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# (4,4′-Dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)-(dimethyl sulfoxide-$\kappa O$)diiodidozinc(II)

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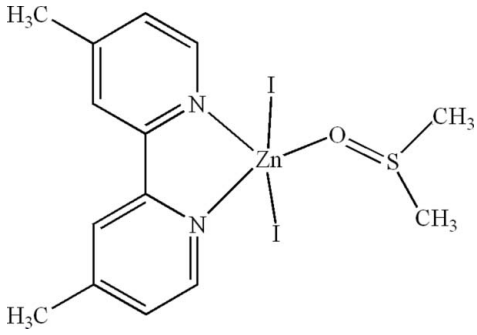
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.076; $wR$ factor = 0.202; data-to-parameter ratio = 27.5.

In the title compound, $[ZnI_2(C_{12}H_{12}N_2)(C_2H_6OS)]$, the $Zn^{II}$ ion is coordinated by two N atoms from a 4,4′-dimethyl-2,2′-bipyridine ligand, one O atom from a dimethyl sulfoxide molecule and two I atoms in a distorted trigonal-bipyramidal geometry. Intramolecular C—H···O hydrogen bonds and intermolecular $\pi$–$\pi$ stacking interactions between the pyridine rings [centroid–centroid distances = 3.637 (4) and 3.818 (4) Å] are present in the crystal structure.

## Related literature

For metal complexes of 4,4′-dimethyl-2,2′-bipyridine, see: Ahmadi *et al.* (2008); Alizadeh *et al.* (2010); Amani *et al.* (2009); Bellusci *et al.* (2008); Hojjat Kashani *et al.* (2008); Kalateh *et al.* (2008, 2010); Sakamoto *et al.* (2004); Sofetis *et al.* (2006); Willett *et al.* (2001); Yoshikawa *et al.* (2003); Yousefi *et al.* (2008).




## Experimental

### Crystal data

$[ZnI_2(C_{12}H_{12}N_2)(C_2H_6OS)]$
$M_r$ = 581.56
Monoclinic, $P2_1/c$
$a$ = 8.6173 (7) Å
$b$ = 15.5424 (11) Å
$c$ = 14.8976 (10) Å
$\beta$ = 102.908 (6)°
$V$ = 1944.9 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 4.54 mm$^{-1}$
$T$ = 298 K
0.40 × 0.20 × 0.10 mm

### Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.350, $T_{max}$ = 0.636
21034 measured reflections
5243 independent reflections
4246 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.113

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.202
$S$ = 1.20
5243 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.87 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Zn1—N1 | 2.135 (5) | Zn1—I1 | 2.6199 (9) |
| Zn1—N2 | 2.167 (6) | Zn1—I2 | 2.6944 (9) |
| Zn1—O1 | 2.112 (5) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O1 | 0.93 | 2.41 | 2.938 (9) | 116 |

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2375).

## References

Ahmadi, R., Kalateh, K., Abedi, A., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m1306–m1307.
Alizadeh, R., Mohammadi Eshlaghi, P. & Amani, V. (2010). *Acta Cryst.* E**66**, m996.
Amani, V., Safari, N., Notash, B. & Khavasi, H. R. (2009). *J. Coord. Chem.* **62**, 1939–1950.
Bellusci, A., Crispini, A., Pucci, D., Szerb, E. I. & Ghedini, M. (2008). *Cryst. Growth Des.* **8**, 3114–3122.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hojjat Kashani, L., Amani, V., Yousefi, M. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m905–m906.
Kalateh, K., Ahmadi, R. & Amani, V. (2010). *Acta Cryst.* E**66**, m512.
Kalateh, K., Ebadi, A., Ahmadi, R., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m1397–m1398.
Sakamoto, J., Yoshikawa, N., Takashima, H., Tsukahara, K., Kanehisa, N., Kai, Y. & Matsumura, K. (2004). *Acta Cryst.* E**60**, m352–m353.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sofetis, A., Raptopoulou, C. P., Terzis, A. & Zafiropoulos, T. F. (2006). *Inorg. Chim. Acta*, **359**, 3389–3395.
Willett, R. D., Pon, G. & Nagy, C. (2001). *Inorg. Chem.* **40**, 4342–4352.
Yoshikawa, N., Sakamoto, J., Kanehisa, N., Kai, Y. & Matsumura-Inoue, (2003). *Acta Cryst.* E**59**, m155–m156.
Yousefi, M., Tadayon Pour, N., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m1259.

# supporting information

*Acta Cryst.* (2010). E**66**, m1594–m1595 [https://doi.org/10.1107/S1600536810046763]

## (4,4′-Dimethyl-2,2′-bipyridine-$\kappa^2N,N'$)(dimethyl sulfoxide-$\kappa O$)diiodidozinc(II)

**Mohammad Yousefi**

### S1. Comment

4,4′-Dimethyl-2,2′-bipyridine (4,4′-dmbipy) is a good bidentate ligand and numerous complexes with 4,4′-dmbipy have been prepared, such as that of mercury (Kalateh *et al.*, 2008; Yousefi *et al.*, 2008), indium (Ahmadi *et al.*, 2008), iron (Amani *et al.*, 2009), platinum (Hojjat Kashani *et al.*, 2008), manganese (Sakamoto *et al.*, 2004), silver (Bellusci *et al.*, 2008), gallium (Sofetis *et al.*, 2006), copper (Willett *et al.*, 2001), zinc (Alizadeh *et al.*, 2010), cadmium (Kalateh *et al.*, 2010) and iridium (Yoshikawa *et al.*, 2003). Here, we report the synthesis and structure of the title compound.

In the title compound (Fig. 1), the $Zn^{II}$ ion is coordinated by two N atoms from a 4,4′-dmbipy ligand, one O atom from a dimethyl sulfoxide molecule and two $I^-$ anions in a distorted trigonal-bipyramidal geometry. The Zn—I, Zn—O and Zn—N bond lengths are collected in Table 1. In the crystal structure, intramolecular C—H···O hydrogen bonds (Table 2) and intermolecular $\pi$–$\pi$ stacking interactions (Fig. 2) between the pyridine rings, $Cg2\cdots Cg2^{i}$ and $Cg2\cdots Cg3^{ii}$ [symmetry codes: (i) 1-x, -y, 1-z; (ii) -x, -y, 1-z; *Cg*2 and *Cg*3 are the centroids of the N1, C1, C2, C3, C5, C6 ring and N2, C7, C8, C9, C11, C12 ring, respectively] may stabilize the structure, with centroid–centroid distances of 3.637 (4) and 3.818 (4) Å.

### S2. Experimental

For the preparation of the title compound, a solution of 4,4′-dmbipy (0.15 g, 0.80 mmol) in methanol (10 ml) was added to a solution of $ZnI_2$ (0.25 g, 0.80 mmol) in methanol (5 ml) at room temperature. Crystals suitable for X-ray diffraction experiment were obtained by methanol diffusion into a colorless solution in DMSO after one week (yield: 0.34 g, 73.1%).

### S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.96 (methyl) Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron density was found 0.81 Å from I2 and the deepest hole 0.86 Å from I1.

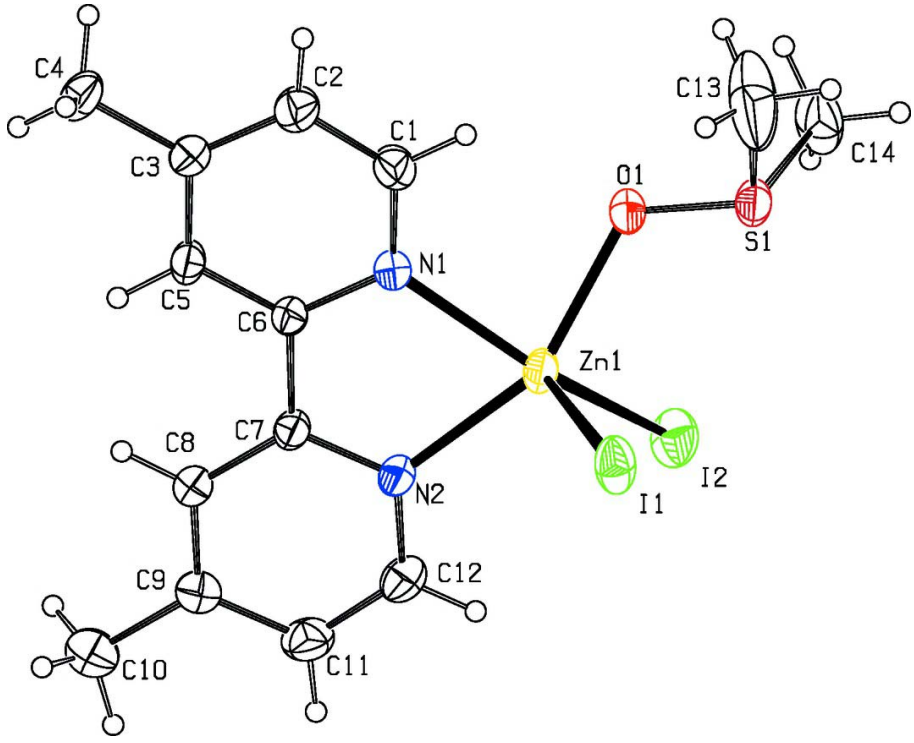


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

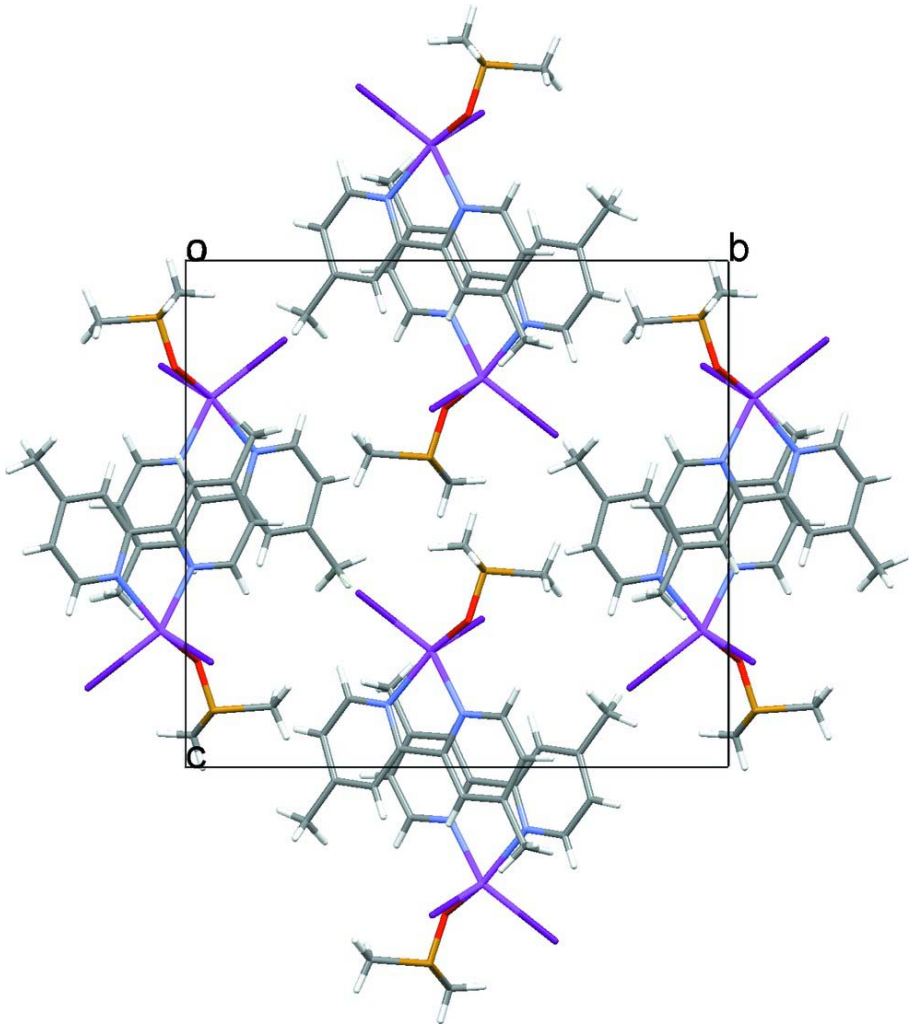


**Figure 2**

Crystal packing diagram for the title compound.

**(4,4′-Dimethyl-2,2′-bipyridine-$\kappa^2$N,N′)(dimethyl sulfoxide-$\kappa$O) diiodidozinc(II)**

*Crystal data*

$[ZnI_2(C_{12}H_{12}N_2)(C_2H_6OS)]$
$M_r$ = 581.56
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 8.6173 (7) Å
$b$ = 15.5424 (11) Å
$c$ = 14.8976 (10) Å
$\beta$ = 102.908 (6)°
$V$ = 1944.9 (3) Å$^3$
$Z$ = 4
$F(000)$ = 1104
$D_x$ = 1.986 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 21034 reflections
$\theta$ = 2.4–29.2°
$\mu$ = 4.54 mm$^{-1}$
$T$ = 298 K
Block, colorless
0.40 × 0.20 × 0.10 mm

*Data collection*

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.350, $T_{max}$ = 0.636
21034 measured reflections
5243 independent reflections
4246 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.113
$\theta_{max}$ = 29.2°, $\theta_{min}$ = 2.4°
$h$ = −11→11
$k$ = −21→21
$l$ = −20→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.202
$S$ = 1.20
5243 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.1105P)^2 + 1.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 2.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.87 e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.3959 (9) | 0.0849 (4) | 0.5994 (5) | 0.0499 (15) |
| H1 | 0.4491 | 0.1110 | 0.6537 | 0.060* |
| C2 | 0.4035 (10) | 0.1229 (5) | 0.5175 (5) | 0.0558 (18) |
| H2 | 0.4613 | 0.1734 | 0.5171 | 0.067* |
| C3 | 0.3249 (8) | 0.0859 (4) | 0.4355 (5) | 0.0434 (13) |
| C4 | 0.3297 (12) | 0.1243 (6) | 0.3445 (5) | 0.060 (2) |
| H4C | 0.2999 | 0.0816 | 0.2972 | 0.072* |
| H4B | 0.4356 | 0.1442 | 0.3456 | 0.072* |
| H4A | 0.2568 | 0.1718 | 0.3320 | 0.072* |
| C5 | 0.2391 (8) | 0.0114 (4) | 0.4415 (4) | 0.0404 (12) |
| H5 | 0.1819 | −0.0146 | 0.3880 | 0.049* |
| C6 | 0.2382 (7) | −0.0246 (4) | 0.5263 (4) | 0.0348 (11) |
| C7 | 0.1490 (7) | −0.1048 (4) | 0.5361 (4) | 0.0371 (11) |
| C8 | 0.0708 (8) | −0.1531 (5) | 0.4614 (4) | 0.0444 (13) |
| H8 | 0.0759 | −0.1363 | 0.4022 | 0.053* |
| C9 | −0.0137 (9) | −0.2252 (5) | 0.4731 (5) | 0.0520 (16) |
| C10 | −0.0965 (13) | −0.2786 (6) | 0.3928 (7) | 0.072 (2) |
| H10C | −0.1468 | −0.3269 | 0.4146 | 0.087* |
| H10B | −0.0202 | −0.2987 | 0.3595 | 0.087* |
| H10A | −0.1755 | −0.2443 | 0.3528 | 0.087* |
| C11 | −0.0155 (10) | −0.2477 (5) | 0.5633 (6) | 0.0578 (18) |
| H11 | −0.0723 | −0.2957 | 0.5749 | 0.069* |
| C12 | 0.0667 (11) | −0.1988 (5) | 0.6351 (5) | 0.0563 (18) |
| H12 | 0.0660 | −0.2157 | 0.6949 | 0.068* |
| C13 | 0.573 (3) | 0.1599 (8) | 0.8800 (9) | 0.148 (9) |

| | | | | |
|---|---|---|---|---|
| H13A | 0.4826 | 0.1882 | 0.8428 | 0.178* |
| H13B | 0.6632 | 0.1665 | 0.8523 | 0.178* |
| H13C | 0.5975 | 0.1849 | 0.9404 | 0.178* |
| C14 | 0.7238 (12) | 0.0134 (10) | 0.9372 (7) | 0.093 (4) |
| H14A | 0.7977 | 0.0373 | 0.9044 | 0.112* |
| H14B | 0.7258 | −0.0482 | 0.9334 | 0.112* |
| H14C | 0.7531 | 0.0307 | 1.0006 | 0.112* |
| N1 | 0.3148 (6) | 0.0114 (3) | 0.6051 (3) | 0.0390 (10) |
| N2 | 0.1480 (7) | −0.1279 (4) | 0.6227 (3) | 0.0408 (11) |
| O1 | 0.4955 (6) | 0.0209 (4) | 0.7891 (3) | 0.0512 (11) |
| Zn1 | 0.28482 (9) | −0.04667 (5) | 0.72994 (5) | 0.0401 (2) |
| I1 | 0.07682 (6) | 0.04536 (4) | 0.79226 (3) | 0.05824 (19) |
| I2 | 0.37974 (8) | −0.18094 (4) | 0.84331 (4) | 0.0642 (2) |
| S1 | 0.5317 (2) | 0.05061 (13) | 0.88831 (11) | 0.0482 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.057 (4) | 0.047 (3) | 0.043 (3) | −0.012 (3) | 0.005 (3) | −0.002 (3) |
| C2 | 0.070 (5) | 0.052 (4) | 0.046 (4) | −0.016 (3) | 0.013 (3) | 0.003 (3) |
| C3 | 0.045 (3) | 0.046 (3) | 0.039 (3) | −0.005 (3) | 0.010 (2) | 0.005 (2) |
| C4 | 0.079 (5) | 0.064 (4) | 0.042 (4) | −0.011 (4) | 0.021 (4) | 0.012 (3) |
| C5 | 0.046 (3) | 0.049 (3) | 0.027 (2) | 0.001 (3) | 0.009 (2) | 0.000 (2) |
| C6 | 0.035 (3) | 0.040 (3) | 0.030 (2) | −0.001 (2) | 0.009 (2) | −0.002 (2) |
| C7 | 0.038 (3) | 0.044 (3) | 0.030 (3) | 0.001 (2) | 0.009 (2) | 0.004 (2) |
| C8 | 0.046 (3) | 0.052 (3) | 0.036 (3) | −0.009 (3) | 0.012 (2) | −0.001 (3) |
| C9 | 0.050 (4) | 0.057 (4) | 0.049 (4) | −0.012 (3) | 0.009 (3) | 0.001 (3) |
| C10 | 0.075 (6) | 0.073 (5) | 0.068 (5) | −0.025 (5) | 0.014 (4) | −0.009 (4) |
| C11 | 0.058 (4) | 0.052 (4) | 0.064 (5) | −0.010 (3) | 0.016 (3) | 0.012 (3) |
| C12 | 0.065 (5) | 0.057 (4) | 0.048 (4) | −0.007 (3) | 0.014 (3) | 0.018 (3) |
| C13 | 0.29 (3) | 0.070 (7) | 0.058 (6) | −0.031 (11) | −0.023 (10) | −0.004 (5) |
| C14 | 0.048 (4) | 0.171 (12) | 0.055 (5) | 0.020 (6) | 0.000 (4) | −0.011 (7) |
| N1 | 0.038 (2) | 0.046 (3) | 0.032 (2) | −0.004 (2) | 0.0059 (19) | 0.000 (2) |
| N2 | 0.041 (3) | 0.051 (3) | 0.031 (2) | −0.002 (2) | 0.0088 (19) | 0.006 (2) |
| O1 | 0.045 (2) | 0.078 (3) | 0.030 (2) | −0.008 (2) | 0.0059 (18) | −0.003 (2) |
| Zn1 | 0.0420 (4) | 0.0511 (4) | 0.0273 (3) | 0.0043 (3) | 0.0079 (3) | 0.0021 (3) |
| I1 | 0.0498 (3) | 0.0841 (4) | 0.0397 (3) | 0.0204 (2) | 0.00761 (19) | −0.0118 (2) |
| I2 | 0.0731 (4) | 0.0624 (3) | 0.0512 (3) | 0.0118 (2) | 0.0009 (2) | 0.0195 (2) |
| S1 | 0.0445 (8) | 0.0693 (11) | 0.0297 (7) | 0.0026 (7) | 0.0062 (6) | 0.0014 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.352 (9) | C10—H10B | 0.9600 |
| C1—C2 | 1.370 (10) | C10—H10A | 0.9600 |
| C1—H1 | 0.9300 | C11—C12 | 1.372 (12) |
| C2—C3 | 1.383 (10) | C11—H11 | 0.9300 |
| C2—H2 | 0.9300 | C12—N2 | 1.341 (9) |
| C3—C5 | 1.388 (9) | C12—H12 | 0.9300 |

| | | | |
|---|---|---|---|
| C3—C4 | 1.490 (9) | C13—S1 | 1.746 (12) |
| C4—H4C | 0.9600 | C13—H13A | 0.9600 |
| C4—H4B | 0.9600 | C13—H13B | 0.9600 |
| C4—H4A | 0.9600 | C13—H13C | 0.9600 |
| C5—C6 | 1.384 (8) | C14—S1 | 1.751 (10) |
| C5—H5 | 0.9300 | C14—H14A | 0.9600 |
| C6—N1 | 1.334 (7) | C14—H14B | 0.9600 |
| C6—C7 | 1.488 (8) | C14—H14C | 0.9600 |
| C7—N2 | 1.341 (7) | Zn1—N1 | 2.135 (5) |
| C7—C8 | 1.387 (9) | Zn1—N2 | 2.167 (6) |
| C8—C9 | 1.368 (10) | O1—S1 | 1.513 (5) |
| C8—H8 | 0.9300 | Zn1—O1 | 2.112 (5) |
| C9—C11 | 1.392 (11) | Zn1—I1 | 2.6199 (9) |
| C9—C10 | 1.498 (12) | Zn1—I2 | 2.6944 (9) |
| C10—H10C | 0.9600 | | |

| | | | |
|---|---|---|---|
| N1—C1—C2 | 123.3 (7) | C12—C11—H11 | 120.0 |
| N1—C1—H1 | 118.3 | C9—C11—H11 | 120.0 |
| C2—C1—H1 | 118.3 | N2—C12—C11 | 122.8 (7) |
| C1—C2—C3 | 119.7 (7) | N2—C12—H12 | 118.6 |
| C1—C2—H2 | 120.2 | C11—C12—H12 | 118.6 |
| C3—C2—H2 | 120.2 | S1—C13—H13A | 109.5 |
| C2—C3—C5 | 117.0 (6) | S1—C13—H13B | 109.5 |
| C2—C3—C4 | 122.0 (6) | H13A—C13—H13B | 109.5 |
| C5—C3—C4 | 121.1 (6) | S1—C13—H13C | 109.5 |
| C3—C4—H4C | 109.5 | H13A—C13—H13C | 109.5 |
| C3—C4—H4B | 109.5 | H13B—C13—H13C | 109.5 |
| H4C—C4—H4B | 109.5 | S1—C14—H14A | 109.5 |
| C3—C4—H4A | 109.5 | S1—C14—H14B | 109.5 |
| H4C—C4—H4A | 109.5 | H14A—C14—H14B | 109.5 |
| H4B—C4—H4A | 109.5 | S1—C14—H14C | 109.5 |
| C6—C5—C3 | 120.5 (6) | H14A—C14—H14C | 109.5 |
| C6—C5—H5 | 119.7 | H14B—C14—H14C | 109.5 |
| C3—C5—H5 | 119.7 | C6—N1—C1 | 117.4 (5) |
| N1—C6—C5 | 122.1 (6) | C6—N1—Zn1 | 117.2 (4) |
| N1—C6—C7 | 115.5 (5) | C1—N1—Zn1 | 125.2 (4) |
| C5—C6—C7 | 122.4 (5) | C12—N2—C7 | 117.9 (6) |
| N2—C7—C8 | 121.4 (6) | C12—N2—Zn1 | 126.3 (5) |
| N2—C7—C6 | 115.7 (5) | C7—N2—Zn1 | 115.7 (4) |
| C8—C7—C6 | 123.0 (5) | S1—O1—Zn1 | 122.0 (3) |
| C9—C8—C7 | 121.3 (6) | O1—Zn1—N1 | 83.89 (19) |
| C9—C8—H8 | 119.4 | O1—Zn1—N2 | 150.80 (19) |
| C7—C8—H8 | 119.4 | N1—Zn1—N2 | 75.84 (19) |
| C8—C9—C11 | 116.7 (7) | O1—Zn1—I1 | 99.96 (15) |
| C8—C9—C10 | 121.6 (7) | N1—Zn1—I1 | 107.68 (15) |
| C11—C9—C10 | 121.8 (7) | N2—Zn1—I1 | 106.06 (15) |
| C9—C10—H10C | 109.5 | O1—Zn1—I2 | 90.64 (15) |
| C9—C10—H10B | 109.5 | N1—Zn1—I2 | 142.63 (15) |

| | | | |
|---|---|---|---|
| H10C—C10—H10B | 109.5 | N2—Zn1—I2 | 92.86 (14) |
| C9—C10—H10A | 109.5 | I1—Zn1—I2 | 109.67 (3) |
| H10C—C10—H10A | 109.5 | O1—S1—C13 | 103.2 (5) |
| H10B—C10—H10A | 109.5 | O1—S1—C14 | 106.0 (4) |
| C12—C11—C9 | 119.9 (7) | C13—S1—C14 | 99.2 (9) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | 0.3 (13) | C8—C7—N2—C12 | −1.0 (10) |
| C1—C2—C3—C5 | 0.9 (12) | C6—C7—N2—C12 | 178.8 (6) |
| C1—C2—C3—C4 | −179.7 (8) | C8—C7—N2—Zn1 | 177.7 (5) |
| C2—C3—C5—C6 | −1.9 (10) | C6—C7—N2—Zn1 | −2.6 (7) |
| C4—C3—C5—C6 | 178.7 (7) | S1—O1—Zn1—N1 | 151.4 (4) |
| C3—C5—C6—N1 | 1.8 (10) | S1—O1—Zn1—N2 | −162.7 (3) |
| C3—C5—C6—C7 | −179.5 (6) | S1—O1—Zn1—I1 | 44.4 (4) |
| N1—C6—C7—N2 | 4.2 (8) | S1—O1—Zn1—I2 | −65.7 (4) |
| C5—C6—C7—N2 | −174.5 (6) | C6—N1—Zn1—O1 | 160.7 (5) |
| N1—C6—C7—C8 | −176.1 (6) | C1—N1—Zn1—O1 | −24.2 (6) |
| C5—C6—C7—C8 | 5.2 (10) | C6—N1—Zn1—N2 | 1.9 (4) |
| N2—C7—C8—C9 | 1.6 (11) | C1—N1—Zn1—N2 | 177.0 (6) |
| C6—C7—C8—C9 | −178.1 (7) | C6—N1—Zn1—I1 | −100.8 (4) |
| C7—C8—C9—C11 | −0.6 (12) | C1—N1—Zn1—I1 | 74.3 (6) |
| C7—C8—C9—C10 | −179.1 (8) | C6—N1—Zn1—I2 | 77.7 (5) |
| C8—C9—C11—C12 | −0.8 (13) | C1—N1—Zn1—I2 | −107.2 (6) |
| C10—C9—C11—C12 | 177.6 (9) | C12—N2—Zn1—O1 | 131.6 (6) |
| C9—C11—C12—N2 | 1.5 (14) | C7—N2—Zn1—O1 | −46.9 (7) |
| C5—C6—N1—C1 | −0.5 (9) | C12—N2—Zn1—N1 | 179.0 (7) |
| C7—C6—N1—C1 | −179.3 (6) | C7—N2—Zn1—N1 | 0.5 (4) |
| C5—C6—N1—Zn1 | 174.9 (5) | C12—N2—Zn1—I1 | −76.3 (6) |
| C7—C6—N1—Zn1 | −3.8 (7) | C7—N2—Zn1—I1 | 105.2 (4) |
| C2—C1—N1—C6 | −0.5 (11) | C12—N2—Zn1—I2 | 35.1 (6) |
| C2—C1—N1—Zn1 | −175.6 (6) | C7—N2—Zn1—I2 | −143.4 (4) |
| C11—C12—N2—C7 | −0.5 (12) | Zn1—O1—S1—C13 | −127.7 (9) |
| C11—C12—N2—Zn1 | −179.0 (6) | Zn1—O1—S1—C14 | 128.5 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O1 | 0.93 | 2.41 | 2.938 (9) | 116 |