Poster Sessions

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**Design and control of hydrogen bonding in DMAN proton sponge complexes**  
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1,8-bis(dimethylamino)naphthalene (DMAN) is commonly known as a proton sponge and is often observed to accept a proton from acidic materials into an N–H–N intramolecular hydrogen bond. We have been using co-crystallisation with a series of benzoic acid derivatives to explore the charge assisted hydrogen bonding induced both within the DMAN and between benzoic acid molecules. X-ray diffraction has been used extensively to determine the resulting crystal structures, with a particular emphasis on attempting to determine accurate hydrogen atom parameters and to define the hydrogen bonding schemes.

In general, DMAN and halogen substituted benzoic acid co-crystals form in a 1:2 ratio where the DMAN molecule deprotonates one benzoic acid molecule taking the hydrogen into a short strong intramolecular hydrogen bond. To compensate for this, the two halogen substituted benzoic acid molecules then form a short, strong, charge assisted hydrogen bond between themselves to stabilise this loss of a proton by forming a single hydrogen bonded dimer motif and with the protonated DMAN molecule acting as building blocks of the complex. This dimer motif is present across almost the entire series of halogen substituted benzoic acid and DMAN molecular complexes with divergence present between the benzoic acids relative position to each other caused mainly by the halogen-halogen interactions occurring in these complexes. Increasing the competition for hydrogen bonds by using hydroxybenzoic acids as the co-molecule induces a different composition ratio and behaviour of the benzoic acid in the complex formed. The 3-hydroxy and 4-hydroxy benzoic acids co-crystallise with DMAN in a hydrated 2:2:1 ratio where the stabilisation of charge assisted hydrogen bond between themselves to stabilise this loss of a proton by forming a single hydrogen bonded dimer motif and with the protonated DMAN molecule acting as building blocks of the complex. This dimer motif is present across almost the entire series of halogen substituted benzoic acid and DMAN molecular complexes with divergence present between the benzoic acids relative position to each other caused mainly by the halogen-halogen interactions occurring in these complexes. Increasing the competition for hydrogen bonds by using hydroxybenzoic acids as the co-molecule induces a different composition ratio and behaviour of the benzoic acid in the complex formed. The 3-hydroxy and 4-hydroxy benzoic acids co-crystallise with DMAN in a hydrated 2:2:1 ratio where the stabilisation of charge assisted hydrogen bond between themselves to stabilise this loss of a proton by forming a single hydrogen bonded dimer motif and with the protonated DMAN molecule acting as building blocks of the complex. This dimer motif is present across almost the entire series of halogen substituted benzoic acid and DMAN molecular complexes with divergence present between the benzoic acids relative position to each other caused mainly by the halogen-halogen interactions occurring in these complexes.

**Keywords:** hydrogen-bonding, neutron, laue

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**Organic and inorganic halogens as HB acceptors in halopyridine complexes of Cu**

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Although interactions involving halogen acceptors have been reported from the early years of hydrogen bonding (HB) research, the primary attention was paid on the oxygen and nitrogen acceptors [1]. Furthermore, due to large partial negative charges in their complexes, fluorine and chlorine are more frequently observed as HB acceptors than less electronegative heavier halogens, e.g. bromine and iodine. The information retrieved from X-ray studies on hydrogen bonding are geometry details of the D–H–A–Y moiety. While the linear D–H–A–Y angles are statistically favoured over bent ones, the preference for the bent angles at accepting halogen atoms originates in the highly anisotropic electron density around the halogen nucleus known as ‘polar flattening’ [2].

Here we report the preparation and characterization of a series of halopyridine complexes of copper(II) with intention to examine the geometry details of weak hydrogen bonding involving organic and inorganic halogens as HB acceptors. In addition to thermal and spectroscopic techniques, the complexes have been characterized using single crystal X-ray diffraction as well.

**Keywords:** Cu(II) complexes, weak H-bonds, supramolecular synthons

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**Structural systematics of fluoro-N-(pyridyl)benzamides and related isomer grids**  
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A 3x3 isomer grid of nine fluoro-N-(pyridyl)benzamides (C12H8N2OF) as Fx (x = para-meta-ortho-) was studied to evaluate and correlate structural relationships from both ab initio calculations and the solid-state. The effect of fluoro (Fx) and pyridine N atom (x) substitution patterns on molecular conformations from calculations and in terms of molecular organization was evaluated.

Eight isomers are forming N-H⋯N hydrogen bonds and only one isomer (Fom) is found to have exclusively N-H⋯O=C interactions. However, the Fpm isomer was found in two polymorphs, Fpm_N and Fpm_O, both in the same space group (P21/n) but with different structures.