



Electron conversion coefficients – today's challenges

T. Kibédi (ANU)

- New theoretical conversion coefficients - BrIcc
- How good are the internal conversion coefficients now?
- Recent conversion electron developments at the ANU

Discovery of monoenergetic electrons (β -rays) in radioactive decay - 100 years on

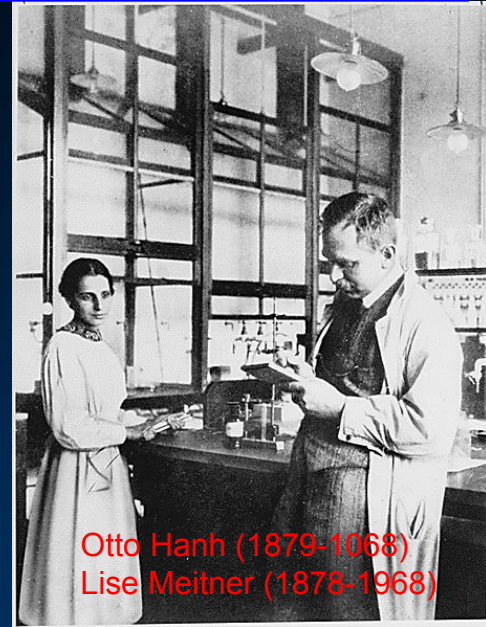
The first "magnetic β -ray spectrometer" (1910)

Von Otto Baeyer and Otto Hahn

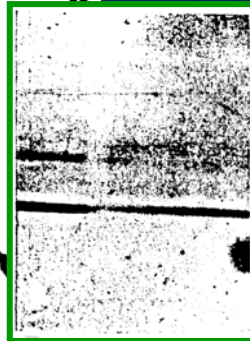
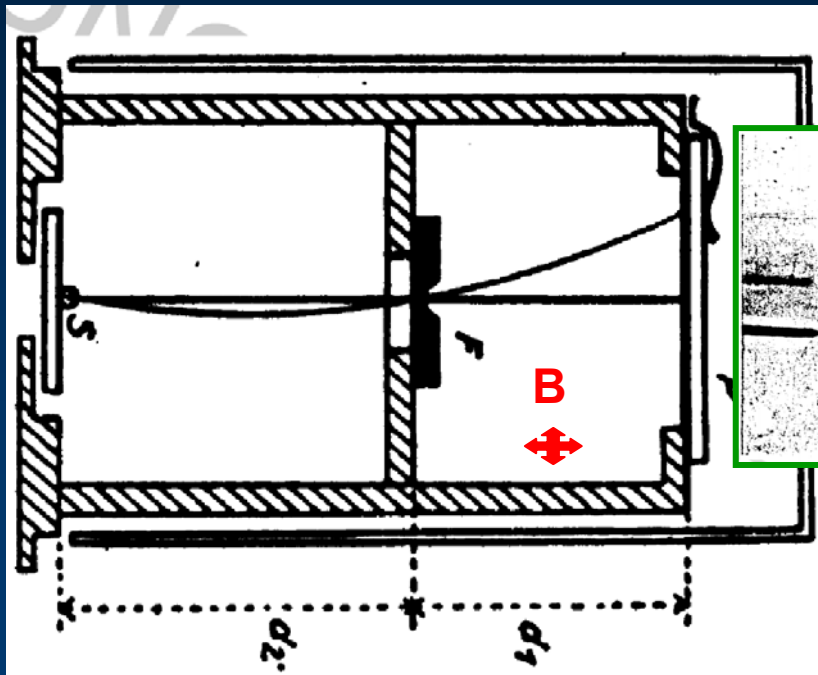
Physikalische Zeitschrift, 11 (1910) 488

Von Otto Baeyer, Otto Hahn and Lise Meitner

Physikalische Zeitschrift 12 (1911) 273



Otto Hahn (1879-1968)
Lise Meitner (1878-1968)



The first monoenergetic β -ray spectrum

For full historical accounts see A. Franklin, "The Spectrum of β Decay: Continuous or Discrete? A Variety of Errors in Experimental Investigation", *Boston Studies in The Phil. of Sci.*, 267 (2008) p211.

Discovery of conversion electron process (1921)

Discovery of conversion electron process

Charles Drummond Ellis,
Proc. of the Royal Soc. of London 99 (1921) 261

Table V.— β -ray Spectrum RaB.

I.	II.	III.	IV.
Origin of Line.	Intensity.	Energy observed.	Energy calculated.
		volts.	
A'	<i>f.</i>	$3 \cdot 851 \times 10^5$	$3 \cdot 843 \times 10^5$
A'	<i>m.s.</i>	3·473	3·482
A'	<i>s.</i>	3·328	3·335
K	<i>v.f.</i>	3·103	3·109
A' } K } K }	<i>m.s.</i>	2·756	{ 2·761 2·748
K	<i>v.s.</i>	2·608	2·601
A'	<i>m.</i>	2·364	2·372
A'	<i>m.s.</i>	2·227	2·228
K	<i>v.s.</i>	2·031	2·027
K	<i>m.s.</i>	1·645	1·638
K	<i>v.s.</i>	1·494	1·494

Introduction of the first level scheme

Charles Drummond Ellis,
Proc. of the Royal Soc. of London 101 (1922) 1

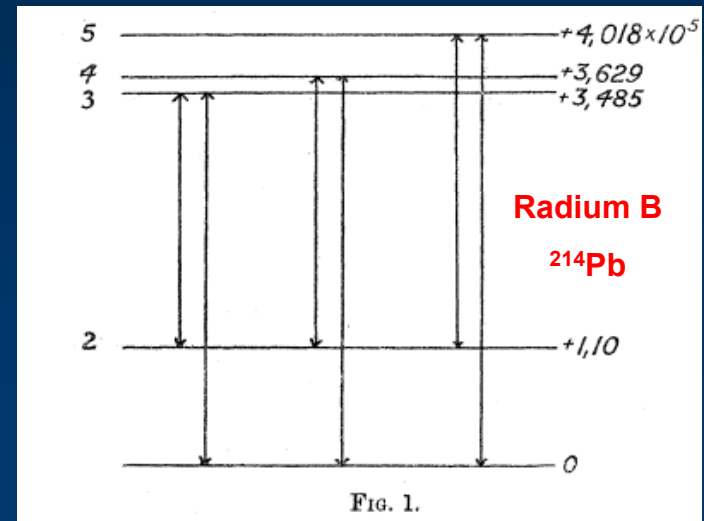


Table IV.— γ -rays of RaB.

I.	II.
Energies in volts.	λ in A.U.
$4 \cdot 000 \times 10^5$	0·0308
3·639	0·0339
3·492	0·0354
2·918	0·0423
2·529	0·0488
2·385	0·0519

FIG. 1.

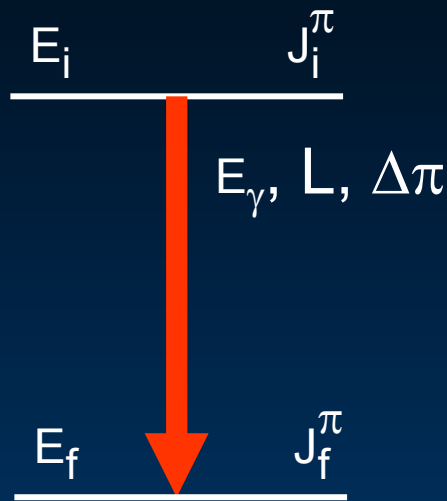
Energetics of γ -decay:

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

$$0 = p_r + p_\gamma$$

where $T_r = (p_r)^2/2M$; usually $T_r/E_\gamma \sim 10^{-5}$

Angular momentum and parity selection rules; multipolarities



Multipolarity known

ΔJ may not be unique

unique $\Delta\pi$

$$|J_i - J_f| \leq L \leq J_i + J_f; L \neq 0$$

$$J_i = J_f$$

$\Delta\pi = \text{no};$

E2, E4, E6

M1, M3, M5

E0

$\Delta\pi = \text{yes};$

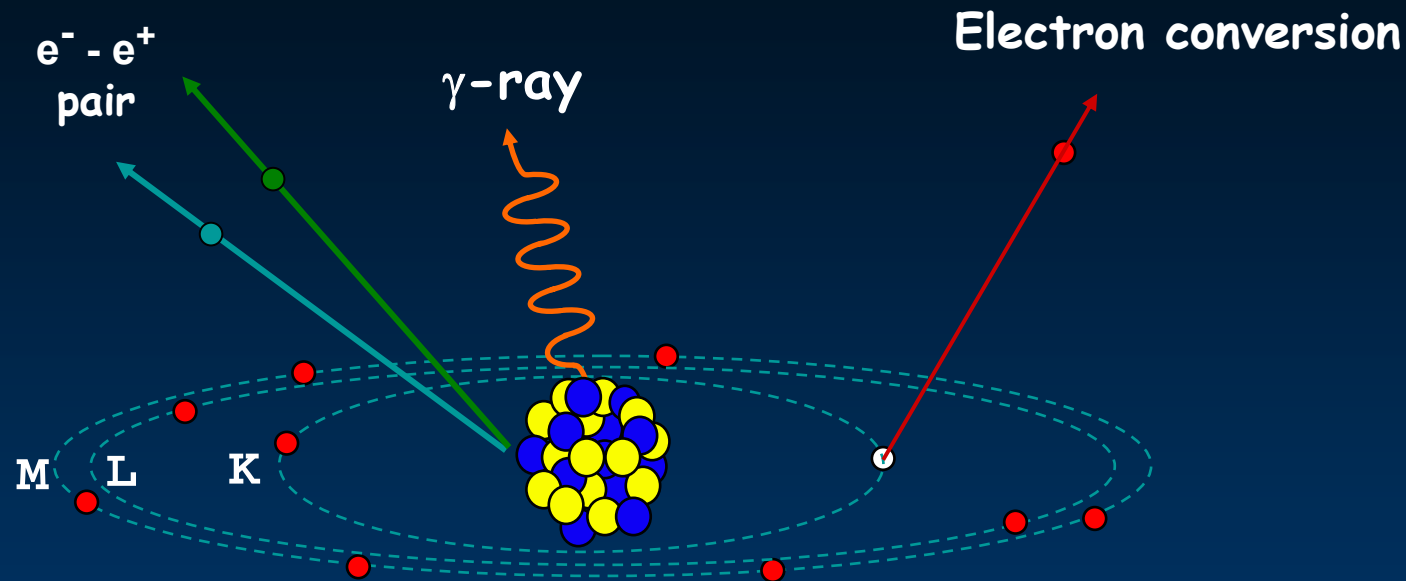
E1, E3, E5

M2, M4, M6

Mixed multipolarity

$$\delta(\pi'L') = I_\gamma(\pi'L') / I_\gamma(\pi L)$$

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

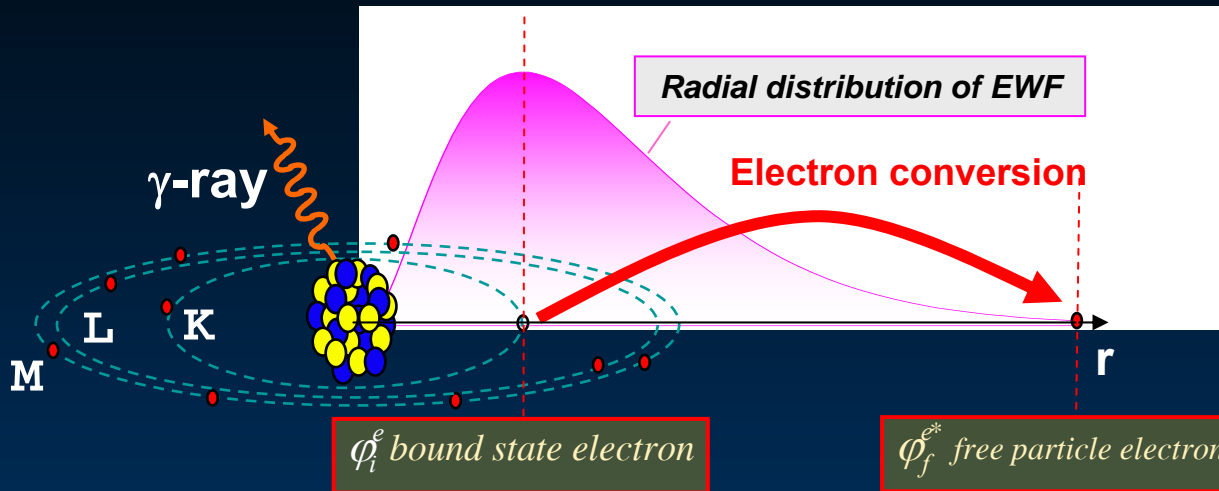


Transition probability

$$\lambda_T = \lambda_\gamma + \lambda_K + \lambda_L + \lambda_M \dots + \lambda_\pi$$

Conversion Coefficient

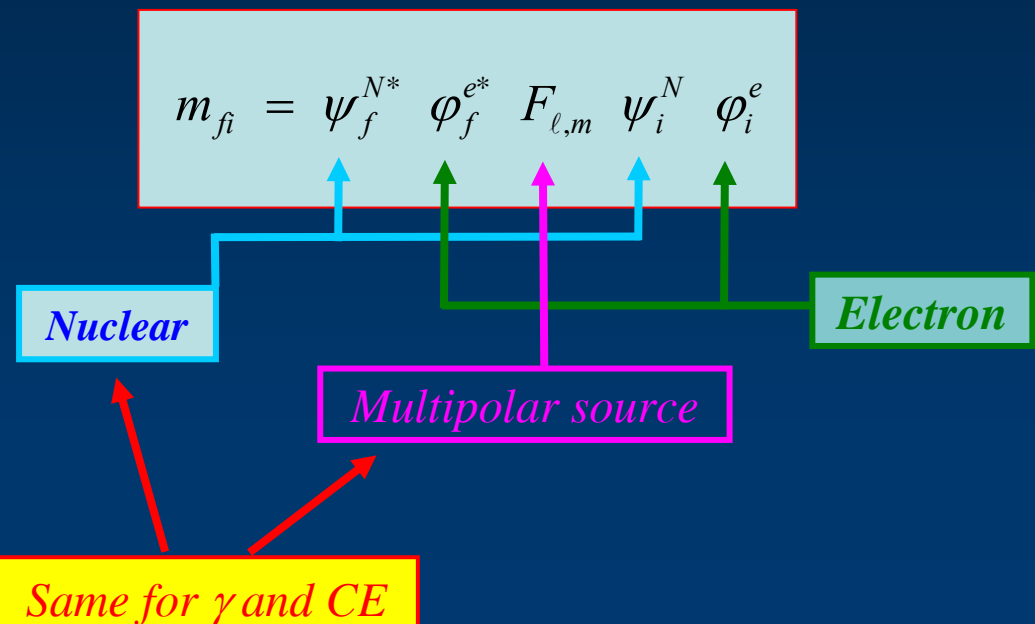
$$\alpha_{ce,\pi} = \lambda_{ce,\pi} / \lambda_\gamma$$

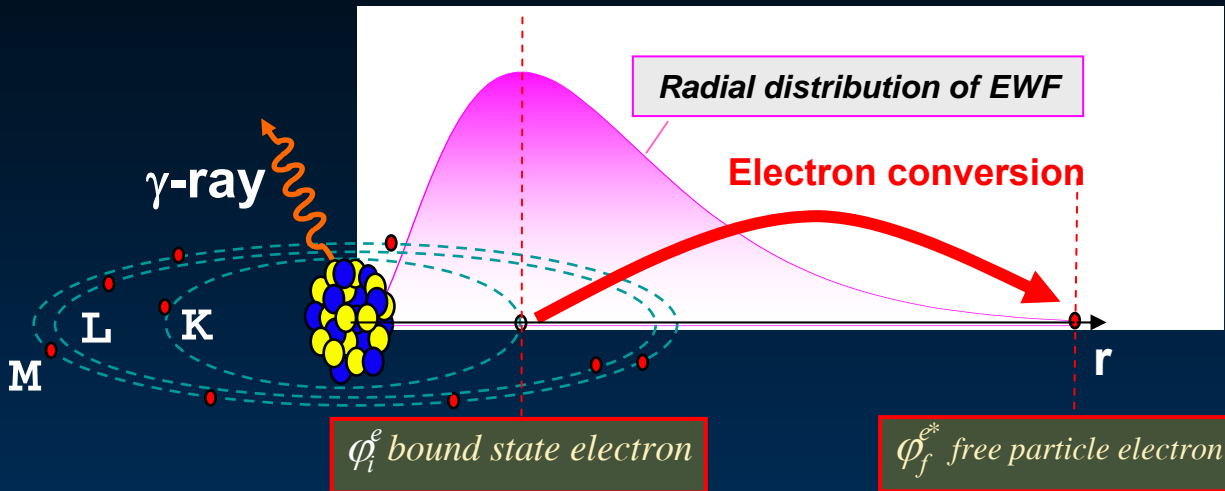


Fermi's golden rule

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

Density of the final electron state (continuum)

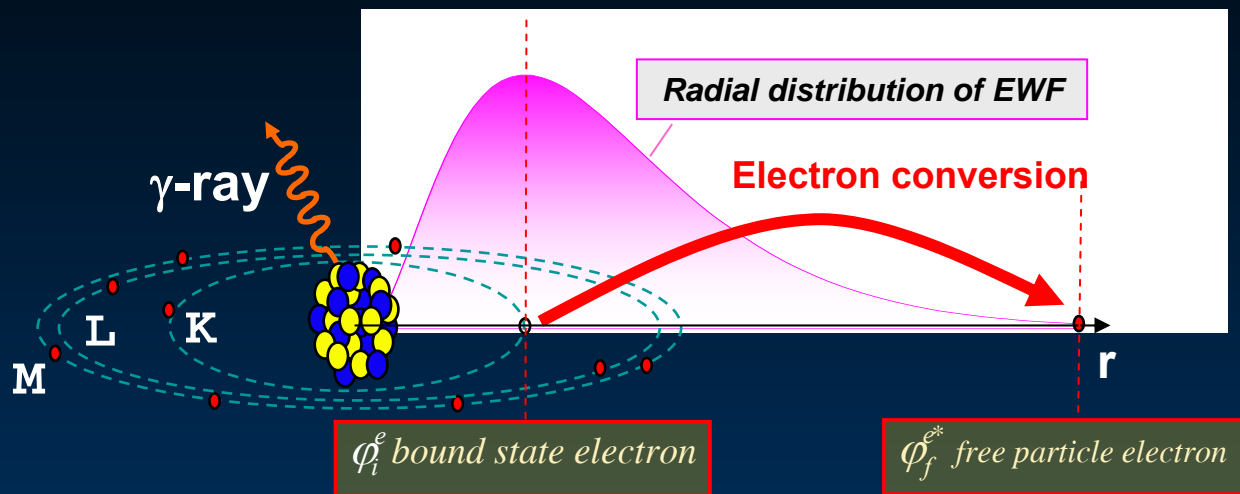




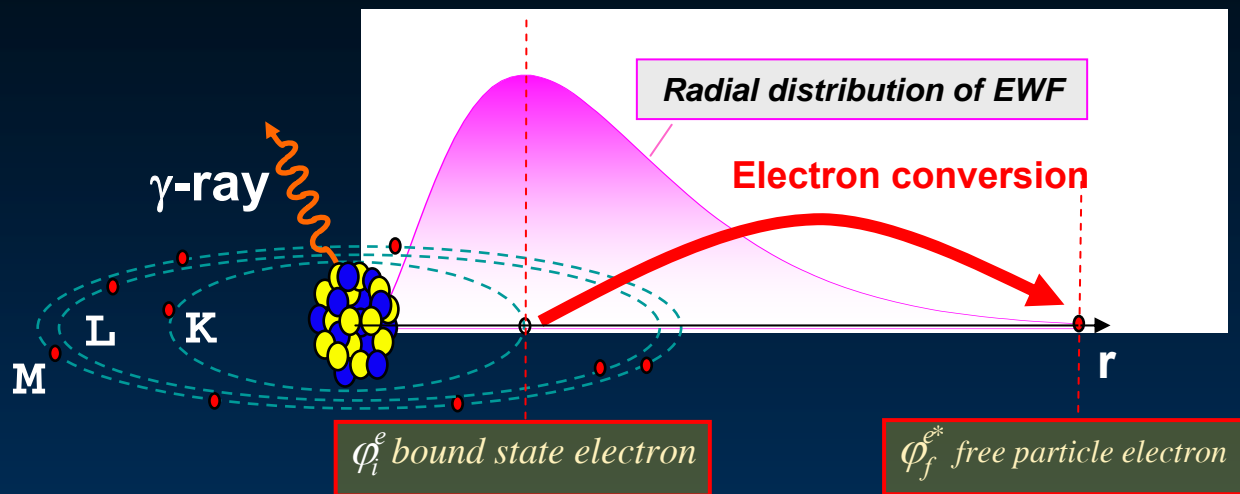
➤ Calculations up to the first nonvanishing order of the perturbation theory

I.M. Band, et al., *Atomic Data and Nuclear Data Tables* **81** (2002) 1

T. Kibèdi, et al., *Nucl. Instr. and Meth. in Physics Research* **A589** (2008) 202



- Relativistic Dirac-Fock method
- One-electron approximation
- Free neutral atom
- Screening of the nuclear field by the atomic electrons
- Spherically symmetric atomic potential
- Experimental ($Z \leq 95$) and theoretical ($Z > 95$) electron binding energies



- Finite nuclear size
- Spherically symmetric nucleus; calculations for the most abundant isotope
- Intranuclear conversion - Penetration effect

Penetration effect

- ^{203}Tl : $E_\gamma = 279.1955(12)$ keV; M1+E2; $\delta = +1.17(5)$

$\alpha_K(\text{Hslcc}) = 0.216$
 $\alpha_K(\text{Brlcc}) = 0.209$

$\alpha_K(\text{exp}) = 0.1642(11)$ from 7 measurements
- “Static effects” is taken into account approximately, but consistently (SC model, Sliv)
- Hindered transitions: correction for “dynamic effects” (Pauli)

Measured ICC

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

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

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

Theoretical ICC

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

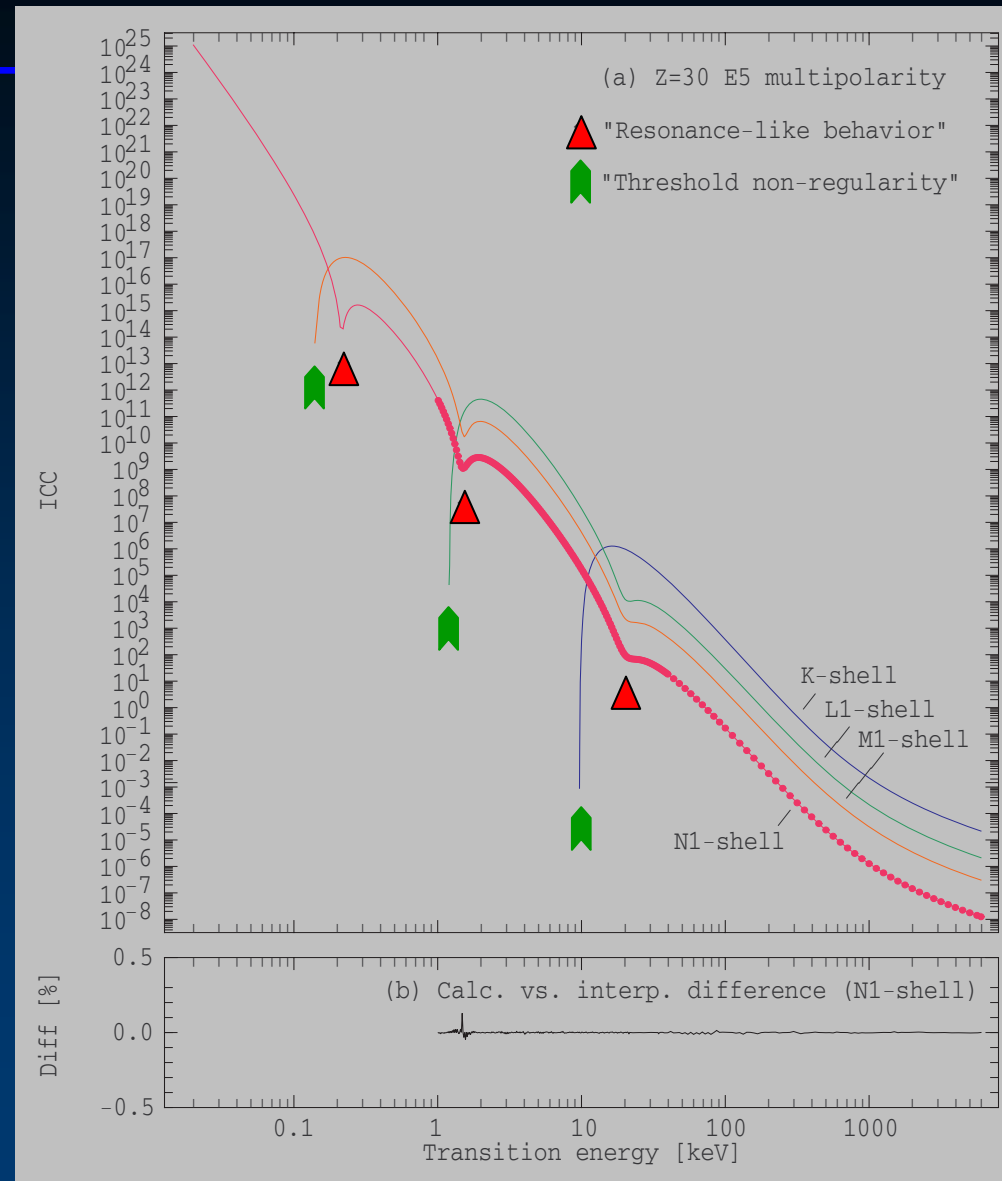


- Atomic many body correlations: factor ~ 2 for $E_{\text{kin}}(\text{ce}) < 1 \text{ keV}$
- Partially filled valence shell: non-spherical atomic field
- Binding energy uncertainty: $< 0.5\%$ for $E_{\text{kin}}(\text{ce}) > 10 \text{ keV}$
- Chemical effects: $\ll 1\%$

$s_{1/2}$ shells, E2-E5 multipolarity

▲ “Resonance-like behavior” above the shell binding energies; effect decreases with Z

▼ “Threshold non-regularity”, sharp up-bend starting at the binding energy. Also for magnetic multipolarities at higher Z



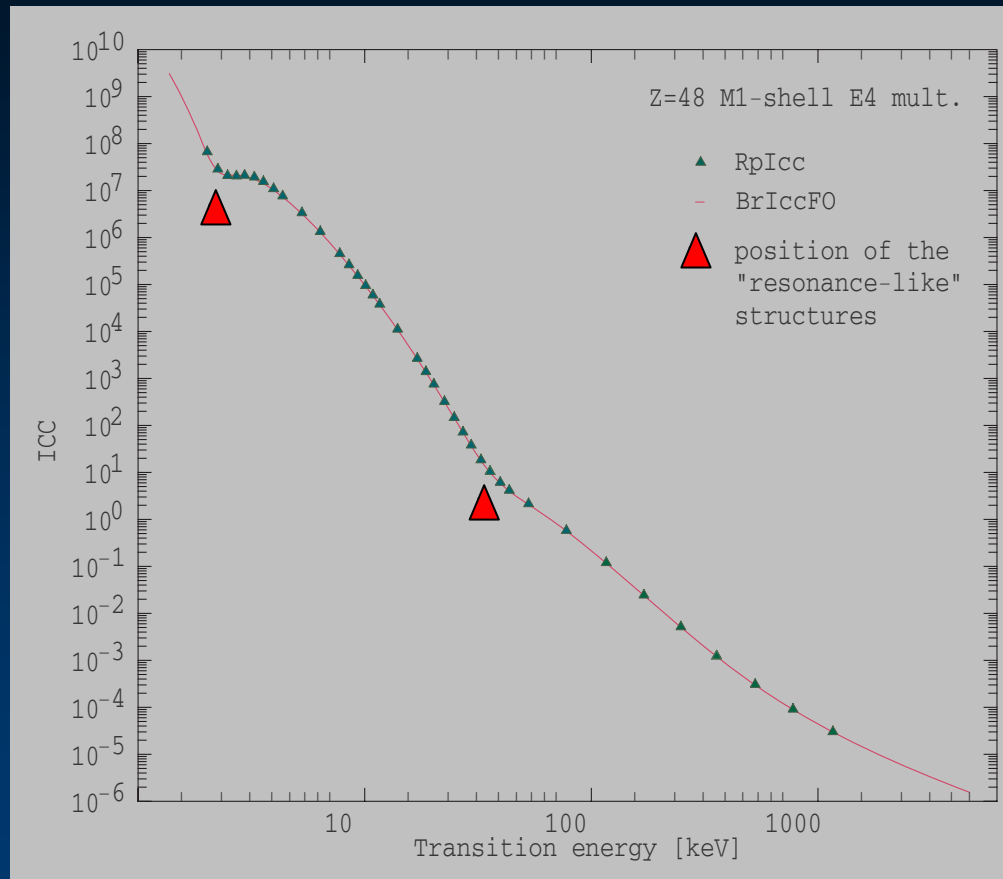
T. Kibèdi et al., Nucl. Instr. and Meth. in Phys. Res. A 589 (2008) 202

Seen in

- Rösel et al.* (\blacktriangle)
- Dirac-Fock-Slater (DFS)*
- Dirack-Fock (DF)*

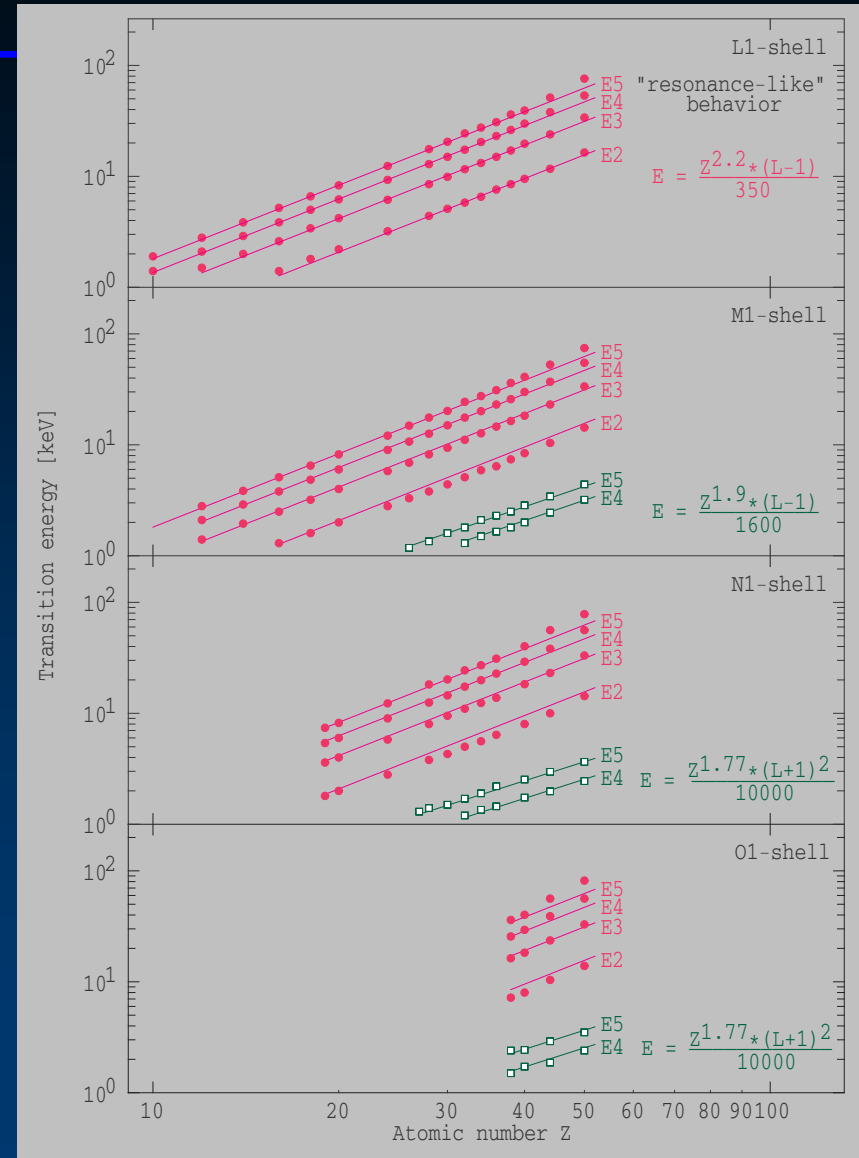
calculations

No suitable experimental ICC is known to us to verify its existence

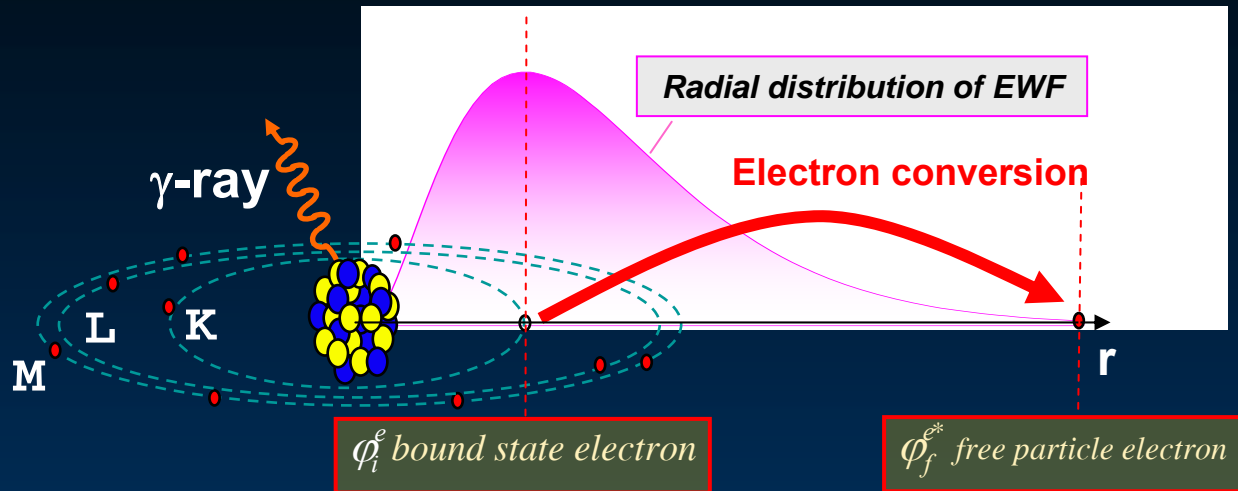


T. Kibèdi et al., Nucl. Instr. and Meth. in Phys. Res. A 589 (2008) 202

Strong correlation with atomic number



T. Kibèdi et al., Nucl. Instr. and Meth. in Phys. Res. A 589 (2008) 202

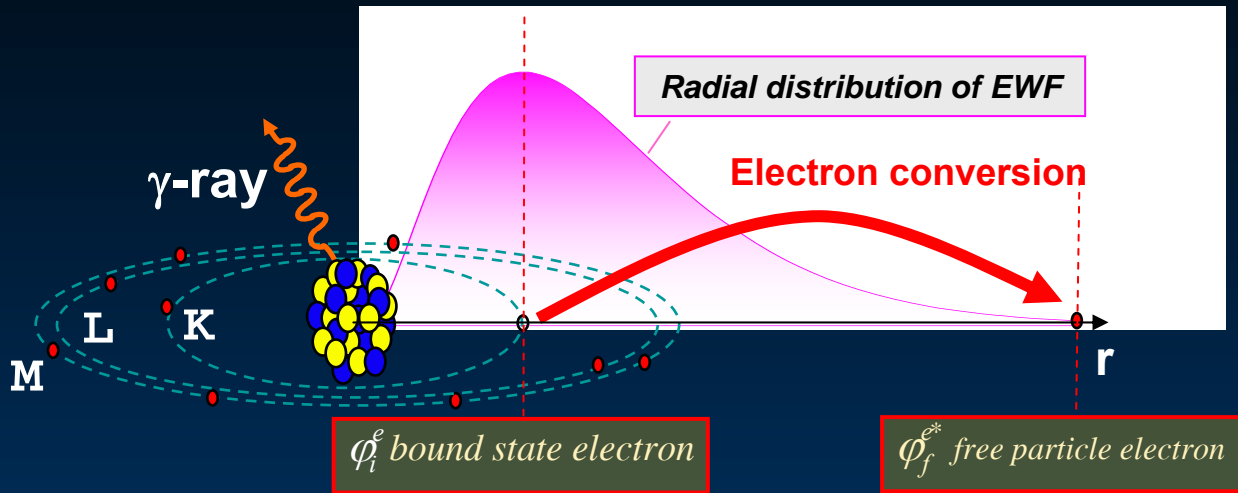


"No Hole" - BTNTR: SCF of a neutral atom

Vacancy disregarded

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

BrIccNH table - extended and revised calculations



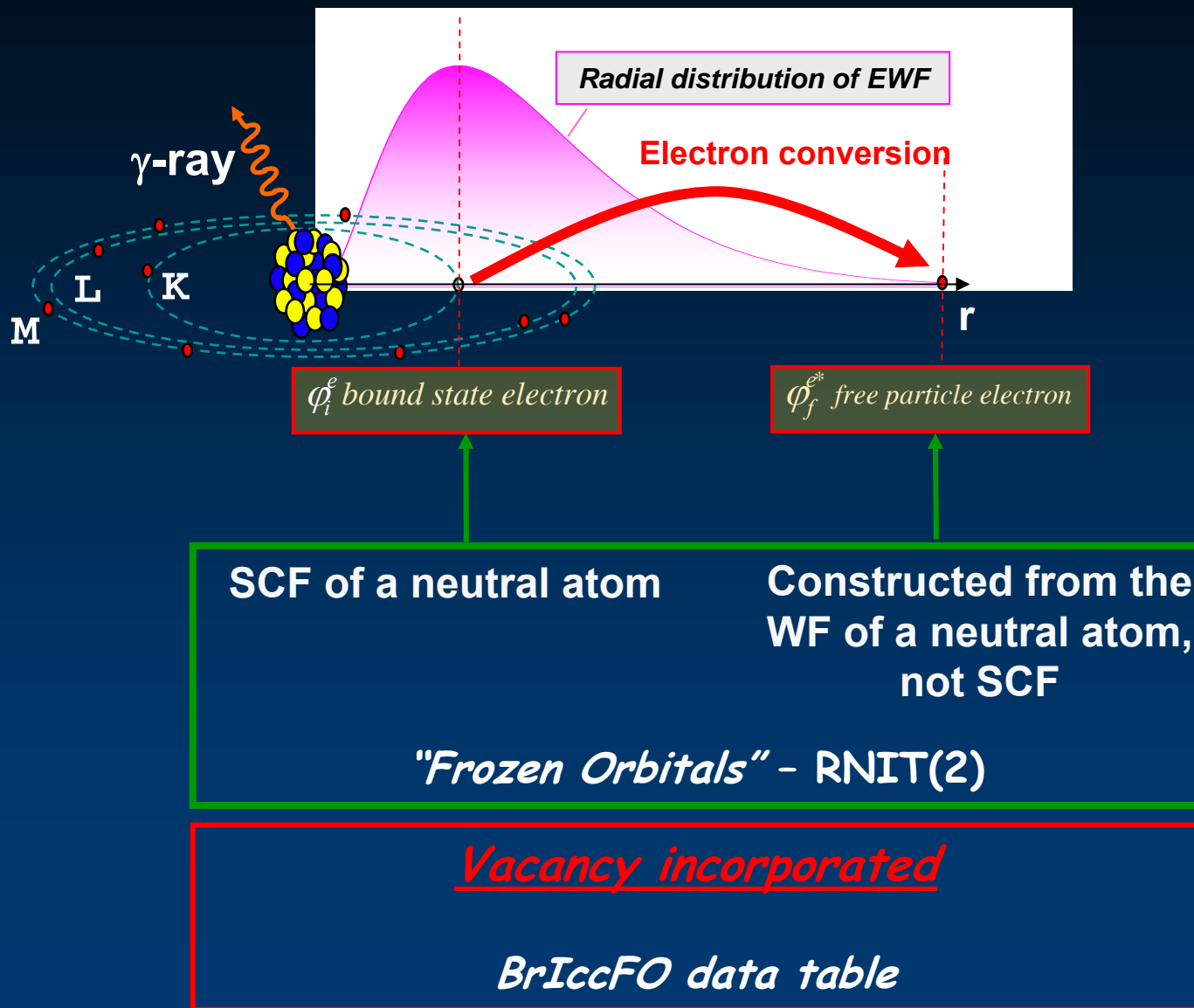
SCF of a neutral atom

SCF of an ion

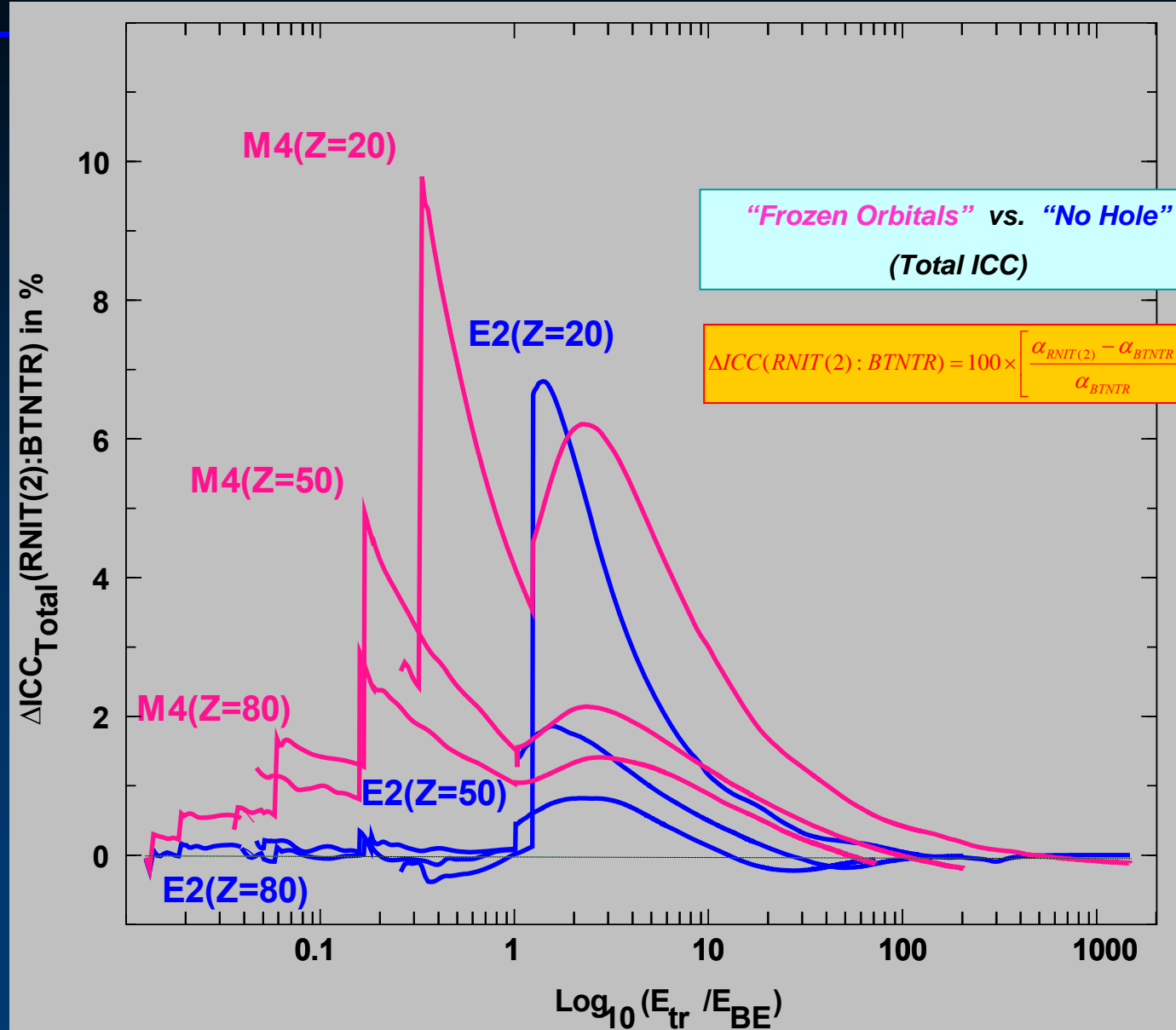
"Self Consistent" - RNIT(1)

Vacancy incorporated

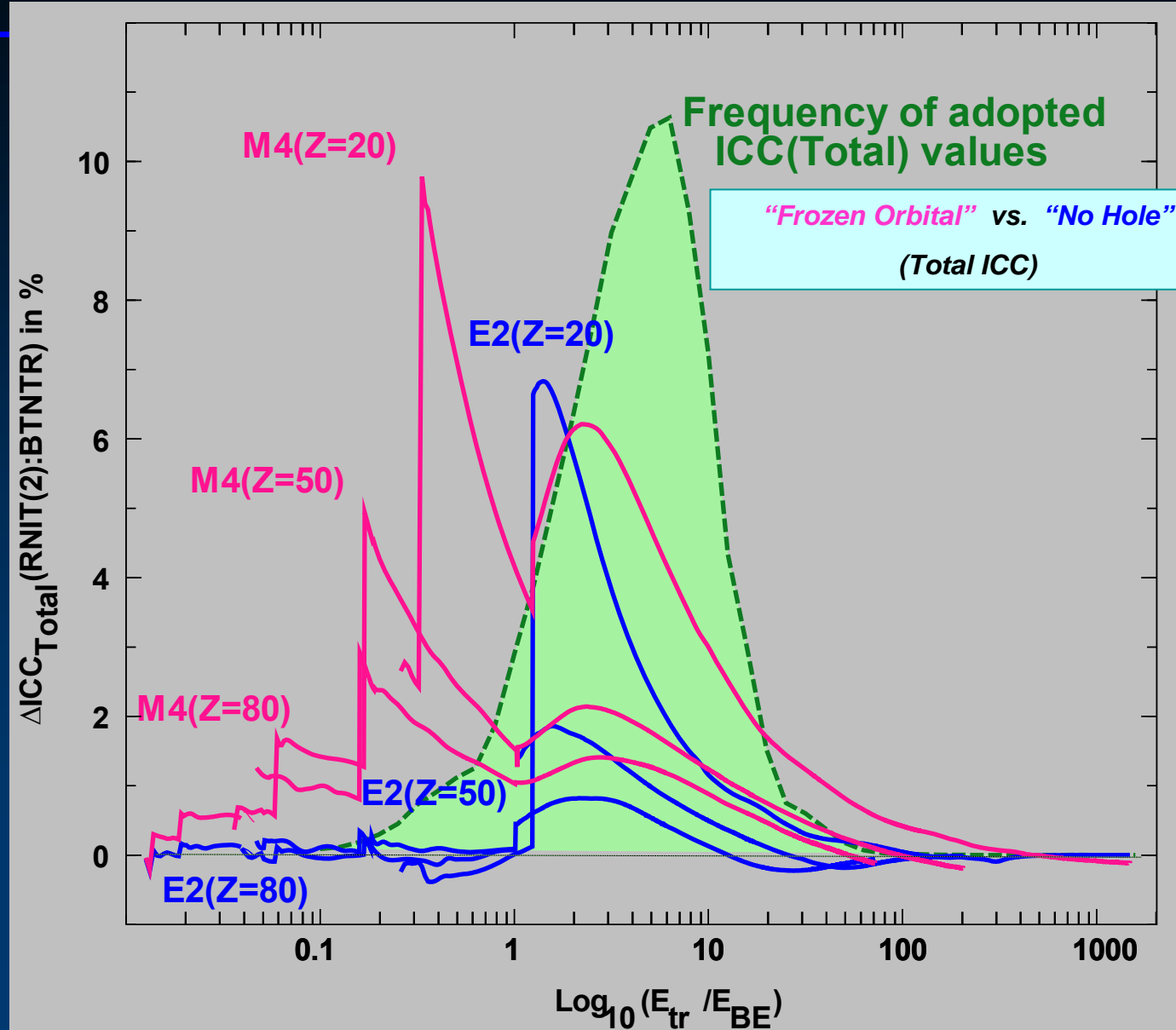
No data table



ICC calculations – Atomic vacancies



ICC calculations – Atomic vacancies



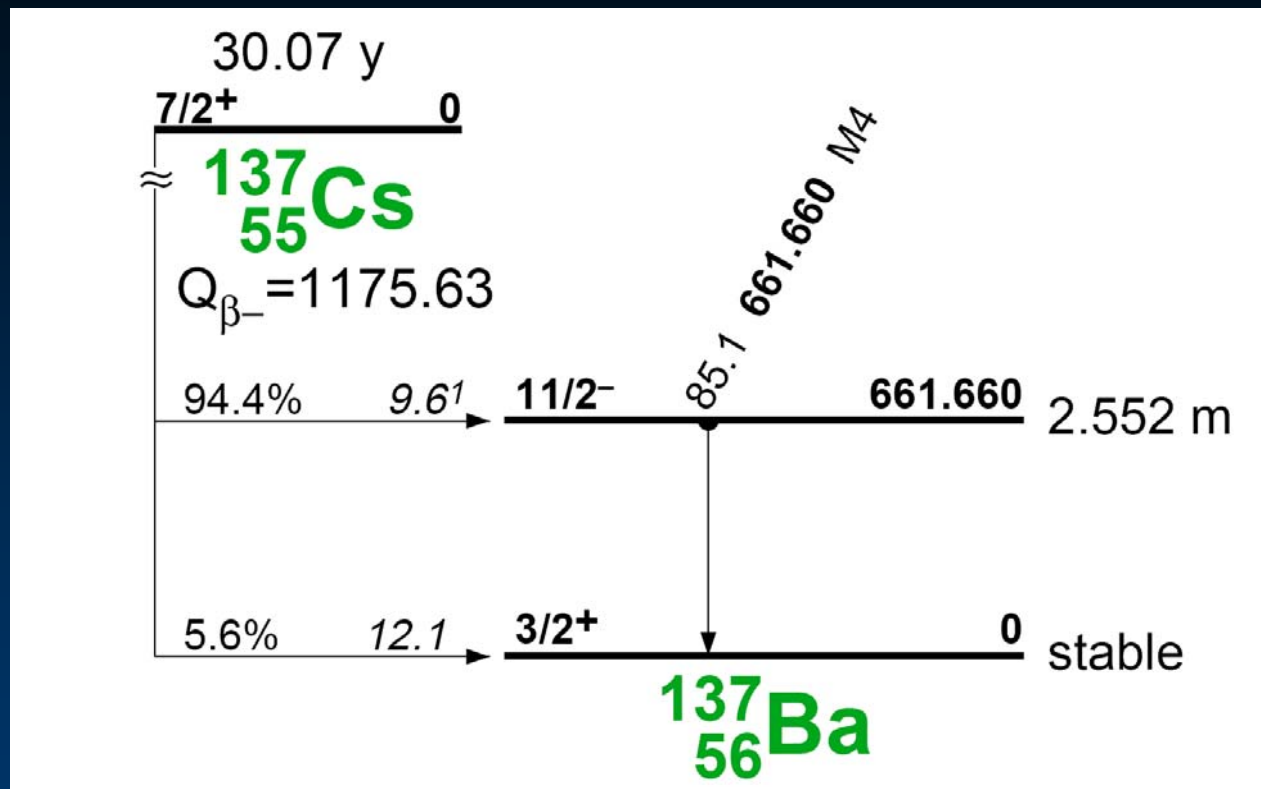
New experiments

- **$\alpha_K(80 \text{ keV } ^{193}\text{Ir M4})$**
Nica, et al., Phys. Rev. C 70 (2004) 054305
- **$\alpha_T(88 \text{ keV } ^{109}\text{Ag E3})$**
Kossert et al., App. Rad. and Isotopes 64 (2006) 1031
- **$\alpha_K(128 \text{ keV } ^{134}\text{Cs E3})/\alpha_K(662 \text{ keV } ^{137}\text{Ba M4})$**
Nica et al., Phys. Rev. C 75, (2007) 024308
- **$\alpha_K(128 \text{ keV } ^{134}\text{Cs E3})$ and $\alpha_K(662 \text{ keV } ^{137}\text{Ba M4})$**
Nica et al., Phys. Rev. C 77, (2008) 034306

Benchmark data sets (compillations)

- **100 α_K and α_T** - *S. Raman, et al., Phys. Rev. C66, 044312 (2002)*
- **1510 ICC ratios** – *S. Raman, et al., Atom. Data and Nucl. Data Tabl. 92, 207 (2006)*
- **194 α_K , α_L , α_T and ICC ratios (L>2)** – *J. Gerl, et al., Atom. Data and Nucl. Data Tabl. 94, 701 (2008)*

^{137}Ba 662 keV M4 K-shell ICC



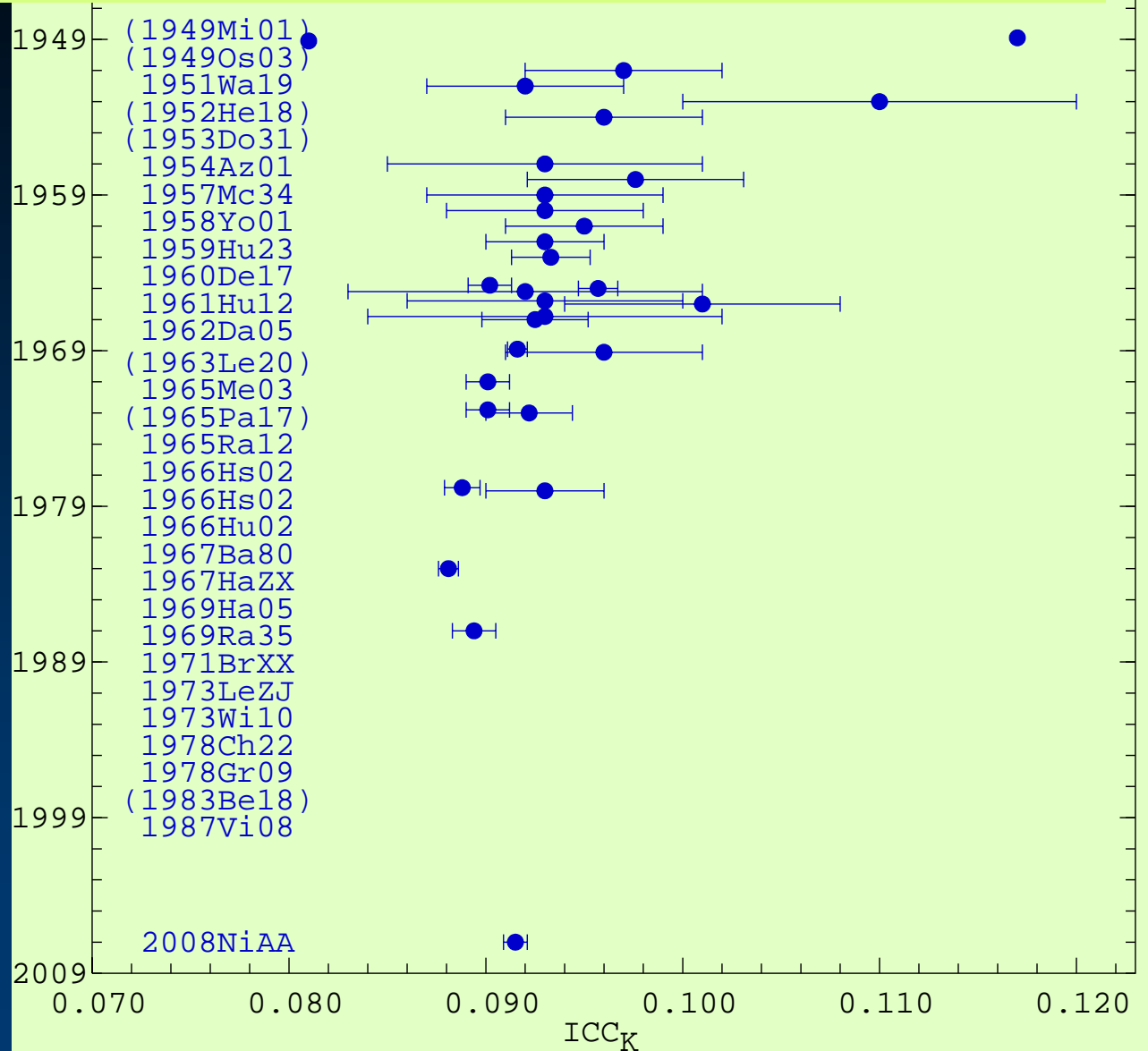
Determining K-shell ICC

$$\alpha_K = \frac{\lambda_K}{\lambda_\gamma} = \frac{A_K}{A_\gamma} \times \frac{\varepsilon_\gamma}{\varepsilon_K} = \frac{A_{KX}}{A_\gamma} \times \frac{\varepsilon_\gamma}{\varepsilon_{KX}} \times \frac{1}{\omega_{KX}}$$

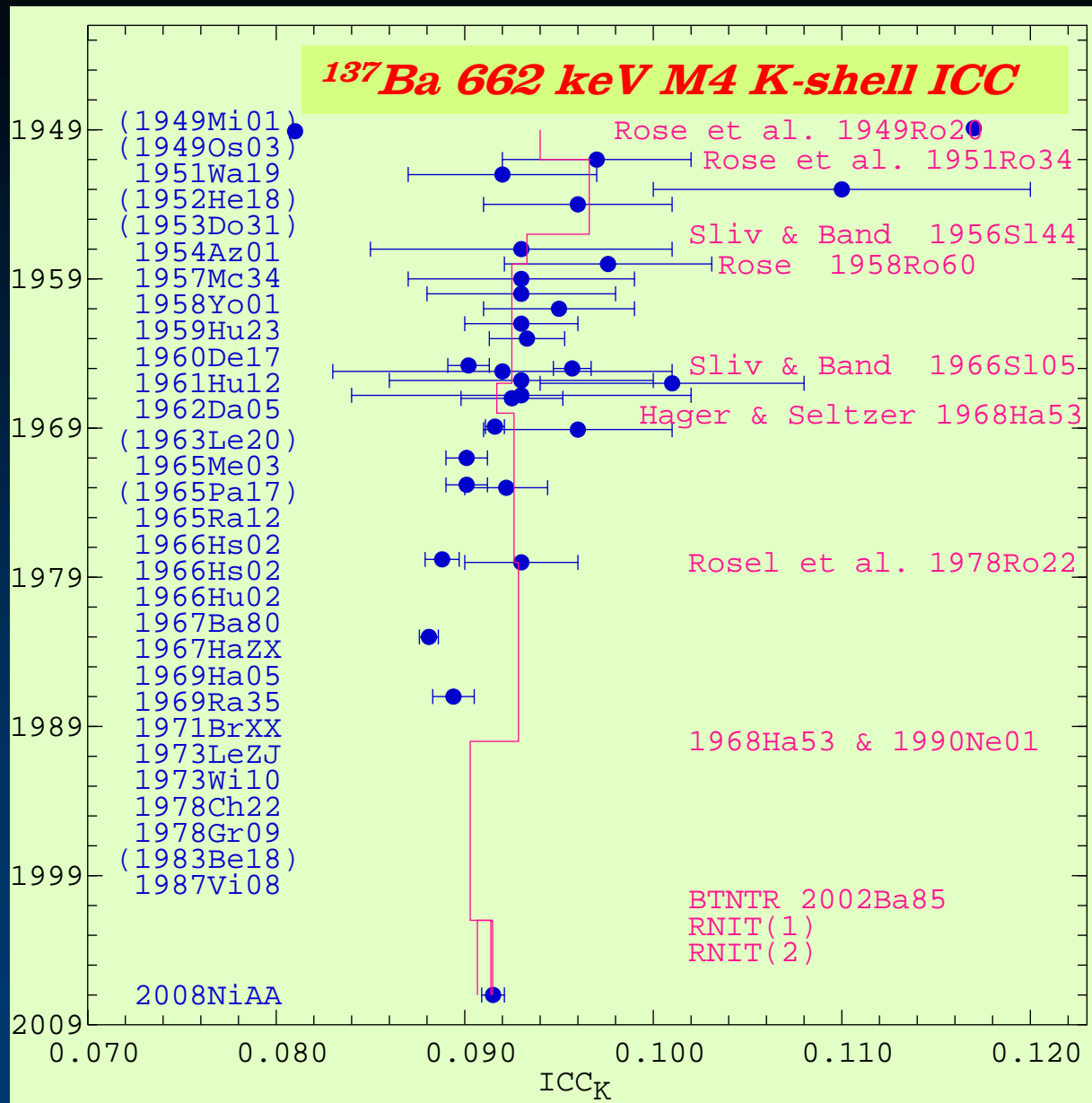
^{137}Ba 662 keV M4 K-shell ICC

α_K (experimental)

(31 data points)



Experiment vs. theory



Aim

- Assemble experimental ICC`s known better than 5% accuracy
- Determine accuracy of ICC calculations (HsIcc, RpIcc, BrIcc) by comparing experimental and theoretical values

General policies

- Primary data: $\Delta\alpha/\alpha \leq 15\%$; Adopted values: $\Delta\alpha/\alpha \leq 5\%$
- Use up-to date atomic and nuclear data to correct experimental ICC`s
- Multipolarity: E2, M3, E3, E4, M4, E5. Excluded: E1 (hindered) and M1 (mixed), M2 (mixed)
- ICCs considered: α_K , α_L , α_{Total} , α_K/α_L
- Energies (uncertainty), mixing ratio from adopted ENSDF data set
- Multipolarity must determined from other quantities
- When more than one measurement is known, three statistical methods used to identify discrepant data points and deduce weighted mean values and assign uncertainties



Adopted

DDEP (2006)

ICC_K = 0.0896(15)

ENSDF (2007)

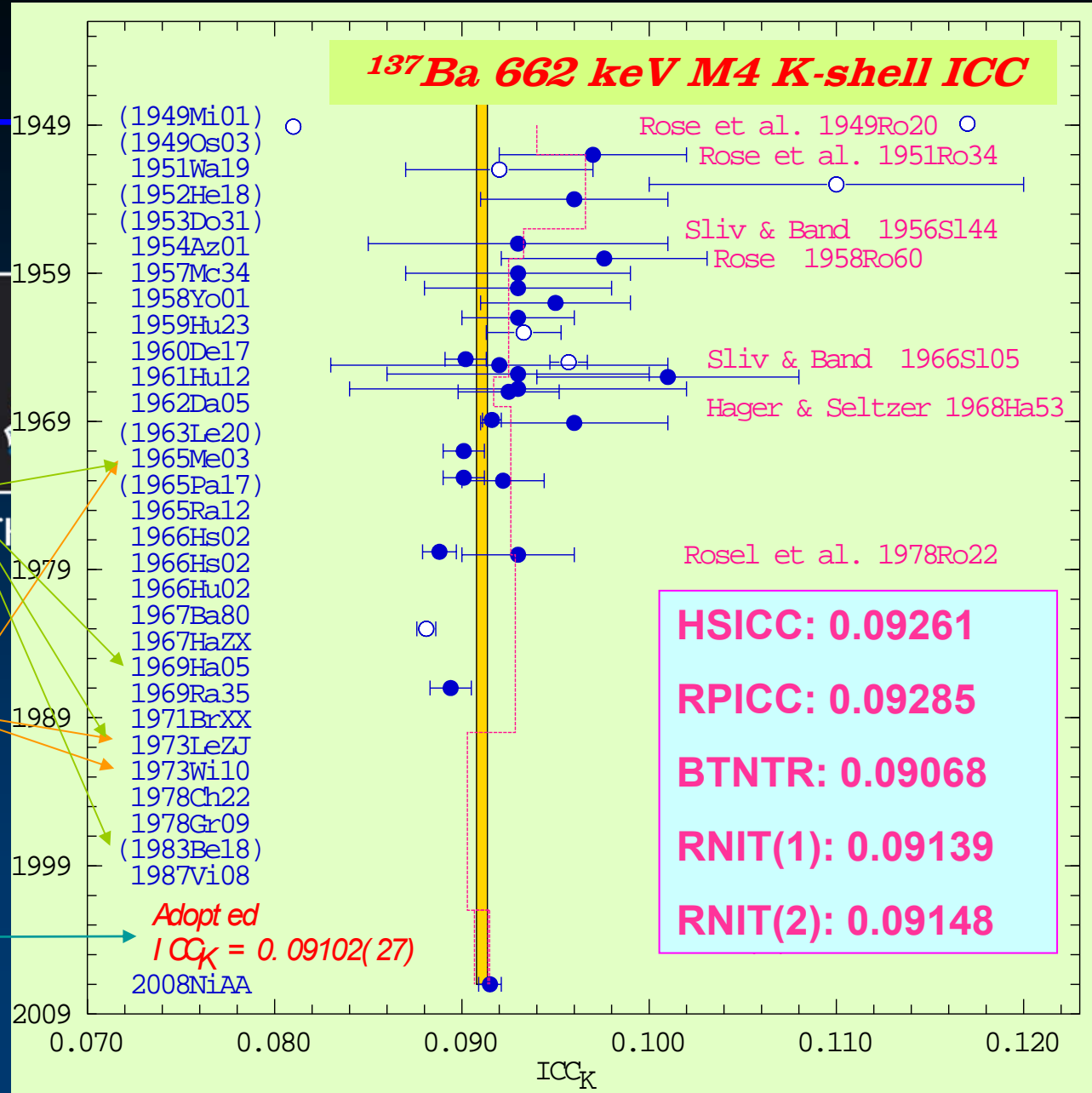
ICC_K = 0.0904(5)

LWM: 0.09102(27)

X²/(N-1)=0.94

NRM: 0.09102(27)

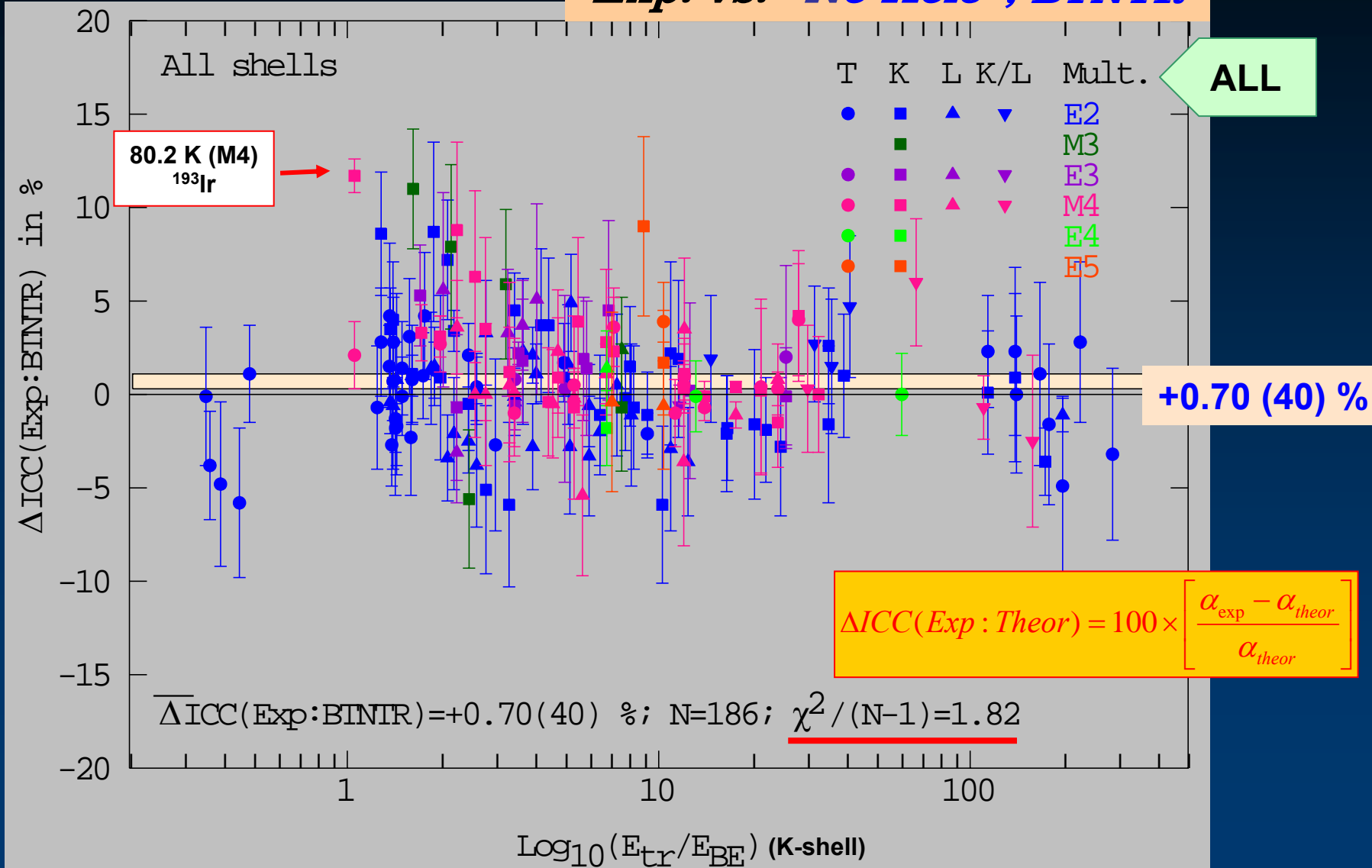
RT: 0.09110(28)





How good are the internal conversion coefficients now?

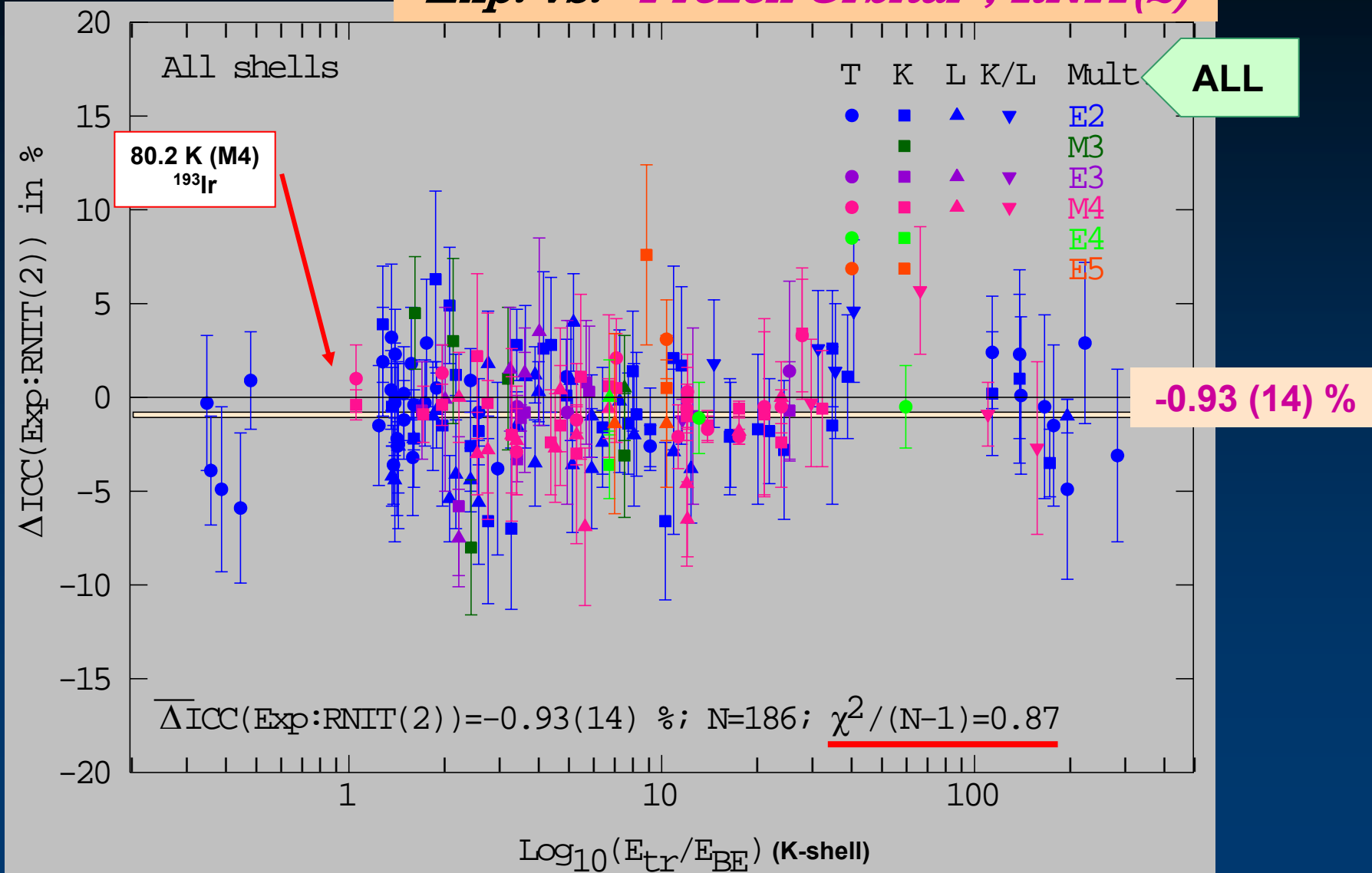
Exp. vs. "No Hole", BTNTR





How good are the internal conversion coefficients now?

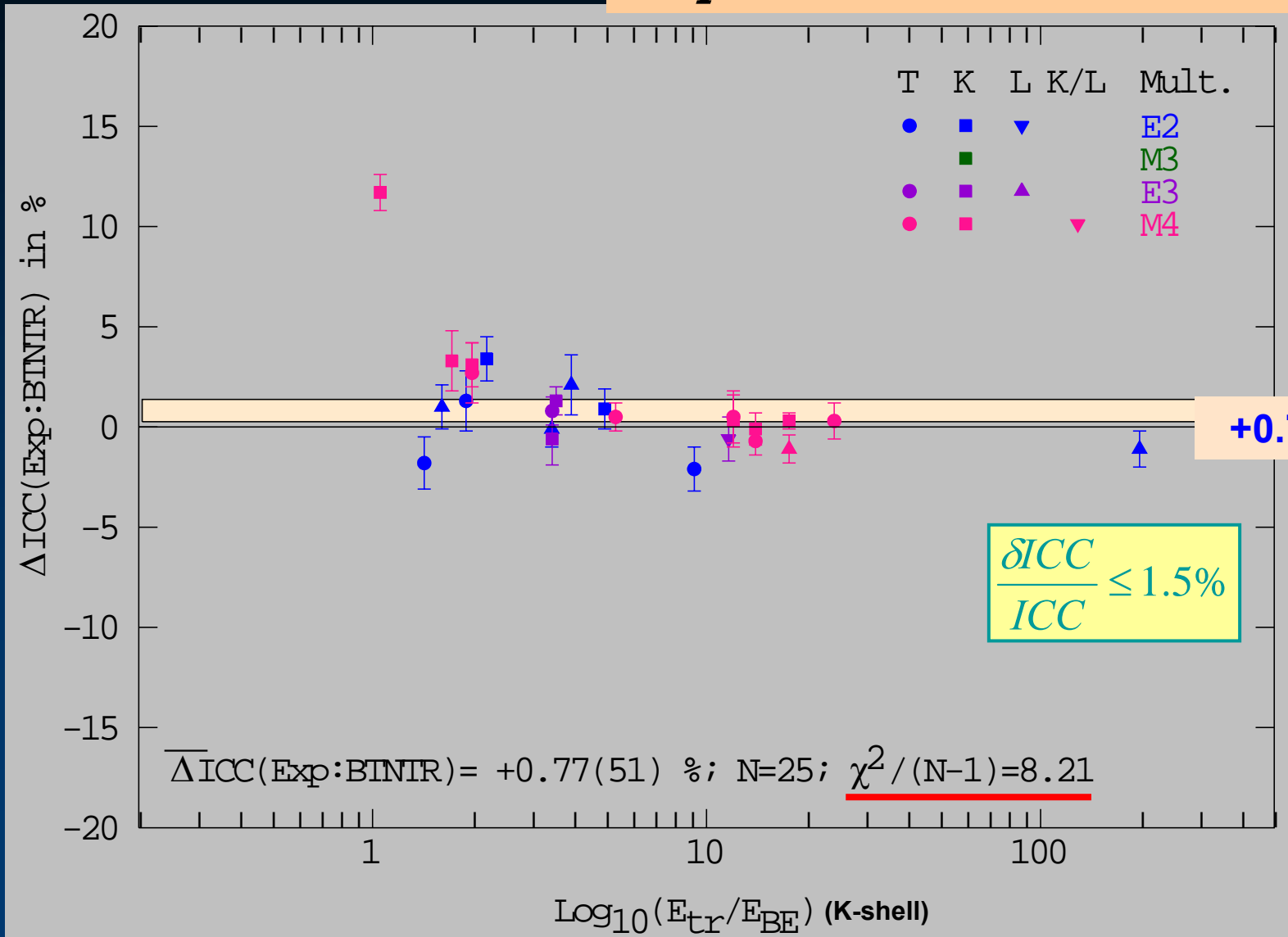
Exp. vs. "Frozen Orbital", RNIT(2)





How good are the internal conversion coefficients now?

Exp. vs. "No Hole", BTNTR



+0.77 (51) %

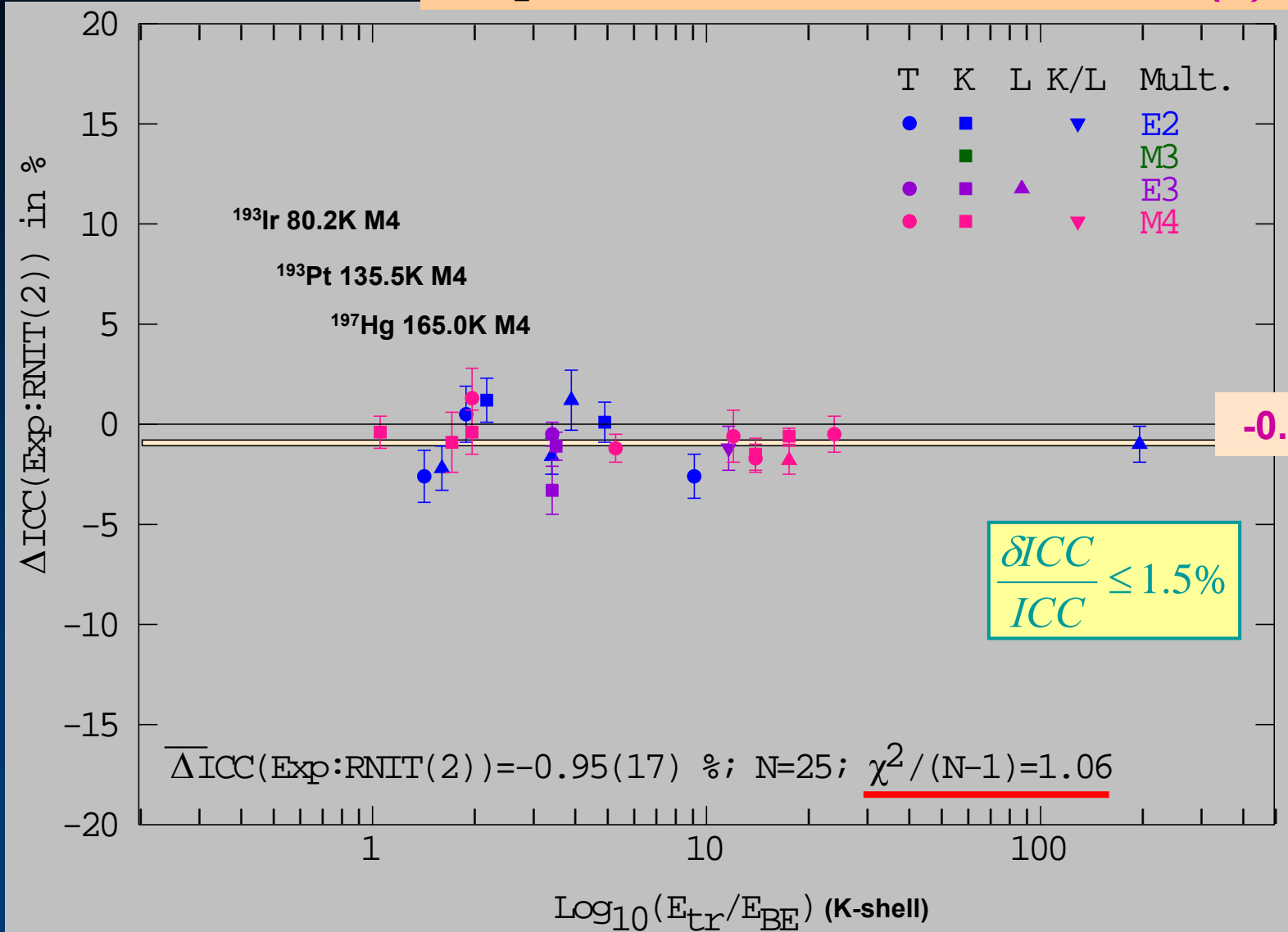
$\frac{\delta ICC}{ICC} \leq 1.5\%$

$\overline{\Delta ICC(\text{Exp:BTNTR})} = +0.77(51) \%$; $N=25$; $\chi^2/(N-1)=8.21$



How good are the internal conversion coefficients now?

Exp. vs. "Frozen Orbital", RNIT(2)



-0.95 (17) %

How good are the internal conversion coefficients now?

Favored

ML	Shell	N	"No Hole" BTNTR		"Self Consistent" RNIT(1)		"Frozen Orbital" RNIT(2)	
			$\Delta\text{ICC}(\text{Exp:Theor})$	$\chi^2/(\text{N}-1)$	$\Delta\text{ICC}(\text{Exp:Theor})$	$\chi^2/(\text{N}-1)$	$\Delta\text{ICC}(\text{Exp:Theor})$	$\chi^2/(\text{N}-1)$
All	All	186	+0.70(40)	1.82	-0.61(14)	1.01	-0.93(14)	0.87
Tot	All	54	+0.32(25)	0.79	-0.55(24)	0.76	-0.71(24)	0.73
K	All	72	+1.50(120)	3.14	-0.18(21)	1.09	-0.72(21)	0.80
K/L	All	46	+0.00(31)	0.83	-1.64(31)	0.96	-1.94(30)	1.02
E2	All	103	+0.21(23)	1.01	-0.77(23)	0.89	-0.93(23)	0.90
M4	All	50	+0.98(68)	3.87	-0.51(20)	1.29	-0.93(20)	0.72
ICCs known better than 1.5% rel. unc.								
All	All	25	+0.77(51)	8.21	-0.56(26)	2.12	-0.95(17)	1.06

Underestimate experiment

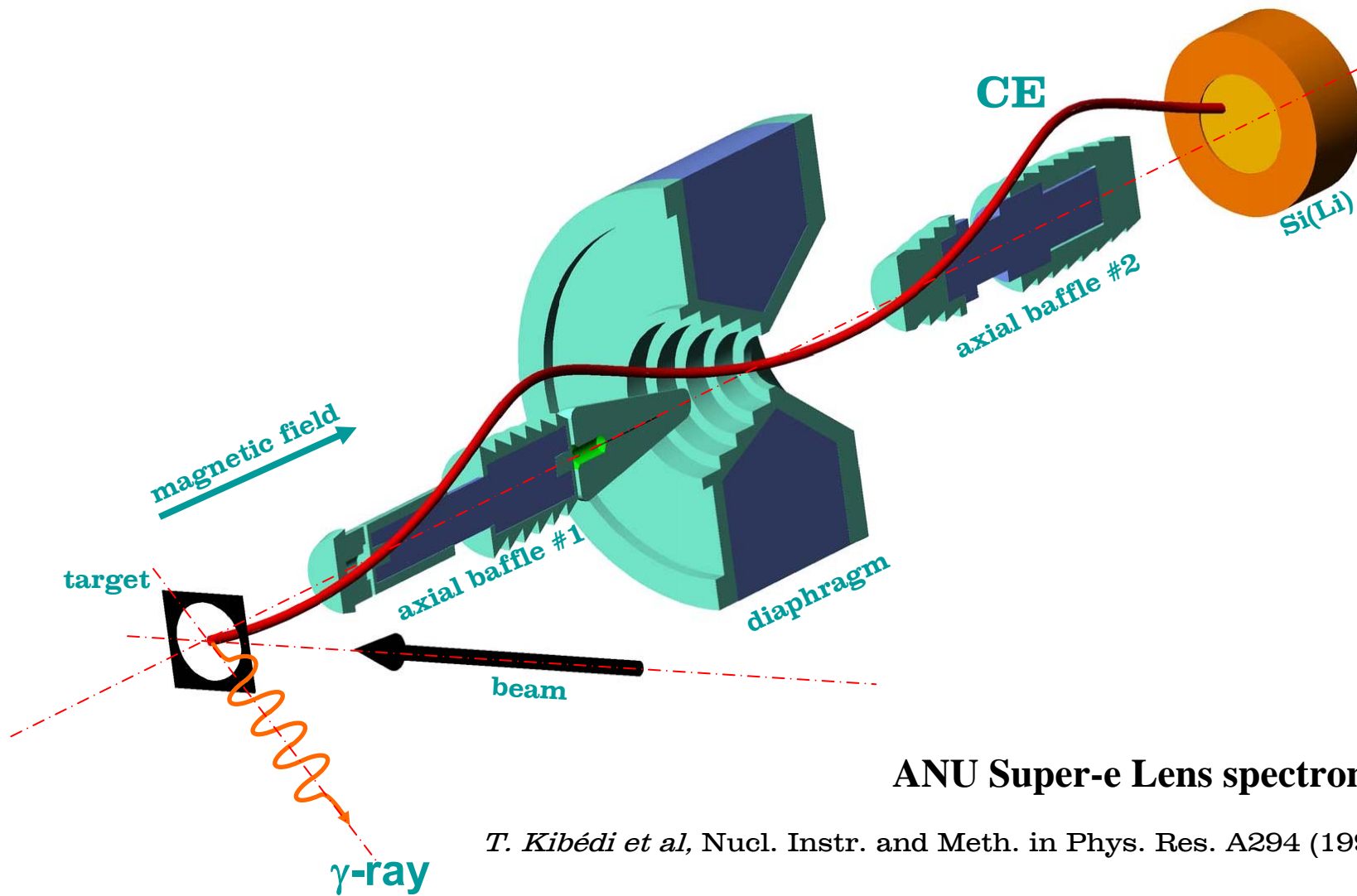
Overestimate experiment

Data Table	Reference	Z	Shells/IPF	L	TranEner [keV]
<i>Internal Conversion Coefficient (ICC)</i>					
BrIccFO	'Frozen Orbitals' approximation	5–110	All shells	1–5	$\epsilon_{ic} + 1 - 6000$
BrIccNH	'No Hole' approximation	5–110	All shells	1–5	$\epsilon_{ic} + 1 - 6000$
<i>Pair Conversion Coefficient (PCC)</i>					
ScPcc	1979Sc31	0–100	IPF	1–3	1100–8000
HoPcc	1996Ho21	50–100	IPF	1–3	1100–8000
<i>Electronic factor $\Omega(E0)$</i>					
HsOmg	1969Ha61	30–42	K, L ₁ , L ₂	0	$\epsilon_{ic} + 6 - 1500$
BeOmg	1970Be87	40–102	K	0	51–2555
		40–102	L ₁ , L ₂	0	51–2555
PaOmg	1986PaZM	8–40	K	0	511–12775
		8–40	IPF	0	1431–12775



In-beam Conversion Electron Spectroscopy

With G.D. Dracoulis (ANU)

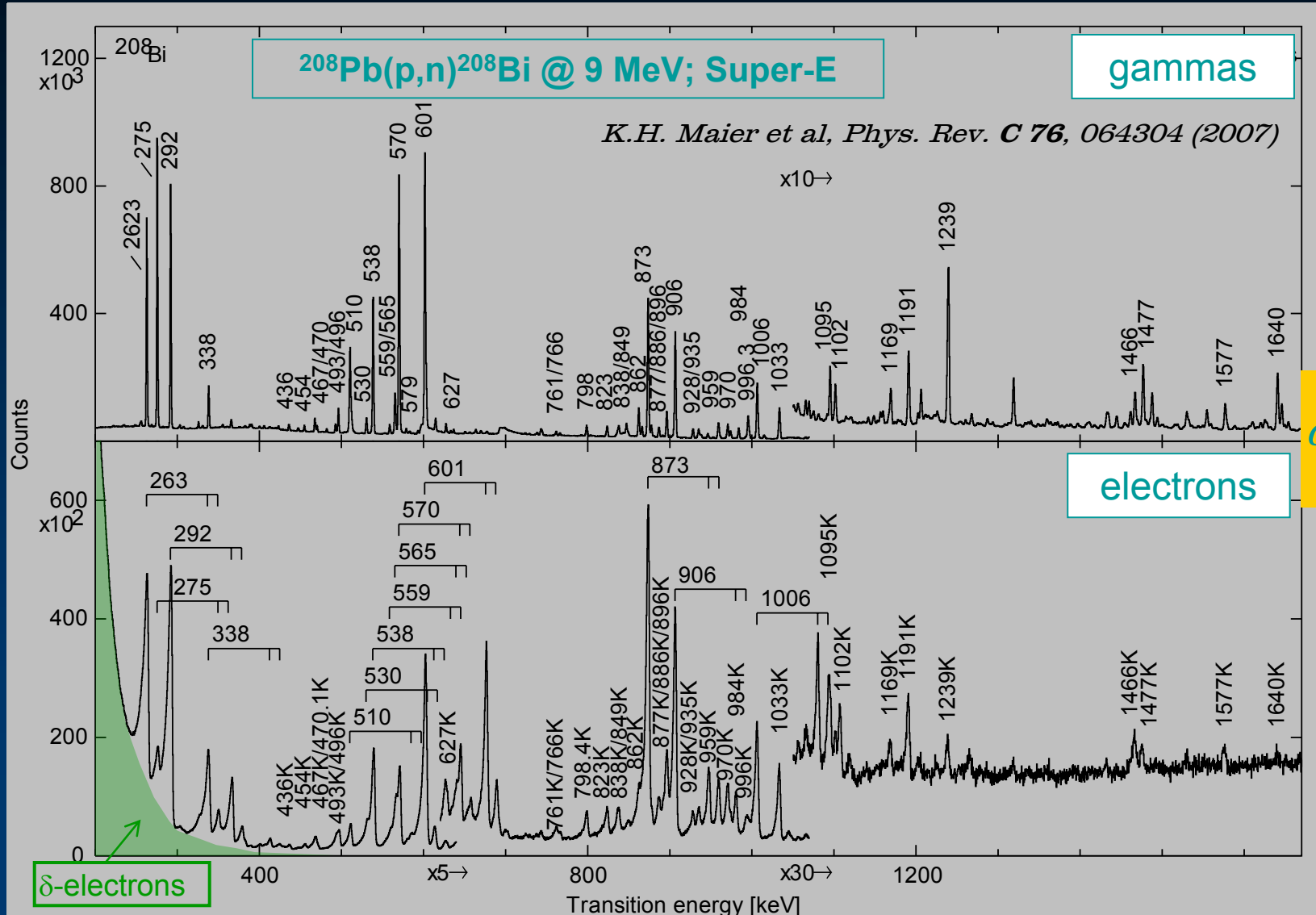


ANU Super-e Lens spectrometer

T. Kibédi et al, Nucl. Instr. and Meth. in Phys. Res. A294 (1990) 523



Conversion Electron Spectroscopy of ^{208}Bi

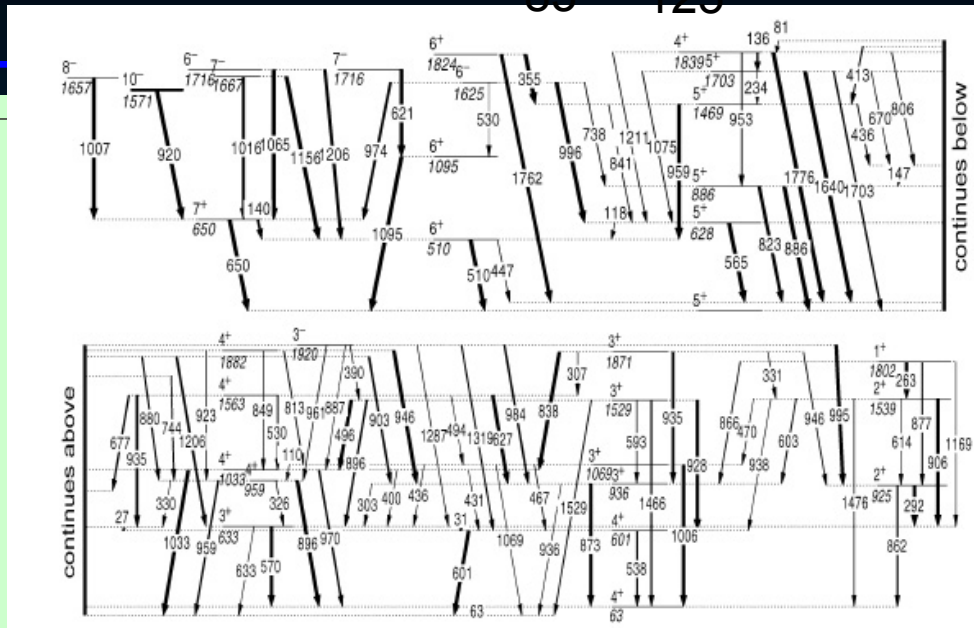
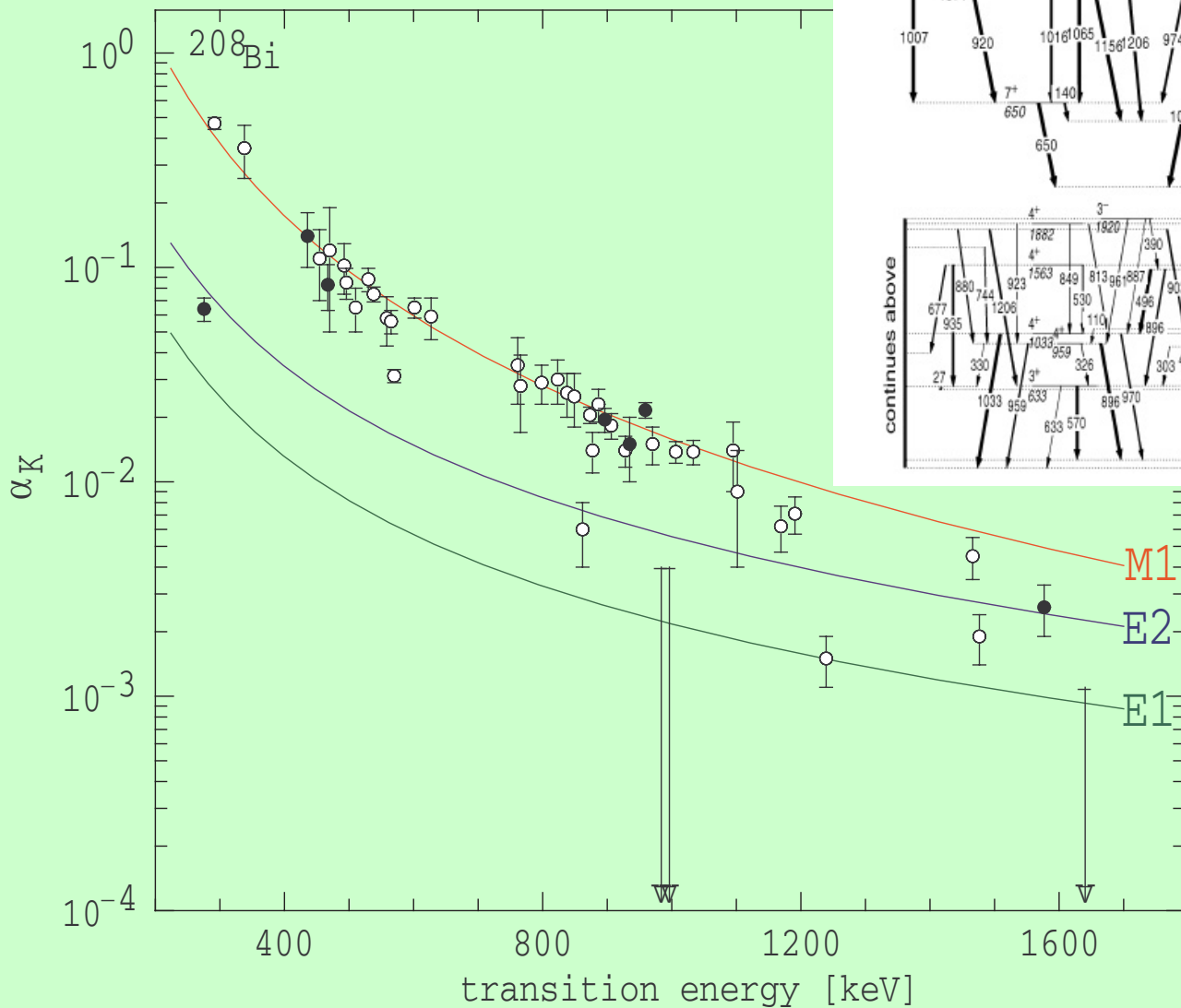


$$\alpha = \frac{I_{\text{electron}}}{I_{\text{gamma}}}$$



Conversion Electron Spectroscopy of ^{208}Bi

83 125



*K.H. Maier et al,
Phys. Rev. C 76, 064304 (2007)*

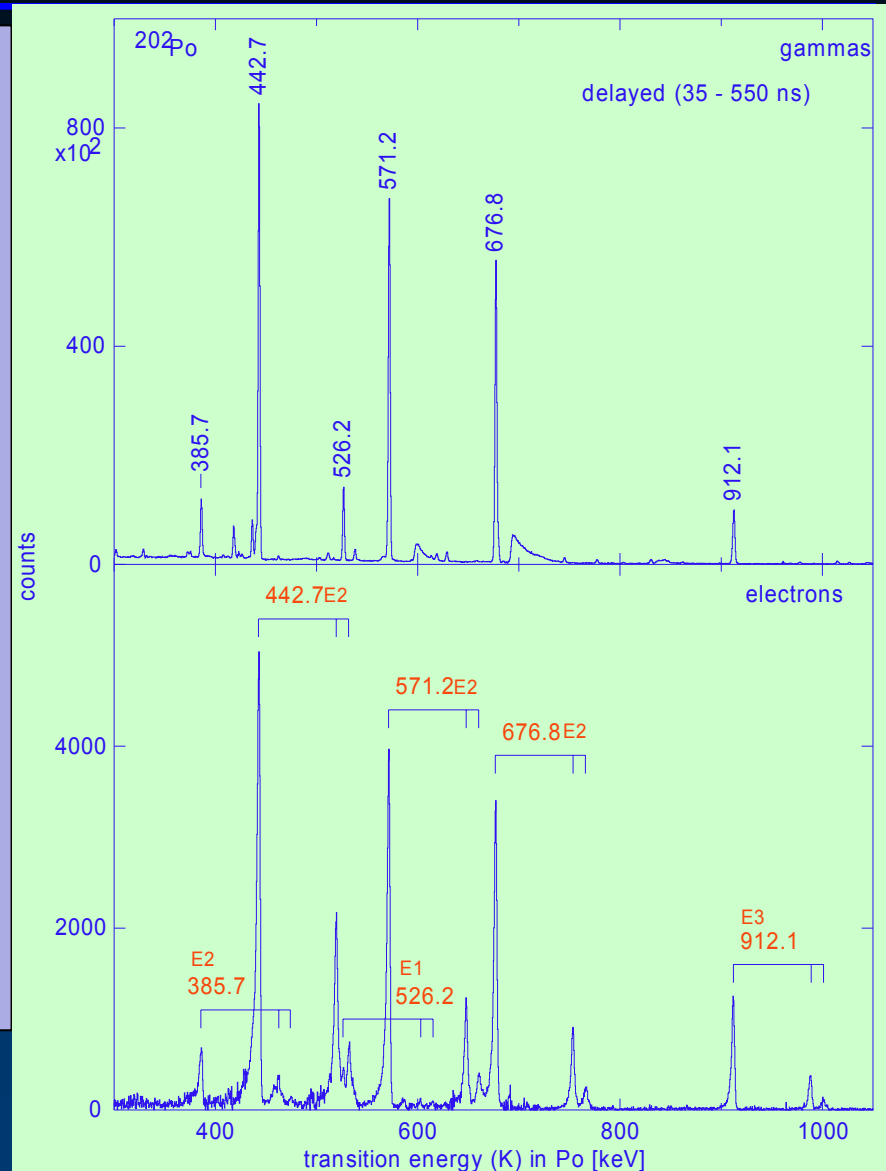
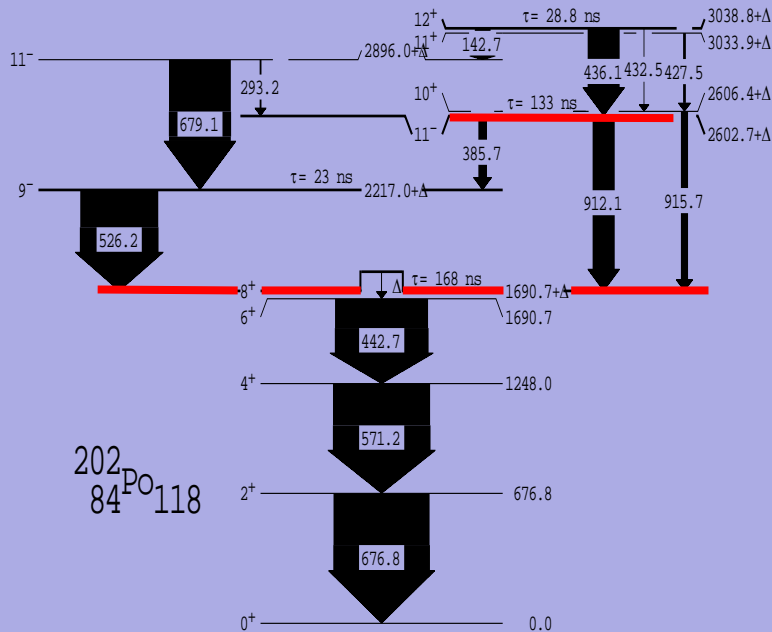


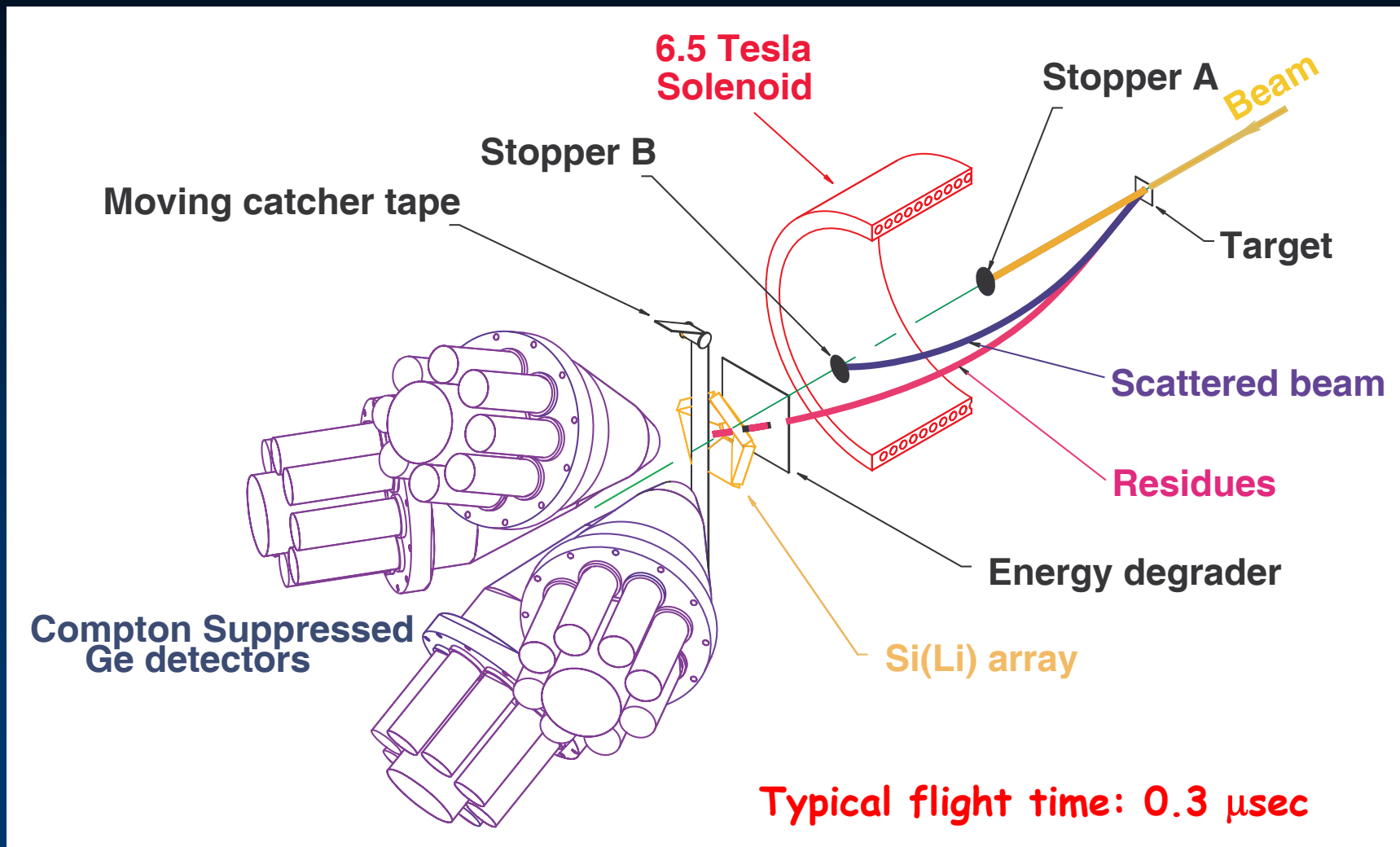
Conversion Electron Spectroscopy of ^{202}Po

83 125

$^{194}\text{Pt}(^{12}\text{C},4n)^{202}\text{Po}$ @ 76 MeV

Pulsed beams (~1 ns) with 1.7 μs separation





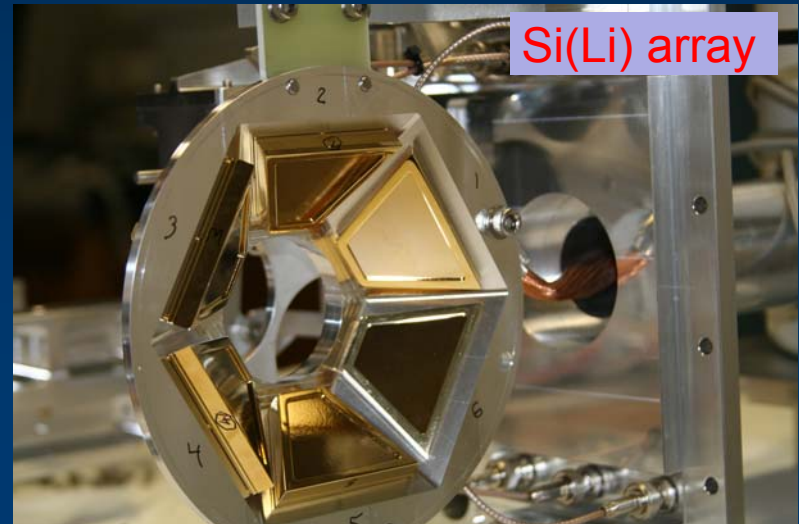
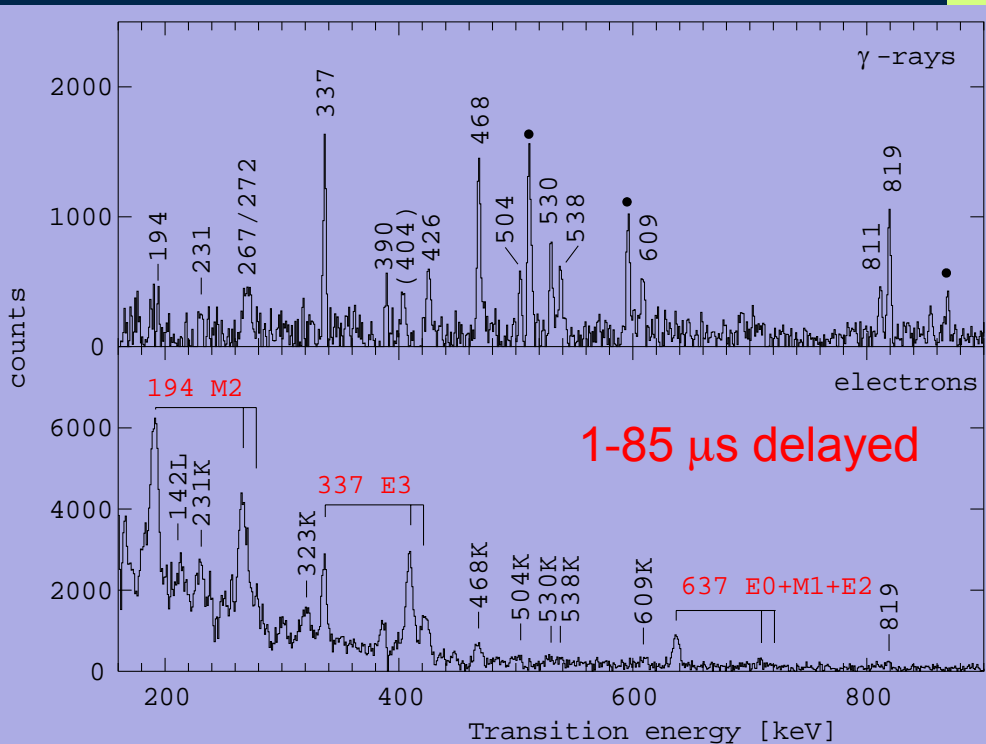
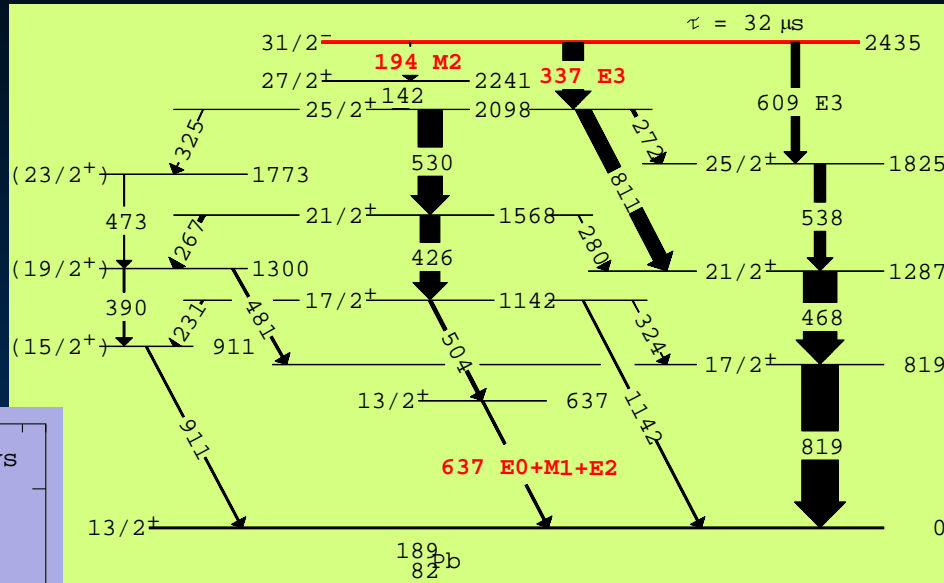
Characterization of the 32 μ s isomer in ^{189}Pb

G.D. Dracoulis, et al., Phys. Rev. C 79, 031302(R) (2009)

$^{164}\text{Er}(^{29}\text{Si},4n)^{189}\text{Pb}$ @145 MeV

Pulsed beam 33 μ s / 170 μ s

700 $\mu\text{g}/\text{cm}^2$ target, $E_{\text{recoils}} \sim 20$ MeV



- Theoretical ICC`s (BrIcc) agree with experiments at ~1% level
- Extend atomic number range beyond Z=110. Requires "*Atomic masses of the most abundant isotope*", atomic binding energies and valence shell electron configurations.
- $\Omega(E0)$ electronic factors for all atomic numbers, shells and energies
$$W_{CE}(E0) + W_{\pi}(E0) = \rho^2(E0) \times [\Omega_{CE}(E0) + \Omega_{\pi}(E0)]$$
- *Treatment of E0 and mixed M1+E2+E0 transitions (ENSDF)*
- Evaluation of energies and intensities of X-ray and Auger electron radiations
- Conversion coefficients for ionized atoms
- Conversion coefficients near electron shell binding energies (<1 keV)

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