JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

**Volume 53 (2020)**

**Supporting information for article:**

# RADDOSE-XFEL: Femtosecond time-resolved dose estimates for macromolecular XFEL experiments

**Joshua L. Dickerson, Patrick McCubbin and Elspeth Garman**

# Supplementary material

## Section 1 – Electron collision stopping power

Collision stopping power is the average energy loss per unit path length as a result of Coulomb collisions with bound atomic electrons, resulting in ionisations and excitations (Berger *et al.*, 2016).

The formula for the collision stopping power ($S_{col}$) for an atom is (Bethe, 1930, 1932):

$$S_{col} = \rho \frac{2\pi N_a r_e mc^2}{\beta^2}\frac{Z}{A}\left(F(\beta) - (2\ln I) - \delta\right) \tag{1}$$

and $F(\beta)$:

$$F(\beta) = \ln\left(\frac{mc^2 E\beta^2}{2(1-\beta^2)}\right) - \left(\left(2\sqrt{1-\beta^2} - 1 + \beta^2\right)\ln 2\right) + 1 - \beta^2 + \frac{1}{8}\left(1 - \sqrt{1-\beta^2}\right)$$

where $\rho$ is the density of the material, $N_a$ is Avogadro's number ($6.022045\times10^{23}$ mol$^{-1}$), $r_e$ is the classical electron radius ($2.817940\times10^{-15}$ m), $m$ is the rest mass of an electron ($9.10956\times10^{-31}$ kg), $c$ is the speed of light ($2.99792458\times10^{8}$ m/s), $Z$ is the atomic number of the atom, $A$ is the atomic mass (g/mol), $I$ is the mean excitation energy (described in main paper equation 7), $\delta$ is the density effect correction (but this is 0 at the energies we are using so is neglected (Berger *et al.*, 2005)) and $E$ is the kinetic energy of the electron (J) being scattered. $\beta = v/c$ where $v$ is the velocity of the electron. $\beta$ is calculated as:

$$\beta = \sqrt{1 - \frac{1}{\gamma^2}} \tag{2}$$

$$\gamma = 1 + \frac{E}{mc^2}$$

The collision stopping power for the entire sample is obtained using the sum Bragg additivity rule (ICRU, 1984), stating that the collision stopping power for a compound is the weighted sum of the atomic constituents. This is equivalent to replacing the $Z/A$ term with:

$$\langle Z/A \rangle = \sum_j \omega_j (\frac{Z_j}{A_j}) \tag{3}$$

where $j$ denotes the $j^{th}$ atomic constituent and $\omega_j$ is the fraction of the total molecular weight in the unit cell that the $j^{th}$ atom contributes. The mean excitation energy and density effect correction are also modified accordingly:

$$\ln I = \left[ \sum_j \omega_j (\frac{Z_j}{A_j}) \ln I_j \right] \times \frac{1}{\langle Z/A \rangle} \tag{4}$$

## *Section 2*

Synchrotron radiation is horizontally polarised, with the intensity of radiation that is polarised being equal to approximately 75% of the total intensity (Rybicki & Lightman, 1979)(Koch *et al.*, 1983). Photoelectrons are preferentially emitted in the same direction as the polarisation vector (Cooper & Zare, 1968). The differential emission cross section $d\sigma/d\Omega$ follows equation 5.

$$d\sigma/_{d\Omega} = \left(\frac{\sigma_{total}}{4\pi}\right) [1 + \beta P_2\,(cos\theta)] \tag{5}$$

Where $P_2(\cos\theta) = 0.5(3\cos^2\theta - 1)$, $\sigma_{total}$ is the total cross section, $\theta$ is the angle between the polarization vector and the direction of the ejected electron, and $\beta$ is an asymmetry parameter.

The asymmetry parameter varies between -1 and 2 depending on the element and the shell. For K shells, the asymmetry parameter is always 2. 75% of the fraction of photoelectrons expected to come from K shells were polarised in their emission by biasing the choice of tracks according to equation 1. 25% of K shell electrons and the fraction of photoelectrons not expected to be produced from K shells were left unpolarised, so the degree of polarisation is expected to be a slight underestimate, but this is a reasonable approximation since K shells dominate the photoelectric cross section (McMaster *et al.*, 1969).

## Supplementary Figure 1

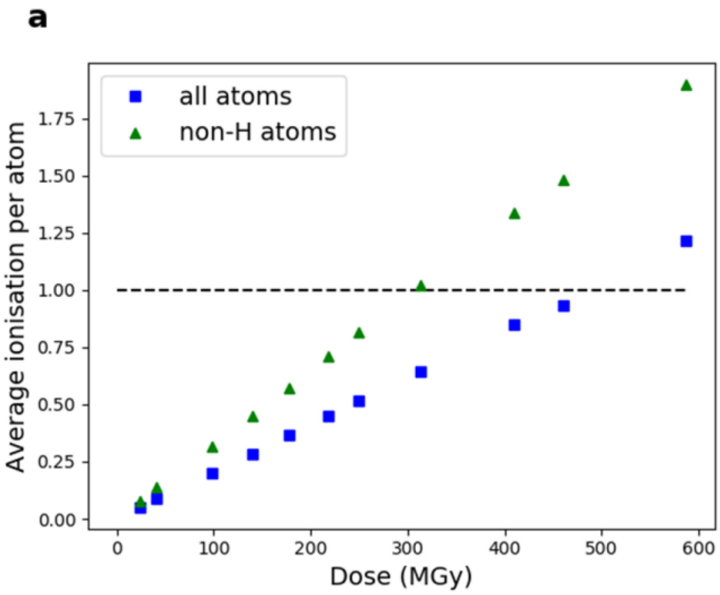

*Figure S1 –* ***Plots demonstrating the increase in average number of ionisations per atom and per non-hydrogen atom with RADDOSE-XFEL calculated doses for lysozyme crystals with a solvent of pure water.*** The dose is ~480 MGy when there is 1 ionisation per atom and ~310 MGy when there is 1 ionisation per non-hydrogen atom.

Berger, M. J., Coursey, J. S., Zucker, M. A. & Chang, J. (2005). *NIST Stand. Ref. Database*.

Berger, M. J., Inokuti, M., Anderson, H. H., Bichsel, H., Dennis, J. A., Powers, D., Seltzer, S. M. & Turner, J. E. (2016). *J. Int. Comm. Radiat. Units Meas.* **os19**, NP-NP.

Bethe, H. A. (1930). *Ann. Phys.* **397**, 325–400.

Bethe, H. A. (1932). *Zeitschrift Für Phys.* **76**, 293–299.

Cooper, J. & Zare, R. N. (1968). *J. Chem. Phys.* **48**, 942.

ICRU (1984). Stopping Powers for Electrons and Positrons 7910 Woodmont Avenue, Suite 400, Bethesda, MD 20814-3095, USA.

Koch, E. E., Eastman, D. E. & Farges, Y. (1983). Synchrotron radiation—a powerful tool in science, in Handbook of Synchrotron Radiation Amsterdam: North-Holland Publishing Company.

McMaster, W. H., Del Grande, N. K., Mallett, J. H. & Hubbell, J. H. (1969). *Lawrence Livermore Natl. Lab. Rep. UCRL-50174*.

Rybicki, G. B. & Lightman, A. P. (1979). Radiaitve Processes In Astrophysics John Wiley & Sons, Inc.