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Crystal structure of catena-poly[(μ₃-5-carboxy-2-(pyridin-4-yl)benzoato-κ⁵O,O’:O’’,O’’’:O’’’)(1,10-phenanthroline-κ²N,N’)cadmium(II)], C₁₀₀H₆₀N₁₂O₁₆Cd₄

https://doi.org/10.1515/ncrs-2017-0299

Received March 4, 2018; accepted June 6, 2018; available online June 20, 2018

Abstract

C₁₀₀H₆₀N₁₂O₁₆Cd₄, monoclinic, I2/a (no. 15), a = 21.2654(5) Å, b = 11.1493(3) Å, c = 17.3039(4) Å, β = 97.774(2)°, V = 4064.96(18) Å³, Z = 2, Rgt(F) = 0.0213, wRref(F²) = 0.0559, T = 289.23(10) K.

CCDC no.: 1847595

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

| Crystal: | Colorless block |
| Size: | 0.41 × 0.35 × 0.28 mm |
| Wavelength: | Mo Kα radiation (0.71073 Å) |
| μ: | 1.12 mm⁻¹ |
| Diffractometer, scan mode: | SuperNova, ω-scans |
| θmax, completeness: | 25.5°, >98% |
| N(hkl)measured, N(hkl)unique, Rint: | 36599, 3728, 0.037 |
| Criterion for Iobs, N(hkl)gt: | Iobs > 2σ(Iobs), 3465 |
| N(param)refined: | 298 |
| Programs: | CrysAlisPRO [1], SHELX [2, 3], OLEX2 [4] |

Source of material

A mixture of Cd(NO₃)₂·2H₂O (0.1 mmol, 0.0272 g), 4-(pyridin-4-yl)-isophthalic acid (0.1 mmol, 0.0243 g), 1,10-phenanthroline (0.1 mmol, 0.0180 g) and distilled water (12 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 423 K for 45 h, followed by slow cooling to room temperature until colourless crystals of the title compound formed.

Discussion

The design and construction of metal-organic frameworks (MOFs) with well regulated network structures has been provoked significant interest on these functional materials with properties, such as electrochemistry, photophysics, catalysis, adsorption and separation [5–8]. The organic ligands, which have their differences in the size, the flexibility, the coordination ability, the number of the carboxylate groups, the positions of the carboxylate groups and so on, are important in the design of frameworks with [9–11]. In addition, N-containing auxiliary ligands [12, 13] are known to be connectors between metal atoms for the propagation of coordination networks.

In this paper we report the crystal structure of a coordination polymer. The asymmetric unit of the title structure contains one Cd(II) metal center, one 4-(4-pyridin-4-ylphenyl)pyridine and one 1,10-phenanthroline ligands to...
construct a new coordination polymer. The cadmium atom is seven-coordinated \([\text{CdN}_5\text{O}_2]\) by five oxygen atoms from 5-carboxy-2-(pyridin-4-yl)benzoato ligands and by two nitrogen atoms from 1,10-phenanthroline. The Cd—O bond lengths range from 2.352(17) Å, 2.3657(17) Å, respectively. The bond angles of O—Cd—O are in the range of 53.78(5)° to 136.20(5)°.

**Acknowledgements**: This work was supported by the Institutions of higher learning key scientific research project of Henan Province (18B150015) and the Natural Science Foundation of Henan Province (182102310909).

**References**


