

Poster Presentation

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Crystal structure and hydrogen bonded network of new cadmium hybrid complex

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Cadmium complexes exhibit extensive potential applications in many fields, such as magnetism materials, biological active materials, optical device and catalysis materials [1]. The reported compound [Tetrakis(5-amino-3-carboxy-1H-1,2,4-triazol-4-ium) hexachloridocadmate (II) tetrahydrate (1)] was prepared as part of our ongoing investigations of hydrogen-bonding interactions in the crystal structures of metal-protonated N-aromatic heterocyclic hybrid frameworks [2]. 5-Amino-1H-1,2,4-triazole-3-carboxylic acid arises as a promising ligand which can be employed in the preparation of coordination compounds as a consequence of its multiple buildings sites and its basic nitrogen capable of associating with a proton H⁺ in acid solution [3]. The single-crystal X-ray structure analysis revealed that (1) crystallizes in the monoclinic P-1 space group, the Cd(II) atom is located at a crystallographic inversion centre. The latter ion is octahedrally coordinated by six chloride anions, Due to the presence of a considerable number of proton donors and acceptors, the crystal structure is rich in hydrogen bonding interactions which led to the formation of discrete cation layers spaced by hexachloridocadmate anions. Examination of the cation-anion interactions reveals that N–H...Cl hydrogen bonding are the major packing interactions, It appears that the layered structure results from the octahedral [CdCl₆]²⁻ anions along with its ability to form hydrogen bonds in different directions, intermolecular hydrogen bonding interactions between the chloride atom and oxygen atoms of water molecules interconnect the layers into a three-dimensional framework.

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