Poster

Different Hydrogen-bond networks in two 1D bimetallic oxalate compounds: $ACr(C_2O_4)_2(H_2O)_4$ (A = Li, Na)

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Single crystals of two new 1D bimetallic oxalate compounds with the formula $[ACr(C_2O_4)_2(H_2O)_4]_n$, A = Li, Na have been synthesized and the crystal structures elucidated by X-ray diffraction analysis and compared [1]. The compound (**I**) with Li atom crystallizes in the monoclinic space group *C2/m*, while the compound (**II**) with Na atom crystallizes in the triclinic space group $P\bar{1}$, however with somewhat similar features. The asymmetric unit of (**I**), contains both Li and Cr atoms on 2/m site symmetry, while only half oxalate ligand is present and two independent water molecules lying on the mirror plane. The oxygen atoms of water molecules around the Li atom are disordered over two equivalent positions separated by 0.539(44) Å. In the asymmetric unit of (**II**), all atoms are on general positions except the metallic atoms (Na and Cr) which are lying on the inversion centre, and there is one ligand $C_2O_4^{2-}$ and two independent water molecules. Both crystal structures are comprised of one-dimensional chains alternating *trans*-$Cr(CO)_4(H_2Ow2)_2$ and *trans*-$A(CO)_4(H_1Ow1)_2$ units μ_2-bridged by bis-chelating oxalato ligands. The resulting linear chains are parallel to the [101] direction for A=Li (**I**) and to $[11\bar{1}]$ direction when A=Na (**II**). Within the two coordination polymers, strong hydrogen-bonds are present as tetrameric synthons $R_4^4(12)$ linked together in order to form H-bonded files, used to extended the metal chains in two-dimensional supramolecular architectures. The two structures differ from each over through the symmetry relations inside the ligand, the role of electrostatic forces in the crystal structure and the molecular interaction H-bonded networks.

[1] Kherfi, H., Benhacine, M. A. A., Hamadène, M. & Balegroune, F. (2019). Acta Cryst. C**75**, 1524.