Poster Presentation

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Radiation Damage in Chemical Crystallography

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Although crystals suffering radiation damage is a well-known and studied phenomena for macromolecular crystallography[1], as far as we are aware there appears to be no such published work relating to chemical crystallography. However, there are numerous anecdotal accounts of disintegrating crystals and resolution progressively dropping off that have been ascribed to radiation damage. Since the start of operations on the small molecule synchrotron beamline I19[2] at Diamond Light Source, there have been multiple comments from several users observing sample damage in the beam. The UK National Crystallography Service[3] handles a wide variety of samples and a number of these have experienced radiation damage. In order to understand the causes and symptoms of this effect in greater detail some controlled experiments were performed. A series of experiments were conducted on crystals that were known to undergo radiation damage in order to determine some quantification of the effect. Additionally the aim is to understand what one might be able to do to mitigate against the damage caused and determine whether the effects observed are similar to those of macromolecular crystallography. The effects of varying the collection temperature, overall dose, dose rate and wavelength of X-ray used were all tested and normalised for each sample. Samples where radiation damage has been observed were chosen and were also required to be air stable and preferably not suffer from solvent loss, in order to minimize problems of non-reproducibility. Those chosen to probe this effect were: 1. A gold complex – has potential to suffer heavily from absorption effects. 2. A nickel complex with significant solvent water – this could to some extent mimic the behaviour exhibited by proteins. 3. A small organic compound – an example of unexpected decay. The poster will summarise the results of these experiments and contrast them with data collected on a high intensity rotating anode laboratory source.

[1] *B. Ravelli, E. Garman, Current Opinion of Structural Biology, 2006, 16, 624-629,* ***[2]*** *H. Nowell, S. Barnett, K. Christensen, et al, J. Synchrotron Rad, 2012, 19, 435-441,* ***[3]*** *S. Coles and P. Gale, Chem. Sci., 2012, 3, 683-689*

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