

E0060

Phasing in the Presence of Severe Site-Specific Radiation Damage Through Dose-Dependent Modeling of Heavy Atoms. M.Schiltz¹, P.Dumas² and G.Bricogne³, ¹Laboratory of Crystallography, EPFL, 1015 Lausanne, Switzerland, ²IBMC, 67084 Strasbourg, France, ³Global Phasing Ltd., Sheraton House, Cambridge CB3 0AX, England.

We re-investigated the case of a brominated RNA structure determination where SAD and MAD phasing were unsuccessful because of fast X-ray induced debromination [Ennifar *et al.* (2002), *Acta Cryst. D***58**, 1262]. We found that if the data are kept unmerged and if a dose-stamp is associated with each reflection measurement, dose-dependent occupancies can be refined for the Br atoms. Such a parametrisation has been implemented in the macromolecular phasing program SHARP. Refining such dose-dependent occupancies on an unmerged dataset gave a dramatic improvement, even for SAD phases and resulted in a good electron-density map after solvent flattening. The crucial difference is made by the use of unmerged data : phasing power is generated through the intensity-differences of symmetry-equivalent reflections recorded at different doses, i.e. corresponding to different states of the x-ray induced debromination. This approach should prove useful in all situations of experimental phasing where site-specific radiation damage occurs unavoidably and undesirably and not only in cases where one is purposely creating radiation damage to demonstrate its potential usefulness.