Open Access

Lei Zhang, Cong-Kui Nie and Dan Zhao*

Crystal structure of *catena*-poly[di-(μ_3-oxido-κ^3*O*:*O*:*O*)-tetraoxido-(μ_2-5′-(pyrazin-2-yl)-1*H*,2′*H*-3,3′-bi(1,2,4-triazole)-κ^2*N*:*N*′)dimolybdenum(VI)], $C_8H_6Mo_2N_8O_6$

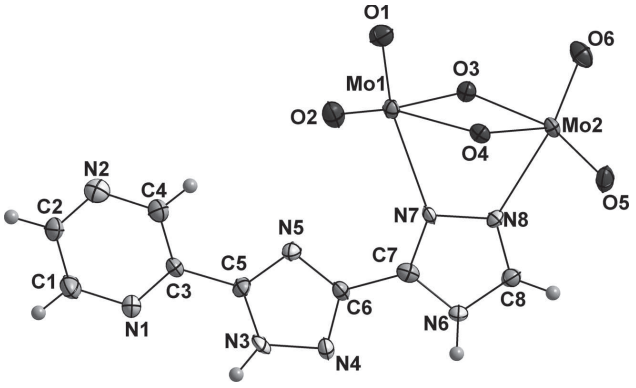

Table 1: Data collection and handling.

Crystal:	Colourless prism
Size:	0.20 × 0.05 × 0.05 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	18.9 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, ω scans
$2\theta_{max}$, completeness:	57°, 93.4%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4588, 3228, 0.029
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2332
$N(param)_{refined}$:	217
Programs:	Bruker programs [1], SHELX [2]

DOI 10.1515/ncrs-2016-0394
Received December 9, 2016; accepted April 12, 2017; available online May 4, 2017

Abstract

$C_8H_6Mo_2N_8O_6$, triclinic, $P\bar{1}$ (no. 2), $a = 7.3053(7)$ Å, $b = 8.7683(9)$ Å, $c = 11.6150(12)$ Å, $\alpha = 87.578(2)°$, $\beta = 74.490(2)°$, $\gamma = 71.912(2)°$, $V = 680.80(12)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.454$, $wR_{ref}(F^2) = 0.1100$, $T = 296$ K.

CCDC no.: 993515

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

Source of material

HCl, KOH and MoO_3 were purchased from Sinopharm Chemical Reagent Co. Ltd; 3-(pyrazin-2-yl)-5-(1*H*-1,2,4-triazol-3-yl)-1,2,4-triazolyl ($C_8H_6N_8$) was purchased from Jinan Camolai Trading Company. All chemicals of analytical grade were obtained from commercial sources and used without further purification. The title compound was synthesized by hydrothermal reaction. A mixture of $C_8H_6N_8$ (0.5 mmol), MoO_3 (2 mmol) and water (10 mL) whose pH value was adjusted to 4 by HCl and KOH was placed in a 30 mL Teflon-lined stainless steel autoclave. Then the autoclave was sealed and heated to 200 °C under autogenously pressure for 5 days. After being slowly cooled to room temperature at a rate of 5 °C/h, colourless prismatic crystals were recovered by filtration, washed with distilled water and air dried.

Experimental details

The H atoms bond to C or N atoms were placed in idealized positions with C—H or N—H bond lengths constrained to 0.93 or 0.86 Å, respectively, and $U_{iso}(H) = 1.2U_{eq}$ (carrier C or N atom).

Comment

In recent years, investigation on coordination polymers (CPs) represents one of the most active areas of material science and chemical research. Major advances have been made in these materials not only because of their fascinating topology and intriguing architectures, but also due to their potential applications in magnetism, luminescence, ion exchange and

***Corresponding author: Dan Zhao,** College of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo, Henan 454000, China, e-mail: iamzd1996@163.com
Lei Zhang and Cong-Kui Nie: College of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo, Henan 454000, China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Mo1	0.45797(7)	0.33867(6)	0.94691(5)	0.01391(15)
Mo2	0.03824(7)	0.63160(6)	1.08741(4)	0.01337(15)
O3	0.1646(6)	0.3926(5)	0.9854(4)	0.0156(9)
O4	0.3258(6)	0.5657(5)	1.0704(3)	0.0146(9)
O1	0.5004(7)	0.2122(5)	1.0564(4)	0.0245(10)
O6	−0.0410(6)	0.5610(6)	1.2235(4)	0.0250(11)
N3	0.7871(7)	0.5002(6)	0.4577(4)	0.0191(12)
H7	0.8476	0.5057	0.3839	0.023*
N1	1.1146(8)	0.2218(6)	0.3708(5)	0.0213(12)
N5	0.7228(8)	0.4071(6)	0.6368(4)	0.0184(11)
C3	1.0222(9)	0.2391(7)	0.4875(5)	0.0160(13)
N4	0.6191(8)	0.6135(6)	0.5195(4)	0.0194(12)
N7	0.3528(7)	0.5689(6)	0.8262(4)	0.0141(10)
C5	0.8460(9)	0.3794(7)	0.5264(5)	0.0161(13)
C1	1.2738(10)	0.0913(8)	0.3363(6)	0.0271(16)
H1	1.3443	0.0747	0.2560	0.033*
C8	0.1437(9)	0.8056(7)	0.8221(5)	0.0183(13)
H8	0.0356	0.8989	0.8438	0.022*
C6	0.5893(9)	0.5487(7)	0.6266(5)	0.0155(12)
N2	1.2461(8)	−0.0018(7)	0.5338(5)	0.0247(13)
C4	1.0874(9)	0.1303(8)	0.5684(6)	0.0223(14)
H4	1.0197	0.1489	0.6491	0.027*
N6	0.2865(8)	0.7785(6)	0.7177(4)	0.0186(11)
H6	0.2950	0.8421	0.6594	0.022*
N8	0.1792(7)	0.6820(6)	0.8882(4)	0.0152(11)
C7	0.4149(9)	0.6296(8)	0.7232(5)	0.0175(13)
O5	−0.0295(6)	0.8312(5)	1.1137(4)	0.0255(11)
O2	0.5282(7)	0.2190(6)	0.8242(4)	0.0274(11)
C2	1.3364(9)	−0.0202(8)	0.4175(6)	0.0227(14)
H2	1.4456	−0.1109	0.3894	0.027*

catalysis [3–6]. Exploring new CP materials with specific networks remains of a particularly important and active subject in the field of crystal engineering and supramolecuar chemistry. The most effective and facile approach for constructing new CPs is the judicious choice of various organic linkers such as aryl carboxylates and *N*-donor ligands. In this work, we introduced a *N*-donor ligand, namely 5′-(pyrazin-2-yl)-1*H*,2′*H*-3,3′-bi(1,2,4-triazole) in our experiment and afforded a new CP compound.

The structure of the title compound features a one-dimensional (1D) structure running along the *a* axis. There is one organic $C_8H_6N_8$ ligand, two molybdenum atoms and six oxygen atoms in an asymmetric unit of the title structure. Each crystallographically unique molybdenum atom is surrounded by five O atoms and one N atom of $C_8H_6N_8$ ligand to form distorted octahedral MoO_5N coordination. Furthermore, the MoO_5N octahedra share common edges or vertices with one another to form a 1D chain running along the aforementioned *a* axis. Adjacent chains are interconnected *via* hydrogen bonds.

Acknowledgements: This work was supported by grants from the Key Research Fund of the Education Department of Henan Province (17A150013).

References

1. Bruker. SMART and SAINT. Bruker AXS Inc., Madison, WI, USA, (2014).
2. Sheldrick, G.: Crystal structure refinement with SHELXL. Acta Crystallogr. **71** (2015) 3–8.
3. Ma, F.-X.; Zhao, D.; Yang, R.-J.; Huang, M.: Crystal structure of poly [tetraaquabis(μ_8-benzene-1,2,4,5-tetracarboxylato-1κ^{3}O^4:O^6:O^8: 2κ^{4}O^2:O^2:O^5:O^5:3κ^{4}O^1:O^3:O^5:O^7)(di-μ_3-hydroxido) pentazinc(II)] decahydrate, $C_{20}H_{34}O_{32}Zn_5$. Z. Kristallogr. – NCS **231** (2016) 897–899.
4. Ma, F.-X.; Zhao, D.; Zhang, R.-H.; Li, F.-F.; Zhang, A.-Y.: A new coordination polymer Pb($C_{12}H_6O_4$): structure resolution of non-merohedral twinning crystal. Chin. J. Struct. Chem. **35** (2016) 437–441.
5. Tan, Y. S.; Azizuddin, A. D.; Campian, M. V.; Haiduc, I.; Tiekink, E. R. T.: Serendipitous compositional and structural diversity in urotropine adducts of binary cadmium xanthates. Z. Kristallogr. – CM **231** (2016) 155–165.
6. Tan, Y. S.; Halim, S. N. A.; Tiekink, E. R. T.: Exploring the crystallization landscape of cadmium bis(*N*-hydroxyethyl, *N*-isopropyldithiocarbamate), Cd[S_2CN(iPr)CH_2CH_2OH]$_2$. Z. Kristallogr. – CM **231** (2016) 113–126.