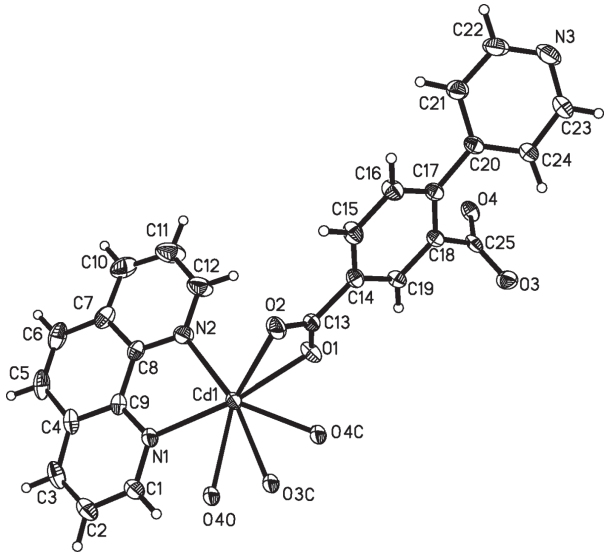
Wei Song*, Xue-Li Xu, Yan-Ju Yang and Shi-Hui Li

Crystal structure of catena-poly[(μ_3-5-carboxy-2-(pyridin-4-yl)benzoato-$\kappa^5O,O':O'',O''':O'''$)(1,10-phenanthroline-$\kappa^2N,N'$)cadmium(II)], $C_{100}H_{60}N_{12}O_{16}Cd_4$



https://doi.org/10.1515/ncrs-2017-0299
Received March 4, 2018; accepted June 6, 2018; available online June 20, 2018

Abstract

$C_{100}H_{60}N_{12}O_{16}Cd_4$, monoclinic, $I2/a$ (no. 15), $a = 21.2654(5)$ Å, $b = 11.1493(3)$ Å, $c = 17.3039(4)$ Å, $\beta = 97.774(2)°$, $V = 4064.96(18)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0213$, $wR_{ref}(F^2) = 0.0559$, $T = 289.23(10)$ 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.

***Corresponding author: Wei Song,** School of Biological and Chemical Engineering, Nanyang institute of Technology, Nanyang 473004, Henan Province, P.R. China, e-mail: zhanglihxx@126.com
Xue-Li Xu and Yan-Ju Yang: School of Biological and Chemical Engineering, Nanyang institute of Technology, Nanyang 473004, Henan Province, P.R. China
Shi-Hui Li: College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, Henan Province, P.R. China

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.41 × 0.35 × 0.28 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.12 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
θ_{max}, completeness:	25.5°, >98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	36599, 3728, 0.037
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3465
$N(param)_{refined}$:	298
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], OLEX2 [4]

Source of material

A mixture of $Cd(NO_3)_2{\cdot}2H_2O$ (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.

Experimental details

All H atoms were positioned geometrically (N-H = 0.86 Å and C-H = 0.93 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

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

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.727175(7)	0.589761(13)	0.724990(8)	0.03225(7)
N1	0.79070(9)	0.50560(16)	0.83331(10)	0.0382(4)
N2	0.77610(9)	0.41304(16)	0.68647(12)	0.0426(5)
N3	0.49186(11)	0.6093(2)	0.09894(13)	0.0628(6)
O1	0.71096(7)	0.65130(15)	0.59764(8)	0.0442(4)
O2	0.63014(8)	0.54919(15)	0.63058(9)	0.0475(4)
O3	0.65605(8)	0.88459(15)	0.32771(9)	0.0474(4)
O4	0.68704(6)	0.72789(14)	0.26565(8)	0.0382(3)
C1	0.79947(13)	0.5536(2)	0.90385(14)	0.0517(6)
H1	0.7768	0.6223	0.9131	0.062*
C2	0.84132(13)	0.5055(3)	0.96477(14)	0.0592(7)
H2	0.8469	0.5422	1.0135	0.071*
C3	0.87385(13)	0.4047(3)	0.95221(16)	0.0587(7)
H3	0.9021	0.3719	0.9923	0.070*
C4	0.86497(11)	0.3501(2)	0.87901(14)	0.0459(6)
C5	0.89659(12)	0.2418(3)	0.86081(18)	0.0613(8)
H5	0.9237	0.2038	0.8999	0.074*
C6	0.88811(12)	0.1945(2)	0.78955(19)	0.0585(7)
H6	0.9091	0.1240	0.7800	0.070*
C7	0.84752(10)	0.2498(2)	0.72794(15)	0.0458(6)
C8	0.81482(9)	0.35559(19)	0.74290(13)	0.0356(5)
C9	0.82286(10)	0.40539(18)	0.82013(13)	0.0358(5)
C10	0.83889(13)	0.2060(3)	0.65117(18)	0.0624(8)
H10	0.8590	0.1359	0.6388	0.075*
C11	0.80116(15)	0.2665(3)	0.59546(19)	0.0780(10)
H11	0.7957	0.2391	0.5442	0.094*
C12	0.77045(14)	0.3698(3)	0.61505(16)	0.0641(8)
H12	0.7447	0.4105	0.5759	0.077*
C13	0.65711(11)	0.60341(18)	0.58132(12)	0.0339(5)
C14	0.62641(10)	0.61100(19)	0.49808(12)	0.0323(4)
C15	0.57484(10)	0.5399(2)	0.47004(12)	0.0406(5)
H15	0.5572	0.4891	0.5039	0.049*
C16	0.54958(10)	0.5439(2)	0.39250(13)	0.0409(5)
H16	0.5148	0.4959	0.3751	0.049*
C17	0.57483(9)	0.61805(19)	0.33925(12)	0.0317(4)
C18	0.62578(9)	0.69246(18)	0.36834(11)	0.0287(4)
C19	0.65084(9)	0.68735(19)	0.44641(11)	0.0320(4)
H19	0.6850	0.7365	0.4647	0.038*
C20	0.54757(9)	0.6164(2)	0.25572(12)	0.0338(5)
C21	0.52478(10)	0.5104(2)	0.21994(13)	0.0449(5)
H21	0.5280	0.4387	0.2477	0.054*
C22	0.49744(12)	0.5121(3)	0.14312(16)	0.0571(7)
H22	0.4819	0.4403	0.1209	0.068*
C23	0.51508(12)	0.7094(3)	0.13273(14)	0.0547(6)
H23	0.5130	0.7786	0.1025	0.066*
C24	0.54206(10)	0.7183(2)	0.20932(13)	0.0407(5)
H24	0.5565	0.7920	0.2298	0.049*
C25	0.65791(9)	0.7748(2)	0.31735(11)	0.0325(5)

construct a new coordination polymer. The cadmium atom is seven-coordinated [CdN_2O_5] 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 2.2891(14)—2.5013(16) Å. The Cd—N bond lengths range from 2.3524(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

1. Agilent Technologies: CrysAlis PRO Software system, version 1.171.38.41r, Agilent Technologies UK Ltd, Oxford, UK (2011).
2. Sheldrick, G. M.: SHELXT-integrated space-group and crystal-structure determination. Acta Crystallogr. **A71** (2015) 3–8.
3. Sheldrick, G. M.: Crystal stucture refinement with SHELXL. Acta Crystallogr. **C71** (2015) 3–8.
4. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Crystallogr. **42** (2009) 339–341.
5. Li, S. H.; Zhao, Y.: Synthesis and crystal structure of a new three-dimensional Co(II) coordination polymer based on 3,3′,4,5′-biphenyl tetracarboxylic acid and 4,4′-bipyridine. Inorg. Nano-Met. Chem. **47** (2017) 256–259.
6. Zhao, Y.; Li, S. H.: Synthesis and crystal structure of a new three-dimensional complex constructed from thiophene-2,5-dicarboxylic acid. Synth. React. Inorg. Met. Org. Chem. **45** (2015) 921–925.
7. Yoneda, K.; Adachi, K.; Nishio, K.; Yamasaki, M.; Fuyuhiro, A.; Katada, M.; Kaizaki, S.; Kawata, S.: Cover picture: organocatalytic highly enantioselective -arylation of -ketoesters/asymmetric organocatalytic -arylation of aldehydes. Angew. Chem. Int. Ed. **45** (2006) 5459–5461.
8. Li, S. H.; Li, X. L.: A cadmium complex based on 5- methylisophthalic acid and 1,6-bis(imidazol-1-yl)hexane: Synthesis, crystal structure, and photoluminescence properties. Synth. React. Inorg. Met. Org. Chem. **43** (2013) 710–713.
9. Li, K.; Olson, D. H.; Seidel, J.; Emge, T. J.; Gong, H.; Zeng, H.; Li, J.: Zeolitic imidazolate frameworks for kinetic separation of propane and propene. J. Am. Chem. Soc. **131** (2009) 10368–10369.
10. Li, S. H.; Zang, J.; Guo, J. B.: Synthesis and crystal structure of a new three-dimensional Ho(II) coordination polymer based on 5′-(4-Carboxyphenyl)-[1,1′:3′,1″-terphenyl] -4,4″-dicarboxylic acid. Inorg. Nano-Met. Chem. **12** (2017) 1746–1749.
11. Li, S. H.; Han, M. L.; Liu, G. Z.; Ma, L. F.; Wang, L. Y.: Guestin-duced single-crystal-to-single-crystal transformations of a new 4-connected 3D cadmium(II) metal-organic framework. RSC Adv. **5** (2015) 17588–17591.
12. Pachfule, P.; Panda, T.; Dey, C.; Banerjee, R.: Structural diversity in a series ofmetal-organic frameworks (MOFs) composed of divalent transition metals, 4,4′-bipyridine and a flexible carboxylic acid. CrystEngComm **12** (2010) 2381–2389.
13. Li, S. H.; Wu, H. X.; Chai, N.: A cobalt(II) complex based on 5-methoxyisophthalic acid and 1,6-bis(1,2,4-triazol-1-yl)hexane: Synthesis, crystal structure and magnetic properties. Synth. React. Inorg. Met. Org. Chem. **43** (2013) 1487–1491.