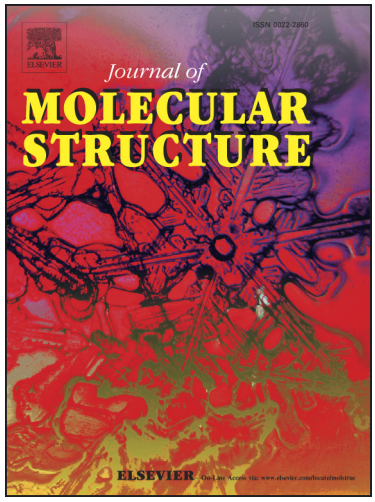

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Exploring the influence of crystal environment on the geometry of bis(pyridine-2,6-dicarboxylato) chromium (III) anionic complexes containing various cationic moieties: Synthesis, structures and Hirshfeld surface analysis

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Abstract

Two chromium (III) complexes with pyridine–2,6–dicarboxylate ligand have been synthesized with various cations yielding new compounds: $(2a4mpy)_2[Cr(pydc)_2]_2 \cdot 9H_2O$ (**I**) and $(bphda)[Cr(pydc)_2]_2 \cdot DMF \cdot 4H_2O$ (**II**) where pydc= pyridine–2,6–dicarbocylate anion, 2a4mpy=2–amino–4–methylpyrimidinium cation and bphda=1,1'–bisphenyl–4,4'–diaminium cation. These compounds have been characterized by IR spectroscopy, CHN microanalysis and X-ray structural studies along with a detailed analysis of Hirshfeld surface and 2D fingerprint plot as an assisting tool for decoding of the intermolecular interactions. In both complex fragments, Cr(III) atoms are surrounded by four oxygen atoms and two nitrogen atoms from two pydc ligands, forming a distorted octahedral environment. Crystal packing in both compounds is mostly governed by strong O—H···O and N—H···O classical hydrogen bond interactions and assisted by the interactions involving π-electrons, namely π···π off-face stacking, carbonyl···π or lone pair···π. All these interactions lead to rather complex three-dimensional structures. In this regard, the fingerprint plots enabled to explore the role of intermolecular interactions types on the distorted geometry of titled complexes and analogous structures retrieved from Cambridge Structural Database (CSD).