Strong Hydrogen Bonding

Jonathan W. Steed*

Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, UK

We have long been interested in the interplay of molecular and crystal structure. Crystal assembly is dominated first and foremost by the minimization of repulsive interactions between core electrons, but there is then a synergy between various attractive intermolecular forces that can represent a continuum of strong and often highly directional forces down to van der Waals interactions. In strongly hydrogen bonded systems, particularly when the strong hydrogen bonds are relatively isolated, subtle manipulation of the hydrogen bonding is reflected in structure change in a way that is predictable and understandable. In this presentation I will discuss several systems in which precise structure determination using data from D19 along with VIVALDI coupled with energy calculations using the PACHA method (in collaboration with Prof. Marc Henry in Strasbourg) represent a very powerful tool for the understanding and modulation of solid state structure. One such example, in which a gradual order-disorder transition is mediated by a well-understood water square is shown in Fig. 1.

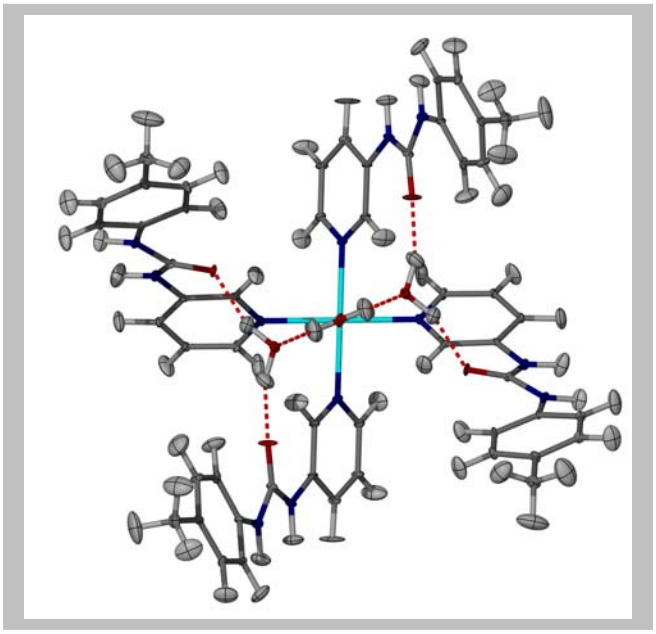

Figure 1: Single crystal neutron structure at 4K for $[Co(TUP)_4(H_2O)_2](SO_4)\cdot 2H_2O$ (TUP = tolyl ureidopyridine).[1]

References

[1] David R. Turner, Marc Henry, Garry S. MacIntyre, Clive Wilkinson, Sax A. Mason Andres E. Goeta and Jonathan W. Steed, *J. Am. Chem. Soc.*, submitted.