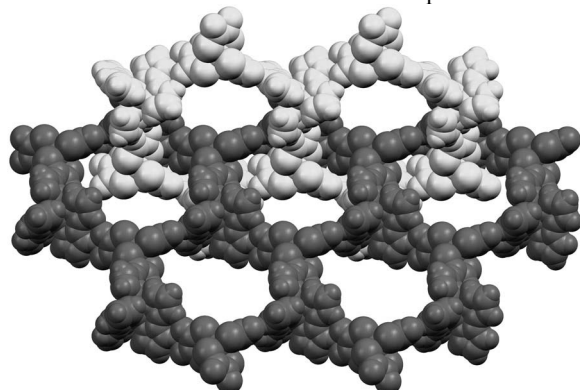


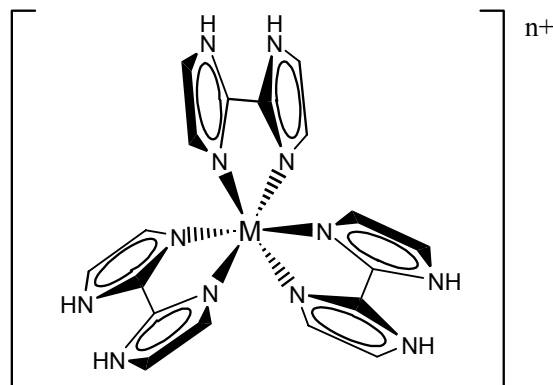
P.09.05.3*Acta Cryst.* (2005). A61, C361**Synthesis of 2D and 3D Nets Using Biimidazole Complexes**Alexandra M. E. Griffin, A. Guy Orpen, *School of Chemistry, University of Bristol, Bristol BS8 1TS*. E-mail: a.griffin@bristol.ac.uk

The use of hydrogen-bonding to control the arrangements of cations and anions has been well documented in previous research.[1]



[2] Here we report tris-chelated metal complexes containing the biimidazole ligand, which are capable of hydrogen-bonding to form three-dimensional and interpenetrated two-dimensional nets.

In particular $[\text{Ni}(\text{H}_2\text{biim})_3]^{2+}$ and $[\text{Cr}(\text{H}_2\text{biim})_3]^{3+}$ (H_2biim = 2,2'-biimidazole) have been crystallized with a variety of anionic tectons capable of hydrogen bonding to these cations.



[1] Podesta T. J., Orpen A. G., *CrystEngComm.*, 2002, 4, 336. [2] Angeloni A., Orpen A. G., *Chem. Commun.*, 2001, 4, 343.

Keywords: crystal synthesis, hydrogen bonding, biimidazole complexes

P.09.05.4*Acta Cryst.* (2005). A61, C361**Bio-mimicking Self Assembly in Materials: Role of Hydrogen and Halogen Bonding**Ashwani Vij, Joseph M. Mabry, Wade W. Grabow, Vandana Vij, *AFRL/PRSP-PRSM, 10 E. Saturn Blvd. Edwards, CA 93524*. E-mail: ashwani.vij@edwards.af.mil

Hydrogen bonding to an electronegative heteroatom is becoming an increasingly interesting area for chemists, biochemists and biologists. Because of such interactions, proteins can interact with drugs, which has enhanced our understanding of various biological processes within the body. We have made similar attempts to investigate the structures and properties of “big” small molecules, especially those containing silicon using a “macromolecular” approach to deal with data quality and diffraction issues. Halogen bonding in molecules containing silicon and tin is a favored process due to the capability of these atoms to expand their coordination spheres. Such an expansion of the coordination sphere can sometimes result in formation of unexpected crystal structures, which impart outstanding physical properties. If these systems contain fluorocarbons or fluorinated ligands, there are domains of hydrophobicity and hydrophilicity. The challenge is, however, to overcome the low temperature phase transitions to obtain meaningful

crystal structures without the destruction of crystal lattice. Data collection employing CCD or GADD detectors utilizing a sealed tube (Copper or Molybdenum) or rotating anode sources and structure solution/refinement strategies will be discussed, time permitting.

Distribution A: Approved for public release, distribution unlimited

Keywords: self assembly, biomimicking, halogen bonding

P.09.05.5*Acta Cryst.* (2005). A61, C361**Benzylidimethylalkylammonium Haloplumbates: Organic/inorganic Composite Materials**Maciej Hodorowicz^a, Katarzyna Stadnicka^a, ^a *Faculty of Chemistry, Jagiellonian University, Kraków, Poland*. E-mail: hodorowm@chemia.uj.edu.pl

In due course of investigations of the relationships between sorption properties of benzylalkylammonium cations and their behaviour in the crystalline phases (the way of packing and the type of interactions), benzylidimethyl-n-alkylammonium haloplumbates(II) with $n = 2 - 6$ and $9 - 10$ were tailored.

In recent years the chemistry of transition metal complexes has been developed towards the construction of different (unusual) structural models in order to rationalize the correlations between structure and physical properties. Halometallates(II) represent interesting systems for designing low-dimensional architecture with specific electronic, thermal, electrical, magnetic and polymorphic properties. Haloplumbates(II) form a particular class of these materials because the flexibility of Pb(II) coordination sphere and non-stereospecific nature of the halide anions. As mixed organic/inorganic materials benzylidimethyl-n-alkylammonium haloplumbates(II) combine properties typical for organic molecular crystals with those associated to inorganic solids. The crystal structures of several benzylidimethyl-n-alkylammonium haloplumbates(II) were determined by X-ray diffraction showing one-dimensional linear chains built of $-\text{[PbBr}_3\text{]}_n-$ mers. The studied structures could easily be modified by the size of ammonium cations, their packing properties and an ability to form weak hydrogen bond systems of C-H... π and C-H...X (X = halogene atom) type.

Keywords: haloplumbates, alkylammonium cations, structure

P.09.05.6*Acta Cryst.* (2005). A61, C361-C362**Crystalline Supramolecular Ladders via Co-Crystals**Tony N Sokolov, Tomislav Frišćić, Leonard R. Mac Gillivray, *Department of Chemistry, University of Iowa*. E-mail: tony-sokolov@uiowa.edu

Controlling the organization of molecules in organic solids is a topic of fundamental importance for the design of supramolecular materials. In this context, methods to dictate the organization of functional molecules in one dimensional arrays are emerging as an important area. The formation of such arrays may be achieved in either two ways: covalent functionalization of a substrate or co-crystallization. While substrate functionalization allows for the packing to be directed solely by the substrate, meaning that the bulk crystal is based purely on the substrate, the method also inherently requires further covalent modification to tune a desired property. In contrast, co-crystallization allows for the use of a “divide and conquer” approach, enabling the substrate to remain untouched while changes to the co-crystallizing agent tune a desired property. In this poster, we demonstrate the ability of 3-aminophenol (3AP) to function as a co-crystallization agent to direct the formation of infinite 1-D ladder-like assemblies in the solid state. The approach utilizes an O-H bond coupled with one N-H bond of 3AP to direct the face-to-face arrangement of a series of bipyridine units, by way of hydrogen bonds, while the second N-H bond of the amine interacts with a neighboring assembly. This approach has been extended to a series of three unsaturated homologues having the 4-pyridyl functionality; namely, 4,4'-dipyridyl(dpy), *trans*-1,2-bis-(4-pyridyl)acetylene(bpa), and *trans*-1,2-bis-(4-pyridyl)ethylene(bpe). X-ray crystal structure analyses of the co-crystals involving (3AP)-(dpy), (3AP)-(bpa), and