Diffraction and Computational Studies of Hydrogen Bonded Base Paired Systems

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Diffraction methods are often utilised to gain a greater insight hydrogen bonding interactions. In work to date the advantages of single crystal variable temperature x-ray and neutron diffraction, coupled with the imaging capabilities of Fourier difference maps, as complementary techniques for anomalous hydrogen bonding investigations have been highlighted [1]. In addition, recent advances in computational chemistry have enabled calculations to be carried out both on isolated molecules and in the periodic (i.e. crystalline) environment [2].

The main aim of this poster is to discuss the use of complementary methods to promote a better understanding of hydrogen bonding within carboxylic acid dimers and nucleic acid base paired systems. One particular system of interest is 3',5'-di-O-acetylthymidine and various techniques have been utilised to determine the presence of anomalous hydrogen behaviour. A crucial part of this has been a multiple temperature high resolution study carried out on station 9.8 at SRS, Daresbury. Alongside experimental work, recent computational work will highlight how these new methods can augment traditional experimental results. Overall it is hoped that the research presented will again highlight the importance of complementary techniques in crystallographic research.

[1] Parkin A., Harte S. M., Goeta A. E., Wilson C. C., *New J. Chem*., 2004, **28**, 718. [2] Wilson C. C., Morrison C. A., *Chem. Phys. Lett.,* 2002, **362**, 85-89.

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