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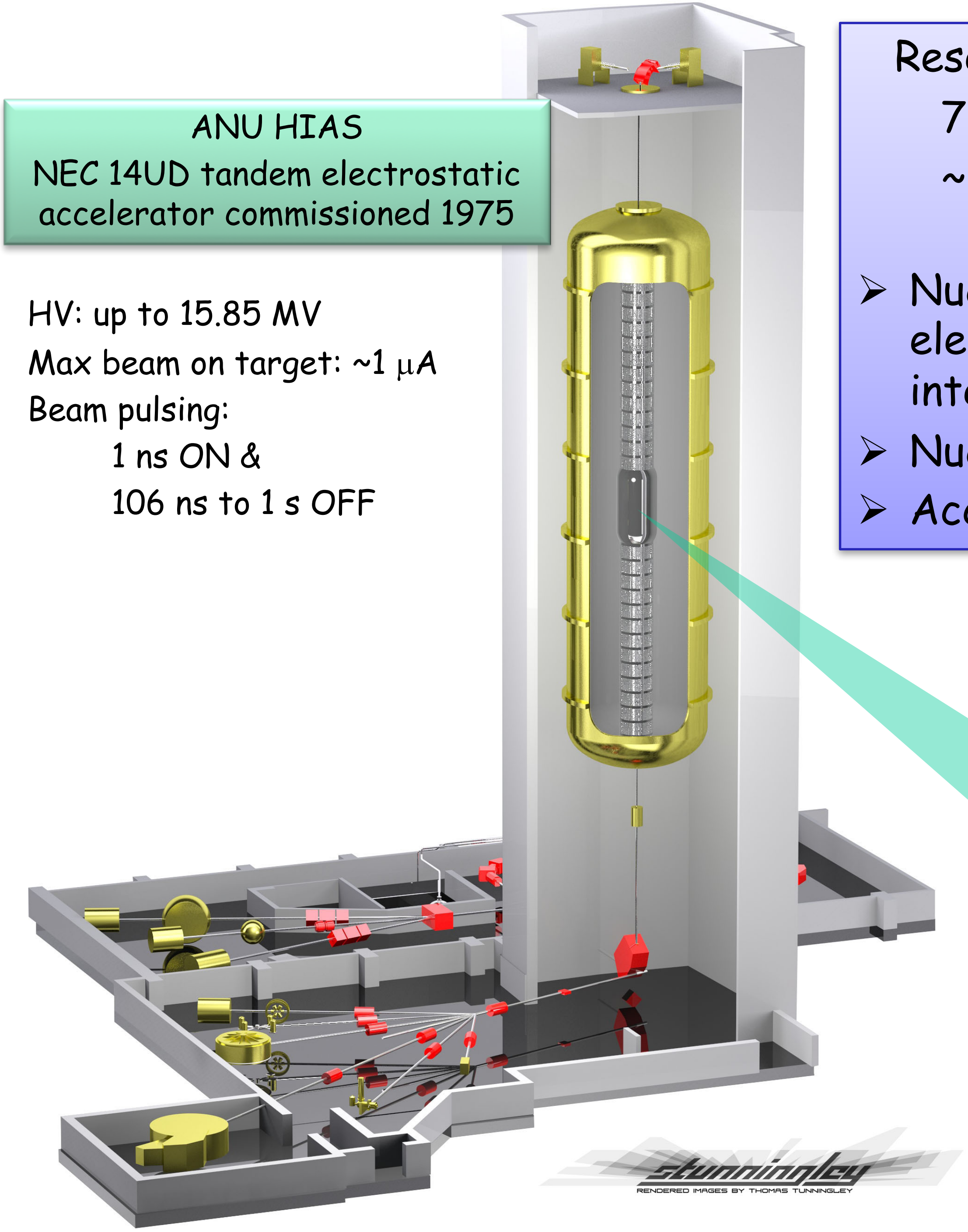
Conversion coefficients and atomic radiations in ENSDF - BrIcc, BrIccMixing and BrIccEmis

Tibor Kibèdi (ANU)

Heavy Ion Accelerator Facility, ANU Canberra

ANU HIAS
NEC 14UD tandem electrostatic accelerator commissioned 1975

HV: up to 15.85 MV
Max beam on target: ~1 μA
Beam pulsing:
1 ns ON &
106 ns to 1 s OFF

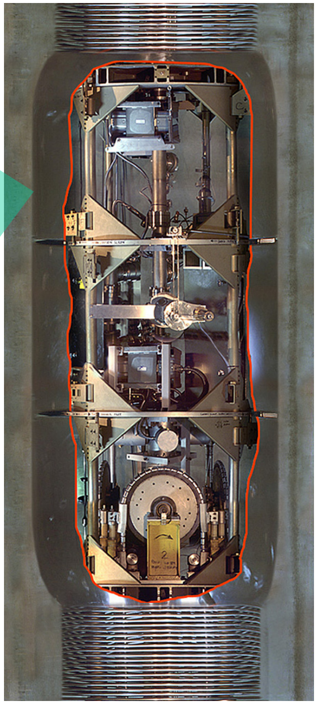


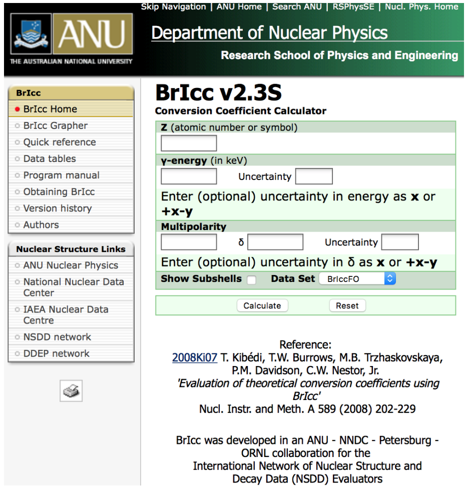
Research areas

7 continuing / 8 postdocs

~20 research students / 60 outside users)

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





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ANU
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Department of Nuclear Physics

Research School of Physics and Engineering

BrIcc
- BrIcc Home
- BrIcc Grapher
- Quick reference
- Data tables
- Program manual
- Obtaining BrIcc
- Version history
- Authors

Nuclear Structure Links
- ANU Nuclear Physics
- National Nuclear Data Center
- IAEA Nuclear Data Centre
- NSDD network
- DDEP network

BrIcc v2.3S

Conversion Coefficient Calculator

Z (atomic number or symbol)

γ-energy (in keV) Uncertainty

Enter (optional) uncertainty in energy as **x** or **+x-y**

Multipolarity δ Uncertainty

Enter (optional) uncertainty in δ as **x** or **+x-y**

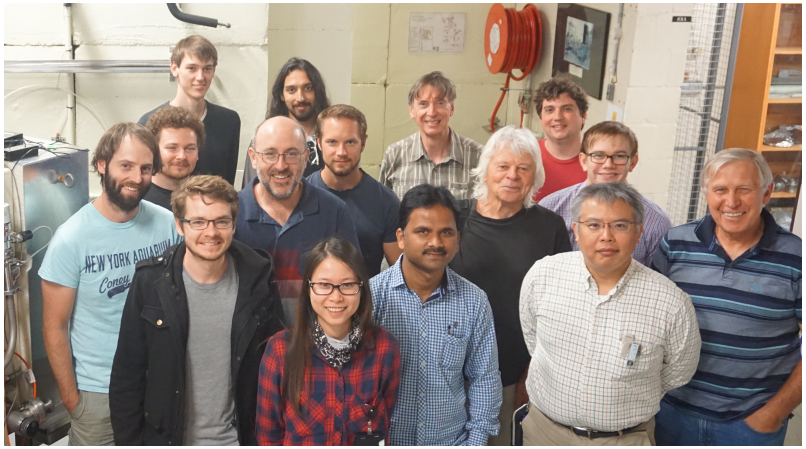
Show Subshells ☐ **Data Set** BrIccFO

Calculate Reset

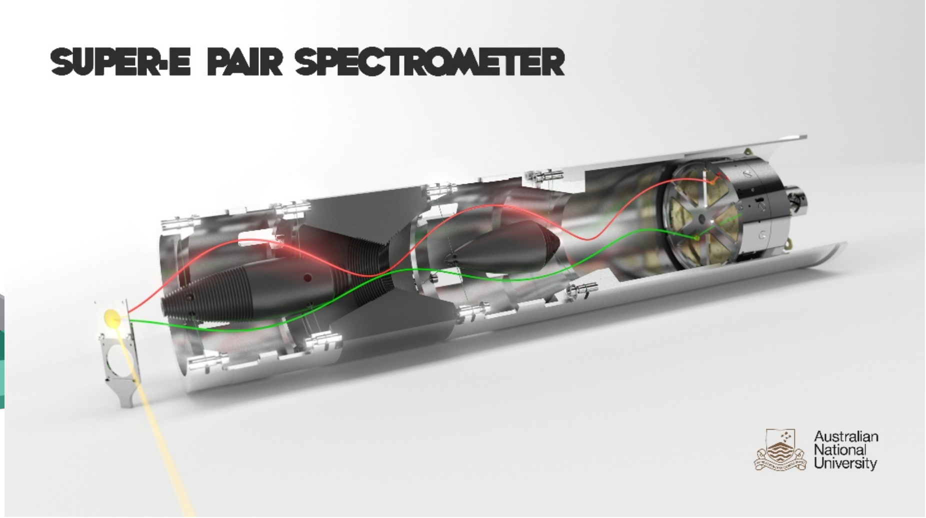
Reference:
2008Ki07 T. Kibédi, T.W. Burrows, M.B. Trzhaskovskaya, P.M. Davidson, C.W. Nestor, Jr.
'Evaluation of theoretical conversion coefficients using BrIcc'
Nucl. Instr. and Meth. A 589 (2008) 202-229

BrIcc was developed in an ANU - NNDC - Petersburg - ORNL collaboration for the International Network of Nuclear Structure and Decay Data (NSDD) Evaluators

stunningley
RENDERED IMAGES BY THOMAS TUNNINGLEY



Looking for E0`s with a ``pair of glasses" in ^{12}C to ^{52}Cr (2018-Apr)



Outline

- ☐ Calculation of conversion coefficients
- ☐ Multipole mixing ratios
- ☐ Electric monopole E0 transitions
- ☐ Measurements and some aspects of extracting information for ENSDF
- ☐ Atomic radiations from nuclear decay

Practice #3:

- ☐ BrIcc, BrIccMixing, Ruler, Gabs

Outline

Electromagnetic Decay Processes

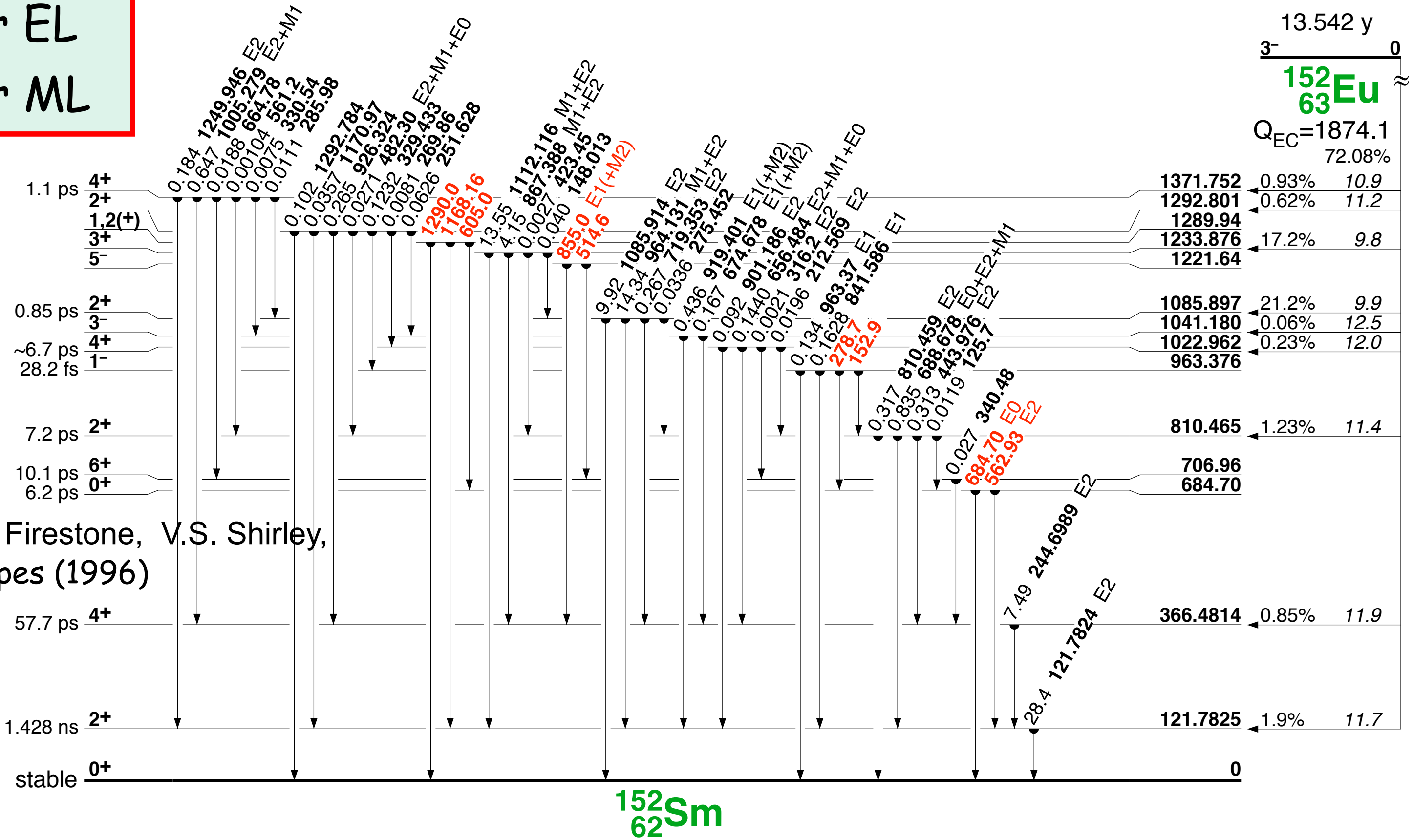
EM decay: energy and momentum carried away

Selection *rules* (πL)

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

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

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



1996FiZY R.B. Firestone, V.S. Shirley, Table of isotopes (1996)

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

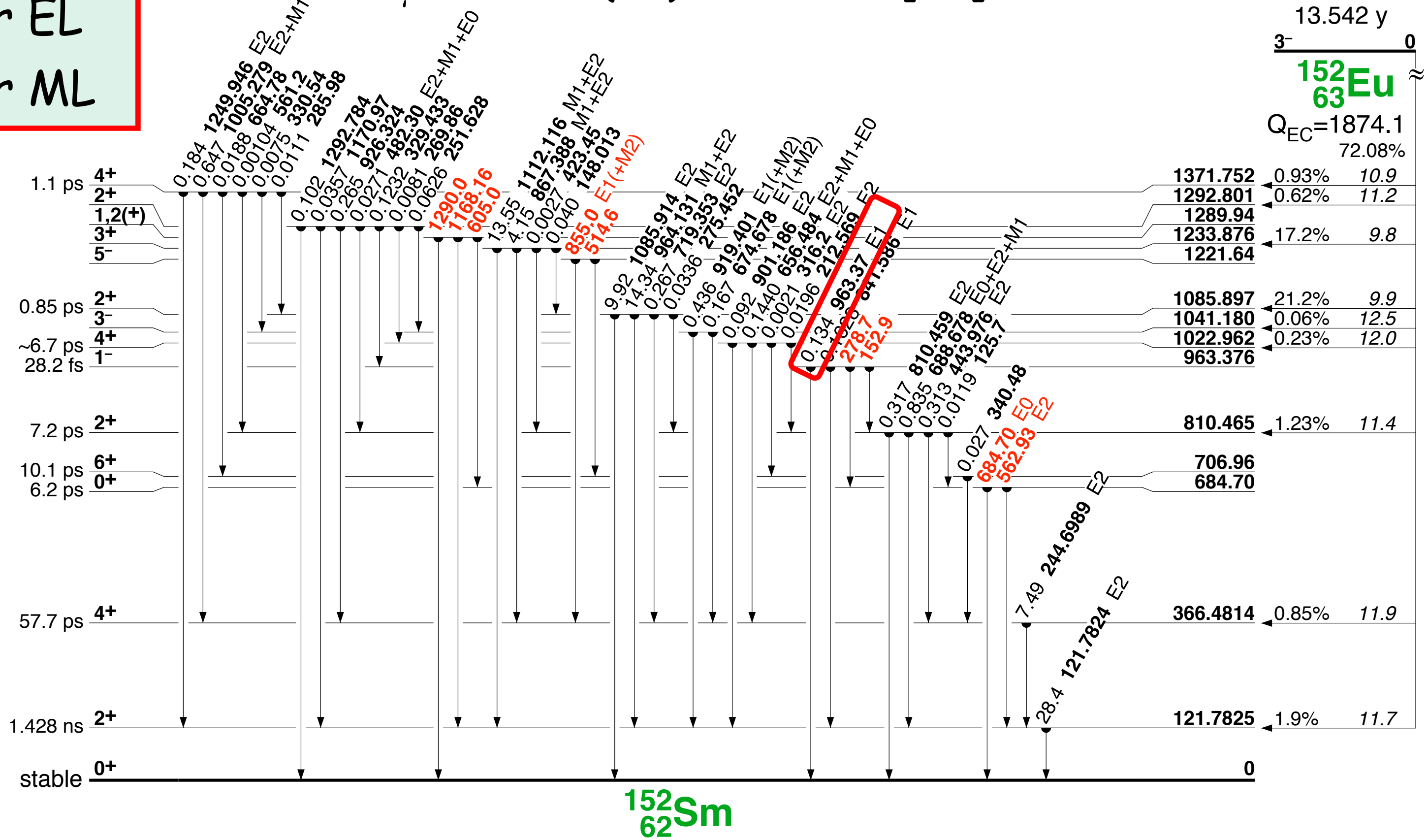
Example (2013Ma77, M.J. Martin, NDSh 114 (2013) 1497):

Initial level: 963.358(3) keV, $J^{\pi}=1^-$

Final level: 810.453(5) keV, $J^{\pi}=2^+$

ΔE=152.905(6) keV, ΔJ=1, $\Delta\pi$=-1

E_{γ}= 152.77(16) keV; ML=[E1]; L=1



Electromagnetic Decay Processes

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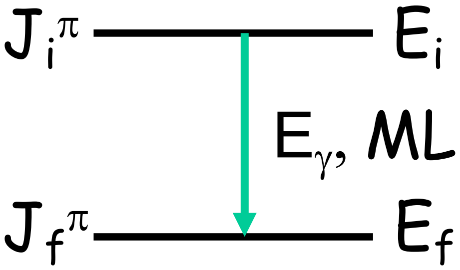

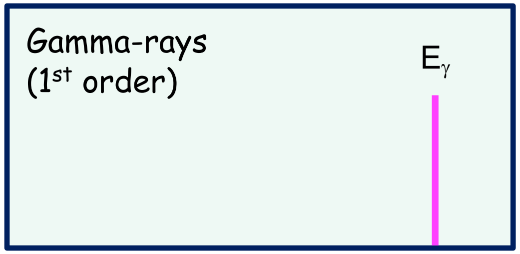

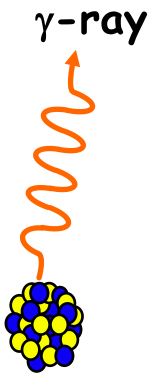

Energetics

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

Electromagnetic Decay Processes

EM decay: energy and momentum carried away

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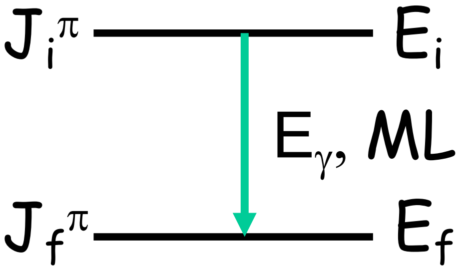

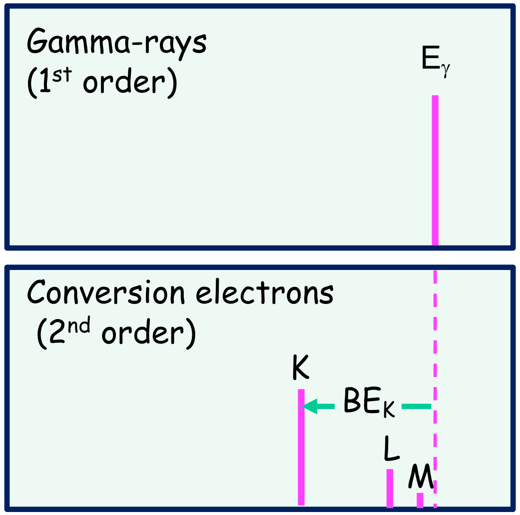

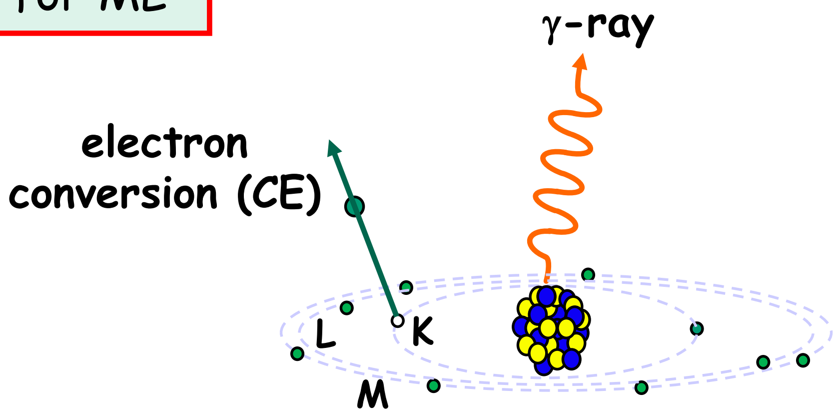

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Electromagnetic Decay Processes

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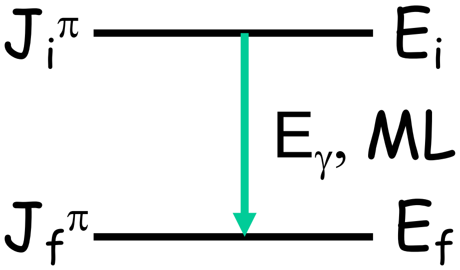

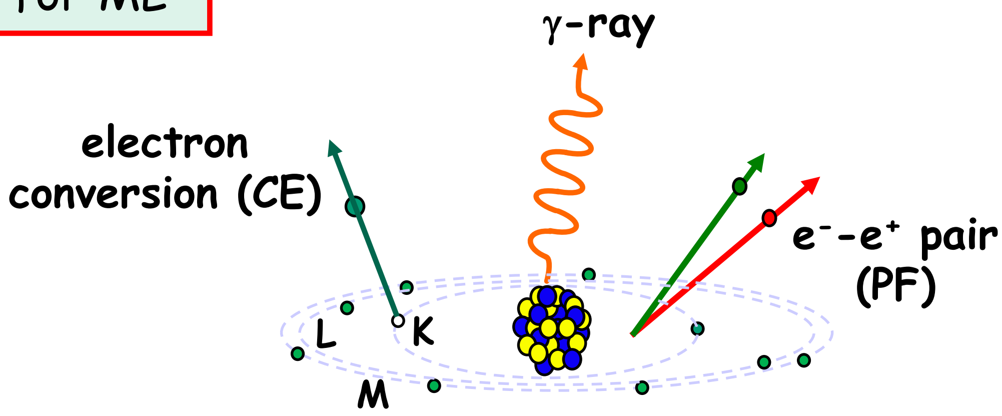

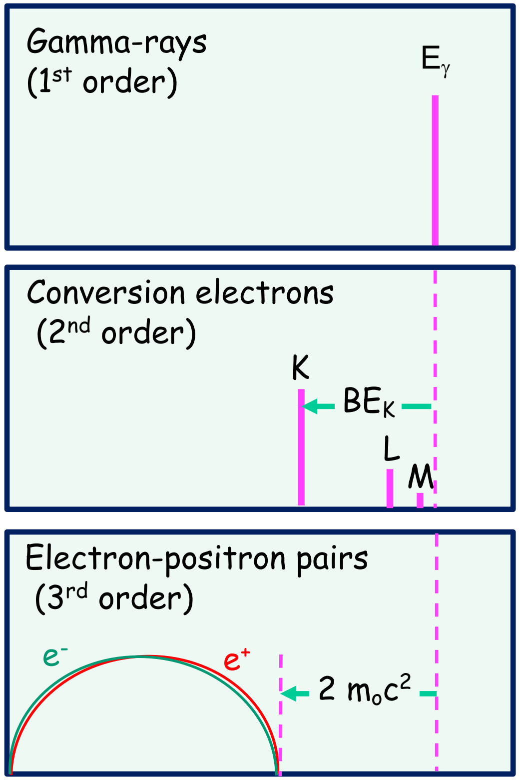

Energetics

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

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

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

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EM decay: energy and momentum carried away

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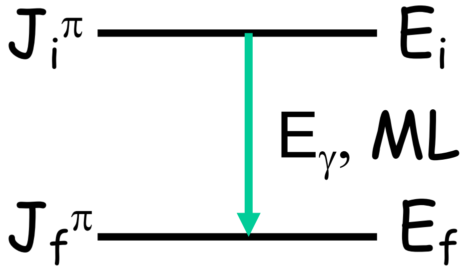

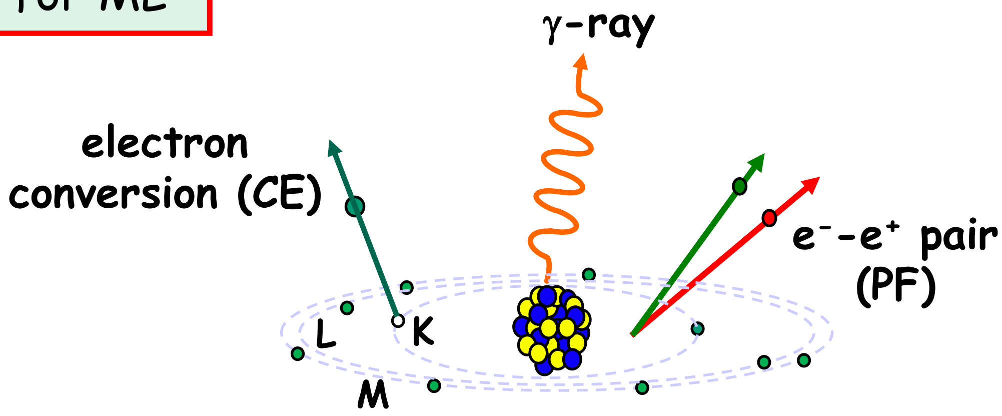

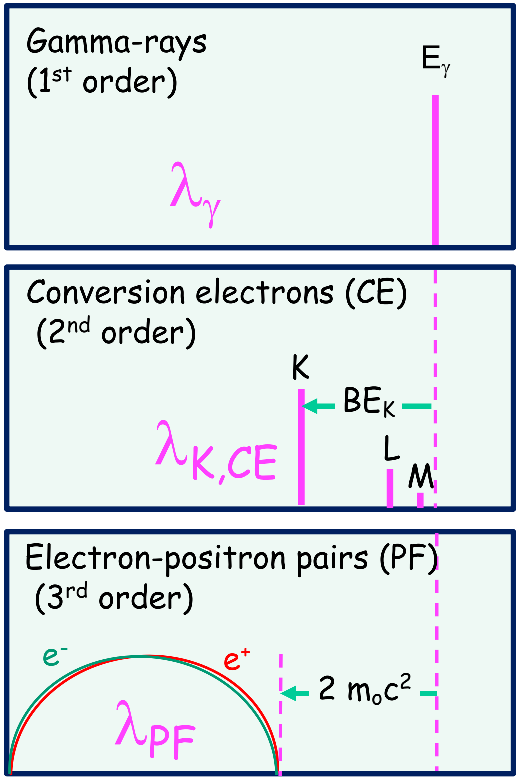

Transition probability

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

Conversion coefficient

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

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

Energetics

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

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Electromagnetic Decay Processes

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Selection *rules* (*πL*)

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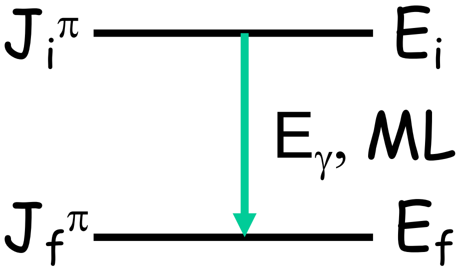
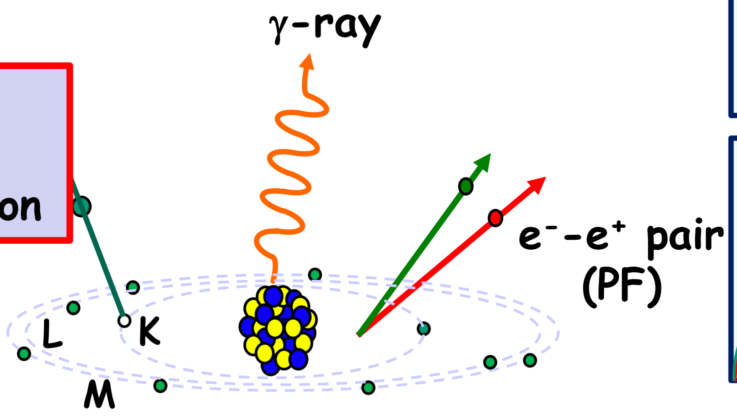
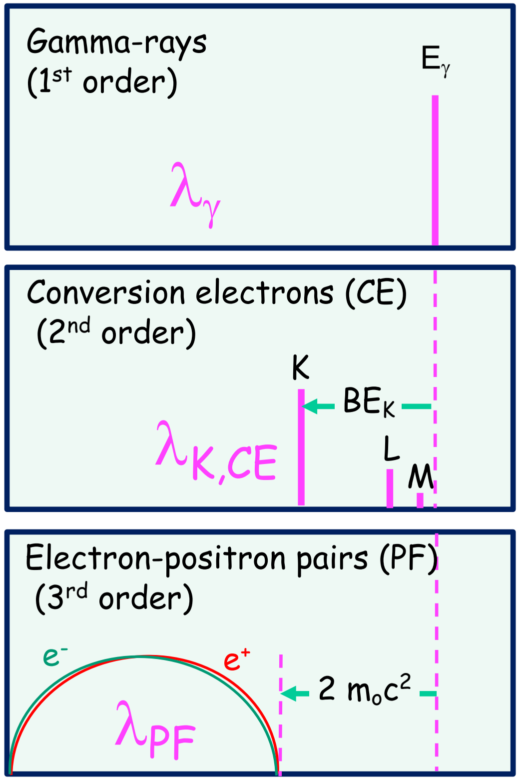
Conversion coefficient: relative probability in comparison to gamma emission







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

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

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Electromagnetic Decay Processes

EM decay: energy and momentum carried away

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

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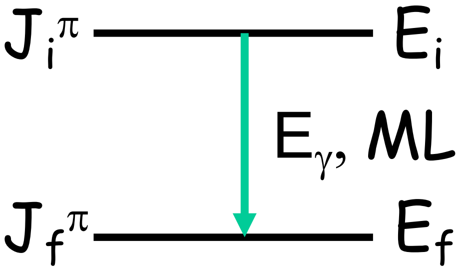
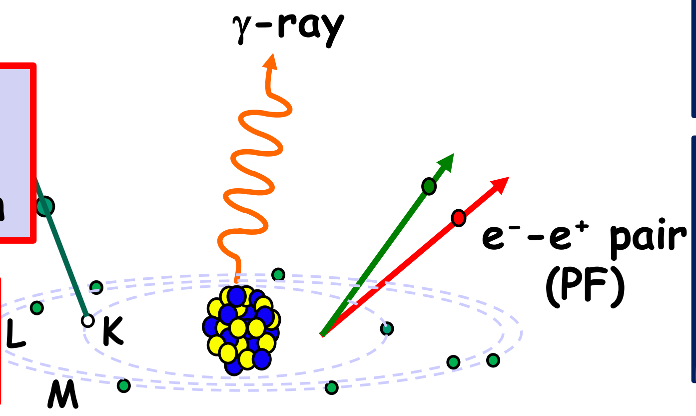
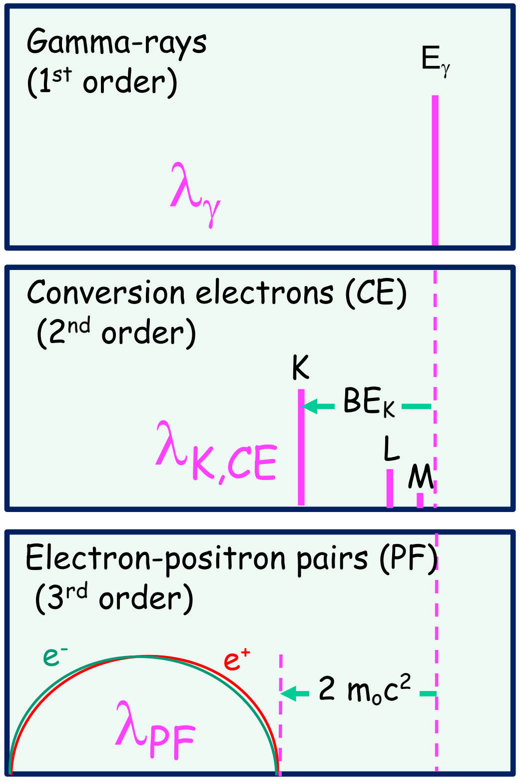


Conversion coefficient: relative probability in comparison to gamma emission

Can be calculated – BrIcc

$\alpha \sim f(Z, E_\gamma, EML, shell)$





Transition probability

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Conversion coefficient

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

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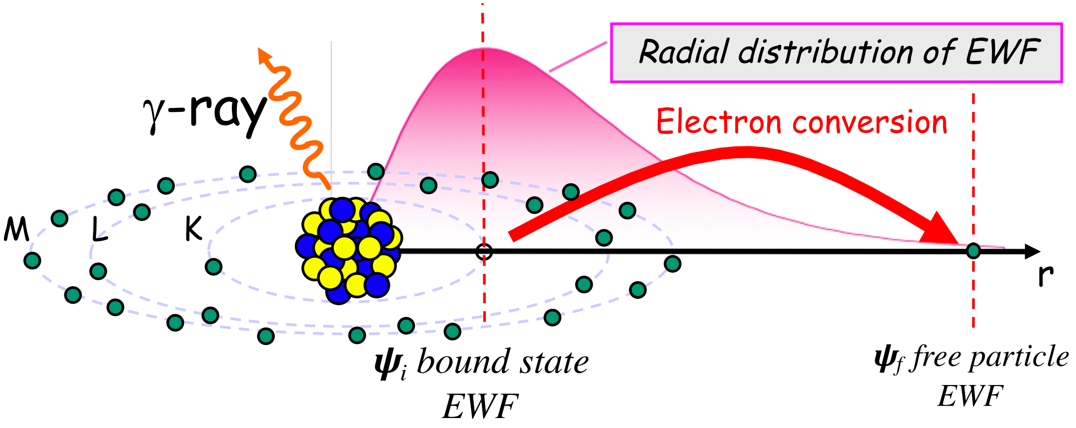
Energetics

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

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

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

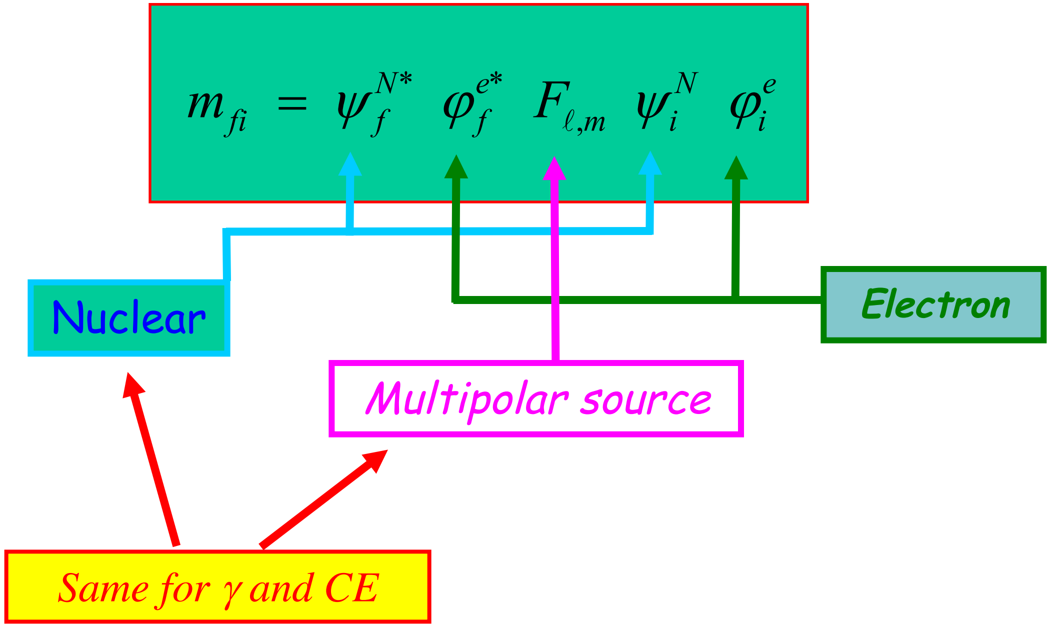
Conversion electron process and electromagnetic interaction



Fermi's golden rule

$$\alpha_e = \frac{\lambda_e}{\lambda_\gamma} \quad \Rightarrow \quad \lambda_e = \frac{2\pi}{\hbar}\left|m_{fi}\right|^2 \frac{d\rho}{dE}$$

Density of the final electron state (continuum)



$$m_{fi} = \psi_f^{N*} \quad \varphi_f^{e*} \quad F_{\ell,m} \quad \psi_i^{N} \quad \varphi_i^{e}$$

Nuclear

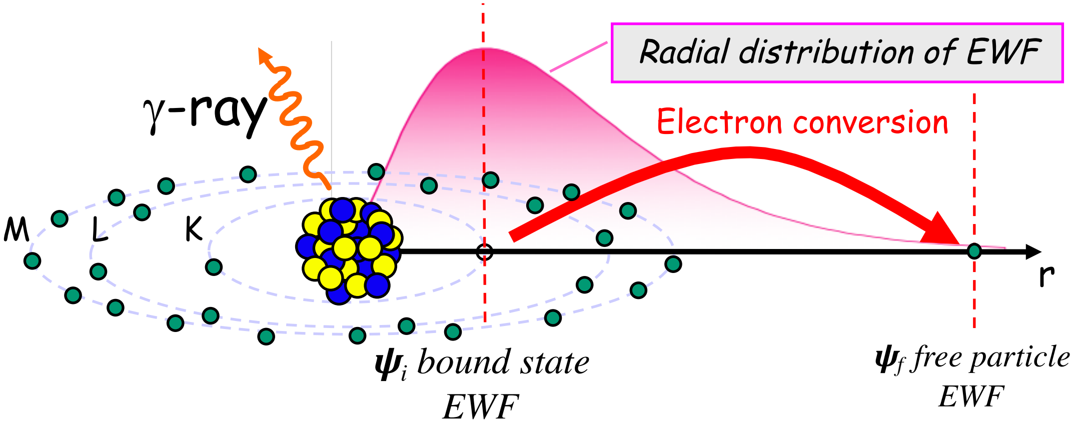
Electron

Multipolar source

Same for γ and CE

ICC calculations – Atomic field model

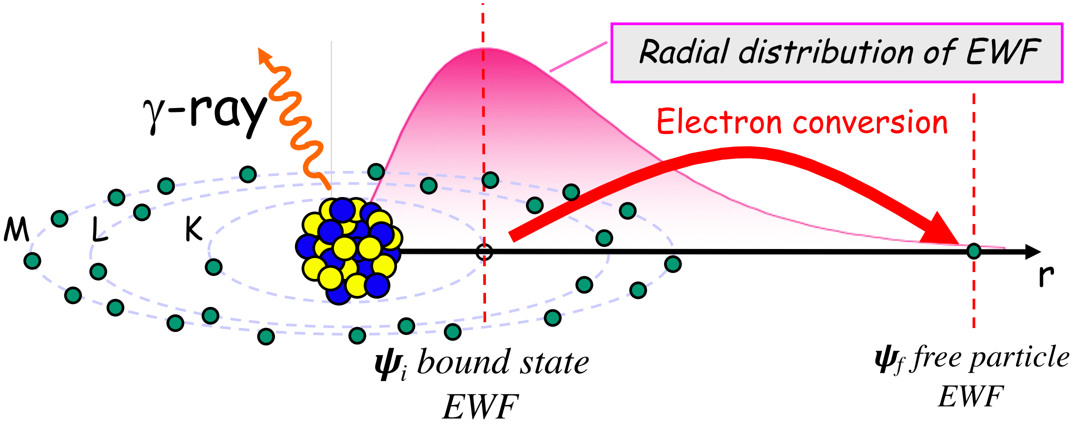
Band et al., ADNDT 81 (2002) 1



- Relativistic Dirac-Fock method
- 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
- Finite nuclear size
- Dynamic (penetration) effects incorporated using the Surface Current model
- Spherically symmetric nucleus; calculations for the most abundant isotope

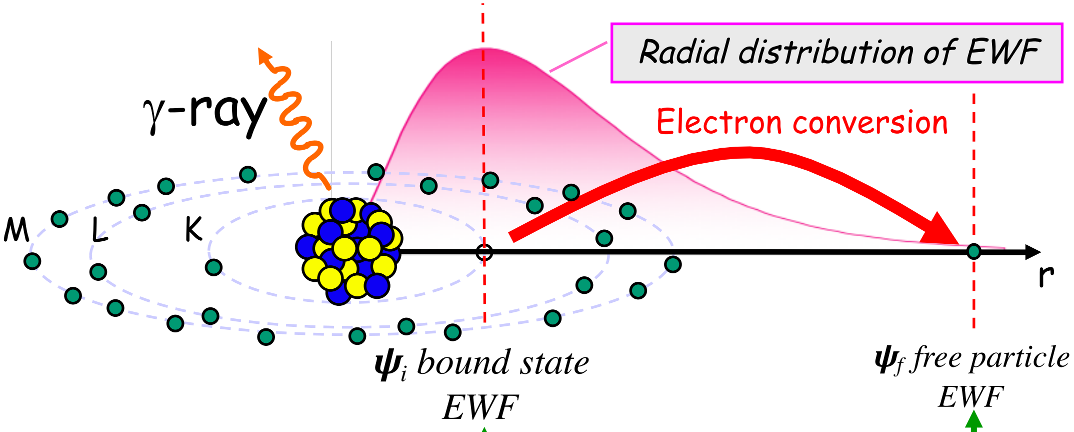
ICC calculations – Higher order effect

Band et al., ADNDT 81 (2002) 1



- 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%

ICC calculations - Atomic vacancies



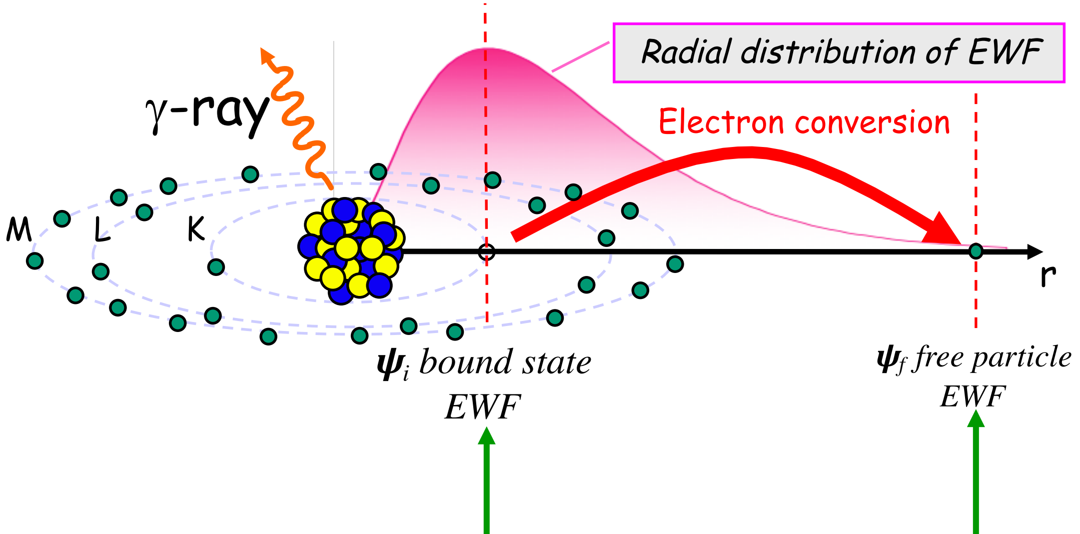
"No Hole" - BTNTR: SCF of a neutral atom

Vacancy disregarded

2002Ba85 numerical tables
(Band et al., ADNDT 81 (2002) 1)

BrIccNH table – extended and revised calculations

ICC calculations – Atomic vacancies



BrIccFO Accuracy:
- 188 α_{tot}, α_K, α_L ICC
- Pure E2, E3, M3 M4 multipolarities (no penetration effect)
- max 10% uncertainty

(Exp-Theor)/Exp ~ +0.8%

SCF of a neutral atom

Constructed from the WF of a neutral atom, not SCF

***"Frozen Orbitals"* – RNIT(2)**

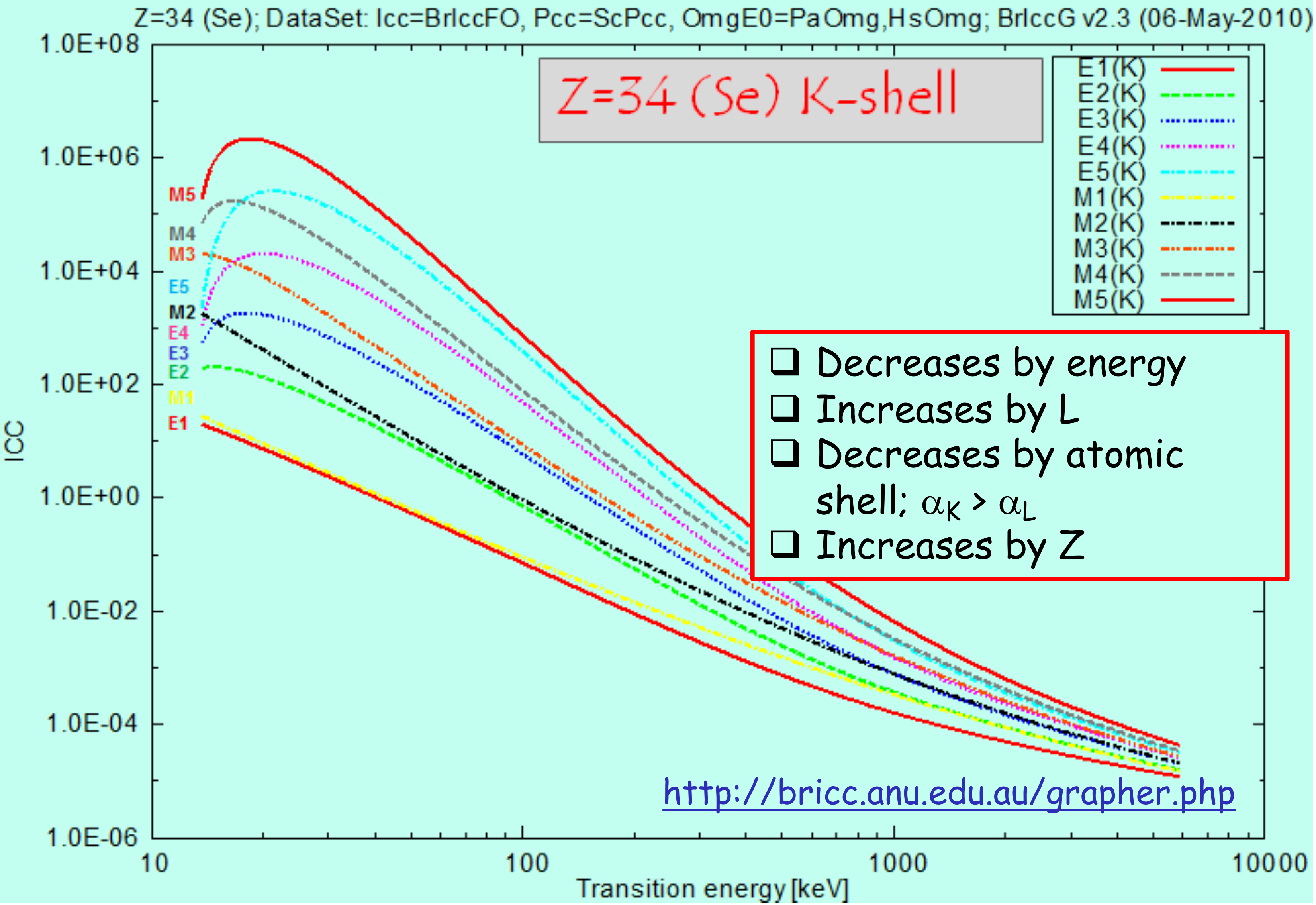
ENSDF pre 2005
Hager and Seltzer
- Hatree-Fock
- Different physical assumptions
- ~4% accuracy

Vacancy incorporated

2008Ki07 *T.* Kibèdi et al., Nucl. Instr. and Meth. **A 589** (2008) 202

BrIccFO – data table

Theoretical conversion coefficients



- ☐ Decreases by energy
- ☐ Increases by L
- ☐ Decreases by atomic shell; $\alpha_K > \alpha_L$
- ☐ Increases by Z

http://bricc.anu.edu.au/grapher.php

Conversion coefficients and nuclear structure

- ☐ Total transition probability (intensity): $\lambda_{total} = I_\gamma \times (1+\alpha_{total})$
- ☐ $\alpha_i(Z, E_\gamma, \pi L, \delta, \lambda)$ function of
  - i - atomic shell / electron-positron pair
  - Z – atomic number
  - E_γ – transition energy
  - πL - multipolarity
  - δ – mixing ratio
  - λ – nuclear penetration parameter (not many cases: E1, M1)
- ☐ Comparing experimental and theoretical conversion coefficients
  - Transition multipolarity (pure/mixed), magnetic or electric character
  - Normalised Peak to Gamma (NPG) method:

$$\alpha_{exp} = N * [A_{CE}/A_\gamma] \times [\varepsilon_\gamma/\varepsilon_{CE}]$$

  - Further details: J.H. Hamilton, *The Electromagnetic Interaction in Nuclear Spectroscopy*, Ch 11, North Holland (1975)

- ☐ E0 transitions – collective excitations and shape co-existence

Mixed transitions

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

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

Special case: mixed transitions with 3 multipolarities:

^{184}W 536.674(15) keV

E1+M2+E3,

ME(M2/E1)=+0.070(6),

MR(E3/M2)=-0.025(4)

λ=-2.1(2);

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

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

γ-ray transition probability:

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

Mixing ratio (MR)

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

Conversion coefficient for CE and PF

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

E0 - electric monopole transitions

EM decay: energy and momentum carried away

Selection *rules* (πL)

$j_i = j_f$

$\Delta\pi = 0$

Pure E0

- ☐ NO gamma-ray
- ☐ Only CE or PF

References:

1997Wo07
J.L. Wood et al.,
NP **A651** (1999) 323

2005Ki02
T. Kibèdi, R.H. Spear,
At. Data Nucl. Data Tabl.
89 (2005) 77

E0 conversion coefficient NOT DEFINED

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

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 (BrIcc)

E0 reduced transition rate

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

Experimental determination

$\rho^2(E0) = 1/[\Omega_{CE}(E0) + \Omega_{PF}(E0)]\times\tau(E0)$

E0+E2+M1 – mixed transitions

EM decay: energy and momentum carried away

Selection *rules* (πL)

$j_i = j_f$

$\Delta\pi = 0$

2⁺ to 2⁺ transition

- ☐ Can proceed with E0 in competition with E2+M1

Transition probability:

$$\lambda(E0+E2+M1) = \lambda_{CE}(E0)+\lambda_{PF}(E0) + \lambda_\gamma(E2) + \lambda_{CE}(E2)+\lambda_{PF}(E2) + \lambda_\gamma(M1) + \lambda_{CE}(M1)+\lambda_{PF}(M1)$$

MR(E2/M1) mixing ratio

$$\delta^2(E2/M1) = \frac{\lambda_\gamma(E2)}{\lambda_\gamma(M1)}$$

MR(E0/E2) mixing ratio

$$q_K^2(E0/E2) = \frac{\lambda_K(E0)}{\lambda_K(E2)}$$

Conversion coefficient (K-shell)

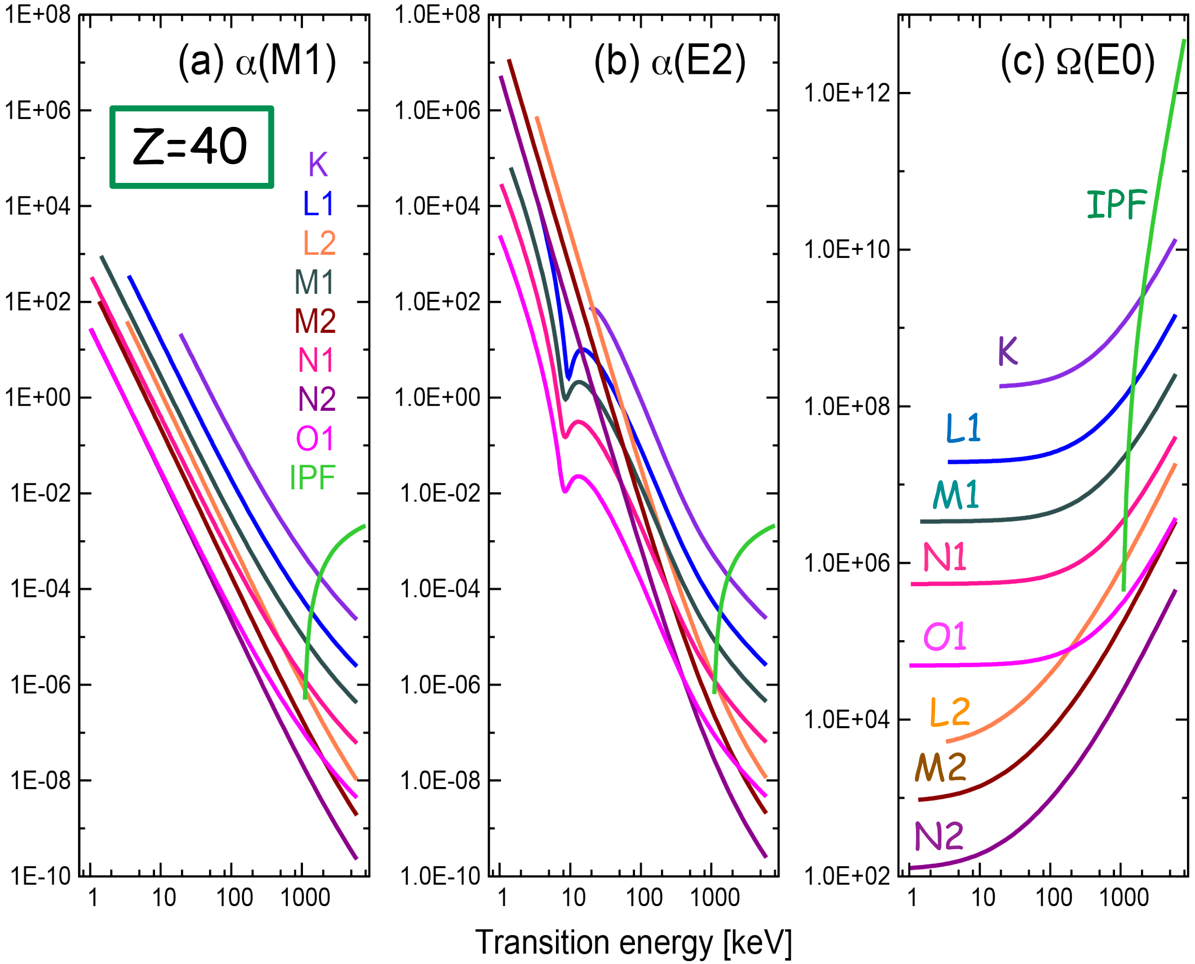
$$\alpha_K(E0+E2+M1) = \frac{\alpha_K(M1) + \delta^2 \times [1 + q_K^2] \times \alpha_K(E2)}{1+\delta^2}$$

ρ^2(E0) can be determined if both E2/M1 and E0/E2 mixing ratios and level half life are known (E0/E2 mixing ratio from α_K)

Conversion coefficients and E0 electronic factors using BrIcc

- E0 conversion on $nS_{1/2}$ and $nP_{1/2}$ shells only
- Energy dependence
  - – α_{CE}(M1,E2): ↓ up 14 orders of magnitude
  - – Ω_{CE}(E0): ↑ 2-3 orders of magnitude
  - - Opposite trend for pair conversion
- Atomic shells (K, L, M): Always decreasing
- Accuracy of the ICC tables:
  - α_{CE} ~ 1.4%
  - α_{PF} – not evaluated, ~3%
  - Ω(E0) ~ 5%

α(M1,E2): from BrIcc (2008Ki07);
$W_{CE,PF}$(E0): J. Dowie and T. Eriksen (2018 ANU)



Conversion coefficients and E0 electronic factors using BrIcc

```
125TE  G 35.4925   5  6.68   13M1+E2     0.029   +3-2  13.68
```

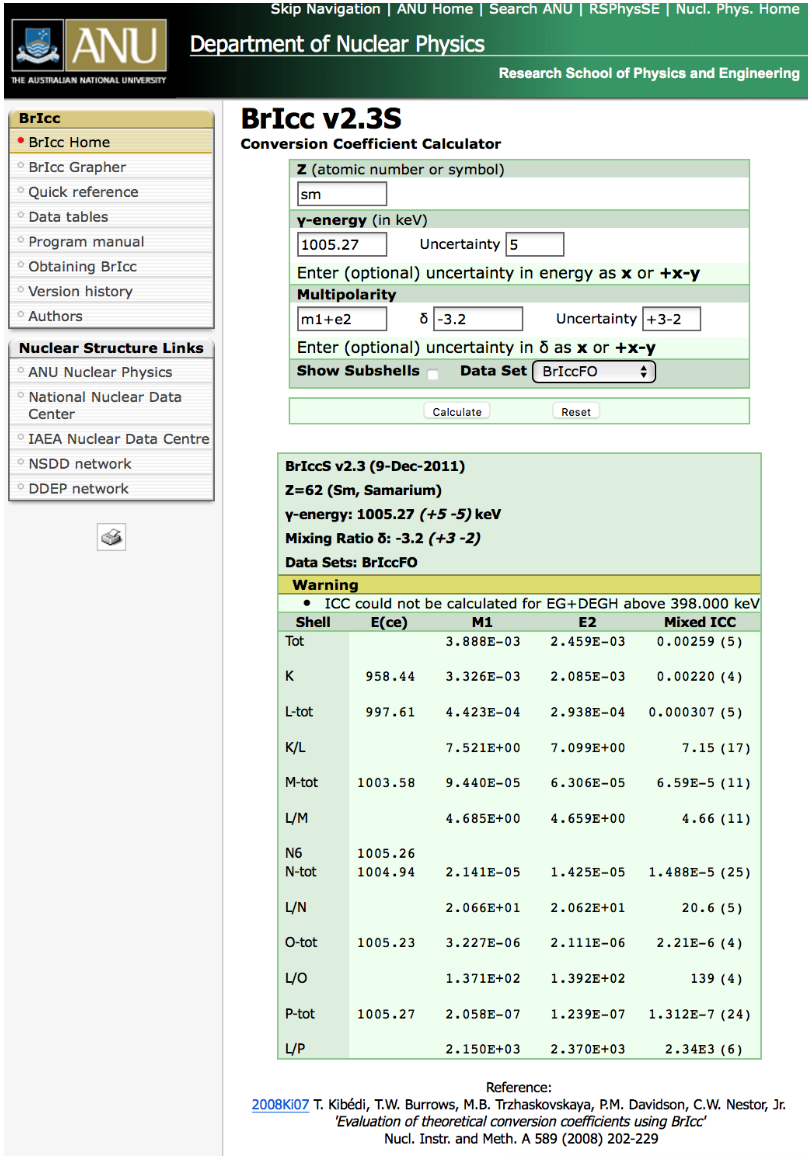
```
125TES G KC=11.69 17$LC=1.596 25$MC=0.319 5$NC+=0.0697 11
125TES G NC=0.0630 10$OC=0.00674 10
```

```
125TE cG E$ From wavelength of 349.328 {I5} m~' (1976Mi18) and
125TE2cG conversion factor of 12398.520 keV|*m~' from 2000He14
125TE cG RI$ From CC deduced by the evaluator from MR and LAMBDA=0.9 {I8}.
125TE2CG    Others: 6.68 {13} (1990Iw04),
125TE3CG            6.8 {I3} (1969Ka08),
125TE4CG            6.51 {I13} (1983De11)
125TE cG M,MR,LAMBDA,CC$ From
125TE2CG    EKC/(1+ECC)=0.80 {I5}, ELC/(1+ECC)=0.11 {I2},
125TE3CG    EMC/(1+ECC)=0.020 {I4} (1952Bo16);
125TE4CG    CEL2/CEL1=0.089 {I4}, CEL3/CEL1=0.024 {I2} (1965Ge04);
125TE5CG    CEK/CEL=12.3 {I25}, CEL2/CEL1=0.106 {I20} (1969Ca01);
125TE6CG    EKC=11.78 {I18}, ECC=12.95 {I28} (1969Ka08);
125TE7CG    EKC/(1+ECC)=0.804 {I10} (1970Ma51);
125TE8CG    ECC=14.25 {I64}, EKC=11.90 {I31}, EM2C/EM1C=0.092 {I5},
125TE9CG    EL2C/EL1C=0.082 {I4}, EL3C/EL1C=0.019 {I3} (1979CoZG);125TEaCG
ELC/EMC=5.21 {I26}, EMC/ENC=4.87 {I20}, EM1C/EM3C=33.6 {I55},
125TEbCG    EM1C/EN1C=4.68 {I14}, EL1C/EL3C=43.7 {I94} (1982Br16);
125TEcCG    ELC=1.4 {I1} (1998Sa55);
125TEdCG    EL2C/EL1C=0.083 {I3}, EL3C/EL1C=0.018 {I4}, EM1C/EL1C=0.20{I1},
125TEeCG    EM2C/EM1C=0.077 {I20}, EN1C/EM1C=0.20 {I1} (2017TeZW).
```

Conversion coefficients and E0 electronic factors using BrIcc

Wednesday Practice #3

- ☐ Gamma records and conversion coefficients in ENSDF
- ☐ How to use BrIcc & BrIccMixing



BrIcc v2.3S

Conversion Coefficient Calculator

Z (atomic number or symbol): sm

γ-energy (in keV): 1005.27 Uncertainty: 5

Enter (optional) uncertainty in energy as **x** or **+x-y**

Multipolarity: m1+e2 δ: -3.2 Uncertainty: +3-2

Enter (optional) uncertainty in δ as **x** or **+x-y**

Show Subshells ☐ **Data Set**: BrIccFO

BrIccS v2.3 (9-Dec-2011)

Z=62 (Sm, Samarium)

γ-energy: 1005.27 *(+5 -5)* keV

Mixing Ratio δ: -3.2 *(+3 -2)*

Data Sets: BrIccFO

Warning

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

Shell	E(ce)	M1	E2	Mixed ICC
Tot		3.888E-03	2.459E-03	0.00259 (5)
K	958.44	3.326E-03	2.085E-03	0.00220 (4)
L-tot	997.61	4.423E-04	2.938E-04	0.000307 (5)
K/L		7.521E+00	7.099E+00	7.15 (17)
M-tot	1003.58	9.440E-05	6.306E-05	6.59E-5 (11)
L/M		4.685E+00	4.659E+00	4.66 (11)
N6	1005.26			
N-tot	1004.94	2.141E-05	1.425E-05	1.488E-5 (25)
L/N		2.066E+01	2.062E+01	20.6 (5)
O-tot	1005.23	3.227E-06	2.111E-06	2.21E-6 (4)
L/O		1.371E+02	1.392E+02	139 (4)
P-tot	1005.27	2.058E-07	1.239E-07	1.312E-7 (24)
L/P		2.150E+03	2.370E+03	2.34E3 (6)

Reference:
2008Ki07 T. Kibédi, T.W. Burrows, M.B. Trzhaskovskaya, P.M. Davidson, C.W. Nestor, Jr.
'Evaluation of theoretical conversion coefficients using BrIcc'
Nucl. Instr. and Meth. A 589 (2008) 202-229

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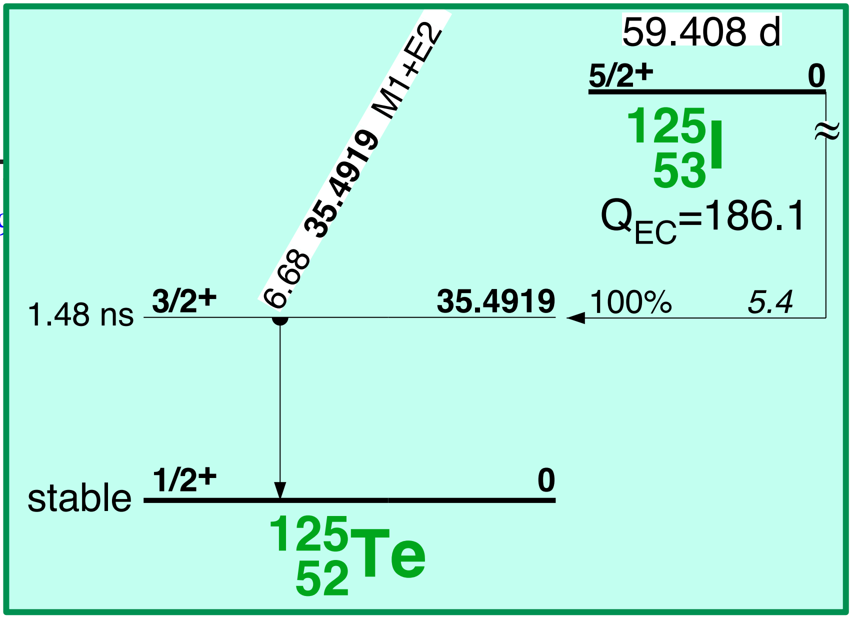
Atomic radiations from nuclear decay



ε radiations

E(decay)	E(level)	I$\varepsilon^{\dagger}$	Log *ft*	
150.27 *6*	35.4925	100	5.4171 *5*	E(decay): Deduced from internal (1986Bo46), 143.8 keV *20* (19 εK(exp)=0.83 *4* (1996Ka48).

[†] Absolute intensity per 100 decays.

$\gamma(^{125}$Te)

Iγ normalization: From Iγ(35γ)=6.68 *13* per decay, no ε feeding to g.s.

E_γ	$I_\gamma^{\dagger}$	E_i(level)	J^π_i	E_f	J^π_f	Mult.	δ	$\alpha^{\ddagger}$	Comments
35.4925 *5*	6.68 *13*	35.4925	3/2$^+$	0.0	1/2$^+$	M1+E2	0.029 +*3*−*2*	13.68	E_γ: From wavelength of 349.328 *5* mÄ (1976Mi18) and conversion factor of 12398.520 keV×mÄ from 2000He14. I_γ: From 1990Iw04. Others: 6.8 *3* (1969Ka08), 6.51 *13* (1983De11). δ: Recommended values from 1977Kr13; δ=0.029 *3* (1982Br16). Mult.: From α(K)exp=12.0 *4*, α(exp)=13.7 *6* (1969Ka08); L1:L2:L3=100 *1*:9.54 *18*:2.3 *5* (1982Br16); see also 1982Br16 for other subshell α.

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Atomic radiations from nuclear decay

ε radiations

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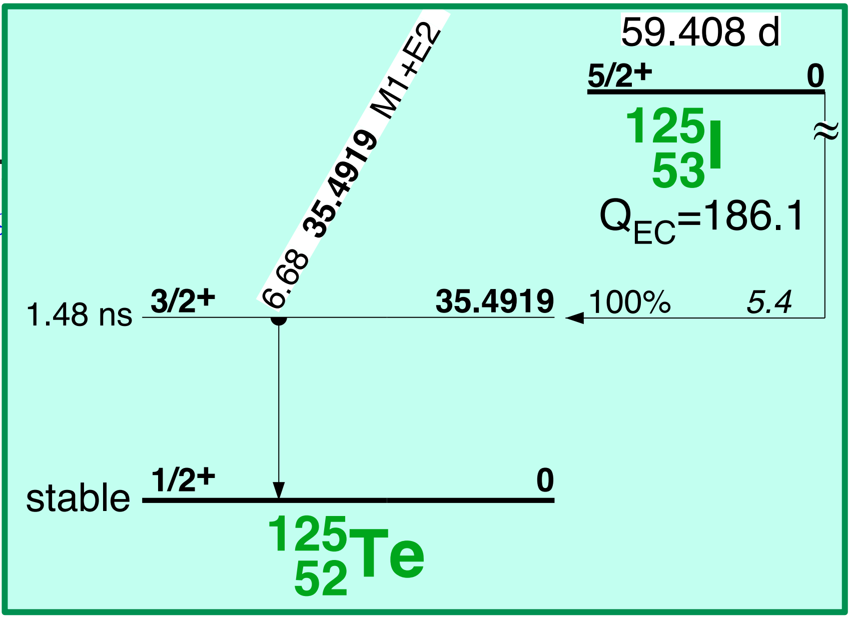
35.4925 *5*	6.68 *13*	35.4925	$3/2^+$	0.0	$1/2^+$	M1+E2	0.029 *+3−2*	13.68	E_γ: From wavelength of 349.328 *5* mÅ (1976Mi18) and conversion factor of 12398.520 keV×mÅ from 2000He14. I_γ: From 1990Iw04. Others: 6.8 *3* (1969Ka08), 6.51 *13* (1983De11). δ: Recommended values from 1977Kr13; δ=0.029 *3* (1982Br16). Mult.: From α(K)exp=12.0 *4*, α(exp)=13.7 *6* (1969Ka08); L1:L2:L3=100 *1*:9.54 *18*:2.3 *5* (1982Br16); see also 1982Br16 for other subshell α.



- ❑ EC decay of ^{125}I: 1.0 atomic vacancy/decay
- ❑ CE decay of the 35.5 keV decay: 0.93 vacancy/decay

X-rays & Auger electrons from the atomic relaxation process are NOT (yet) in ENSDF

The biological effect of Auger electrons

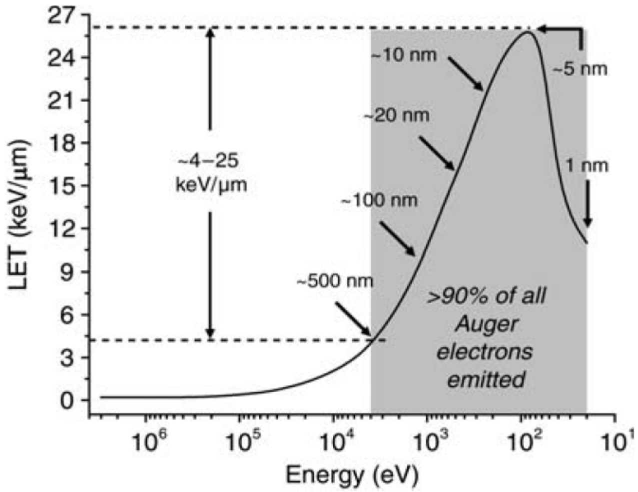
Interaction of ionizing radiation:

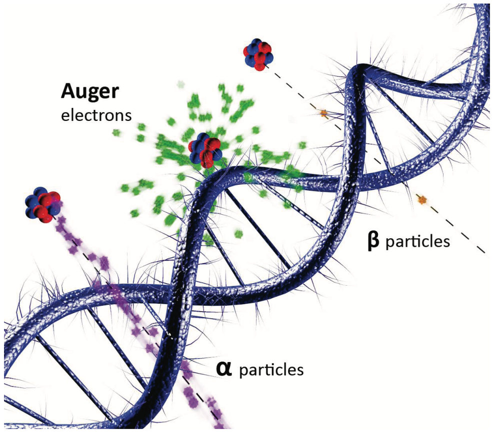
☐ Spectrum of energy loss

☐ Generation of secondary electrons

☐ Low energy electrons are the ideal tool

☐ *Auger electrons from radioisotopes – decay at close proximity to the DNA*





The biological effect of Auger electrons

Interaction of ionizing radiation:

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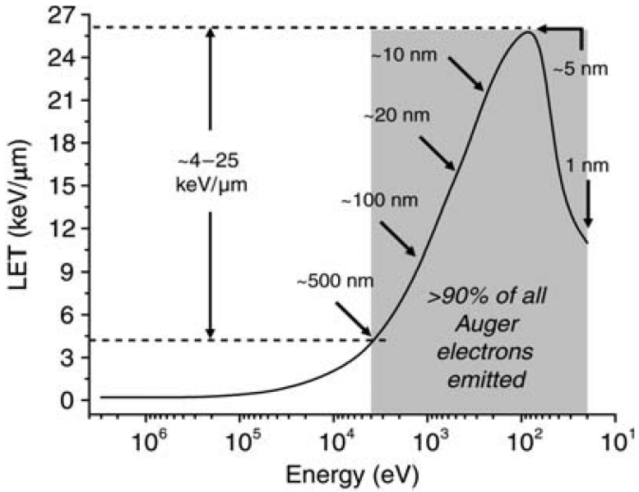


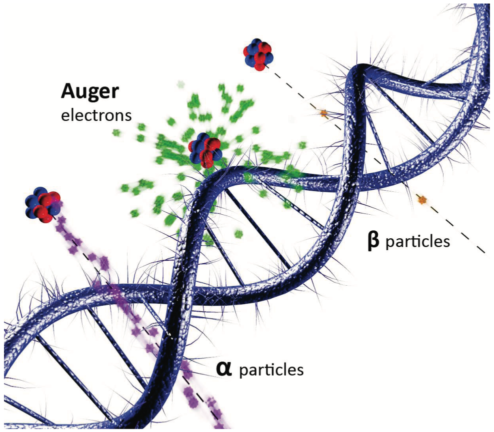
Which Isotope?

☐ Number of electrons per decay

☐ Ratio of X & γ vs. e^- & β

☐ Physical vs. effective half life

☐ Suitable radiochemistry



Physics input to dose calculations:

☐ Radiation spectra

☐ Energy loss

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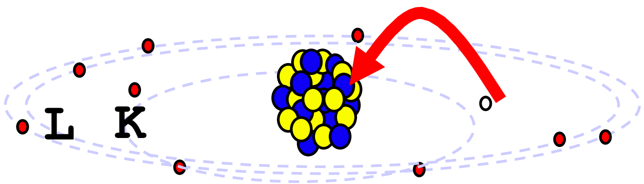
Auger electron yields – how well are known?

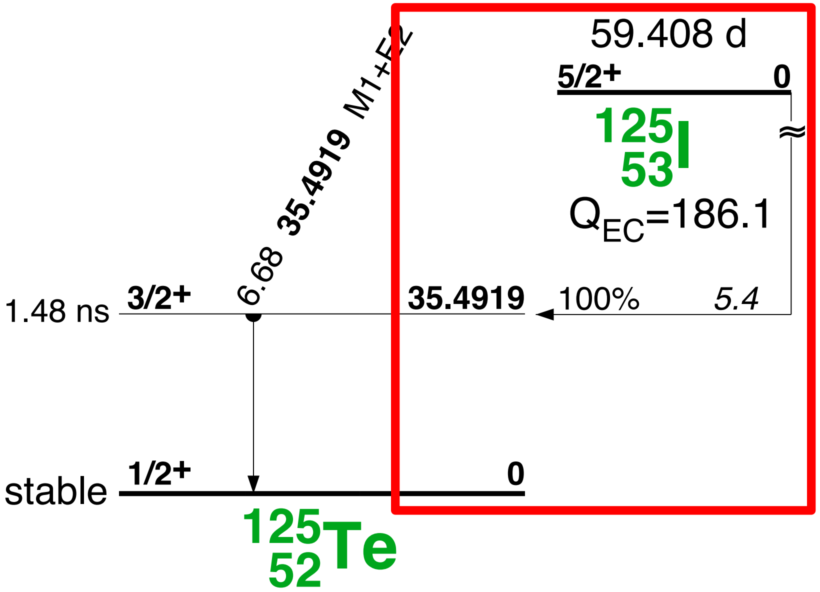
	RADAR	DDEP	Eckerman & Endo (2007)	Howell (1992)	Stepanek (2000)	Pomplun (2012)
^{99m}Tc (6.007 h)	0.869	0.13	4.363	4.0		2.5
^{111}In (2.805 d)	1.136	1.16	7.215	14.7	6.05	
^{123}I (13.22 h)	1.064	1.08	13.71	14.9		6.4
^{125}I (59.4 d)	1.77	1.78	23.0	24.9	15.3	12.2
^{201}Tl (3.04 d)	0.773	0.614	20.9	36.9		
Vacancy propagation	**Deterministic**	**Deterministic**	**Deterministic** (+++)	**Monte Carlo** with charge neutralization	**Monte Carlo**	**Monte Carlo**

Electron capture rates

Electron capture



$${}^{A}_{Z}X_{N} + e = {}^{A}_{Z-1}X_{N+1} + \nu_e$$



Electron capture rates:

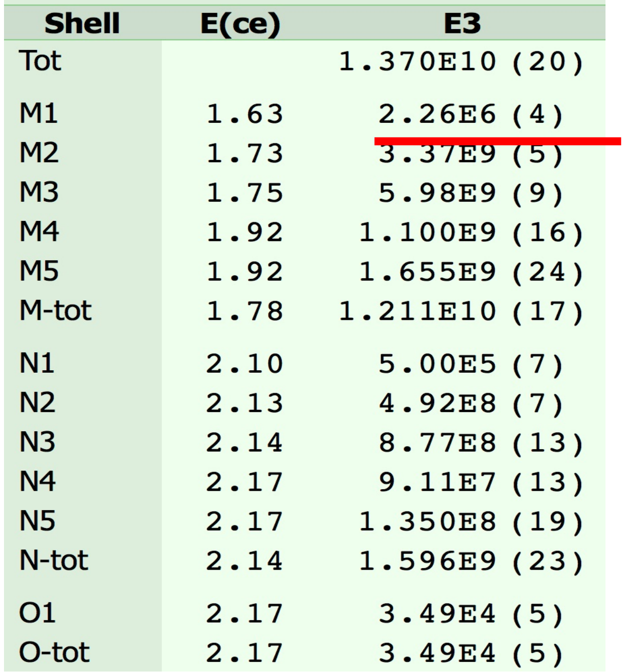
$$P_K+P_L+P_M+P_N+P_O+P_{\beta+} = 1$$

Tables: $3 \leqq Z \leqq 103$; E. Schönfeld, PTB-6.33-95-2 (1995)

Calculation of subshell ratios: E. Schönfeld,
Appl. Rad. And Isot. 49 (1998) 1353

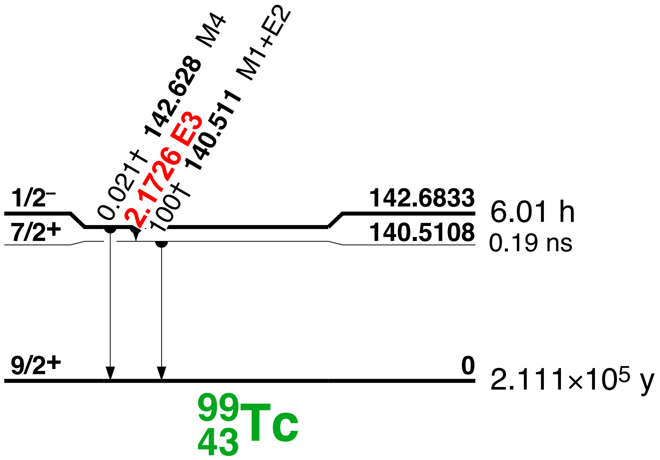
Accuracy: P_K: 0.3%, P_L: 3%, subshell ratios: up to 25%

BrIcc - Internal conversion coefficients



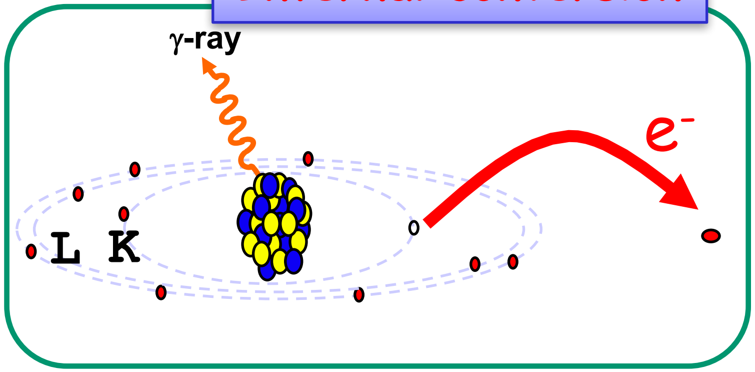
Shell	E(ce)	E3
Tot		1.370E10 (20)
M1	1.63	2.26E6 (4)
M2	1.73	3.37E9 (5)
M3	1.75	5.98E9 (9)
M4	1.92	1.100E9 (16)
M5	1.92	1.655E9 (24)
M-tot	1.78	1.211E10 (17)
N1	2.10	5.00E5 (7)
N2	2.13	4.92E8 (7)
N3	2.14	8.77E8 (13)
N4	2.17	9.11E7 (13)
N5	2.17	1.350E8 (19)
N-tot	2.14	1.596E9 (23)
O1	2.17	3.49E4 (5)
O-tot	2.17	3.49E4 (5)

Conversion coefficient
= $N(e^-)/N(\gamma)$

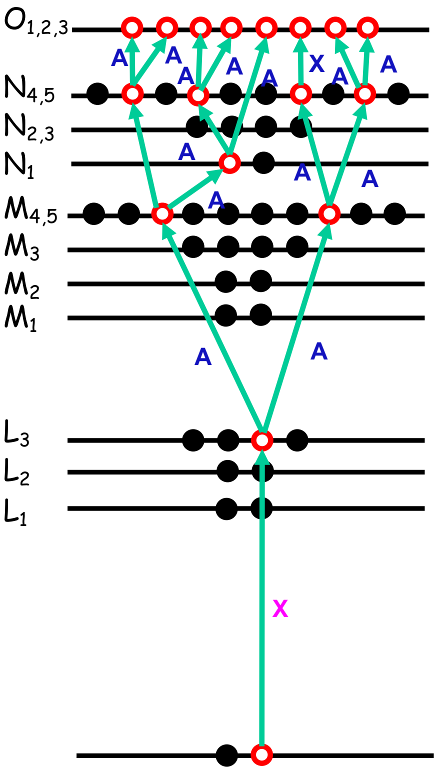


- ☐ Relativistic Dirac-Fock atomic model; Band et al. ADNDT 81 (2002) 1
- ☐ Frozen orbital approximation
- ☐ ICC ~1.3% accurate
- ☐ Z=5-110; 1-6000 keV; E1-E5, M1-M5, All subshells; Electron/Pair ICC, E0
- ☐ Tabulations:
  Z=5-110: T. Kibedi, et al, NIM **A589** (2008) 202
  Z=111-126: T. Kibedi, et al, ADNDT 98 (2012) 313

Internal conversion

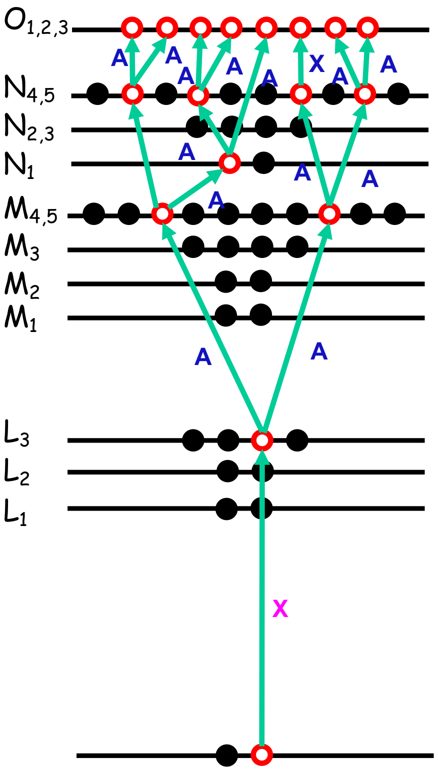


Atomic radiations and transition energies



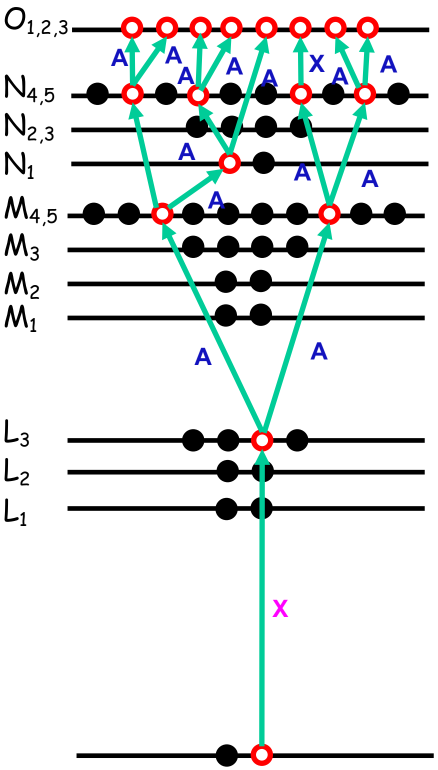
- ☐ Transition energies from Dirac-Fock atomic model
  - ❖ RAINE code (Band 2002)
  - ❖ No QED or Breit corrections; energies overestimated
- ☐ Transition rates from EADL (Perkins 1991)
  - ❖ Calculated for single initial vacancies
  - ❖ Krause-Carlson statistical correction, PR 158 (1967) 18
  - ❖ No shaking or double Auger process

BrIccEmis - Propagation of the vacancies



- ❑ X-ray or Auger electron emission to fill vacancy
- ❑ Multi step, stochastic process; Monte Carlo
- ❑ Transition energies and transition probabilities are needed for every propagation step
- ❑ Transition energies from Dirac-Fock atomic model
- ❑ Transition rates from EADL (Perkins 1991)
- ❑ Krause-Carlson correction to transition rates to take into account multiple vacancies
- ❑ STOP: Vacancy in valence shell / no transition is possible

BrIccEmis - Fast vs. Slow neutralisation



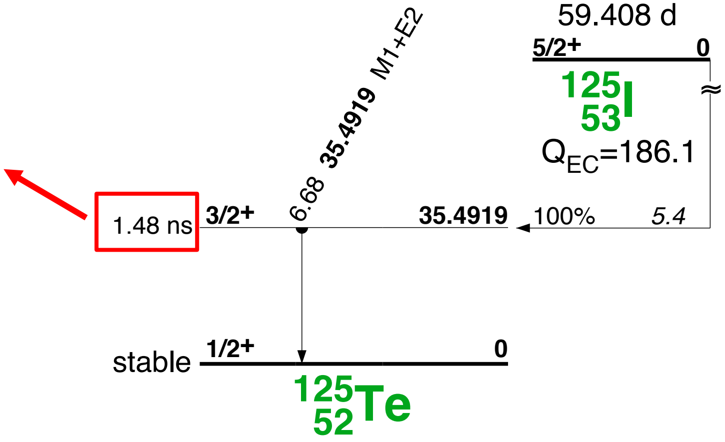
- Is the atom ISOLATED or in CONDENSED PHASE?
- Auger cascade very fast: 10^{-14} to 10^{-16} s
- Condensed phase: vacancies filled from environment (Charlton and Booz 1981, Humm 1984, Howell 1992)
- Neutralization is a slow process (Pomplun 2012)
- BrIccEmis: fast or slow neutralization option
  <u>Correct treatment: condensed physics model</u>

EC

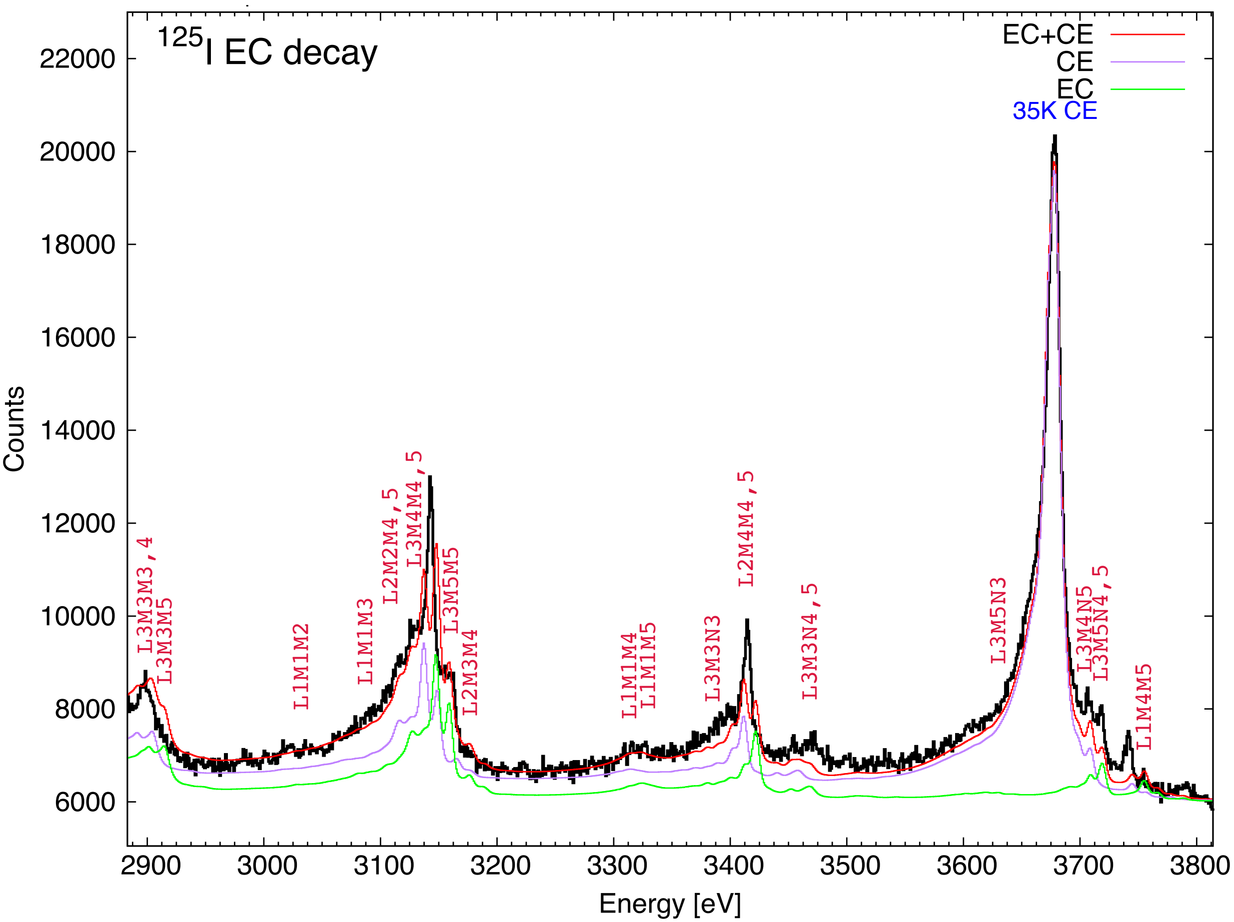
Relaxation

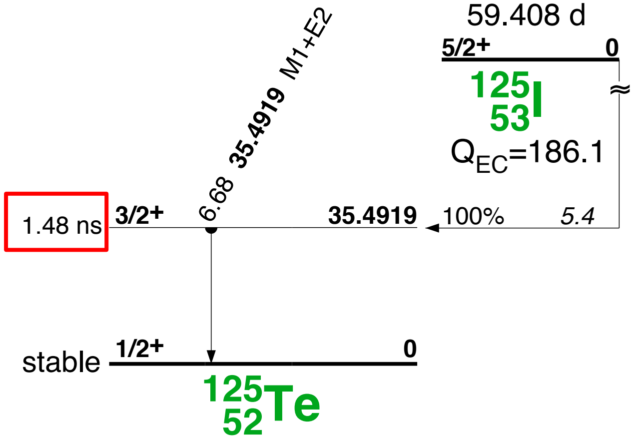
Internal conversion

Relaxation



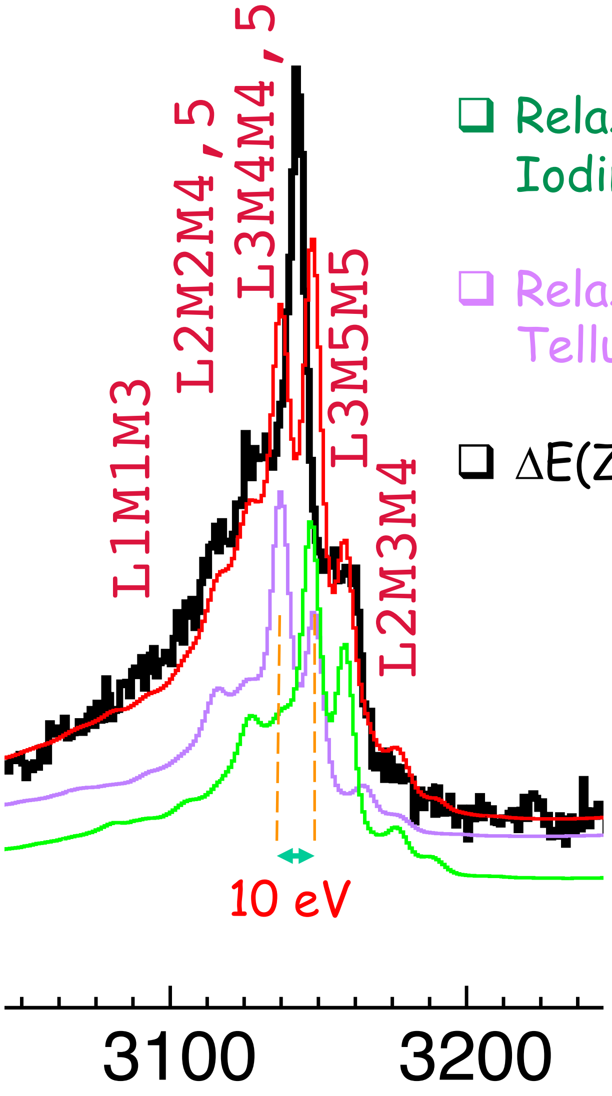
Benchmarking BrIccEmis using low energy electron measurements



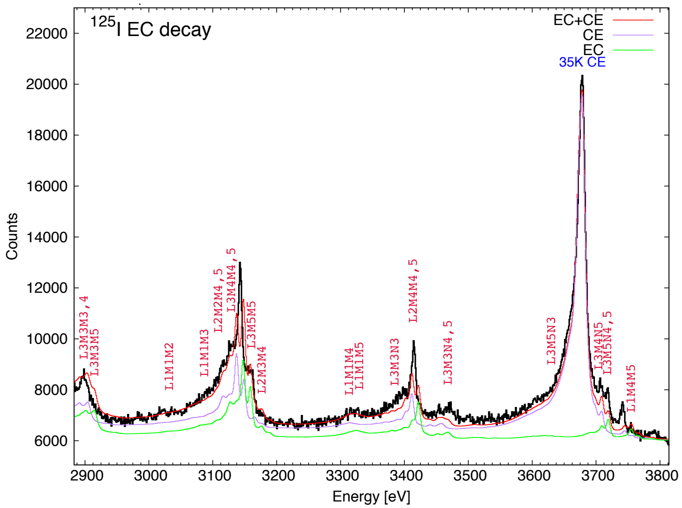


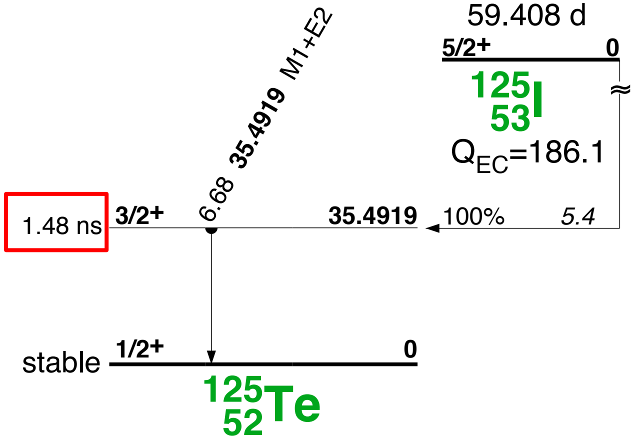
- Monolayer source, FWHM=7 eV! (with M. Vos, ANU 2018)
- See Bryan Tee`s talk on Friday

Benchmarking BrIccEmis using low energy electron measurements

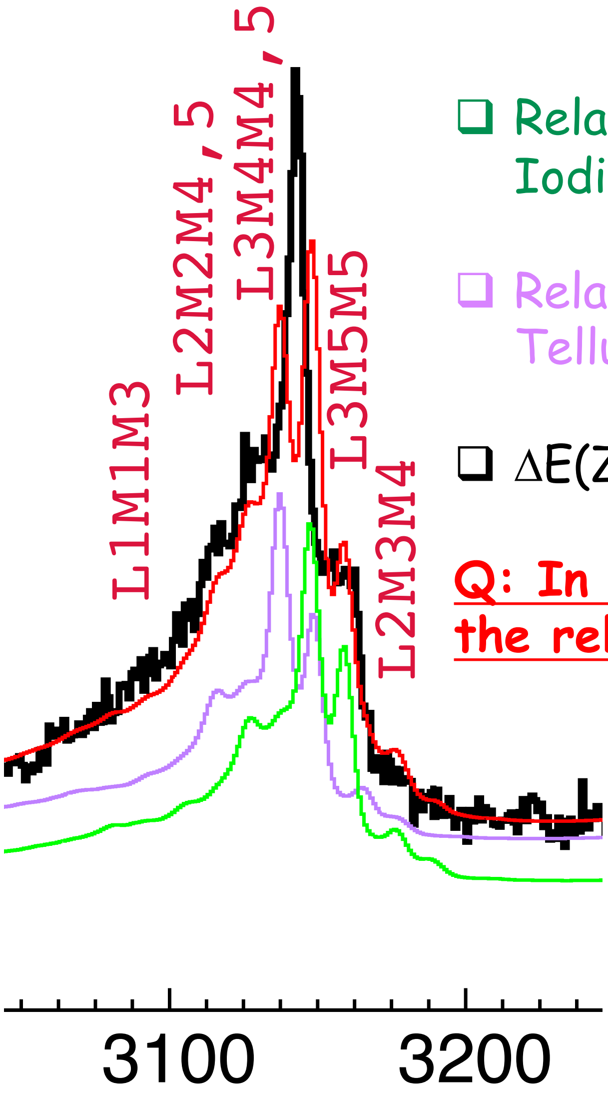


- ☐ Relaxation following EC in Iodine (Z=53)
- ☐ Relaxation following CE in Tellurium (Z=52)
- ☐ ΔE(Z=53 vs Z=52) ~10 eV



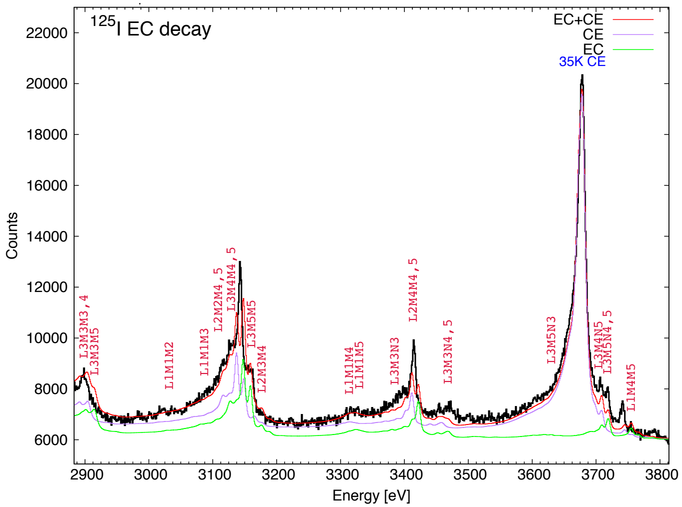


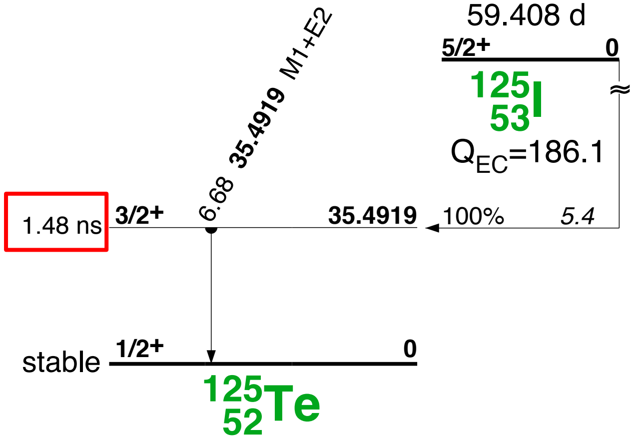
Benchmarking BrIccEmis using low energy electron measurements



- ☐ Relaxation following EC in Iodine (Z=53)
- ☐ Relaxation following CE in Tellurium (Z=52)
- ☐ ΔE(Z=53 vs Z=52) ~10 eV

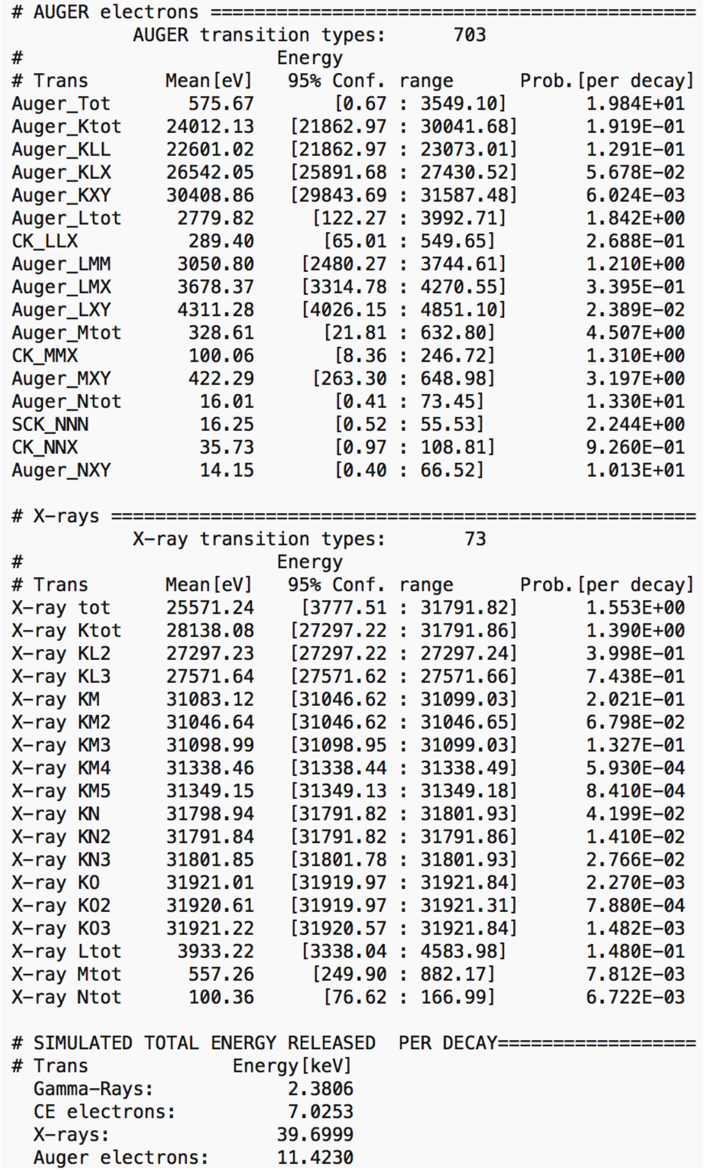
Q: In which atomic field the relaxation take place





Atomic radiations in ENSDF

- ☐ BrIccEmis atomic radiations data base and programs – under development
- ☐ NSDD 2017: new ENSDF record types adopted
- ☐ ^{125}I: Energy release keV) per decay:
  - Gamma-Rays: 2.3806
  - CE electrons: 7.0253
  - X-rays: 39.6999
  - Auger electrons: 11.4230



```
# AUGER electrons ============================================
           AUGER transition types:     703
#                       Energy
# Trans        Mean[eV]   95% Conf. range     Prob.[per decay]
Auger_Tot       575.67       [0.67 : 3549.10]       1.984E+01
Auger_Ktot    24012.13   [21862.97 : 30041.68]      1.919E-01
Auger_KLL     22601.02   [21862.97 : 23073.01]      1.291E-01
Auger_KLX     26542.05   [25891.68 : 27430.52]      5.678E-02
Auger_KXY     30408.86   [29843.69 : 31587.48]      6.024E-03
Auger_Ltot     2779.82     [122.27 : 3992.71]       1.842E+00
CK_LLX          289.40      [65.01 : 549.65]        2.688E-01
Auger_LMM      3050.80    [2480.27 : 3744.61]       1.210E+00
Auger_LMX      3678.37    [3314.78 : 4270.55]       3.395E-01
Auger_LXY      4311.28    [4026.15 : 4851.10]       2.389E-02
Auger_Mtot      328.61      [21.81 : 632.80]        4.507E+00
CK_MMX          100.06       [8.36 : 246.72]        1.310E+00
Auger_MXY       422.29     [263.30 : 648.98]        3.197E+00
Auger_Ntot       16.01       [0.41 : 73.45]         1.330E+01
SCK_NNN          16.25       [0.52 : 55.53]         2.244E+00
CK_NNX           35.73       [0.97 : 108.81]        9.260E-01
Auger_NXY        14.15       [0.40 : 66.52]         1.013E+01

# X-rays =====================================================
           X-ray transition types:      73
#                       Energy
# Trans        Mean[eV]   95% Conf. range     Prob.[per decay]
X-ray tot     25571.24    [3777.51 : 31791.82]      1.553E+00
X-ray Ktot    28138.08   [27297.22 : 31791.86]      1.390E+00
X-ray KL2     27297.23   [27297.22 : 27297.24]      3.998E-01
X-ray KL3     27571.64   [27571.62 : 27571.66]      7.438E-01
X-ray KM      31083.12   [31046.62 : 31099.03]      2.021E-01
X-ray KM2     31046.64   [31046.62 : 31046.65]      6.798E-02
X-ray KM3     31098.99   [31098.95 : 31099.03]      1.327E-01
X-ray KM4     31338.46   [31338.44 : 31338.49]      5.930E-04
X-ray KM5     31349.15   [31349.13 : 31349.18]      8.410E-04
X-ray KN      31798.94   [31791.82 : 31801.93]      4.199E-02
X-ray KN2     31791.84   [31791.82 : 31791.86]      1.410E-02
X-ray KN3     31801.85   [31801.78 : 31801.93]      2.766E-02
X-ray KO      31921.01   [31919.97 : 31921.84]      2.270E-03
X-ray KO2     31920.61   [31919.97 : 31921.31]      7.880E-04
X-ray KO3     31921.22   [31920.57 : 31921.84]      1.482E-03
X-ray Ltot     3933.22    [3338.04 : 4583.98]       1.480E-01
X-ray Mtot      557.26     [249.90 : 882.17]        7.812E-03
X-ray Ntot      100.36      [76.62 : 166.99]        6.722E-03

# SIMULATED TOTAL ENERGY RELEASED  PER DECAY=================
# Trans             Energy[keV]
  Gamma-Rays:            2.3806
  CE electrons:          7.0253
  X-rays:               39.6999
  Auger electrons:      11.4230
```