

# catena-Poly[[diaqua(2,2'-bipyridine- $\kappa^2N,N'$ )zinc]- $\mu$ -2,2'-[1,4-phenylenebis(sulfanediy)]diacetato- $\kappa^2O:O'$ ]

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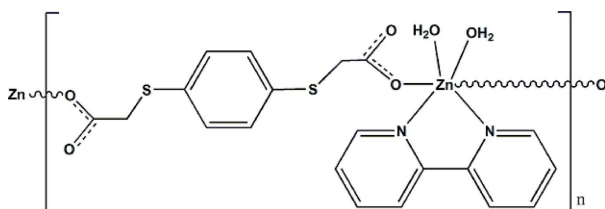
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.002$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.070; data-to-parameter ratio = 16.7.

In the polymeric title complex,  $[Zn(C_{10}H_8O_4S_2)(C_{10}H_8N_2)(H_2O)_2]_n$ , the  $Zn^{2+}$  ion lies on a twofold rotation axis and exhibits an octahedral environment, in which it is coordinated by two *trans* O atoms from two symmetry-related 2,2'-[1,4-phenylenebis(sulfanediy)]diacetate anions, two N atoms from one 2,2'-bipyridine ligand, and two *cis* O atoms from water molecules. The dihedral angle between the two pyridine rings is  $11.5(1)^\circ$ . Adjacent  $Zn^{2+}$  ions are bridged in a monodentate manner by the diacetate anions, forming a chain structure extending parallel to  $[101]$ , and are further linked into the final three-dimensional structure by  $O-H\cdots O$  hydrogen bonds between the coordinating water molecules as donor and the non-coordinating carboxylate O atoms as acceptor atoms.

## Related literature

For background to 1,4-benzenebis(thioacetic acid), including its synthesis and coordination behaviour, see: Yin & Feng (2009); Yin *et al.* (2009); Chen *et al.* (2010); Wang *et al.* (2011a,b); Jiang *et al.* (2012).



## Experimental

### Crystal data

$[Zn(C_{10}H_8O_4S_2)(C_{10}H_8N_2)(H_2O)_2]$   
 $M_r = 513.87$   
Monoclinic,  $C2/c$

$a = 20.4396(8)$  Å  
 $b = 12.8695(8)$  Å  
 $c = 7.9798(4)$  Å

$\beta = 90.765(3)^\circ$   
 $V = 2098.88(19)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation

$\mu = 1.41$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.22 \times 0.16 \times 0.11$  mm

### Data collection

Bruker APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.761$ ,  $T_{\max} = 0.853$

16253 measured reflections  
2448 independent reflections  
2237 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.070$   
 $S = 1.04$   
2448 reflections  
147 parameters  
3 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.31$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Zn1—O1W	2.0896 (11)	Zn1—O1	2.1529 (10)
Zn1—N1	2.1477 (13)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA $\cdots$ O2 <sup>i</sup>	0.83 (1)	1.90 (2)	2.7107 (15)	170 (2)
O1W—H1WB $\cdots$ O2	0.82 (1)	1.86 (2)	2.6582 (16)	164 (2)

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

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008) and DIAMOND (Crystal Impact, 2008); software used to prepare material for publication: publCIF (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2568).

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## supporting information

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**catena-Poly[[diaqua(2,2'-bipyridine- $\kappa^2N,N'$ )zinc]- $\mu$ -2,2'-[1,4-phenylenebis(sulfanediyl)]diacetato- $\kappa^2O:O'$ ]****Hong Lin and Xiao-Juan Wang****S1. Comment**

1,4-Benzenebis(thioacetic acid), (C<sub>10</sub>H<sub>10</sub>O<sub>4</sub>S<sub>2</sub>), is a flexible aromatic multi-carboxylate ligand, which can be prepared from 1,4-benzenebisthiol (Yin & Feng, 2009). Compared with rigid ligands, these flexible aromatic carboxylate ligands contain more coordination sites (*viz.* S and O atoms) to construct various extended structures with different metal ions. Recently, some complexes derived from 1,4-benzenebis(thioacetic acid) with bipyridine ligands have been reported (Yin *et al.*, 2009; Chen *et al.*, 2010; Wang *et al.*, 2011*a,b*; Jiang *et al.*, 2012). Here we report the synthesis and structure of a new complex, [Zn(C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>S<sub>2</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>, (I).

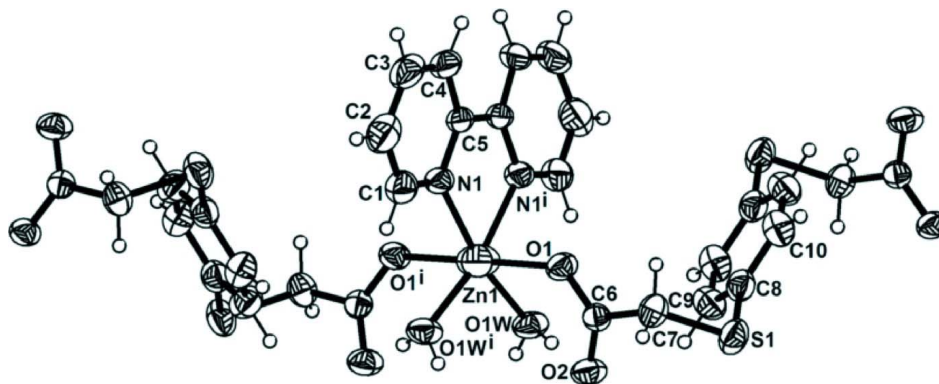
Complex (I) is isotypic with its Co(II) analogue (Jiang *et al.*, 2012). A view on the molecular structure of (I), showing the coordination environment of the Zn<sup>2+</sup> ion, is presented in Fig. 1. The asymmetric unit consists of one Zn<sup>2+</sup> ion (situated on a twofold rotation axis), half of a [C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>S<sub>2</sub>]<sup>2-</sup> anion, half of a 2,2'-bipy molecule, and one coordinating water molecule. The Zn<sup>2+</sup> ion is six-coordinated by two O atoms from two symmetry-related [C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>S<sub>2</sub>]<sup>2-</sup> anions (Zn—O 2.1529 (10) Å), two N atoms from one chelating 2,2'-bipy molecule (Zn—N 2.1477 (13) Å), and two water molecules (Zn—O 2.0896 (11) Å) to form a slightly distorted octahedral geometry. The two pyridine rings in the bipy ligand are almost parallel with a dihedral angle of 11.5 (1)°. As shown in Fig. 2, adjacent Zn<sup>2+</sup> ions are monodentately linked by the [C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>S<sub>2</sub>]<sup>2-</sup> anions to form a chain structure running parallel to [101]. The chains are further linked by O—H...O hydrogen bonds to form the final three-dimensional supramolecular architecture (Fig. 3).

**S2. Experimental**

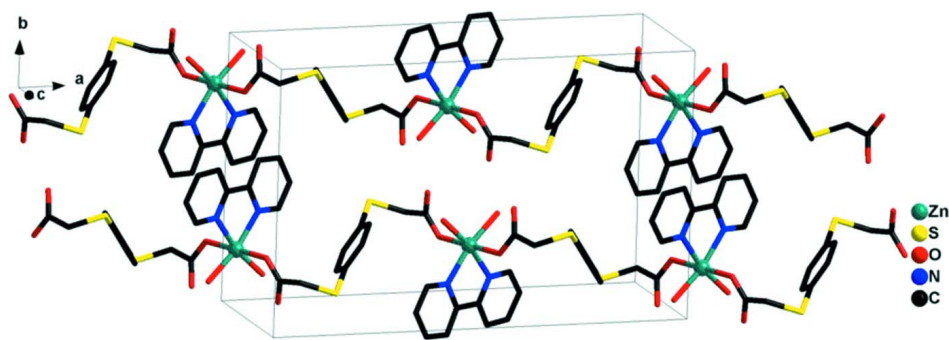
A mixture of 1,4-benzenebis(thioacetic acid) (0.103 g, 0.4 mmol), ZnCl<sub>2</sub>·6H<sub>2</sub>O (0.054 g, 0.4 mmol), 2,2'-bipy (0.031 g, 0.2 mmol), and Na<sub>2</sub>CO<sub>3</sub> (0.042 g, 0.4 mmol) in H<sub>2</sub>O (16 ml)/C<sub>2</sub>H<sub>5</sub>OH (2 ml) was placed in a 25 ml Teflon-lined stainless steel vessel and heated at 433 K for 72 h, then cooled to room temperature over 3 d. Colourless crystals suitable for X-ray analysis were obtained.

**S3. Refinement**

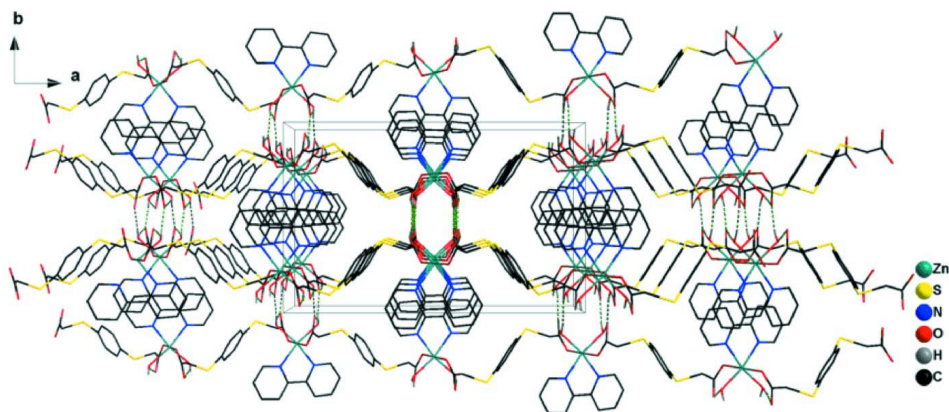
The carbon-bound H-atoms were positioned geometrically and included in the refinement using a riding model [aromatic C—H 0.93 Å and aliphatic C—H 0.97 Å,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ ]. The oxygen-bound H-atoms were located in difference Fourier maps and refined with an O—H distance restrained to 0.85 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ .


**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i)  $-x + 1, y, -z + 1/2$ .]


**Figure 2**

The chain structure of the title complex. All H atoms have been omitted for clarity.


**Figure 3**

The three-dimensional supramolecular structure built through O—H...O hydrogen bonds (dashed lines).

**catena-Poly[[diaqua(2,2'-bipyridine- $\kappa^2N,N'$ )zinc]- $\mu$ -2,2'-[1,4-phenylenebis(sulfanediy)]diacetato- $\kappa^2O:O'$ ]**

*Crystal data*

$[\text{Zn}(\text{C}_{10}\text{H}_8\text{O}_4\text{S}_2)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]$   
 $M_r = 513.87$

Monoclinic,  $C2/c$   
 Hall symbol:  $-C 2yc$

$a = 20.4396 (8) \text{ \AA}$   
 $b = 12.8695 (8) \text{ \AA}$   
 $c = 7.9798 (4) \text{ \AA}$   
 $\beta = 90.765 (3)^\circ$   
 $V = 2098.88 (19) \text{ \AA}^3$   
 $Z = 4$   
 $F(000) = 1056$   
 $D_x = 1.626 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 7952 reflections  
 $\theta = 1.9\text{--}27.7^\circ$   
 $\mu = 1.41 \text{ mm}^{-1}$   
 $T = 296 \text{ K}$   
 Block, colourless  
 $0.22 \times 0.16 \times 0.11 \text{ mm}$

*Data collection*

Bruker APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.761, T_{\max} = 0.853$

16253 measured reflections  
 2448 independent reflections  
 2237 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\max} = 27.7^\circ, \theta_{\min} = 1.9^\circ$   
 $h = -26 \rightarrow 26$   
 $k = -15 \rightarrow 16$   
 $l = -10 \rightarrow 10$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.070$   
 $S = 1.04$   
 2448 reflections  
 147 parameters  
 3 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.7442P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.31 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.31 \text{ e \AA}^{-3}$

*Special details*

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.5000	0.725191 (16)	0.2500	0.03569 (9)
S1	0.676748 (19)	0.62114 (4)	0.78141 (5)	0.04863 (12)
N1	0.44065 (7)	0.85617 (9)	0.31662 (16)	0.0391 (3)
O1W	0.57320 (6)	0.61941 (8)	0.18683 (14)	0.0435 (3)
H1WA	0.5703 (10)	0.5693 (13)	0.123 (2)	0.052*
H1WB	0.5785 (10)	0.5933 (15)	0.2793 (18)	0.052*
O1	0.54190 (6)	0.72445 (7)	0.49896 (13)	0.0398 (2)
O2	0.57240 (6)	0.55857 (8)	0.50514 (13)	0.0446 (3)

C1	0.38250 (9)	0.85086 (14)	0.3913 (2)	0.0484 (4)
H1A	0.3633	0.7861	0.4061	0.058*
C2	0.34980 (10)	0.93842 (17)	0.4477 (2)	0.0597 (5)
H2A	0.3089	0.9329	0.4966	0.072*
C3	0.37950 (11)	1.03389 (15)	0.4292 (3)	0.0618 (5)
H3A	0.3594	1.0937	0.4688	0.074*
C4	0.43876 (10)	1.03996 (13)	0.3523 (2)	0.0532 (4)
H4A	0.4592	1.1040	0.3391	0.064*
C5	0.46836 (8)	0.94978 (11)	0.29374 (19)	0.0403 (3)
C6	0.56711 (6)	0.64669 (10)	0.56961 (17)	0.0319 (3)
C7	0.59312 (7)	0.66315 (13)	0.74760 (18)	0.0395 (3)
H7A	0.5652	0.6258	0.8245	0.047*
H7B	0.5901	0.7365	0.7746	0.047*
C8	0.71752 (7)	0.69346 (13)	0.6228 (2)	0.0408 (3)
C9	0.71738 (8)	0.65950 (13)	0.4586 (2)	0.0479 (4)
H9A	0.6958	0.5983	0.4300	0.057*
C10	0.75080 (8)	0.78402 (14)	0.6640 (2)	0.0475 (4)
H10A	0.7518	0.8070	0.7745	0.057*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.04999 (16)	0.02228 (13)	0.03467 (14)	0.000	-0.00485 (10)	0.000
S1	0.0406 (2)	0.0562 (3)	0.0490 (2)	0.00141 (17)	-0.00659 (17)	0.01881 (18)
N1	0.0518 (7)	0.0284 (6)	0.0367 (6)	0.0019 (5)	-0.0129 (5)	-0.0020 (5)
O1W	0.0664 (7)	0.0291 (5)	0.0349 (5)	0.0064 (5)	-0.0039 (5)	-0.0045 (4)
O1	0.0540 (6)	0.0316 (5)	0.0336 (5)	0.0051 (4)	-0.0085 (5)	-0.0008 (4)
O2	0.0661 (7)	0.0290 (5)	0.0385 (5)	0.0007 (5)	-0.0048 (5)	0.0043 (4)
C1	0.0531 (9)	0.0449 (9)	0.0468 (9)	0.0033 (7)	-0.0084 (7)	-0.0017 (7)
C2	0.0590 (11)	0.0643 (12)	0.0555 (11)	0.0169 (9)	-0.0085 (8)	-0.0076 (9)
C3	0.0744 (13)	0.0478 (10)	0.0626 (11)	0.0254 (9)	-0.0234 (9)	-0.0171 (8)
C4	0.0680 (11)	0.0309 (8)	0.0600 (10)	0.0107 (7)	-0.0274 (9)	-0.0082 (7)
C5	0.0546 (8)	0.0258 (6)	0.0398 (7)	0.0028 (6)	-0.0231 (6)	-0.0023 (5)
C6	0.0324 (6)	0.0328 (7)	0.0304 (6)	-0.0034 (5)	0.0012 (5)	0.0042 (5)
C7	0.0400 (7)	0.0479 (8)	0.0307 (7)	0.0045 (6)	-0.0003 (6)	0.0028 (6)
C8	0.0310 (7)	0.0437 (8)	0.0475 (8)	0.0024 (6)	-0.0010 (6)	0.0051 (7)
C9	0.0418 (8)	0.0454 (9)	0.0564 (10)	-0.0066 (7)	0.0025 (7)	-0.0064 (7)
C10	0.0420 (8)	0.0553 (10)	0.0452 (9)	-0.0039 (7)	0.0003 (7)	-0.0075 (7)

*Geometric parameters (Å, °)*

Zn1—O1W <sup>i</sup>	2.0896 (11)	C2—C3	1.379 (3)
Zn1—O1W	2.0896 (11)	C2—H2A	0.9300
Zn1—N1 <sup>i</sup>	2.1477 (13)	C3—C4	1.367 (3)
Zn1—N1	2.1477 (13)	C3—H3A	0.9300
Zn1—O1 <sup>i</sup>	2.1529 (10)	C4—C5	1.392 (2)
Zn1—O1	2.1529 (10)	C4—H4A	0.9300
S1—C8	1.7861 (16)	C5—C5 <sup>i</sup>	1.478 (4)

S1—C7	1.8095 (15)	C6—C7	1.5247 (19)
N1—C1	1.339 (2)	C7—H7A	0.9700
N1—C5	1.3447 (19)	C7—H7B	0.9700
O1W—H1WA	0.825 (14)	C8—C9	1.382 (2)
O1W—H1WB	0.817 (14)	C8—C10	1.387 (2)
O1—C6	1.2557 (16)	C9—C10 <sup>ii</sup>	1.388 (2)
O2—C6	1.2506 (17)	C9—H9A	0.9300
C1—C2	1.388 (3)	C10—C9 <sup>ii</sup>	1.388 (2)
C1—H1A	0.9300	C10—H10A	0.9300
O1W <sup>i</sup> —Zn1—O1W	98.69 (7)	C1—C2—H2A	120.8
O1W <sup>i</sup> —Zn1—N1 <sup>i</sup>	168.43 (5)	C4—C3—C2	119.51 (17)
O1W—Zn1—N1 <sup>i</sup>	92.47 (5)	C4—C3—H3A	120.2
O1W <sup>i</sup> —Zn1—N1	92.47 (5)	C2—C3—H3A	120.2
O1W—Zn1—N1	168.43 (5)	C3—C4—C5	119.63 (17)
N1 <sup>i</sup> —Zn1—N1	76.59 (7)	C3—C4—H4A	120.2
O1W <sup>i</sup> —Zn1—O1 <sup>i</sup>	86.70 (4)	C5—C4—H4A	120.2
O1W—Zn1—O1 <sup>i</sup>	92.97 (4)	N1—C5—C4	121.03 (16)
N1 <sup>i</sup> —Zn1—O1 <sup>i</sup>	89.66 (4)	N1—C5—C5 <sup>i</sup>	115.91 (9)
N1—Zn1—O1 <sup>i</sup>	90.74 (4)	C4—C5—C5 <sup>i</sup>	123.05 (11)
O1W <sup>i</sup> —Zn1—O1	92.97 (4)	O2—C6—O1	125.11 (13)
O1W—Zn1—O1	86.70 (4)	O2—C6—C7	118.57 (12)
N1 <sup>i</sup> —Zn1—O1	90.74 (4)	O1—C6—C7	116.32 (12)
N1—Zn1—O1	89.66 (4)	C6—C7—S1	114.48 (10)
O1 <sup>i</sup> —Zn1—O1	179.49 (5)	C6—C7—H7A	108.6
C8—S1—C7	100.80 (7)	S1—C7—H7A	108.6
C1—N1—C5	118.97 (14)	C6—C7—H7B	108.6
C1—N1—Zn1	125.31 (11)	S1—C7—H7B	108.6
C5—N1—Zn1	115.42 (11)	H7A—C7—H7B	107.6
Zn1—O1W—H1WA	127.8 (14)	C9—C8—C10	119.04 (15)
Zn1—O1W—H1WB	97.9 (14)	C9—C8—S1	120.80 (13)
H1WA—O1W—H1WB	104.3 (17)	C10—C8—S1	120.15 (13)
C6—O1—Zn1	125.00 (9)	C8—C9—C10 <sup>ii</sup>	120.52 (16)
N1—C1—C2	122.49 (17)	C8—C9—H9A	119.7
N1—C1—H1A	118.8	C10 <sup>ii</sup> —C9—H9A	119.7
C2—C1—H1A	118.8	C8—C10—C9 <sup>ii</sup>	120.43 (16)
C3—C2—C1	118.3 (2)	C8—C10—H10A	119.8
C3—C2—H2A	120.8	C9 <sup>ii</sup> —C10—H10A	119.8
O1W <sup>i</sup> —Zn1—N1—C1	7.41 (13)	C2—C3—C4—C5	0.0 (3)
O1W—Zn1—N1—C1	-157.1 (2)	C1—N1—C5—C4	2.5 (2)
N1 <sup>i</sup> —Zn1—N1—C1	-176.39 (15)	Zn1—N1—C5—C4	-171.45 (11)
O1 <sup>i</sup> —Zn1—N1—C1	94.13 (13)	C1—N1—C5—C5 <sup>i</sup>	-178.37 (15)
O1—Zn1—N1—C1	-85.55 (13)	Zn1—N1—C5—C5 <sup>i</sup>	7.63 (19)
O1W <sup>i</sup> —Zn1—N1—C5	-179.03 (10)	C3—C4—C5—N1	-2.3 (2)
O1W—Zn1—N1—C5	16.4 (3)	C3—C4—C5—C5 <sup>i</sup>	178.72 (18)
N1 <sup>i</sup> —Zn1—N1—C5	-2.82 (7)	Zn1—O1—C6—O2	1.0 (2)
O1 <sup>i</sup> —Zn1—N1—C5	-92.30 (10)	Zn1—O1—C6—C7	-179.21 (9)

O1—Zn1—N1—C5	88.01 (10)	O2—C6—C7—S1	51.79 (17)
O1W <sup>i</sup> —Zn1—O1—C6	63.39 (12)	O1—C6—C7—S1	-128.01 (12)
O1W—Zn1—O1—C6	-35.15 (12)	C8—S1—C7—C6	55.61 (13)
N1 <sup>i</sup> —Zn1—O1—C6	-127.58 (12)	C7—S1—C8—C9	-80.93 (14)
N1—Zn1—O1—C6	155.84 (12)	C7—S1—C8—C10	100.14 (14)
O1 <sup>i</sup> —Zn1—O1—C6	14.13 (13)	C10—C8—C9—C10 <sup>ii</sup>	-1.0 (3)
C5—N1—C1—C2	-0.6 (2)	S1—C8—C9—C10 <sup>ii</sup>	-179.94 (13)
Zn1—N1—C1—C2	172.80 (13)	C9—C8—C10—C9 <sup>ii</sup>	1.0 (3)
N1—C1—C2—C3	-1.7 (3)	S1—C8—C10—C9 <sup>ii</sup>	179.95 (13)
C1—C2—C3—C4	1.9 (3)		

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

*Hydrogen-bond geometry (Å, °)*

<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>
O1W—H1WA $\cdots$ O2 <sup>iii</sup>	0.83 (1)	1.90 (2)	2.7107 (15)	170 (2)
O1W—H1WB $\cdots$ O2	0.82 (1)	1.86 (2)	2.6582 (16)	164 (2)

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