Structure Determination of a novel Metal-Organic Compound synthesized from Aluminum and 2,5-Pyridinedicarboxylic Acid.

The structure of \[
[\text{Al}_2(\text{pydc})_2(\text{OH})_2(\text{H}_2\text{O})_2]_n \quad (\text{pydc}=2,5\text{-pyridinedicarboxylate})
\]
determined from powder X-ray diffraction data. The compound crystallizes in the triclinic system (space group P -1) with \(a = 6.7813(1) \ \text{\AA}, \quad b=7.4944(1) \ \text{\AA}, \quad c=8.5013(1) \ \text{\AA}, \ \alpha = 95.256(1)\%\), \(\beta =102.478(1)\%\), \(\gamma =108.979(1)\%\). The structure consists of aluminum ions coordinating N and O in distorted octahedra, sharing an edge through two hydroxide ions. These dinuclear complexes are connected by pydc ions, which at one end coordinate by nitrogen and oxygen and only by oxygen at the other end. The pydc orientation is reversed in the neighboring pydc, forming double stranded chains interconnected by the aluminum dinuclear complexes in a ladder-like arrangement along (001).

Liang, Y., Hong, M., Cao, R., Weng, J. (2001). Hydrothermal Synthesis and Structure Characterization of Compound \(\text{Zn}(\text{H}_2\text{pydc})_2(\text{H}_2\text{O})_2\) \(\text{pydc}=\text{pyridine-2,5-dicarboxylate})\),? Chinese J. Struct. Chem, 20, 455-458.

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- Mounting mode: 'transmission'
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diffcorr_measurement_device =
Department of Chemistry
Technical University of Denmark
Lyngby, Denmark

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Sample spinning by appr. 1 turn/sec during measurements

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Expected bond lengths of pydc (Liang et al., 2001) were used as restraints.

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ITO, Visser, 1969 (j.appl.cryst.2,89(1969))
EXPO, Altorami et al., 1994, 1995

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computing_molecular_graphics = 'ATOMS 6.2, Shape Software, USA'
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C5 C7 O3 112.2(5) \ldots 
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