Consistent atomic relaxations and new photo-electric cross sections in EGSnrc

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Ionizing Radiation Standards
Measurement Science and Standards

National Research Council Canada | Conseil national de recherches Canada
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To renormalize or not to renormalize photo-electric cross sections?

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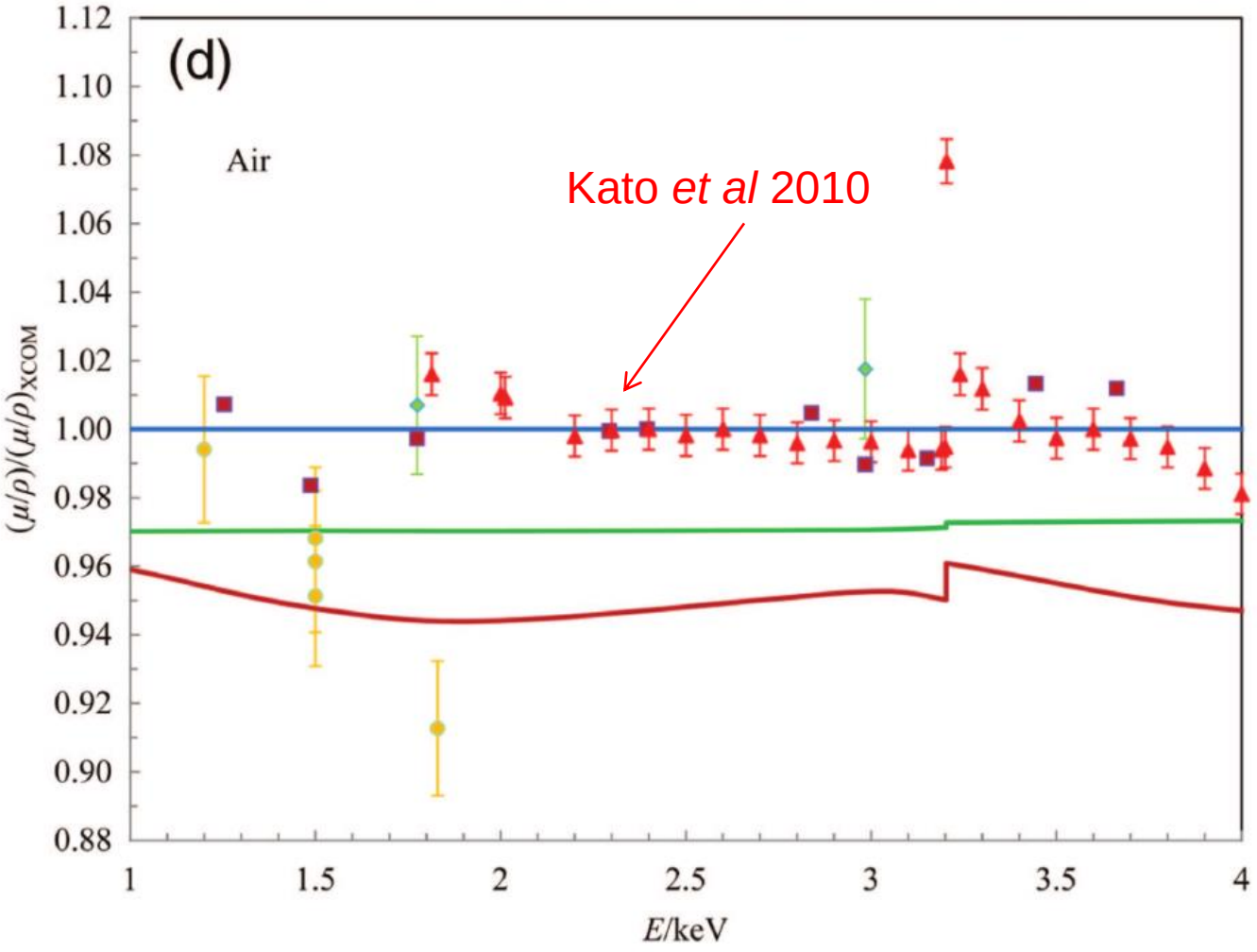
State of the art

- Independent electrons model in a self-consistent DHFS potential (Scoffield 1973). Interaction of the atom with electromagnetic field treated as a first order perturbation.
- Scoffield used energy-independent normalization screening approximation to correct for multi-configuration effects (1973).
- Sabbatucci and Salvat (2016) calculated PE cross sections using a more robust numerical algorithm with an adaptive energy grid around the atomic edges.
- Sabbatucci and Salvat applied MCDF corrections to their calculated cross sections.
- Both calculations are in excellent agreement

Photo-electric cross section libraries

- Better agreement of uncorrected photo-electric cross sections with experimental data below 1 keV lead NIST to use these in XCOM.
- EPDL library also uses un-renormalized cross sections.
- XCOM and EPDL use slightly different ionization energies
- PENELOPE uses currently renormalized cross sections and yet another set of ionization energies

Motivation: ICRU 90 report



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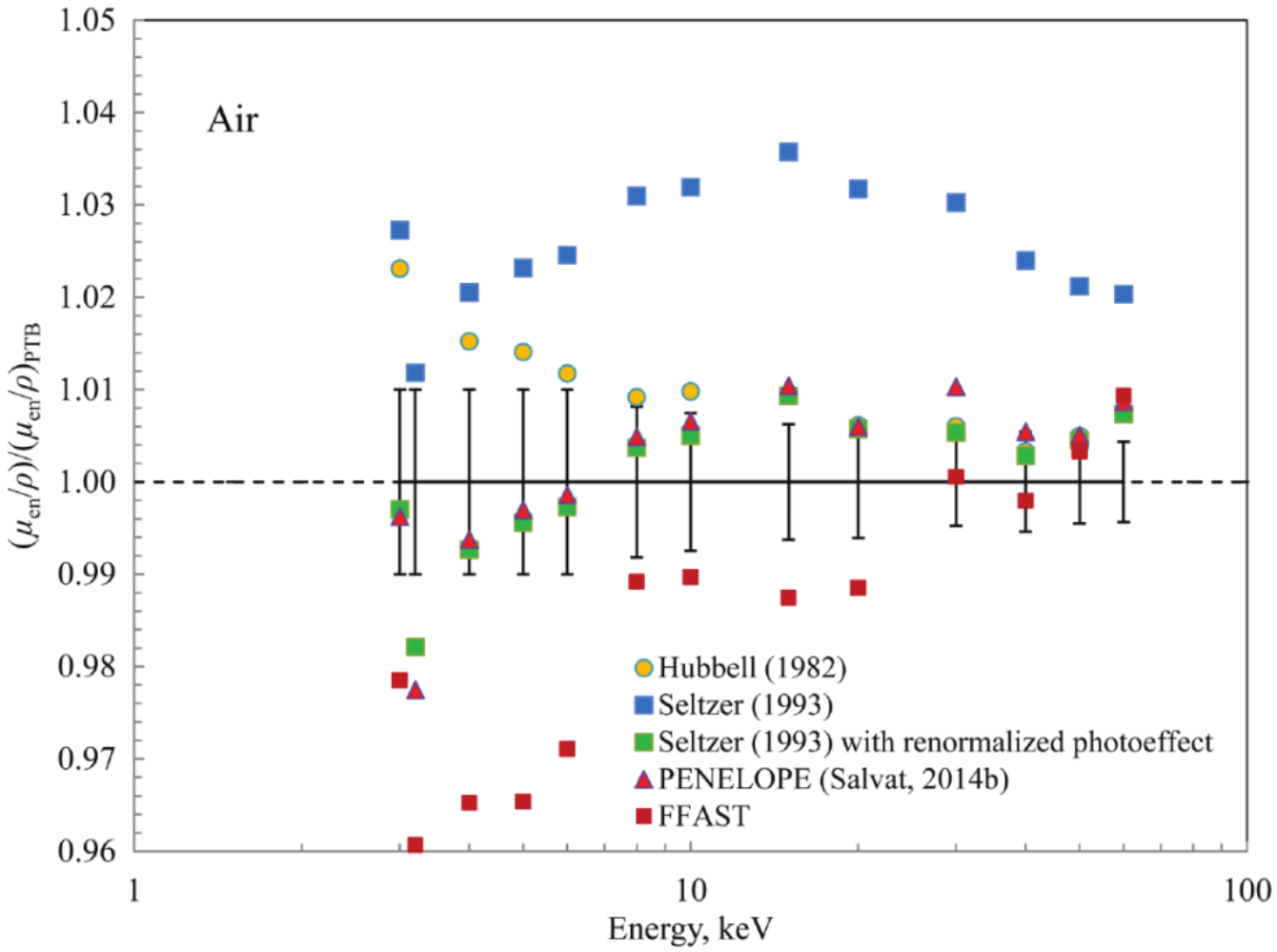
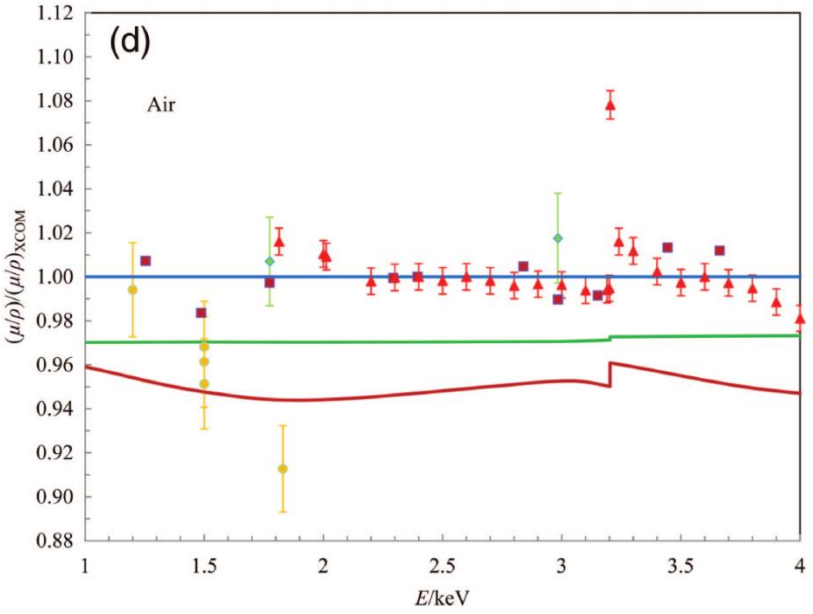
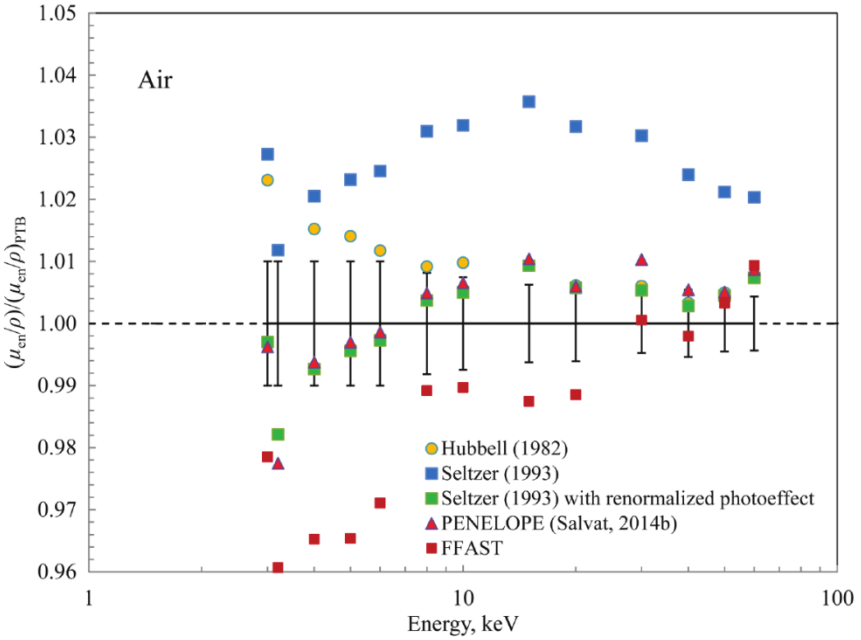


PTB: Buermann et al 2006, Buhr et al 2012

Motivation: ICRU 90 report





Must include renormalized photo-electric cross sections in EGSnrc

Inconsistency in atomic relaxations

- Binding energies used in the atomic relaxation routine from EADL library
- Binding energies in Compton, photo-effect and EII from XCOM library
- Creates a small inconsistency violating energy conservation
- User reported total energy deposited in an infinite CdWO4 phantom differed from initial energy by 0.5% for 1 MeV photons

Inconsistency in atomic relaxations

Medium	Z	Edep
Oxygen	8	0.9999992
Manganese	25	0.9999706
Copper	29	0.9999541
Tin	50	1.0001120
Terbium	65	1.0006940
Lead	82	1.0018390
Einstenium	99	1.0031970
Water	-	0.9999993
Air	-	0.9999949

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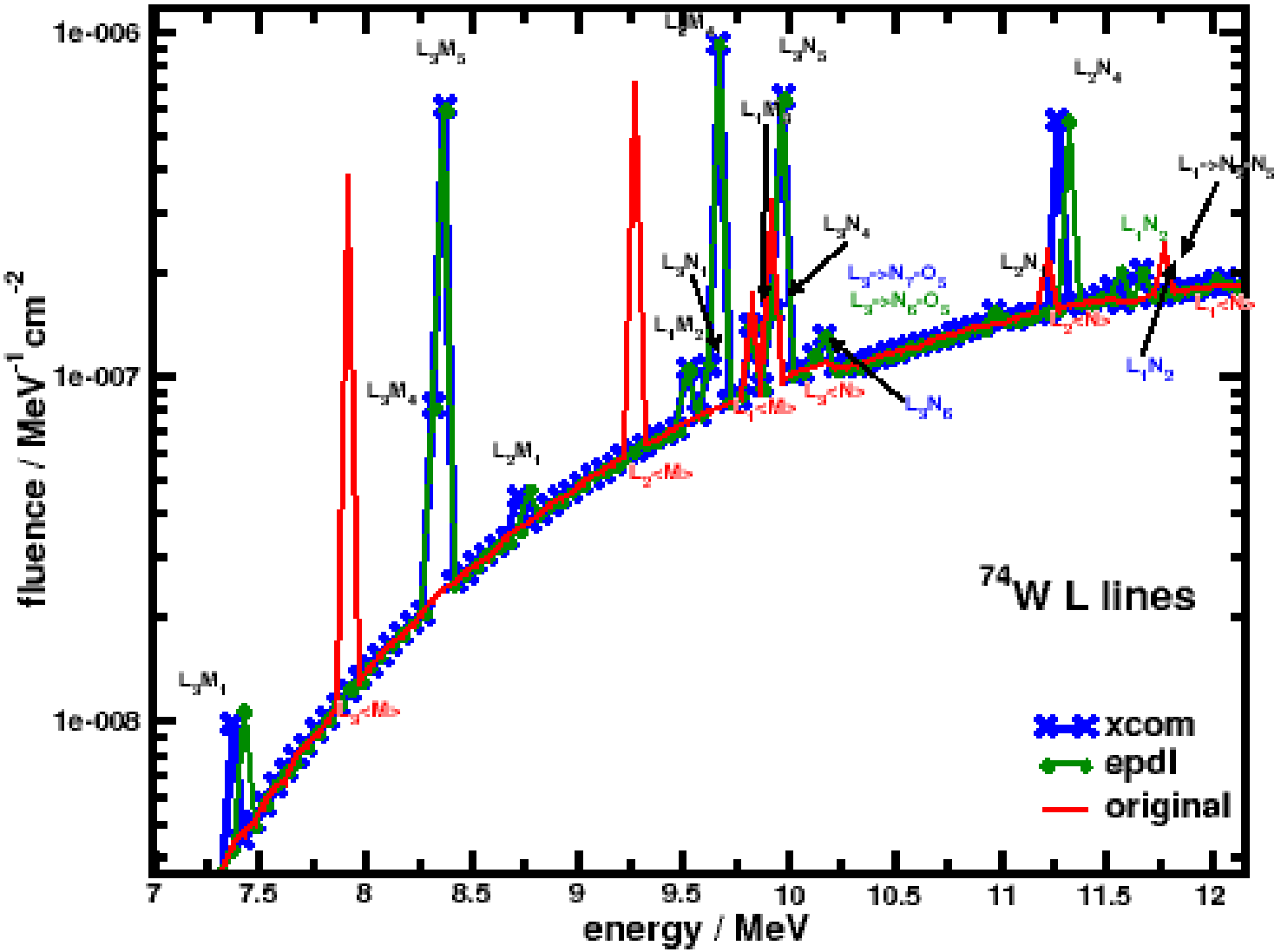
Removing inconsistency

- Use consistent set of binding energies throughout the code.
- Binding energies selected depending on the photon cross section libraries requested by the user, i.e., xcom or epdl.
- Transition probabilities are still taken from the EADL library.
- Position of the x-ray lines match either the EADL radiative transitions (epdl) or the radiative transitions from the Table of Isotopes (8th Edition) (xcom).

Consistency in atomic relaxations

Medium	Z	0.1 MeV	1.0 MeV	10 MeV
Oxygen	8	0.100000	1.000000	10.000000
Manganese	25	0.100000	1.000000	10.000000
Copper	29	0.100000	1.000000	10.000000
Tin	50	0.100000	0.999999	10.000000
Terbium	65	0.100000	0.999998	10.000000
Lead	82	0.100000	1.000000	9.999887
Thorium	90	0.100000	1.000000	9.999900
Einstenium	99	0.100000	0.999998	9.999983
Water	-	0.100000	0.999997	10.000000
Air	-	0.100000	1.000000	10.000000

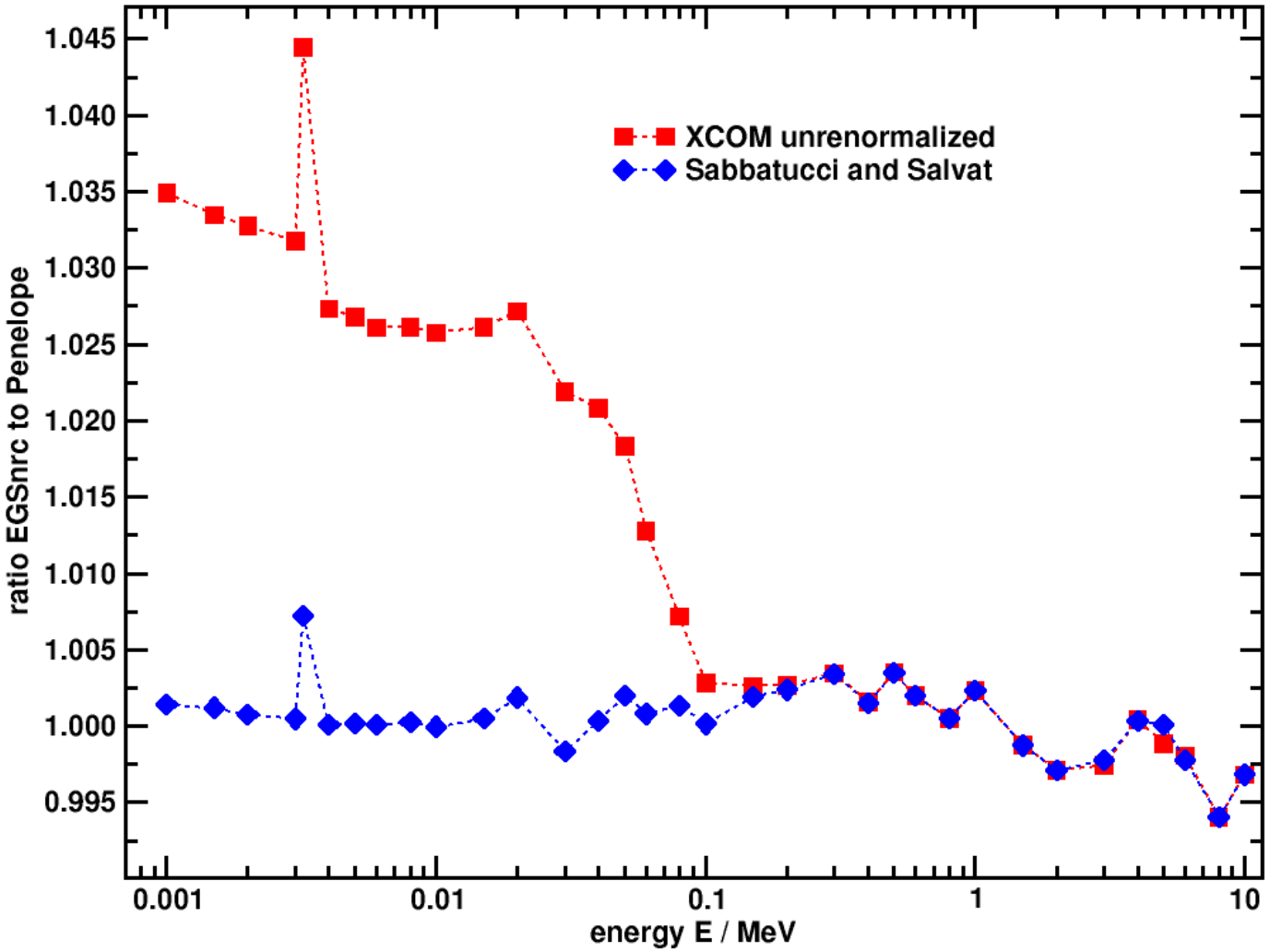
20 kV spectrum



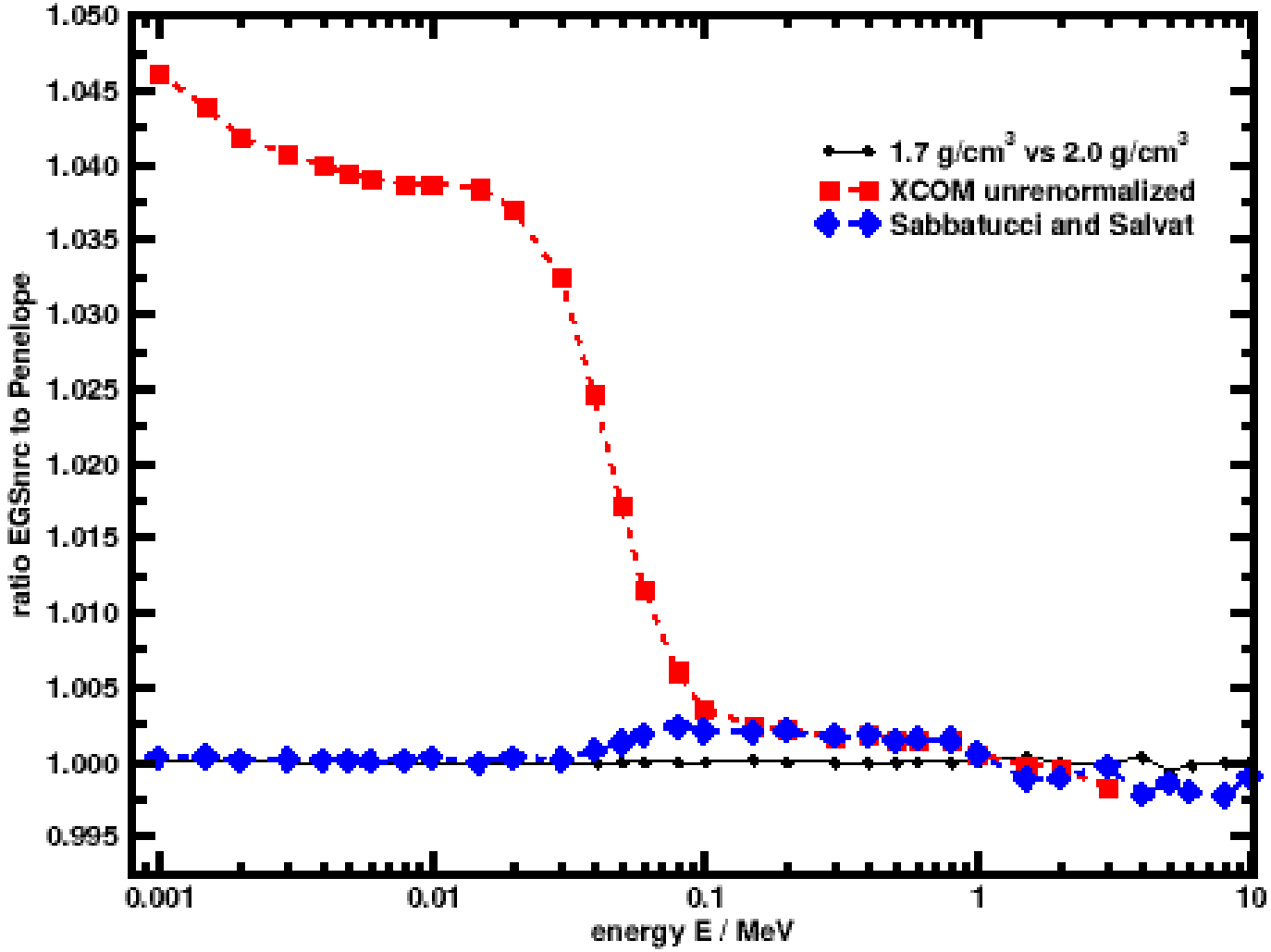
A more detailed photoelectric model

- Renormalized shell-wise photoelectric cross sections by Sabbatucci and Salvat up to 1 GeV
- Atomic sub-shells up to N7 for elements from Z=1 to Z=99 available, but only shells with binding energies above 1 keV considered.
- Medium elements sorted in decreasing Z order and inner shells sampled starting from the K shell.
- Binary search used for interpolating the shell cross sections to preserve the original adaptive energy grid.

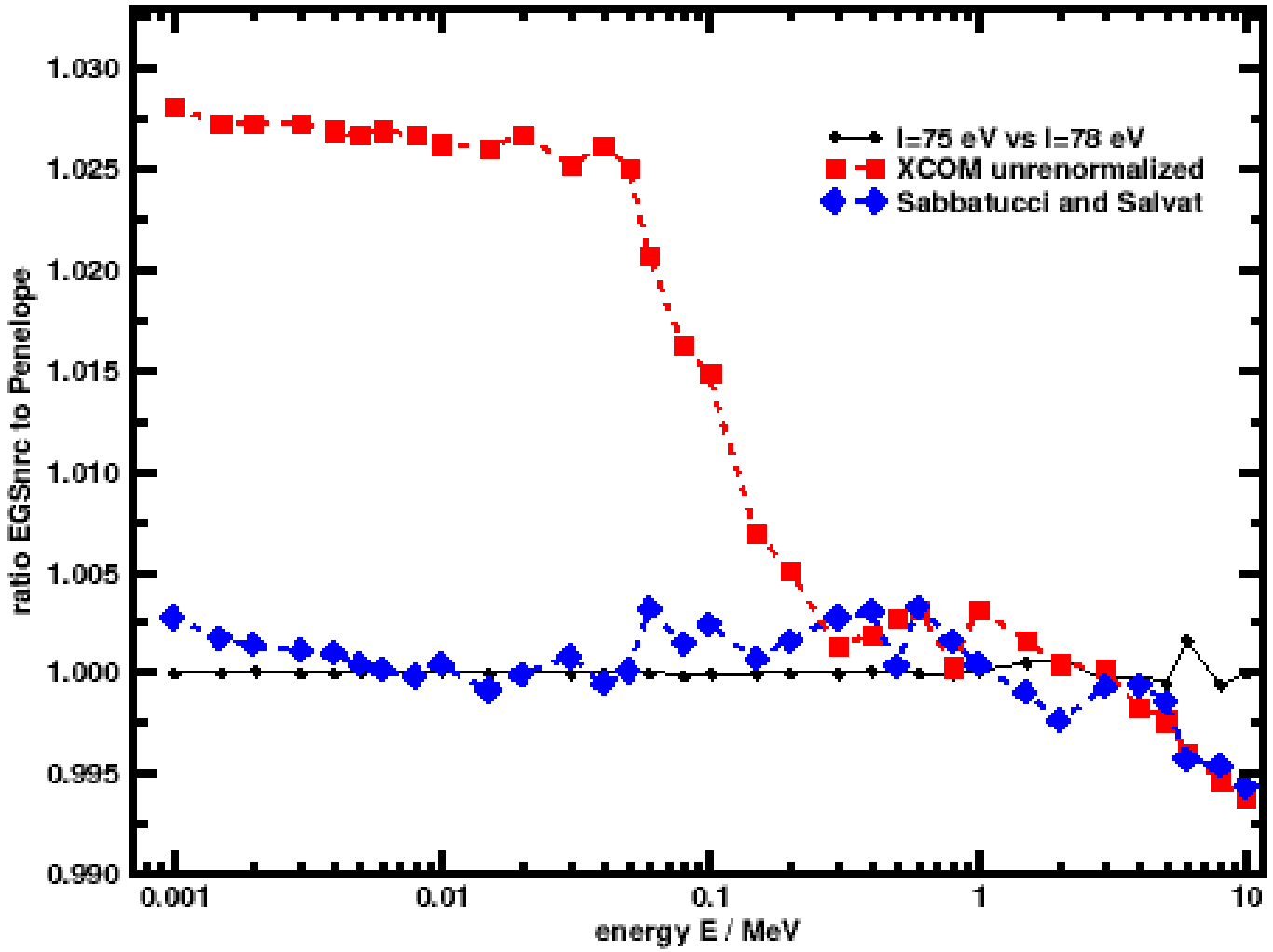
EGSnrc vs Penelope: Air mass-energy absorption coefficients



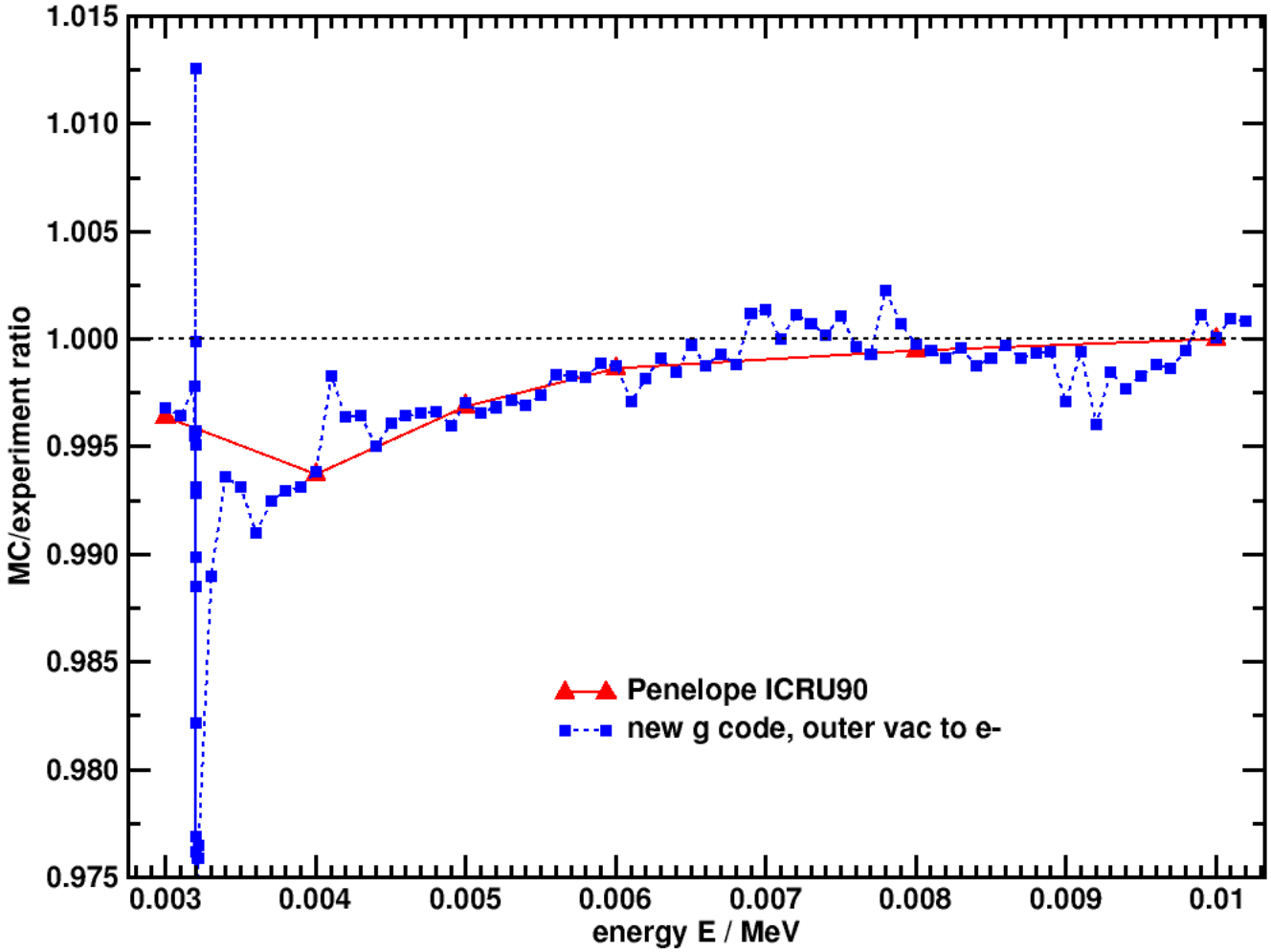
EGSnrc vs Penelope: graphite



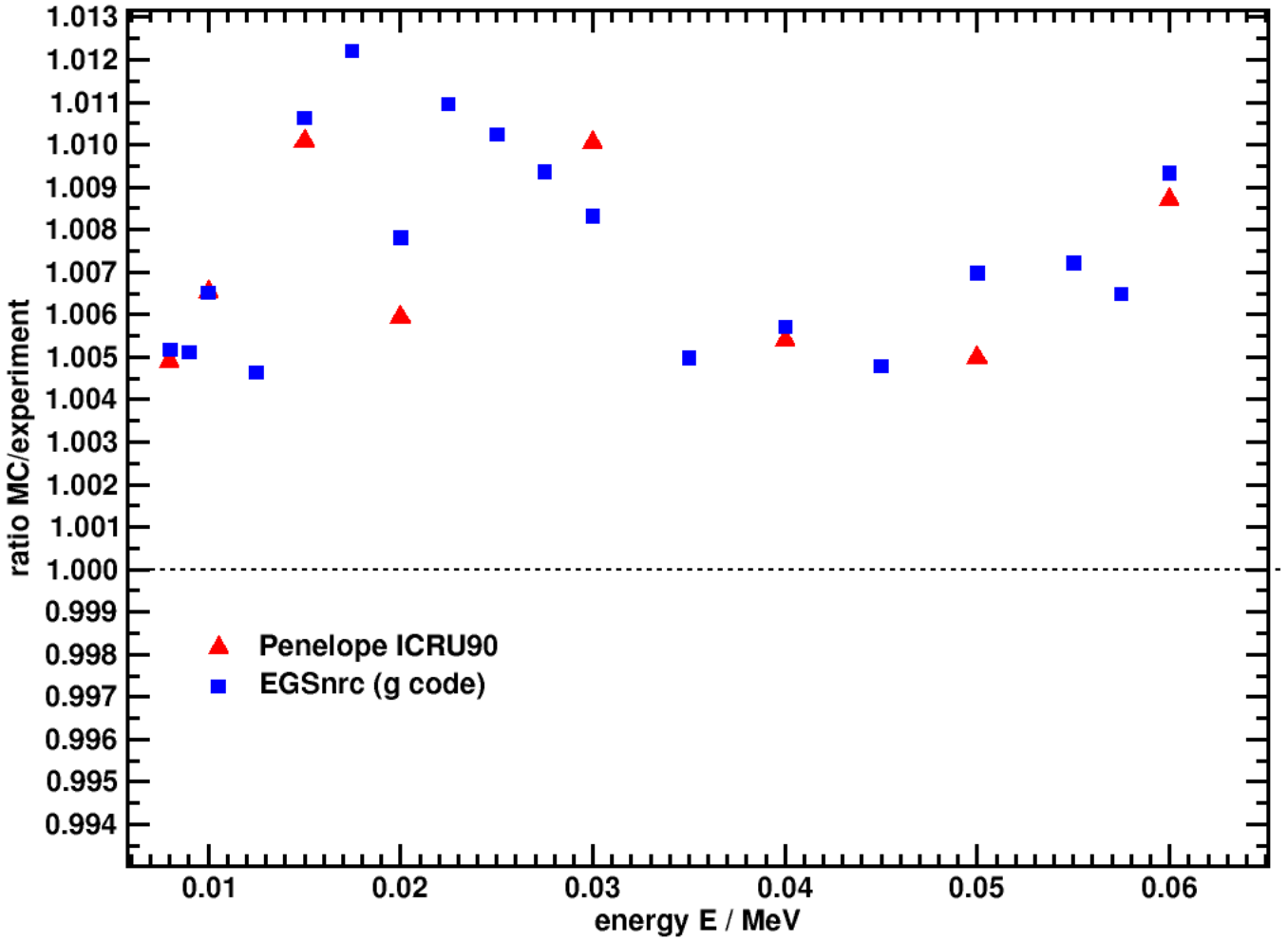
EGSnrc vs Penelope: water



MC vs Büermann (2006,2012): Air

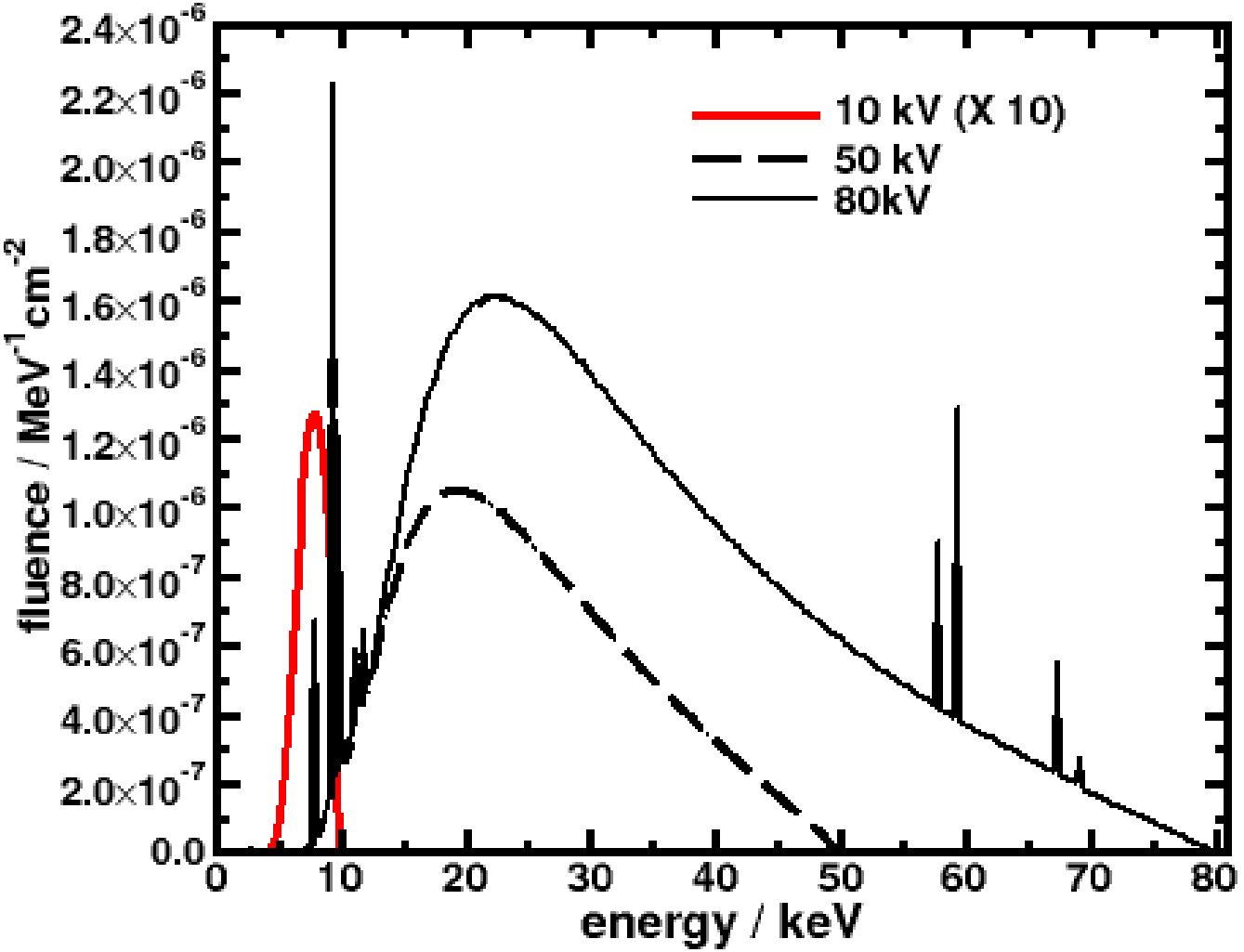


MC vs Buhr (2012): Air

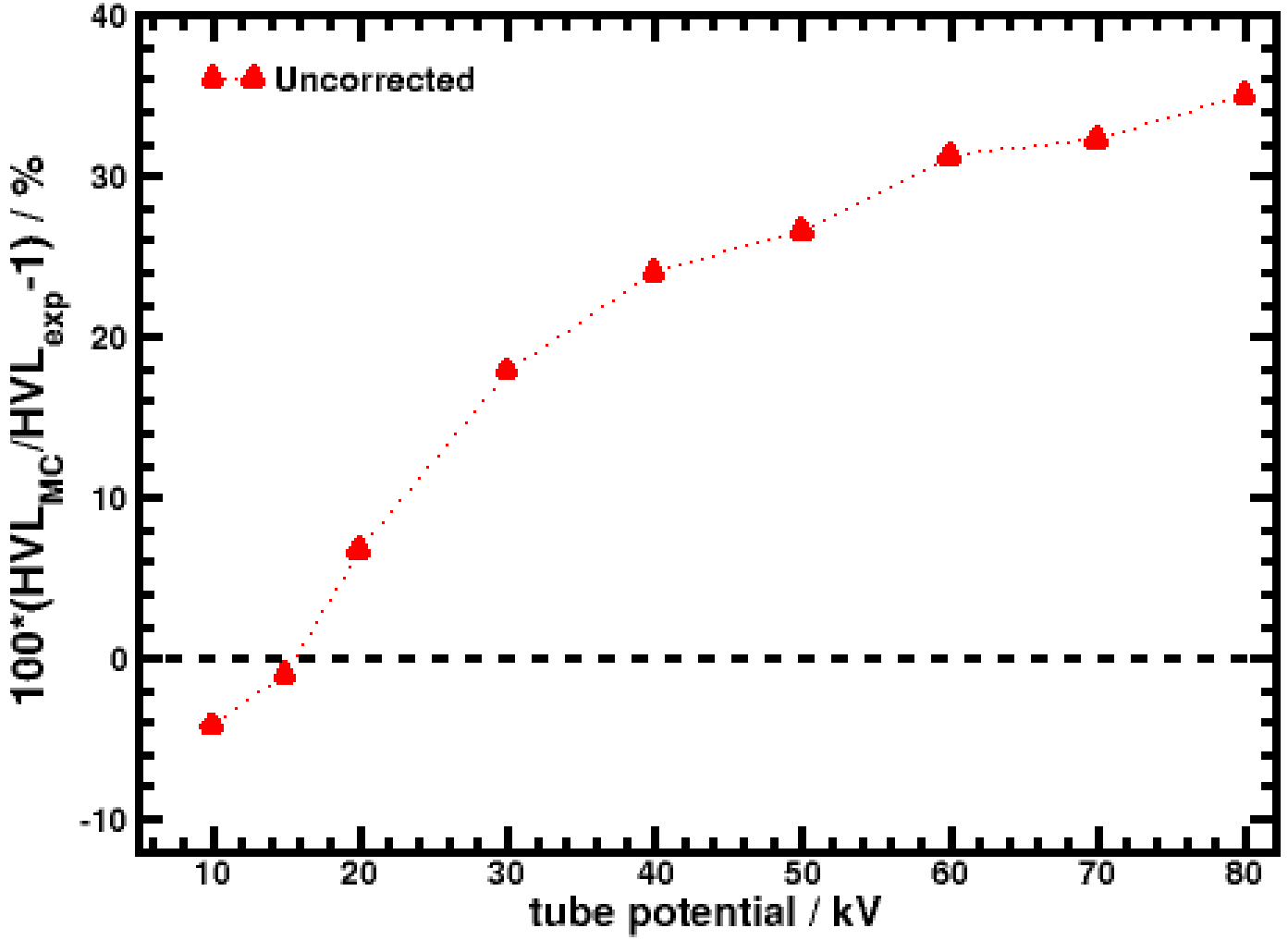


Comparison to experiments with lightly filtered x-ray beams

Lightly filtered x-ray beams



MC vs Experimental Al HVL



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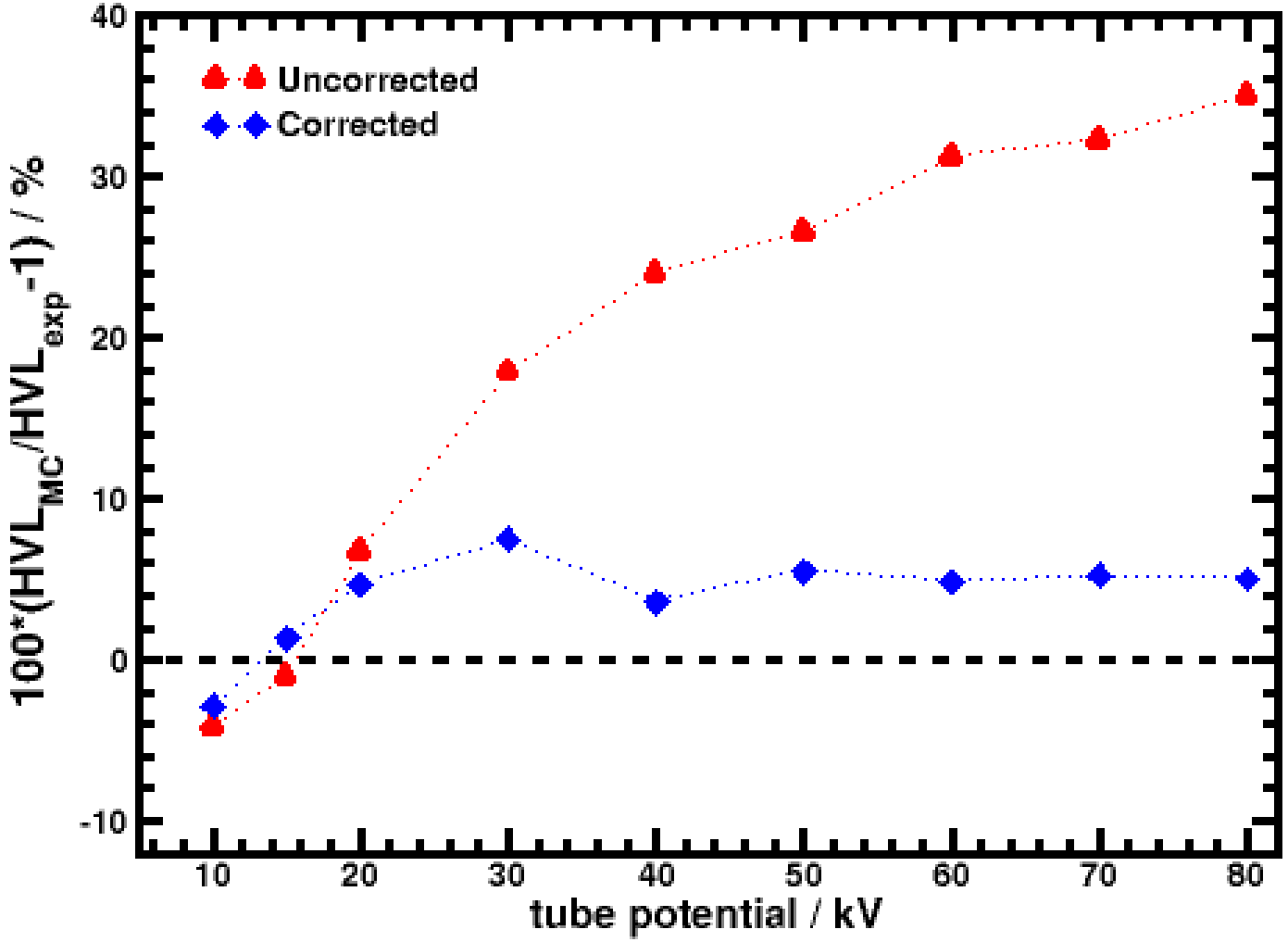
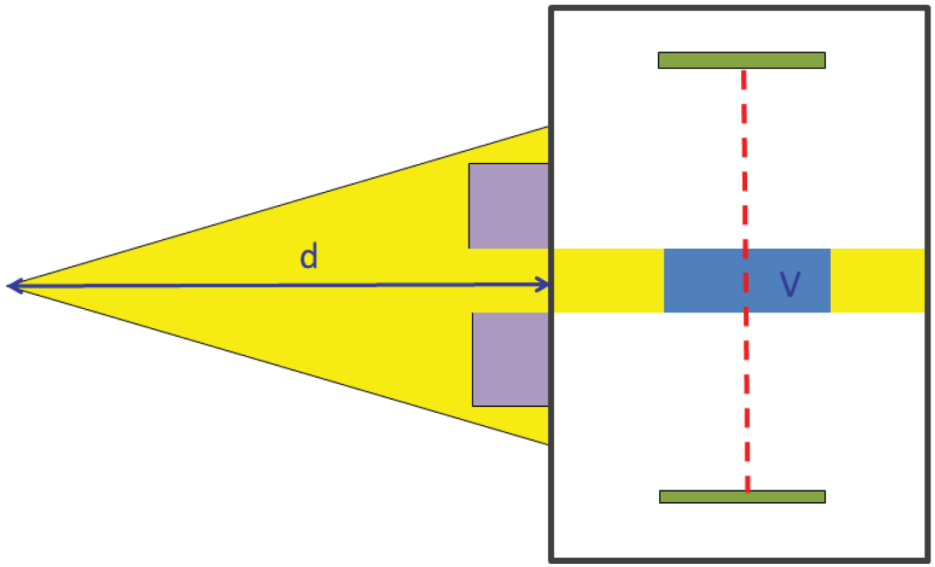


FAC correction factors

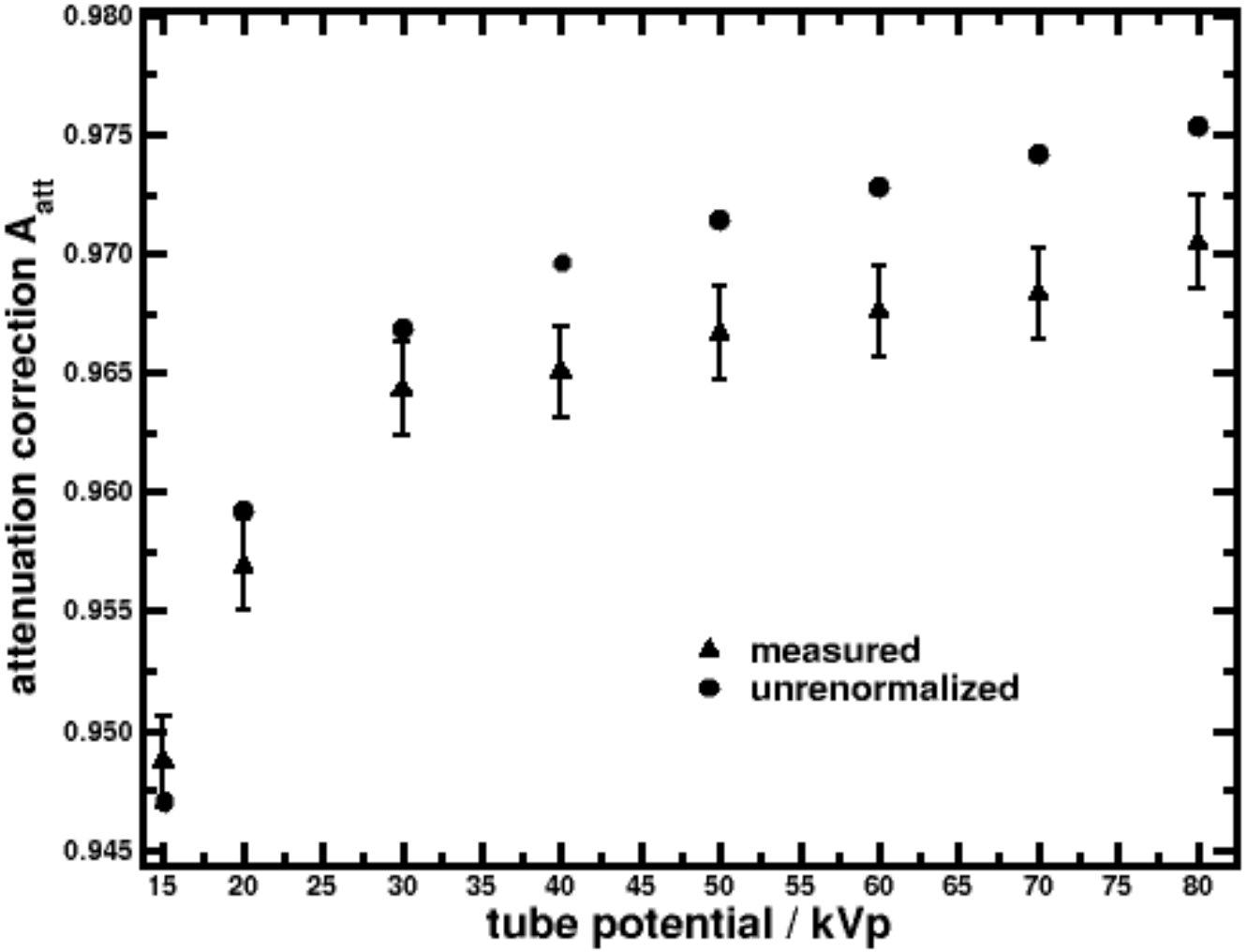
› Do not use MC-calculated corrections

› Experimentally determined attenuation correction

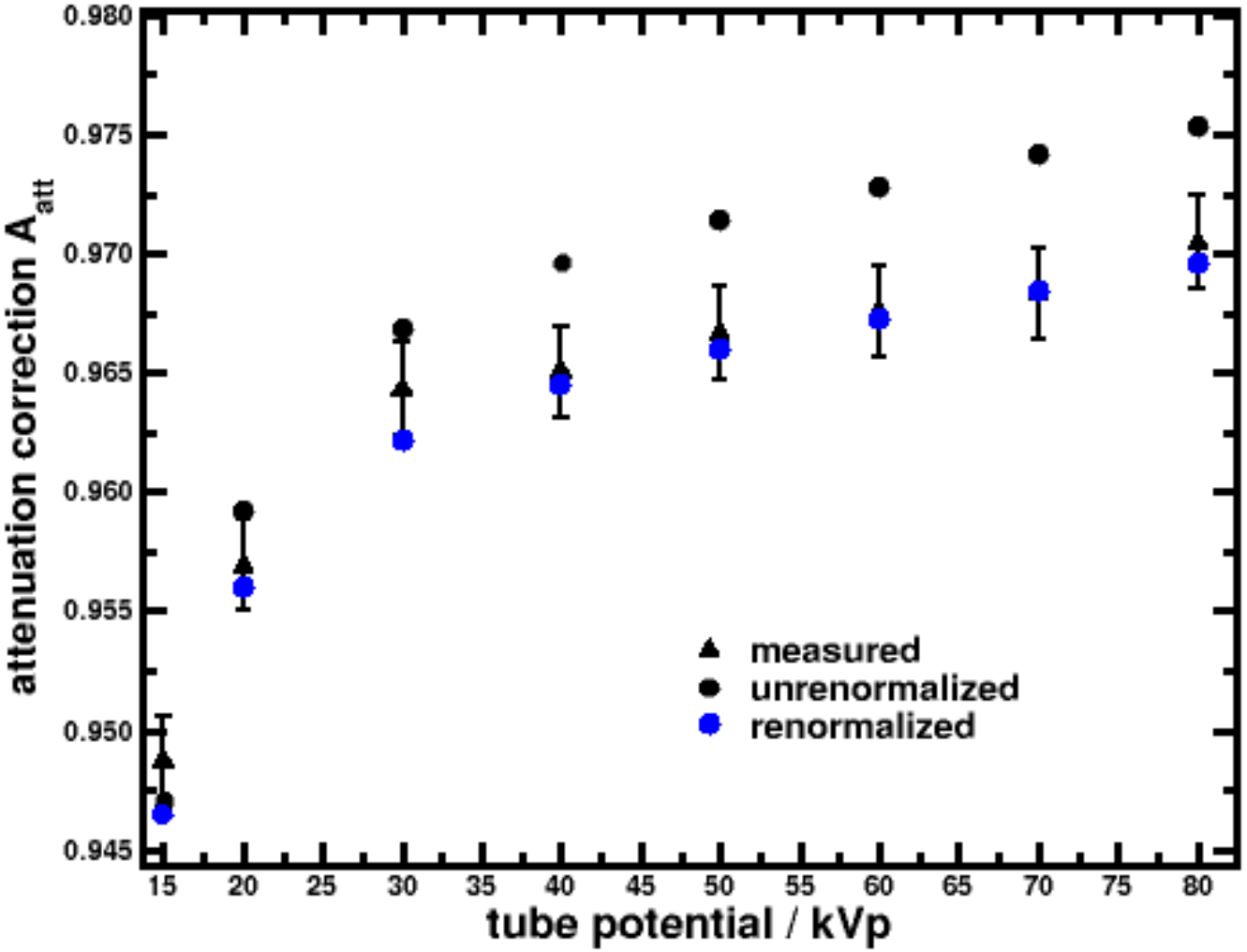
$$\frac{Q}{m_V}\left(\frac{W}{e}\right) = A_{eloss} A_{scat} A_{att,exp} A_x A_{ap} A_{cpe} A_g A_b K_{col}(d)$$



MC vs Experimental A_{att}



MC vs Experimental A_{att}



Conclusions

- Measured mass-energy attenuation coefficients are reproduced to better than 1% when using renormalized photo-electric cross sections
- Renormalized photo-electric cross sections improve agreement with experimental data for lightly filtered x-ray beams