Combined Experimental and Theoretical Studies of Solid State Proton Migration

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Hydrogen bonds are of great interest, due to their importance in structural, functional and dynamical properties of chemical systems, ranging from inorganic to biological chemistry [1]. The very strong hydrogen bonds are of current interest because they enable charge and energy to be transferred between molecules in the solid state.

Recent work has focused on urea-acid complexes, which contain a rich variety of short, strong hydrogen bonds in a relatively simple framework. It has been demonstrated that the combination of cutting edge computational techniques (MD/PW-DFT) with variable temperature neutron diffraction results was successful in showing the migration of the proton with increasing temperature and a plausible explanation for the effect has been presented [2].

A collaborative project with the aim of continuing this work has now begun. A series of hydrogen-bonded adducts have been prepared in a systematic manner for experimental and theoretical investigation. In particular, the effects of temperature and pressure on proton migration and disorder in these adducts are being explored to shed light on the factors that influence proton migration. In this poster presentation we will describe some of our most recent results, which include studies on periodic acid-urea and ammonium iodate.

[1] Steiner T., *Angew. Chem. Int. Ed.*, 2002, **41**, 48. [2] Morrison C. A., Siddick M. M., Camp P. J., Wilson C. C., *J. Am. Chem. Soc.*, *in press*.

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