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catena-Poly[[(1,10-phenanthroline-κ^2N,N')zinc]-μ-4-sulfonatobenzotriazolido-$\kappa^3N^3,O:N^1$]

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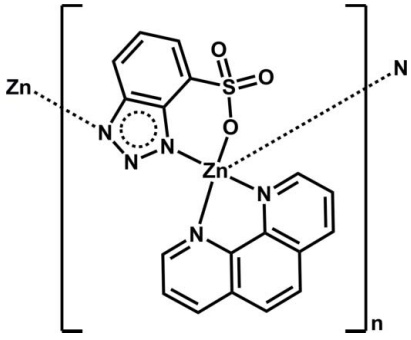
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.147; data-to-parameter ratio = 15.1.

In the title complex, $[Zn(C_6H_3N_3O_3S)(C_{12}H_8N_2)]_n$, the Zn^{2+} cation is coordinated by two N atoms from two 4-sulfonatobenzotriazolide dianions, two N atoms from a 1,10-phenanthroline molecule and a sulfonate O atom from a 4-sulfonatobenzotriazolide anion, displaying a distorted ZnN_4O trigonal–bipyramidal geometry. Each 1,10-phenanthroline ligand displays a bidentate chelating coordinating mode and the 4-sulfonatobenzotriazolide ions act as μ_2-bridges, linking different Zn^{2+} cations into a chain along the b axis. The crystal structure is consolidated by C—H···O hydrogen-bonding interactions.

Related literature

For related structures, see: Xia *et al.* (2010).



Experimental

Crystal data

$[Zn(C_6H_3N_3O_3S)(C_{12}H_8N_2)]$
M_r = 442.75
Orthorhombic, *Pccn*
a = 14.5562 (19) Å
b = 25.903 (3) Å
c = 8.9239 (12) Å
V = 3364.8 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.62 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.738, T_{max} = 0.738
19596 measured reflections
3819 independent reflections
2895 reflections with $I > 2\sigma(I)$
R_{int} = 0.092

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.147
S = 1.10
3819 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2^{i}	0.93	2.49	3.351 (5)	154
C12—H12···O2^{ii}	0.93	2.55	3.369 (5)	148

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2482).

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supporting information

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catena-Poly[[(1,10-phenanthroline-κ^2N,N')zinc]-μ-4-sulfonatobenzotriazolido-$\kappa^3N^3,O:N^1$]

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S1. Comment

Benzotriazole-4-sulfonic acid is often used as a ligand to synthesize complexes for its variable coordination modes. Herein, we report the crystal structure of the title complex. The asymmetric unit consists of one zinc ion, one 1,10-phenanthroline molecule, and one 4-sulfonatobenzotriazolide anion. each Zn ion is coordinated by two N atoms from two different 4-sulfonatobenzotriazolide anions, two N atoms from one 1,10-phenanthroline molecule, and one sulfonate O atoms from one 4-sulfonatobenzotriazolide anions, displaying a distorted ZnN_4O trigonal bipyramidal geometry (Fig. 1). Each 1,10-phenanthroline displays a bidentate coordinating mode. And every 4-sulfonatobenzotriazolide acts as a μ_2-bridge, linking different zinc ions to form a one-dimensional chain along the *b* axis direction. The crystal structure is consolidated by hydrogen bonding interactions of the type C—H···O (Table 1).

S2. Experimental

A mixture of zinc nitrate hexahydrate (59.4 mg, 0.2 mmol), benzotriazole-4-sulfonic acid (39.8 mg, 0.2 mmol), 1,10-phenanthroline (36.0 mg, 0.2 mmol) and potassium hydroxide (22.4 mg, 0.4 mmol) in 12 ml H_2O was sealed in a 16 ml Teflon-lined stainless steel container and heated to 413 K for 3 days. After cooling the container to the room temperature, colorless block crystals of the title complex were obtained.

S3. Refinement

The hydrogen atoms were located in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

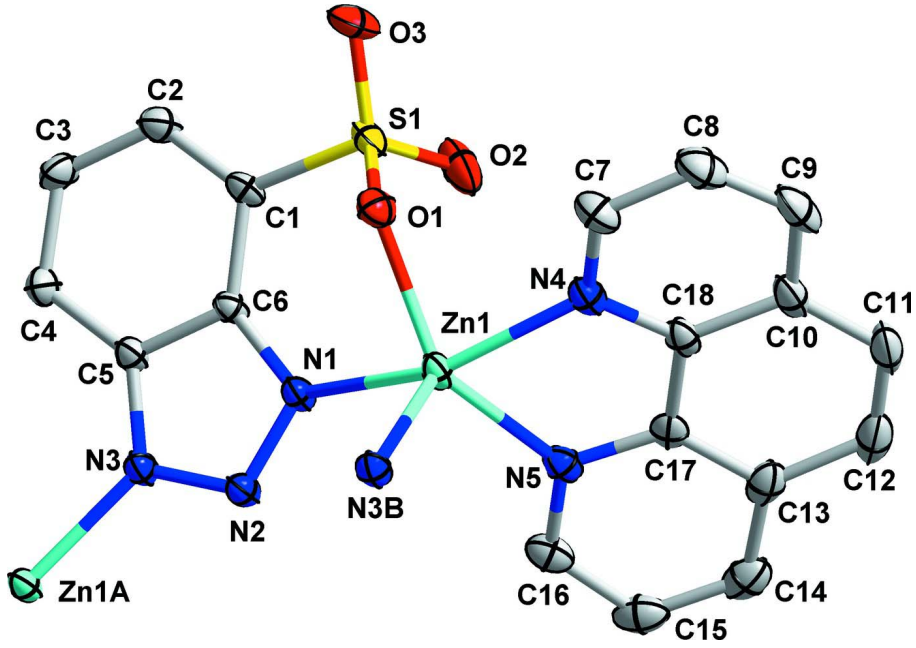

Figure 1

The coordination environment of zinc ion in the title complex with the ellipsoids drawn at the 30% probability level. The hydrogen atoms are omitted for clarity. Symmetry codes: A = *x*, -*y* + 1/2, *z* + 1/2; B = *x*, -*y* + 1/2, *z* - 1/2.

***catena*-Poly[[(1,10-phenanthroline-κ^2N,N')zinc]-μ- 4-sulfonatobenzotriazolido-$\kappa^3N^3,O:N^1$]**

Crystal data

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Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
a = 14.5562 (19) Å
b = 25.903 (3) Å
c = 8.9239 (12) Å
V = 3364.8 (8) Å^3
Z = 8
F(000) = 1792
D_x = 1.748 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2885 reflections
θ = 2.7–25.0°
μ = 1.62 mm^{-1}
T = 293 K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.738, T_{max} = 0.738
19596 measured reflections
3819 independent reflections
2895 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
θ_{max} = 27.4°, θ_{min} = 1.6°
h = −18→18
k = −33→33
l = −7→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.147
S = 1.10
3819 reflections
253 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
$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 1.2933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.97927 (3)	0.330127 (13)	0.19495 (5)	0.02895 (17)
N5	0.8384 (2)	0.34450 (11)	0.1826 (3)	0.0334 (7)
C17	0.8148 (2)	0.38273 (12)	0.0857 (4)	0.0333 (8)
C9	0.9411 (4)	0.47031 (16)	−0.1724 (5)	0.0581 (13)
H9	0.9313	0.4973	−0.2392	0.070*
C10	0.8673 (3)	0.44934 (14)	−0.0912 (5)	0.0454 (10)
C13	0.7232 (3)	0.39803 (14)	0.0600 (5)	0.0421 (9)
C14	0.6559 (3)	0.36901 (16)	0.1331 (5)	0.0497 (11)
H14	0.5942	0.3767	0.1170	0.060*
C7	1.0419 (3)	0.41028 (15)	−0.0526 (5)	0.0459 (10)
H7	1.1012	0.3977	−0.0398	0.055*
C18	0.8878 (3)	0.40801 (12)	0.0054 (4)	0.0337 (8)
C16	0.7712 (3)	0.31927 (15)	0.2529 (5)	0.0420 (9)
H16	0.7865	0.2937	0.3216	0.050*
C15	0.6784 (3)	0.32995 (16)	0.2270 (6)	0.0508 (12)
H15	0.6328	0.3105	0.2735	0.061*
N4	0.9732 (2)	0.38901 (11)	0.0256 (4)	0.0356 (7)
S1	1.10686 (6)	0.40039 (3)	0.37277 (12)	0.0366 (2)
N1	0.99027 (19)	0.29840 (10)	0.4183 (3)	0.0279 (6)
N2	0.9579 (2)	0.25262 (10)	0.4630 (3)	0.0312 (6)
C1	1.1157 (2)	0.35655 (11)	0.5213 (4)	0.0293 (7)
C2	1.1777 (3)	0.35925 (14)	0.6343 (5)	0.0392 (9)
H2	1.2171	0.3875	0.6391	0.047*
C3	1.1841 (3)	0.32053 (16)	0.7447 (5)	0.0441 (10)
H3	1.2267	0.3242	0.8217	0.053*
O1	1.10445 (18)	0.36563 (10)	0.2416 (3)	0.0391 (6)
O3	1.1878 (2)	0.43226 (10)	0.3728 (4)	0.0511 (8)
O2	1.0199 (2)	0.42648 (11)	0.3896 (4)	0.0628 (10)
N3	1.0018 (2)	0.23706 (11)	0.5874 (3)	0.0307 (6)

C6	1.0567 (2)	0.31302 (11)	0.5174 (4)	0.0257 (7)
C5	1.0640 (2)	0.27433 (12)	0.6254 (4)	0.0294 (7)
C4	1.1290 (3)	0.27760 (15)	0.7414 (4)	0.0375 (8)
H4	1.1344	0.2517	0.8130	0.045*
C12	0.7058 (3)	0.44058 (16)	−0.0377 (6)	0.0551 (12)
H12	0.6456	0.4514	−0.0526	0.066*
C11	0.7738 (3)	0.46542 (16)	−0.1083 (6)	0.0581 (13)
H11	0.7602	0.4935	−0.1692	0.070*
C8	1.0273 (3)	0.45068 (18)	−0.1525 (6)	0.0553 (12)
H8	1.0764	0.4644	−0.2059	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0395 (3)	0.0203 (2)	0.0271 (3)	0.00316 (14)	−0.00219 (17)	−0.00023 (15)
N5	0.0423 (17)	0.0270 (14)	0.0309 (17)	−0.0015 (12)	−0.0001 (13)	−0.0032 (12)
C17	0.0427 (19)	0.0239 (16)	0.033 (2)	0.0031 (13)	−0.0079 (16)	−0.0106 (14)
C9	0.100 (4)	0.032 (2)	0.043 (3)	−0.005 (2)	−0.005 (3)	0.0132 (18)
C10	0.074 (3)	0.0236 (17)	0.038 (2)	0.0022 (17)	−0.016 (2)	0.0010 (16)
C13	0.045 (2)	0.041 (2)	0.041 (2)	0.0082 (17)	−0.0131 (19)	−0.0133 (17)
C14	0.041 (2)	0.052 (2)	0.055 (3)	0.0053 (18)	−0.006 (2)	−0.022 (2)
C7	0.054 (2)	0.036 (2)	0.048 (3)	−0.0056 (17)	0.007 (2)	0.0085 (18)
C18	0.048 (2)	0.0231 (16)	0.0296 (19)	0.0012 (14)	−0.0052 (16)	−0.0027 (14)
C16	0.051 (2)	0.0347 (19)	0.041 (2)	−0.0063 (17)	0.007 (2)	−0.0041 (17)
C15	0.046 (2)	0.047 (3)	0.059 (3)	−0.0087 (18)	0.008 (2)	−0.018 (2)
N4	0.0468 (18)	0.0287 (15)	0.0312 (17)	0.0009 (12)	−0.0005 (14)	0.0031 (13)
S1	0.0427 (5)	0.0234 (4)	0.0437 (6)	−0.0010 (3)	0.0040 (4)	0.0088 (4)
N1	0.0386 (15)	0.0217 (13)	0.0232 (14)	0.0007 (11)	−0.0012 (12)	0.0012 (11)
N2	0.0422 (16)	0.0241 (14)	0.0273 (15)	−0.0041 (11)	−0.0026 (13)	0.0017 (12)
C1	0.0381 (18)	0.0188 (15)	0.0311 (18)	−0.0014 (12)	0.0053 (15)	−0.0012 (13)
C2	0.045 (2)	0.0339 (19)	0.038 (2)	−0.0103 (15)	−0.0016 (18)	−0.0019 (16)
C3	0.045 (2)	0.051 (2)	0.036 (2)	−0.0136 (18)	−0.016 (2)	0.0041 (19)
O1	0.0430 (14)	0.0394 (15)	0.0350 (14)	−0.0068 (11)	0.0000 (12)	0.0070 (12)
O3	0.0644 (18)	0.0334 (14)	0.0557 (19)	−0.0201 (13)	0.0057 (15)	0.0051 (13)
O2	0.060 (2)	0.0438 (17)	0.084 (3)	0.0201 (14)	0.0185 (17)	0.0227 (17)
N3	0.0406 (16)	0.0248 (14)	0.0267 (16)	−0.0011 (11)	−0.0032 (13)	0.0029 (12)
C6	0.0327 (17)	0.0222 (14)	0.0221 (16)	−0.0027 (12)	0.0009 (14)	−0.0006 (12)
C5	0.0370 (18)	0.0223 (15)	0.0288 (18)	−0.0012 (13)	−0.0008 (15)	0.0001 (13)
C4	0.042 (2)	0.038 (2)	0.032 (2)	−0.0055 (15)	−0.0067 (17)	0.0088 (16)
C12	0.059 (3)	0.051 (3)	0.056 (3)	0.021 (2)	−0.025 (2)	−0.011 (2)
C11	0.078 (3)	0.035 (2)	0.061 (3)	0.015 (2)	−0.028 (3)	0.006 (2)
C8	0.073 (3)	0.046 (2)	0.048 (3)	−0.014 (2)	0.006 (2)	0.010 (2)

Geometric parameters (Å, º)

Zn1—N3^{i}	2.014 (3)	C15—H15	0.9300
Zn1—O1	2.083 (3)	S1—O3	1.439 (3)
Zn1—N5	2.086 (3)	S1—O2	1.443 (3)

Zn1—N4	2.149 (3)	S1—O1	1.477 (3)
Zn1—N1	2.162 (3)	S1—C1	1.750 (4)
N5—C16	1.334 (5)	N1—N2	1.337 (4)
N5—C17	1.359 (5)	N1—C6	1.364 (4)
C17—C13	1.410 (5)	N2—N3	1.343 (4)
C17—C18	1.440 (5)	C1—C2	1.355 (5)
C9—C8	1.365 (7)	C1—C6	1.418 (4)
C9—C10	1.405 (7)	C2—C3	1.409 (6)
C9—H9	0.9300	C2—H2	0.9300
C10—C18	1.407 (5)	C3—C4	1.372 (5)
C10—C11	1.431 (6)	C3—H3	0.9300
C13—C14	1.397 (6)	N3—C5	1.366 (4)
C13—C12	1.427 (6)	N3—Zn1^{ii}	2.014 (3)
C14—C15	1.354 (7)	C6—C5	1.395 (4)
C14—H14	0.9300	C5—C4	1.405 (5)
C7—N4	1.338 (5)	C4—H4	0.9300
C7—C8	1.391 (6)	C12—C11	1.338 (7)
C7—H7	0.9300	C12—H12	0.9300
C18—N4	1.349 (5)	C11—H11	0.9300
C16—C15	1.398 (6)	C8—H8	0.9300
C16—H16	0.9300		

N3^{i}—Zn1—O1	109.52 (12)	C18—N4—Zn1	113.0 (2)
N3^{i}—Zn1—N5	106.80 (12)	O3—S1—O2	116.73 (18)
O1—Zn1—N5	142.30 (11)	O3—S1—O1	111.69 (17)
N3^{i}—Zn1—N4	106.53 (12)	O2—S1—O1	110.3 (2)
O1—Zn1—N4	82.14 (11)	O3—S1—C1	108.17 (18)
N5—Zn1—N4	78.21 (11)	O2—S1—C1	106.83 (18)
N3^{i}—Zn1—N1	95.67 (11)	O1—S1—C1	101.91 (15)
O1—Zn1—N1	85.34 (11)	N2—N1—C6	107.6 (3)
N5—Zn1—N1	100.92 (11)	N2—N1—Zn1	125.9 (2)
N4—Zn1—N1	157.12 (11)	C6—N1—Zn1	123.0 (2)
C16—N5—C17	118.1 (3)	N1—N2—N3	110.2 (3)
C16—N5—Zn1	127.5 (3)	C2—C1—C6	117.6 (3)
C17—N5—Zn1	114.4 (2)	C2—C1—S1	125.4 (3)
N5—C17—C13	123.2 (4)	C6—C1—S1	116.9 (3)
N5—C17—C18	117.5 (3)	C1—C2—C3	121.9 (3)
C13—C17—C18	119.3 (3)	C1—C2—H2	119.1
C8—C9—C10	119.4 (4)	C3—C2—H2	119.1
C8—C9—H9	120.3	C4—C3—C2	121.5 (4)
C10—C9—H9	120.3	C4—C3—H3	119.2
C9—C10—C18	116.6 (4)	C2—C3—H3	119.2
C9—C10—C11	124.0 (4)	S1—O1—Zn1	116.64 (16)
C18—C10—C11	119.3 (4)	N2—N3—C5	108.0 (3)
C14—C13—C17	115.8 (4)	N2—N3—Zn1^{ii}	125.1 (2)
C14—C13—C12	125.3 (4)	C5—N3—Zn1^{ii}	126.9 (2)
C17—C13—C12	118.9 (4)	N1—C6—C5	107.6 (3)
C15—C14—C13	121.4 (4)	N1—C6—C1	131.8 (3)

C15—C14—H14	119.3	C5—C6—C1	120.5 (3)
C13—C14—H14	119.3	N3—C5—C6	106.6 (3)
N4—C7—C8	122.0 (4)	N3—C5—C4	132.2 (3)
N4—C7—H7	119.0	C6—C5—C4	121.1 (3)
C8—C7—H7	119.0	C3—C4—C5	117.3 (3)
N4—C18—C10	123.7 (4)	C3—C4—H4	121.3
N4—C18—C17	116.6 (3)	C5—C4—H4	121.3
C10—C18—C17	119.6 (3)	C11—C12—C13	121.9 (4)
N5—C16—C15	122.3 (4)	C11—C12—H12	119.1
N5—C16—H16	118.9	C13—C12—H12	119.1
C15—C16—H16	118.9	C12—C11—C10	120.9 (4)
C14—C15—C16	119.0 (4)	C12—C11—H11	119.6
C14—C15—H15	120.5	C10—C11—H11	119.6
C16—C15—H15	120.5	C9—C8—C7	120.3 (4)
C7—N4—C18	117.9 (3)	C9—C8—H8	119.9
C7—N4—Zn1	128.9 (3)	C7—C8—H8	119.9

N3^{i}—Zn1—N5—C16	70.4 (3)	N3^{i}—Zn1—N1—C6	117.1 (3)
O1—Zn1—N5—C16	−125.6 (3)	O1—Zn1—N1—C6	7.9 (3)
N4—Zn1—N5—C16	174.3 (3)	N5—Zn1—N1—C6	−134.6 (3)
N1—Zn1—N5—C16	−29.0 (3)	N4—Zn1—N1—C6	−49.0 (4)
N3^{i}—Zn1—N5—C17	−106.6 (2)	C6—N1—N2—N3	−0.4 (4)
O1—Zn1—N5—C17	57.5 (3)	Zn1—N1—N2—N3	158.8 (2)
N4—Zn1—N5—C17	−2.6 (2)	O3—S1—C1—C2	12.6 (4)
N1—Zn1—N5—C17	154.0 (2)	O2—S1—C1—C2	−113.8 (4)
C16—N5—C17—C13	2.1 (5)	O1—S1—C1—C2	130.4 (3)
Zn1—N5—C17—C13	179.4 (3)	O3—S1—C1—C6	−163.3 (3)
C16—N5—C17—C18	−177.2 (3)	O2—S1—C1—C6	70.3 (3)
Zn1—N5—C17—C18	0.0 (4)	O1—S1—C1—C6	−45.5 (3)
C8—C9—C10—C18	−1.1 (6)	C6—C1—C2—C3	0.0 (6)
C8—C9—C10—C11	−177.1 (4)	S1—C1—C2—C3	−175.9 (3)
N5—C17—C13—C14	−4.2 (5)	C1—C2—C3—C4	1.3 (7)
C18—C17—C13—C14	175.2 (3)	O3—S1—O1—Zn1	−165.49 (16)
N5—C17—C13—C12	176.5 (3)	O2—S1—O1—Zn1	−33.9 (2)
C18—C17—C13—C12	−4.2 (5)	C1—S1—O1—Zn1	79.25 (19)
C17—C13—C14—C15	2.3 (6)	N3^{i}—Zn1—O1—S1	−152.98 (16)
C12—C13—C14—C15	−178.3 (4)	N5—Zn1—O1—S1	43.2 (3)
C9—C10—C18—N4	1.6 (6)	N4—Zn1—O1—S1	102.19 (18)
C11—C10—C18—N4	177.9 (4)	N1—Zn1—O1—S1	−58.61 (17)
C9—C10—C18—C17	−176.5 (3)	N1—N2—N3—C5	0.7 (4)
C11—C10—C18—C17	−0.2 (5)	N1—N2—N3—Zn1^{ii}	−178.7 (2)
N5—C17—C18—N4	4.5 (5)	N2—N1—C6—C5	0.0 (4)
C13—C17—C18—N4	−174.8 (3)	Zn1—N1—C6—C5	−160.0 (2)
N5—C17—C18—C10	−177.2 (3)	N2—N1—C6—C1	177.1 (3)
C13—C17—C18—C10	3.4 (5)	Zn1—N1—C6—C1	17.1 (5)
C17—N5—C16—C15	1.8 (6)	C2—C1—C6—N1	−177.8 (4)
Zn1—N5—C16—C15	−175.0 (3)	S1—C1—C6—N1	−1.6 (5)
C13—C14—C15—C16	1.2 (7)	C2—C1—C6—C5	−1.0 (5)

N5—C16—C15—C14	−3.5 (7)	S1—C1—C6—C5	175.3 (3)
C8—C7—N4—C18	−0.2 (6)	N2—N3—C5—C6	−0.7 (4)
C8—C7—N4—Zn1	−175.8 (3)	Zn1^{ii}—N3—C5—C6	178.7 (2)
C10—C18—N4—C7	−1.0 (5)	N2—N3—C5—C4	−178.1 (4)
C17—C18—N4—C7	177.2 (3)	Zn1^{ii}—N3—C5—C4	1.3 (6)
C10—C18—N4—Zn1	175.3 (3)	N1—C6—C5—N3	0.5 (4)
C17—C18—N4—Zn1	−6.6 (4)	C1—C6—C5—N3	−177.1 (3)
N3^{i}—Zn1—N4—C7	−75.0 (3)	N1—C6—C5—C4	178.2 (3)
O1—Zn1—N4—C7	33.1 (3)	C1—C6—C5—C4	0.6 (5)
N5—Zn1—N4—C7	−179.2 (4)	C2—C3—C4—C5	−1.6 (6)
N1—Zn1—N4—C7	90.6 (4)	N3—C5—C4—C3	177.7 (4)
N3^{i}—Zn1—N4—C18	109.2 (3)	C6—C5—C4—C3	0.7 (6)
O1—Zn1—N4—C18	−142.6 (3)	C14—C13—C12—C11	−177.5 (4)
N5—Zn1—N4—C18	5.0 (2)	C17—C13—C12—C11	1.8 (6)
N1—Zn1—N4—C18	−85.2 (4)	C13—C12—C11—C10	1.5 (7)
N3^{i}—Zn1—N1—N2	−39.2 (3)	C9—C10—C11—C12	173.7 (5)
O1—Zn1—N1—N2	−148.4 (3)	C18—C10—C11—C12	−2.3 (6)
N5—Zn1—N1—N2	69.1 (3)	C10—C9—C8—C7	0.0 (7)
N4—Zn1—N1—N2	154.7 (3)	N4—C7—C8—C9	0.7 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{iii}	0.93	2.49	3.351 (5)	154
C12—H12···O2^{iv}	0.93	2.55	3.369 (5)	148

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