

КРАТКИЕ СООБЩЕНИЯ

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CRYSTAL STRUCTURE OF COBALT(II) 1,12-DODECANEDIOATE TRIHYDRATE:
A NEW LAYERED COORDINATION NETWORKD.J. Price¹, S.J. Coles², M.B. Hursthouse^{2,3}¹WestCHEM, School of Chemistry, University of Glasgow, Glasgow, United Kingdom

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Reaction of cobalt hydroxide with the α,ω -dicarboxylic acid and 1,12-dodecanedioic acid under ambient conditions results in the formation of a trihydrate $\text{Co}(\text{C}_{12}\text{H}_{20}\text{O}_4)(\text{H}_2\text{O})_3$ (**1**). Single crystal X-ray diffraction studies show **1** to crystallise in the orthorhombic space group *Pccn* with cell parameters $a = 40.2343(7)$ Å, $b = 8.1519(1)$ Å, $c = 9.1011(2)$ Å. The structure has a very pronounced two dimensional character, with a separation of hydrophobic *n*-alkyl chains from the carboxylate groups, the Co^{2+} cations and the water of crystallisation. The structure is discussed in respect of the structures of other known compositionally related compounds, including the dihydrate $\text{Co}(\text{C}_{12}\text{H}_{20}\text{O}_4)(\text{H}_2\text{O})_2$.

Keywords: cobalt, layered compound, carboxylate bridge, pseudopolymorphism.

The interest in the chemical and physical properties of transition metal coordination networks (now often referred to as MOFs — metal organic frameworks) is rapidly increasing. This is because many have characteristics that make them appealing as candidate materials in areas such as gas absorption [1], gas separation [2], catalysis [3], luminescence [4], and magnetism [5, 6]. In the design of new materials there are many strategies and parameters that can be exploited. We can use ligands with well defined chelating coordination modes to produce well defined arrays of metal ions, whether they are discreet clusters [7] or infinite arrays [8]. A reduction of specificity of the coordination mode introduces some flexibility in the possible metal coordination geometries, but can still retain predictable gross structural features in the metal atom distribution. This is certainly seen with aryl carboxylate ligands such as the rigid 1,2,4,5-benzene tetracarboxylate [9]. With alkyl carboxylates we introduce a conformational flexibility to the ligand, and we also introduce the hydrophobic alkyl-alkyl interactions which when the alkyl chain is long enough, result in a layered 2D lamella character to a material. We describe here the structure of $\text{Co}(\text{O}_2\text{C}(\text{CH}_2)_{10}\text{CO}_2)(\text{H}_2\text{O})_3$ (**1**) and comment on its structural relationship to a growing family of transition metal soaps.

Experimental. C and H analysis was obtained using an Exeter Analytical Inc. CE-440 Elemental Analyser. Infrared spectra were recorded on a Perkin Elmer Spectrum One FTIR spectrometer as pressed KBr pellets; UV-visible spectra were recorded on a Perkin Elmer Lambda 19 spectrometer in diffuse reflectance mode, using powdered BaSO_4 as a diluting matrix. Powder X-ray diffraction was performed using a Bruker D5000 instrument with $\text{CuK}\alpha$ radiation.

Synthesis of $\text{Co}[\text{O}_2\text{C}(\text{CH}_2)_{10}\text{CO}_2](\text{H}_2\text{O})_3$ (1**).** A solution of NaOH (0.033 g, 0.83 mmol) in distilled water (4 ml) was added to a solution of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.152 g, 0.64 mmol) in distilled water (3 ml), producing a blue precipitate of $\text{Co}(\text{OH})_2$. To this mixture, 1,12-dodecanedioic acid (0.096 g,