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Synthesis and crystal structure compound Adeninium Bis(pyridine-2,6-dicarboxylate) Chromate(III) pyridine-2,6-dicarboxylic acid tetra hydrate

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Abstract: A new supramolecular compound of adeninium bis(pyridine-2,6-dicarboxylate) Chromate(III) pyridine-2,6-dicarboxylic acid tetrahydrate $(AdH^+)[Cr(pydc)_2](H_2pydc).4H_2O$ (**1**) (where Ad and H_2pydc are adenine and pyridine-2,6-dicarboxylic acid, respectively) was synthesized *via* proton transfer method and its structure was determined using single crystal X-ray diffraction technique. This compound crystallizes in the orthorhombic crystal system with *Pbca* space group and the unit cell parameters are a = 14.180(14), b = 13.036(12), c = 33.98(3) Å and $\alpha = \beta = \gamma = 90^\circ$. The final R value is 0.053 for 2523 independent reflections. The asymmetric unit of compound **1** contains anionic, cationic and neutral species. The anionic part is a complex of Cr(III) with two coordinated pyridine-2,6-dicarboxylate groups and the cationic part is a protonated adenine. The neutral part has one molecule of pyridine-2,6-dicarboxylic acid and four hydration water molecules. The Cr(III) atom in compound **1** adopts a distorted octahedral coordination geometry. All six coordination sites have been occupied by two deprotonated pyridine-2,6-dicarboxylate ligands. Non-covalent and intermolecular interactions i.e. Hydrogen bonds and C = O…π interactions are responsible for the self-assembled and regular structure of **1**.

Keyword: *Supramolecular compounds; proton transfer compounds*; *adenine; hydrogen bonds;* C = O…π *interaction.*

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