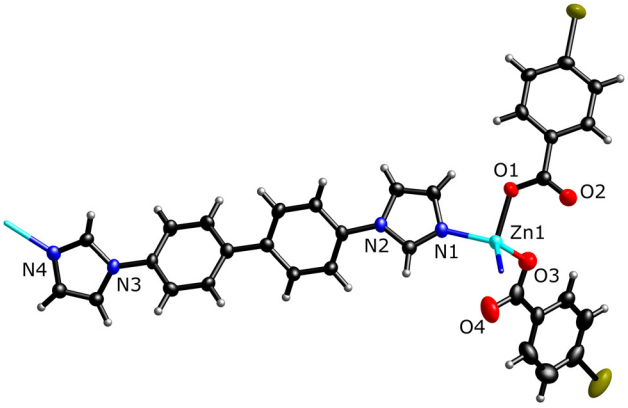
Xiao-Hui Bai, Yan Xing and Si-Jie Liu*

Crystal structure of *catena*-poly[(μ_2-1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol)-κ^2*N*:*N*′)-bis(4-bromobenzoate-κ^1*O*)zinc(II)], $C_{64}H_{44}Br_4N_8O_8Zn_2$



https://doi.org/10.1515/ncrs-2021-0413
Received October 24, 2021; accepted December 2, 2021; published online December 14, 2021

Abstract

$C_{64}H_{44}Br_4N_8O_8Zn_2$, monoclinic, $P2_1/c$ (No. 14), a = 6.6263(5) Å, b = 24.355(2) Å, c = 18.2418(15) Å, β = 96.433(2)°, V = 2925.4(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0400, $wR_{ref}(F^2)$ = 0.1302, T = 296(2) K.

CCDC no.: 2125833

A part of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.25 × 0.22 × 0.18 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	3.62 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14,841, 5141, 0.037
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 3836
$N(param)_{refined}$:	388
Programs:	Bruker [1], SHELX [2]

Source of material

The mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (1 mmol, 297.5 mg), 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) (bibp) (1 mmol, 286.3 mg), 4-bromobenzoic acid (2 mmol, 402.0 mg), dimethylformamide (1 mL) and H_2O (3 mL) were placed in a 10 mL Teflon-lined autoclave at 373 K for 72 h, then cooled to room temperature. Colourless block crystals were obtained.

Experimental details

The hydrogen atoms were positioned geometrically with C–H = 0.93 Å. Their U_{iso} values were set to be 1.2U_{eq} of the parent atoms.

Comment

As an imidazole derivative, 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) (bibp) is a good neutral N-donor organic ligand to construct coordination polymers because of its versatile coordination modes [3–11]. In order to expand this research area, the title compound based on bibp ligand and the auxiliary ligand 4-bromobenzoic acid (BBA) was synthesised and its crystal structure determined.

In the title compound, the fundamental unit contains one Zn(II) cation, one bibp ligand, and two 4-bromobenzoate ligands. The Zn(II) cation is four coordinated by two O atoms from two crystallographically independent 4-bromobenzoate ligands (Zn–O = 1.959(3)–1.967(3) Å), and two N atoms from two symmetry related bibp ligands (Zn–N = 1.996(3)–2.032(3) Å), forming a distorted tetrahedral geometry (see the

***Corresponding author: Si-Jie Liu,** College of Chemical Engineering, Shijiazhuang University, 050035, Shijiazhuang, Hebei, People's Republic of China, E-mail: liusijie1982@163.com. https://orcid.org/0000-0001-7003-8061
Xiao-Hui Bai and Yan Xing, School of Chemistry and Chemical Engineering, Yulin University, 719000, Yulin, Shannxi, People's Republic of China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Br1	−0.76816 (8)	0.21102 (2)	0.58783 (3)	0.0566 (2)
Br2	−0.57573 (12)	0.44537 (3)	−0.11702 (3)	0.0808 (3)
C1	−0.2321 (7)	0.36584 (19)	0.4241 (2)	0.0343 (10)
C2	−0.3587 (6)	0.32803 (17)	0.4660 (2)	0.0291 (9)
C3	−0.2935 (7)	0.27553 (19)	0.4867 (2)	0.0357 (11)
H3	−0.167762	0.263428	0.475150	0.043*
C4	−0.4112 (7)	0.24100 (19)	0.5241 (2)	0.0385 (11)
H4	−0.364248	0.206418	0.539411	0.046*
C5	−0.6016 (7)	0.25912 (19)	0.5382 (2)	0.0365 (11)
C6	−0.6711 (7)	0.31017 (18)	0.5170 (2)	0.0338 (10)
H6	−0.800177	0.321361	0.526105	0.041*
C7	−0.5489 (7)	0.34491 (18)	0.4820 (2)	0.0336 (10)
H7	−0.594245	0.380086	0.469009	0.040*
C8	−0.0570 (8)	0.3985 (2)	0.1799 (3)	0.0453 (13)
C9	−0.1857 (7)	0.41048 (19)	0.1077 (3)	0.0363 (11)
C10	−0.3933 (7)	0.4026 (2)	0.0995 (3)	0.0445 (12)
H10	−0.456723	0.390002	0.139269	0.053*
C11	−0.5083 (8)	0.4132 (2)	0.0330 (3)	0.0540 (14)
H11	−0.648037	0.407698	0.028133	0.065*
C12	−0.4169 (9)	0.4318 (2)	−0.0250 (3)	0.0531 (14)
C13	−0.2115 (10)	0.4412 (2)	−0.0189 (3)	0.0621 (16)
H13	−0.150119	0.454539	−0.058661	0.074*
C14	−0.0981 (8)	0.4303 (2)	0.0478 (3)	0.0596 (15)
H14	0.041209	0.436445	0.052412	0.071*
C15	0.4202 (6)	0.29685 (17)	0.2894 (2)	0.0313 (10)
H15	0.494078	0.322288	0.265287	0.038*
C16	0.1879 (7)	0.25870 (17)	0.3451 (3)	0.0353 (11)
H16	0.068910	0.253858	0.366899	0.042*
C17	0.3279 (7)	0.21989 (18)	0.3396 (2)	0.0350 (11)
H17	0.324499	0.183837	0.356265	0.042*
C18	0.6530 (6)	0.21531 (17)	0.2829 (2)	0.0287 (10)
C19	0.7298 (6)	0.17200 (18)	0.3265 (2)	0.0345 (10)
H19	0.681428	0.165228	0.371588	0.041*
C20	0.8787 (7)	0.13883 (18)	0.3027 (3)	0.0361 (11)
H20	0.927446	0.109257	0.331723	0.043*
C21	0.9571 (6)	0.14865 (17)	0.2366 (2)	0.0299 (10)
C22	0.8835 (7)	0.19386 (19)	0.1961 (2)	0.0341 (10)
H22	0.937485	0.202149	0.152446	0.041*
C23	0.7326 (7)	0.22711 (18)	0.2182 (2)	0.0347 (11)
H23	0.685449	0.257108	0.189772	0.042*
C24	1.1159 (6)	0.11215 (16)	0.2118 (2)	0.0282 (9)
C25	1.1064 (6)	0.05530 (18)	0.2193 (3)	0.0333 (10)
H25	0.998225	0.040017	0.240601	0.040*
C26	1.2522 (6)	0.02102 (18)	0.1962 (2)	0.0345 (11)
H26	1.240297	−0.016892	0.200052	0.041*
C27	1.4168 (6)	0.04417 (16)	0.1673 (2)	0.0270 (9)
C28	1.4328 (7)	0.10033 (17)	0.1597 (2)	0.0340 (10)
H28	1.544067	0.115435	0.140126	0.041*
C29	1.2816 (6)	0.13409 (17)	0.1814 (2)	0.0310 (10)
H29	1.291190	0.171898	0.175584	0.037*
C30	1.6501 (6)	−0.03478 (16)	0.1826 (2)	0.0305 (10)
H30	1.606079	−0.047450	0.226169	0.037*
C31	1.6783 (7)	0.01509 (18)	0.0844 (2)	0.0341 (10)
H31	1.659815	0.042244	0.048429	0.041*
C32	1.8123 (7)	−0.02684 (18)	0.0872 (3)	0.0357 (11)
H32	1.902534	−0.033593	0.052666	0.043*

Table 2: (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2452 (5)	0.30712 (14)	0.31357 (19)	0.0294 (8)
N2	0.4797 (5)	0.24438 (14)	0.30403 (18)	0.0287 (8)
N3	1.5745 (5)	0.00971 (14)	0.14526 (19)	0.0294 (8)
N4	1.7946 (5)	−0.05807 (13)	0.1492 (2)	0.0305 (8)
O1	−0.0915 (5)	0.34167 (13)	0.39403 (18)	0.0454 (9)
O2	−0.2708 (5)	0.41479 (14)	0.4199 (2)	0.0586 (10)
O3	−0.1497 (5)	0.38258 (14)	0.23303 (19)	0.0482 (9)
O4	0.1289 (5)	0.40361 (18)	0.1836 (2)	0.0648 (11)
Zn1	0.05911 (7)	0.37310 (2)	0.31760 (3)	0.02964 (16)

figure). Geometric parameters are all in the expected ranges [12]. The bridging bibp ligands link adjacent Zn(II) cations to form a chain structure with the Zn–Zn distance of 17.797 Å along the *b* axis.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This work was financial supported by research project of Yulin Science and Technology Bureau (2019-83-3 and 2019-83-5) and Natural Science Youth Foundation of Hebei Province (H2018106015).

Conflict of interest statement: The authors declare 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. Li H., Han X., Cao B. Crystal structure of *catena*-poly[*trans*-tetraaqua(μ_2-1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol)-κ^2N:N') cobalt(II)] dinitrate – 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) – water (1/3/2), $C_{72}H_{68}CoN_{18}O_{12}$. *Z. Kristallogr. NCS.* 2021, *236*, 463–465.
4. Yang X., Ren Y., Chai H., Hou X., Wang Z., Wang J. Highly sensitive detection of nitrobenzene by a series of fluorescent 2D zinc(II) metal-organic frameworks with a flexible triangular ligand. *RSC Adv.* 2021, *11*, 23975–23984.
5. Fan C., Xu C., Zhu B., Wang L., Zong Z., Wu R., Zhang X., Fan Y. New topological Zn metal organic frameworks as multi-responsive fluorescent sensing materials for detecting Fe^{3+}, $Cr_2O_7^{2-}$, CrO_4^{2-} and tetracycline in aqueous system. *J. Solid State Chem.* 2021, *298*, 122157.
6. Lozan V., Makhloufi G., Druta V., Bourosh P., Kravtsov V.-Ch., Marangoci N., Heering C., Janiak C. Synthesis and structure of zinc(II) and cobalt(II) coordination polymers involving the elongated 2′,3′,5′,6′ tetramethylterphenyl-4,4″-dicarboxylate ligand. *Inorg. Chim. Acta* 2020, *506*, 119500.
7. Meng L., Zhao L., Guo G., Liu X. Multifunctional polymers with interpenetrating structures: luminescent sensing, ECL behaviors, selective detection of Fe^{3+} ion and rapid removal of anionic dyes. *New J. Chem.* 2020, *44*, 9025–9036.
8. Fan C., Zhang X., Li N., Xu C., Wu R., Zhu B., Zhang G., Bi S., Fan Y. Zn-MOFs based luminescent sensors for selective and highly sensitive detection of Fe^{3+} and tetracycline antibiotic. *J. Pharmaceut. Biomed. Anal.* 2020, *188*, 113444.
9. Voda I., Makhloufi G., Druta V., Lozan V., Shova S., Bourosh P., Kravtsov V., Janiak C. Mixed-ligand coordination compounds based on the rigid 4,4′-bis(1-imidazolyl)biphenyl and pyridinedicarboxylate ligands. *Inorg. Chim. Acta* 2018, *482*, 526–534.
10. Zhu Z., Meng X., Zhang D., Zhang X., Wang M., Jin F., Fan Y. Syntheses, structures and selective dye adsorption of five formic-based coordination polymers prepared by in-situ hydrolysis of *N*,*N*′-dimethylformamide. *J. Solid State Chem.* 2017, *248*, 109–118.
11. Ning Y.-X., Fan W., Xie G. *catena*-poly[[(dichloridozinc)-μ-4,4′-bis(1*H*-imidazol-1-yl)biphenyl-κ$^2N^3$:$N^{3'}$] 0.25 -hydrate]. *Acta Crystallogr.* 2012, *E68*, m406.
12. Liu G.-Z., Chen H.-T., Zhang X.-T. Syntheses, crystal structures, and fluorescence properties of three coordination polymers constructed based on benzoic acid and its derivatives. *Huaxue J.* 2017, *36*, 2058.