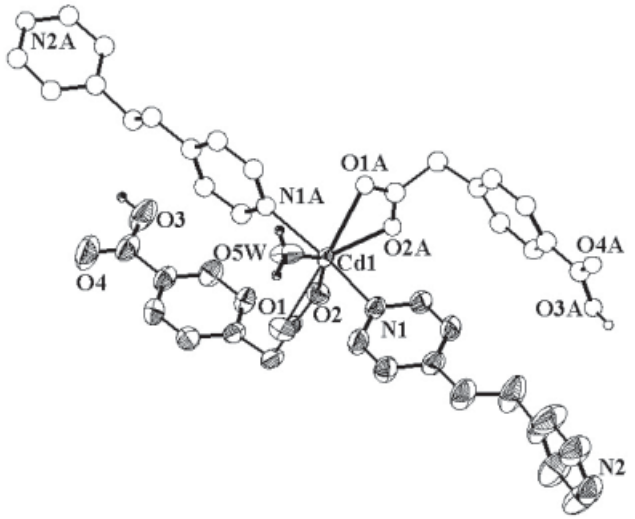
Crystal structure of aqua-bis(2-(4-carboxyphenyl)acetato-$\kappa^2 O,O'$)-bis(1,2-di-(pyridin-4-yl)ethane-κN)-cadmium(II), $Cd(C_9H_7O_4)_2(C_{12}H_{12}N_2)_2(H_2O)$, $C_{42}H_{40}CdN_4O_9$

Gui-Lian Li* and Wei-Dong Yin

College of Chemistry and Chemical Engineering, LuoYang Normal University, Luoyang 471022, Henan Province, P. R. China

Received October 18, 2012, accepted January 22, 2013, available online April 12, 2013, CCDC no. 1267/3944



Abstract

$C_{42}H_{40}CdN_4O_9$, monoclinic, *C*2/*c* (no. 15), $a = 42.518(6)$ Å, $b = 9.945(2)$ Å, $c = 9.062(1)$ Å, $\beta = 94.674(2)°$, $V = 3819.2$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0241$, $wR_{ref}(F^2) = 0.0613$, $T = 296$ K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.11×0.24×0.36 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.35 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	13755, 3541
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3250
$N(param)_{refined}$:	255
Programs:	SHELX [10]

Source of material

The mixtures of 4-carboxyphenylacetic acid (0.1 mmol, 18.0 mg), *bpa* (1,2-di(pyridin-4-yl)-ethane, 0.1 mmol, 39.7 mg), $Cd(OAC)_2{\cdot}2H_2O$ (0.1 mmol, 18.4 mg), NaOH (0.1 mmol), and H_2O (7.0 ml) were placed in a 23 ml Teflon lined stainless steel reactor. The vessel was heated to 393K for 4 days, and then slowly cooled to room temperature. Colourless crystals were obtained, and further crystals were filtered off, washed with mother liquid, and dried under ambient conditions. Yield 39%.

Discussion

The current focus on metal-organic frameworks (MOFs) is rapidly expanding not only for their intriguing architectures and fascinating topologies but also for their great potential in catalysis, gas sorption, magnetic, photoluminescent properties and so on [1-5]. In this regard, the effective and facile approach for the synthesis of such complexes is still the appropriate choice of well-designed organic ligands as bridges or terminal groups (building blocks) with metal ions as nodes. Among various organic ligands, multi-carboxylates have attracted considerable attention due to their various coordination modes to metal atoms [6,7]. On the other hand, the introduction of additional *N*-donor ligands to such synthetic systems can modify the structures and properties of the resulting materials [8, 9]. The asymmetric unit of the title complex contains one *bpa* molecule, one half Cd ion, one 2-(4-carboxyphenyl)acetato ligand and one half coordinated water molecule. The Cd ion is seven-coordinated by two N atoms of two symmetry-related *bpa* ligands, four carboxylate oxygen atoms of two 2-(4-carboxyphenyl)acetato ligand coordinating in a bidentatly chelating mode and one oxygen atom of coordinated water. The Cd–O bond lengths are in the range of 2.295(2)-2.4881(15) Å and the Cd–N bond lengths is 2.4022(16) Å. The $[CdO_5N_2]$ environment is best described as distorted pentagonal bipyramid geometry. In the complex, there are two kinds of hydrogen bonds. Firstly, the coordinated water acts as a twofold donor and the carboxylate oxygen in the adjacent 2-(4-carboxyphenyl)acetato ligand as acceptor (O5W–H3W···O1#2 distances are 1.821 Å) alternately connect to favor the formation of 2D layer structure. Secondly, the hydrogen bonding interactions of carboxylate hydrogen act as a donor to the nitrogen atoms in *bpa* (O3–H3···N2#1 distances are 1.825 Å) resulting in a 3D structure.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(3)	8*f*	–0.1949	0.5664	0.2887	0.120
H(3W)	8*f*	0.0047	1.0844	0.3218	0.098
H(2A)	8*f*	–0.0279	0.5381	0.6520	0.051
H(2B)	8*f*	–0.0321	0.6809	0.7225	0.051
H(4)	8*f*	–0.0710	0.4561	0.4619	0.057
H(5)	8*f*	–0.1237	0.4604	0.3764	0.062
H(7)	8*f*	–0.1366	0.7812	0.6301	0.071
H(8)	8*f*	–0.0839	0.7793	0.7113	0.064
H(10)	8*f*	0.0441	0.9597	0.5058	0.062
H(11)	8*f*	0.0945	1.0038	0.5962	0.068
H(13)	8*f*	0.1245	0.7426	0.3061	0.065
H(14)	8*f*	0.0731	0.7055	0.2229	0.059
H(15A)	8*f*	0.1550	0.9972	0.4935	0.088
H(15B)	8*f*	0.1495	0.9093	0.6318	0.088
H(16A)	8*f*	0.1751	0.8188	0.3802	0.112
H(16B)	8*f*	0.1681	0.7259	0.5132	0.112
H(18)	8*f*	0.2168	1.0033	0.4333	0.112
H(19)	8*f*	0.2660	1.0434	0.5463	0.100
H(20)	8*f*	0.2563	0.7576	0.8239	0.107
H(21)	8*f*	0.2072	0.7072	0.7185	0.107

* Correspondence author (e-mail: yligl@163.com)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	4*e*	0	0.80036(2)	$\frac{1}{4}$	0.0240(1)	0.0365(1)	0.0374(1)	0	–0.00210(7)	0
N(1)	8*f*	0.05339(4)	0.8292(2)	0.3537(2)	0.0293(8)	0.045(1)	0.047(1)	0.0007(7)	–0.0028(7)	–0.0016(8)
N(2)	8*f*	0.26598(4)	0.9045(2)	0.6955(3)	0.033(1)	0.080(2)	0.085(2)	–0.001(1)	–0.011(1)	–0.017(1)
O(1)	8*f*	–0.01271(4)	0.8132(2)	0.5128(2)	0.061(1)	0.046(1)	0.0450(8)	–0.0102(7)	0.0080(7)	–0.0029(7)
O(2)	8*f*	–0.01919(3)	0.6247(2)	0.3900(2)	0.0470(8)	0.0485(9)	0.0417(8)	–0.0006(7)	0.0040(6)	–0.0043(7)
O(3)	8*f*	–0.17715(4)	0.5487(2)	0.3254(2)	0.0392(9)	0.091(1)	0.105(2)	0.0034(9)	–0.023(1)	–0.009(1)
O(4)	8*f*	–0.18722(5)	0.7154(2)	0.4764(3)	0.042(1)	0.122(2)	0.125(2)	0.024(1)	–0.008(1)	–0.024(2)
O(5W)	4*e*	0	1.0312(2)	$\frac{1}{4}$	0.107(2)	0.036(1)	0.048(1)	0	–0.022(1)	0
C(1)	8*f*	–0.02122(4)	0.6921(2)	0.5049(2)	0.0223(9)	0.046(1)	0.036(1)	0.0036(8)	–0.0041(7)	0.0037(9)
C(2)	8*f*	–0.03639(4)	0.6275(2)	0.6335(2)	0.033(1)	0.055(1)	0.039(1)	–0.0009(9)	–0.0048(8)	0.010(1)
C(3)	8*f*	–0.07152(4)	0.6198(2)	0.5927(2)	0.032(1)	0.050(1)	0.038(1)	–0.0022(9)	0.0008(8)	0.0107(9)
C(4)	8*f*	–0.08406(5)	0.5232(2)	0.4944(3)	0.034(1)	0.045(1)	0.064(1)	0.0020(9)	0.001(1)	0.001(1)
C(5)	8*f*	–0.11576(5)	0.5250(2)	0.4437(3)	0.038(1)	0.048(1)	0.067(1)	–0.007(1)	–0.004(1)	0.001(1)
C(6)	8*f*	–0.13554(5)	0.6224(2)	0.4927(2)	0.030(1)	0.057(1)	0.057(1)	–0.001(1)	0.0007(9)	0.013(1)
C(7)	8*f*	–0.12334(6)	0.7165(3)	0.5943(3)	0.041(1)	0.074(2)	0.062(2)	0.014(1)	0.005(1)	–0.006(1)
C(8)	8*f*	–0.09173(5)	0.7151(2)	0.6433(3)	0.043(1)	0.067(2)	0.049(1)	0.002(1)	0.000(1)	–0.008(1)
C(9)	8*f*	–0.16927(5)	0.6337(3)	0.4326(3)	0.034(1)	0.072(2)	0.074(2)	0.003(1)	–0.001(1)	0.012(1)
C(10)	8*f*	0.06050(5)	0.9156(2)	0.4642(3)	0.034(1)	0.059(1)	0.062(1)	0.006(1)	–0.002(1)	–0.012(1)
C(11)	8*f*	0.09081(5)	0.9424(2)	0.5193(3)	0.043(1)	0.061(2)	0.065(2)	0.003(1)	–0.010(1)	–0.021(1)
C(12)	8*f*	0.11599(5)	0.8794(2)	0.4617(3)	0.033(1)	0.053(1)	0.057(1)	–0.003(1)	–0.0079(9)	–0.003(1)
C(13)	8*f*	0.10851(5)	0.7889(2)	0.3487(3)	0.030(1)	0.074(2)	0.059(1)	0.007(1)	–0.001(1)	–0.013(1)
C(14)	8*f*	0.07744(5)	0.7671(2)	0.2990(2)	0.034(1)	0.062(1)	0.050(1)	0.002(1)	–0.0059(9)	–0.013(1)
C(15)	8*f*	0.14939(5)	0.9077(3)	0.5247(3)	0.038(1)	0.084(2)	0.096(2)	–0.001(1)	–0.015(1)	–0.025(2)
C(16)	8*f*	0.17385(6)	0.8166(3)	0.4866(4)	0.036(1)	0.097(2)	0.142(3)	0.003(1)	–0.026(2)	–0.031(2)
C(17)	8*f*	0.20604(5)	0.8487(3)	0.5618(4)	0.032(1)	0.075(2)	0.099(2)	0.003(1)	–0.013(1)	–0.024(2)
C(18)	8*f*	0.22432(7)	0.9503(4)	0.5130(4)	0.052(2)	0.126(3)	0.097(2)	–0.013(2)	–0.025(2)	0.014(2)
C(19)	8*f*	0.25397(6)	0.9743(4)	0.5821(4)	0.043(1)	0.111(2)	0.093(2)	–0.015(2)	–0.011(1)	0.005(2)
C(20)	8*f*	0.24832(8)	0.8080(3)	0.7430(4)	0.063(2)	0.089(2)	0.108(3)	–0.006(2)	–0.034(2)	0.007(2)
C(21)	8*f*	0.21858(7)	0.7769(3)	0.6802(4)	0.054(2)	0.082(2)	0.128(3)	–0.015(2)	–0.021(2)	0.005(2)

Acknowledgments. This work was supproted by the Foundation of Science and Technology of Henan province (grant no. 112102310638)

References

1. Xu, H. B.; Wang, B. W.; Pan, F.; Wang, Z. M.; Gao, S.: Stringing Oxo-Centered Trinuclear [Mn^{III}_3O] Units into Single-Chain Magnets with Formate or Azide Linkers. Angew. Chem. Int. Ed. **46** (2007) 7388-7392.
2. Seo, J. S.; Whang, D.; Lee, H.; Jun, S. I.; Oh, J.; Jeon, Y. J.; Kim, K.: A Homochiral Metal-Organic Porous Material for Enantioselective Separation and Catalysis. Nature **404** (2000) 982-986.
3. Zhang, Y. B.; Zhang, W. X.; Feng, F. Y.; Zhang, J. P.; Chen, X. M.: A Highly Connected Porous Coordination Polymer with Unusual Channel Structure and Sorption Properties. Angew. Chem., Int. Ed. **48** (2009) 5287-5290.
4. Yaghi, O. M.; Li, H.: T-Shaped Molecular Building Units in the Porous Structure of Ag(4,4'-bpy)·NO_3. J. Am. Chem. Soc. **118** (1996) 295-296.
5. Liu, G. Z.; Xin, L. Y.; Wang, L. Y.: Ancillary Ligand-Mediated Syntheses and Fluorescence Properties of Zinc(II) Complexes Based on Flexible Benzene Dicarboxylic Acid. CrystEngComm. **13** (2011) 3013-3020.
6. Ma, L. F.; Wang, L. Y.; Wang, Y. Y.; Batten, S. R.; Wang, J. G.: Self-Assembly of a Series of Cobalt(II) Coordination Polymers Constructed from H_2tbip and Dipyridyl-Based Ligands. Inorg. Chem. **48** (2009) 915-924.
7. Yang, F.; Ren, Y. X.; Li, D. S.; Fu, F.; Qi, G. C.; Wang, Y. Y.: 1D Zigzag Chain and 0D Monomer Cd(II)/Zn(II) Compounds Based on Flexible Phenylenediacetic Ligand: Synthesis, Crystal Structure and Fluorescent Properties. J. Mol. Struct. **892** (2008) 283-288.
8. Wang, F.; Zhang, J.; Yu, R.; Chen, S. M.; Wu, X. Y.; Chen, S. C.; Xie, Y. M.; Zhou, W. W.; Lu, C. Z.: Topological Derivation from Centrosymmetry to Noncentrosymmetry in a Three-dimensional Polar Framework Material. CrystEngComm. **12** (2010) 671-673.
9. Xin, L. Y.; Liu, G. Z.; Wang, L. Y.: New Coordination Polymers from 1D Chain, 2D Layer to 3D Framework Constructed from 1,2-Phenylenediacetic Acid and 1,3-Bis(4-pyridyl)propane Flexible Ligands. J. Solid State Chem. **184** (2011) 1387-1392.
10. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.