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BrIcc – recent developments in theoretical conversion coefficients

T. Kibédi (ANU)

Outline

BrIcc status

Conversion coefficients for superheavy elements

Electronic factors for E0 transitions

Collaborators

M.B. Trzhaskovskaya (Petersburg Nuclear Physics Institute, Russia)

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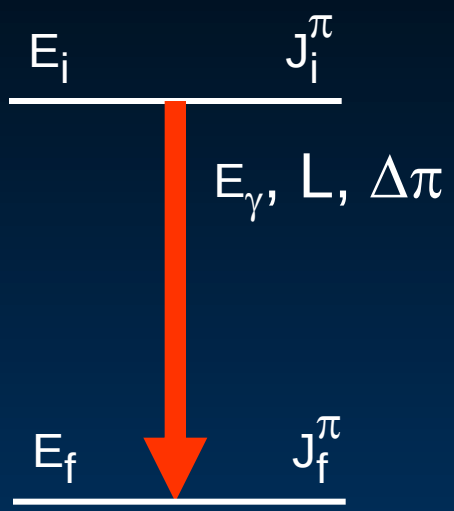
A.E. Stuchbery and D. Tsifakis (ANU)

Electromagnetic Decay and Nuclear Structure



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

	$\lvert J_i - J_f\rvert \le L \le J_i + J_f$; $L \neq 0$		$J_i = J_f$
$\Delta\pi$ = no;	E2, E4, E6	M1, M3, M5	E0
$\Delta\pi$ = yes;	E1, E3, E5	M2, M4, M6	

Multipolarity known

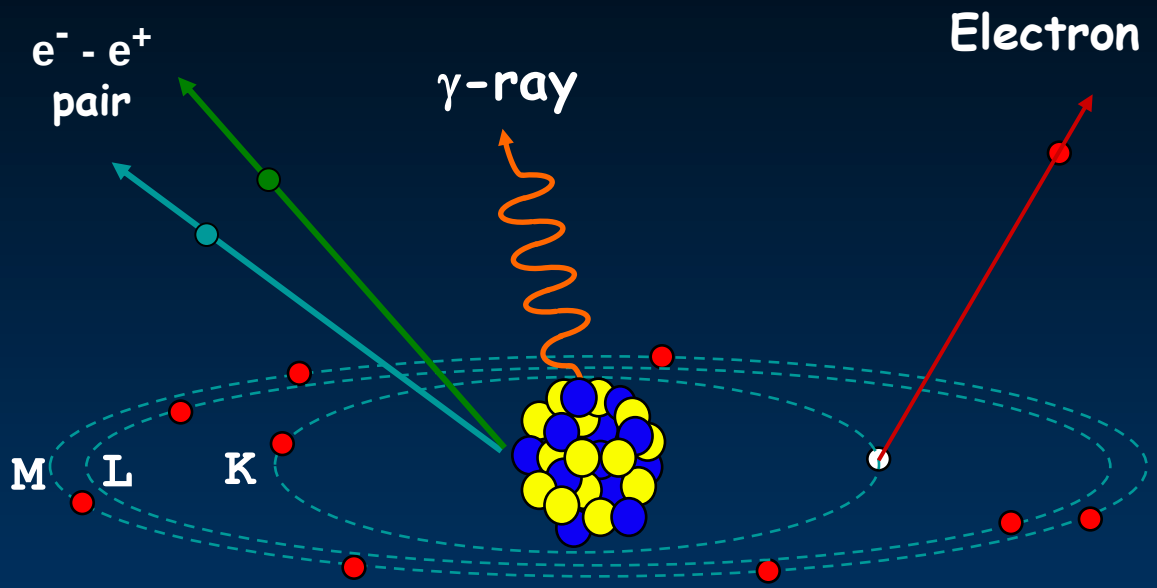
ΔJ may not be unique

unique Δπ

Mixed multipolarity

$$\delta^2(\pi`L`) = I_\gamma(\pi`L`) / I_\gamma(\pi L)$$

Basic concept



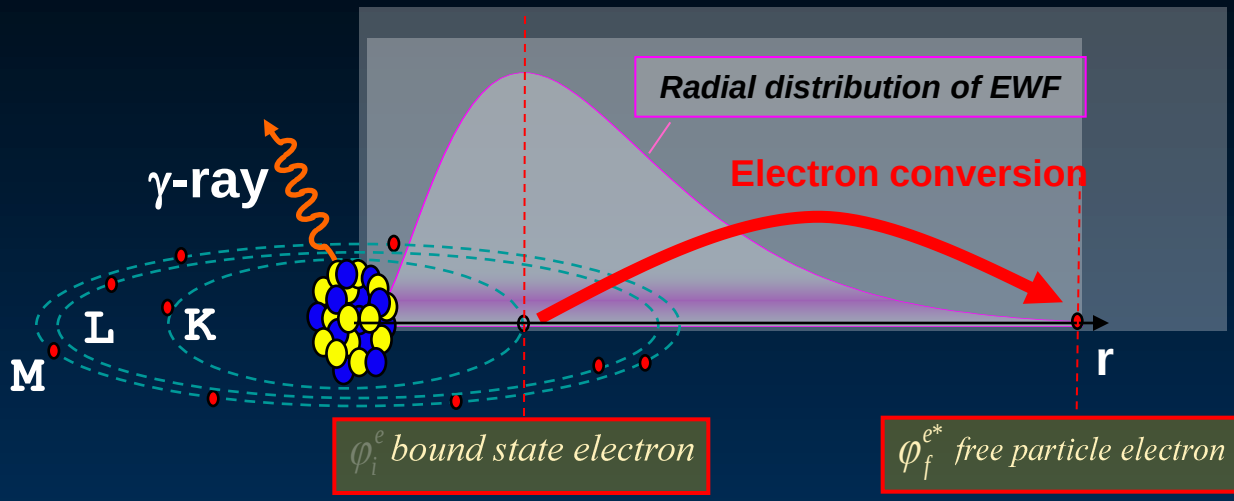
Transition probability

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

Conversion Coefficient

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

Conversion electron process and electromagnetic interaction



Fermi's golden rule

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

Density of the final electron state (continuum)

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

Nuclear

Electron

Multipolar source

Same for γ and CE

ICC calculations – Atomic field model

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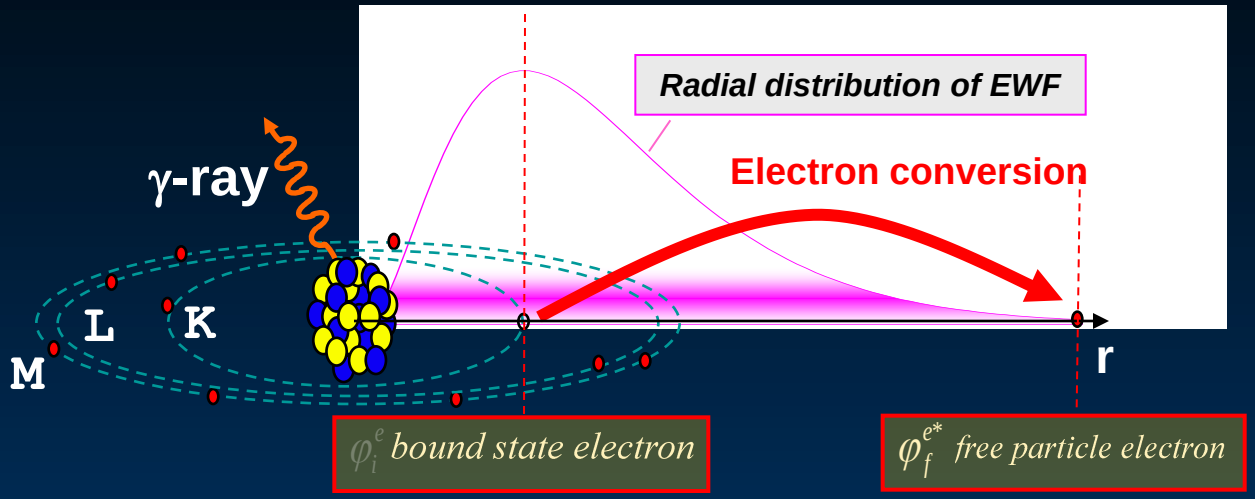
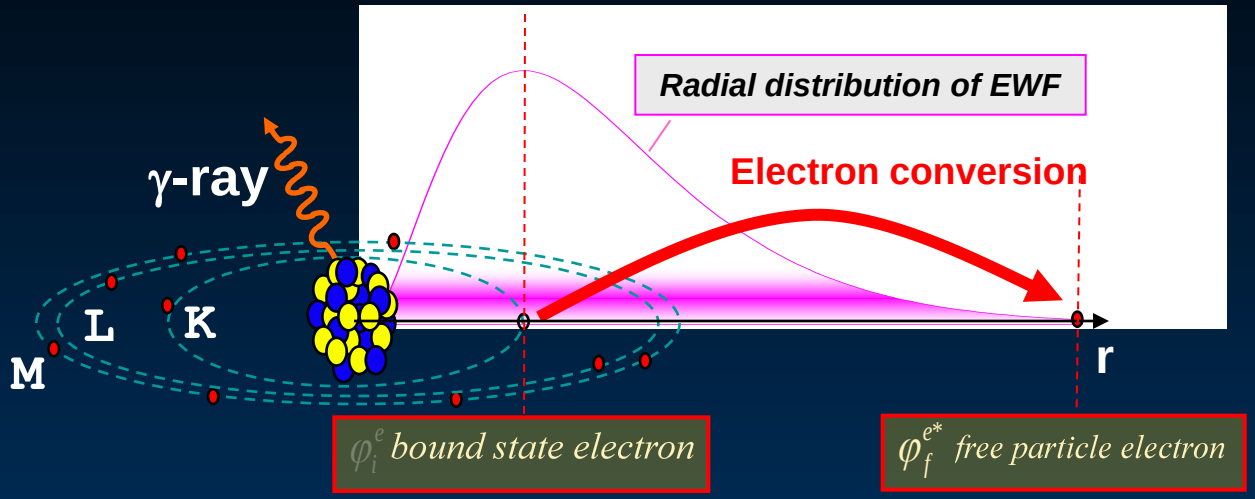
Band et al., ADNDT 81 (2002) 1



- 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

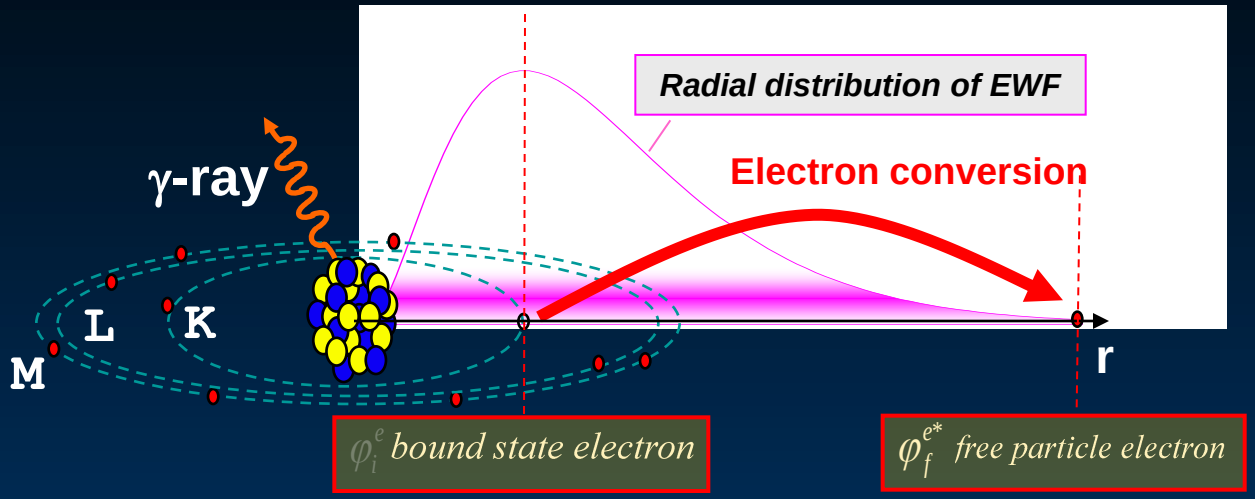
ICC calculations – Nuclear model

Band et al., ADNDT 81 (2002) 1



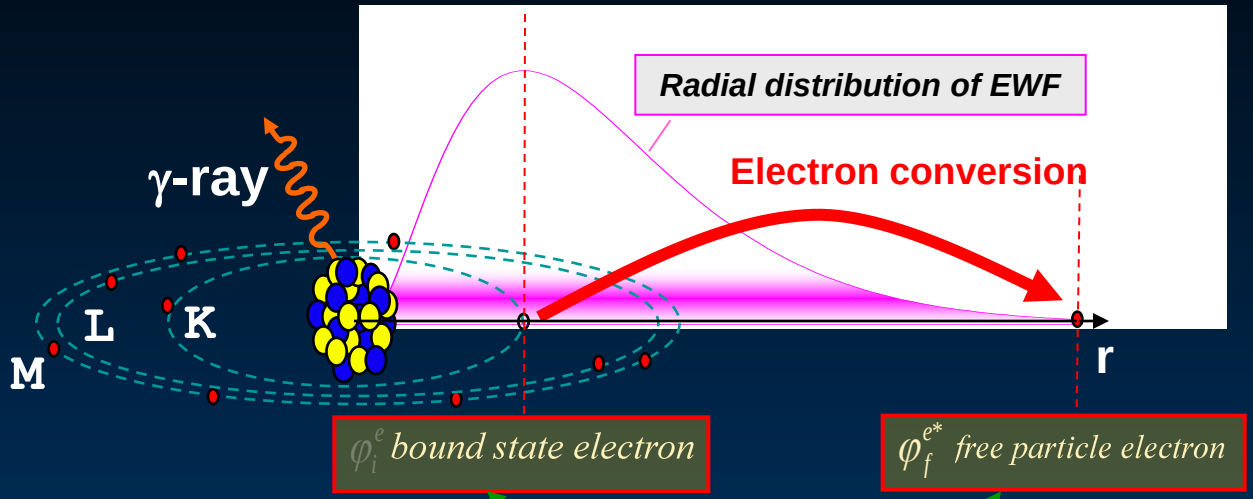
- Finite nuclear size
- Dynamic (penetration) effects incorporated using the Surface Current model
- Spherically symmetric nucleus; most abundant isotope

ICC calculations – Higher order effects



- 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



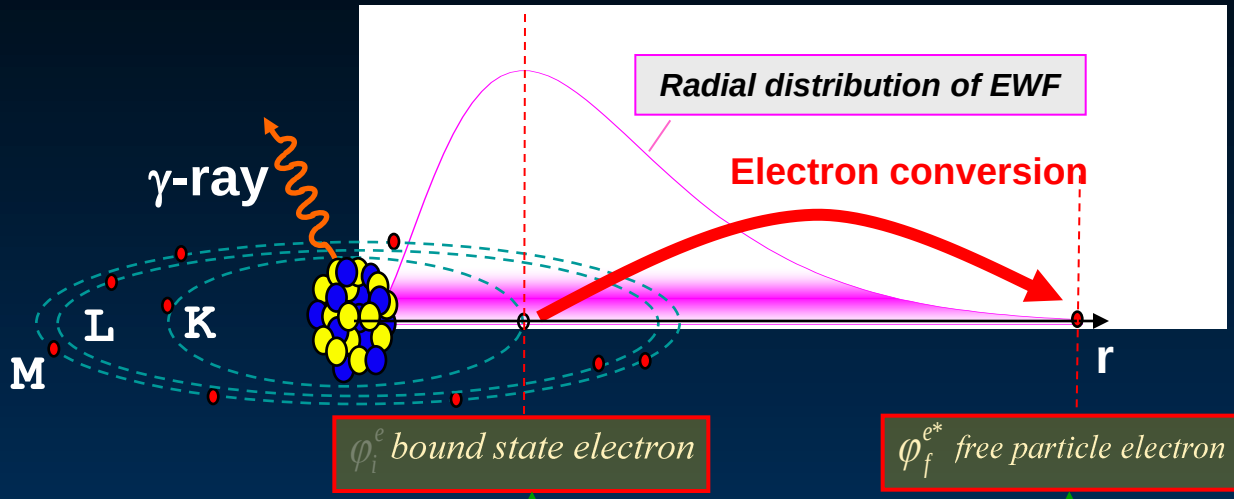
"No Hole" - BTNTR: SCF of a neutral atom

Vacancy disregarded

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

BrIccNH table - extended and revised calculations

ICC calculations – Atomic vacancies



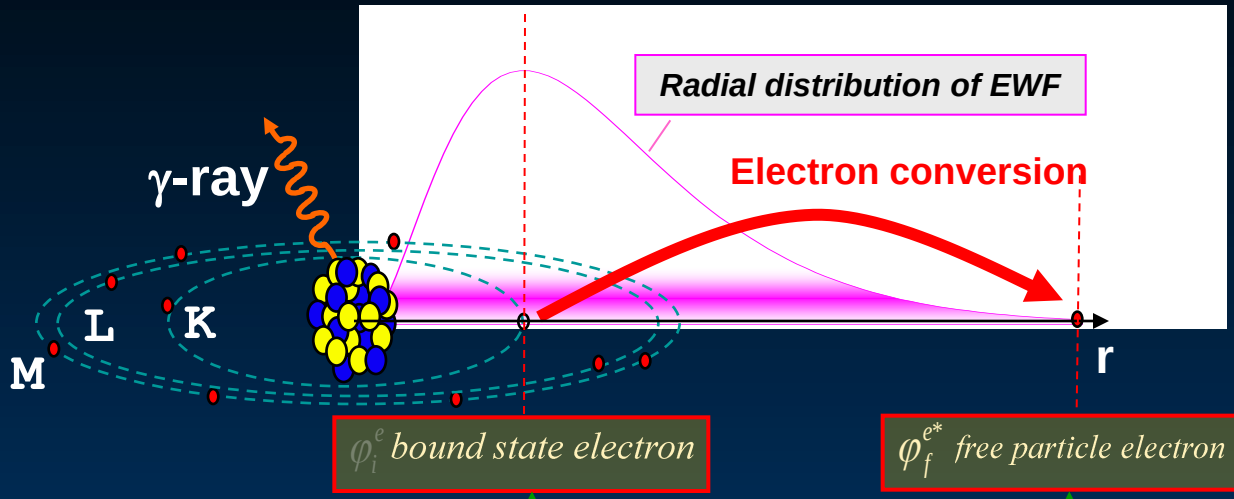
SCF of a neutral atom SCF of an ion

"Self Consistent" – RNIT(1)

Vacancy incorporated

No data table

ICC calculations – Atomic vacancies



SCF of a neutral atom

Constructed from the WF of a neutral atom, not SCF

"Frozen Orbitals" – RNIT(2)

Vacancy incorporated

BrIccFO data table

Kibedi et al., Nucl. Instr. and Meth. A 589 (2008) 202

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Which atomic model to choose

ML	Shell	N	"No Hole" BTNTR		*"Self Consistent" RNIT(1)*		"Frozen Orbital" RNIT(2)	
				$\chi^2/(N-1)$		$\chi^2/(N-1)$		$\chi^2/(N-1)$
All	All	229	+0.70*(40)*	1.82	**-0.61*(14)***	1.01	−0.93(14)	0.87
Tot	All	63	+0.32(25)	0.79	−0.55(24)	0.76	−0.71(24)	0.73
K	All	91	+1.50(120)	3.14	−0.18(21)	1.09	−0.72(21)	0.80
K/L	All	56	+0.00(31)	0.83	−1.64(31)	0.96	−1.94(30)	1.02
E2	All	115	+0.21(23)	1.01	−0.77(23)	0.89	−0.93(23)	0.90
M4	All	49	+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

BrIcc computer program

- General tool to obtain
  - electron conversion coefficients: α_i; i=K, L1, L2, …R2 shells; L=1-5
  - electron-positron pair conversion coefficients: L=1-3
  - E0 electronic factors: Ω_i (K,L1,L2) and Ω_π
- ENSDF evaluation tool to calculate:
  - $\alpha_i \pm \Delta\alpha_i$ for the GAMMA records for a given Z, E_γ and for pure or mixed multipolarities.
  - Correct treatment of Uncertainties in E and MR; symmetric, asymmetric or limits
  - GAMMA & GAMMA continuation records scanned for E, DE, M, MR, DMR, RI, DRI, TI & DTI, CC, DCC
  - Calculation report
  - New G cards with CC and DCC values
  - New S_G cards for other applications
  - MERGE option to combine new cards with ENSDF file, old records removed

BrIccFO(Default) and BrIccNH data tables

Data Table	Reference	Z	Shells/IPF	L	TranEner [keV][a]
Internal Conversion Coefficient (ICC)					
BrIccFO	2008Ki07 - based on the model using the *'Frozen Orbitals'* approximation of 2002Ba85	5–110	All shells	1–5	ε_{ic}+1–6000
BrIccNH	2008Ki07 - based on the model using the *'No Hole'* approximation of 2002Ba85	5–110	All shells	1–5	ε_{ic}+1–6000
Pair Conversion Coefficient (PCC)					
ScPcc	1979Sc31	0–100[b]	IPF	1–3	1100–8000
HoPcc	1996Ho21	50–100	IPF	1–3	1100–8000
Electronic factor Ω(E0)[c]					
HsOmg	1969Ha61	30–42	K[d],L_1[e],L_2[f]	0	ε_{ic}+6–1500
BeOmg	1970Be87	40–102	K	0	51[f]–2555
		40–102	L_1,L_2	0	51–2555
PaOmg	1986PaZM	8–40	K[e]	0	511–12775
		8–40	IPF	0	1431–12775

[a] ε_{ic} is the binding energy for the ic-shell
[b] Used for Z < 50
[c] Electronic factors are only calculated for even Z values at present
[d] Not used
[e] Used for Z < 40
[f] For Z=40–58: 51.1 keV; for Z=60–82: 102.2 keV; for Z=84–96: 153.3 keV and for Z=98–102: 204.4 keV

BrIcc – Recent developments

Version	Date	
0.0	15-Nov-2003	Project initiated at the NSDD coordination meeting (Vienna)
1.0	6-Apr-2004	Tabulations using the *'No Hole'* approximation completed for ε_{ic}+1–6000 keV energies and Z=10–95 atomic numbers.
1.3	20-Dec-2004	BrIcc relesed for ENSDF evaluators.
	6-Jun-2005	NSDD coordination meeting (McMaster) adopted the *'Frozen Orbitals'* approximation.
2.0	1-Sep-2005	Tabulations using the *'Frozen Orbitals'* approximation completed. BrIcc program logic, exception and error handling improved.
2.1	1-Oct-2005	BrIccS (*'slave'*) version developed and the new ANU web interface created.
2.0a	19-Dec-2005	Corrected a bug in the BrIcc *MERGE* operation.
2.0b	12-Jan-2006	Corrected a bug in the BrIcc *MERGE* operation.
2.1	28-Feb-2007	User selectable data tables, including *BrIccFO*, *BrIccNH*, *HsIcc* and *RpIcc* were added to the ANU web interface.
2.2	4-Jan-2008	The *BrIccFO* and the *BrIccNH* data tables have been recalculated for several chemical elements and the range of the tables have been extended for Z=5–110.
2.2a	13-Jul-2008	The lowest tabulated point in the *BrIccFO* and the *BrIccNH* data tables for Z=88, 98, 100, 101 and 102 K-shell was 2 keV above the binding energies.
	27-Nov-2008	Minor bug in the Slave version fixed. For pure and mixed ICC`s and for transition energy within 1 keV to the binding energy incorrect XML code was returned.
2.2b	20-Jan-2009	For Z=34 incorrect Ω_{IPF}(E0) values were used for the PaOmg data table.

BrIcc (v2.3) – Current programs

- Intel Fortran compiler on Windows, Linux, Mac
- Improvements in the code, fixed several bugs
- 32/64 bit
- **BrIcc** – ENSDF evaluation tool / desktop application to obtain ICC`s
- **BrIccS** – slave program to be used from other programs (DDEP, Web)
- **BrIccG** – to chart ICC values vs. transition energy
- **BrIccMixing** – to deduce mixing ratio from CE data
- **BrIccEmis** – under development

BrIcc (v2.3) evaluation tool – new features

If no MR is given use NEW DEFAULT values of

MR=1 for E2/M1 and E3/M2

MR=0.1 for M2/E1, M3/E2, E4/M3, M5/E4, M4/E3 and E5/M4

MRE0E2=EK(E0)/EK(E2) experimental E0/E2 mixing ratio

BrIcc will read from Continuation G records

If CC > 0.0001 total ICC will be put on G record (56-64)

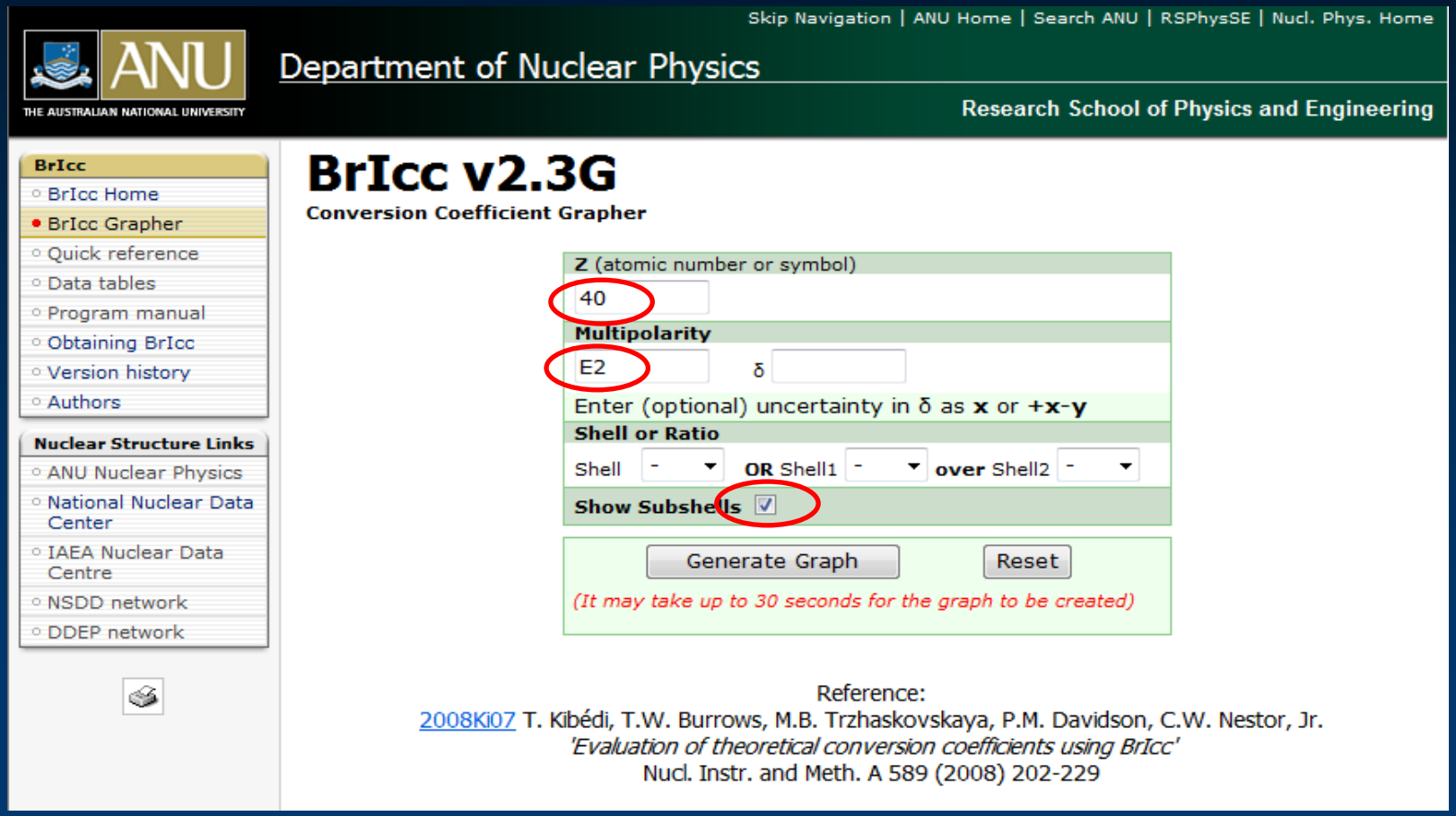
Otherwise CC will be put on the S_G record

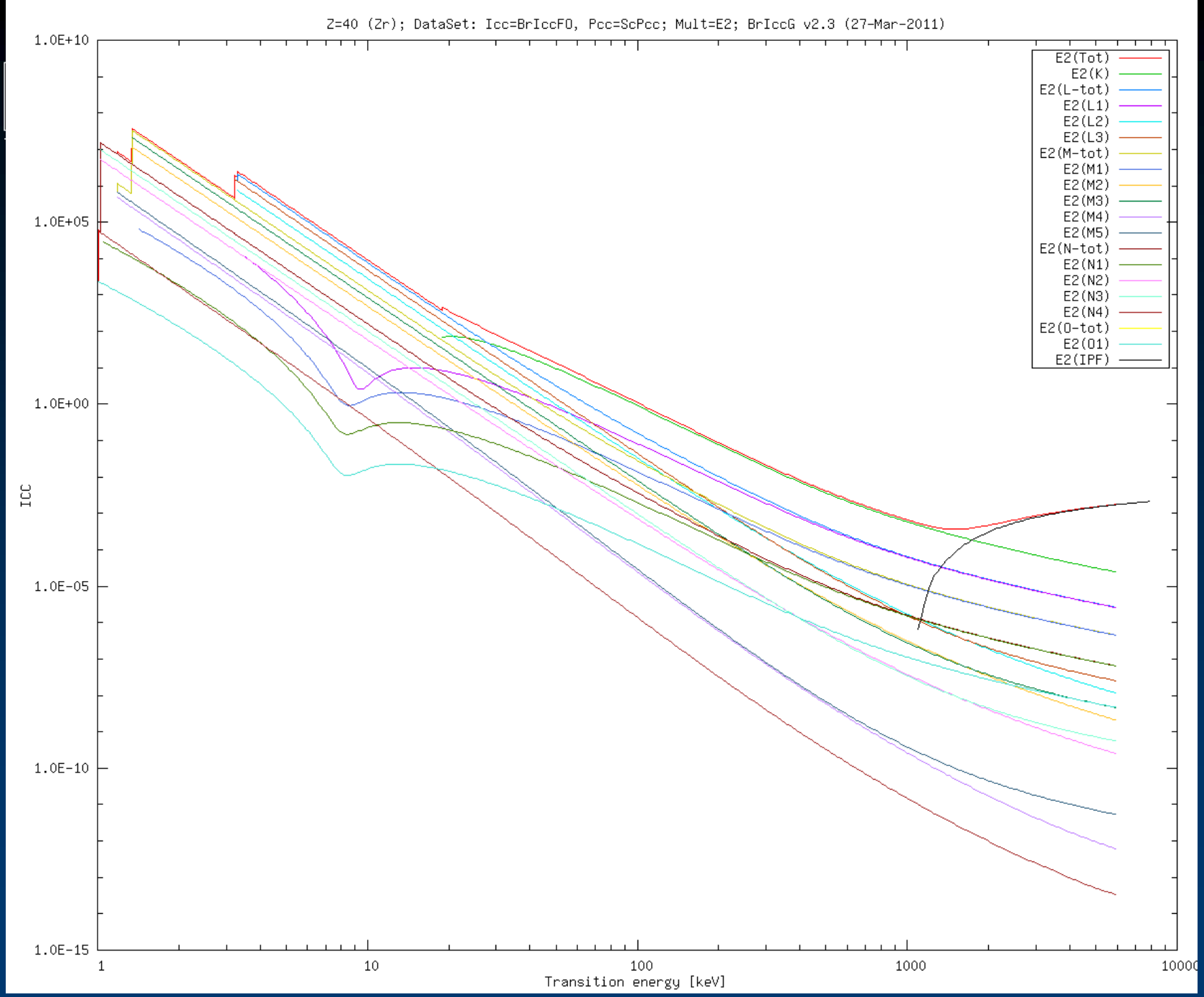
NEW: Let user select cut-off value of CC

BrIccG (v2.3) on the web: Calculator & Grapher

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

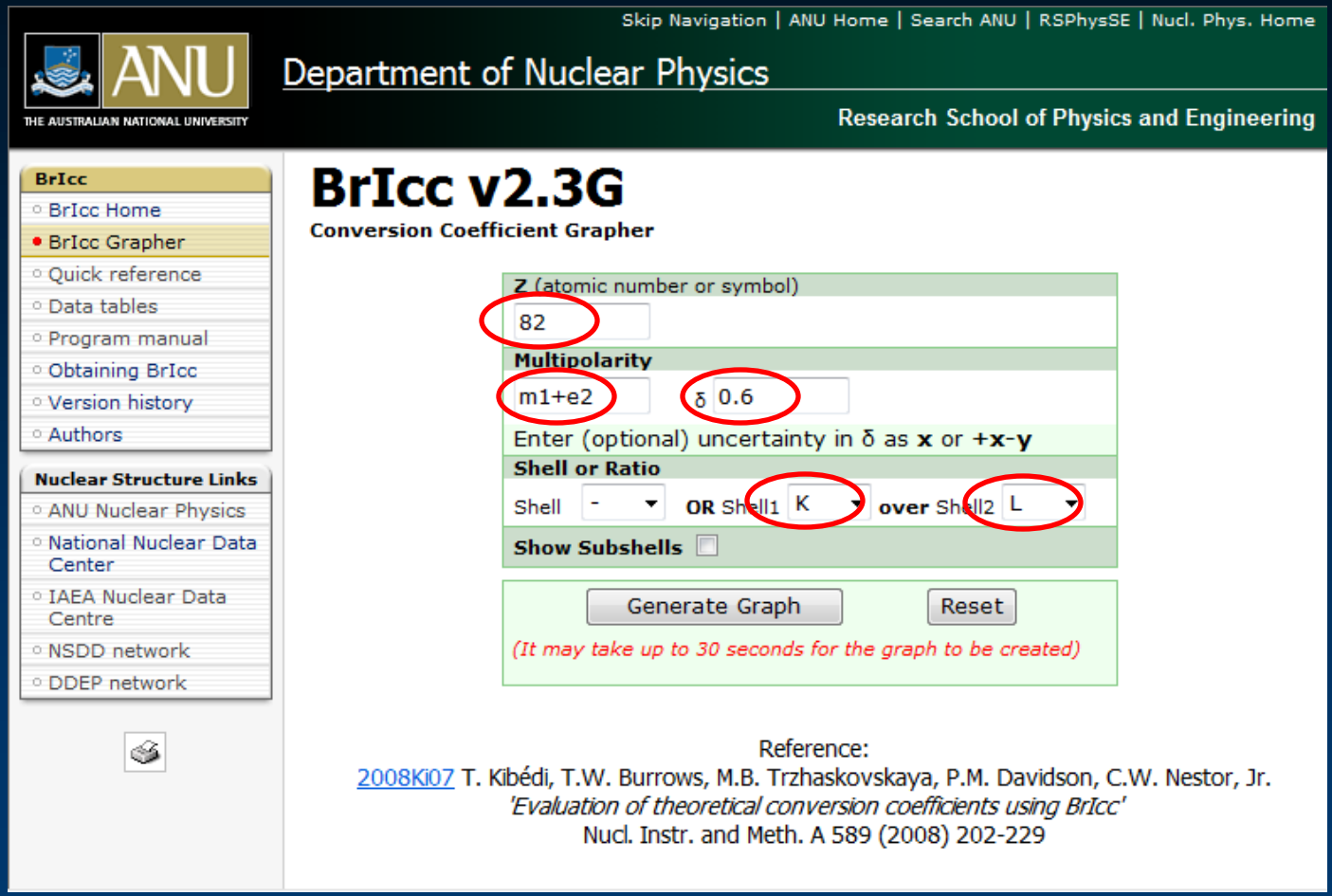
Unique users since 2005: 24815 (95k page loads)




Z=40 (Zr); DataSet: Icc=BrIccFO, Pcc=ScPcc; Mult=E2; BrIccG v2.3 (27-Mar-2011)
E2(Tot)
E2(K)
E2(L-tot)
E2(L1)
E2(L2)
E2(L3)
E2(M-tot)
E2(M1)
E2(M2)
E2(M3)
E2(M4)
E2(M5)
E2(N-tot)
E2(N1)
E2(N2)
E2(N3)
E2(N4)
E2(O-tot)
E2(O1)
E2(IPF)
1.0E+10
1.0E+05
1.0E+00
1.0E-05
1.0E-10
1.0E-15
ICC
1
10
100
1000
10000
Transition energy [keV]

BrIccG (v2.3) - Grapher

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



Conversion coefficients for superheavy elements Z=111 to 126

With M.B. Trzhaskovskaya, M. Gupta and A.E. Stuchbery
Accepted in ADNDT

Existing ICC tables

- Rysavy and Dragoun, ADNDT 78 (2001) 129
  Dirac-Slater atomic model, few energy points
- Band et al., ADNDT *81 (2002) 1*
  Relativistic Dirac-Fock atomic model, “No-Hole” approximation, from L1 shell binding energy

Conversion coefficients for superheavy elements Z=111 to 126

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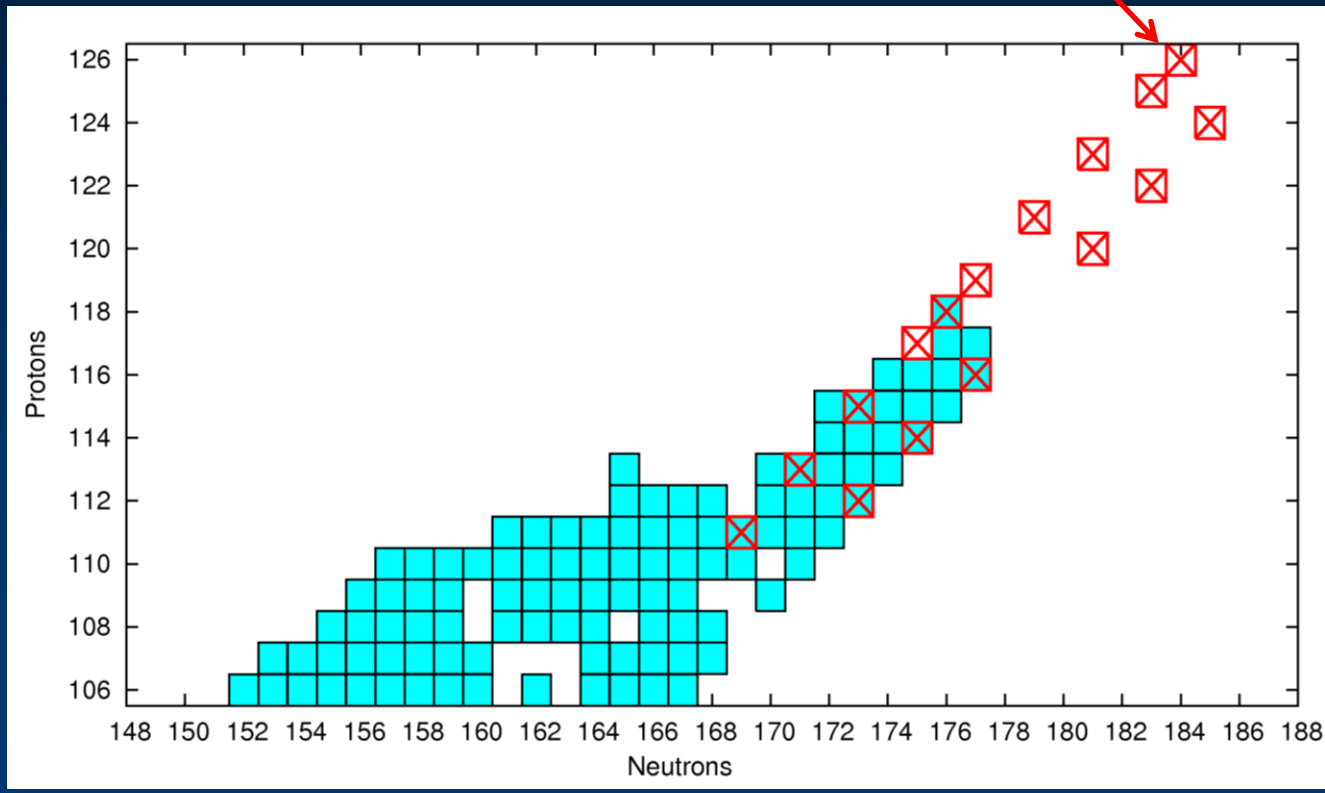
Input parameters

- Adopted atomic masses
- Valence electron configurations
- Neutral atom binding energies

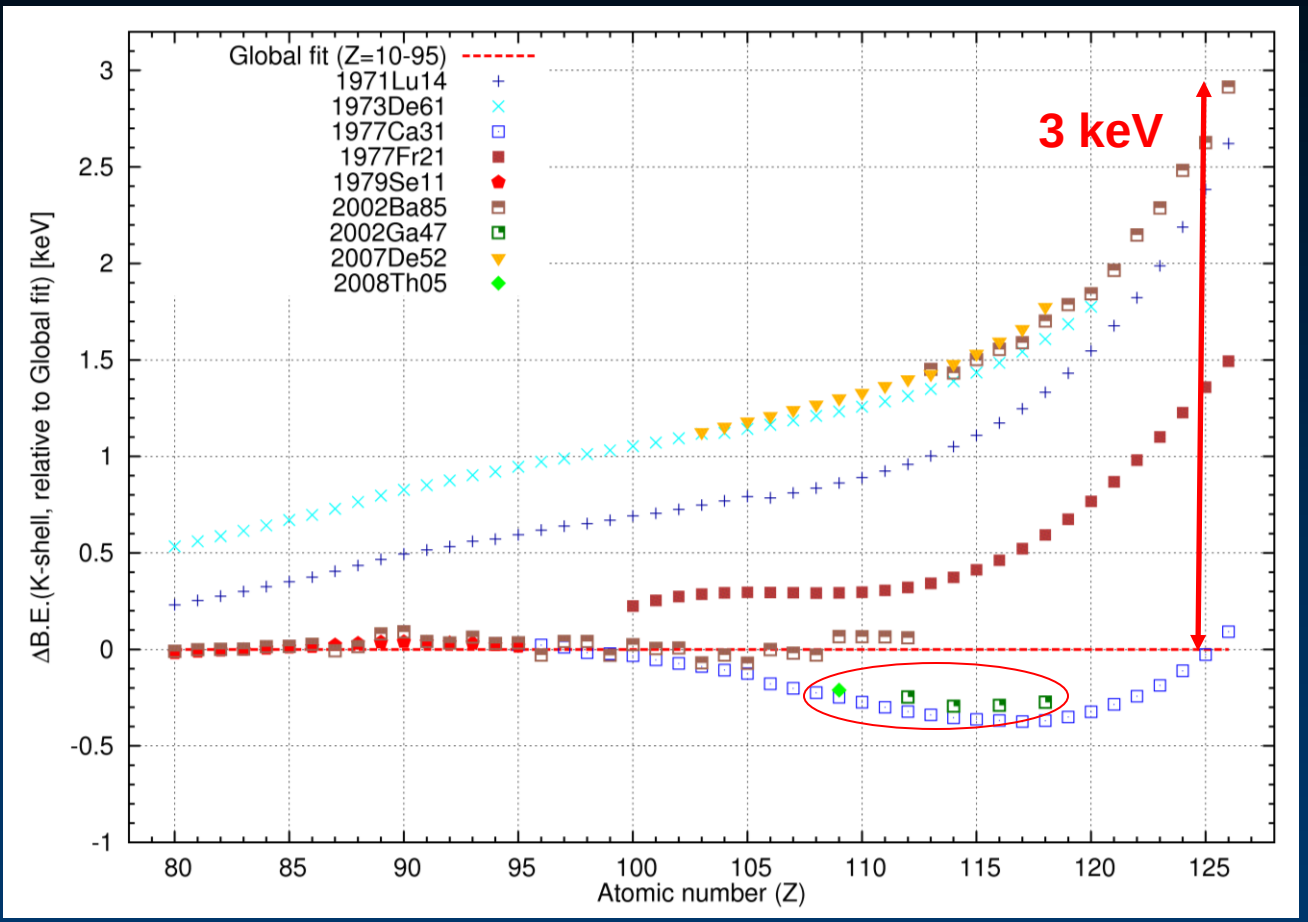
Next shell closure at Z=114, 120 or **126** N=184

IUPAC Atomic Weights and Isotopic Abundances: Z=111-116, 118

Z=117 new isotopes 2010Og01



K-shell binding energies



Global fit
1979Se11 Sevier Z=10-95
2002Ba85 Band et al. Z>95

Adopted
1977Ca31 Carlson & Nestor relativistic Dirac-Fock with semi-empirical corrections

New systematic calculations needed!

New relativistic Dirack-Fock calculations with QED corrections (2002Ga47, 2007De52)

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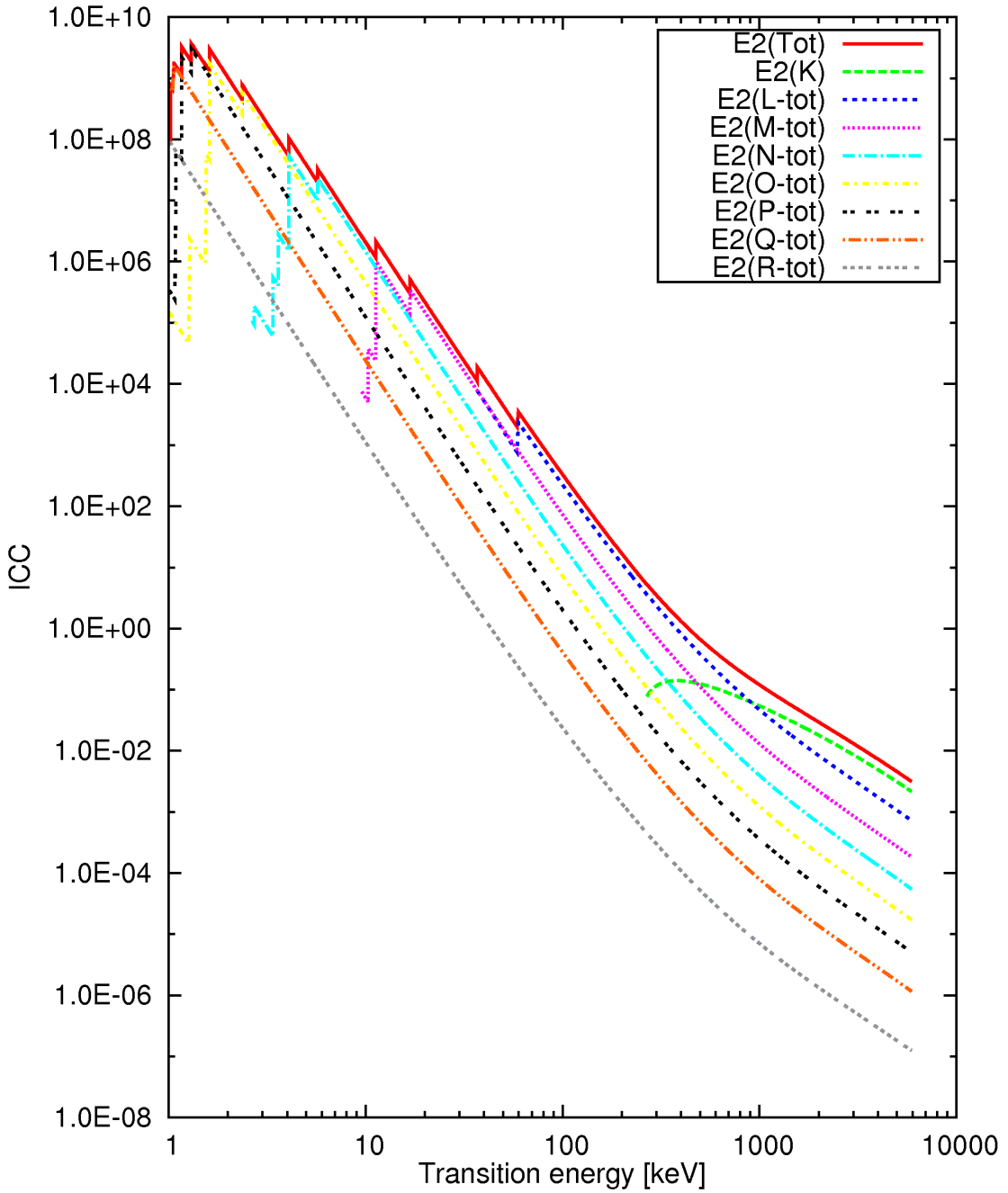
Z=126
E2 multipolarity
1 – 6000 keV
All shells
E1-E5 M1-M5

More electron shells used
Not compatible with current BrIcc



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NICC
Rysavy and Dragoun, ADNDT 78 (2001) 129
Systematically larger by 5-10%

BrIccV1.3 (2002Ba85) Band et al., ADNDT *81 (2002) 1*
Up to 5% for E2 in K and L1

BrIccFO / BrIccNH
"Frozen orbitals" vs. "No-Hole"
Up to 5% for E2 in K and L1

Selected conversion coefficients (ICC) for $Z = 126$ obtained from various theoretical calculations.

Shell	E_{tr}	ICC(M1)				ICC(E2)			
	[keV]	NICC [24]	BrIcc V1.3 [8]	BrIccNH[a]	BrIccFO[b]	NICC [24]	BrIcc V1.3 [8]	BrIccNH[a]	BrIccFO[b]
Total	10	1.883E+4	–	1.670E+4	1.673E+4	2.248E+6	–	2.070E+6	2.072E+6
	50	5.128E+2	–	4.647E+2	4.650E+2	4.555E+3	–	4.368E+3	4.374E+3
	100	2.445E+2	2.24E+2	2.238E+2	2.243E+2	3.419E+2	3.30E+2	3.300E+2	3.319E+2
	300	3.075E+1	2.84E+1	2.841E+1	2.852E+1	3.552E+0	3.48E+0	3.475E+0	3.493E+0
	1000	9.807E-1	8.82E-1	8.814E-1	8.817E-1	1.236E-1	1.19E-1	1.193E-1	1.199E-1
K	270	–	–	2.554E+1	2.576E+1	–	–	7.434E-2	7.895E-2
	300	2.079E+1	1.92E+1	1.919E+1	1.929E+1	1.079E-1	1.04E-1	1.107E-1	1.154E-1
	1000	6.639E-1	5.99E-1	5.984E-1	5.986E-1	5.526E-2	5.37E-2	5.392E-2	5.441E-2
L1	61	–	5.13E+2	5.153E+2	5.183E+2	–	5.27E+1	5.337E+1	5.513E+1
	100	1.323E+2	1.21E+2	1.214E+2	1.217E+2	1.115E+1	1.09E+1	1.091E+1	1.110E+1
	300	5.262E+0	4.89E+0	4.890E+0	4.895E+0	3.532E-1	3.50E-1	3.500E-1	3.525E-1
	1000	1.648E-1	1.48E-1	1.479E-1	1.479E-1	1.970E-2	1.92E-2	1.915E-2	1.920E-2
M1	18	–	–	4.896E+3	4.919E+3	–	–	4.155E+3	4.240E+3
	50	2.597E+2	–	2.365E+2	2.367E+2	7.018E+1	–	6.772E+1	6.834E+1
	100	3.328E+1	3.04E+1	3.037E+1	3.040E+1	4.956E+0	4.82E+0	4.817E+0	4.845E+0
	300	1.320E+0	1.22E+0	1.215E+0	1.215E+0	1.170E-1	1.15E-1	1.151E-1	1.154E-1
	1000	4.110E-2	3.66E-2	3.658E-2	3.658E-2	5.300E-3	5.12E-3	5.117E-3	5.121E-3
N1	7	–	–	2.473E+4	2.483E+4	–	–	1.298E+5	1.311E+5
	10	9.595E+3	–	8.555E+3	8.572E+3	2.704E+4	–	2.518E+4	2.541E+4
	50	7.841E+1	–	7.063E+1	7.063E+1	2.569E+1	–	2.457E+1	2.466E+1
	100	1.004E+1	9.09E+0	9.063E+0	9.066E+0	1.702E+0	1.64E+0	1.639E+0	1.643E+0
	300	3.984E-1	3.62E-1	3.620E-1	3.620E-1	3.783E-2	3.67E-2	3.673E-2	3.678E-2
	1000	1.237E-2	1.09E-2	1.088E-2	1.089E-2	1.627E-3	1.55E-3	1.554E-3	1.554E-3

E0 Electronic factors for Z=10-95

with G. Gosselin, V. Meot, and M. Pascal

E0 Transition probability

$$W_{ic}(E0) = \rho^2(E0) \times \Omega_{ic}(E0)$$

$\rho^2(E0)$: Nuclear

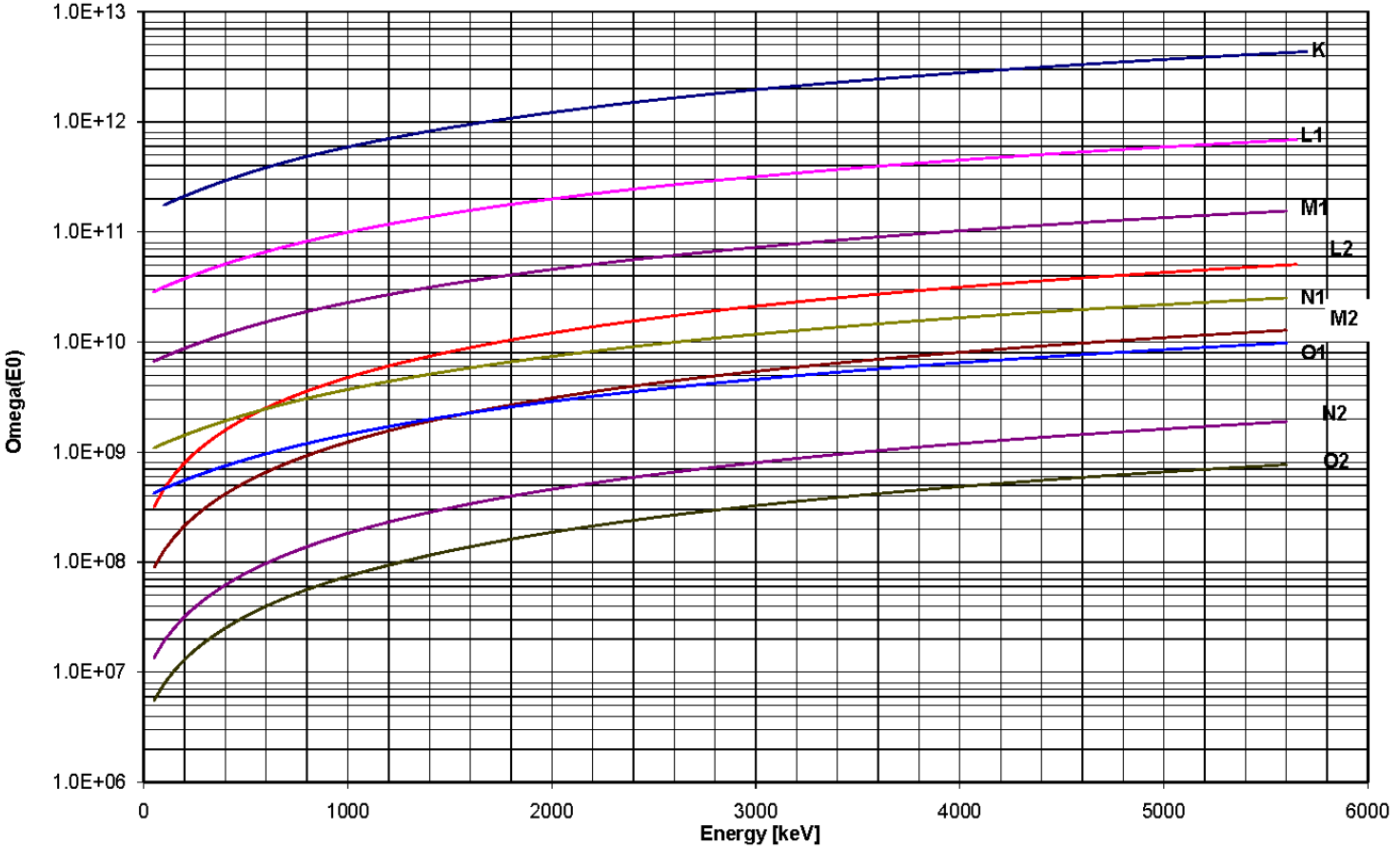
$\Omega_{ic}(E0)$: Atomic

Current BrIcc Table

- composed from 3 tabulations
- Do not cover all energies and atomic shells
- Ω(E0) and ICC tables are incompatible

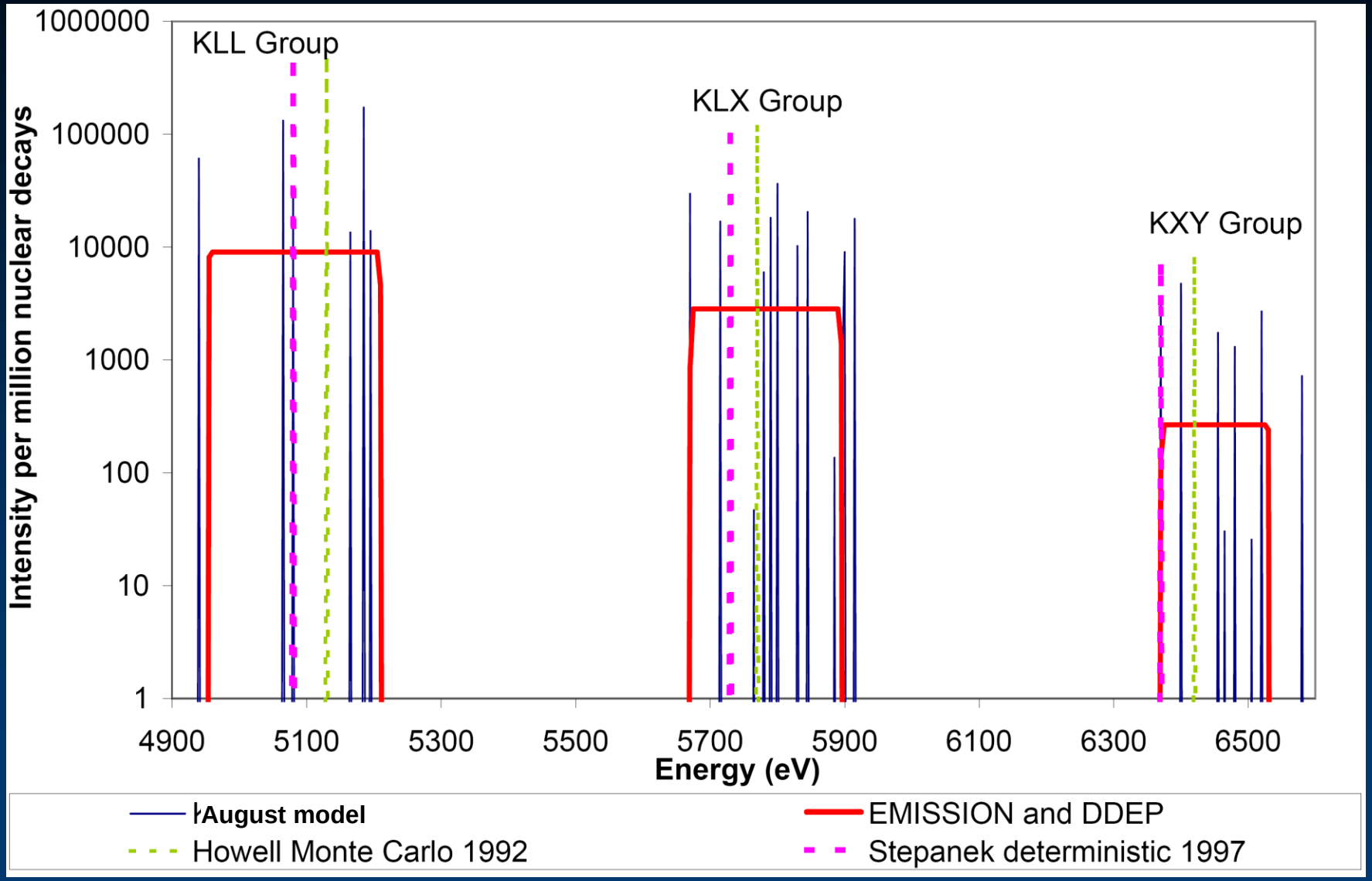
New calculations using CATAR (H.C.Pauli, U.Raff 1975Pa26)

Z=82 E0 electronic factors



Need to compare with existing tabulations and ratios of sub-shell CE intensities of E0 transitions (K/L, L1/L2)

$^{55}Fe + e^- \rightarrow {}^{55}Mn + \nu$: *K*-Auger electrons (5 eV bins)



Slide courtesy of Kalman Robertson

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$^{55}Fe + e^- \rightarrow {}^{55}Mn + \nu$

3.7 x 10^6 Auger electrons and 2.8 x 10^5 X-rays per 10^6 nuclear decays

L- and *M*- Auger electrons (5 eV bins)

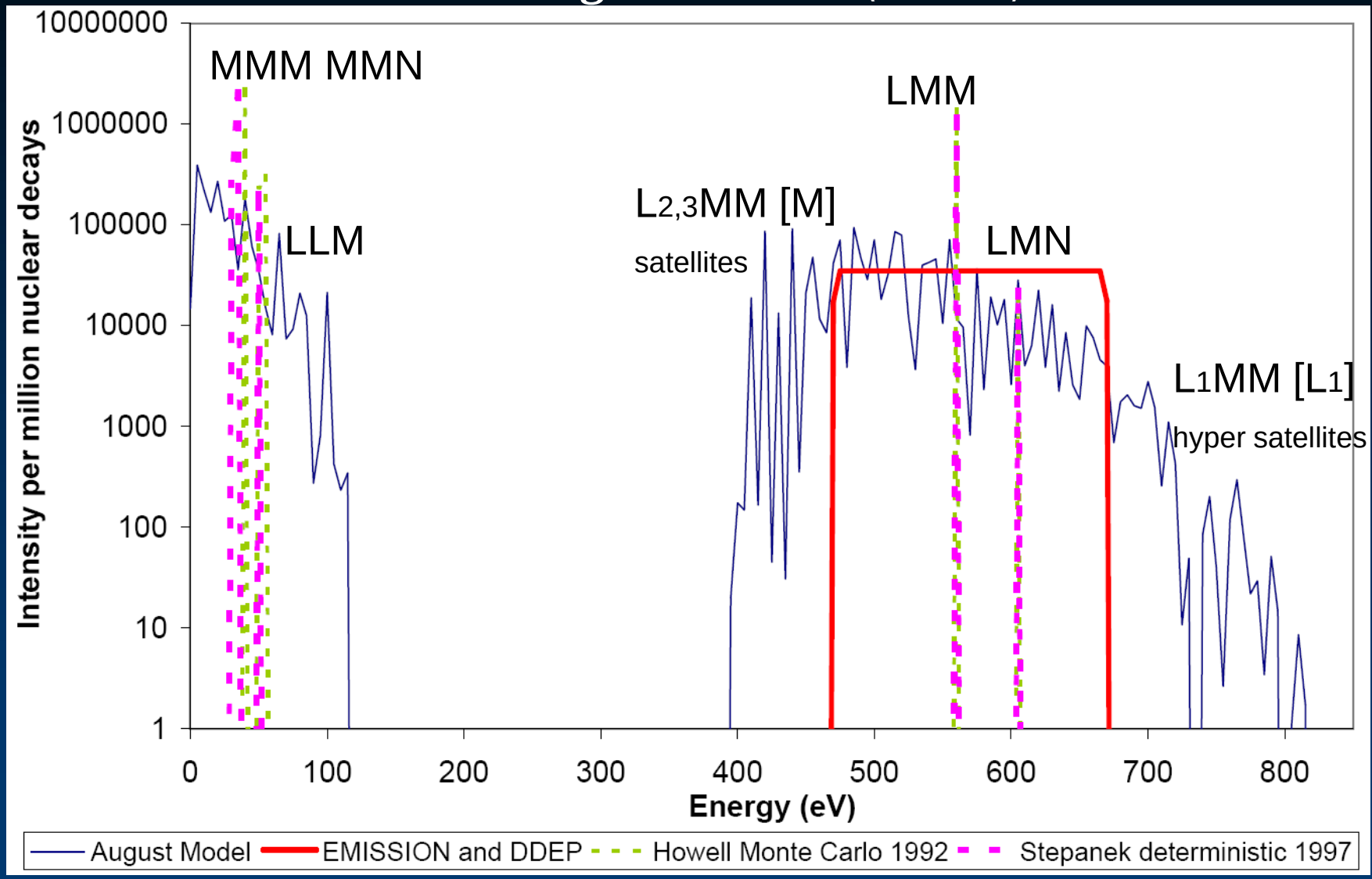

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Table 6.1: Mean energy and intensity (per million nuclear disintegrations) of groups of atomic radiations in nuclear decay of ^{55}Fe in condensed phase. The August Model results are calculated using Approach 2 as explained in Section 6.3. For each transition group in the August Model results, the uncertainty in the mean energies is less than 30 eV and the uncertainty in intensity is less than 5%. The DDEP values agree with the EMISSION values except for the *LXY* transition intensity (indicated by *), which is 1.40 E 6 according to DDEP and 1.31 E 6 by running the EMISSION program. "Bound-bound X-rays" and "free-bound X-rays" are abbreviated "b-b X" and "f-b X." The bound-bound X-ray, Auger, CK and free-bound X-ray totals are the total energies released in these respective forms per million nuclear decays. The average energy released through atomic transitions per nuclear decay is (5890 ± 50) eV (see section 6.6).

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Radiation	August Model		EMISSION/DDEP		Howell		Stepanek	
	Energy	Intensity	Energy	Intensity	Energy	Intensity	Energy	Intensity
K_α	5925 eV	2.492E5	5895 eV	2.50E5	5895 eV	2.44E5	5860 eV	2.44E5
K_β	6530 eV	3.389E4	6512 eV	3.40E4	6490 eV	2.97E4	6450 eV	2.91E4
L b-b X	665 eV	4.340E3	565 eV	4.90E3	635 eV	3.30E3	585 eV	6.90E3
M b-b X	50 eV	< 1E2	N/A	N/A	N/A	N/A	N/A	N/A
b-b X total	1701 MeV		1700 MeV		1636 MeV		1566 MeV	
KLL	5100 eV	4.212E5	5080 eV	4.66E5	5130 eV	4.87E5	5080 eV	4.87E5
KLX	5790 eV	1.653E5	5780 eV	1.27E5	5770 eV	1.20E5	5730 eV	1.19E5
KXY	6440 eV	1.469E4	6450 eV	8.62E3	6420 eV	8.20E3	6370 eV	7.30E3
LXY	513 eV	1.346E6	570 eV	1.40E6*	564 eV	1.43E 6	561 eV	1.42E6
LLX	44 eV	3.563E5	N/A	N/A	55.2 eV	3.10E5	31.4 eV	2.63E5
M and *N* Auger/CK	23 eV	1.396E6	N/A	N/A	42 eV	2.77E6	38 eV	2.83E6
Auger/CK total	3938 MeV		3950 MeV		4170 MeV		4240 MeV	
f-b X	40 eV	4.699E6	N/A	N/A	N/A	N/A	11 eV	6.13E6
f-b X total	189 MeV		N/A		N/A		68.3 MeV	