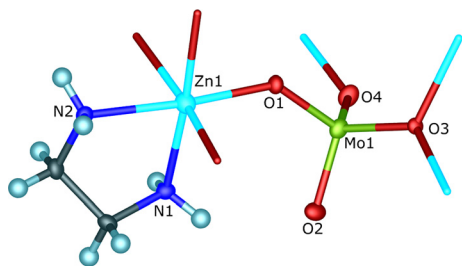


Xin Zhuo*

Crystal structure of *catena*-poly[(ethylenediamine- κ^2N,N')- μ -tetraoxomolybdato(VI) zinc(II)], $C_2H_8MoN_2O_4Zn$



<https://doi.org/10.1515/ncrs-2025-0088>

Received February 22, 2025; accepted April 16, 2025;

published online April 30, 2025

Abstract

$C_2H_8MoN_2O_4Zn$, monoclinic, $P2_1/c$ (no. 4), $a = 10.3133(6)$ Å, $b = 9.6996(5)$ Å, $c = 7.2740(4)$ Å, $\beta = 106.088(1)^\circ$, $V = 699.16(7)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0191$, $wR_{ref}(F^2) = 0.0512$, $T = 296(2)$ K.

CCDC no.: 2444266

A part of the title polymeric structure is shown in the figure. Table 1 contains crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of material

A mixture of $Na_2MoO_4 \cdot 2H_2O$ (0.243 g, 1.0 mmol), $Zn(NO_3)_2 \cdot 6H_2O$ (0.2989 g, 1.0 mmol) was dissolved in 10 mL distilled water and stirred briefly for 0.5 h. When the pH value was adjusted to about 7.2 with ethylenediamine, the mixture was sealed into a 20 mL Teflon-lined autoclave and then kept under autogenous pressure at 433 K for 3 days. After slowly cooling to room temperature, colorless block crystals were isolated and washed with distilled water (57 % yield, based on Mo).

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.20 \times 0.18 \times 0.16$ mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	5.18 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max} , completeness:	25.0°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	3607, 1232, 0.029
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1,184
$N(param)_{refined}$:	91
Programs:	Bruker, ¹ SHELX ²

2 Experimental details

All H atoms were located in calculated positions (C–H = 0.97 Å, N–H = 0.89 Å) and were included in the refinement using the riding model approximation with $U_{iso}(H)$ set to $1.2U_{eq}(C,N)$.

3 Discussion

Polyoxomolybdate-based metal-organic complexes (MOCs) are important class of inorganic/organic hybrid compounds and have drawn continuous significant interest not only because of their various structures but also their extensive applications (catalysis, magnetism, electrode materials and fluorescent materials, *et. al.*).^{3–10} In addition, ethylenediamine (en) is one of the most extensively used bidentate ligands in coordination chemistry.^{4,11–15} In order to synthesize new MOCs, the title compound based on MoO_4^{2-} and ethylenediamine was synthesized and its crystal structure determined.

Single-crystal X-ray diffraction structure analysis shows that the title compound has the similar structure of its analogous compound poly[(ethylenediamine- κ^2N,N')-cobalt(II)]- μ -tetraoxomolybdato(VI)].⁴ The title compound exhibited the same two-dimensional configuration. The title compound crystallizes in the monoclinic space group $P2_1/c$ (no. 14), and its unit cell is filled with one complex containing one Zn^{2+} , one MoO_4^{2-} , and one en ligand (see the figure). The Zn^{2+} has a distorted octahedral coordination geometry, which is coordinated by two nitrogen atoms from one en

*Corresponding author: Xin Zhuo, School of Chemistry and Chemical Engineering, Suzhou University, 234000, Suzhou, Anhui, People's Republic of China, E-mail: szxyzx@163.com. <https://orcid.org/0000-0002-7186-4362>

ligand and four oxygen atoms from three symmetry related MoO₄^{2−}. The bond lengths and angles are all within the normal ranges. A binuclear [Zn₂O₂] unit is formed by the two adjacent Zn²⁺ cations and the bridging oxygen atoms, which are further connected by the bridging MoO₄^{2−} anions, giving rise to a two-dimensional network.

Author contribution: The author has accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: Scientific research and Development Fund Project of Suzhou University (2021fzjj07), Action for the Training of Middle-aged and Young Teachers in Disciplines (Specialties) Leading Personnel (DTR2023056), and Anhui Provincial Key Project of Quality Engineering for Higher Education Institutions (2023jyxm0764).

Conflict of interest: The author declares no conflicts of interest regarding this article.

References

1. Bruker APEX2, SAINT and SADABS; Bruker AXS Inc.: Madison, Wisconsin, USA, 2008.
2. Sheldrick, G. M. A Short History of SHELX. *Acta Crystallogr.* **2008**, A64, 112–122.
3. Xu, L.-J.; Wang, C.-M.; Yu, K.; Wang, C.-X.; Zhou, B.-B. Research Progress of POMs Constructed by 1,3,5-benzene-Tricarboxylic Acid: From Synthesis to Application. *Coord. Chem. Rev.* **2023**, 481, 215044.
4. Lin, B.-Z. Layered (ethylenediamine-κ²N,N')-Cobalt(II) Molybdate(VI). *Acta Crystallogr.* **2002**, C62, m261–m263.
5. Bazargan, M.; Mirzaei, M.; Franconetti, A.; Frontera, A. On the Preferences of Five-Membered Chelate Rings in Coordination Chemistry: Insights from the Cambridge Structural Database and Theoretical Calculations. *Dalton Trans.* **2019**, 48, 5476–5490.
6. Chan, L.; Hutchison, G. R.; Morris, G. M. Understanding Ring Puckering in Small Molecules and Cyclic Peptides. *J. Chem. Inf. Model.* **2021**, 61, 743–755.
7. Sun, X.; Ban, R.; Ma, P.; Wang, J.; Zhang, D.; Niu, J.; Wang, J. Four Transition-Metal-Bridging Risedronate-Based Polyoxomolybdates: Syntheses, Structures, Characterizations and Magnetic Properties. *Synthetic Met.* **2017**, 223, 19–25.
8. Zhang, L.; Jiang, H.; Wang, C.; Yu, K.; Lv, J.; Wang, C.; Zhou, B. Improved Supercapacitors and Water Splitting Performances of Anderson-type Manganese(III)-polyoxomolybdate through Assembly with Zn-MOF in a Host-Guest Structure. *J. Colloid Interf. Sci.* **2025**, 654, 1393–1404.
9. Gao, Q.; Dong, X.-R.; Lin, Z.; Liu, W.; Hu, D.-H.; Xu, L. 3D Organic-Inorganic Hybrid Based on Strandberg-type Cluster of [(P^{III}O₃)₂Mo₅O₁₅]^{6−}: Synthesis, Crystal Structure and Electrochemical Properties. *J. Mol. Struct.* **2025**, 1321, 140171.
10. Hou, Y.; Sun, Y.; Zhang, S.; Han, P.; Li, H.; Wang, X.; Chen, H.; Cheng, Y. Two 2D Phosphomolybdate-Based on Cu-Organic Complexes for the Heterogeneous Catalysis of Various Sulfides. *J. Mol. Struct.* **2025**, 1328, 141358.
11. Ndlangamandla, N. G.; Clayton, H. S. The Crystal Structure of *trans*-Dichlorido-(ethylenediamine-κ²N,N')-bis(triphenylphosphine-κ¹P) ruthenium(II), C₃₈H₃₈Cl₂N₂P₂Ru. *Z. Kristallogr. NCS.* **2022**, 237, 1175–1179.
12. Uemura, K. Binding Ability of Chloride Ion with Platinum and Rhodium Dinuclear Complex Containing Ethylenediamine as Co-ligand. *Inorg. Chim. Acta* **2024**, 570, 122171.
13. Chen, A.-N.; Liu, L.; Pan, C.-Y. Synthesis, Structure, and Oxygen Reduction Reaction of Three Copper Complexes Supported by Ethylenediamine Derivatives with Outer-Sphere Oxoboron Clusters. *Inorg. Chim. Acta* **2024**, 570, 122179.
14. Zhou, C.-Y.; Du, Y.-J.; Su, F.; Zhang, B.-X.; Li, S.-D. Crystal Structure of Poly [bis(μ₂-1,4-di(1*H*-Imidazol-1-yl)benzene-κ²N,N')-(μ₂-tetraoxidomolybdate(VI)-κ²O:O')cobalt(II)], C₂₄H₂₀N₈O₄MoCo. *Z. Kristallogr. NCS.* **2020**, 235, 1555–1557.
15. Rohde, D.; Kondracka, M.; Merzweiler, K. Synthesis and Properties of Triphenyltin Molybdates with Chainlike Anions of the Type ¹_∞[(Ph₃Sn)MoO₄][−]. The Crystal Structures of (Pr₄N)[(Ph₃Sn)MoO₄][−]·CH₃CN, (tBu₄N)[(Ph₃Sn)MoO₄], [Zn(en)₂(Ph₃Sn)₂(MoO₄)₂]-2DMF-EtOH, and [Cu(en)₂(Ph₃Sn)₂(MoO₄)₂]-2DMF-EtOH. *Z. Anorg. Allg. Chem.* **2012**, 638, 2213.