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# Tetraaqua(5,5′-dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)zinc(II) sulfate

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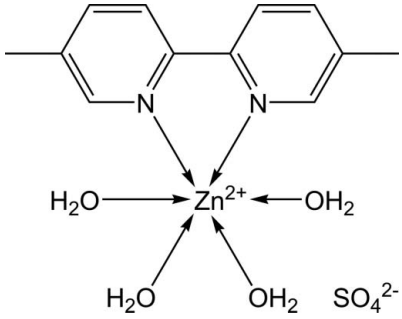
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.037; $wR$ factor = 0.091; data-to-parameter ratio = 14.9.

The asymmetric unit of the title compound, $[Zn(C_{12}H_{12}N_2)(H_2O)_4]SO_4$, consists of a $Zn^{II}$ complex cation, a sulfate anion and four molecules of water coordinated to the $Zn^{II}$ atom. The $Zn^{II}$ complex cation, with approximate twofold symmetry, displays a slightly distorted octahedral geometry around the $Zn^{II}$ atom, which is coordinated by two N atoms from a 5,5′-dimethyl-2,2′-bipyridine ligand and by the O atoms of four water molecules. In the crystal, O—H···O hydrogen bonds help to establish the packing.

## Related literature

For related structures, see: Schubert, Eschbaumer *et al.* (1999); Schubert, Hochwimmer *et al.* (1999); Shi *et al.* (2009); Zhang *et al.* (2009); Momeni *et al.* (2009); Kim *et al.* (2009); Yang *et al.* (2001).




## Experimental

### Crystal data

$[Zn(C_{12}H_{12}N_2)(H_2O)_4]SO_4$
$M_r$ = 417.73
Monoclinic, $P2_1/c$
$a$ = 9.5648 (17) Å
$b$ = 9.6050 (17) Å
$c$ = 18.477 (3) Å
$\beta$ = 102.453 (4)°
$V$ = 1657.5 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.65 mm$^{-1}$
$T$ = 296 K
0.30 × 0.26 × 0.25 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.637, $T_{max}$ = 0.683
9462 measured reflections
3263 independent reflections
2648 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.085

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.091
$S$ = 1.04
3263 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.40 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4$W$—H4$WB$···O6$^{i}$ | 0.85 | 1.84 | 2.695 (3) | 179 |
| O4$W$—H4$WA$···O5 | 0.85 | 1.87 | 2.722 (3) | 178 |
| O3$W$—H3$WB$···O5$^{ii}$ | 0.85 | 1.90 | 2.748 (3) | 178 |
| O3$W$—H3$WA$···O6 | 0.85 | 1.96 | 2.804 (3) | 170 |
| O2$W$—H2$WB$···O8$^{i}$ | 0.85 | 1.99 | 2.831 (3) | 170 |
| O2$W$—H2$WA$···O7$^{iii}$ | 0.85 | 1.92 | 2.766 (3) | 173 |
| O1$W$—H1$WB$···O8$^{iii}$ | 0.85 | 1.87 | 2.717 (3) | 175 |
| O1$W$—H1$WA$···O7$^{ii}$ | 0.85 | 1.93 | 2.772 (3) | 169 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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); 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: PV2173).

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# supporting information

*Acta Cryst.* (2009). E**65**, m866 [doi:10.1107/S160053680902488X]

## Tetraaqua(5,5′-dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)zinc(II) sulfate

**Qing-Lan Zhao and Hui-Feng Bai**

### S1. Comment

As a contribution to structural characterization of 5,5′-dimethyl-2,2′-bipyridine complexes (Schubert, Eschbaumer *et al.* 1999; Schubert, Hochwimmer *et al.* 1999; Yang *et al.*, 2001) we present here the crystal structure of the title complex, $[ZnL(H_2O)_4].SO_4$ (*L* = 5,5′-dimethyl-2,2′-bipyridine).

The molecular structure of the title compound (Fig. 1) is made up of a $[ZnL(H_2O)_4]^{2+}$ cation and a sulfate anion; the cation shows an approximate two fold rotational symmetry. The Zinc atom is coordinated totwo N atoms of a 5,5′-dimethyl-2,2′-bipyridine ligand and four aqua ligands to form distorted octahedral geometry.

With O—H···O and O—H···S hydrogen bonds (Table 1), a three-dimensional network is formed as shown in Fig. 2.

### S2. Experimental

The title compound was synthesized hydrothermally in a Teflon-lined autoclave (25 ml) by heating a mixture of 5,5′-dimethyl-2,2′-bipyridine (0.2 mmol), $ZnSO_4$ (0.2 mmol) and one drop of $Et_3N$ (pH ≃ 8–9) in water (10 ml) at 393 K for 3 d. Crystals suitable for X-ray analysis were obtained.

### S3. Refinement

All H atoms were included in calculated positions, with C—H bond lengths fixed at 0.96 Å (methyl $CH_3$), 0.93Å (aryl group) and O—H = 0.85 Å and were refined in the riding-model approximation. $U_{iso}$(H) values were calculated at 1.5 $U_{eq}$(C) for methyl groups and 1.2 $U_{eq}$(C) otherwise.

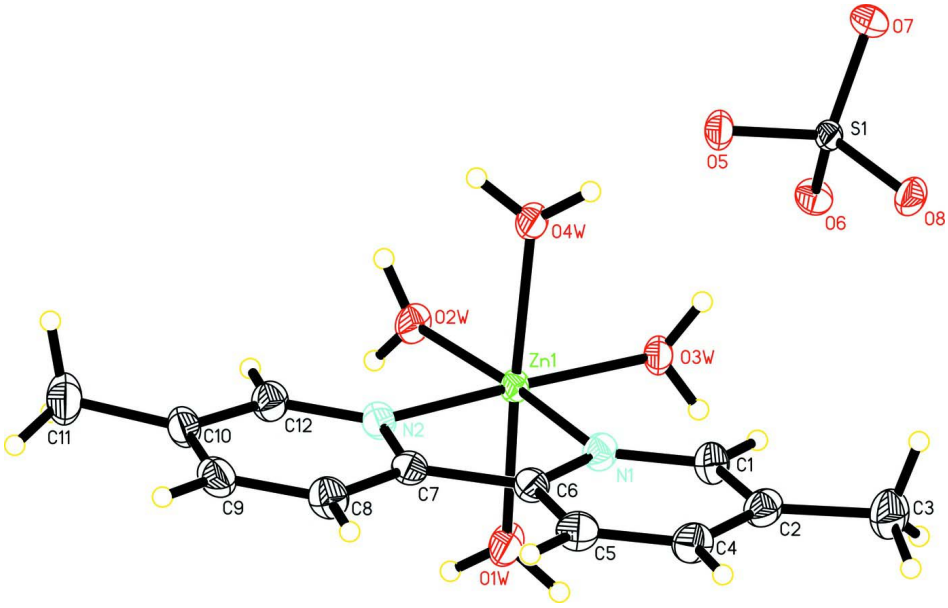


**Figure 1**

The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

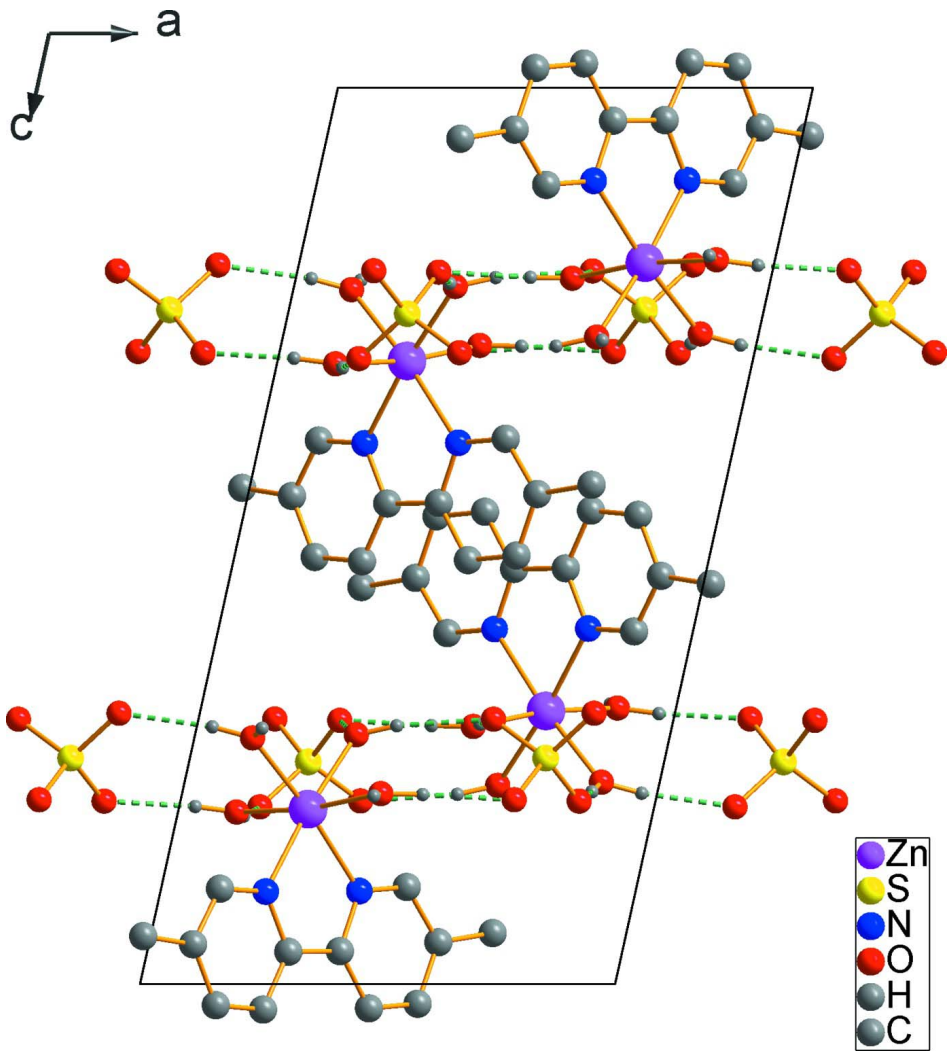


**Figure 2**

Crystal packing of the title complound. Hydrogen-bond interactions are drawn with dashed lines.

**Tetraaqua(5,5′-dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)zinc(II) sulfate**

*Crystal data*

$[Zn(C_{12}H_{12}N_2)(H_2O)_4]SO_4$
$M_r = 417.73$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.5648$ (17) Å
$b = 9.6050$ (17) Å
$c = 18.477$ (3) Å
$\beta = 102.453$ (4)°
$V = 1657.5$ (5) Å$^3$
$Z = 4$
$F(000) = 864$
$D_x = 1.674$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4417 reflections
$\theta = 2.2$–27.9°
$\mu = 1.65$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.30 × 0.26 × 0.25 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.637, $T_{max}$ = 0.683
9462 measured reflections
3263 independent reflections
2648 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.085
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.2°
$h$ = −11→11
$k$ = −11→10
$l$ = −22→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.091
$S$ = 1.04
3263 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.52 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.40 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 | 0.27251 (3) | 0.86942 (3) | 0.804800 (16) | 0.02610 (12) |
| S1 | 0.74896 (6) | 0.86596 (7) | 0.74789 (4) | 0.02499 (17) |
| N1 | 0.4185 (2) | 0.7784 (2) | 0.89612 (12) | 0.0321 (5) |
| N2 | 0.2216 (2) | 0.9768 (2) | 0.89671 (12) | 0.0324 (5) |
| O1W | 0.1234 (2) | 0.7150 (2) | 0.80803 (15) | 0.0632 (7) |
| H1WA | 0.1400 | 0.6281 | 0.8125 | 0.076* |
| H1WB | 0.0336 | 0.7268 | 0.8018 | 0.076* |
| O2W | 0.12257 (18) | 0.9747 (2) | 0.72531 (10) | 0.0378 (5) |
| H2WA | 0.0329 | 0.9606 | 0.7130 | 0.045* |
| H2WB | 0.1381 | 1.0586 | 0.7146 | 0.045* |
| O3W | 0.33946 (19) | 0.7568 (2) | 0.72175 (10) | 0.0347 (5) |
| H3WA | 0.4203 | 0.7743 | 0.7118 | 0.042* |
| H3WB | 0.3264 | 0.6693 | 0.7182 | 0.042* |
| O4W | 0.4183 (2) | 1.0182 (2) | 0.78745 (13) | 0.0486 (6) |
| H4WA | 0.5066 | 1.0052 | 0.7884 | 0.058* |
| H4WB | 0.4049 | 1.1053 | 0.7901 | 0.058* |

| | | | | |
|---|---|---|---|---|
| O5 | 0.70202 (19) | 0.9743 (2) | 0.79426 (10) | 0.0335 (4) |
| O6 | 0.62104 (18) | 0.7951 (2) | 0.70442 (10) | 0.0343 (4) |
| O7 | 0.83003 (19) | 0.9308 (2) | 0.69779 (11) | 0.0359 (5) |
| O8 | 0.83933 (19) | 0.7631 (2) | 0.79580 (10) | 0.0358 (5) |
| C1 | 0.5164 (3) | 0.6810 (3) | 0.89163 (17) | 0.0369 (7) |
| H1A | 0.5233 | 0.6498 | 0.8449 | 0.044* |
| C2 | 0.6085 (3) | 0.6240 (3) | 0.95322 (17) | 0.0379 (7) |
| C3 | 0.7185 (3) | 0.5184 (4) | 0.9430 (2) | 0.0527 (9) |
| H3A | 0.6773 | 0.4559 | 0.9036 | 0.079* |
| H3B | 0.7494 | 0.4667 | 0.9881 | 0.079* |
| H3C | 0.7991 | 0.5652 | 0.9308 | 0.079* |
| C4 | 0.5934 (3) | 0.6713 (3) | 1.02187 (17) | 0.0409 (7) |
| H4A | 0.6511 | 0.6351 | 1.0648 | 0.049* |
| C5 | 0.4932 (3) | 0.7720 (3) | 1.02696 (15) | 0.0393 (7) |
| H5 | 0.4843 | 0.8043 | 1.0732 | 0.047* |
| C6 | 0.4054 (3) | 0.8254 (3) | 0.96315 (15) | 0.0311 (6) |
| C7 | 0.2972 (3) | 0.9349 (3) | 0.96385 (15) | 0.0303 (6) |
| C8 | 0.2708 (3) | 0.9936 (3) | 1.02828 (16) | 0.0399 (7) |
| H8 | 0.3214 | 0.9634 | 1.0743 | 0.048* |
| C9 | 0.1693 (3) | 1.0966 (3) | 1.02349 (18) | 0.0419 (7) |
| H9 | 0.1517 | 1.1360 | 1.0666 | 0.050* |
| C10 | 0.0931 (3) | 1.1423 (3) | 0.95547 (18) | 0.0384 (7) |
| C11 | −0.0155 (4) | 1.2571 (4) | 0.9464 (2) | 0.0544 (9) |
| H11A | −0.0502 | 1.2665 | 0.9911 | 0.082* |
| H11B | −0.0938 | 1.2353 | 0.9060 | 0.082* |
| H11C | 0.0281 | 1.3428 | 0.9362 | 0.082* |
| C12 | 0.1239 (3) | 1.0770 (3) | 0.89353 (17) | 0.0371 (7) |
| H12 | 0.0732 | 1.1048 | 0.8470 | 0.045* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.01825 (17) | 0.02401 (18) | 0.0354 (2) | 0.00040 (12) | 0.00430 (11) | −0.00115 (13) |
| S1 | 0.0161 (3) | 0.0206 (3) | 0.0387 (4) | 0.0001 (2) | 0.0068 (2) | −0.0004 (3) |
| N1 | 0.0287 (12) | 0.0324 (12) | 0.0335 (13) | 0.0039 (10) | 0.0029 (9) | 0.0026 (11) |
| N2 | 0.0292 (12) | 0.0330 (12) | 0.0359 (14) | 0.0003 (10) | 0.0089 (10) | −0.0031 (11) |
| O1W | 0.0231 (11) | 0.0266 (12) | 0.143 (2) | −0.0025 (10) | 0.0252 (12) | −0.0011 (13) |
| O2W | 0.0200 (9) | 0.0340 (11) | 0.0553 (13) | 0.0050 (8) | −0.0006 (8) | 0.0072 (10) |
| O3W | 0.0266 (10) | 0.0263 (10) | 0.0534 (12) | 0.0023 (8) | 0.0134 (8) | −0.0075 (9) |
| O4W | 0.0229 (10) | 0.0246 (10) | 0.1025 (18) | −0.0007 (9) | 0.0230 (10) | 0.0024 (11) |
| O5 | 0.0294 (10) | 0.0277 (10) | 0.0452 (12) | 0.0053 (8) | 0.0116 (8) | −0.0061 (9) |
| O6 | 0.0203 (9) | 0.0336 (11) | 0.0478 (12) | −0.0079 (8) | 0.0050 (8) | −0.0051 (9) |
| O7 | 0.0282 (10) | 0.0343 (11) | 0.0480 (12) | −0.0060 (9) | 0.0148 (8) | 0.0016 (9) |
| O8 | 0.0270 (10) | 0.0270 (10) | 0.0522 (13) | 0.0076 (8) | 0.0058 (8) | 0.0053 (9) |
| C1 | 0.0317 (15) | 0.0394 (16) | 0.0392 (17) | 0.0061 (13) | 0.0064 (12) | −0.0003 (14) |
| C2 | 0.0318 (15) | 0.0325 (16) | 0.0469 (19) | −0.0001 (13) | 0.0033 (12) | 0.0034 (14) |
| C3 | 0.0392 (18) | 0.052 (2) | 0.064 (2) | 0.0148 (16) | 0.0058 (14) | 0.0063 (18) |
| C4 | 0.0316 (16) | 0.0439 (17) | 0.0438 (19) | 0.0053 (14) | 0.0006 (12) | 0.0127 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0425 (17) | 0.0427 (17) | 0.0320 (17) | −0.0004 (15) | 0.0062 (12) | 0.0031 (14) |
| C6 | 0.0264 (14) | 0.0307 (14) | 0.0361 (16) | −0.0012 (12) | 0.0065 (11) | 0.0012 (13) |
| C7 | 0.0261 (14) | 0.0304 (14) | 0.0340 (16) | −0.0036 (12) | 0.0057 (11) | −0.0008 (12) |
| C8 | 0.0412 (17) | 0.0450 (18) | 0.0337 (18) | 0.0020 (15) | 0.0083 (13) | −0.0008 (14) |
| C9 | 0.0440 (18) | 0.0430 (17) | 0.0437 (19) | −0.0030 (15) | 0.0205 (14) | −0.0076 (15) |
| C10 | 0.0296 (15) | 0.0363 (16) | 0.0520 (19) | 0.0004 (13) | 0.0149 (13) | −0.0077 (14) |
| C11 | 0.049 (2) | 0.049 (2) | 0.068 (2) | 0.0133 (17) | 0.0188 (16) | −0.0089 (17) |
| C12 | 0.0306 (15) | 0.0380 (16) | 0.0417 (17) | 0.0036 (13) | 0.0053 (12) | 0.0017 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—O1W | 2.068 (2) | C1—H1A | 0.9300 |
| Zn1—O4W | 2.0693 (19) | C2—C4 | 1.384 (4) |
| Zn1—O2W | 2.0806 (18) | C2—C3 | 1.502 (4) |
| Zn1—O3W | 2.0880 (17) | C3—H3A | 0.9600 |
| Zn1—N2 | 2.131 (2) | C3—H3B | 0.9600 |
| Zn1—N1 | 2.132 (2) | C3—H3C | 0.9600 |
| S1—O7 | 1.4682 (19) | C4—C5 | 1.379 (4) |
| S1—O8 | 1.4756 (19) | C4—H4A | 0.9300 |
| S1—O6 | 1.4772 (19) | C5—C6 | 1.389 (4) |
| S1—O5 | 1.4779 (19) | C5—H5 | 0.9300 |
| N1—C1 | 1.339 (3) | C6—C7 | 1.477 (4) |
| N1—C6 | 1.349 (3) | C7—C8 | 1.388 (4) |
| N2—C12 | 1.334 (4) | C8—C9 | 1.376 (4) |
| N2—C7 | 1.355 (3) | C8—H8 | 0.9300 |
| O1W—H1WA | 0.8496 | C9—C10 | 1.381 (4) |
| O1W—H1WB | 0.8495 | C9—H9 | 0.9300 |
| O2W—H2WA | 0.8497 | C10—C12 | 1.392 (4) |
| O2W—H2WB | 0.8497 | C10—C11 | 1.499 (4) |
| O3W—H3WA | 0.8497 | C11—H11A | 0.9600 |
| O3W—H3WB | 0.8498 | C11—H11B | 0.9600 |
| O4W—H4WA | 0.8498 | C11—H11C | 0.9600 |
| O4W—H4WB | 0.8499 | C12—H12 | 0.9300 |
| C1—C2 | 1.392 (4) | | |
| | | | |
| O1W—Zn1—O4W | 172.74 (10) | C2—C1—H1A | 118.3 |
| O1W—Zn1—O2W | 89.68 (9) | C4—C2—C1 | 116.5 (3) |
| O4W—Zn1—O2W | 86.56 (8) | C4—C2—C3 | 123.5 (3) |
| O1W—Zn1—O3W | 88.40 (9) | C1—C2—C3 | 120.0 (3) |
| O4W—Zn1—O3W | 85.42 (8) | C2—C3—H3A | 109.5 |
| O2W—Zn1—O3W | 90.41 (8) | C2—C3—H3B | 109.5 |
| O1W—Zn1—N2 | 92.68 (9) | H3A—C3—H3B | 109.5 |
| O4W—Zn1—N2 | 93.82 (9) | C2—C3—H3C | 109.5 |
| O2W—Zn1—N2 | 94.95 (8) | H3A—C3—H3C | 109.5 |
| O3W—Zn1—N2 | 174.54 (8) | H3B—C3—H3C | 109.5 |
| O1W—Zn1—N1 | 91.22 (10) | C5—C4—C2 | 120.3 (3) |
| O4W—Zn1—N1 | 93.29 (9) | C5—C4—H4A | 119.9 |
| O2W—Zn1—N1 | 172.85 (8) | C2—C4—H4A | 119.9 |

| | | | |
|---|---|---|---|
| O3W—Zn1—N1 | 96.70 (8) | C4—C5—C6 | 120.2 (3) |
| N2—Zn1—N1 | 77.93 (9) | C4—C5—H5 | 119.9 |
| O7—S1—O8 | 109.97 (11) | C6—C5—H5 | 119.9 |
| O7—S1—O6 | 109.92 (12) | N1—C6—C5 | 119.8 (3) |
| O8—S1—O6 | 109.07 (11) | N1—C6—C7 | 116.8 (2) |
| O7—S1—O5 | 109.56 (11) | C5—C6—C7 | 123.5 (3) |
| O8—S1—O5 | 109.62 (11) | N2—C7—C8 | 120.3 (3) |
| O6—S1—O5 | 108.68 (11) | N2—C7—C6 | 116.1 (2) |
| C1—N1—C6 | 119.7 (2) | C8—C7—C6 | 123.6 (3) |
| C1—N1—Zn1 | 125.80 (19) | C9—C8—C7 | 119.5 (3) |
| C6—N1—Zn1 | 114.48 (17) | C9—C8—H8 | 120.2 |
| C12—N2—C7 | 119.0 (2) | C7—C8—H8 | 120.2 |
| C12—N2—Zn1 | 126.3 (2) | C8—C9—C10 | 120.9 (3) |
| C7—N2—Zn1 | 114.67 (18) | C8—C9—H9 | 119.5 |
| Zn1—O1W—H1WA | 126.3 | C10—C9—H9 | 119.5 |
| Zn1—O1W—H1WB | 125.8 | C9—C10—C12 | 116.2 (3) |
| H1WA—O1W—H1WB | 107.8 | C9—C10—C11 | 123.6 (3) |
| Zn1—O2W—H2WA | 127.8 | C12—C10—C11 | 120.3 (3) |
| Zn1—O2W—H2WB | 119.8 | C10—C11—H11A | 109.5 |
| H2WA—O2W—H2WB | 107.8 | C10—C11—H11B | 109.5 |
| Zn1—O3W—H3WA | 119.6 | H11A—C11—H11B | 109.5 |
| Zn1—O3W—H3WB | 120.4 | C10—C11—H11C | 109.5 |
| H3WA—O3W—H3WB | 107.8 | H11A—C11—H11C | 109.5 |
| Zn1—O4W—H4WA | 126.5 | H11B—C11—H11C | 109.5 |
| Zn1—O4W—H4WB | 123.8 | N2—C12—C10 | 124.0 (3) |
| H4WA—O4W—H4WB | 107.7 | N2—C12—H12 | 118.0 |
| N1—C1—C2 | 123.5 (3) | C10—C12—H12 | 118.0 |
| N1—C1—H1A | 118.3 | | |

| | | | |
|---|---|---|---|
| O1W—Zn1—N1—C1 | 88.9 (2) | C1—N1—C6—C5 | −0.2 (4) |
| O4W—Zn1—N1—C1 | −85.4 (2) | Zn1—N1—C6—C5 | 178.9 (2) |
| O3W—Zn1—N1—C1 | 0.3 (2) | C1—N1—C6—C7 | 178.8 (2) |
| N2—Zn1—N1—C1 | −178.6 (2) | Zn1—N1—C6—C7 | −2.1 (3) |
| O1W—Zn1—N1—C6 | −90.20 (19) | C4—C5—C6—N1 | −0.1 (4) |
| O4W—Zn1—N1—C6 | 95.50 (19) | C4—C5—C6—C7 | −178.9 (3) |
| O3W—Zn1—N1—C6 | −178.73 (18) | C12—N2—C7—C8 | 1.4 (4) |
| N2—Zn1—N1—C6 | 2.29 (18) | Zn1—N2—C7—C8 | −177.9 (2) |
| O1W—Zn1—N2—C12 | −90.7 (2) | C12—N2—C7—C6 | −179.0 (2) |
| O4W—Zn1—N2—C12 | 86.1 (2) | Zn1—N2—C7—C6 | 1.8 (3) |
| O2W—Zn1—N2—C12 | −0.8 (2) | N1—C6—C7—N2 | 0.2 (4) |
| N1—Zn1—N2—C12 | 178.6 (2) | C5—C6—C7—N2 | 179.1 (2) |
| O1W—Zn1—N2—C7 | 88.50 (19) | N1—C6—C7—C8 | 179.9 (3) |
| O4W—Zn1—N2—C7 | −94.72 (19) | C5—C6—C7—C8 | −1.2 (4) |
| O2W—Zn1—N2—C7 | 178.41 (18) | N2—C7—C8—C9 | −1.3 (4) |
| N1—Zn1—N2—C7 | −2.17 (18) | C6—C7—C8—C9 | 179.1 (3) |
| C6—N1—C1—C2 | −0.4 (4) | C7—C8—C9—C10 | 0.1 (4) |
| Zn1—N1—C1—C2 | −179.4 (2) | C8—C9—C10—C12 | 0.9 (4) |
| N1—C1—C2—C4 | 1.1 (4) | C8—C9—C10—C11 | −178.0 (3) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | −178.0 (3) | C7—N2—C12—C10 | −0.3 (4) |
| C1—C2—C4—C5 | −1.3 (4) | Zn1—N2—C12—C10 | 178.9 (2) |
| C3—C2—C4—C5 | 177.8 (3) | C9—C10—C12—N2 | −0.9 (4) |
| C2—C4—C5—C6 | 0.8 (4) | C11—C10—C12—N2 | 178.1 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4*W*—H4*WB*···S1$^{i}$ | 0.85 | 2.91 | 3.701 (2) | 155 |
| O4*W*—H4*WB*···O6$^{i}$ | 0.85 | 1.84 | 2.695 (3) | 179 |
| O4*W*—H4*WA*···S1 | 0.85 | 2.91 | 3.697 (2) | 155 |
| O4*W*—H4*WA*···O5 | 0.85 | 1.87 | 2.722 (3) | 178 |
| O3*W*—H3*WB*···O5$^{ii}$ | 0.85 | 1.90 | 2.748 (3) | 178 |
| O3*W*—H3*WA*···O6 | 0.85 | 1.96 | 2.804 (3) | 170 |
| O2*W*—H2*WB*···O8$^{i}$ | 0.85 | 1.99 | 2.831 (3) | 170 |
| O2*W*—H2*WA*···O7$^{iii}$ | 0.85 | 1.92 | 2.766 (3) | 173 |
| O1*W*—H1*WB*···S1$^{iii}$ | 0.85 | 3.00 | 3.801 (2) | 157 |
| O1*W*—H1*WB*···O8$^{iii}$ | 0.85 | 1.87 | 2.717 (3) | 175 |
| O1*W*—H1*WA*···O7$^{ii}$ | 0.85 | 1.93 | 2.772 (3) | 169 |

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*−1, *y*, *z*.