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# (Dimethyl sulfoxide-$\kappa O$)bis(thiosemicarbazide-$\kappa^2 N^1,S$)zinc dipicrate dimethyl sulfoxide solvate monohydrate

**R. Shanthakumari,[a]* Ramu Hema,[b] K. Ramamurthy,[c] Balasubramnian Sridar[d] and Helen Stoeckli-Evans[e]***

[a]Department of Physics, Government Arts College for Women, Pudukottai 622 001, Tamil Nadu, India, [b]Department of Physics, Seethalakshmi Ramaswami College (Autonomous), Tiruchirappalli 620 002, India, [c]Crystal Growth and Thin Film Laboratory, School of Physics, Bharathidasan University, Tiruchirapalli 620 024, India, [d]Laboratory of Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, and [e]Institute of Physics, University of Neuchâtel, Rue Emile-Argand 11, CH-2000, Neuchâtel, Switzerland
Correspondence e-mail: santhasrinthi@yahoo.co.in, helen.stoeckli-evans@unine.ch

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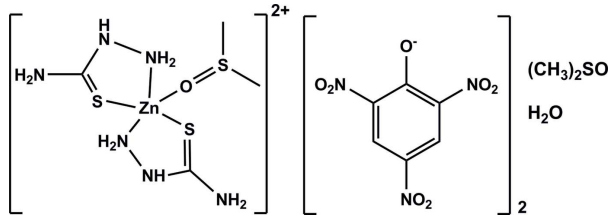
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.034; $wR$ factor = 0.095; data-to-parameter ratio = 14.1.

The title complex, $[Zn(CH_5N_3S)_2(C_2H_6OS)](C_6H_2N_3O_7)_2\cdot C_2H_6OS\cdot H_2O$, is composed of a $[Zn(thiosemicarbazide)_2(DMSO)]^{2+}$ cation (where DMSO is dimethyl sulfoxide), and two picrate anions. In the asymmetric unit, there is also a solvent molecule of DMSO and a water molecule of crystallization. In the cation, the $Zn^{II}$ atom is five-coordinated in a distorted square–pyramidal geometry. It coordinates to the O atom of a DMSO molecule and to the S and one N atom of two thiosemicarbazide molecules, which behave as bidentate ligands coordinating in a *trans* arrangement. In the crystal, a number of N—H···O, O—H···O and N—H···S hydrogen bonds link the molecules into two-dimensional networks. These networks are further linked *via* weak C—H···O interactions, forming a three-dimensional arrangement. Positional disorder in one methyl group of the coordinated DMSO molecule and in the two picrate anions was observed.

## Related literature

For the biological activity of thiosemicarbazides, see: Gowda & Mahadevappa (1977); Pillai *et al.* (1977). For the use of thiosemicarbazide as a masking agent, see: Kirkbright & Taddia (1978). For the crystal structure of a similar five-coordinate zinc(II)–thiosemicarbazide complex, see: Babb *et al.* (2003). For a description of five-coordinate metal atoms, see: Addison *et al.* (1984).




## Experimental

### Crystal data

$[Zn(CH_5N_3S)_2(C_2H_6OS)](C_6H_2N_3O_7)_2\cdot C_2H_6OS\cdot H_2O$
$M_r$ = 878.13
Triclinic, $P\overline{1}$
$a$ = 10.8762 (11) Å
$b$ = 11.2559 (12) Å
$c$ = 14.4859 (15) Å
$\alpha$ = 81.124 (2)°
$\beta$ = 77.063 (2)°
$\gamma$ = 81.168 (2)°
$V$ = 1694.6 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.06 mm$^{-1}$
$T$ = 294 K
0.24 × 0.24 × 0.20 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
18781 measured reflections
7719 independent reflections
6573 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
$S$ = 1.05
7719 reflections
546 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*NA*···O1*W*$^{i}$ | 0.87 (2) | 2.20 (2) | 2.974 (3) | 148 (2) |
| N2—H*N2*···O15*A*$^{i}$ | 0.80 (2) | 2.41 (3) | 3.01 (2) | 133 (2) |
| N2—H*N2*···O16$^{i}$ | 0.80 (2) | 1.96 (2) | 2.693 (2) | 152 (2) |
| N3—H3*NA*···O10$^{i}$ | 0.87 (3) | 2.44 (3) | 3.166 (2) | 141 (2) |
| N3—H3*NA*···O16$^{i}$ | 0.87 (3) | 2.03 (3) | 2.790 (3) | 146 (3) |
| N3—H3*NB*···O5$^{ii}$ | 0.77 (2) | 2.24 (2) | 3.004 (3) | 173 (2) |
| N5—H5*N*···O7$^{iii}$ | 0.84 (2) | 2.37 (2) | 3.007 (3) | 133 (2) |
| N5—H5*N*···O9*A*$^{iii}$ | 0.84 (2) | 1.94 (3) | 2.698 (17) | 150 (2) |
| N4—H4*NA*···O2$^{iii}$ | 0.88 (2) | 2.20 (2) | 2.933 (3) | 141 (2) |
| N4—H4*NB*···S1$^{iv}$ | 0.84 (3) | 2.63 (3) | 3.457 (2) | 170 (2) |
| N6—H6*NA*···O6$^{iii}$ | 0.82 (3) | 2.41 (3) | 3.081 (3) | 140 (2) |
| N6—H6*NA*···O9*A*$^{iii}$ | 0.82 (3) | 2.05 (5) | 2.76 (3) | 145 (3) |
| N6—H6*NB*···O11$^{v}$ | 0.82 (3) | 2.22 (3) | 3.034 (3) | 172 (3) |
| O1*W*—H1*WA*···O8 | 0.819 (19) | 2.27 (2) | 3.059 (3) | 163 (3) |
| O1*W*—H1*WB*···O2 | 0.80 (2) | 2.02 (2) | 2.806 (3) | 171 (3) |
| C6—H6*B*···O2$^{iii}$ | 0.96 | 2.52 | 3.347 (3) | 145 |
| C8—H8···O4$^{vi}$ | 0.93 | 2.47 | 3.390 (3) | 168 |
| C4*A*—H4*A*2···O1*W* | 0.96 | 2.48 | 3.430 (7) | 170 |

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -y+1, -z$; (iii) $-x, -y+1, -z+1$; (iv) $-x, -y, -z+1$; (v) $x, y-1, z+1$; (vi) $-x+1, -y+1, -z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2775).

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# supporting information

*Acta Cryst.* (2011). E**67**, m133–m134 [doi:10.1107/S160053681005378X]

# (Dimethyl sulfoxide-$\kappa O$)bis(thiosemicarbazide-$\kappa^2 N^1,S$)zinc dipicrate dimethyl sulfoxide solvate monohydrate

**R. Shanthakumari, Ramu Hema, K. Ramamurthy, Balasubramnian Sridar and Helen Stoeckli-Evans**

## S1. Comment

Thosemicarbazide, a well known chelating agent, is used to characterize aldehydes, ketones, and polysaccharides. Some thiosemicarbazide derivatives are potential anti-tumor, anti-hypertensive agents, and are active against influenza, protozoa and smallpox (Gowda & Mahadevappa, 1977; Pillai *et al.*, 1977). Thiosemicarbazide is also used as a masking agent to minimize interference from metals such as copper, nickel and platinum in the determination of arsenic by atomic absorption methods (Kirkbright & Taddia, 1978). The conformational preferences of thiosemicarbazide in metal-complex formation are therefore of some interest. The reaction of zinc chloride with thiosemicarbazide in the presence of picric acid gave a yellow powder that was recrystallized using DMSO. This lead to the formation of yellow crystals of the title compoud, a DMSO-water solvate.

The molecular structure of the title complex is illustrated in Fig. 1. In the cation $[Zn(thiosemicarbazide)_2(DMSO)]^{2+}$ the thiosemicarbazide ligands coordinate in a bidentate mode, bonding to atom Zn1 through atoms S1, N1 and S2, N4, in a *trans* arrangment. Atom Zn1 is also coordinated to a DMSO molecule through the O-atom, O1. The zinc atom has a distorted square pyramidal coordination sphere with a $\tau$ value of 0.17 [$\tau$ = 0 for square pyramidal, $\tau$ = 1 for trigonal bipyramidal; Addison *et al.*, 1984]. The bond distances are comparable to those in a related penta-coordinated complex, (Citraconato-*O*)-bis(thiosemicarbazide-N,*S*)-zinc(II) monohydrate (Babb *et al.*, 2003). Interestingly, here the thiosemicarbazide ligands are in a *cis* disposition, and the zinc coordination sphere has a $\tau$ value of 0.72, hence it can be described as a distorted trigonal bipyramid.

In the crystal a sheet-like network is formed, propagating in the *ac*-plane, as a result of a number of intermolecular N—H···O, O—H···O and N—H···S hydrogen bonds. These sheets are then linked *via* weak C—H···O interactions to form a three-dimensional arrangement (Table 1 and Fig. 2).

## S2. Experimental

A mixture of supersaturated solutions of thiosemicarbazide, picric acid and zinc chloride were added in the molar ratio of 1:1:1 (0.9 g: 2.5 g: 2.8 g). The calculated amount of thiosemicarbazide and zinc chloride were dissolved in distilled water and picric acid dissolved in acetone was added. Within a few minutes, the solution became turbid. The reaction was ensured with continuous stirring and after 1 h a yellow product was deposited at the bottom of the beaker, it was filtered off and dried. This yellow solid was recrystallized from DMSO to afford yellow block-like crystals of the title compound (yield: 4 g, 66.6%)

### S3. Refinement

There is a certain positional disorder in one of the methyl groups of the coordinated DMSO molecule, and in the two picrate anions. Methyl C4 was refined with occupanices of C4A/C4B = 0.5/0.5, with C—S distance restraints of 1.76 (2) Å and their ADP's were made equal to those of atom C3. O-atom O9 in one of the picrate anions was refined with occupancies of O9A/O9B = 0.56 (8)/0.44 (8), while O-atoms O14 and O15 of a $NO_2$ group in the second picrate anion where refined with occupancies of O14A/O14B = O15A/O15B = 0.67 (3)/0.33 (7). There is a short O13···O13$^{i}$ contact involving a $NO_2$ O-atom [symmetry code (i) = -*x* + 2, -*y* + 1, -*z*]. This contact was refined with a distance restraint of 2.95 (3) Å. The $NH_2$ and NH H atoms were located in difference electron density maps and were freely refined. The water molecule H-atoms could also be located in a difference electron density map and were refined with distance restraints of 0.84 (2) Å. The C-bound H atoms were included in calculated positions and treated as riding atoms; C—H = 0.93 and 0.96 Å for CH and methyl H-atoms, respectively, with $U_{iso}$(H) = k ×$U_{eq}$(C), where k =1.5 for methyl H-atoms and k = 1.2 for all other H-atoms.

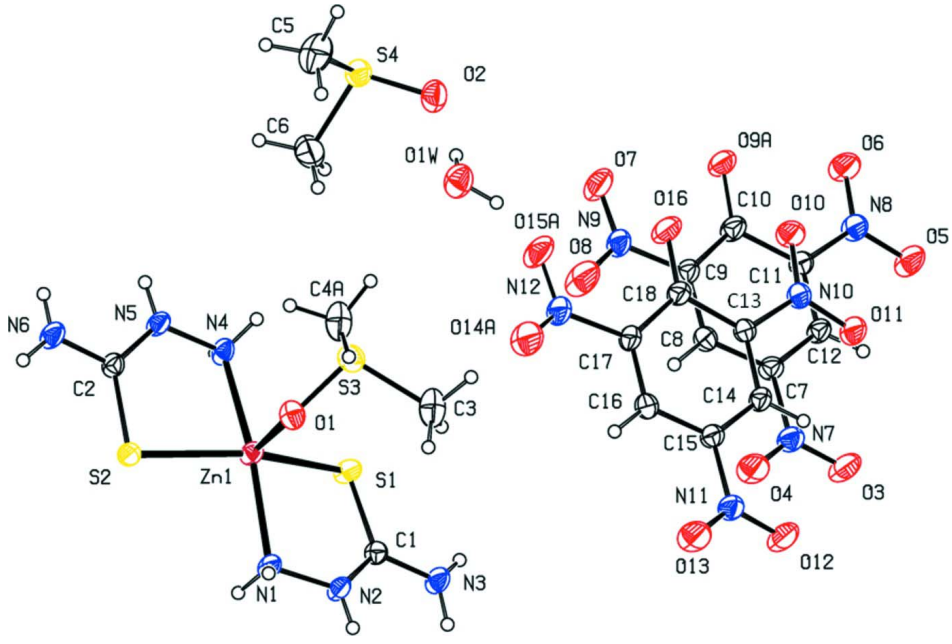


**Figure 1**

View of the asymmetric unit of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Only the principal components of the disordered atoms are shown.

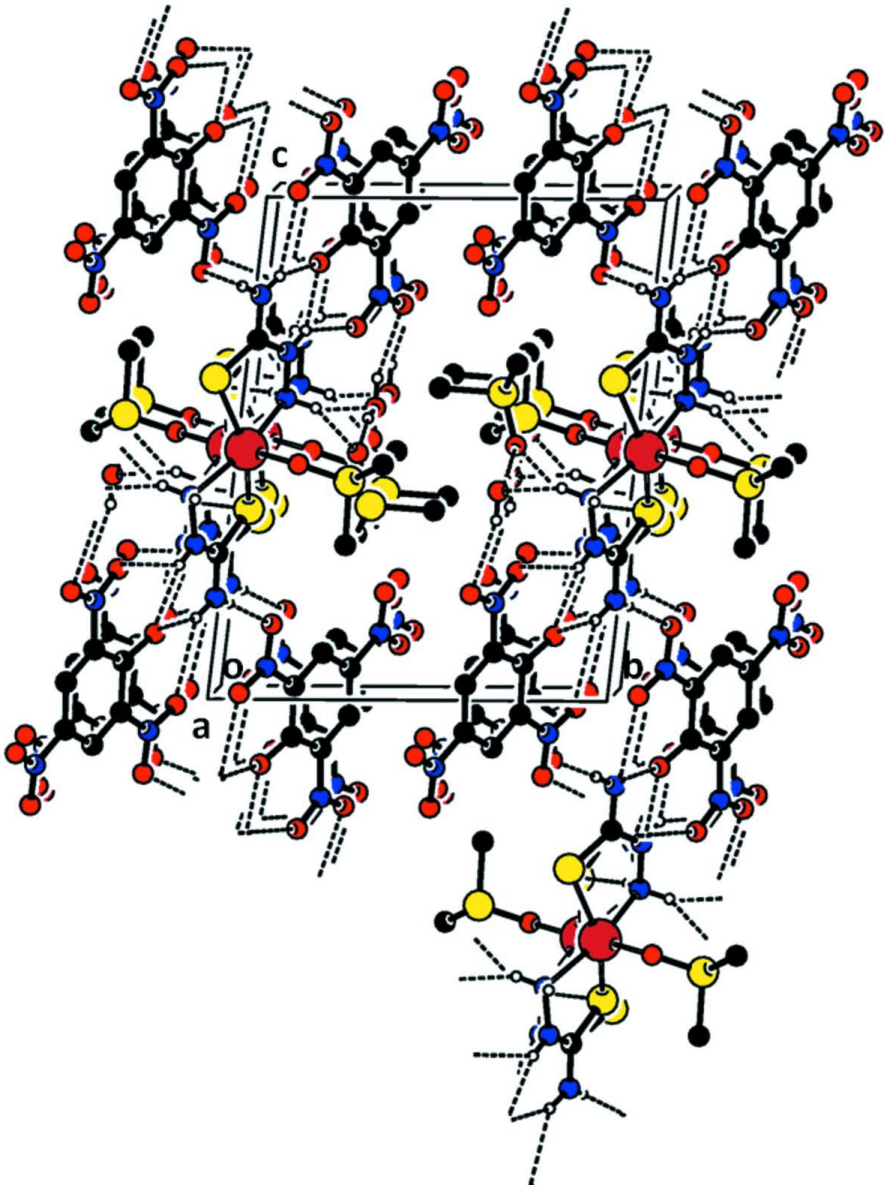


**Figure 2**

A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines [details are given in Table 1; C-bound H-atoms have been omitted for clarity].

**(Dimethyl sulfoxide-*κO*)bis(thiosemicarbazide-$\kappa^2N^1,S$)zinc dipicrate dimethyl sulfoxide solvate monohydrate**

*Crystal data*

$[Zn(CH_5N_3S)_2(C_2H_6OS)]$
$(C_6H_2N_3O_7)_2\cdot C_2H_6OS\cdot H_2O$
$M_r = 878.13$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.8762\ (11)$ Å
$b = 11.2559\ (12)$ Å
$c = 14.4859\ (15)$ Å
$\alpha = 81.124\ (2)°$
$\beta = 77.063\ (2)°$
$\gamma = 81.168\ (2)°$
$V = 1694.6\ (3)$ Å$^3$
$Z = 2$
$F(000) = 900$
$D_x = 1.721$ Mg m$^{-3}$
Melting point: 469 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5926 reflections

$\theta$ = 1.9–25.0°
$\mu$ = 1.06 mm$^{-1}$
$T$ = 294 K

Block, yellow
0.24 × 0.24 × 0.20 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
18781 measured reflections
7719 independent reflections

6573 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 28.0°, $\theta_{min}$ = 1.9°
$h$ = −14→13
$k$ = −14→14
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
$S$ = 1.05
7719 reflections
546 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2 + 0.4578P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Zn1 | 0.26667 (2) | 0.03164 (2) | 0.50488 (1) | 0.0319 (1) | |
| S1 | 0.14900 (4) | 0.05204 (5) | 0.38255 (3) | 0.0384 (1) | |
| S2 | 0.32467 (5) | −0.06515 (5) | 0.64778 (3) | 0.0377 (1) | |
| S3 | 0.33061 (5) | 0.30032 (5) | 0.44415 (4) | 0.0427 (2) | |
| O1 | 0.37531 (13) | 0.16931 (13) | 0.47872 (10) | 0.0403 (4) | |
| N1 | 0.39527 (17) | −0.08894 (18) | 0.41352 (11) | 0.0353 (5) | |
| N2 | 0.37816 (15) | −0.06488 (16) | 0.31838 (11) | 0.0356 (5) | |
| N3 | 0.25503 (19) | −0.00172 (19) | 0.20917 (12) | 0.0425 (6) | |
| N4 | 0.10145 (16) | 0.11037 (18) | 0.60253 (11) | 0.0357 (5) | |
| N5 | 0.12502 (16) | 0.10238 (17) | 0.69507 (11) | 0.0392 (5) | |
| N6 | 0.23281 (19) | 0.0216 (2) | 0.81157 (13) | 0.0464 (6) | |
| C1 | 0.26914 (17) | −0.01021 (16) | 0.29808 (13) | 0.0304 (5) | |
| C2 | 0.22014 (17) | 0.02636 (17) | 0.72219 (13) | 0.0323 (5) | |
| C3 | 0.3683 (3) | 0.3103 (3) | 0.31805 (18) | 0.0625 (8) | |

| | | | | | |
|---|---|---|---|---|---|
| C4A | 0.4290 (6) | 0.3825 (6) | 0.4800 (4) | 0.0625 (8) | 0.500 |
| C4B | 0.4667 (6) | 0.3781 (6) | 0.4444 (4) | 0.0625 (8) | 0.500 |
| O10 | 0.37612 (15) | 0.93032 (16) | 0.00119 (11) | 0.0523 (5) | |
| O11 | 0.46364 (16) | 0.86421 (16) | −0.13237 (11) | 0.0530 (5) | |
| O12 | 0.83363 (17) | 0.59567 (19) | −0.17971 (11) | 0.0648 (6) | |
| O13 | 0.95110 (17) | 0.5539 (2) | −0.07638 (13) | 0.0719 (7) | |
| O14A | 0.7817 (12) | 0.655 (3) | 0.2427 (8) | 0.083 (4) | 0.67 (7) |
| O15A | 0.604 (2) | 0.7437 (19) | 0.2841 (6) | 0.074 (3) | 0.67 (7) |
| O16 | 0.48564 (19) | 0.8581 (2) | 0.14820 (12) | 0.0727 (7) | |
| N10 | 0.46168 (16) | 0.86917 (15) | −0.04741 (12) | 0.0373 (5) | |
| N11 | 0.85340 (17) | 0.60065 (17) | −0.10083 (12) | 0.0432 (5) | |
| N12 | 0.6796 (2) | 0.69437 (19) | 0.22324 (13) | 0.0535 (7) | |
| C13 | 0.56306 (18) | 0.79722 (17) | −0.00584 (13) | 0.0335 (5) | |
| C14 | 0.65550 (18) | 0.73364 (17) | −0.06708 (13) | 0.0344 (5) | |
| C15 | 0.75575 (18) | 0.66393 (18) | −0.03405 (13) | 0.0355 (5) | |
| C16 | 0.76483 (19) | 0.65359 (18) | 0.06125 (14) | 0.0384 (6) | |
| C17 | 0.6701 (2) | 0.71427 (19) | 0.12300 (13) | 0.0386 (6) | |
| C18 | 0.5638 (2) | 0.79503 (19) | 0.09423 (14) | 0.0393 (6) | |
| O15B | 0.575 (3) | 0.709 (4) | 0.2800 (14) | 0.070 (5) | 0.33 (7) |
| O14B | 0.759 (4) | 0.607 (4) | 0.2468 (12) | 0.076 (5) | 0.33 (7) |
| O3 | 0.35471 (17) | 0.59850 (19) | −0.20375 (12) | 0.0616 (6) | |
| O4 | 0.47002 (16) | 0.55050 (18) | −0.09782 (13) | 0.0644 (6) | |
| O5 | −0.02160 (17) | 0.8604 (2) | −0.15007 (12) | 0.0684 (7) | |
| O6 | −0.10969 (17) | 0.91940 (19) | −0.01512 (12) | 0.0648 (6) | |
| O7 | 0.12595 (19) | 0.7413 (2) | 0.26100 (12) | 0.0690 (7) | |
| O8 | 0.3023 (2) | 0.6364 (2) | 0.22031 (14) | 0.0917 (9) | |
| O9A | 0.002 (3) | 0.849 (3) | 0.1297 (7) | 0.059 (4) | 0.56 (8) |
| N7 | 0.37299 (16) | 0.59932 (17) | −0.12325 (12) | 0.0422 (5) | |
| N8 | −0.02350 (16) | 0.86148 (17) | −0.06498 (12) | 0.0432 (6) | |
| N9 | 0.20614 (17) | 0.69458 (17) | 0.20037 (12) | 0.0417 (5) | |
| C7 | 0.27455 (18) | 0.66079 (18) | −0.05566 (13) | 0.0349 (5) | |
| C8 | 0.28479 (17) | 0.64976 (17) | 0.03925 (14) | 0.0352 (5) | |
| C9 | 0.19018 (18) | 0.70787 (18) | 0.10207 (13) | 0.0356 (6) | |
| C10 | 0.0773 (2) | 0.7806 (2) | 0.07608 (14) | 0.0434 (6) | |
| C11 | 0.07928 (18) | 0.78936 (18) | −0.02508 (14) | 0.0367 (6) | |
| C12 | 0.17383 (18) | 0.73076 (18) | −0.08814 (13) | 0.0355 (5) | |
| O9B | −0.0239 (12) | 0.803 (4) | 0.1378 (10) | 0.047 (3) | 0.44 (8) |
| S4 | −0.00366 (5) | 0.64929 (5) | 0.61310 (4) | 0.0427 (2) | |
| O2 | 0.03790 (16) | 0.69781 (16) | 0.50943 (11) | 0.0524 (5) | |
| C5 | 0.1098 (3) | 0.6799 (3) | 0.6734 (2) | 0.0726 (11) | |
| C6 | 0.0343 (4) | 0.4902 (2) | 0.6228 (2) | 0.0740 (12) | |
| O1W | 0.29788 (19) | 0.67515 (18) | 0.42553 (14) | 0.0576 (6) | |
| H1NA | 0.385 (2) | −0.164 (2) | 0.4348 (18) | 0.049 (7)* | |
| H1NB | 0.465 (3) | −0.076 (2) | 0.4097 (15) | 0.047 (7)* | |
| HN2 | 0.429 (2) | −0.097 (2) | 0.2780 (15) | 0.039 (6)* | |
| H3A | 0.45390 | 0.27340 | 0.29780 | 0.0940* | |
| H3B | 0.36070 | 0.39390 | 0.29120 | 0.0940* | |
| H3C | 0.31090 | 0.26890 | 0.29680 | 0.0940* | |

| | | | | | |
|---|---|---|---|---|---|
| H3NA | 0.312 (3) | −0.043 (2) | 0.1701 (19) | 0.053 (7)* | |
| H3NB | 0.192 (2) | 0.030 (2) | 0.1965 (17) | 0.041 (6)* | |
| H5N | 0.074 (2) | 0.139 (2) | 0.7368 (16) | 0.037 (6)* | |
| H4NA | 0.080 (2) | 0.187 (2) | 0.5829 (18) | 0.050 (7)* | |
| H4NB | 0.035 (3) | 0.077 (2) | 0.6116 (18) | 0.050 (7)* | |
| H6NA | 0.179 (3) | 0.061 (2) | 0.8477 (19) | 0.054 (7)* | |
| H6NB | 0.290 (3) | −0.026 (2) | 0.8302 (18) | 0.050 (7)* | |
| H4B1 | 0.47740 | 0.37480 | 0.50880 | 0.0940* | 0.500 |
| H4B2 | 0.45180 | 0.46110 | 0.41740 | 0.0940* | 0.500 |
| H4B3 | 0.54210 | 0.33900 | 0.40720 | 0.0940* | 0.500 |
| H4A1 | 0.42610 | 0.36100 | 0.54720 | 0.0940* | 0.500 |
| H4A2 | 0.40120 | 0.46750 | 0.46740 | 0.0940* | 0.500 |
| H4A3 | 0.51460 | 0.36480 | 0.44540 | 0.0940* | 0.500 |
| H16 | 0.83350 | 0.60660 | 0.08270 | 0.0460* | |
| H14 | 0.65030 | 0.73770 | −0.13070 | 0.0410* | |
| H8 | 0.35460 | 0.60380 | 0.05970 | 0.0420* | |
| H12 | 0.16980 | 0.73830 | −0.15230 | 0.0430* | |
| H5A | 0.10470 | 0.76580 | 0.67340 | 0.1090* | |
| H5B | 0.19340 | 0.64940 | 0.64160 | 0.1090* | |
| H5C | 0.09310 | 0.64110 | 0.73800 | 0.1090* | |
| H6A | 0.12030 | 0.47020 | 0.58990 | 0.1110* | |
| H6B | −0.02230 | 0.45630 | 0.59490 | 0.1110* | |
| H6C | 0.02570 | 0.45780 | 0.68890 | 0.1110* | |
| H1WA | 0.305 (3) | 0.679 (3) | 0.3677 (13) | 0.079 (10)* | |
| H1WB | 0.2231 (18) | 0.688 (3) | 0.445 (2) | 0.079 (11)* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0304 (1) | 0.0402 (1) | 0.0272 (1) | −0.0032 (1) | −0.0084 (1) | −0.0087 (1) |
| S1 | 0.0272 (2) | 0.0551 (3) | 0.0363 (2) | 0.0046 (2) | −0.0122 (2) | −0.0176 (2) |
| S2 | 0.0387 (2) | 0.0412 (3) | 0.0309 (2) | 0.0088 (2) | −0.0099 (2) | −0.0067 (2) |
| S3 | 0.0398 (3) | 0.0435 (3) | 0.0471 (3) | 0.0000 (2) | −0.0169 (2) | −0.0063 (2) |
| O1 | 0.0408 (7) | 0.0413 (7) | 0.0431 (8) | −0.0097 (6) | −0.0171 (6) | −0.0016 (6) |
| N1 | 0.0323 (9) | 0.0488 (10) | 0.0277 (8) | 0.0042 (7) | −0.0144 (6) | −0.0107 (7) |
| N2 | 0.0304 (8) | 0.0515 (10) | 0.0240 (7) | 0.0058 (7) | −0.0072 (6) | −0.0102 (7) |
| N3 | 0.0393 (10) | 0.0588 (11) | 0.0301 (8) | 0.0083 (8) | −0.0152 (8) | −0.0103 (8) |
| N4 | 0.0290 (8) | 0.0517 (10) | 0.0263 (8) | 0.0013 (7) | −0.0105 (6) | −0.0038 (7) |
| N5 | 0.0348 (9) | 0.0560 (10) | 0.0254 (8) | 0.0115 (8) | −0.0103 (7) | −0.0117 (7) |
| N6 | 0.0416 (10) | 0.0673 (13) | 0.0288 (8) | 0.0150 (9) | −0.0145 (8) | −0.0121 (8) |
| C1 | 0.0297 (8) | 0.0333 (9) | 0.0305 (8) | −0.0034 (7) | −0.0099 (7) | −0.0060 (7) |
| C2 | 0.0287 (8) | 0.0398 (10) | 0.0285 (9) | −0.0011 (7) | −0.0083 (7) | −0.0039 (7) |
| C3 | 0.0726 (16) | 0.0699 (13) | 0.0501 (13) | −0.0240 (12) | −0.0251 (11) | 0.0108 (11) |
| C4A | 0.0726 (16) | 0.0699 (13) | 0.0501 (13) | −0.0240 (12) | −0.0251 (11) | 0.0108 (11) |
| C4B | 0.0726 (16) | 0.0699 (13) | 0.0501 (13) | −0.0240 (12) | −0.0251 (11) | 0.0108 (11) |
| O10 | 0.0416 (8) | 0.0646 (10) | 0.0461 (9) | 0.0187 (7) | −0.0124 (7) | −0.0132 (7) |
| O11 | 0.0544 (9) | 0.0681 (11) | 0.0376 (8) | 0.0168 (8) | −0.0242 (7) | −0.0121 (7) |
| O12 | 0.0578 (10) | 0.0959 (14) | 0.0380 (9) | 0.0225 (10) | −0.0137 (7) | −0.0260 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O13 | 0.0516 (10) | 0.0996 (15) | 0.0582 (11) | 0.0363 (10) | −0.0204 (8) | −0.0229 (10) |
| O14A | 0.088 (4) | 0.106 (10) | 0.058 (3) | 0.038 (5) | −0.046 (2) | −0.023 (4) |
| O15A | 0.078 (5) | 0.108 (6) | 0.035 (2) | 0.028 (4) | −0.027 (3) | −0.026 (3) |
| O16 | 0.0752 (12) | 0.0983 (15) | 0.0355 (8) | 0.0452 (11) | −0.0187 (8) | −0.0257 (9) |
| N10 | 0.0357 (8) | 0.0421 (9) | 0.0349 (8) | 0.0023 (7) | −0.0136 (7) | −0.0050 (7) |
| N11 | 0.0393 (9) | 0.0509 (10) | 0.0361 (9) | 0.0071 (8) | −0.0073 (7) | −0.0084 (7) |
| N12 | 0.0645 (13) | 0.0628 (12) | 0.0340 (9) | 0.0129 (10) | −0.0239 (9) | −0.0088 (8) |
| C13 | 0.0337 (9) | 0.0361 (9) | 0.0312 (9) | 0.0037 (7) | −0.0126 (7) | −0.0048 (7) |
| C14 | 0.0367 (10) | 0.0398 (10) | 0.0275 (8) | −0.0008 (8) | −0.0102 (7) | −0.0056 (7) |
| C15 | 0.0341 (9) | 0.0400 (10) | 0.0318 (9) | 0.0021 (8) | −0.0081 (7) | −0.0076 (7) |
| C16 | 0.0383 (10) | 0.0418 (10) | 0.0364 (10) | 0.0046 (8) | −0.0165 (8) | −0.0050 (8) |
| C17 | 0.0453 (11) | 0.0437 (11) | 0.0279 (9) | 0.0027 (9) | −0.0142 (8) | −0.0058 (8) |
| C18 | 0.0416 (11) | 0.0446 (11) | 0.0305 (9) | 0.0067 (8) | −0.0108 (8) | −0.0084 (8) |
| O15B | 0.066 (7) | 0.122 (12) | 0.021 (4) | 0.010 (8) | −0.012 (4) | −0.019 (5) |
| O14B | 0.106 (11) | 0.075 (11) | 0.039 (4) | 0.041 (9) | −0.036 (5) | −0.008 (5) |
| O3 | 0.0527 (10) | 0.0909 (13) | 0.0397 (9) | 0.0133 (9) | −0.0087 (7) | −0.0270 (8) |
| O4 | 0.0427 (9) | 0.0877 (13) | 0.0552 (10) | 0.0275 (9) | −0.0122 (8) | −0.0176 (9) |
| O5 | 0.0597 (11) | 0.1050 (15) | 0.0401 (9) | 0.0329 (10) | −0.0282 (8) | −0.0239 (9) |
| O6 | 0.0496 (10) | 0.0909 (14) | 0.0490 (9) | 0.0321 (9) | −0.0181 (8) | −0.0228 (9) |
| O7 | 0.0631 (11) | 0.1053 (15) | 0.0325 (8) | 0.0230 (10) | −0.0140 (8) | −0.0171 (9) |
| O8 | 0.0740 (13) | 0.147 (2) | 0.0503 (11) | 0.0524 (14) | −0.0364 (10) | −0.0318 (12) |
| O9A | 0.057 (6) | 0.078 (9) | 0.0335 (19) | 0.029 (6) | −0.012 (2) | −0.018 (3) |
| N7 | 0.0368 (9) | 0.0498 (10) | 0.0376 (9) | 0.0026 (7) | −0.0047 (7) | −0.0104 (7) |
| N8 | 0.0364 (9) | 0.0570 (11) | 0.0379 (9) | 0.0079 (8) | −0.0166 (7) | −0.0116 (8) |
| N9 | 0.0425 (9) | 0.0521 (10) | 0.0323 (8) | 0.0006 (8) | −0.0153 (7) | −0.0064 (7) |
| C7 | 0.0296 (9) | 0.0408 (10) | 0.0336 (9) | 0.0004 (7) | −0.0059 (7) | −0.0085 (7) |
| C8 | 0.0298 (9) | 0.0397 (10) | 0.0359 (9) | 0.0020 (7) | −0.0112 (7) | −0.0040 (8) |
| C9 | 0.0351 (10) | 0.0435 (10) | 0.0294 (9) | −0.0008 (8) | −0.0105 (7) | −0.0065 (7) |
| C10 | 0.0377 (10) | 0.0595 (13) | 0.0321 (10) | 0.0103 (9) | −0.0117 (8) | −0.0127 (9) |
| C11 | 0.0325 (9) | 0.0463 (11) | 0.0328 (9) | 0.0055 (8) | −0.0138 (8) | −0.0092 (8) |
| C12 | 0.0337 (9) | 0.0447 (10) | 0.0295 (9) | −0.0007 (8) | −0.0097 (7) | −0.0088 (8) |
| O9B | 0.037 (3) | 0.069 (9) | 0.033 (3) | 0.011 (4) | −0.007 (2) | −0.020 (4) |
| S4 | 0.0414 (3) | 0.0479 (3) | 0.0403 (3) | −0.0013 (2) | −0.0136 (2) | −0.0069 (2) |
| O2 | 0.0545 (9) | 0.0617 (10) | 0.0409 (8) | −0.0040 (8) | −0.0163 (7) | 0.0005 (7) |
| C5 | 0.083 (2) | 0.093 (2) | 0.0590 (16) | −0.0320 (17) | −0.0335 (15) | −0.0139 (14) |
| C6 | 0.122 (3) | 0.0469 (14) | 0.0635 (16) | −0.0030 (15) | −0.0447 (17) | −0.0084 (12) |
| O1W | 0.0559 (11) | 0.0734 (12) | 0.0472 (10) | −0.0066 (9) | −0.0200 (9) | −0.0065 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—S1 | 2.3728 (5) | N3—H3NB | 0.77 (2) |
| Zn1—S2 | 2.3554 (6) | N4—H4NA | 0.88 (2) |
| Zn1—O1 | 2.0302 (15) | N4—H4NB | 0.84 (3) |
| Zn1—N1 | 2.1662 (19) | N5—H5N | 0.84 (2) |
| Zn1—N4 | 2.1852 (18) | N6—H6NA | 0.82 (3) |
| S1—C1 | 1.7214 (19) | N6—H6NB | 0.82 (3) |
| S2—C2 | 1.718 (2) | N10—C13 | 1.452 (3) |
| S3—O1 | 1.5240 (16) | N11—C15 | 1.446 (3) |

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|---|---|---|---|
| S3—C3 | 1.770 (3) | N12—C17 | 1.459 (3) |
| S3—C4A | 1.724 (7) | N7—C7 | 1.448 (3) |
| S3—C4B | 1.833 (7) | N8—C11 | 1.452 (3) |
| S4—C5 | 1.764 (3) | N9—C9 | 1.455 (3) |
| S4—C6 | 1.766 (2) | C3—H3C | 0.9600 |
| S4—O2 | 1.5088 (17) | C3—H3A | 0.9600 |
| O10—N10 | 1.223 (2) | C3—H3B | 0.9600 |
| O11—N10 | 1.236 (2) | C4A—H4A3 | 0.9600 |
| O12—N11 | 1.220 (2) | C4A—H4A1 | 0.9600 |
| O13—N11 | 1.213 (3) | C4A—H4A2 | 0.9600 |
| O14A—N12 | 1.208 (17) | C4B—H4B3 | 0.9600 |
| O14B—N12 | 1.26 (4) | C4B—H4B2 | 0.9600 |
| O15A—N12 | 1.203 (16) | C4B—H4B1 | 0.9600 |
| O15B—N12 | 1.25 (3) | C13—C14 | 1.373 (3) |
| O16—C18 | 1.235 (3) | C13—C18 | 1.448 (3) |
| O3—N7 | 1.228 (2) | C14—C15 | 1.374 (3) |
| O4—N7 | 1.219 (3) | C15—C16 | 1.392 (3) |
| O5—N8 | 1.230 (2) | C16—C17 | 1.374 (3) |
| O6—N8 | 1.217 (3) | C17—C18 | 1.454 (3) |
| O7—N9 | 1.211 (3) | C14—H14 | 0.9300 |
| O8—N9 | 1.214 (3) | C16—H16 | 0.9300 |
| O9A—C10 | 1.25 (3) | C7—C8 | 1.389 (3) |
| O9B—C10 | 1.272 (19) | C7—C12 | 1.376 (3) |
| O1W—H1WB | 0.80 (2) | C8—C9 | 1.368 (3) |
| O1W—H1WA | 0.819 (19) | C9—C10 | 1.457 (3) |
| N1—N2 | 1.411 (2) | C10—C11 | 1.449 (3) |
| N2—C1 | 1.322 (3) | C11—C12 | 1.373 (3) |
| N3—C1 | 1.318 (3) | C8—H8 | 0.9300 |
| N4—N5 | 1.407 (2) | C12—H12 | 0.9300 |
| N5—C2 | 1.328 (3) | C5—H5B | 0.9600 |
| N6—C2 | 1.325 (3) | C5—H5C | 0.9600 |
| N1—H1NB | 0.78 (3) | C5—H5A | 0.9600 |
| N1—H1NA | 0.87 (2) | C6—H6C | 0.9600 |
| N2—HN2 | 0.80 (2) | C6—H6A | 0.9600 |
| N3—H3NA | 0.87 (3) | C6—H6B | 0.9600 |

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|---|---|---|---|
| S1—Zn1—S2 | 152.59 (2) | S3—C4A—H4A3 | 109.00 |
| S1—Zn1—O1 | 108.71 (4) | C4B—C4A—H4A1 | 137.00 |
| S1—Zn1—N1 | 82.09 (5) | S3—C4A—H4A2 | 110.00 |
| S1—Zn1—N4 | 91.39 (5) | C4B—C4A—H4B2 | 54.00 |
| S2—Zn1—O1 | 98.68 (4) | S3—C4A—H4B1 | 141.00 |
| S2—Zn1—N1 | 95.55 (5) | S3—C4A—H4B2 | 106.00 |
| S2—Zn1—N4 | 82.99 (5) | H4B2—C4A—H4A3 | 71.00 |
| O1—Zn1—N1 | 97.42 (7) | H4A1—C4A—H4A2 | 109.00 |
| O1—Zn1—N4 | 99.60 (7) | H4A1—C4A—H4A3 | 109.00 |
| N1—Zn1—N4 | 162.94 (7) | H4A2—C4A—H4A3 | 109.00 |
| Zn1—S1—C1 | 97.02 (7) | C4B—C4A—H4B1 | 93.00 |
| Zn1—S2—C2 | 96.46 (7) | H4B1—C4A—H4A2 | 109.00 |

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|---|---|---|---|
| O1—S3—C3 | 104.91 (12) | H4B1—C4A—H4A3 | 65.00 |
| O1—S3—C4A | 103.8 (2) | H4B2—C4A—H4A1 | 142.00 |
| O1—S3—C4B | 102.5 (2) | C4B—C4A—H4A2 | 97.00 |
| C3—S3—C4A | 108.6 (2) | H4B1—C4A—H4B2 | 108.00 |
| C3—S3—C4B | 91.3 (2) | S3—C4B—H4B3 | 109.00 |
| C5—S4—C6 | 97.69 (17) | S3—C4B—H4A3 | 136.00 |
| O2—S4—C5 | 106.85 (12) | S3—C4B—H4A2 | 93.00 |
| O2—S4—C6 | 107.24 (12) | H4B2—C4B—H4B3 | 110.00 |
| Zn1—O1—S3 | 124.56 (9) | S3—C4B—H4B1 | 109.00 |
| H1WA—O1W—H1WB | 104 (3) | S3—C4B—H4B2 | 109.00 |
| Zn1—N1—N2 | 112.09 (13) | H4B2—C4B—H4A3 | 112.00 |
| N1—N2—C1 | 121.00 (16) | H4B3—C4B—H4A2 | 150.00 |
| Zn1—N4—N5 | 111.38 (13) | H4A2—C4B—H4A3 | 129.00 |
| N4—N5—C2 | 121.32 (17) | C4A—C4B—H4B2 | 96.00 |
| Zn1—N1—H1NB | 108.9 (16) | C4A—C4B—H4B3 | 152.00 |
| H1NA—N1—H1NB | 112 (2) | C4A—C4B—H4A3 | 120.00 |
| N2—N1—H1NA | 109.0 (16) | H4B1—C4B—H4B2 | 110.00 |
| N2—N1—H1NB | 103.8 (16) | H4B1—C4B—H4B3 | 109.00 |
| Zn1—N1—H1NA | 110.6 (16) | H4B1—C4B—H4A2 | 79.00 |
| C1—N2—HN2 | 118.8 (16) | H4B1—C4B—H4A3 | 71.00 |
| N1—N2—HN2 | 118.9 (16) | N10—C13—C18 | 120.67 (17) |
| C1—N3—H3NB | 118.7 (18) | C14—C13—C18 | 123.49 (18) |
| H3NA—N3—H3NB | 123 (3) | N10—C13—C14 | 115.84 (16) |
| C1—N3—H3NA | 117.8 (19) | C13—C14—C15 | 119.81 (17) |
| Zn1—N4—H4NA | 111.4 (16) | N11—C15—C16 | 119.95 (18) |
| Zn1—N4—H4NB | 116.2 (17) | C14—C15—C16 | 121.52 (18) |
| N5—N4—H4NB | 103.2 (17) | N11—C15—C14 | 118.52 (17) |
| H4NA—N4—H4NB | 106 (2) | C15—C16—C17 | 118.52 (19) |
| N5—N4—H4NA | 108.2 (16) | C16—C17—C18 | 124.12 (18) |
| C2—N5—H5N | 117.6 (15) | N12—C17—C18 | 119.41 (18) |
| N4—N5—H5N | 120.6 (15) | N12—C17—C16 | 116.47 (19) |
| H6NA—N6—H6NB | 122 (3) | C13—C18—C17 | 112.38 (17) |
| C2—N6—H6NA | 119 (2) | O16—C18—C17 | 123.79 (19) |
| C2—N6—H6NB | 119.0 (17) | O16—C18—C13 | 123.8 (2) |
| O10—N10—C13 | 120.59 (16) | C13—C14—H14 | 120.00 |
| O11—N10—C13 | 117.81 (17) | C15—C14—H14 | 120.00 |
| O10—N10—O11 | 121.59 (18) | C15—C16—H16 | 121.00 |
| O12—N11—O13 | 122.5 (2) | C17—C16—H16 | 121.00 |
| O12—N11—C15 | 118.43 (19) | N7—C7—C12 | 118.57 (16) |
| O13—N11—C15 | 119.08 (17) | C8—C7—C12 | 121.73 (18) |
| O14B—N12—C17 | 116.3 (10) | N7—C7—C8 | 119.69 (18) |
| O15B—N12—C17 | 113.9 (12) | C7—C8—C9 | 118.72 (18) |
| O14A—N12—O15A | 115.6 (12) | C8—C9—C10 | 124.08 (17) |
| O14B—N12—O15B | 117 (2) | N9—C9—C8 | 116.57 (18) |
| O14A—N12—C17 | 118.3 (6) | N9—C9—C10 | 119.35 (17) |
| O15A—N12—C17 | 123.0 (8) | O9A—C10—C11 | 122.6 (10) |
| O3—N7—C7 | 118.38 (18) | C9—C10—C11 | 112.28 (18) |
| O4—N7—C7 | 118.72 (17) | O9B—C10—C9 | 122.0 (11) |

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|---|---|---|---|
| O3—N7—O4 | 122.90 (19) | O9B—C10—C11 | 123.0 (7) |
| O5—N8—C11 | 117.93 (18) | O9A—C10—C9 | 123.3 (12) |
| O6—N8—C11 | 120.77 (17) | C10—C11—C12 | 123.67 (19) |
| O5—N8—O6 | 121.3 (2) | N8—C11—C12 | 116.06 (17) |
| O8—N9—C9 | 118.53 (18) | N8—C11—C10 | 120.26 (18) |
| O7—N9—O8 | 120.53 (19) | C7—C12—C11 | 119.44 (17) |
| O7—N9—C9 | 120.93 (19) | C9—C8—H8 | 121.00 |
| S1—C1—N2 | 122.28 (14) | C7—C8—H8 | 121.00 |
| S1—C1—N3 | 119.89 (16) | C7—C12—H12 | 120.00 |
| N2—C1—N3 | 117.81 (18) | C11—C12—H12 | 120.00 |
| S2—C2—N5 | 123.28 (14) | S4—C5—H5A | 109.00 |
| S2—C2—N6 | 119.36 (16) | S4—C5—H5B | 109.00 |
| N5—C2—N6 | 117.36 (18) | H5A—C5—H5B | 109.00 |
| S3—C4A—C4B | 91.2 (9) | H5A—C5—H5C | 109.00 |
| S3—C4B—C4A | 70.1 (9) | S4—C5—H5C | 109.00 |
| S3—C3—H3C | 109.00 | H5B—C5—H5C | 109.00 |
| S3—C3—H3A | 109.00 | S4—C6—H6B | 109.00 |
| S3—C3—H3B | 109.00 | S4—C6—H6C | 109.00 |
| H3B—C3—H3C | 110.00 | S4—C6—H6A | 109.00 |
| H3A—C3—H3B | 109.00 | H6A—C6—H6C | 109.00 |
| H3A—C3—H3C | 109.00 | H6B—C6—H6C | 110.00 |
| S3—C4A—H4A1 | 109.00 | H6A—C6—H6B | 110.00 |

| | | | |
|---|---|---|---|
| S2—Zn1—S1—C1 | −101.75 (7) | O15A—N12—C17—C18 | −1.3 (13) |
| O1—Zn1—S1—C1 | 80.25 (8) | O4—N7—C7—C8 | −8.4 (3) |
| N1—Zn1—S1—C1 | −14.95 (8) | O3—N7—C7—C8 | 171.5 (2) |
| N4—Zn1—S1—C1 | −179.13 (8) | O3—N7—C7—C12 | −9.7 (3) |
| S1—Zn1—S2—C2 | −94.78 (8) | O4—N7—C7—C12 | 170.5 (2) |
| O1—Zn1—S2—C2 | 83.31 (8) | O6—N8—C11—C10 | 3.1 (3) |
| N1—Zn1—S2—C2 | −178.29 (8) | O5—N8—C11—C10 | −175.7 (2) |
| N4—Zn1—S2—C2 | −15.39 (8) | O5—N8—C11—C12 | 3.3 (3) |
| S1—Zn1—O1—S3 | 41.44 (11) | O6—N8—C11—C12 | −177.9 (2) |
| S2—Zn1—O1—S3 | −137.63 (9) | O7—N9—C9—C10 | 1.3 (3) |
| N1—Zn1—O1—S3 | 125.56 (10) | O7—N9—C9—C8 | −178.8 (2) |
| N4—Zn1—O1—S3 | −53.34 (11) | O8—N9—C9—C8 | 1.9 (3) |
| S1—Zn1—N1—N2 | 21.71 (13) | O8—N9—C9—C10 | −178.1 (2) |
| S2—Zn1—N1—N2 | 174.21 (13) | N10—C13—C14—C15 | 179.42 (18) |
| O1—Zn1—N1—N2 | −86.26 (14) | C14—C13—C18—C17 | −2.4 (3) |
| S1—Zn1—N4—N5 | 172.48 (13) | N10—C13—C18—O16 | −4.8 (3) |
| S2—Zn1—N4—N5 | 19.39 (13) | N10—C13—C18—C17 | 177.75 (18) |
| O1—Zn1—N4—N5 | −78.28 (14) | C18—C13—C14—C15 | −0.4 (3) |
| Zn1—S1—C1—N2 | 9.21 (17) | C14—C13—C18—O16 | 175.0 (2) |
| Zn1—S1—C1—N3 | −169.23 (16) | C13—C14—C15—N11 | −178.34 (18) |
| Zn1—S2—C2—N5 | 13.08 (18) | C13—C14—C15—C16 | 1.5 (3) |
| Zn1—S2—C2—N6 | −167.45 (16) | N11—C15—C16—C17 | −179.62 (19) |
| C3—S3—O1—Zn1 | −89.65 (14) | C14—C15—C16—C17 | 0.5 (3) |
| C4A—S3—O1—Zn1 | 156.5 (2) | C15—C16—C17—N12 | 176.16 (19) |
| C4B—S3—O1—Zn1 | 175.6 (2) | C15—C16—C17—C18 | −3.8 (3) |

| | | | |
|---|---|---|---|
| O1—S3—C4A—C4B | 88.3 (9) | C16—C17—C18—O16 | −172.9 (2) |
| C3—S3—C4A—C4B | −22.9 (10) | C16—C17—C18—C13 | 4.6 (3) |
| O1—S3—C4B—C4A | −96.1 (9) | N12—C17—C18—C13 | −175.37 (19) |
| C3—S3—C4B—C4A | 158.3 (9) | N12—C17—C18—O16 | 7.2 (3) |
| Zn1—N1—N2—C1 | −23.6 (2) | N7—C7—C8—C9 | −179.51 (18) |
| N1—N2—C1—S1 | 8.4 (3) | C12—C7—C8—C9 | 1.7 (3) |
| N1—N2—C1—N3 | −173.14 (19) | N7—C7—C12—C11 | 179.74 (18) |
| Zn1—N4—N5—C2 | −17.8 (2) | C8—C7—C12—C11 | −1.4 (3) |
| N4—N5—C2—S2 | 1.8 (3) | C7—C8—C9—N9 | −179.32 (18) |
| N4—N5—C2—N6 | −177.69 (19) | C7—C8—C9—C10 | 0.6 (3) |
| O10—N10—C13—C14 | −178.90 (18) | N9—C9—C10—O9A | 12.0 (17) |
| O10—N10—C13—C18 | 0.9 (3) | N9—C9—C10—C11 | 177.15 (18) |
| O11—N10—C13—C14 | 2.7 (3) | C8—C9—C10—O9A | −168.0 (17) |
| O11—N10—C13—C18 | −177.51 (19) | C8—C9—C10—C11 | −2.8 (3) |
| O12—N11—C15—C14 | −11.4 (3) | O9A—C10—C11—N8 | −12.7 (18) |
| O12—N11—C15—C16 | 168.7 (2) | O9A—C10—C11—C12 | 168.4 (18) |
| O13—N11—C15—C14 | 169.1 (2) | C9—C10—C11—N8 | −178.05 (18) |
| O13—N11—C15—C16 | −10.8 (3) | C9—C10—C11—C12 | 3.0 (3) |
| O14A—N12—C17—C16 | 19.5 (17) | N8—C11—C12—C7 | 179.91 (18) |
| O14A—N12—C17—C18 | −160.6 (17) | C10—C11—C12—C7 | −1.1 (3) |
| O15A—N12—C17—C16 | 178.7 (12) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*NA*···O1*W*$^{i}$ | 0.87 (2) | 2.20 (2) | 2.974 (3) | 148 (2) |
| N2—H*N*2···O15*A*$^{i}$ | 0.80 (2) | 2.41 (3) | 3.01 (2) | 133 (2) |
| N2—H*N*2···O16$^{i}$ | 0.80 (2) | 1.96 (2) | 2.693 (2) | 152 (2) |
| N3—H3*NA*···O10$^{i}$ | 0.87 (3) | 2.44 (3) | 3.166 (2) | 141 (2) |
| N3—H3*NA*···O16$^{i}$ | 0.87 (3) | 2.03 (3) | 2.790 (3) | 146 (3) |
| N3—H3*NB*···O5$^{ii}$ | 0.77 (2) | 2.24 (2) | 3.004 (3) | 173 (2) |
| N5—H5*N*···O7$^{iii}$ | 0.84 (2) | 2.37 (2) | 3.007 (3) | 133 (2) |
| N5—H5*N*···O9*A*$^{iii}$ | 0.84 (2) | 1.94 (3) | 2.698 (17) | 150 (2) |
| N4—H4*NA*···O2$^{iii}$ | 0.88 (2) | 2.20 (2) | 2.933 (3) | 141 (2) |
| N4—H4*NB*···S1$^{iv}$ | 0.84 (3) | 2.63 (3) | 3.457 (2) | 170 (2) |
| N6—H6*NA*···O6$^{iii}$ | 0.82 (3) | 2.41 (3) | 3.081 (3) | 140 (2) |
| N6—H6*NA*···O9*A*$^{iii}$ | 0.82 (3) | 2.05 (5) | 2.76 (3) | 145 (3) |
| N6—H6*NB*···O11$^{v}$ | 0.82 (3) | 2.22 (3) | 3.034 (3) | 172 (3) |
| O1*W*—H1*WA*···O8 | 0.819 (19) | 2.27 (2) | 3.059 (3) | 163 (3) |
| O1*W*—H1*WB*···O2 | 0.80 (2) | 2.02 (2) | 2.806 (3) | 171 (3) |
| C6—H6*B*···O2$^{iii}$ | 0.96 | 2.52 | 3.347 (3) | 145 |
| C8—H8···O4$^{vi}$ | 0.93 | 2.47 | 3.390 (3) | 168 |
| C12—H12···O5 | 0.93 | 2.31 | 2.636 (3) | 100 |
| C14—H14···O11 | 0.93 | 2.30 | 2.631 (3) | 101 |
| C4*A*—H4*A*2···O1*W* | 0.96 | 2.48 | 3.430 (7) | 170 |

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*, −*y*+1, −*z*; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*, −*y*, −*z*+1; (v) *x*, *y*−1, *z*+1; (vi) −*x*+1, −*y*+1, −*z*.