

molecule of water. These cations adopt a typical chair conformation and are alternate with hexachloridoindiumate 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.

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Effect of the anion on cation chain geometry in hexamethylenediammonium salts

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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 diammonium cation geometry. Four crystal structures are presented – the chloride, bromide, iodide and nitrate salts of hexamethylenediamine. Significant deviations from diammonium 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 dication 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.

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

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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 Bis adeninium hexafluorosilicate(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 by 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 NH₂ groups and the H atom of the protonated N atom of the five membered ring forming respectively centrosymmetric R₂²(10) and R₂²(8) rings. Then 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 R₄⁴(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 R₃³(10) graph set motif.

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D-H...X Contacts Performed by N-Heterocycles: a Practical View
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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 which in most cases would be the dominating forces in the corresponding crystal structures. As a matter of fact in many of our obtained solid state structures hydrogen bonds between different donors and halogens 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.