Poster Presentation

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An X-ray study of new hybrid systems of Fe(III) and Cu(II) based anions

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Organic-inorganic hybrid compounds represent one of the most important developments in materials chemistry in recent years [1]. The role of weak intermolecular interactions in the stabilization of these hybrid systems is one of the main targets of our investigation in crystal engineering study. In continuation of our research on N-aromatic heterocyclic-metal halide salts, the X-ray crystal structures of 4-dimethylaminopyridinium (HDMAP) cation with tetrachlorocuprate (II) (1) and tetrachloroferrate (III) (2) anions is reported [2,3]. In (1), Cu(II) is situated on a twofold rotation axis (4 e). The [CuCl4]2- ions are highly distorted with a mean trans angle of 141.02(1)° as a result of hydrogen bonding interactions with two nearly planar HDMAP cations (0.0295 Å mean deviation). The crystal structure of (1) is stabilized by N—H…Cl and C—H…Cl hydrogen bonds. In the three dimensional network, cations and anions pack in the lattice so as to generate chains of [CuCl4]2- anions separated by two orientations of cation layers, which are interlocked through π–π tacking contacts between pairs of pyridine rings, with centroid–centroid distances of 3.7874 (7) Å. In (2), the protonoted 4-(dimethylamino) pyridine cation is essentially planar (the r.m.s deviation for all non-H atoms being 0.004 Å). The packing of the ionic entities is realized by alternating layers of cations and [FeCl4]- anions parallel to (010) whereby the cations are oriented in a zig-zag fashion. The crystal packing is stabilized by N—H…Cl and C—H…Cl hydrogen bonds forming a three-dimensional network.

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