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Bis(2,2′-bipyridyl-κ^2N,N')(sulfato-κ^2O,O')zinc(II) ethane-1,2-diol solvate

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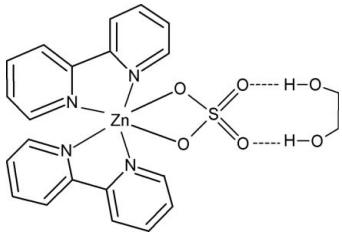
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.088; data-to-parameter ratio = 16.0.

The title compound, $[Zn(SO_4)(C_{10}H_8N_2)_2]\cdot C_2H_6O_2$, is a six-coordinate zinc(II) complex with a distorted octahedral coordination geometry. The Zn^{II} atom is bonded by two O atoms of the bidentate chelating sulfate ligand and four N atoms of the two chelating 2,2′-bipyridine ligands. The Zn—N bond distances range from 2.1287 (17) to 2.1452 (17) Å and the Zn—O bond distance is 2.1811 (15) Å. The two chelating NCCN groups subtend a dihedral angle of 81.1 (1)°. In the crystal structure, the $[ZnSO_4(C_{10}H_8N_2)_2]$ and $C_2H_6O_2$ units are connected by intermolecular O—H···O hydrogen bonding, which leads to additional stabilization of the structure.

Related literature

For related compounds, see: Liu & Arora (1993); Harvey *et al.* (2001, 2002); Jian *et al.* (2004); Rodrigues (2004); Juric *et al.* (2006); Zhu *et al.* (2006); Yu *et al.* (2007); Zhong *et al.* (2007).



Experimental

Crystal data

$[Zn(SO_4)(C_{10}H_8N_2)_2]\cdot C_2H_6O_2$
M_r = 535.90
Monoclinic, $C2/c$
a = 17.017 (3) Å
b = 11.890 (2) Å
c = 12.831 (3) Å
β = 122.14 (3)°
V = 2198.3 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 223 K
0.55 × 0.45 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.747, T_{max} = 1.000
6138 measured reflections
2489 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.088
S = 1.08
2489 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.1287 (17)	S1—O2	1.4683 (15)
Zn1—N1	2.1452 (17)	S1—O1	1.4915 (15)
Zn1—O1	2.1811 (15)		
N2—Zn1—N1	76.61 (7)	O1^{i}—Zn1—O1	65.64 (8)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.82	1.97	2.746 (2)	158

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2188).

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supporting information

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Bis(2,2′-bipyridyl-κ^2N,N')(sulfato-κ^2O,O')zinc(II) ethane-1,2-diol solvate

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S1. Comment

2,2′-bipyridyl(2,2′-bipy) is a well known neutral didentate ligand. Many metal zinc complexes with 2,2′-bipy have been previously synthesized and reported, such as bis(2,2′-bipyridyl) zinc(II) with diperchlorate (Liu & Arora, 1993), uranyl phosphate (Yu *et al.*, 2007), thiocyanate (Zhong *et al.*, 2007), oxalate (Juric *et al.*, 2006), azide (Jian *et al.*, 2004), acetate (Rodrigues, 2004). Moreover, the crystal structures of zinc complexes with monodente (Harvey *et al.*, 2003), bidentate chelating (Zhu *et al.*, 2006) and bidentate bridging sulfate (Harvey *et al.*, 2000) have been structurally characterized. Recently, we attempt to utilize polydentate and mixed ligands for the design of coordination networks. The title compound $[ZnSO_4(C_{10}H_8N_2)_2].C_2H_6O_2$, (I), which is very similar to the zinc complex with 1,10-phenanthroline instead of 2,2′-bipyridine (Zhu *et al.*, 2006), was obtained unitentionally during an attempt to synthesize mixed-ligand complex of Zn(II) with 2,2′-bipy and melamine *via* a solvothermal reaction. The crystal structure of the title complex has not hitherto been reported.

Single crystal X-ray diffraction experiment reveal that a twofold rotation axis (symmetry code: -*x*, *y*, - *z* + 1/2) passes through the Zn, S atoms, and also through the mid-point of C—C bond of the solvent, 1,2-ethanediol molecule. The Zn (II) ions are coordinated by four N atoms from two chelating 2,2′-bipy ligands and two O atoms from a bidentate-chelating salfate ligand, in a distorted octahedral geometry (Fig. 1. and Table 1.). The Zn—N bond distances range from 2.1287 (17)Å to 2.1452 (17)Å and Zn—O bond distance is 2.1811 (15) Å. The N—Zn—N bite angle, O—Zn—O bite angle and the dihedral angle between the two chelating NCCN groups is 76.61 (7) Å, 65.64 (8) Å and 81.1 (1) Å, respectively. The metal complex and solvent components of the title compound are held together by intermolecular O3—H3···O2 hydrogen bonding, which contribute to the stabilization of the structure (Fig.1 and Table 2.).

S2. Experimental

The title compound was obtained unexpectedly during an attempt to synthesize mixed-ligand complex of Zn(II) with phenol and melamine *via* a solvo-thermal reaction. Colorless prism-shaped single crystals of the title compound for X-ray diffraction determination were prepared by 0.2 mmol mixing 2,2′-bipyridine, 0.1 mmol melamine, 0.1 mmol $ZnSO_4.7H_2O$, 2.0 ml 1,3-propanediol and 1.0 ml water and then placing them in a thick Pyrex tube, which was sealed and heated to 423 K for 3 days.

S3. Refinement

All H atoms of 2,2′-bipyridyl were positioned geometrically and allowed to ride on their attached atoms, with C—H =0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms of 1,2-ethanediol were locate in a difference map and then allowed to ride on their parent atoms, with C—H =0.97 Å and O—H =0.82 Å; U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

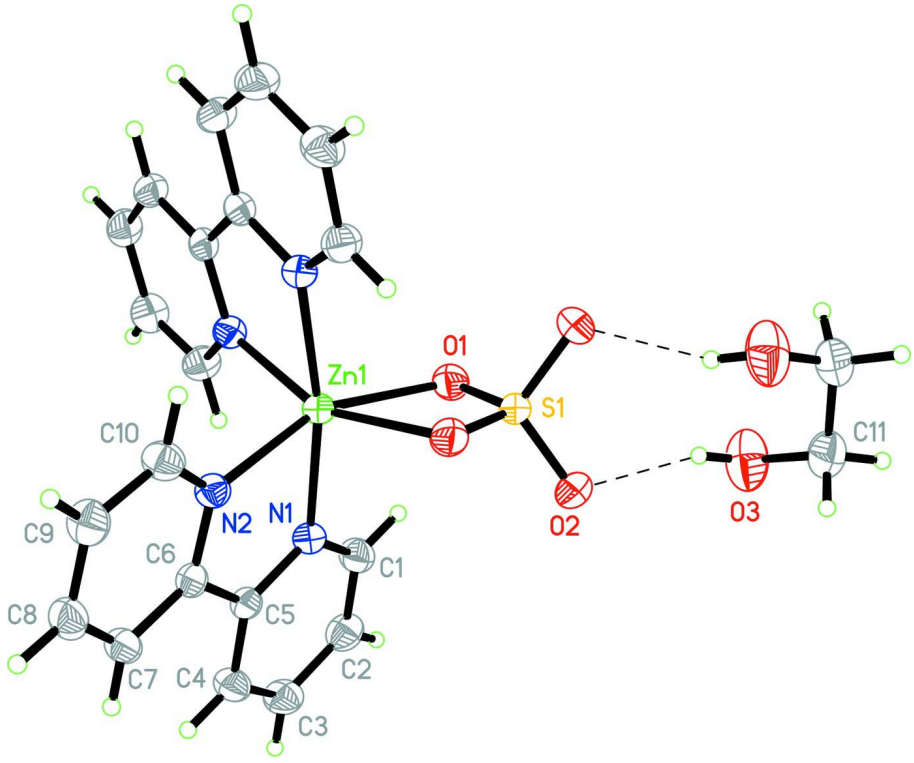

Figure 1

The molecular structure of (I) showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. The dashed lines represent O—H···O interactions. Unlabeled atoms are related to the labeled atoms by the symmetry operator(-*x*, *y*, -*z* + 1/2).

Bis(2,2′-bipyridyl-κ^2N,N')(sulfato-κ^2O,O')zinc(II) ethane-1,2-diol solvate

Crystal data

$[Zn(SO_4)(C_{10}H_8N_2)_2]\cdot C_2H_6O_2$
M_r = 535.90
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 17.017 (3) Å
b = 11.890 (2) Å
c = 12.831 (3) Å
β = 122.14 (3)°
V = 2198.3 (10) Å^3
Z = 4
F(000) = 1104
D_x = 1.619 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5954 reflections
θ = 3.4–27.5°
μ = 1.26 mm^{-1}
T = 223 K
Prism, colorless
0.55 × 0.45 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite Monochromator monochromator
Detector resolution: 28.5714 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (REQAB; Jacobson, 1998)
T_{min} = 0.747, T_{max} = 1.000
6138 measured reflections
2489 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −22→22
k = −12→15
l = −16→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.088$
$S = 1.08$
2489 reflections
156 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0173 (10)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.0000	0.30659 (2)	0.2500	0.02342 (14)
S1	0.0000	0.53723 (5)	0.2500	0.02518 (18)
N2	0.09876 (11)	0.19245 (12)	0.38322 (15)	0.0241 (4)
O1	−0.04900 (9)	0.46074 (12)	0.14153 (13)	0.0304 (3)
O2	0.06823 (10)	0.60723 (12)	0.24320 (15)	0.0359 (4)
C9	0.16178 (16)	0.07532 (17)	0.5611 (2)	0.0327 (5)
H9A	0.1567	0.0452	0.6242	0.039*
C7	0.24124 (14)	0.09388 (16)	0.45508 (19)	0.0280 (4)
H7A	0.2911	0.0771	0.4469	0.034*
C8	0.23603 (14)	0.04818 (17)	0.55093 (19)	0.0316 (5)
H8A	0.2821	−0.0001	0.6074	0.038*
C10	0.09473 (14)	0.14816 (18)	0.47609 (19)	0.0307 (4)
H10A	0.0450	0.1670	0.4839	0.037*
C6	0.17124 (13)	0.16470 (15)	0.37204 (18)	0.0233 (4)
N1	0.10086 (11)	0.29012 (13)	0.19914 (16)	0.0246 (4)
C5	0.17129 (13)	0.21769 (16)	0.26699 (18)	0.0234 (4)
C4	0.23903 (15)	0.19633 (16)	0.2402 (2)	0.0299 (4)
H4A	0.2869	0.1461	0.2880	0.036*
C1	0.09742 (14)	0.34294 (18)	0.1043 (2)	0.0297 (4)
H1A	0.0494	0.3935	0.0581	0.036*
C2	0.16244 (16)	0.32515 (18)	0.0724 (2)	0.0326 (5)
H2A	0.1578	0.3625	0.0057	0.039*
C3	0.23444 (15)	0.25072 (19)	0.1417 (2)	0.0336 (5)

H3A	0.2791	0.2374	0.1223	0.040*
O3	0.02134 (16)	0.82127 (14)	0.14925 (19)	0.0535 (5)
H3	0.0243	0.7602	0.1809	0.080*
C11	0.03464 (18)	0.90768 (19)	0.2313 (3)	0.0437 (6)
H11A	0.0316	0.9794	0.1934	0.052*
H11B	0.0963	0.9006	0.3045	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02046 (19)	0.0218 (2)	0.0288 (2)	0.000	0.01361 (15)	0.000
S1	0.0204 (3)	0.0203 (3)	0.0342 (4)	0.000	0.0141 (3)	0.000
N2	0.0227 (8)	0.0242 (8)	0.0248 (8)	−0.0007 (6)	0.0122 (7)	−0.0012 (6)
O1	0.0258 (7)	0.0285 (7)	0.0321 (8)	0.0005 (6)	0.0120 (6)	−0.0016 (6)
O2	0.0303 (8)	0.0280 (7)	0.0520 (10)	−0.0042 (6)	0.0236 (7)	0.0030 (7)
C9	0.0364 (11)	0.0338 (11)	0.0273 (11)	0.0006 (9)	0.0166 (9)	0.0038 (9)
C7	0.0228 (9)	0.0263 (10)	0.0312 (11)	0.0022 (8)	0.0118 (8)	−0.0011 (8)
C8	0.0284 (10)	0.0290 (10)	0.0289 (11)	0.0030 (9)	0.0094 (9)	0.0030 (8)
C10	0.0296 (10)	0.0346 (11)	0.0303 (10)	0.0027 (9)	0.0176 (9)	0.0011 (9)
C6	0.0223 (9)	0.0195 (8)	0.0256 (9)	−0.0022 (7)	0.0111 (8)	−0.0042 (7)
N1	0.0219 (8)	0.0242 (8)	0.0287 (9)	−0.0002 (7)	0.0140 (7)	0.0004 (7)
C5	0.0213 (9)	0.0208 (9)	0.0261 (9)	−0.0025 (7)	0.0112 (8)	−0.0037 (7)
C4	0.0256 (10)	0.0307 (10)	0.0348 (11)	0.0036 (8)	0.0170 (9)	−0.0013 (9)
C1	0.0292 (10)	0.0297 (10)	0.0327 (11)	0.0033 (9)	0.0182 (9)	0.0056 (9)
C2	0.0358 (11)	0.0344 (11)	0.0337 (11)	−0.0045 (9)	0.0227 (10)	−0.0008 (9)
C3	0.0323 (11)	0.0372 (12)	0.0396 (12)	−0.0011 (10)	0.0247 (10)	−0.0045 (10)
O3	0.0912 (15)	0.0382 (9)	0.0511 (11)	0.0008 (9)	0.0513 (11)	0.0052 (8)
C11	0.0494 (14)	0.0302 (11)	0.0551 (16)	−0.0024 (10)	0.0301 (13)	0.0025 (10)

Geometric parameters (Å, º)

Zn1—N2^{i}	2.1287 (17)	C8—H8A	0.9300
Zn1—N2	2.1287 (17)	C10—H10A	0.9300
Zn1—N1	2.1452 (17)	C6—C5	1.488 (3)
Zn1—N1^{i}	2.1452 (17)	N1—C1	1.343 (3)
Zn1—O1^{i}	2.1811 (15)	N1—C5	1.351 (3)
Zn1—O1	2.1811 (15)	C5—C4	1.390 (3)
Zn1—S1	2.7424 (8)	C4—C3	1.385 (3)
S1—O2	1.4683 (15)	C4—H4A	0.9300
S1—O2^{i}	1.4683 (14)	C1—C2	1.385 (3)
S1—O1	1.4915 (15)	C1—H1A	0.9300
S1—O1^{i}	1.4915 (15)	C2—C3	1.384 (3)
N2—C10	1.338 (3)	C2—H2A	0.9300
N2—C6	1.356 (3)	C3—H3A	0.9300
C9—C8	1.376 (3)	O3—C11	1.401 (3)
C9—C10	1.385 (3)	O3—H3	0.8200
C9—H9A	0.9300	C11—C11^{i}	1.490 (5)
C7—C6	1.383 (3)	C11—H11A	0.9700

C7—C8	1.390 (3)	C11—H11B	0.9700
C7—H7A	0.9300		

N2^{i}—Zn1—N2	100.78 (9)	C6—C7—C8	119.04 (19)
N2^{i}—Zn1—N1	96.61 (7)	C6—C7—H7A	120.5
N2—Zn1—N1	76.61 (7)	C8—C7—H7A	120.5
N2^{i}—Zn1—N1^{i}	76.61 (7)	C9—C8—C7	119.1 (2)
N2—Zn1—N1^{i}	96.61 (7)	C9—C8—H8A	120.4
N1—Zn1—N1^{i}	169.52 (9)	C7—C8—H8A	120.4
N2^{i}—Zn1—O1^{i}	156.73 (6)	N2—C10—C9	122.5 (2)
N2—Zn1—O1^{i}	98.79 (6)	N2—C10—H10A	118.8
N1—Zn1—O1^{i}	100.06 (6)	C9—C10—H10A	118.8
N1^{i}—Zn1—O1^{i}	88.78 (6)	N2—C6—C7	121.72 (19)
N2^{i}—Zn1—O1	98.79 (6)	N2—C6—C5	115.57 (17)
N2—Zn1—O1	156.73 (6)	C7—C6—C5	122.69 (18)
N1—Zn1—O1	88.78 (6)	C1—N1—C5	118.56 (17)
N1^{i}—Zn1—O1	100.06 (6)	C1—N1—Zn1	125.22 (14)
O1^{i}—Zn1—O1	65.64 (8)	C5—N1—Zn1	116.18 (13)
N2^{i}—Zn1—S1	129.61 (4)	N1—C5—C4	121.68 (19)
N2—Zn1—S1	129.61 (4)	N1—C5—C6	115.19 (17)
N1—Zn1—S1	95.24 (4)	C4—C5—C6	123.12 (18)
N1^{i}—Zn1—S1	95.24 (4)	C3—C4—C5	119.26 (19)
O1^{i}—Zn1—S1	32.82 (4)	C3—C4—H4A	120.4
O1—Zn1—S1	32.82 (4)	C5—C4—H4A	120.4
O2—S1—O2^{i}	110.95 (12)	N1—C1—C2	122.7 (2)
O2—S1—O1	110.94 (9)	N1—C1—H1A	118.7
O2^{i}—S1—O1	109.50 (8)	C2—C1—H1A	118.7
O2—S1—O1^{i}	109.50 (8)	C3—C2—C1	118.8 (2)
O2^{i}—S1—O1^{i}	110.94 (9)	C3—C2—H2A	120.6
O1—S1—O1^{i}	104.85 (12)	C1—C2—H2A	120.6
O2—S1—Zn1	124.53 (6)	C2—C3—C4	119.0 (2)
O2^{i}—S1—Zn1	124.53 (6)	C2—C3—H3A	120.5
O1—S1—Zn1	52.43 (6)	C4—C3—H3A	120.5
O1^{i}—S1—Zn1	52.43 (6)	C11—O3—H3	109.5
C10—N2—C6	118.62 (17)	O3—C11—C11^{i}	113.7 (2)
C10—N2—Zn1	125.01 (14)	O3—C11—H11A	108.8
C6—N2—Zn1	116.37 (13)	C11^{i}—C11—H11A	108.8
S1—O1—Zn1	94.75 (8)	O3—C11—H11B	108.8
C8—C9—C10	119.0 (2)	C11^{i}—C11—H11B	108.8
C8—C9—H9A	120.5	H11A—C11—H11B	107.7
C10—C9—H9A	120.5		

N2^{i}—Zn1—S1—O2	−114.55 (10)	N1^{i}—Zn1—O1—S1	84.03 (8)
N2—Zn1—S1—O2	65.45 (10)	O1^{i}—Zn1—O1—S1	0.0
N1—Zn1—S1—O2	−11.49 (9)	C10—C9—C8—C7	−0.5 (3)
N1^{i}—Zn1—S1—O2	168.51 (9)	C6—C7—C8—C9	−0.5 (3)
O1^{i}—Zn1—S1—O2	88.97 (11)	C6—N2—C10—C9	0.1 (3)
O1—Zn1—S1—O2	−91.03 (11)	Zn1—N2—C10—C9	−179.13 (15)

N2^{i}—Zn1—S1—O2^{i}	65.45 (10)	C8—C9—C10—N2	0.8 (3)
N2—Zn1—S1—O2^{i}	−114.55 (10)	C10—N2—C6—C7	−1.2 (3)
N1—Zn1—S1—O2^{i}	168.51 (9)	Zn1—N2—C6—C7	178.11 (14)
N1^{i}—Zn1—S1—O2^{i}	−11.49 (9)	C10—N2—C6—C5	−179.68 (17)
O1^{i}—Zn1—S1—O2^{i}	−91.03 (11)	Zn1—N2—C6—C5	−0.4 (2)
O1—Zn1—S1—O2^{i}	88.97 (11)	C8—C7—C6—N2	1.4 (3)
N2^{i}—Zn1—S1—O1	−23.52 (9)	C8—C7—C6—C5	179.77 (18)
N2—Zn1—S1—O1	156.48 (9)	N2^{i}—Zn1—N1—C1	80.70 (17)
N1—Zn1—S1—O1	79.54 (9)	N2—Zn1—N1—C1	−179.74 (18)
N1^{i}—Zn1—S1—O1	−100.46 (9)	N1^{i}—Zn1—N1—C1	129.77 (17)
O1^{i}—Zn1—S1—O1	180.0	O1^{i}—Zn1—N1—C1	−83.00 (17)
N2^{i}—Zn1—S1—O1^{i}	156.48 (9)	O1—Zn1—N1—C1	−18.01 (17)
N2—Zn1—S1—O1^{i}	−23.52 (9)	S1—Zn1—N1—C1	−50.23 (17)
N1—Zn1—S1—O1^{i}	−100.46 (9)	N2^{i}—Zn1—N1—C5	−97.15 (14)
N1^{i}—Zn1—S1—O1^{i}	79.54 (9)	N2—Zn1—N1—C5	2.41 (13)
O1—Zn1—S1—O1^{i}	180.0	N1^{i}—Zn1—N1—C5	−48.08 (13)
N2^{i}—Zn1—N2—C10	−87.46 (16)	O1^{i}—Zn1—N1—C5	99.15 (14)
N1—Zn1—N2—C10	178.23 (17)	O1—Zn1—N1—C5	164.14 (14)
N1^{i}—Zn1—N2—C10	−9.89 (17)	S1—Zn1—N1—C5	131.92 (13)
O1^{i}—Zn1—N2—C10	79.90 (16)	C1—N1—C5—C4	−0.5 (3)
O1—Zn1—N2—C10	125.73 (18)	Zn1—N1—C5—C4	177.47 (15)
S1—Zn1—N2—C10	92.54 (16)	C1—N1—C5—C6	178.66 (17)
N2^{i}—Zn1—N2—C6	93.31 (13)	Zn1—N1—C5—C6	−3.3 (2)
N1—Zn1—N2—C6	−1.00 (13)	N2—C6—C5—N1	2.5 (2)
N1^{i}—Zn1—N2—C6	170.88 (13)	C7—C6—C5—N1	−176.01 (17)
O1^{i}—Zn1—N2—C6	−99.33 (13)	N2—C6—C5—C4	−178.35 (18)
O1—Zn1—N2—C6	−53.5 (2)	C7—C6—C5—C4	3.2 (3)
S1—Zn1—N2—C6	−86.69 (13)	N1—C5—C4—C3	0.1 (3)
O2—S1—O1—Zn1	118.12 (8)	C6—C5—C4—C3	−179.02 (18)
O2^{i}—S1—O1—Zn1	−119.09 (8)	C5—N1—C1—C2	0.8 (3)
O1^{i}—S1—O1—Zn1	0.0	Zn1—N1—C1—C2	−177.02 (15)
N2^{i}—Zn1—O1—S1	161.88 (7)	N1—C1—C2—C3	−0.6 (3)
N2—Zn1—O1—S1	−51.09 (18)	C1—C2—C3—C4	0.1 (3)
N1—Zn1—O1—S1	−101.62 (8)	C5—C4—C3—C2	0.1 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.82	1.97	2.746 (2)	158