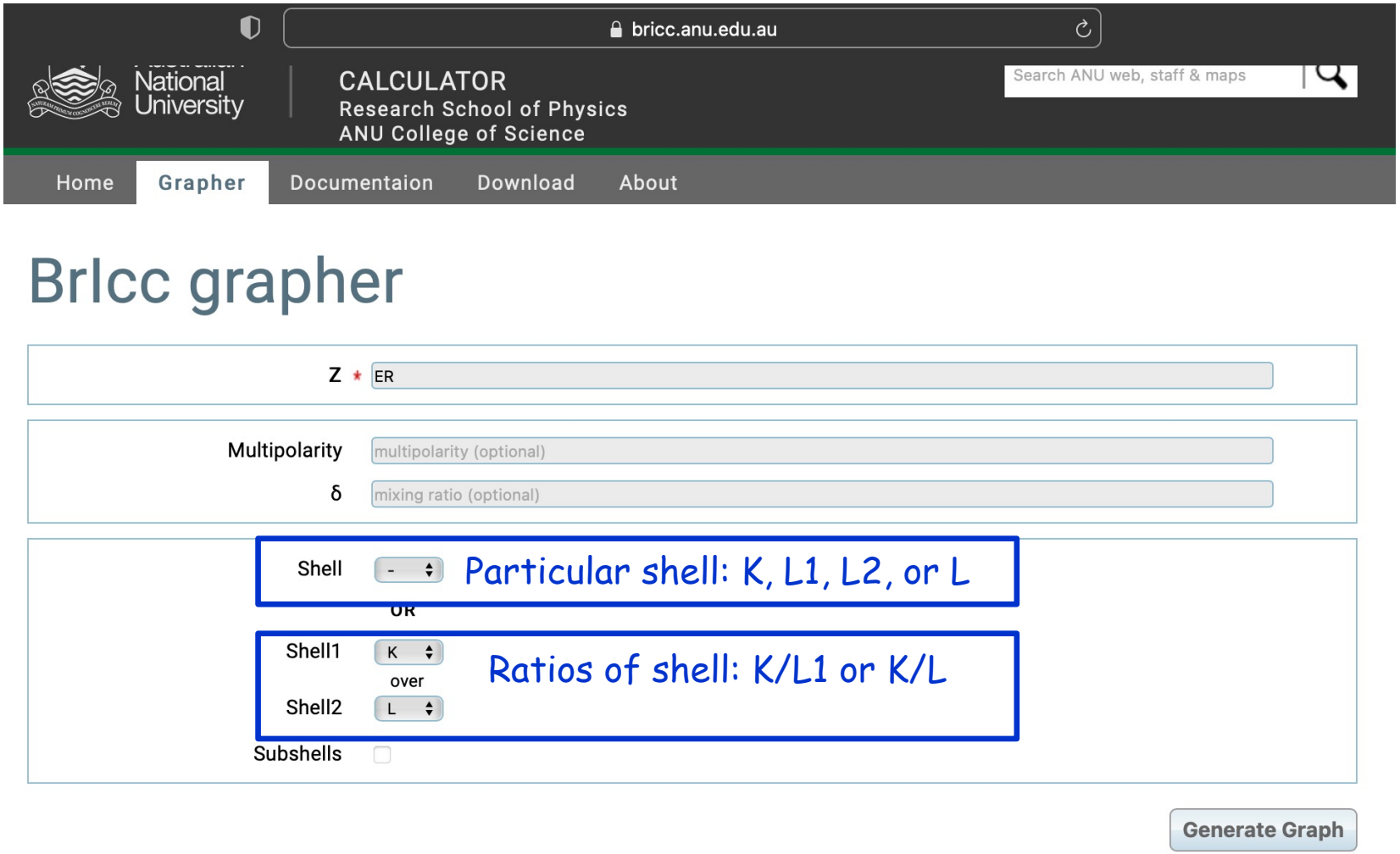
```
MacBook-Pro-6:~ tibor$ briccs -S Er -g 1447.820 -e 25 -L M1+E2 -d +0.5 -u 3
<BRICC version="BrIccS v2.3d (23-May-2020)">
  <ELEM z="68" symb="Er"> Erbium </ELEM>
  <DATASET icc="BrIccFO" pcc="HoPcc"> </DATASET>
  <MULT mult1="M1" mult2="E2"> M1+E2 </MULT>
  <MR dmrh="+3" dmrl="-3"> +0.5 </MR>
  <E deh="+25" del="-25"> 1447.820 </E>
  <MixedCC
    Shell="Tot"
    CCmult1="2.603E-03"
    CCmult2="1.673E-03"
    DCC="18">
    0.00242
  </MixedCC>
```

XML output

```
<MixedCC
  Shell="K"
  Eic="1390.334"
  DEic="25"
  CCmult1="2.152E-03"
  CCmult2="1.367E-03"
  DCC="15">
  0.00200
</MixedCC>
```

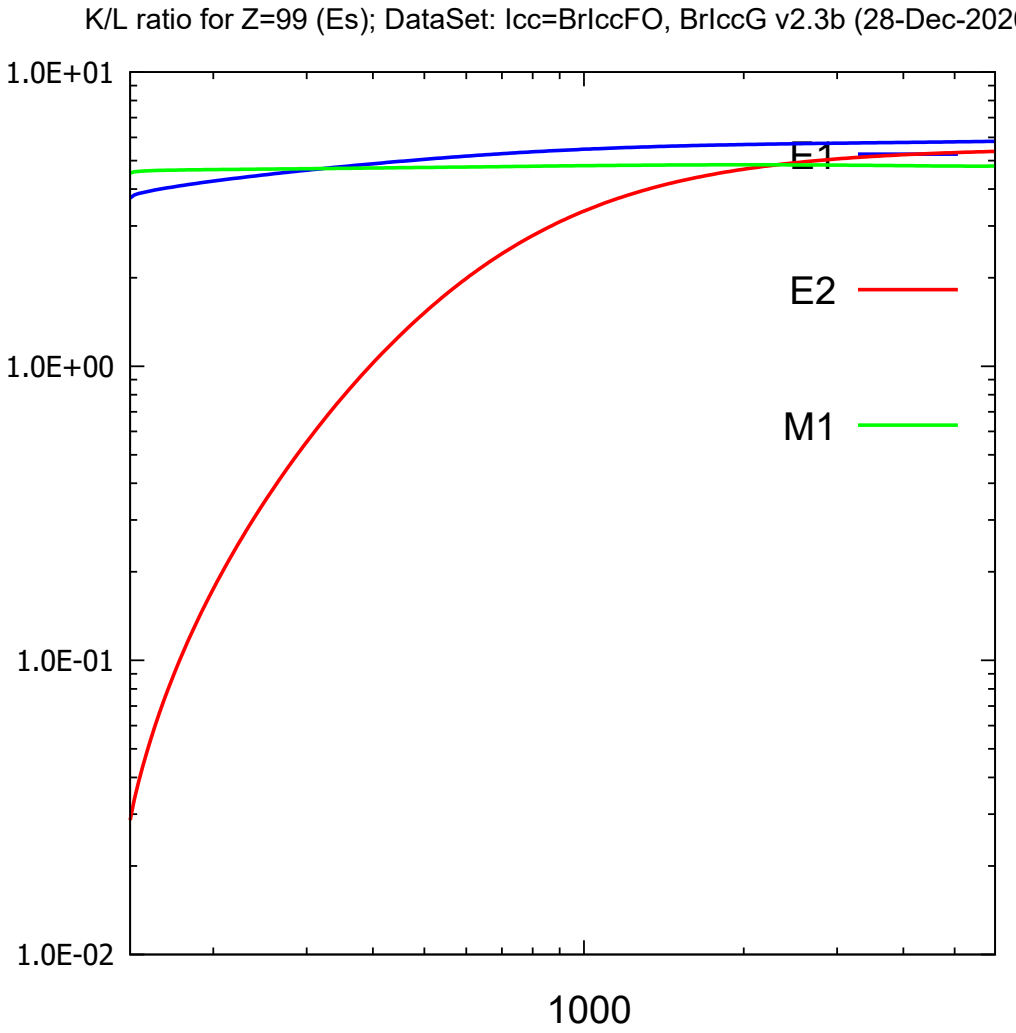
Obtaining conversion coefficients

BrIccG – plot conversion coefficients and ratios
from ANU: https://bricc.anu.edu.au/grapher.php



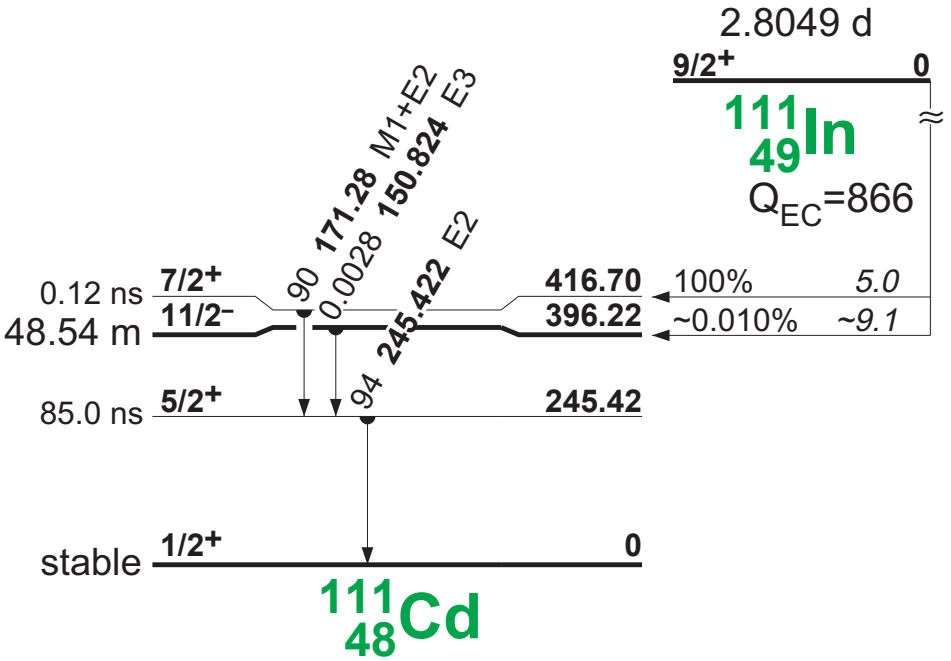
Obtaining conversion coefficients

BrIccG – plot conversion coefficients and ratios
from ANU: https://bricc.anu.edu.au/grapher.php



K/L for Z=99

Using ICC values – intensity balance of decay schemes



Transition probability

$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M \ldots\ldots + \lambda_{PF}$

Total transition intensity

$I_{tot} = I\gamma * (1+\alpha_{tot})$

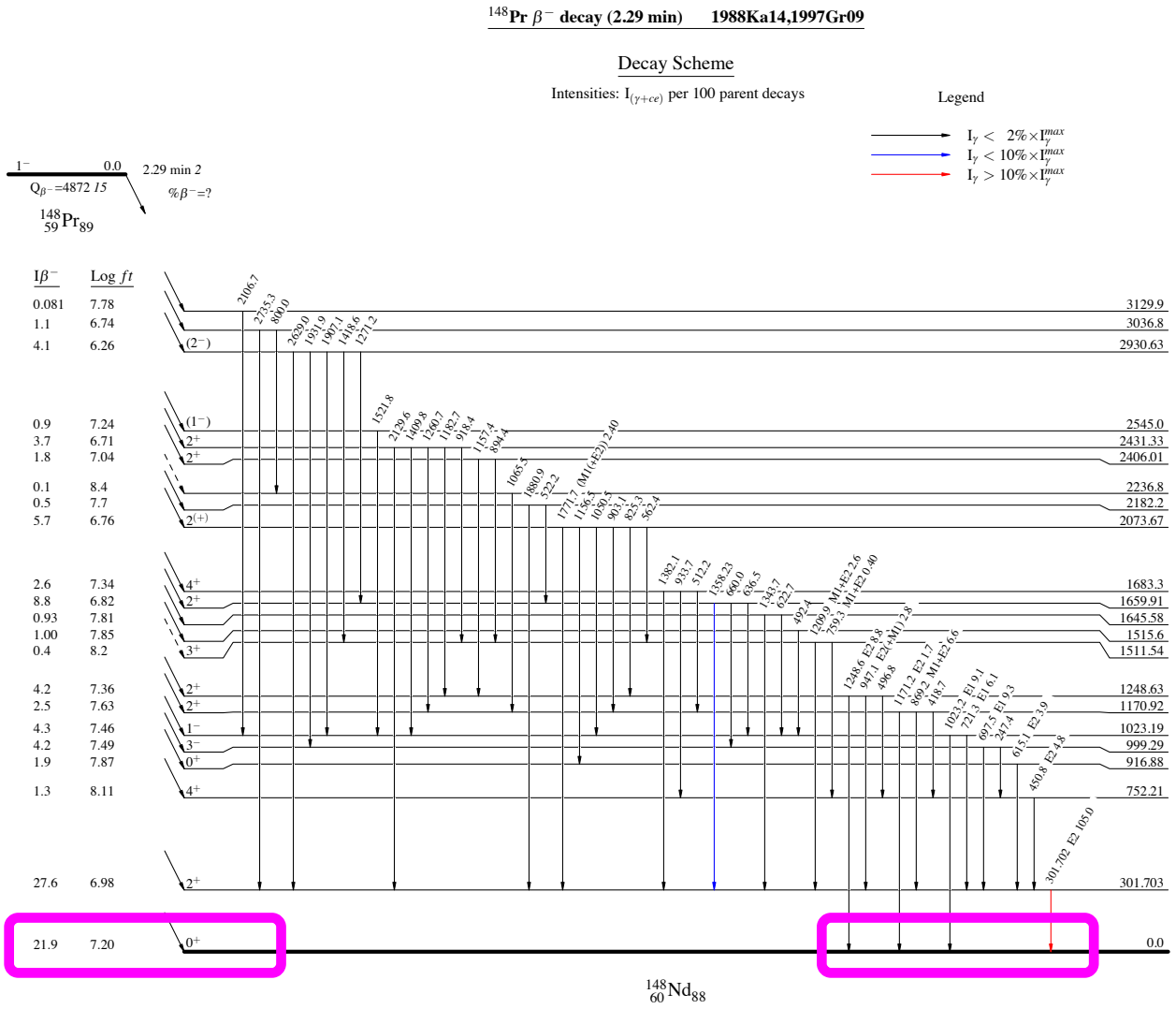
Intensity balance

$I_{tot}(245) = I_{tot}(151) + I_{tot}(171)$

$I_\gamma(171)$ from $\alpha_{tot}(171)$]

$I\gamma(171) = (100 - I_\beta(396) / [1 + \alpha_{tot}(171)]$

Using ICC values –decay schemes normalization



Total decay intensity to g.s. = 100

Experimental determination of ICC`s

Definition: $\alpha_{i,exp} = I_{i,CE} / I_\gamma$

- Absolute detector efficiency for CE and γ-rays: hard to do
- Most ICCs from PNG (i: K, L,...)

$$\alpha_{i,exp} = N * [A_{i,CE} / \varepsilon_{CE}(E_{CE})] / [A\gamma / \varepsilon_\gamma(E_\gamma)]$$

Using a known conversion coefficient or assumed multipolarity

$$N = \alpha_{i,cal} * I_{\gamma,cal} / I_{i,cal}$$

- α_K from singles γ and K X-rays

$$\alpha_K \omega_K = [N_K / N_\gamma] * [\varepsilon_\gamma/\varepsilon_K]$$

- α_{tot} from intensity balance (singles/coincidence measurements)

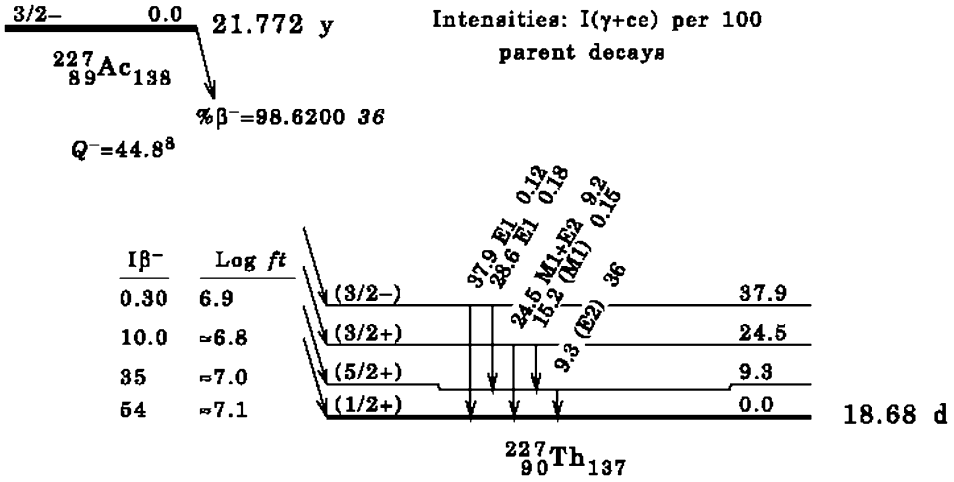
$$I_\gamma(1) * [1+\alpha_{tot}(1)] = I_\gamma(2) * [1+\alpha_{tot}(2)]$$

For low energy / highly converted transitions

- etc ...

<u>Always report details of the calibration</u>

BrIccMixing - Multipolarity mixing ratio from ICC`s



ICC for CE and IPF

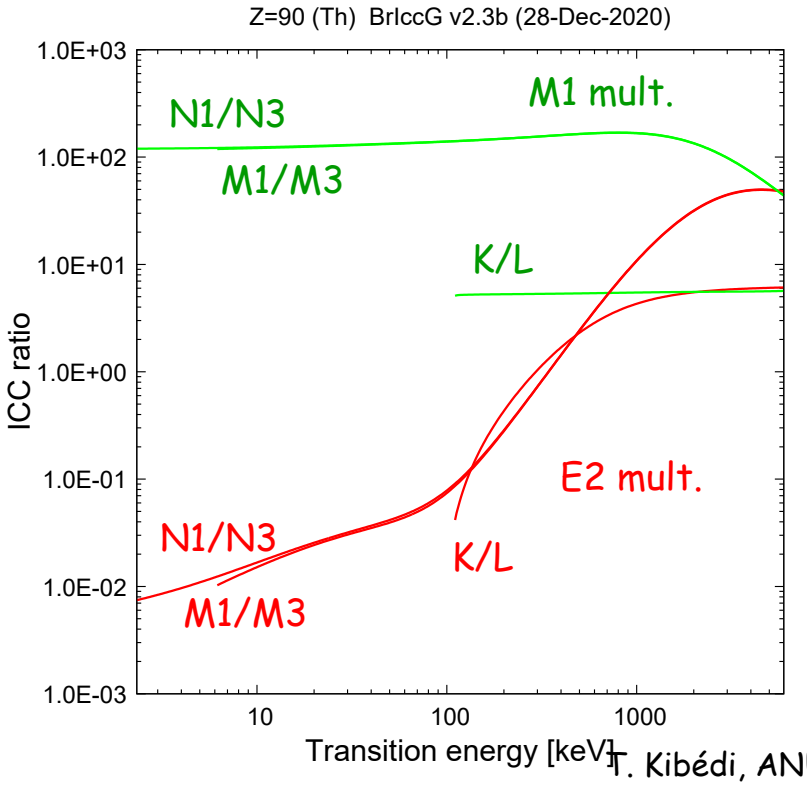
$$\alpha(\pi' L'/\pi L) = \frac{\alpha(\pi L) + \delta^2 \alpha(\pi' L')}{1 + \delta^2}$$

ELSEVIER

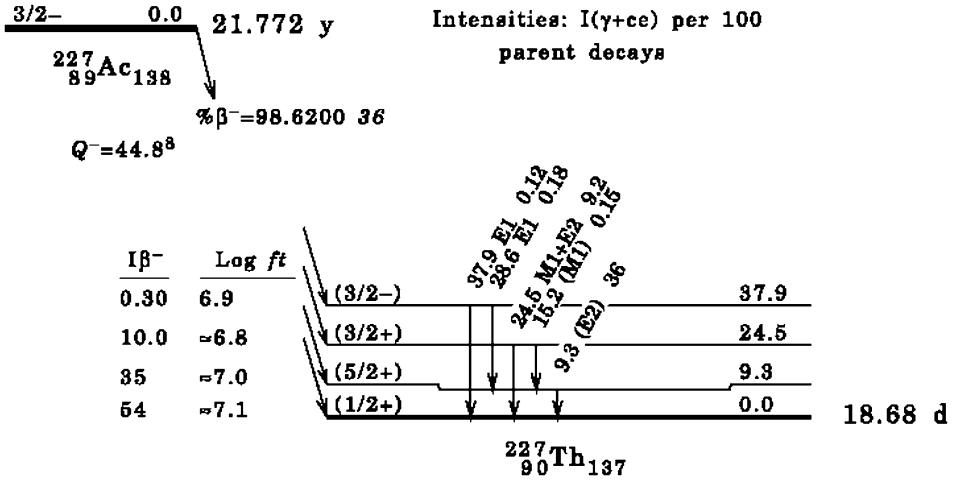
Physics Letters B
Volume 820, 10 September 2021, 136593

The first experimental evidence for the (M1 + E2) mixed character of the 9.2 keV transition in ^{227}Th

A. Kovalík [a, b] ✉, A.Kh. Inoyatov [a, c] ✉, L.L. Perevoshchikov [a] ✉, M. Ryšavý [b] ✉, D.V. Filosofov [a] ✉, P. Alexa [d] ✉, J. Kvasil [e] ✉



BrIccMixing - Multipolarity mixing ratio from ICC`s



ICC for CE and IPF

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

ELSEVIER

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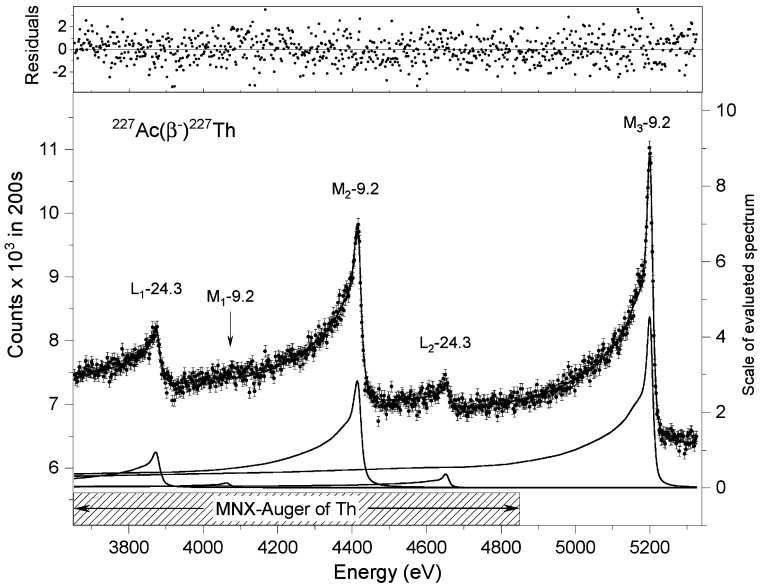
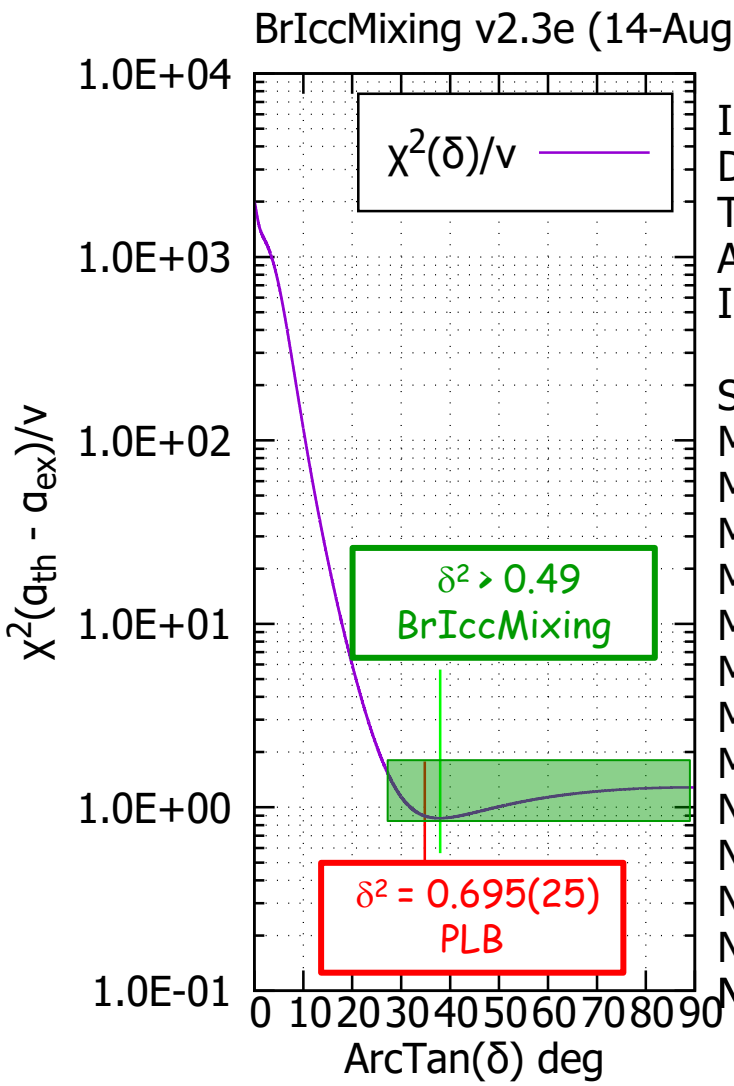


BrIccMixing – Multipolarity mixing ratio from ICC`s



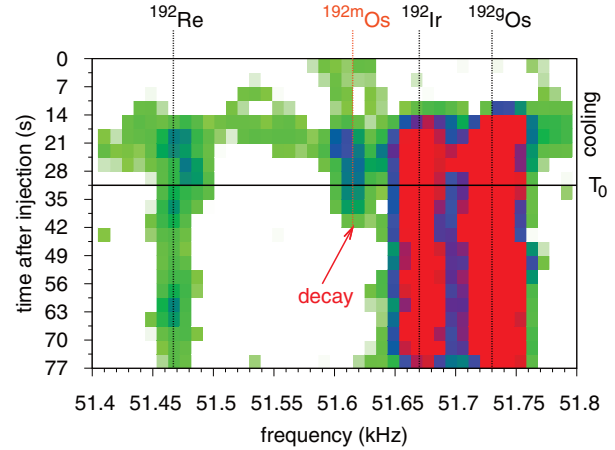
Input file: 227Th$_M$R.in
Data set: 227TH G 9.3 1 0.00011 M1+E2
Transition: 9.245 (1) keV
Adopted from fit: δ=0.78(-29); χ^2/v= 8.72E-01
Input data ----------

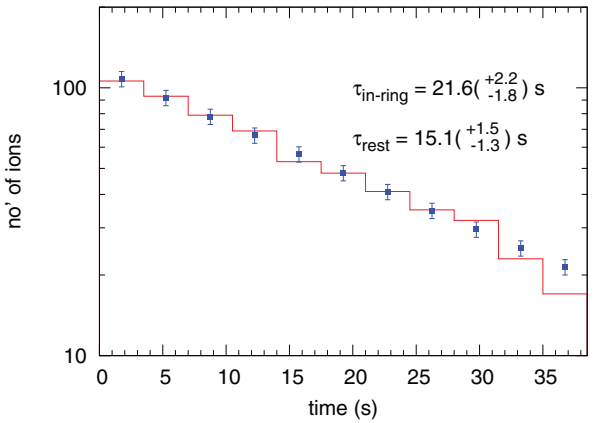
Shell	Experiment Icc(Unc)	Fit Icc(Unc)	Type
M1/M2	0.031(11)	0.0271(5)	R
M1/M2	0.027(9)	0.0271(5)	R
M1/M3	0.025(9)	0.0227(4)	R
M1/M3	0.023(7)	0.0227(4)	R
M2/M3	0.852(10)	0.836(17)	R
M4/M3	0.019(6)	0.01595(32)	R
M4/M3	0.021(4)	0.01595(32)	R
M5/M3	0.019(4)	0.01197(24)	R
N1/N3	0.02(3)	0.0244(5)	R
N1/N3	0.012(13)	0.0244(5)	R
N2/N3	0.84(7)	0.832(16)	R
N2/N3	0.84(2)	0.832(16)	R
N5/N3	0.044(17)	0.01155(23)	R

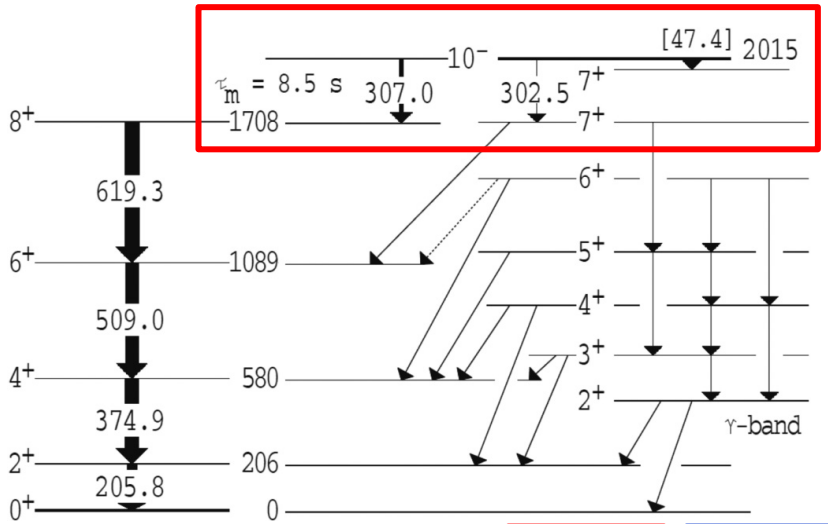
ICC of a Hydrogen-like ^{192m}Os

A. Akber et al., Phys.Rev. C 91, 031301 (2015)

- ^{197}Au @ 478-492 MeV on 221 mg/cm2 ^{9}Be; relativistic projectile fragmentation UNILAC & SIS-18 GSI
- Hydrogen like (one K electron only, Z=76) ^{192m}Os in storage ring







Energy (kev)	I_γ	$\sigma\lambda$	BrIcc α_T^{neut}	RAINE α_T^{H-like}
47.4	0.0031(6)	*E*3	7760	0
302.6	100(6)	*E*3	0.433	0.084
307.0	13.3(3)	*M*2	0.975	0.374
K_{BE}(Os)[keV]			73.87	85.7

$\tau_{H\text{-like}}$ = 13.0 (24) s (calc)
τ_{rest} = 15.1(+15-13) s (measured)

Angular distributions and correlations

- Gamma-gamma angular correlation well understood, widely used

$$W(\gamma\gamma, E2+M1) = P_0 + \frac{1}{1+\delta^2}[A_2^e + 2\delta A_2 + \delta^2 A_2^m]P_2 + \frac{1}{1+\delta^2}[A_4^e]P_4$$

A_2 A_4 can be calculated; "e" E2, "m" M1

- Electron-gamma angular correlation

$$W(e\gamma, E2+M1) = P_0 + \frac{1}{1+p^2}[b_2^e A_2^e + 2pb_2A_2 + p^2 b_2^m A_2^m]P_2 + \frac{1}{1+p^2}[b_4^e A_4^e]P_4$$

b_2 b_4 particle parameters need to be calculated

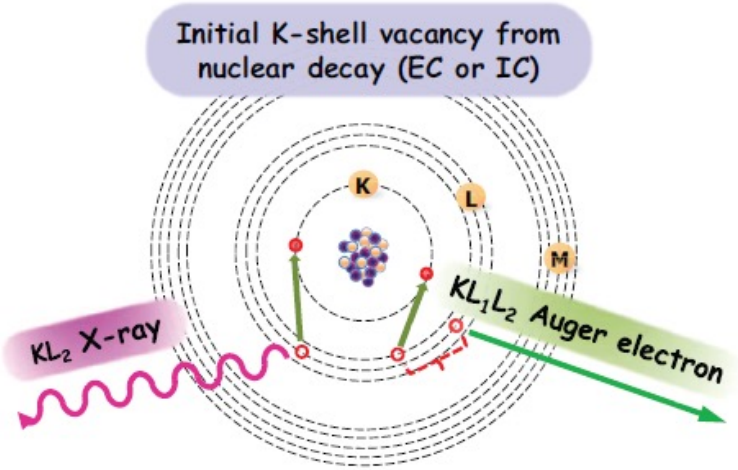
Hager-Seltzer Nucl. Data **A4**, 1 (1968)

$p^2 = \delta^2 \times \alpha_{M1} / \alpha_{E2}$

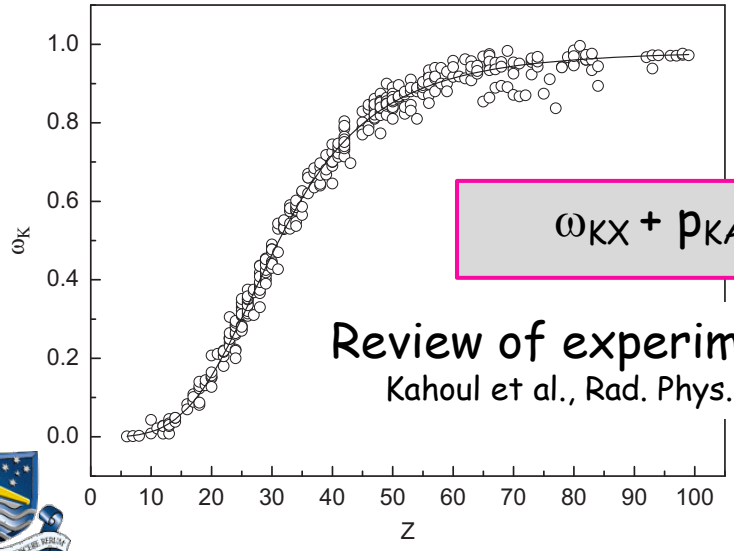
- Corrections using Monte Carlo
  - SINGLES: for angular distribution
  - COINCIDENCES: for angular correlation
  - PAIR CONVERSION: see T.K. Eriksen, PhD (ANU) 2018

BrIccEmis – atomic relaxation following nuclear decay

B.Q. Lee & B.P.E. Tee



K-shell fluorescence probability

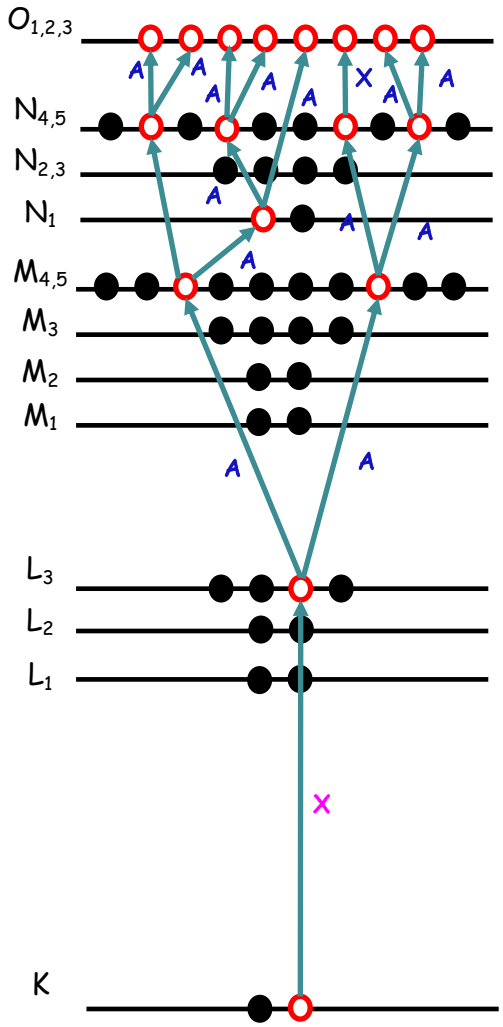


$$\omega_{KX} + p_{KA} = 1$$

Review of experiments & global fit

Kahoul et al., Rad. Phys. Chem. **80** (2011) 369

Vacancy cascade



T. Kibédi, ANU

BrIccEmis – atomic relaxation following nuclear decay

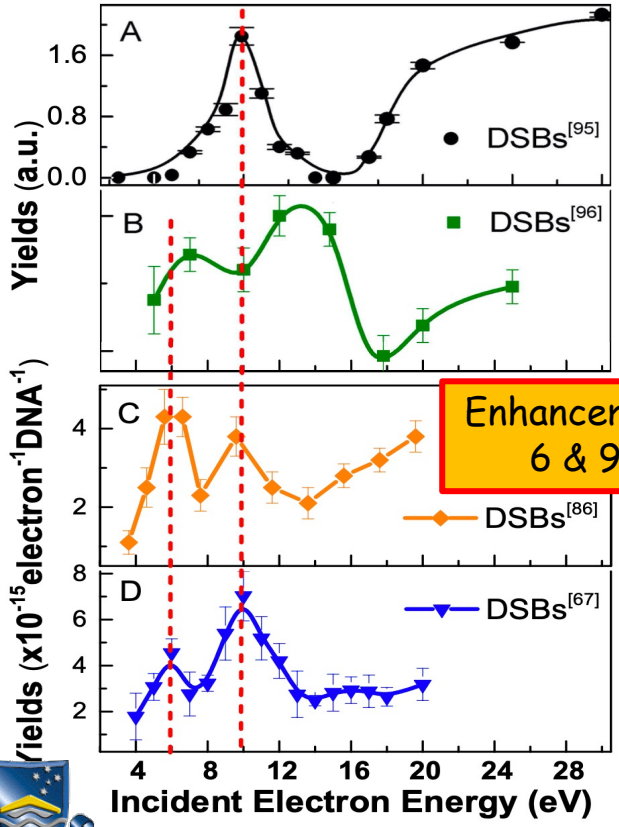
B.Q. Lee & B.P.E. Tee

International Journal of *Molecular Sciences* 2019

Review

Clustered DNA Damages induced by 0.5 to 30 eV Electrons

Yi Zheng [1,*] and Léon Sanche [2]

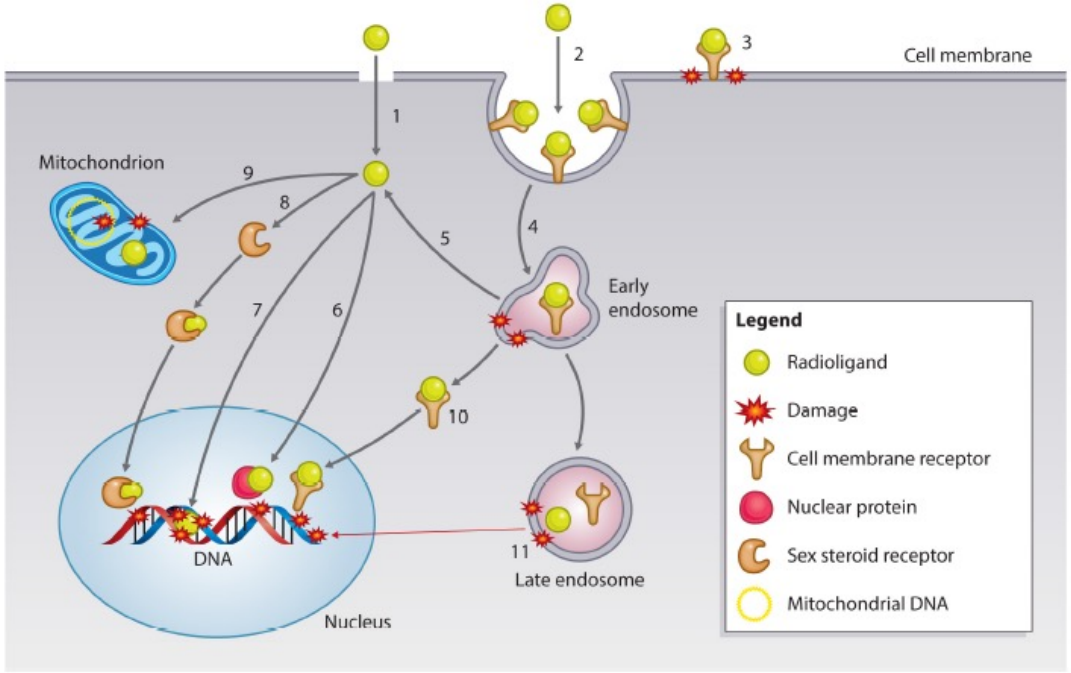


Enhancement at 6 & 9 eV

Subcellular Targeting of Theranostic Radionuclides

*Bas M. Bavelaar, Boon Q. Lee, Martin R. Gill, Nadia Falzone and Katherine A. Vallis**

Frontiers in Pharmacology 2018, 9, 996.

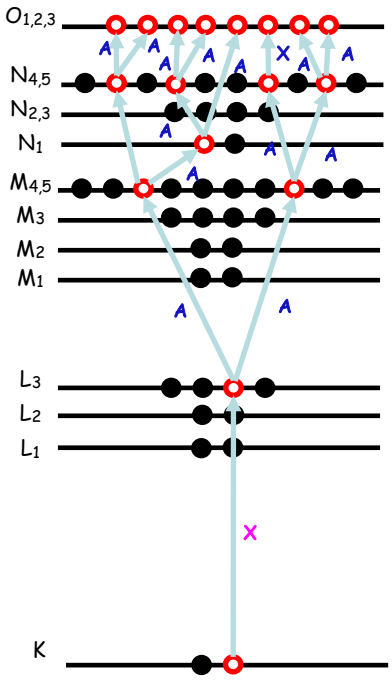


New bread of delivery agents: subcellular targeted cancer treatment is a reality

T. Kibédi, ANU

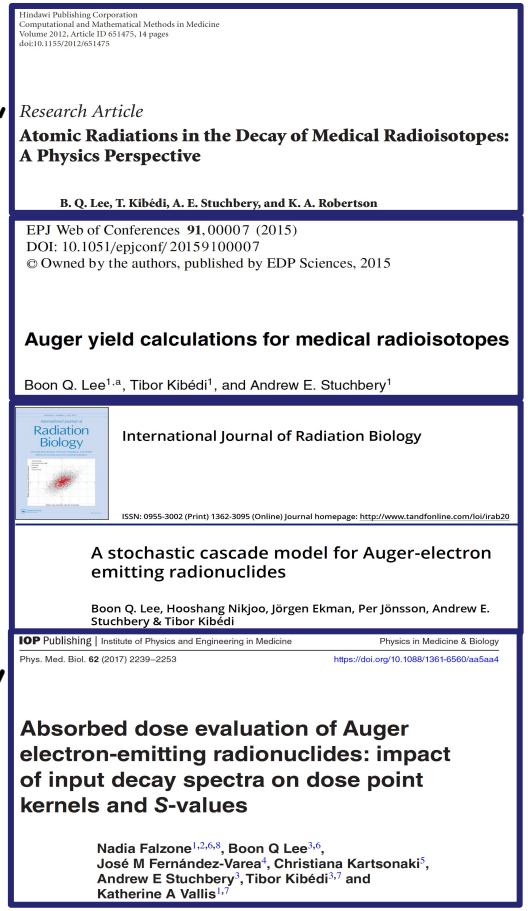
BrIccEmis – atomic relaxation following nuclear decay

B.Q. Lee & B.P.E. Tee



- ❑ Step 1: Evaluate distribution of atomic vacancies from nuclear decay latest nuclear data and models (ENSDF, BrIcc, BetaShape)
- ❑ Step 2: Propagate vacancies using a full Monte Carlo approach
  - Transition energies: from atomic model calculations (Raine DF)
  - Transition rates: from Evaluated Atomic Data Library
- ❑ Step 3: Full energy spectrum from sorting data of 1 Million (or more) decay events

BrIccEmis data base: quick retrieval of the full atomic spectra
In seconds instead of hours


Hindawi Publishing Corporation
Computational and Mathematical Methods in Medicine
Volume 2012, Article ID 651475, 14 pages
doi:10.1155/2012/651475

Research Article

Atomic Radiations in the Decay of Medical Radioisotopes: A Physics Perspective

B. Q. Lee, T. Kibédi, A. E. Stuchbery, and K. A. Robertson

EPJ Web of Conferences **91**, 00007 (2015)
DOI: 10.1051/epjconf/20159100007
© Owned by the authors, published by EDP Sciences, 2015

Auger yield calculations for medical radioisotopes

Boon Q. Lee[1,a], Tibor Kibédi[1], and Andrew E. Stuchbery[1]

International Journal of Radiation Biology

ISSN: 0955-3002 (Print) 1362-3095 (Online) Journal homepage: http://www.tandfonline.com/loi/irab20

A stochastic cascade model for Auger-electron emitting radionuclides

Boon Q. Lee, Hooshang Nikjoo, Jörgen Ekman, Per Jönsson, Andrew E. Stuchbery & Tibor Kibédi

IOP Publishing | Institute of Physics and Engineering in Medicine — Physics in Medicine & Biology

Phys. Med. Biol. **62** (2017) 2239–2253 https://doi.org/10.1088/1361-6560/aa5aa4

Absorbed dose evaluation of Auger electron-emitting radionuclides: impact of input decay spectra on dose point kernels and *S*-values

Nadia Falzone[1,2,6,8], Boon Q Lee[3,6], José M Fernández-Varea[4], Christiana Kartsonaki[5], Andrew E Stuchbery[3], Tibor Kibédi[3,7] and Katherine A Vallis[1,7]

BrIccEmis – atomic relaxation following nuclear decay

B.Q. Lee & B.P.E. Tee

For a single ionized system:

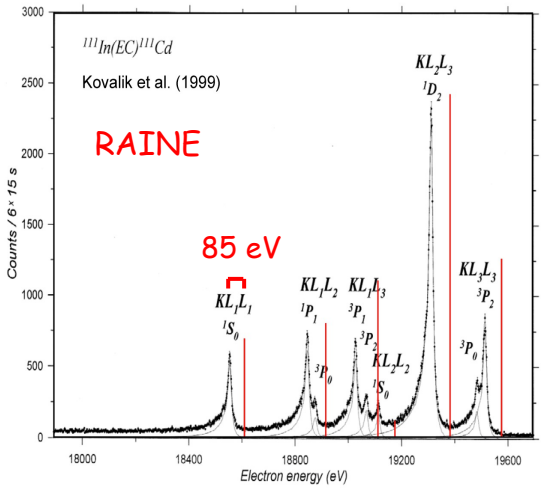
Neutral binding energies

$E(X,YZ) = BE(X) - BE(Y) - BE(Z) + \Phi$

hole-hole coupling

Breit and QED corrections not in RAINE

- ❑ semi-empirical corrections using literature values of BE
- ❑ Grasp2K BE calculations (preferably)



Kovalik, et al., J. of Electron Spect. and Rel. Phen. **105** (1999) 219

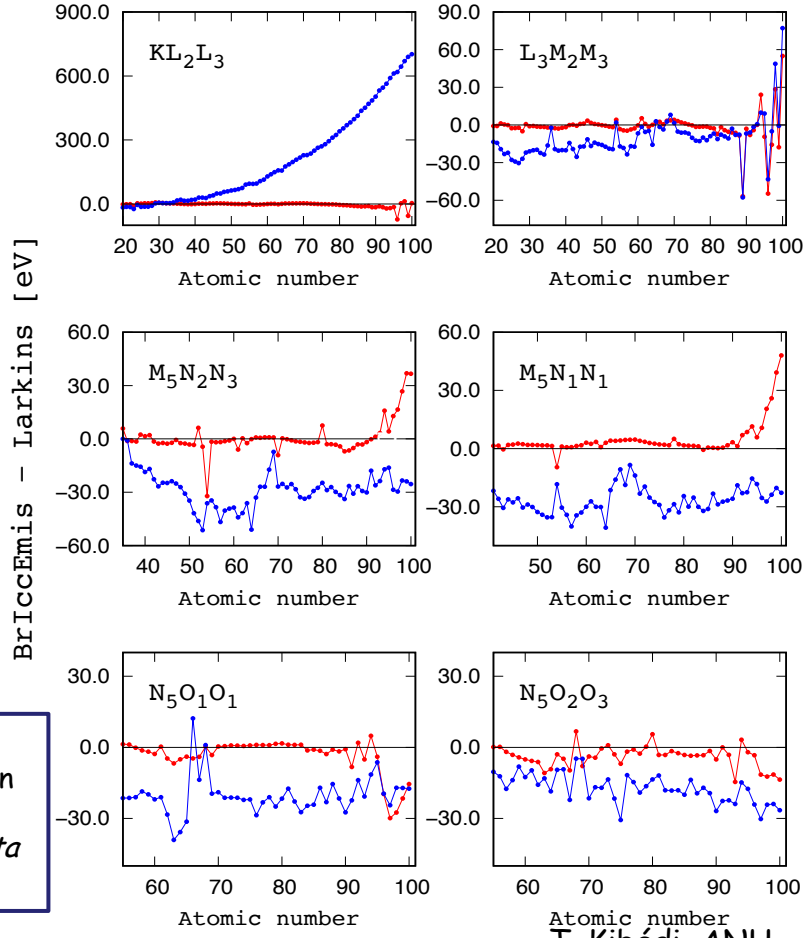
Semi-empirical corrections of calculated Auger energies

F.P. Larkins, Semi-empirical Auger electron energies *Atomic Data and Nuclear Data Tables*, *20*(4) (1977) 311.

Auger energies

No correction

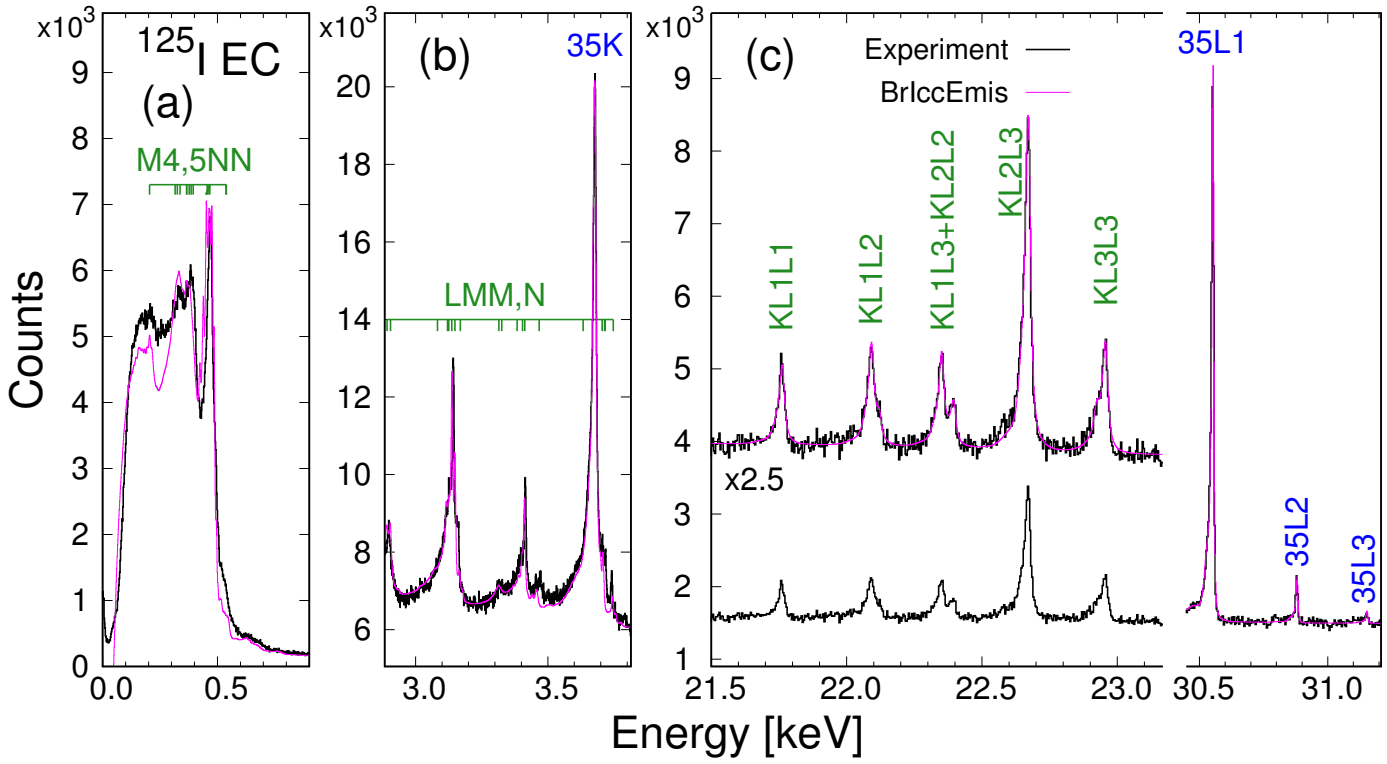
With correction



T. Kibédi, ANU

BrIccEmis – atomic relaxation following nuclear decay

B.Q. Lee & B.P.E. Tee



M. Alotiby, et al., J. Elect. Spectr. Rel. Phenom. 232 (2019) 73
B.P.E. Tee, et al., PRC 100 (2019) 034313

Thanks