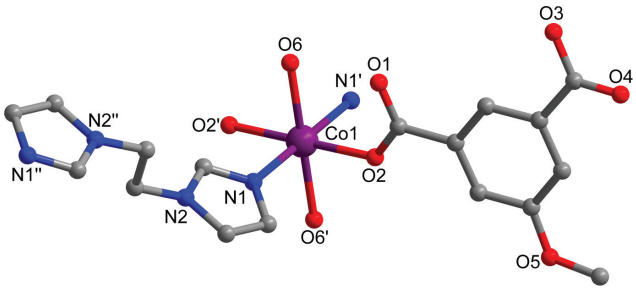
Min-Le Han*

Crystal structure of *catena*-poly[diaqua-bis(3-carboxy-5-methoxybenzoato-κO)-(1,2-bis(imidazol-1-yl)ethane-κ^2*N*:*N*′)cobalt(II)], $C_{26}H_{28}CoN_4O_{12}$, $[Co(C_9H_6O_5)_2(H_2O)_2(C_8H_{10}N_4)]$



https://doi.org/10.1515/ncrs-2018-0555
Received December 6, 2018; accepted February 11, 2019; available online March 26, 2019

Abstract

$C_{26}H_{28}CoN_4O_{12}$, triclinic, $P\bar{1}$ (no. 2), $a = 6.5186(10)$ Å, $b = 9.4111(14)$ Å, $c = 12.1777(18)$ Å, $\alpha = 79.365(2)°$, $\beta = 77.535(2)°$, $\gamma = 89.226(2)°$, $V = 716.66(19)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0304$, $wR_{ref}(F^2) = 0.0778$, T = 296.15 K.

CCDC no.: 1896510

A part of the title 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.

Source of material

A mixture of 5-methoxyisophthalic acid (H_2moip, 19.3 mg, 0.1 mmol), $Co(OAc)_2 \cdot 2H_2O$ (24 mg, 0.1 mmol), and 1,2-bis(imidazol-1-yl)ethane (bia, 16.2 mg, 0.1 mmol) were added to water (9 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 413 K for 3 days and then slowly cooled to room temperature. Pink block crystals were obtained.

Experimental details

The hydrogen atoms were placed in calculated positions riding on attached atoms with isotropic thermal parameters 1.2 and 1.5 times those of their carrier atoms (Table 2).

Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.23 × 0.18 × 0.14 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.67 mm^{-1}
Diffractometer, scan mode:	CCD, φ and ω
θ_{max}, completeness:	25.5°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5365, 2650, 0.018
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2401
$N(param)_{refined}$:	198
Programs:	Bruker [1], Olex2 [2], SHELX [3]

Comment

In the last two decades, the design and construction of Co(II)-based metal-organic coordination complexes is of interest in the field of molecular magnetism and materials chemistry due to their potential applications as functional materials [4–8]. Among *N*-donor co-ligands, 1,2-bis(imidazol-1-yl)ethane (bia), a flexible ligand, serves as bridging ligand, which can act as bidentate ligand to coordinate to two metal ions [9–13]. Herein, we report a Co(II) supramolecular coordination polymer with 3-carboxy-5-methoxybenzoate (H moip) and bia. There is one Co(II) ion, two Hmoip ligands, and one bia ligand, in the asymmetric unit of the title complex (figure top). Co1 is six-coordinated with a distorted octahedral geometry by two O atoms from two Hmoip and a pair of N atoms of two bia ligands, located at the basal equatorial plane, and two coordinated water molecules from the axial positions with a O6—Co1—O6′ angle of 180°. The Co—N bond lengths are 2.1011(16) Å and the Co—O ones are in the range of 2.1184(12) and 2.1407(13) Å. Co(II) ions are linked by bia ligands to form a 1-D polymer known for related compounds [14]. In the title complex, there are four kinds of hydrogen bonds: (*a*) intramolecular hydrogen bonding between water and carboxylate O atoms with d(O···O) = 2.65 Å; (*b*) intermolecular hydrogen bonding between water and carboxylate O atoms with d(O···O) = 2.91 Å; (*c*) intermolecular hydrogen bonding between carboxy O atoms and carboxylate O atoms with d(O···O) = 2.62 Å; (*d*) weak intermolecular ones between methyl C atoms and water with d(C···O) = 3.06 Å. An extended three-dimensional network of hydrogen bonds contributes to the stability of the structure.

***Corresponding author: Min-Le Han,** College of Chemistry and Chemical Engineering, Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang, Henan 471934, P.R. China, e-mail: minle_han@163.com

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.0000	0.0000	0.02376(12)
O1	0.0439(2)	0.12543(17)	0.12938(12)	0.0401(4)
O2	0.3547(2)	0.04776(15)	0.16172(10)	0.0331(3)
O3	−0.3740(3)	0.41740(19)	0.38224(13)	0.0527(4)
H3	−0.4729	0.4666	0.4056	0.079*
O4	−0.3160(2)	0.41339(18)	0.55699(12)	0.0491(4)
O5	0.3543(2)	0.13195(19)	0.55305(12)	0.0519(4)
O6	0.2385(2)	0.07371(15)	−0.07337(11)	0.0343(3)
H1W	0.1599	0.0910	−0.0122	0.051*
H2W	0.1823	0.0031	−0.0918	0.051*
N1	0.3799(3)	−0.21383(18)	0.04767(14)	0.0365(4)
N2	0.2260(3)	−0.4160(2)	0.03794(19)	0.0553(6)
C1	0.1803(3)	0.10381(19)	0.18968(15)	0.0261(4)
C2	0.1296(3)	0.15257(19)	0.30346(15)	0.0270(4)
C3	0.2613(3)	0.1220(2)	0.37973(16)	0.0339(4)
H3A	0.3819	0.0699	0.3609	0.041*
C4	0.2151(3)	0.1684(2)	0.48418(16)	0.0352(5)
C5	0.0383(3)	0.2491(2)	0.51156(16)	0.0338(4)
H5	0.0068	0.2809	0.5811	0.041*
C6	−0.0915(3)	0.2821(2)	0.43410(16)	0.0316(4)
C7	−0.0488(3)	0.2326(2)	0.33167(15)	0.0292(4)
H7	−0.1393	0.2528	0.2816	0.035*
C8	−0.2724(3)	0.3758(2)	0.46275(17)	0.0359(5)
C9	0.2961(4)	0.1586(3)	0.66652(17)	0.0464(6)
H9A	0.2922	0.2610	0.6647	0.070*
H9B	0.3970	0.1171	0.7093	0.070*
H9C	0.1597	0.1156	0.7023	0.070*
C10	0.3298(5)	−0.2983(3)	0.1545(2)	0.0625(8)
H10	0.3569	−0.2737	0.2206	0.075*
C11	0.2359(5)	−0.4218(3)	0.1492(3)	0.0790(10)
H11	0.1867	−0.4973	0.2100	0.095*
C12	0.3148(3)	−0.2887(2)	−0.01966(19)	0.0417(5)
H12	0.3286	−0.2572	−0.0980	0.050*
C13	0.1151(4)	−0.5162(3)	−0.0090(3)	0.0690(8)
H13A	0.1327	−0.6147	0.0281	0.083*
H13B	0.1746	−0.5078	−0.0902	0.083*

Acknowledgements: This work was supported financially by the Natural Science Foundation of Henan province (No. 182300410238) and Henan tackle key problem of science and technology (No. 182102310620).

References

1. BRUKER. SAINT, APEX2 and SADABS. Bruker AXS Inc., Madison, WI, USA (2009).
2. 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.
3. Sheldrick, G. M.: Crystal structure refinement with SHELXL. Acta Crystallogr. **C71** (2015) 3–8.
4. Wu, Y.-P.; Zhou, W.; Zhao, J.; Dong, W.-W.; Lan, Y.-Q.; Li, D.-S.; Sun, C.; Bu, X.: Surfactant-assisted phase-selective synthesis of new cobalt MOFs and their efficient electrocatalytic hydrogen evolution reaction. Angew. Chem. Int. Ed. **56** (2017) 13001–13005.
5. Gogol, A.; Nashre-ul-Islam, S. M.; Frontera, A.; Bhattacharyya, M. K.: Supramolecular association in Cu(II) and Co(II) coordination complexes of 3,5-dimethylpyrazole: experimental and theoretical studies. Inorg. Chim. Acta **484** (2019) 133–141.
6. Li, Y.; Xie, M.; Zhang, X.; Liu, Q.; Lin, D.; Xu, C.; Xie, F.; Sun, X.: Co-MOF nanosheet array: a high-performance electrochemical sensor for non-enzymatic glucose detection. Sens. Actuators, B **278** (2019) 126–132.
7. Wei, X.; Li, Y.; Peng, H.; Gao, D.; Ou, Y.; Yang, Y.; Hu, J.; Zhang, Y.; Xiao, P.: A novel functional material of Co_3O_4/Fe_2O_3 nanocubes derived from a MOF precursor for high-performance electrochemical energy storage and conversion application. Chem. Eng. J. **355** (2019) 336–340.
8. Han, M.-L.; Duan, Y.-P.; Li, D.-S.; Xu, G.-W.; Wu, Y.-P.; Zhao, J.: A series of divalent metal coordination polymers based on isomeric tetracarboxylic acids: synthesis, structures and magnetic properties. Dalton Trans. **43** (2014) 17519–17527.
9. Niu, D.; Yang, J.; Guo, J.; Kan, W.-Q.; Song, S.-Y.; Du, P.; Ma, J.-F.: Syntheses, structures, and photoluminescent properties of 12 new metal-organic frameworks constructed by a flexible dicarboxylate and various *N*-donor ligands. Cryst. Growth Des. **12** (2012) 2397–2410.
10. Guo, J.-B.; Li, S.-H.: Crystal structure of *catena*-diaqua (5-methoxyisophthalate)[1,2-bis-(imidazol-1-yl)ethane]-cadmium(II)-water (1:1), $C_{13}H_{17}CdN_2O_8$. Z. Kristallogr. NCS **227** (2012) 295–296.
11. Han, M.-L.; Wang, S.-T.; Li, Z.-Q.: Crystal structure of *catena*-(μ_3-5-bromoisophthatato-κ*O*,*O′*:*O′*, *O″*)-(1,2-bis-(imidazol-1-yl)ethane-κ*N*:*N′*)- cobalt(II), $C_{16}H_{13}CoN_4O_4Br$. Z. Kristallogr. NCS **233** (2018) 79–81.
12. Niu, D.; Yang, J.; Guo, J.; Kan, W.-Q.; Song, S.-Y.; Du, P.; Ma, J.-F.: Syntheses, structures, and photoluminescent properties of 12 new metal-organic frameworks constructed by a flexible dicarboxylate and various *N*-donor ligands. Cryst. Growth Des. **12** (2012) 2379–2410.
13. Chang, X.-H.; Han, M.-L.: A Cu(II) coordination polymer with 5-*tert*-butyl isophthalate linker: synthesis, crystal structure, and magnetic properties. Chin. J. Struct. Chem. **34** (2015) 1895–1900.
14. Li, X.; Su, Y.; Li, X.; Ma, G.; Ling, Q.: Syntheses, structures, and characteristics of six coordination polymers based on 1,4-bis(imidazol-1-yl)benzene and isophthalates containing coordination-inert substituents. Eur. J. Inorg. Chem. **2015** (2015) 3274–3284.