Quantifying differences between theoretical models in calculations of Compton mass energy-transfer coefficients

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Background and Objective: Basic photon interaction data used in dosimetry, such as mass energy-transfer and mass energy-absorption coefficients, require as a main component the incoherent scattering energy-transfer fractions [1]. The simplest approach for calculating incoherent scattering cross sections is the Klein-Nishina (KN) model, in which the photon is scattered by a free electron initially at rest. As an improvement on KN, a well-known and frequently-used approximation is the Waller-Hartree (WH) model which accounts for binding effects approximately through the incoherent scattering function, but which neglects the spread in energy of photons scattered at a given angle. The relativistic impulse approximation (RIA) incorporates both binding effects and Doppler broadening and yields an expression for the DDCS differential in outgoing photon angle and energy. The key ingredient to the calculation of the RIA cross sections is the Compton profile (CP) of each atomic or molecular orbital, which is computed from the corresponding linear momentum distribution. The atomic CPs typically used are from the tabulation of Biggs et al [2].

An important and frequently cited source of photon interaction data is from Seltzer [3], who derived mass energy-absorption coefficients for elements and compounds using the WH model for Compton binding effects. In addition, interaction coefficients for compounds used in dosimetry were modeled using an independent-atom approach.

In this work we investigated for three materials of dosimetric interest (air, water, and carbon) the impact of using a molecular CP on the Compton energy-transfer cross section derived within the RIA. We also studied the difference between the RIA and the WH approach to modelling binding effects. The new energy-transfer cross sections are relevant for $\mu_{\square\square}/\square$ values in the tens of keV range, where for these materials Compton becomes the dominant interaction.

Methods: We calculated Compton cross sections within the RIA [4], which includes relativistic effects. The CPs were integrated from momentum densities obtained through self-consistent Hartree-Fock calculations, with wave functions expanded in a cc-pVTZ Gaussian basis set [5]. We performed the RIA calculations employing both molecular and atomic CPs in order to quantify the effect of using more accurate CPs to describe molecules. The atomic and molecular binding energies were taken from tabulated experimental data.

It should be noted that in our calculations of mass energy-transfer coefficients, we neglected for now the emission of characteristic x-rays in the relaxation process after the Compton interaction, as the magnitude of this effect is very small for low-*Z* atoms below 1 MeV.

Results: Figure 1 shows the Compton component of the mass energy-transfer coefficients for air and water calculated in the different formalisms discussed above, with insets showing each $\mu_{\square\square}/\square$ normalized by the $\mu_{\square\square}/\square$ for KN. Both RIA curves (molecular and atomic) are significantly closer to the KN mass energy-transfer coefficients than the WH model. The latter can differ by a large amount from the other models in the tens of keV range (e.g. ~6-10% at 20 keV).
We find that there is very little difference between the RIA with atomic and molecular CPs, thus the RIA does not seem to be particularly sensitive to the specific shape of the CPs. However, it can be

slightly more sensitive to the choice of binding energies. Nevertheless, by far the biggest impact comes from the type of formalism which is employed.

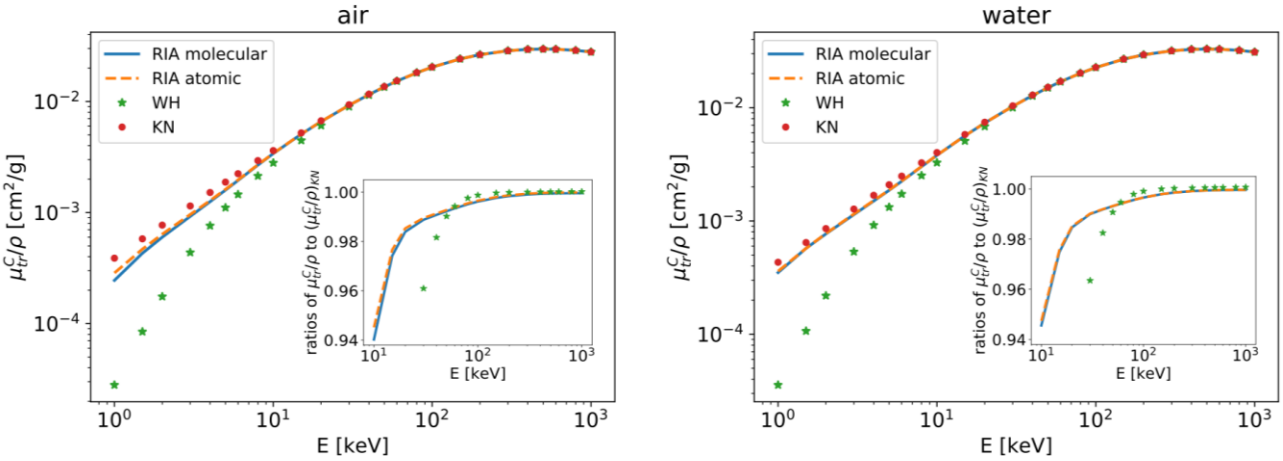

Figure 1: Mass energy-transfer coefficients for air (left) and water (right) calculated within KN, WH, and RIA (atomic & molecular CPs). The insets show data normalized to KN μ_{tr}/ρ.

Conclusions: In calculating the mass energy-transfer coefficient, the RIA using a variety of different CPs is always much closer to KN than to WH. In the immediate future we will continue with the main goal of this project, which is to determine the differences in the mass energy-absorption coefficient μ_{en}/ρ from using the various Compton cross sections. We will incorporate fluorescence emissions and radiative losses, and include all other relevant photon interactions, to fully quantify the dosimetric impact.

Relevance to CIRMS: Basic photon cross section data is essential to accurately model and measure most dosimetry quantities, and is at the foundation of established standards for ionizing radiation. Any potential improvement in such data therefore contributes to the core of the CIRMS mission. This work is especially of interest for techniques using lower energy radiation, such as brachytherapy or intraoperative radiotherapy. It represents one part of a broader doctoral project involving theoretical calculations in atomic and molecular physics with the aim of expanding the existing interaction cross section data sets for photons and electrons. The first author hopes to follow a primarily research-focused career in either an academic or clinical environment, and the CIRMS meeting provides an excellent opportunity to no only present this work, but also to foster future ideas and collaborations.

References:

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