Benchmarking study of Geant4 Auger electrons emitted by medical radioisotopes

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Goal of the project

Validate Geant4 Auger e- emission with respect to calculated and experimental data.

	Calculations	Experimental
^{123}I	BrIccEmis [4] Pomplun [44]	-
^{124}I	BrIccEmis [4]	-
^{125}I	BrIccEmis [4] Stepanek [27] Pomplun (KLL spectrum) [26]	ANU (KLL spectrum) [8]
^{131}Cs	-	JINR (KLL spectrum) [42]

Reference data

[4] B. Q. Lee, H. Nikjoo, J. Ekman, P. Jonsson, A. E. Stuchbery, and T. Kibedi, "A stochastic cascade model for Auger-electron emitting radionuclides," Int J Radiat Biol, vol. 92, no. 11, pp. 641–653, 2016.

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[26] E. Pomplun, "Auger Electron Spectra - The Basic Data for Understanding the Auger Effect," Acta Oncol. (Madr)., vol. 39, no. 6, pp. 673–679, 2000.

[27] J. Stepanek, "Methods to determine the fluorescence and Auger spectra due to decay of radionuclides or due to a single atomic-subshell ionization and comparisons with experiments," Med. Phys., vol. 27, no. 7, pp. 1544–1554, 2000.

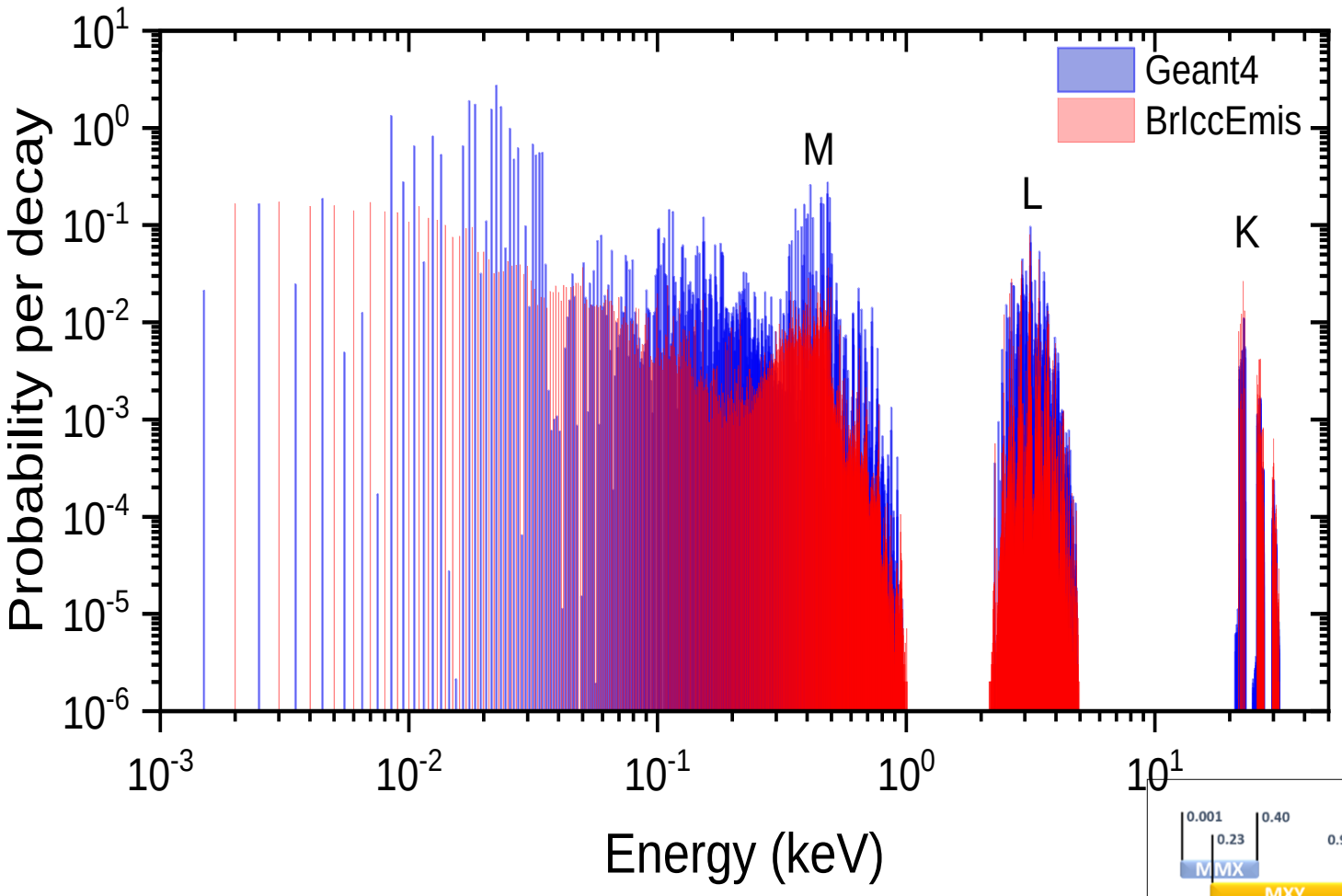
[42] A. Kovalik et al., "The electron spectrum from the atomic deexcitation of Xe-131(54)," J. Electron Spectros. Relat. Phenomena, vol. 95, no. 2–3, pp. 231–254, 1998.

[44] E. Pomplun, "Monte Carlo-simulated Auger electron spectra for nuclides of radiobiological and medical interest – a validation with noble gas ionization data," Int. J. Radiat. Biol., vol. 88, no. 1–2, pp. 108–114, Jan. 2012.

Methodology

- **Geant4 rdecay01 extended example (Geant4 10.05.p01)**
  - 20 mm, cube of galactic material, point source of (I-123, I-124, I-125 and Cs-131) in centre
  - The radioactive decay and the full atomic relaxation are modelled
  - Auger-electron cascade switched on
  - Output: energy spectra of electrons

Geant4 vs other theoretical approaches: I-123



Line	Geant4		BrIccEmis [4]		Pomplun [43]	
	$\bar{E}$ (keV)	Yield	$\bar{E}$ (keV)	Yield	$\bar{E}$ (keV)	Yield
Auger MXY	0.446	2.261	0.411	1.94	0.394	1.93
Auger LMM	3.065	0.486	3.047	0.736	3.028	0.711
Auger LMX	3.524	0.298	3.676	0.206	3.656	0.200
Auger KLL	22.662	0.0808	22.525	0.0811	22.52	0.0731
Auger KLX	26.528	0.0356	26.459	0.0356	26.43	0.0328
Auger KXY	30.387	0.00373	30.313	0.00365	30.30	0.00280
Auger total	0.376	28.7	0.932	7.4	-	7.3

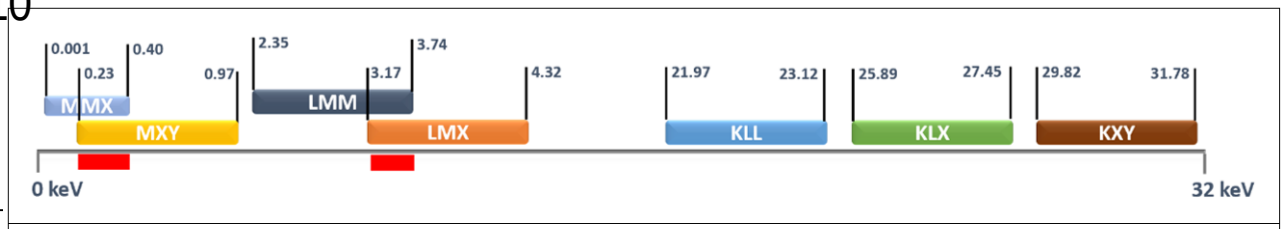
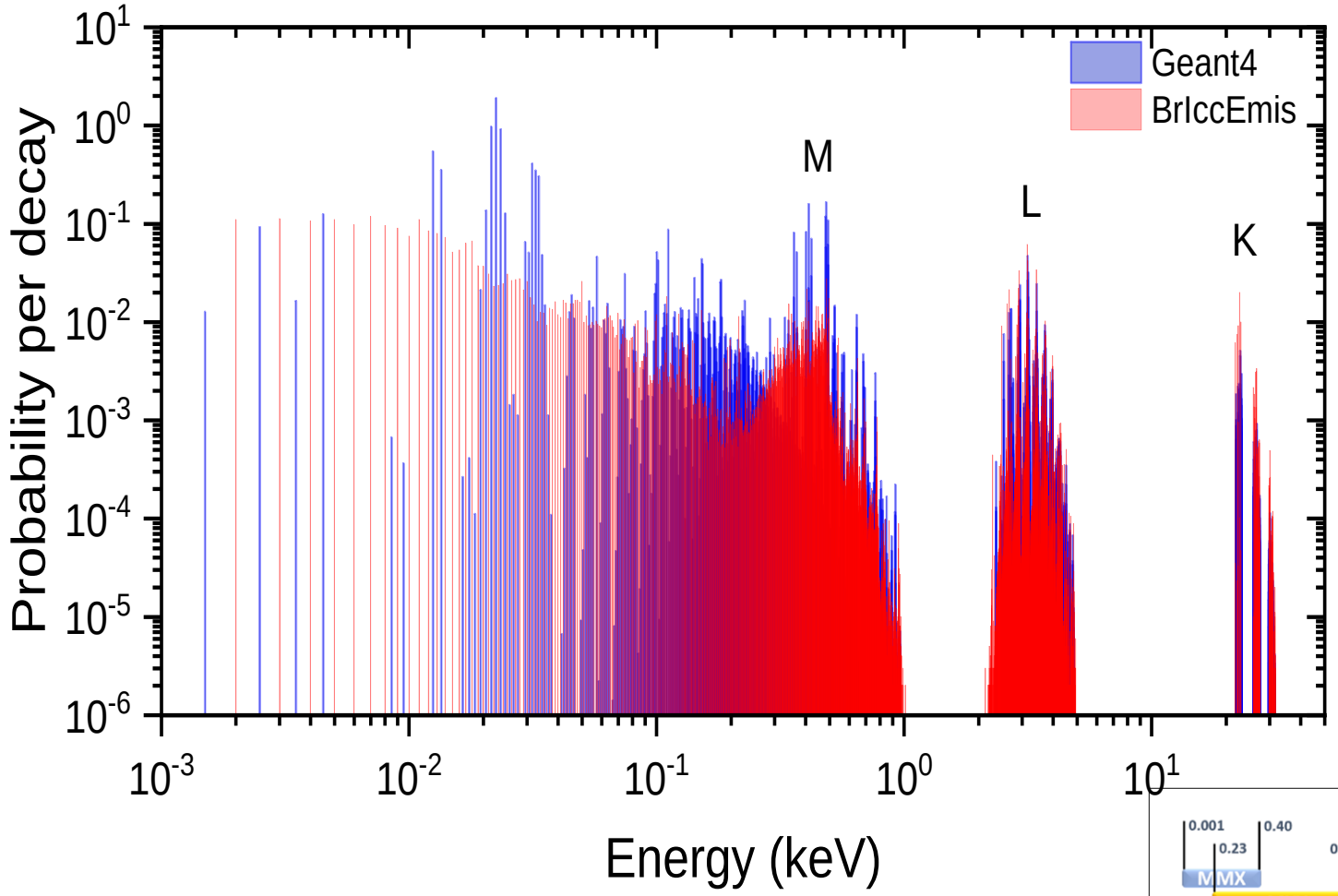


Fig. 1 Energy ranges for Auger electron groups in tellurium according to EADL [21].

Geant4 vs other theoretical approaches: I-124



Line	Geant4		BrIccEmis [4]	
	$\overline{E}$ (keV)	Yield	$\overline{E}$ (keV)	Yield
Auger MXY	0.450	1.171	0.413	1.30
Auger LMM	3.060	0.226	3.049	0.493
Auger LMX	3.544	0.139	3.676	0.139
Auger KLL	22.676	0.0541	22.525	0.0504
Auger KLX	26.529	0.0238	26.461	0.0238
Auger KXY	30.381	0.00251	30.322	0.00255
Auger total	0.499	10	0.920	5.04

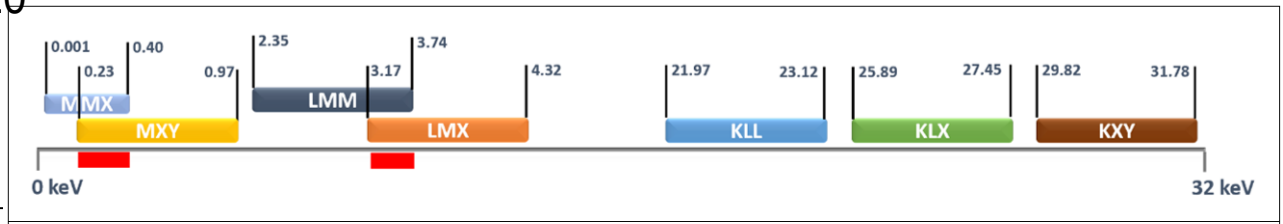
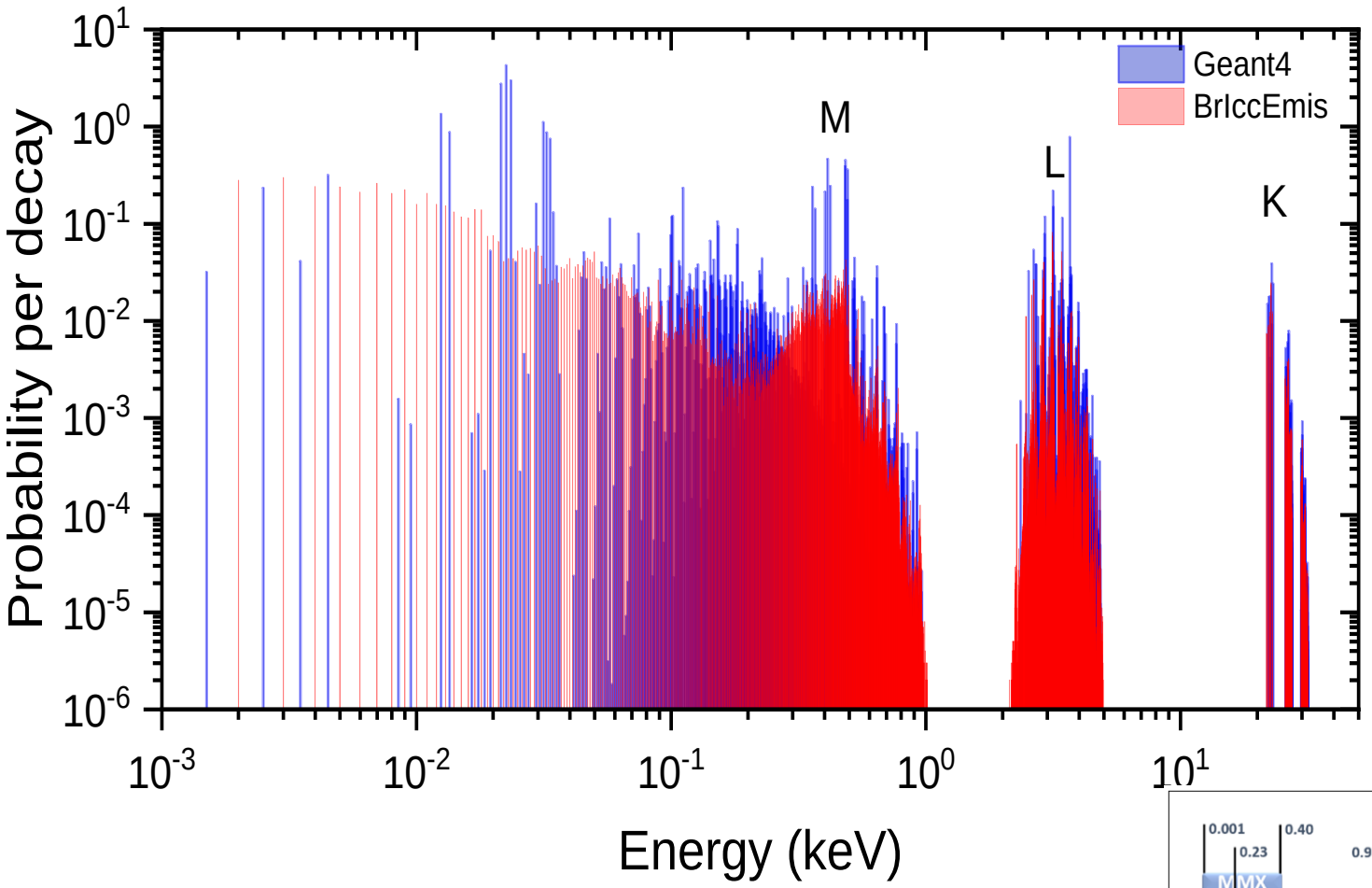


Fig. 1 Energy ranges for Auger electron groups in tellurium according to EADL [21].

Geant4 vs other theoretical approaches: I-125



Line	Geant4		BrIccEmis [4]		Stepanek [25]	
	$\bar{E}$ (keV)	Yield	$\bar{E}$ (keV)	Yield	$\bar{E}$ (keV)	Yield
Auger MXY	0.452	3.366	0.408	3.20	0.380	3.24
Auger LMM	3.058	0.952	3.047	1.21	3.01	1.22
Auger LMX	3.532	0.551	3.676	0.338	3.63	0.339
Auger KLL	22.655	0.129	22.522	0.129	22.6	0.126
Auger KLX	26.541	0.0565	26.457	0.0568	26.5	0.0580
Auger KXY	30.345	0.00600	30.322	0.00596	30.3	0.00550
Auger total	0.734	25.8	0.955	11.8	-	8.92

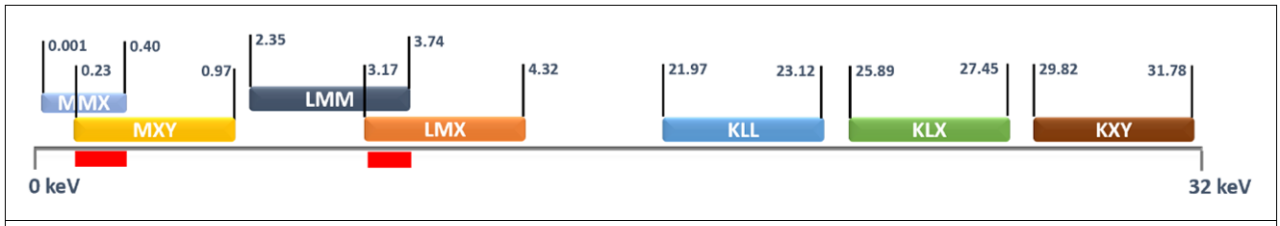
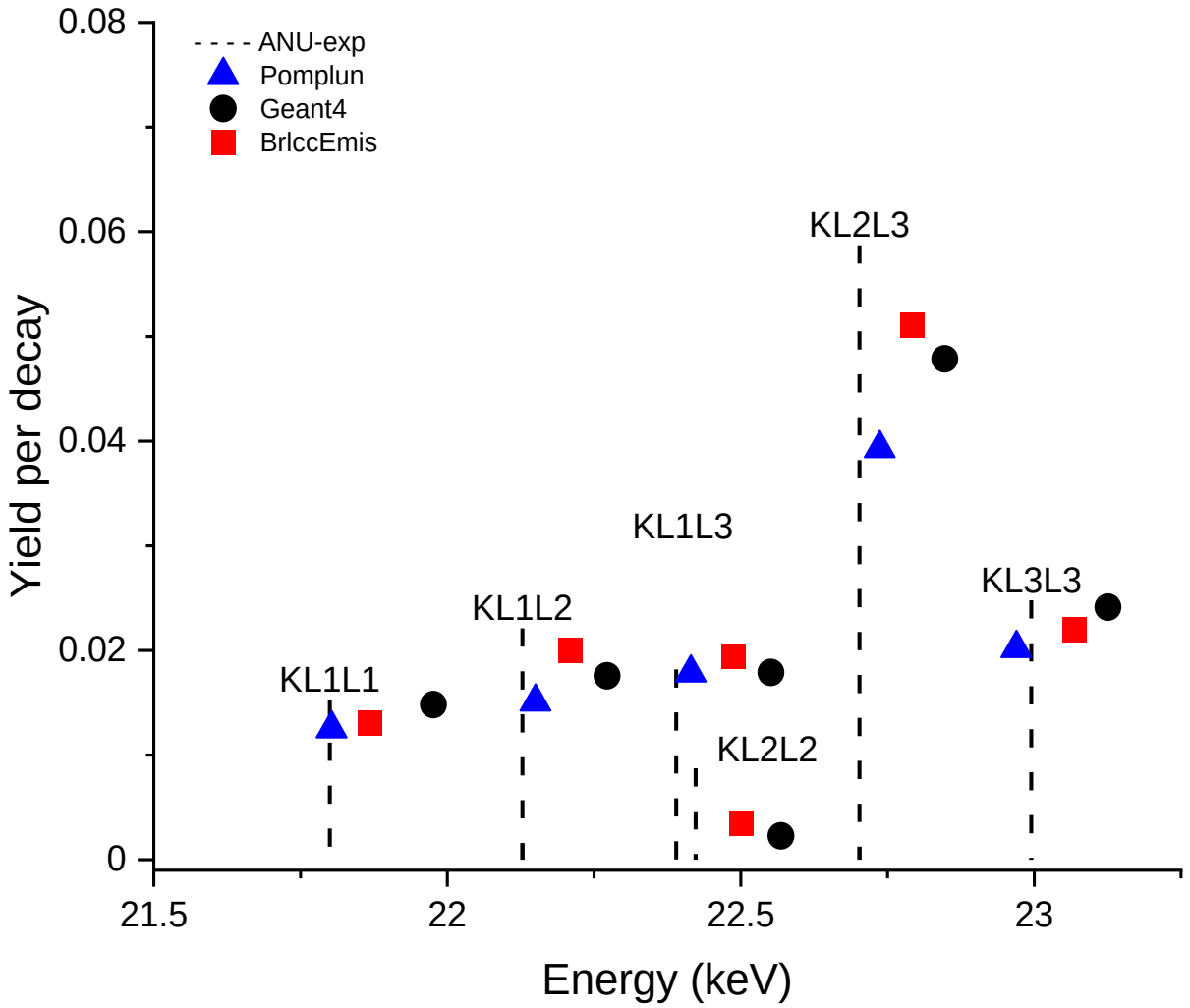


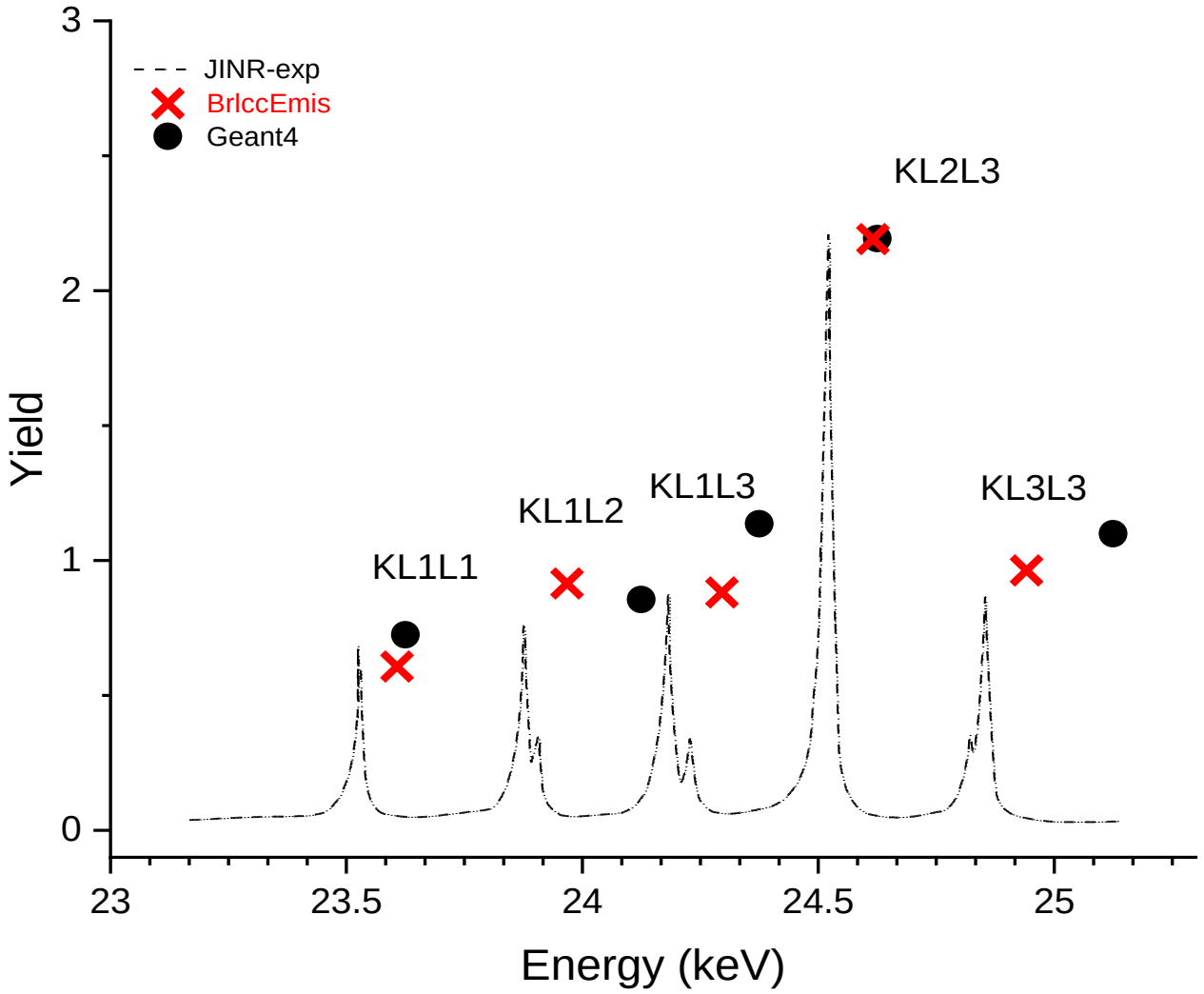
Fig. 1 Energy ranges for Auger electron groups in tellurium according to EADL [21].

Geant4 vs experimental data: I-125



Line	Geant4		BrIccEmis [4]		Pomplun [26]		Experimental [8]	
	Energy (keV)	Yield	Energy (keV)	Yield	Energy (keV)	Yield	Energy (keV)	Yield
KL1L1	21.9765	0.311	21.868	0.263	21.803	0.319	21.890	0.262(5)
KL1L2	22.2725	0.366	22.209	0.397	22.151	0.384	22.118	0.382(12)
KL1L3	22.5515	0.373	22.488	0.457	22.4153	0.454	22.480	0.462(9)
KL2L2	22.5685	0.047	22.501	0.046	-	-	-	-
KL2L3	22.8475	1.000	22.792	1.000	22.737	1.000	22.792	1.000
KL3L3	23.1255	0.503	23.068	0.436	22.970	0.514	23.085	0.435(9)

Geant4 vs experimental data: Cs-131



Line	Geant4		BrIccEmis [45]		Experimental	
	Energy (keV)	Yield	Energy (keV)	Yield	Energy (keV)	Yield
KL1L1	23.625	0.329	23.521	0.330	23.526(2)	0.269(21)
KL1L2	24.125	0.388	23.876	0.379	23.883(2)	0.387(31)
KL1L3	24.375	0.516	24.200	0.471	24.196(3)	0.37(5)
KL2L2	-	-	24.178	0.047	24.187(3)	0.12(4)
KL2L3	24.625	1.000	24.516	1.000	24.522(20)	1.000
KL3L3	25.125	0.502	24.838	0.498	24.850(2)	0.421(34)

Conclusion

- Benchmarked the emission of Auger electrons deriving from ^{123}I, ^{124}I, ^{125}I and ^{131}Cs decays.
  - Against other theoretical approaches: Good agreement for K and M shells. However, larger differences for L shell.
  - Against experimental data: a shift in the Auger kinetic energies was found.
    - Possible due to (QED) effects, Breit magnetic electron interaction corrections, atomic structure effects.
    - Generally, good agreement (within 15%).
- Finalising paper to be submitted to NIMA