

Crystal structure and Hirshfeld surface analysis of a zinc xanthate complex containing the 2,2'-bipyridine ligand

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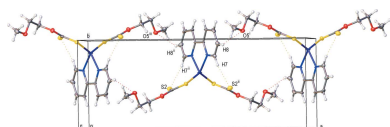
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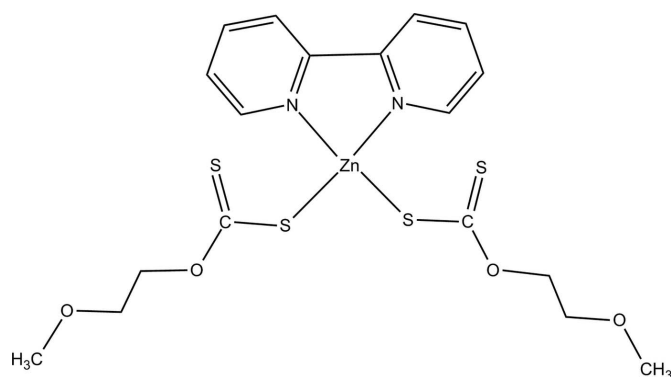
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In the title compound, (2,2'-bipyridine- κ^2N,N')bis(2-methoxyethyl xanthato- κS)zinc(II), $[Zn(C_4H_7O_2S_2)_2(C_{10}H_8N_2)]$, the Zn^{II} ion is coordinated to two N atoms of the 2,2'-bipyridine ligand and two S atoms from two 2-methoxyethyl xanthate ligands. The Zn^{II} ion lies on a crystallographic twofold rotation axis and has distorted tetrahedral coordination geometry. In the crystal, molecules are linked by weak C—H...O hydrogen bonds, forming supramolecular chains propagating along the *a*-axis direction. Weak intramolecular C—H...S hydrogen bonds are also observed. The intermolecular contacts in the crystal were further analysed using Hirshfeld surface analysis, which indicates that the most significant contacts are H...H (36.3%), followed by S...H/H...S (24.7%), C...H/H...C (15.1%), O...H/H...O (14.4%), N...H/H...N (4.1%) and C...C (2.9%).

1. Chemical context

Xanthates (dithiocarbonates, $ROCS_2^-$) have attracted the attention of scientific groups of researchers due to their diverse applications. Metal xanthates have been used as single-source precursors to metal sulfide materials (Kociok-Köhn *et al.*, 2015). It was reported that metal xanthates have cytotoxic activity on human cancer cells (Efrima *et al.*, 2003; Friebolin *et al.*, 2005). Cellulose xanthate have been used for the column separation of alcohols by chromatographic methods (Friebolin *et al.*, 2004). Zinc(II) xanthate complexes have a tetrahedral geometry, while zinc(II) xanthate complexes with neutral bidentate nitrogen donor ligands are either strongly distorted octahedral or tetrahedral. In our previous work, Zn^{II} 2-methoxyethylxanthate with *N,N,N',N'*-tetramethylethylenediamine was synthesized, structurally characterized and studied by density functional theory (Qadir *et al.*, 2019). The complex showed a tetrahedral environment around metal center and the HOMO–LUMO band gap was 3.9 eV. Aromatic heterocyclic nitrogen donor ligands have been used by researchers to prepare mixed-ligand complexes of transition metals with supramolecular architectures. In this work, the synthesis and crystal structure of a zinc(II) 2-methoxyethyl xanthate involving 2,2'-bipyridine is reported. Hirshfeld surface analysis was used to further investigate the intermolecular interactions.





2. Structural commentary

The title complex (Fig. 1) comprises one Zn^{II} ion, one 2,2'-bipyridine ligand and two 2-methoxyethyl xanthate ligands. The Zn^{II} ion is coordinated to two N atoms of the 2,2'-bipyridine ligand and two S atoms from two 2-methoxyethyl xanthate ligands in a distorted tetrahedral environment and lies on a crystallographic twofold rotation axis. The Zn–N and Zn–S bond lengths are 2.083 (5) and 2.295 (2) Å, respectively, whereas the bond angles around the central Zn^{II} ion are in the range 78.7 (3)–126.64 (10)° (Table 1). The bond lengths and angles of the ZnN_2S_2 coordination units correspond to those in the structures of mixed-ligand Zn^{II} coordination compounds (see; *Database Survey*). The C–O bond lengths range from 1.346 (8) to 1.453 (8) Å although all of the C–O bonds show single-bond character. In the $\{\text{S}_2\text{C}\}$ part of the xanthate ligands, the C1–S1 distance is 1.727 (7) Å, which is typical of a single bond whereas the C1–S2 distance of 1.652 (7) Å is typical of a carbon-to-sulfur double bond. The C–N and C–C bond lengths in 2,2'-bipyridine are normal for 2-substituted pyridine derivatives (Strotmeyer *et al.*, 2003; Iskenderov *et al.*, 2009; Golenya *et al.*, 2012).

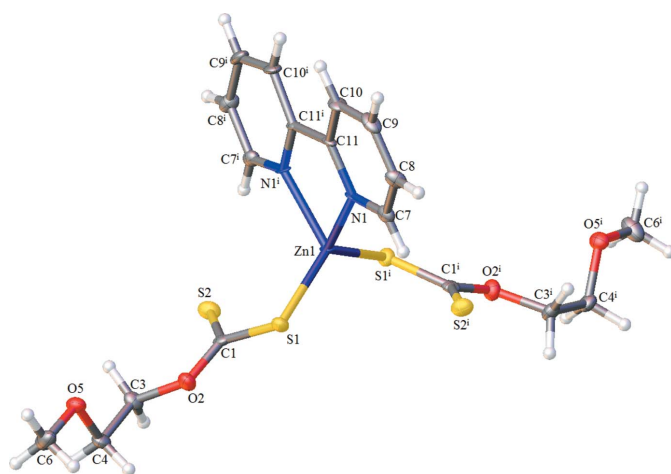


Figure 1
The molecular structure of the title complex, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.

Table 1
Selected geometric parameters (Å, °).

Zn1–S1	2.2954 (18)	Zn1–N1	2.083 (5)
S1 ⁱ –Zn1–S1	126.64 (10)	N1–Zn1–S1	100.54 (15)
N1 ⁱ –Zn1–S1	120.78 (15)	N1–Zn1–N1 ⁱ	78.7 (3)

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

3. Supramolecular features

The crystal packing of the title compound (Fig. 2) features intermolecular C8–H8···O5ⁱⁱ hydrogen bonds (Table 2), which connect the molecules into supramolecular chains propagating along the *a*-axis direction. Weak intramolecular C–H···S hydrogen bonds are also observed.

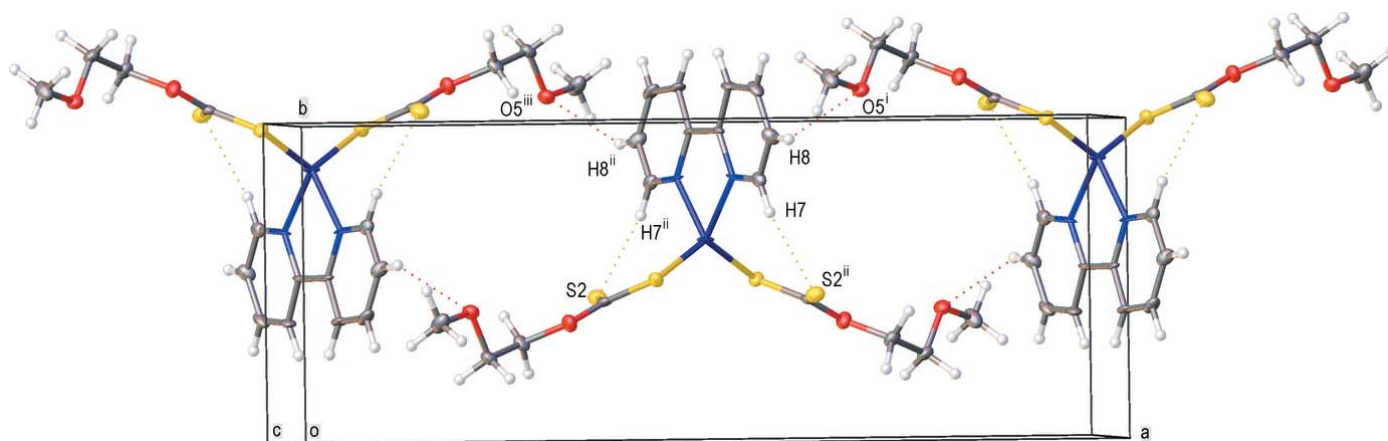
4. Hirshfeld surface analysis

The Hirshfeld surface analysis and the associated two-dimensional fingerprint plots were performed with *Crystal-Explorer17.5* (Turner *et al.*, 2017). The Hirshfeld surface of the title complex is shown in Fig. 3*a* and 3*b*. The intermolecular interactions are represented using different colours, red indicating distances closer than the sum of the van der Waals radii, white indicating distances near the van der Waals radii separation, and blue indicating distances longer than the van der Waals radii (McKinnon *et al.*, 2007). The weak C–H···O and C–H···S hydrogen bonding in the crystal of the title complex are represented as red spots on d_{norm} . Selected two-dimensional fingerprint plots are shown in Fig. 4 for all contacts as well as those delineated into H···H, S···H/H···S and C···H/H···C contacts, whose percentage contribution is also given. H···H intermolecular contacts make the highest percentage contribution (36.3%), a result of the prevalence of hydrogen from the organic ligands. The S···H/H···S and O···H/H···O intermolecular contacts are due to the attractive C–H···S and C–H···O hydrogen-bonding interactions and make percentage contributions of 24.7 and 14.4%, respectively, indicating these to be the dominant stabilizing interactions in this crystal. In addition, C···H/H···C contacts contribute 15.1% to the Hirshfeld surface. The small percentage contributions from the other different interatomic contacts to the Hirshfeld surfaces are as follows: N···H/H···N (4.1%), C···C (2.9%), S···S (1.1%), S···O/O···S (0.8%) and S···C/C···S (0.3%).

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

<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>
C8–H8···O5 ⁱ	0.95	2.51	3.246 (9)	134
C7–H7···S2 ⁱⁱ	0.95	2.90	3.552 (7)	127

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

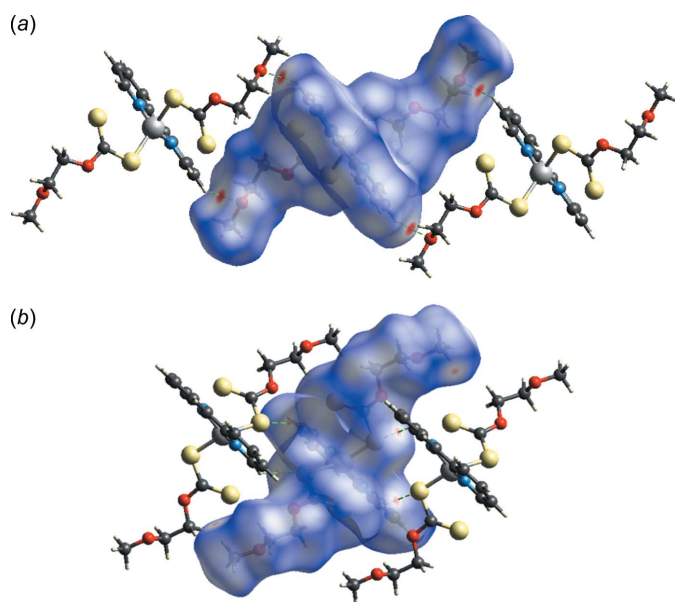

Figure 2

A view of the crystal packing of the title complex. Dashed lines denote the intermolecular hydrogen bonds (Table 2). Symmetry codes: (i) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$, (ii) $1 - x, y, \frac{1}{2} - z$, (iii) $\frac{1}{2} - x, \frac{3}{2} - y, -z$.

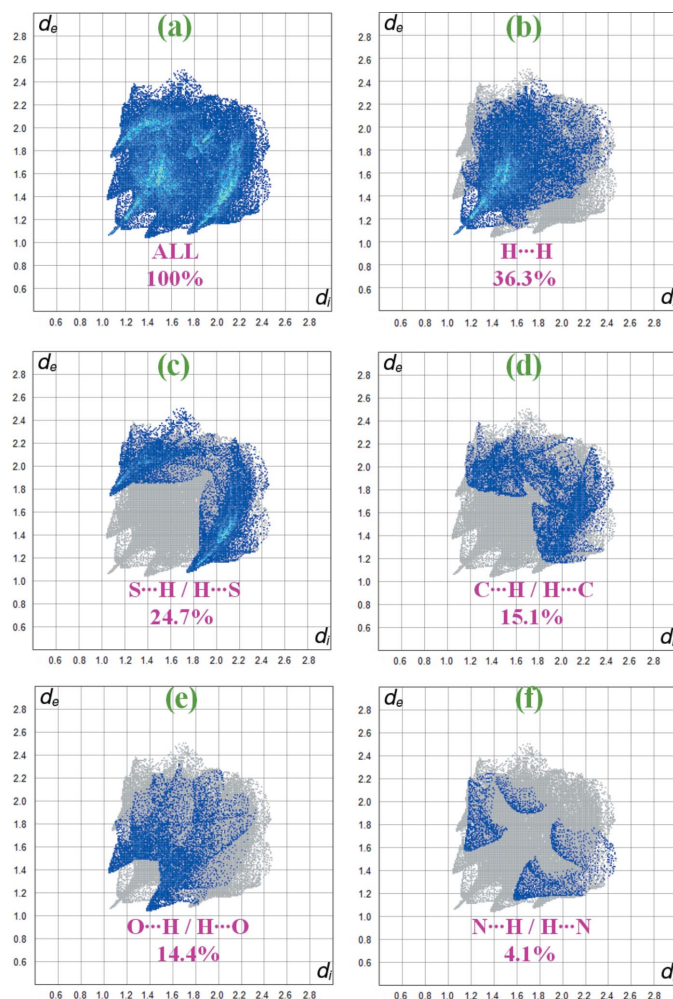
5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update of February 2019; Groom *et al.*, 2016) for compounds related to the title complex revealed five hits: (2,2'-dipyridyl)bis(butylxanthato)zinc(II) (DIFBOK; Klevtsova *et al.*, 2006), (2,2'-bipyridine)(*O-n*-propyldithiocarbonato- κ^2S,S')(*O-n*-propyldithiocarbonato-*S*)zinc(II) (IGUGUO; Jeremias *et al.*, 2014), (2,2'-bipyridine)-bis(*O-isopropylxanthato*)zinc(II) and (2,2'-bipyridine)bis(*O-isobutylxanthato*)zinc(II) (with refcodes MUJJOQ and MUJJUW, respectively; Klevtsova *et al.*, 2002) and (2,2'-bipyridyl)bis(ethylxanthato)zinc(II) (WITLAM; Glinskaya *et al.*, 2000). All of these complexes except IGUGUO have tetrahedral environments around the metal center. The Zn–N and Zn–S bond lengths

range from 2.065 to 2.147 Å and 2.284 to 2.341 Å, respectively. The Zn–N and Zn–S bond lengths in the title complex [2.083 (5) and 2.295 (2) Å, respectively] fall within these limits.


Figure 3

The Hirshfeld surfaces mapped over d_{norm} in the range -0.1353 to $+1.0127$ (arbitrary units) for visualizing the weak intermolecular (a) C–H...O and (b) C–H...S hydrogen bonding.


Figure 4

Hirshfeld surface fingerprint plots for the H...H, S...H/H...S, C...H/H...C and N...H/H...N contacts of the title complex.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Zn(C ₄ H ₇ O ₂ S ₂) ₂ (C ₁₀ H ₈ N ₂)]
<i>M_r</i>	523.98
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	22.869 (4), 8.3212 (12), 12.5627 (19)
β (°)	115.348 (4)
<i>V</i> (Å ³)	2160.5 (6)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.55
Crystal size (mm)	0.42 × 0.36 × 0.04
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2009)
<i>T_{min}</i> , <i>T_{max}</i>	0.599, 0.745
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	11173, 2119, 1954
<i>R_{int}</i>	0.061
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.618
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.087, 0.155, 1.43
No. of reflections	2119
No. of parameters	134
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.55, -1.00

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

The structure with refcode IGUGUO has a distorted trigonal-bipyramidal coordination environment.

6. Synthesis and crystallization

To a hot solution of Zn(CH₃CO₂)₂·2H₂O (10 mmol, 2.20 g) in 2-methoxyethanol, was added a hot solution of 2,2'-bipy (10 mmol, 1.56 g) in 2-methoxyethanol. A hot solution of potassium 2-methoxyethylxanthate (20 mmol, 3.81 g) in 2-methoxyethanol was added under stirring. Colourless crystals were formed after 30 minutes. The crystals were washed with small amounts of 2-methoxyethanol and water and air-dried.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound H atoms were

positioned geometrically and refined using a riding model, with C–H = 0.95, 0.98 and 0.99 Å with *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl H atoms and 1.2*U*_{eq}(C) otherwise. The crystal was a weak diffractor (*I*/ σ at 0.81 resolution was 5.1) and refined as a two-component twin with HKLF 4 data (twin law -1 0 0 0 - 1 0 0 0 - 1) but this had little effect. The anisotropy of N1 was restrained with ISOR 0.01 0.02 in *SHELXL* (Sheldrick, 2015).

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supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *S SAINT* (Bruker, 2009); data reduction: *S SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

(2,2'-Bipyridine- κ^2N,N')bis(2-methoxyethyl xanthato- κS)zinc(II)

Crystal data

[Zn(C₄H₇O₂S₂)₂(C₁₀H₈N₂)]

$M_r = 523.98$

Monoclinic, *C2/c*

$a = 22.869$ (4) Å

$b = 8.3212$ (12) Å

$c = 12.5627$ (19) Å

$\beta = 115.348$ (4)°

$V = 2160.5$ (6) Å³

$Z = 4$

$F(000) = 1080$

$D_x = 1.611$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2844 reflections

$\theta = 3.0$ – 25.4 °

$\mu = 1.55$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.42 \times 0.36 \times 0.04$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2009)

$T_{\min} = 0.599$, $T_{\max} = 0.745$

11173 measured reflections

2119 independent reflections

1954 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\max} = 26.1$ °, $\theta_{\min} = 2.6$ °

$h = -28 \rightarrow 28$

$k = -9 \rightarrow 10$

$l = -14 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.087$

$wR(F^2) = 0.155$

$S = 1.43$

2119 reflections

134 parameters

6 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 39.0236P]$

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

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

$\Delta\rho_{\max} = 0.55$ e Å⁻³

$\Delta\rho_{\min} = -1.00$ e Å⁻³

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.

Refinement. Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.5000	0.63086 (13)	0.2500	0.0085 (3)
S1	0.44329 (8)	0.5070 (2)	0.33978 (16)	0.0164 (4)
S2	0.36008 (9)	0.4541 (2)	0.08028 (17)	0.0208 (4)
O2	0.3340 (2)	0.3748 (7)	0.2598 (4)	0.0203 (11)
O5	0.2155 (2)	0.4123 (6)	0.2833 (4)	0.0193 (11)
N1	0.5396 (3)	0.8245 (6)	0.3634 (5)	0.0101 (11)
C1	0.3750 (3)	0.4405 (8)	0.2208 (6)	0.0153 (15)
C3	0.2717 (3)	0.3151 (9)	0.1750 (6)	0.0186 (16)
H3A	0.2775	0.2208	0.1325	0.022*
H3B	0.2481	0.3996	0.1169	0.022*
C4	0.2350 (4)	0.2688 (9)	0.2455 (7)	0.0192 (16)
H4A	0.1966	0.2038	0.1964	0.023*
H4B	0.2630	0.2037	0.3146	0.023*
C6	0.1815 (4)	0.3775 (11)	0.3521 (7)	0.0289 (19)
H6A	0.1441	0.3094	0.3067	0.043*
H6B	0.1666	0.4780	0.3731	0.043*
H6C	0.2102	0.3211	0.4240	0.043*
C7	0.5764 (3)	0.8146 (9)	0.4798 (6)	0.0165 (15)
H7	0.5905	0.7116	0.5138	0.020*
C8	0.5948 (4)	0.9481 (9)	0.5521 (6)	0.0191 (16)
H8	0.6204	0.9372	0.6345	0.023*
C9	0.5751 (4)	1.0972 (9)	0.5021 (7)	0.0214 (17)
H9	0.5874	1.1913	0.5494	0.026*
C10	0.5371 (3)	1.1084 (8)	0.3815 (7)	0.0189 (16)
H10	0.5229	1.2103	0.3455	0.023*
C11	0.5204 (3)	0.9708 (8)	0.3151 (6)	0.0113 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0137 (6)	0.0030 (5)	0.0118 (6)	0.000	0.0084 (4)	0.000
S1	0.0169 (9)	0.0160 (9)	0.0181 (9)	-0.0021 (7)	0.0091 (7)	0.0031 (7)
S2	0.0285 (10)	0.0198 (10)	0.0198 (10)	-0.0027 (8)	0.0158 (8)	-0.0026 (8)
O2	0.018 (3)	0.022 (3)	0.023 (3)	-0.002 (2)	0.011 (2)	0.003 (2)
O5	0.022 (3)	0.016 (3)	0.023 (3)	-0.001 (2)	0.013 (2)	0.002 (2)
N1	0.016 (3)	0.003 (3)	0.017 (3)	-0.004 (2)	0.011 (2)	-0.004 (2)
C1	0.019 (4)	0.007 (3)	0.022 (4)	0.004 (3)	0.011 (3)	0.004 (3)
C3	0.020 (4)	0.019 (4)	0.017 (4)	-0.006 (3)	0.008 (3)	-0.005 (3)

C4	0.020 (4)	0.014 (4)	0.023 (4)	-0.005 (3)	0.009 (3)	-0.001 (3)
C6	0.028 (4)	0.029 (4)	0.038 (5)	0.009 (4)	0.022 (4)	0.015 (4)
C7	0.017 (4)	0.018 (4)	0.020 (4)	-0.002 (3)	0.013 (3)	-0.003 (3)
C8	0.025 (4)	0.021 (4)	0.016 (4)	-0.006 (3)	0.013 (3)	-0.003 (3)
C9	0.021 (4)	0.018 (4)	0.030 (4)	-0.008 (3)	0.015 (3)	-0.014 (3)
C10	0.020 (4)	0.006 (3)	0.032 (4)	-0.002 (3)	0.013 (3)	-0.005 (3)
C11	0.012 (3)	0.004 (3)	0.021 (4)	-0.002 (3)	0.011 (3)	-0.002 (3)

Geometric parameters (Å, °)

Zn1—S1	2.2954 (18)	C4—H4A	0.9900
Zn1—S1 ⁱ	2.2954 (18)	C4—H4B	0.9900
Zn1—N1 ⁱ	2.083 (5)	C6—H6A	0.9800
Zn1—N1	2.083 (5)	C6—H6B	0.9800
S1—C1	1.727 (7)	C6—H6C	0.9800
S2—C1	1.652 (7)	C7—H7	0.9500
O2—C1	1.346 (8)	C7—C8	1.382 (10)
O2—C3	1.453 (8)	C8—H8	0.9500
O5—C4	1.426 (9)	C8—C9	1.377 (11)
O5—C6	1.418 (8)	C9—H9	0.9500
N1—C7	1.342 (9)	C9—C10	1.390 (11)
N1—C11	1.347 (8)	C10—H10	0.9500
C3—H3A	0.9900	C10—C11	1.371 (9)
C3—H3B	0.9900	C11—C11 ⁱ	1.497 (13)
C3—C4	1.506 (10)		
S1 ⁱ —Zn1—S1	126.64 (10)	C3—C4—H4A	110.0
N1 ⁱ —Zn1—S1	120.78 (15)	C3—C4—H4B	110.0
N1—Zn1—S1 ⁱ	120.78 (15)	H4A—C4—H4B	108.4
N1—Zn1—S1	100.54 (15)	O5—C6—H6A	109.5
N1 ⁱ —Zn1—S1 ⁱ	100.54 (15)	O5—C6—H6B	109.5
N1—Zn1—N1 ⁱ	78.7 (3)	O5—C6—H6C	109.5
C1—S1—Zn1	102.2 (2)	H6A—C6—H6B	109.5
C1—O2—C3	119.3 (5)	H6A—C6—H6C	109.5
C6—O5—C4	111.4 (6)	H6B—C6—H6C	109.5
C7—N1—Zn1	125.7 (5)	N1—C7—H7	118.7
C7—N1—C11	118.5 (6)	N1—C7—C8	122.7 (7)
C11—N1—Zn1	115.4 (4)	C8—C7—H7	118.7
S2—C1—S1	126.8 (4)	C7—C8—H8	120.8
O2—C1—S1	109.1 (5)	C9—C8—C7	118.4 (7)
O2—C1—S2	124.0 (5)	C9—C8—H8	120.8
O2—C3—H3A	110.5	C8—C9—H9	120.4
O2—C3—H3B	110.5	C8—C9—C10	119.2 (7)
O2—C3—C4	105.9 (6)	C10—C9—H9	120.4
H3A—C3—H3B	108.7	C9—C10—H10	120.4
C4—C3—H3A	110.5	C11—C10—C9	119.2 (7)
C4—C3—H3B	110.5	C11—C10—H10	120.4
O5—C4—C3	108.3 (6)	N1—C11—C10	121.9 (6)

O5—C4—H4A	110.0	N1—C11—C11 ⁱ	115.0 (4)
O5—C4—H4B	110.0	C10—C11—C11 ⁱ	123.1 (4)
Zn1—S1—C1—S2	4.2 (5)	C3—O2—C1—S2	-1.8 (9)
Zn1—S1—C1—O2	-175.3 (4)	C6—O5—C4—C3	-179.0 (6)
Zn1—N1—C7—C8	-172.1 (5)	C7—N1—C11—C10	-0.5 (9)
Zn1—N1—C11—C10	173.2 (5)	C7—N1—C11—C11 ⁱ	179.9 (6)
Zn1—N1—C11—C11 ⁱ	-6.4 (9)	C7—C8—C9—C10	0.7 (10)
O2—C3—C4—O5	73.0 (7)	C8—C9—C10—C11	-0.3 (10)
N1—C7—C8—C9	-0.9 (10)	C9—C10—C11—N1	0.2 (10)
C1—O2—C3—C4	-173.4 (6)	C9—C10—C11—C11 ⁱ	179.8 (7)
C3—O2—C1—S1	177.8 (5)	C11—N1—C7—C8	0.8 (10)

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

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>
C8—H8 \cdots O5 ⁱⁱ	0.95	2.51	3.246 (9)	134
C7—H7 \cdots S2 ⁱ	0.95	2.90	3.552 (7)	127

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