Jia-Le Li, Zhang-Fan Chen and Shui-Sheng Chen*

Crystal structure of *catena*-poly[*diaqua*-bis(μ_2 -5-(3-(1*H*-imidazol-5-yl)phenyl)tetrazol-2-ido- $\kappa^2 N:N'$)cobalt(II)], $C_{20}H_{18}CoN_{12}O_2$

Table 1: Data collection and handling.

Crystal:	Purple block
Size:	0.24 × 0.20 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.90 mm ⁻¹
Diffractometer, scan mode:	Bruker Apex, φ and ω
$\theta_{\max}$, completeness:	25.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5322, 1779, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1608
$N(\text{param})_{\text{refined}}$:	164
Programs:	Bruker [1], SHELX [2, 3]

<https://doi.org/10.1515/ncrs-2018-0148>

Received June 25, 2018; accepted August 14, 2018; available online September 5, 2018

Abstract

$C_{20}H_{18}CoN_{12}O_2$, monoclinic, $C2/c$ (no. 15), $a = 17.6924(15)$ Å, $b = 11.3253(10)$ Å, $c = 12.8536(11)$ Å, $\beta = 128.029(10)^\circ$, $V = 2028.7(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0258$, $wR_{\text{ref}}(F^2) = 0.0890$, $T = 296(2)$ K.

CCDC no.: 1862080

A part of the polymeric title crystal structure is shown in the figure ($a = 0.5 - x, 1.5 - y, -z$; $b = x, y - 1, z$; $c = 0.5 - x, 0.5 - y, -z$). 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 materials

All reagents and solvents were used as obtained without further purification. A mixture containing Cobalt(II) chloride hexahydrate (0.023 g, 0.1 mmol), 1-(1*H*-imidazol-4-yl)-3-(4*H*-tetrazol-5-yl)benzene (HL) (0.021 mg, 0.1 mmol), DMF (1 mL), 10 mL H₂O was sealed in a 16 mL Teflon-lined stainless steel

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.250000	0.250000	0.000000	0.01885(16)
C1	0.44090(13)	0.85089(17)	0.04833(18)	0.0213(4)
C2	0.53791(14)	0.87934(17)	0.13885(19)	0.0277(4)
H2	0.557177	0.957950	0.154012	0.033*
C3	0.60504(13)	0.7913(2)	0.2056(2)	0.0319(5)
H3	0.669826	0.810586	0.263930	0.038*
C4	0.57729(13)	0.67413(18)	0.18710(19)	0.0267(4)
H4	0.623348	0.615332	0.233771	0.032*
C5	0.48073(13)	0.64403(16)	0.09887(17)	0.0206(4)
C6	0.41337(13)	0.73363(16)	0.0275(2)	0.0222(4)
H6	0.348942	0.714215	−0.035058	0.027*
C7	0.36969(13)	0.94588(16)	−0.02047(18)	0.0221(4)
C8	0.44866(12)	0.52176(16)	0.08262(17)	0.0209(4)
C9	0.36021(13)	0.47629(17)	0.02707(19)	0.0239(4)
H9	0.304502	0.520933	−0.013874	0.029*
C10	0.45505(13)	0.32806(16)	0.10178(18)	0.0225(4)
H10	0.479076	0.251459	0.123003	0.027*
N1	0.29323(11)	1.10390(13)	−0.05730(15)	0.0235(4)
N2	0.24868(11)	1.04857(14)	−0.17092(16)	0.0258(4)
N3	0.29627(11)	0.94745(13)	−0.15023(16)	0.0260(4)
N4	0.37002(11)	1.04133(14)	0.03979(16)	0.0252(4)
N5	0.36416(11)	0.35517(14)	0.03956(15)	0.0224(4)
N6	0.50861(11)	0.42456(13)	0.13072(15)	0.0220(4)
H6A	0.569552	0.425791	0.171959	0.026*
O1	0.34393(10)	0.17563(13)	0.19713(13)	0.0275(3)
H1	0.311541	0.145628	0.215907	0.041*
H1A	0.3668(16)	0.119(2)	0.185(2)	0.033*

*Corresponding author: Shui-Sheng Chen, College of Chemistry and Chemical Engineering, Fuyang Normal University, Fuyang, Anhui 236041, China, e-mail: sscfync@163.com

Jia-Le Li: College of Chemistry and Chemical Engineering, Fuyang Normal University, Fuyang, Anhui 236041, China

Zhang-Fan Chen: Department of Chemistry, Fuyang Normal College, Fuyang, Anhui 236041, China

container and heated at 453 K for 72 h. After cooling to room temperature within 12 h, purple crystals were obtained in 62% yield. Analysis calculated (%): C, 46.43; H, 3.51; N, 32.49%; Found: C, 46.62; H, 3.36; N, 32.28%.

Experimental details

H atoms bonded to C atoms were placed geometrically and treated as riding, with C—H distances 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the CH while $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ for the NH group. The water H atoms were located from difference maps and refined with the O—H distances restrained to 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

Comment

Design and synthesis of porous MOFs has been attracted continuous and increasing attention over the past few decades [4–6]. Generally, rational design/choice of organic linkers and inorganic moieties are crucial for the assembly of targeted MOFs with desired structures and properties. Among the various organic ligands, the classes of polydentate N-heterocyclic bases (such as imidazoles, triazoles, tetrazoles and pyrazoles) and aromatic polycarboxylic acids have been broadly explored as building blocks and linkers for the construction of coordination networks [7–9]. In this context, we are particularly interested in the design and construction of MOFs from polydentate N-heterocyclic bases with specific functions such as gas adsorption, luminescence and magnetic properties [10–12]. In our previous study, we have synthesized a novel multi-N containing ligand HL and constructed a series of novel MOFs together with carboxylate ligands [13].

In the title compound, the asymmetric unit contains one 1-(1*H*-imidazol-4-yl)-3-(4*H*-tetrazol-5-yl)benzene organic molecule, a half of cobalt(II) cation and one coordinated water molecule (figure). The Co1 is located on an inversion center and has octahedral coordination geometry defined by four nitrogen atoms from four *L*[−] ligands and two oxygen donors from two water molecules. Each organic deprotonated *L*[−] as a linear ditopic linker connects two Co(II) atom, leading to an infinite chain with Co···Co distances of 11.325 Å.

Acknowledgements: We gratefully acknowledge support by the Natural Science Foundation of Anhui Provincial Education Commission (No. KH2016B123).

References

1. BRUKER. SAINT, APEX2 and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA (2009).
2. Sheldrick, G. M.: SHELXT – Integrated space-group and crystal-structure determination. *Acta Crystallogr.* **A71** (2015) 3–8.
3. Sheldrick, G. M.: Crystal structure refinement with SHELXL. *Acta Crystallogr.* **C71** (2015) 3–8.
4. Hu, F.; Di, Z.; Lin, P.; Huang, P.; Wu, M.; Jiang, F.; Hong, M.: An anionic uranium-based metal-organic framework with ultralarge nanocages for selective dye adsorption. *Cryst. Growth Des.* **18** (2018) 576–580.
5. Furukawa, H.; Ko, N.; Go, Y. B.; Aratani, N.; Choi, S. B.; Choi, E.; Yazaydin, A.; Snurr, R. Q.; O’Keeffe, M.; Kim, J.; Yaghi, O. M.: Ultrahigh porosity in metal-organic frameworks. *Science* **329** (2010) 424–428.
6. Song, F.; Wang, C.; Falkowski, J. M.; Ma, L.; Lin, W.: Isorecticular chiral metal-organic frameworks for asymmetric alkene epoxidation: tuning catalytic activity by controlling framework catenation and varying open channel sizes. *J. Am. Chem. Soc.* **132** (2010) 15390–15398.
7. Zhu, M. A.; Guo, X. Z.; Chen, S. S.: Synthesis, crystal structure and luminescent property of a Zn(II) complex based on 4-imidazole-carboxylate ligand. *Chin. J. Struct. Chem.* **36** (2017) 1348–1354.
8. Zhu, M. A.; Guo, X. Z.; Xiao, L.; Chen, S. S.: A new Cd(II) coordination compound based on 4-(1,2,4-triazol-4-yl)phenylacetic acid: synthesis, structure and photoluminescence property. *Chin. J. Struct. Chem.* **37** (2018) 437–444.
9. Zhang, Z. Y.; Xiao, L.; Chen, S. S.; Qiao, R.; Yang, S.: A novel Zn(II) complex with 4-connected umc topology: synthesis, crystal structure and luminescent property. *Chin. J. Struct. Chem.* **36** (2017) 819–824.
10. Chen, S. S.; Liu, Q.; Zhao, Y.; Qiao, R.; Sheng, L. Q.; Liu, Z. D.; Yang, S.; Song, C. F.: New metal-organic frameworks constructed from the 4-imidazole-carboxylate ligand: structural diversities, luminescence, and gas adsorption properties. *Cryst. Growth Des.* **14** (2014) 3727–3741.
11. Chen, S. S.; Wang, P.; Takamizawa, S.; Okamura, T. A.; Chen, M.; Sun, W. Y.: Zinc^{II} and cadmium^{II} metal-organic frameworks with 4-imidazole containing tripodal ligand: sorption and anion exchange properties. *Dalton Trans.* **43** (2014) 6012–6020.
12. Xiao, L.; Li, W. D.; Fang, X.; Jiang, L. Y.; Chen, S. S.: Two three-dimensional supramolecular polymer built from mixed N-donor and carboxylate ligands. *Chin. J. Struct. Chem.* **35** (2016) 781–788.
13. Chen, S. S.; Qiao, R.; Sheng, L. Q.; Zhao, Y.; Yang, S.; Chen, M. M.; Liu, Z. D.; Wang, D. H.: Cadmium^{II} and zinc^{II} complexes with rigid 1-(1*H*-imidazol-4-yl)-3-(4*H*-tetrazol-5-yl) benzene and varied carboxylate ligands. *CrystEngComm* **15** (2013) 5713–5725.