Poster Presentation

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Interplay of Packing, Proton Transfer and Hydrogen Bonding on Crystal Properties

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The designed creation of crystalline materials with desired physical properties is a key objective of crystal engineering. Currently the development of multi-component crystals such as salts and co-crystals as a route for the modification of physicochemical properties has been a major focus within the field. However, while the creation of such materials has been repeatedly demonstrated, understanding the structure-property relationships between the component molecules and the final crystal form is great challenge, so limiting the ability to design new materials. Controlling the proton transfer process is vital for the designed creation of protonic conductive materials but also important in other fields as the proton location alters the physical properties of other systems such as pharmaceutical or photochromic materials. The interaction between chemical structure and local crystallographic environment has been shown to alter the energy landscape of the proton transfer process [1,2] This presentation will report on work investigating the relationships between changes in molecular and crystal structure on proton transfer processes in multi-component materials. Both experimental crystal growth and computational modelling have been used to study proton transfer in binary and ternary systems based on the carboxylic acid…pyridine hydrogen bond. Understanding the interplay between packing forces and proton transfer in controlling the observed photochromism in bipy/rac-mandelic acid system and how this can be used to design new material based on these concepts.

[1] *Jones A. O. F., Blagden N., McIntyre G. J., et al., (2013). Crystal Growth & Design. 13, 497–509.,* ***[2]*** *Seaton C. C., Blagden N., Munshi T., et al. (2013). Chem. - Eur. J. 19, 10663–10671.*

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