MS35.P26

Single crystal synchrotron X-ray diffraction for imaging hydrogen bond evolution

L. Saunders[1], H. Nowell[2], L. Thomas[1], P. Raithby[1], C. Wilson[1]
[1]University of Bath, Department of Chemistry, Bath, U.K., [2]Diamond Light Source, I19, Oxon, U.K.

Hydrogen bonding is a valuable intermolecular interaction in “engineering” solid-state materials. This is because of the directionality and relative strength (1) of these bonds. Hydrogen bonds enable charge and energy transfer, via H-bond evolution, in a range of biological and chemical systems (2). Recent work has demonstrated that single crystal X-ray diffraction can be used to image the evolution of hydrogen bonds, including variable temperature proton migration and proton disorder processes. In particular, in a recent study of the temperature dependent proton disorder in hydrogen bonded 3,5-dinitrobenzoic acid (3,5-DNBA) dimers, the proton disorder deduced from data collected on an X-ray laboratory source is in agreement with that found from neutron data (3). This work focuses on variable temperature single crystal synchrotron X-ray diffraction, for the imaging of evolving hydrogen bonds. The development of appropriate methodology is important here, particularly as previous studies have involved laboratory X-ray sources only. Results will be presented from variable temperature data collections on I19, at the Diamond Light Source, and on beamline 11.3.1, at the Advanced Light Source (ALS), on systems such as 3,5-DNBA and co-crystals of benzimidazole, both exhibiting proton disorder across hydrogen bonding interactions. Synchrotron X-ray diffraction measurements have also been used to follow the change in the position of a proton within an intramolecular [N—H•••N]+ hydrogen bond across a range of proton-sponge molecular complexes. Importantly, it has been possible to visualise the evolving hydrogen atom position in Fourier difference electron density maps generated from the synchrotron data. In particular, for the 35-DNBA study, the clearest picture of the evolving hydrogen atom position is observed in those generated from data collected at the ALS; even clearer than that observed in X-ray laboratory and neutron measurements on the same system.

***[1]** G. R. Desiraju, Angew. Chem. Int. Ed. Engl., 1995, 21, 34, 2311-2327, **[2]** S. Horiuchi, R. Kumai, and Y. Tokura, Angew. Chem. Int. Ed., 2007, 46, 3497-3501, **[3]** A. O. F. Jones, N. Blagden, G. J. McIntyre, et al., Cryst. Growth Des., 2013, 13, 497-509*

Keywords: Hydrogen bond, synchrotrons, electron density visualisation