molecule of water. These cations adopt a typical chair conformation and are alternate with hexachloroindiumate complex forming layers parallel to the (10-1) plane (Fig.1). In the crystal, the components of the structure are linked via intra and intermolecular N---H-O, O-H...Cl, C-H...O and N-H...Cl hydrogen bonds to form a complex three-dimensional network. Additional stabilization within these layers is provided by weak intermolecular C-H...Cl interactions.


Keywords: hexamethylenediammonium salts, hydrogen bonding, chain geometry.

**MS73.P08**


Effect of the anion on cation chain geometry in hexamethylenediammonium salts

Charmaine Ardene, Gert J. Kruger, Department of Chemistry, University of Johannesburg, PO Box 524, Auckland Park, Johannesburg (South Africa), 2006. E-mail: carderne@uj.ac.za

The investigation of structure-property relationships and applications of N-alkyldiammonium salts are of continued importance and form the basis of our ongoing studies [1], [2] of these materials. In particular, we have focused on the structural characteristics of the N-alkyldiammonium salts as they are precursors to layered inorganic-organic perovskite-type hybrids [3]; they are bidentate ligands in transition metal complexes that have applications in propellants, explosives and pyrotechnic compositions [4]; they have structure directing properties in the synthesis of a number of zeolites [5]; and many have biological applications [6].

This work focuses on the effect of variation of the anion in hexamethylenediammonium salts on the diamonium cation geometry. Four crystal structures are presented – the chloride, bromide, iodide and nitrate salts of hexamethylenediamine. Significant deviations from diamonium cation chain planarity become evident as the anion is varied. The smaller spherical anions (such as chloride and bromide) showed minor deviations from dication chain planarity while larger spherical anions (such as iodide) and large trigonal planar anions (such as nitrate) showed major deviations from di cation chain planarity – resulting in kinked and buckled dication chain conformations.

The variation in anion type in the crystal structures resulted in significantly different types of hydrogen bonding interactions being identified. These interactions were found to be strong N-H-...X bonds (X = anion type) as well as weak C-H-...X bonds. All relevant bonds were found to be directly related to the observed aberration in dication chain geometry.


Keywords: hexamethylenediammonium salts, hydrogen bonding, structural chemistry.

**MS73.P09**


New hybrid compound based on fluorosilicate with complex hydrogen-bonding scheme.

Ratiba Belhouas, a Sofia Bouacida, a Chaouki Boudren, a and Jean-Claude Daran,* a Unité de recherche CHEMS, Université Constantine, Algeria b Département SM, Université LBM, Oum El Bouaghi, (Alegria). Laboratoire de Chimie de Coordination, Université de Toulouse, (France). E-mail: Belhouas_ratiba@yahoo.fr

Fluorosilicate salts involving onium cations of N- and O-containing organic bases and amino acids have practical applications as ionic liquids (Katayama et al., 2001), dielectrics with cryptocrystalline structure (Kalem, 2004) and layered organic-inorganic hybrid materials (Airoldi & De Farias, 2000). This new hybrid compound has been prepared by slow evaporation of an aqueous solution of adenine, SiO₂ and hydrofluoric acid in a molar ratio of 10:5:1.

The asymmetric unit of Bisadeniniumhexafluorosilicate(VI)hydrate consists of one adeninium cation, half of a fluorosilicate anion located on inversion center and a solvent water molecule which are connected through the water molecules with N-H...O and O-H...F hydrogen bonds to the (10-1) plane. The adeninium cations are connected by N-H...N hydrogen bonds involving one H atom of the NH₃ groups and the H atom of the protonated N atom of the five membered ring forming respectively centrosymmetric R₂(10) and R₂(8) rings. These N-H...N hydrogen bonds build up an infinite planar ribbon parallel to the (1 2 2) plane. The H atoms of the water molecules interact with the F2 and F3 atoms of the fluorosilicate building R₃(12) graph set motif. These O-H...F hydrogen bonds form infinite chains parallel to the[1 0 0] axis.

The adeninium ribbons and the chains formed by the water and fluorosilicate are further connected through N-H...O1W, N-H...F and O1W-H...F building a R₂(10) graph set motif.


Keywords: hybrid materials, single crystal, hydrogen bond.

**MS73.P10**


D-H-...X Contacts Performed by N-Heterocycles: a Practical View

Yu Sun, Werner R. Thiel, Fachbereich Chemie, TU Kaiserslautern, 67663 Kaiserslautern (Germany). E-mail: sun@chemie.uni-kl.de

N-Heterocycles are important structural motifs in organic syntheses, coordination chemistry and also in various catalytically active compounds. For quite some time our group has been working on the development of novel N-heterocyclic ligands based on pyrazoles, pyrimidines and related structures.

The existence of N-H(s) groups obviously provides a good opportunity to form hydrogen bonds with other molecules and structures between different donors and acceptors as the acceptors were observed. These hydrogen bond acceptors could be halide anions (X⁻), metal-halides (X-M) and carbon-halides (X-C), most of them serving at the same time as counter anions, templates and solvents.

In order to better understand the roles of these counter anions, templates and solvents in the nucleation processes and sometimes even in the synthesis procedures, a brief study of the hydrogen bonds involving halogens as the acceptors in these structures was carried out.