A one-dimensional coordination polymer with a pseudo face-centred monoclinic lattice: Structural and intermolecular insights

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The present work reports the crystal structure study of a 1D coordination polymer, $LiCr(C_2O_4)_2(H_2O)_4$ (**I**), determined by single crystal X-ray diffraction [1], along with an investigation of its intermolecular interactions via Hirshfeld surface analysis. The compound was prepared using reflex method in deionized water. It belongs to the monoclinic system, space group *C*2/*m*, with unit cell parameters, *a* = 10.097 (8) Å, *b* = 7.787 (8) Å, *c* = 6.737 (6) Å and β = 104.3 (1)°. The asymmetric unit contains both Li and Cr atoms on 2/*m* site symmetry leading to a pseudo face-centred monoclinic lattice, a half oxalate ligand and two independent water molecules lying on the mirror plane. The crystal structure is built up from octahedral *trans*-$Cr(CO)_4(H_2O)_2$ and *trans*-$Li(CO)_4(H_2O)_2$ units, bridged by the oxalate ligands, forming one-dimensional linear chains parallel to the [101] direction. Strong hydrogen-bonds are observed, involving tetrameric synthons $R_4^4(12)$, linked together to form H-bonded files that play a key role in the extension of the 2D supramolecular architecture. These noncovalent interactions were further highlighted through Hirshfeld surface analysis [2] and the corresponding 2D fingerprint plots [3]. The results confirmed their critical contribution to the crystal packing stabilization, with O···O contacts being the most dominant, accounting for 59.9% of the total interatomic interactions.

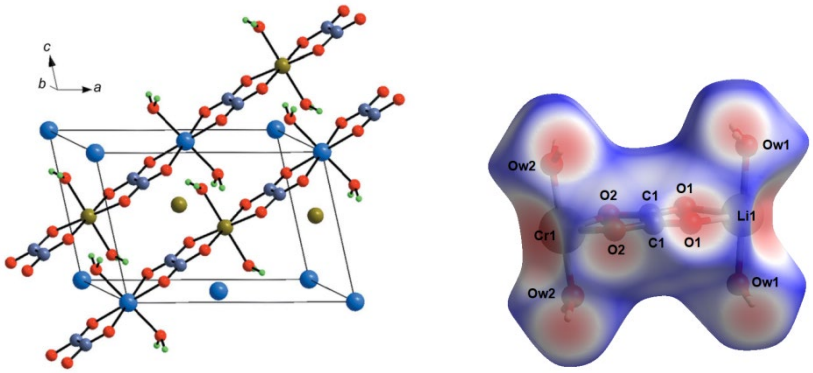

Figure 1. The face-centred monoclinic lattice in $LiCr(C_2O_4)_2(H_2O)_4$ (Li blue and Cr olive-green), and its Hirshfeld surface plotted over d_{norm}.

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[2] Spackman, M. A., Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19.

[3] Spackman, M. A., McKinnon, J. J. (2002). *CrystEngComm*, **4**, 378.