

# Synthesis and crystal structure of *catena*-poly-[[aquazinc(II)]-bis[ $\mu_2$ -4-(phenyldiazenyl)benzoato- $\kappa^2$ O:O']]

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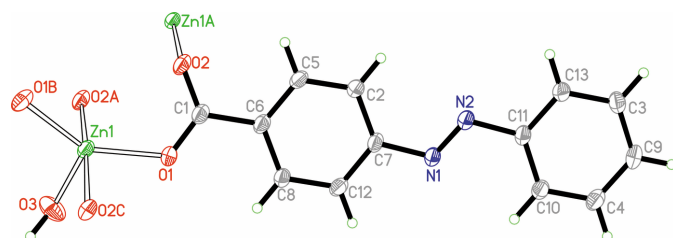
In the title compound,  $[\text{Zn}(\text{C}_{13}\text{H}_9\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})]_n$  or  $[\text{Zn}(\text{pba})_2(\text{H}_2\text{O})]_n$  ( $\text{pba}^- = 4\text{-(phenyldiazenyl)benzoate}$ ), the  $\text{Zn}^{2+}$  ions are coordinated by one water molecule and four oxygen atoms from four different  $\text{pba}^-$  ligands to form a  $[\text{ZnO}_5]$  trigonal bipyramid. The Zn ion and the water O atom lie on a twofold axis. The trigonal bipyramids are bridged by the  $\text{pba}^-$  ligands, extending the structure into chains propagating along the *b*-axis direction. The chains are connected through hydrogen-bonding interactions.

## 1. Chemical context

Azobenzene, as a classical photoswitchable molecule, has gained great attention in designing stimuli-responsive supramolecular system due to its unique photochromic properties arising from reversible *E* and *Z* geometric isomerism (Feng *et al.*, 2025; Golzani *et al.*, 2026; Hao *et al.*, 2017). In recent years, metal–organic frameworks (MOFs) and their derivatives have become widely used in many fields such as separation, catalysis, detection and electrochemical reduction (Liang *et al.*, 2024; Zhao *et al.*, 2022, 2026; Zhong *et al.*, 2025). Incorporating azobenzene derivatives into MOFs represents a frontier strategy for constructing stimuli responsive systems in materials science. For example, Nitschke and co-workers successfully developed light-responsive metal–organic capsules by incorporating azobenzene-based ligands (Ghosh *et al.*, 2026) while Tadjarodi and co-workers fabricated a sacrificial nanozyme-based MOF capable of detecting and quantifying  $\text{Hg}^{2+}$  ions in aqueous solutions by using an azobenzene-4,4-dicarboxylate ligand (Golzani *et al.*, 2026). However, theoretically, the molecular motion will be certainly restricted by steric constraints and lattice strain in crystalline MOFs. To supply more examples of functional compounds incorporation by azobenzene derivatives, the title compound, **(1)**, with a one-dimensional chain structure, was obtained.

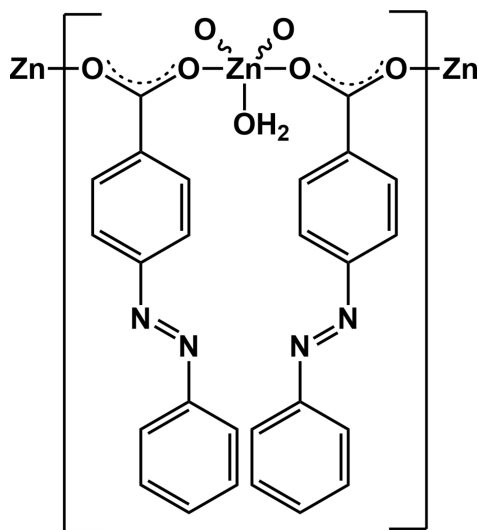
## 2. Structural commentary

The asymmetric unit of **(1)** one Zn ion (site symmetry 2), one  $\text{pba}^-$  anion and one water molecule (O atom site symmetry 2) (Fig. 1). The Zn–O bond lengths are in the range 1.954 (5)–2.150 (3) Å (Table 1). All the data are comparable to those reported for other related  $\text{Zn}^{\text{II}}$ -polycarboxylate compounds (Gu *et al.*, 2023; Liu *et al.*, 2025; Zhao *et al.*, 2024). Each Zn center is five-coordinated by four oxygen from four different  $\text{pba}^-$  anions and one coordinated water molecule, forming a



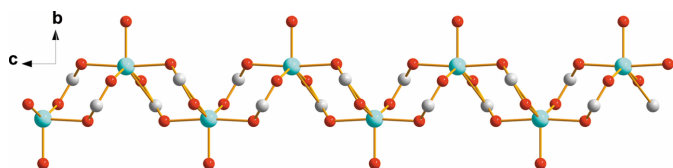
**Figure 1**  
The extended asymmetric unit of (**1**) showing the coordination environment of the  $\text{Zn}^{2+}$  cation and the ligand. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A)  $-x + 1, -y + 1, -z + 1$ ; (B)  $-x + 1, y, -z + \frac{3}{2}$ ; (C)  $x, -y + 1, z + \frac{1}{2}$ .]

trigonal–bipyramidal geometry. The equatorial plane is occupied by atoms O1, O1<sup>i</sup> and O3. The pba<sup>−</sup> ligand bridges two  $\text{Zn}^{\text{II}}$  ions through its carboxyl O atoms, and two  $\text{Zn}^{\text{II}}$  ions are bridged by two pba<sup>−</sup> ligands to form a binuclear  $\text{Zn}_2(\text{COO})_2$  unit. The two  $\text{Zn}^{\text{II}}$  ions and the two carboxyl carbon atoms are in the same plane. The neighboring  $\text{Zn}_2(\text{COO})_2$  unit is distorted and the angle between the binuclear units is  $77.3 (1)^\circ$  (the plane is defined by two  $\text{Zn}^{\text{II}}$  ions and two carboxyl carbon atoms).



### 3. Supramolecular features

In the crystal, The units are extended along the *c*-axis direction, generating a one-dimensional zigzag chain (Fig. 2). The ligand hangs along the chain towards different directions (Fig. 3). O–H...O hydrogen bonds are observed (Table 2). The packing is shown in Fig. 4.



**Figure 2**  
The one-dimensional zigzag chain.

**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Zn1–O1	1.964 (3)	Zn1–O2 <sup>iii</sup>	2.150 (3)
Zn1–O1 <sup>i</sup>	1.964 (3)	Zn1–O3	1.954 (5)
Zn1–O2 <sup>ii</sup>	2.150 (3)		
O1–Zn1–O1 <sup>i</sup>	142.3 (2)	O3–Zn1–O1 <sup>i</sup>	108.85 (11)
O1–Zn1–O2 <sup>iii</sup>	87.11 (12)	O3–Zn1–O1	108.85 (10)
O1 <sup>i</sup> –Zn1–O2 <sup>iii</sup>	94.66 (13)	O3–Zn1–O2 <sup>iii</sup>	87.26 (9)
O1 <sup>i</sup> –Zn1–O2 <sup>ii</sup>	87.11 (12)	O3–Zn1–O2 <sup>ii</sup>	87.26 (9)
O1–Zn1–O2 <sup>ii</sup>	94.66 (13)	C1–O1–Zn1	121.4 (3)
O2 <sup>iii</sup> –Zn1–O2 <sup>ii</sup>	174.51 (18)	C1–O2–Zn1 <sup>ii</sup>	125.4 (3)

Symmetry codes: (i)  $-x + 1, y, -z + \frac{3}{2}$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $x, -y + 1, z + \frac{1}{2}$ .

**Table 2**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O3–H3...O2 <sup>iv</sup>	0.87	1.78	2.588 (4)	154

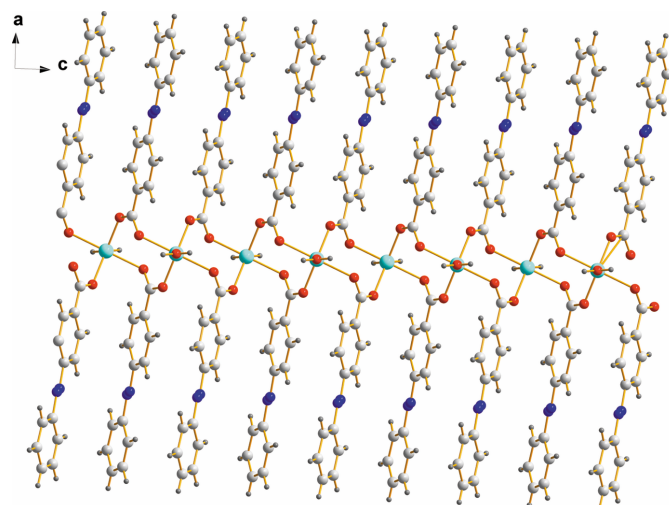
Symmetry code: (iv)  $-x + 1, y + 1, -z + \frac{3}{2}$ .

### 4. Synthesis and crystallization

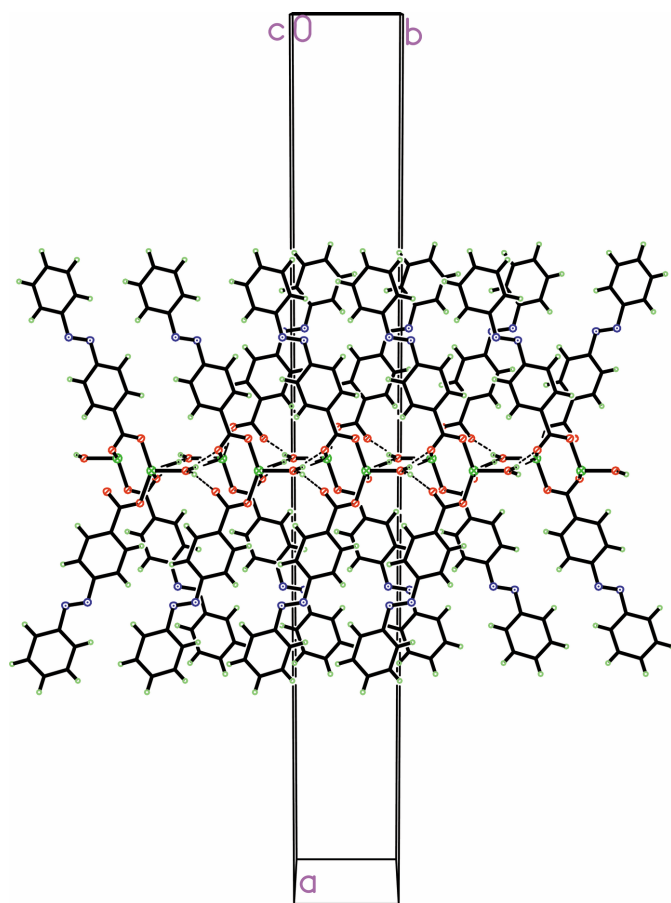
A mixture of  $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (29.5 mg, 0.1 mmol) and pba (45.2 mg, 0.2 mmol) in 5 mL DMF was sealed in a Teflon lined autoclave and heated to 393 K for 48 h, then gradually cooled down to room temperature. Pale-yellow block-shaped crystals were obtained.

### 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atom of the coordinated water molecule was located from a difference-Fourier map, and refined using a riding model with isotropic displacement parameters  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . C-bound H atoms were positioned geometrically (C–H = 0.95  $\text{\AA}$ ) and refined with as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .



**Figure 3**  
The one-dimensional chain constructed by  $\text{Zn}^{\text{II}}$  ions and the carboxyl groups.



**Figure 4**  
Packing diagram of (1), showing hydrogen-bonding interactions (dashed lines).

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**Table 3**  
Experimental details.

Crystal data	
Chemical formula	[Zn(C <sub>13</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O)]
<i>M<sub>r</sub></i>	533.83
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	51.1233 (13), 6.1213 (2), 7.2534 (3)
$\beta$ (°)	90.788 (3)
<i>V</i> (Å <sup>3</sup> )	2269.68 (13)
<i>Z</i>	4
Radiation type	Cu <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.91
Crystal size (mm)	0.35 × 0.34 × 0.34
Data collection	
Diffractometer	ROD, Synergy Custom DW system, HyPix
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku Oxford Diffraction, 2023)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.683, 1.000
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	12079, 2310, 1997
<i>R<sub>int</sub></i>	0.074
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.629
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.064, 0.188, 1.09
No. of reflections	2310
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.98, -0.79

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

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## supporting information

*Acta Cryst.* (2026). E82 [https://doi.org/10.1107/S2056989026005177]

## Synthesis and crystal structure of *catena*-poly[[aquazinc(II)]-bis[ $\mu_2$ -4-(phenyldiazenyl)benzoato- $\kappa^2$ O:O']]

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### Computing details

*catena*-Poly[[aquazinc(II)]-bis[ $\mu_2$ -4-(phenyldiazenyl)benzoato- $\kappa^2$ O:O']]

#### Crystal data

[Zn(C<sub>13</sub>H<sub>9</sub>N<sub>2</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)]

$M_r = 533.83$

Monoclinic,  $C2/c$

$a = 51.1233$  (13) Å

$b = 6.1213$  (2) Å

$c = 7.2534$  (3) Å

$\beta = 90.788$  (3)°

$V = 2269.68$  (13) Å<sup>3</sup>

$Z = 4$

$F(000) = 1096$

$D_x = 1.562$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54184$  Å

Cell parameters from 5128 reflections

$\theta = 1.7\text{--}75.3^\circ$

$\mu = 1.91$  mm<sup>-1</sup>

$T = 100$  K

Block, colourless

0.35 × 0.34 × 0.34 mm

#### Data collection

ROD, Synergy Custom DW system, HyPix diffractometer

Radiation source: Rotating-anode X-ray tube, Rigaku (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku Oxford Diffraction, 2023)

$T_{\min} = 0.683$ ,  $T_{\max} = 1.000$

12079 measured reflections

2310 independent reflections

1997 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.074$

$\theta_{\max} = 75.8^\circ$ ,  $\theta_{\min} = 1.7^\circ$

$h = -63 \rightarrow 63$

$k = -7 \rightarrow 7$

$l = -9 \rightarrow 9$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.064$

$wR(F^2) = 0.188$

$S = 1.09$

2310 reflections

164 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2 + 14.3419P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.98$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.78$  e Å<sup>-3</sup>

#### Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.500000	0.68636 (12)	0.750000	0.0348 (3)
O1	0.46580 (5)	0.5827 (6)	0.6597 (5)	0.0429 (8)
O2	0.48302 (5)	0.2968 (5)	0.5191 (4)	0.0395 (7)
O3	0.500000	1.0056 (8)	0.750000	0.0614 (15)
H3	0.501450	1.091918	0.844860	0.092*
N1	0.35958 (6)	0.1029 (6)	0.4436 (5)	0.0366 (8)
N2	0.35633 (7)	-0.0988 (6)	0.4260 (5)	0.0380 (8)
C1	0.46353 (8)	0.4063 (8)	0.5720 (6)	0.0363 (9)
C2	0.40772 (8)	0.0371 (7)	0.4283 (6)	0.0363 (9)
H2	0.405238	-0.105117	0.378553	0.044*
C3	0.29970 (9)	-0.4379 (8)	0.2927 (7)	0.0428 (10)
H3A	0.296645	-0.578410	0.241022	0.051*
C4	0.28344 (8)	-0.0956 (9)	0.4070 (7)	0.0437 (11)
H4	0.269101	-0.003491	0.435632	0.052*
C5	0.43271 (8)	0.1173 (8)	0.4591 (7)	0.0377 (10)
H5	0.447401	0.030593	0.427714	0.045*
C6	0.43656 (8)	0.3233 (7)	0.5352 (6)	0.0353 (9)
C7	0.38625 (8)	0.1666 (7)	0.4710 (6)	0.0345 (9)
C8	0.41509 (8)	0.4531 (7)	0.5779 (6)	0.0357 (9)
H8	0.417655	0.593238	0.631425	0.043*
C9	0.27874 (9)	-0.3010 (9)	0.3321 (7)	0.0461 (11)
H9	0.261314	-0.347783	0.307790	0.055*
C10	0.30859 (8)	-0.0238 (8)	0.4405 (6)	0.0381 (10)
H10	0.311607	0.117081	0.491508	0.046*
C11	0.32956 (8)	-0.1596 (7)	0.3988 (6)	0.0366 (10)
C12	0.38991 (8)	0.3773 (8)	0.5420 (6)	0.0369 (10)
H12	0.375247	0.467940	0.565622	0.044*
C13	0.32514 (9)	-0.3678 (8)	0.3294 (7)	0.0399 (10)
H13	0.339470	-0.462513	0.306996	0.048*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.0210 (4)	0.0272 (4)	0.0562 (6)	0.000	0.0029 (3)	0.000
O1	0.0247 (14)	0.0444 (19)	0.060 (2)	-0.0063 (13)	0.0040 (12)	-0.0118 (15)
O2	0.0221 (13)	0.0465 (19)	0.0500 (18)	0.0000 (12)	0.0034 (12)	0.0032 (14)
O3	0.096 (4)	0.027 (2)	0.061 (3)	0.000	-0.017 (3)	0.000
N1	0.0252 (16)	0.0325 (19)	0.052 (2)	-0.0029 (14)	0.0021 (14)	-0.0003 (16)
N2	0.0267 (17)	0.036 (2)	0.052 (2)	-0.0029 (15)	0.0044 (14)	0.0000 (16)
C1	0.0256 (19)	0.039 (2)	0.044 (2)	-0.0017 (17)	0.0039 (16)	0.0033 (19)
C2	0.0277 (19)	0.032 (2)	0.049 (2)	-0.0001 (16)	0.0024 (17)	-0.0010 (18)
C3	0.038 (2)	0.036 (2)	0.054 (3)	-0.0103 (19)	0.0004 (19)	0.001 (2)
C4	0.029 (2)	0.049 (3)	0.054 (3)	0.0010 (19)	0.0047 (18)	0.005 (2)
C5	0.0241 (19)	0.037 (2)	0.053 (3)	0.0038 (17)	0.0060 (17)	0.0018 (19)
C6	0.0241 (19)	0.035 (2)	0.047 (2)	-0.0017 (16)	0.0042 (16)	0.0042 (18)

C7	0.0231 (18)	0.034 (2)	0.046 (2)	-0.0031 (16)	0.0027 (16)	0.0051 (17)
C8	0.0269 (19)	0.034 (2)	0.047 (2)	-0.0034 (16)	0.0026 (16)	0.0004 (18)
C9	0.029 (2)	0.056 (3)	0.053 (3)	-0.011 (2)	0.0004 (19)	0.003 (2)
C10	0.0284 (19)	0.037 (2)	0.049 (2)	-0.0006 (17)	0.0032 (17)	0.0022 (19)
C11	0.028 (2)	0.036 (2)	0.046 (3)	-0.0060 (16)	0.0035 (17)	0.0014 (18)
C12	0.0259 (19)	0.036 (2)	0.049 (3)	0.0034 (16)	0.0058 (17)	0.0035 (19)
C13	0.034 (2)	0.032 (2)	0.054 (3)	-0.0024 (17)	0.0068 (19)	0.0020 (19)

*Geometric parameters (Å, °)*

Zn1—O1	1.964 (3)	C3—C9	1.393 (7)
Zn1—O1 <sup>i</sup>	1.964 (3)	C3—C13	1.392 (6)
Zn1—O2 <sup>ii</sup>	2.150 (3)	C4—H4	0.9500
Zn1—O2 <sup>iii</sup>	2.150 (3)	C4—C9	1.389 (7)
Zn1—O3	1.954 (5)	C4—C10	1.377 (6)
O1—C1	1.258 (6)	C5—H5	0.9500
O2—C1	1.265 (5)	C5—C6	1.390 (6)
O3—H3	0.8700	C6—C8	1.393 (6)
O3—H3 <sup>i</sup>	0.8700	C7—C12	1.400 (6)
N1—N2	1.252 (5)	C8—H8	0.9500
N1—C7	1.430 (5)	C8—C12	1.389 (6)
N2—C11	1.429 (5)	C9—H9	0.9500
C1—C6	1.490 (6)	C10—H10	0.9500
C2—H2	0.9500	C10—C11	1.393 (6)
C2—C5	1.384 (6)	C11—C13	1.388 (6)
C2—C7	1.392 (6)	C12—H12	0.9500
C3—H3A	0.9500	C13—H13	0.9500
O1—Zn1—O1 <sup>i</sup>	142.3 (2)	C10—C4—C9	120.9 (4)
O1—Zn1—O2 <sup>iii</sup>	87.11 (12)	C2—C5—H5	119.6
O1 <sup>i</sup> —Zn1—O2 <sup>iii</sup>	94.66 (13)	C2—C5—C6	120.8 (4)
O1 <sup>i</sup> —Zn1—O2 <sup>ii</sup>	87.11 (12)	C6—C5—H5	119.6
O1—Zn1—O2 <sup>ii</sup>	94.66 (13)	C5—C6—C1	120.4 (4)
O2 <sup>iii</sup> —Zn1—O2 <sup>ii</sup>	174.51 (18)	C5—C6—C8	119.9 (4)
O3—Zn1—O1 <sup>i</sup>	108.85 (11)	C8—C6—C1	119.7 (4)
O3—Zn1—O1	108.85 (10)	C2—C7—N1	124.5 (4)
O3—Zn1—O2 <sup>iii</sup>	87.26 (9)	C2—C7—C12	120.3 (4)
O3—Zn1—O2 <sup>ii</sup>	87.26 (9)	C12—C7—N1	115.1 (4)
C1—O1—Zn1	121.4 (3)	C6—C8—H8	120.0
C1—O2—Zn1 <sup>ii</sup>	125.4 (3)	C12—C8—C6	119.9 (4)
Zn1—O3—H3	127.4	C12—C8—H8	120.0
Zn1—O3—H3 <sup>i</sup>	127.408 (2)	C3—C9—H9	120.1
H3—O3—H3 <sup>i</sup>	105.2	C4—C9—C3	119.7 (4)
N2—N1—C7	114.1 (4)	C4—C9—H9	120.1
N1—N2—C11	113.4 (4)	C4—C10—H10	120.3
O1—C1—O2	122.7 (4)	C4—C10—C11	119.4 (4)
O1—C1—C6	117.5 (4)	C11—C10—H10	120.3
O2—C1—C6	119.8 (4)	C10—C11—N2	123.6 (4)

C5—C2—H2	120.3	C13—C11—N2	116.1 (4)
C5—C2—C7	119.4 (4)	C13—C11—C10	120.3 (4)
C7—C2—H2	120.3	C7—C12—H12	120.2
C9—C3—H3A	120.2	C8—C12—C7	119.7 (4)
C13—C3—H3A	120.2	C8—C12—H12	120.2
C13—C3—C9	119.6 (4)	C3—C13—H13	120.0
C9—C4—H4	119.5	C11—C13—C3	120.0 (4)
C10—C4—H4	119.5	C11—C13—H13	120.0
Zn1—O1—C1—O2	-7.8 (6)	C2—C5—C6—C8	-1.3 (7)
Zn1—O1—C1—C6	170.5 (3)	C2—C7—C12—C8	-3.0 (7)
Zn1 <sup>ii</sup> —O2—C1—O1	-95.8 (5)	C4—C10—C11—N2	179.1 (4)
Zn1 <sup>ii</sup> —O2—C1—C6	86.0 (5)	C4—C10—C11—C13	-1.9 (7)
O1—C1—C6—C5	-172.2 (4)	C5—C2—C7—N1	179.3 (4)
O1—C1—C6—C8	7.6 (6)	C5—C2—C7—C12	0.8 (7)
O2—C1—C6—C5	6.1 (7)	C5—C6—C8—C12	-0.8 (7)
O2—C1—C6—C8	-174.0 (4)	C6—C8—C12—C7	2.9 (7)
N1—N2—C11—C10	-17.8 (7)	C7—N1—N2—C11	180.0 (4)
N1—N2—C11—C13	163.1 (4)	C7—C2—C5—C6	1.3 (7)
N1—C7—C12—C8	178.5 (4)	C9—C3—C13—C11	-2.3 (7)
N2—N1—C7—C2	18.8 (6)	C9—C4—C10—C11	-0.2 (7)
N2—N1—C7—C12	-162.7 (4)	C10—C4—C9—C3	1.0 (7)
N2—C11—C13—C3	-177.8 (4)	C10—C11—C13—C3	3.1 (7)
C1—C6—C8—C12	179.3 (4)	C13—C3—C9—C4	0.2 (7)
C2—C5—C6—C1	178.5 (4)		

Symmetry codes: (i)  $-x+1, y, -z+3/2$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $x, -y+1, z+1/2$ .

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3 $\cdots$ O2 <sup>iv</sup>	0.87	1.78	2.588 (4)	154

Symmetry code: (iv)  $-x+1, y+1, -z+3/2$ .