Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Bis[$\mu$-1,2-bis(1*H*-imidazol-1-ylmethyl)benzene-$\kappa^2N^3:N^{3'}$]disilver(I) bis(4-amino-2,5-dichlorobenzenesulfonate) tetrahydrate

**Hai-Yan Liu,* Yun-Chao Chi and Guang-Hui Wang**

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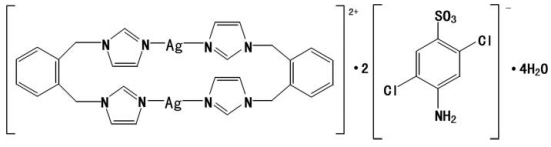
Received 18 July 2008; accepted 22 July 2008

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.044; $wR$ factor = 0.153; data-to-parameter ratio = 16.3.

The asymmetric unit of the title compound, $[Ag_2(C_{14}H_{14}N_4)_2](C_6H_4Cl_2NO_3S)_2\cdot4H_2O$, contains one-half of each of two independent dicationic units, two 4-amino-2,5-dichlorobenzenesulfonate anions and four water molecules. Each centrosymmetric dicationic unit has a dinuclear structure in which two $Ag^I$ atoms are bridged by two 1,2-bis(1*H*-imidazol-1-ylmethyl)benzene ligands in a slightly distorted linear coordination geometry. The 4-amino-2,5-dichlorobenzenesulfonate anion does not coordinate with the $Ag^I$ center, acting only as a counteranion. In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds form a three-dimensional network.

## Related literature

For related literature, see: Aakeröy & Beatty (1998); Cote & Shimizu (2004); Feazell *et al.* (2006); Li *et al.* (2006); Liu *et al.* (2007); Ma *et al.* (2005).




## Experimental

### Crystal data

$[Ag_2(C_{14}H_{14}N_4)_2](C_6H_4Cl_2NO_3S)_2\cdot4H_2O$
$M_r$ = 1246.51
Triclinic, $P\overline{1}$
$a$ = 11.732 (6) Å
$b$ = 14.598 (6) Å
$c$ = 15.718 (6) Å
$\alpha$ = 79.068 (12)°
$\beta$ = 72.843 (19)°
$\gamma$ = 70.991 (17)°
$V$ = 2418.8 (18) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.18 mm$^{-1}$
$T$ = 293 (2) K
0.35 × 0.25 × 0.24 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.716, $T_{max}$ = 0.753
19762 measured reflections
10576 independent reflections
6897 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.152
$S$ = 0.96
10576 reflections
649 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N2—Ag2 | 2.092 (3) | N8—Ag1 | 2.103 (3) |
| N3—Ag2 | 2.090 (4) | N9—Ag1 | 2.100 (3) |
| N9—Ag1—N8 | 175.91 (13) | N3—Ag2—N2 | 178.95 (15) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2$W$—H2$A$···O6 | 0.81 (6) | 2.15 (7) | 2.868 (5) | 148 (7) |
| O3$W$—H3$A$···O2 | 0.82 (7) | 2.00 (7) | 2.819 (6) | 172 (9) |
| O1$W$—H1$A$···O4$^{i}$ | 0.80 (6) | 1.99 (6) | 2.762 (5) | 165 (7) |
| N6—H6$B$···O2$^{ii}$ | 0.80 (3) | 2.19 (4) | 2.928 (5) | 154 (6) |
| N5—H5$B$···O5$^{iii}$ | 0.81 (6) | 2.28 (6) | 2.913 (5) | 136 (5) |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank the Science Foundation of Suihua University (grant No. K071001) for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2638).

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# supporting information

*Acta Cryst.* (2008). E**64**, m1071 [doi:10.1107/S1600536808023052]

# Bis[$\mu$-1,2-bis(1*H*-imidazol-1-ylmethyl)benzene-$\kappa^2N^3$:$N^{3'}$]disilver(I) bis(4-amino-2,5-dichlorobenzenesulfonate) tetrahydrate

**Hai-Yan Liu, Yun-Chao Chi and Guang-Hui Wang**

## S1. Comment

$Ag^I$ complexes have shown versatility of their coordination geometry (Aakeröy & Beatty, 1998; Ma *et al.*, 2005). Some silver(I) sulfonate compounds, modified by secondary nitrogen-based ligands, have been reported (Cote & Shimizu, 2004; Liu *et al.*, 2007). Herein, we present a new silver-sulfonate complex, namely $[Ag_2(IBI)_2]L_2.4H_2O$, where IBI is 1,2-bis ((1*H*-imidazol-1-yl)methyl)benzene and *L* is 4-amino-2,5-dichlorobenzenesulfonic acid.

Selected bond distances and angles are listed in Table 1. The asymmetric unit of the title compound contains one-half each of two independent dicationic units, two 4-amino-2,5-dichlorobenzenesulfonate anions and four water molecules. Each $Ag^I$ ion is two-coordinated by two N atoms from two IBI ligands, showing a slightly distorted linear geometry. The Ag—N bond distances are within the normal range observed in N-containing $Ag^I$ complexes (Li *et al.*, 2006; Feazell *et al.*, 2006). The *L* anion does not coordinate with silver ion but acts as a counteranion.

N—H···O and O—H···O hydrogen bonds between water molecules and *L* ligands result in the formation of a three-dimensional supramolecular structure (Table 2).

## S2. Experimental

An aqueous solution (10 ml) of 4-amino-2,5-dichlorobenzenesulfonic acid (1 mmol) was added to solid $Ag_2CO_3$ (0.5 mmol) and stirred for several minutes until no further $CO_2$ was given off. 1-(3-(1*H*-Imidazol-1-yl)methyl)benzyl)-1*H*-imidazole (1 mmol) was then added and a precipitate was formed. The precipitate was dissolved by ammonium hydroxide. Single crystals of the title compound were obtained by slow evaporation of the solution for 6 d at room temperature.

## S3. Refinement

H atoms bonded to N atoms were located in a difference map and refined with a N—H distance restraint of 0.85 (3) Å and with $U_{iso}$(H) = 1.5$U_{eq}$(N). Water H atoms were located in a difference Fourier map and refined with O—H and H···H distance restraints of 0.85 (3) Å and 1.30 (3) Å, respectively, and with $U_{iso}$(H) = 1.5$U_{eq}$(O). H atoms bonded to C atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C). The highest residual density peak is located 0.89 Å from atom Ag2 and the deepest hole is located 1.54 Å from atom Ag1.

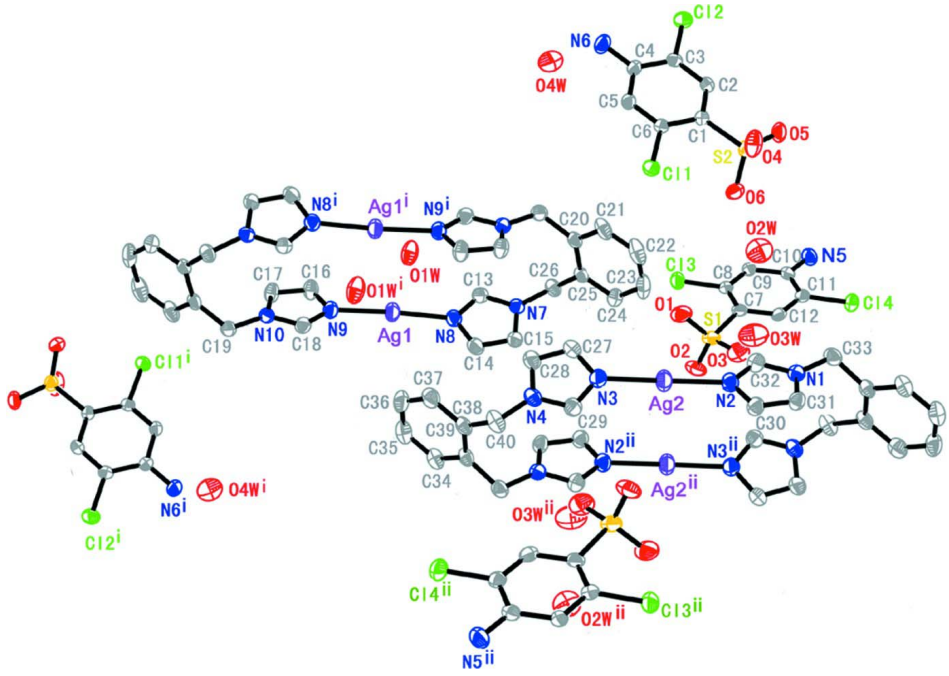


**Figure 1**

The structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) 1-x, 1-y, 2-z; (ii) 2-x, -y, 1-z.

**Bis[$\mu$-1,2-bis(1*H*-imidazol-1-ylmethyl)benzene- $\kappa^2N^3$:$N^{3'}$]disilver(I) bis(4-amino-2,5-dichlorobenzenesulfonate) tetrahydrate**

*Crystal data*

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Hall symbol: -P 1
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$c = 15.718\ (6)$ Å
$\alpha = 79.068\ (12)°$
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$\gamma = 70.991\ (17)°$
$V = 2418.8\ (18)$ Å$^3$
$Z = 2$
$F(000) = 1256$
$D_x = 1.712$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 10576 reflections
$\theta = 3.0–27.5°$
$\mu = 1.18$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.35 × 0.25 × 0.24 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.716$, $T_{max} = 0.753$
19762 measured reflections
10576 independent reflections
6897 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -15\rightarrow15$
$k = -18\rightarrow18$
$l = -20\rightarrow19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.152$
$S = 0.96$
10576 reflections
649 parameters
13 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
$w = 1/[\sigma^2(F_o^2) + (0.0975P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.92$ e Å$^{-3}$
$\Delta\rho_{min} = -0.36$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.8198 (3) | 0.6791 (2) | 0.2186 (2) | 0.0354 (7) |
| C2 | 0.7330 (3) | 0.7577 (2) | 0.1876 (2) | 0.0366 (7) |
| H2 | 0.7202 | 0.7590 | 0.1317 | 0.044* |
| C3 | 0.6652 (3) | 0.8340 (2) | 0.2383 (2) | 0.0388 (7) |
| C4 | 0.6792 (4) | 0.8342 (2) | 0.3238 (2) | 0.0438 (8) |
| C5 | 0.7666 (3) | 0.7540 (2) | 0.3548 (2) | 0.0427 (8) |
| H5 | 0.7784 | 0.7516 | 0.4113 | 0.051* |
| C6 | 0.8349 (3) | 0.6793 (2) | 0.3037 (2) | 0.0356 (7) |
| C7 | 0.3133 (4) | 0.2224 (2) | 0.3052 (2) | 0.0443 (8) |
| C8 | 0.1970 (4) | 0.2875 (2) | 0.3230 (2) | 0.0475 (9) |
| C9 | 0.1282 (4) | 0.3219 (3) | 0.2605 (2) | 0.0480 (9) |
| H9 | 0.0505 | 0.3674 | 0.2751 | 0.058* |
| C10 | 0.1729 (4) | 0.2898 (3) | 0.1759 (2) | 0.0474 (9) |
| C11 | 0.2901 (4) | 0.2236 (2) | 0.1576 (2) | 0.0470 (9) |
| C12 | 0.3595 (4) | 0.1902 (2) | 0.2207 (3) | 0.0458 (8) |
| H12 | 0.4380 | 0.1457 | 0.2062 | 0.055* |
| C13 | 0.4409 (4) | 0.3953 (3) | 0.8315 (3) | 0.0484 (9) |
| H13 | 0.3734 | 0.4511 | 0.8355 | 0.058* |
| C14 | 0.5857 (4) | 0.2737 (3) | 0.8637 (3) | 0.0601 (11) |
| H14 | 0.6393 | 0.2289 | 0.8953 | 0.072* |
| C15 | 0.5879 (4) | 0.2697 (3) | 0.7782 (3) | 0.0538 (10) |
| H15 | 0.6413 | 0.2227 | 0.7406 | 0.065* |
| C16 | 0.2850 (4) | 0.5007 (3) | 1.1974 (3) | 0.0592 (11) |
| H16 | 0.2168 | 0.5300 | 1.1731 | 0.071* |

| | | | | |
|---|---|---|---|---|
| C17 | 0.2902 (4) | 0.5130 (3) | 1.2789 (3) | 0.0562 (10) |
| H17 | 0.2282 | 0.5513 | 1.3207 | 0.067* |
| C18 | 0.4640 (4) | 0.4143 (3) | 1.2125 (3) | 0.0525 (9) |
| H18 | 0.5443 | 0.3719 | 1.2019 | 0.063* |
| C19 | 0.4582 (5) | 0.4438 (3) | 1.3650 (3) | 0.0597 (12) |
| H19A | 0.5467 | 0.4372 | 1.3440 | 0.072* |
| H19B | 0.4481 | 0.3839 | 1.4012 | 0.072* |
| C20 | 0.6035 (4) | 0.4727 (3) | 0.5778 (2) | 0.0473 (9) |
| C21 | 0.7006 (5) | 0.4807 (4) | 0.5034 (3) | 0.0672 (13) |
| H21 | 0.7272 | 0.5363 | 0.4912 | 0.081* |
| C22 | 0.7575 (5) | 0.4091 (5) | 0.4482 (3) | 0.0814 (17) |
| H22 | 0.8223 | 0.4163 | 0.3988 | 0.098* |
| C23 | 0.7203 (5) | 0.3264 (5) | 0.4645 (3) | 0.0805 (16) |
| H23 | 0.7600 | 0.2772 | 0.4268 | 0.097* |
| C24 | 0.6223 (5) | 0.3165 (3) | 0.5383 (3) | 0.0597 (11) |
| H24 | 0.5958 | 0.2609 | 0.5494 | 0.072* |
| C25 | 0.5645 (4) | 0.3890 (3) | 0.5949 (2) | 0.0426 (8) |
| C26 | 0.4588 (4) | 0.3750 (3) | 0.6729 (2) | 0.0513 (9) |
| H26A | 0.3906 | 0.4347 | 0.6767 | 0.062* |
| H26B | 0.4293 | 0.3241 | 0.6629 | 0.062* |
| C27 | 0.9272 (5) | 0.2163 (3) | 0.6345 (3) | 0.0624 (11) |
| H27 | 0.8772 | 0.2668 | 0.6042 | 0.075* |
| C28 | 0.9248 (4) | 0.2116 (3) | 0.7213 (3) | 0.0602 (11) |
| H28 | 0.8742 | 0.2564 | 0.7616 | 0.072* |
| C29 | 1.0624 (4) | 0.0856 (3) | 0.6622 (3) | 0.0555 (10) |
| H29 | 1.1252 | 0.0270 | 0.6561 | 0.067* |
| C30 | 1.2267 (4) | −0.0007 (3) | 0.2968 (3) | 0.0548 (10) |
| H30 | 1.2907 | −0.0338 | 0.3246 | 0.066* |
| C31 | 1.2282 (4) | −0.0092 (3) | 0.2127 (3) | 0.0529 (9) |
| H31 | 1.2920 | −0.0478 | 0.1721 | 0.064* |
| C32 | 1.0534 (4) | 0.0933 (3) | 0.2743 (3) | 0.0556 (10) |
| H32 | 0.9746 | 0.1379 | 0.2823 | 0.067* |
| C33 | 1.0740 (5) | 0.0685 (3) | 0.1172 (3) | 0.0587 (11) |
| H33A | 1.1058 | 0.1188 | 0.0771 | 0.070* |
| H33B | 0.9837 | 0.0920 | 0.1323 | 0.070* |
| C34 | 0.8843 (4) | 0.0216 (3) | 0.9298 (2) | 0.0479 (9) |
| C35 | 0.7849 (5) | 0.0306 (4) | 1.0058 (3) | 0.0628 (12) |
| H35 | 0.7457 | −0.0184 | 1.0247 | 0.075* |
| C36 | 0.7438 (5) | 0.1089 (4) | 1.0529 (3) | 0.0759 (14) |
| H36 | 0.6781 | 0.1127 | 1.1039 | 0.091* |
| C37 | 0.7994 (6) | 0.1817 (4) | 1.0251 (3) | 0.0802 (15) |
| H37 | 0.7705 | 0.2360 | 1.0567 | 0.096* |
| C38 | 0.8985 (5) | 0.1757 (4) | 0.9501 (3) | 0.0682 (13) |
| H38 | 0.9360 | 0.2257 | 0.9318 | 0.082* |
| C39 | 0.9421 (4) | 0.0953 (3) | 0.9020 (2) | 0.0525 (10) |
| C40 | 1.0505 (4) | 0.0916 (4) | 0.8221 (3) | 0.0634 (12) |
| H40A | 1.0991 | 0.1308 | 0.8293 | 0.076* |
| H40B | 1.1034 | 0.0249 | 0.8190 | 0.076* |

| | | | | |
|---|---|---|---|---|
| N1 | 1.1171 (3) | 0.0505 (2) | 0.1992 (2) | 0.0470 (7) |
| N2 | 1.1180 (4) | 0.0633 (3) | 0.3353 (2) | 0.0544 (8) |
| N3 | 1.0130 (4) | 0.1370 (3) | 0.5975 (2) | 0.0584 (9) |
| N4 | 1.0121 (3) | 0.1272 (2) | 0.7374 (2) | 0.0509 (8) |
| N5 | 0.1005 (4) | 0.3204 (3) | 0.1159 (3) | 0.0668 (11) |
| H5A | 0.041 (4) | 0.371 (3) | 0.130 (4) | 0.100* |
| H5B | 0.140 (6) | 0.309 (4) | 0.066 (4) | 0.100* |
| N6 | 0.6122 (5) | 0.9084 (3) | 0.3745 (3) | 0.0742 (13) |
| H6A | 0.622 (6) | 0.912 (4) | 0.424 (3) | 0.111* |
| H6B | 0.580 (6) | 0.960 (3) | 0.351 (4) | 0.111* |
| N7 | 0.4956 (3) | 0.3487 (2) | 0.75842 (19) | 0.0425 (7) |
| N8 | 0.4938 (3) | 0.3527 (2) | 0.8973 (2) | 0.0516 (8) |
| N9 | 0.3948 (3) | 0.4387 (2) | 1.1558 (2) | 0.0516 (8) |
| N10 | 0.4063 (3) | 0.4572 (2) | 1.2871 (2) | 0.0457 (7) |
| O1 | 0.4075 (4) | 0.2441 (2) | 0.4284 (2) | 0.0799 (11) |
| O2 | 0.5249 (3) | 0.1193 (2) | 0.3297 (2) | 0.0792 (10) |
| O1W | 0.2170 (4) | 0.5412 (3) | 0.9721 (2) | 0.0832 (11) |
| H1A | 0.169 (7) | 0.563 (5) | 1.016 (4) | 0.125* |
| H1B | 0.178 (6) | 0.515 (4) | 0.953 (4) | 0.125* |
| O3 | 0.3444 (3) | 0.1006 (2) | 0.4441 (2) | 0.0727 (10) |
| O2W | 0.7688 (5) | 0.3506 (4) | 0.1994 (4) | 0.1072 (15) |
| H2A | 0.810 (8) | 0.375 (6) | 0.216 (5) | 0.161* |
| H2B | 0.794 (8) | 0.356 (6) | 0.144 (2) | 0.161* |
| O4 | 1.0322 (3) | 0.5854 (3) | 0.1273 (2) | 0.0742 (9) |
| O3W | 0.7592 (4) | 0.1554 (4) | 0.2732 (4) | 0.1118 (16) |
| H3A | 0.691 (5) | 0.145 (5) | 0.285 (6) | 0.168* |
| H3B | 0.746 (7) | 0.214 (3) | 0.254 (5) | 0.168* |
| O5 | 0.8507 (3) | 0.6085 (2) | 0.07362 (17) | 0.0578 (7) |
| O4W | 0.2819 (6) | 0.9250 (4) | 0.5166 (4) | 0.1301 (19) |
| H4A | 0.299 (8) | 0.963 (6) | 0.542 (6) | 0.195* |
| H4B | 0.354 (5) | 0.902 (7) | 0.480 (5) | 0.195* |
| O6 | 0.8852 (3) | 0.49480 (18) | 0.2017 (2) | 0.0645 (8) |
| S1 | 0.40489 (11) | 0.16866 (7) | 0.38332 (8) | 0.0534 (3) |
| S2 | 0.90401 (9) | 0.58453 (7) | 0.15024 (6) | 0.0444 (2) |
| Ag1 | 0.44041 (4) | 0.40061 (3) | 1.02509 (2) | 0.06083 (13) |
| Ag2 | 1.06711 (4) | 0.09945 (3) | 0.46655 (2) | 0.06964 (14) |
| Cl1 | 0.94358 (9) | 0.58423 (6) | 0.34728 (6) | 0.0462 (2) |
| Cl2 | 0.55802 (10) | 0.93124 (7) | 0.19615 (7) | 0.0550 (3) |
| Cl3 | 0.12837 (12) | 0.33250 (8) | 0.42796 (7) | 0.0687 (3) |
| Cl4 | 0.35254 (12) | 0.17913 (8) | 0.05280 (7) | 0.0663 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0315 (18) | 0.0399 (16) | 0.0357 (15) | −0.0105 (14) | −0.0085 (13) | −0.0052 (14) |
| C2 | 0.0325 (18) | 0.0433 (17) | 0.0334 (15) | −0.0118 (14) | −0.0083 (13) | −0.0006 (14) |
| C3 | 0.0345 (19) | 0.0360 (16) | 0.0422 (17) | −0.0089 (14) | −0.0091 (14) | 0.0014 (15) |
| C4 | 0.049 (2) | 0.0370 (16) | 0.0439 (18) | −0.0071 (15) | −0.0124 (16) | −0.0087 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.048 (2) | 0.0433 (17) | 0.0387 (17) | −0.0096 (16) | −0.0154 (16) | −0.0070 (15) |
| C6 | 0.0338 (18) | 0.0354 (15) | 0.0388 (16) | −0.0109 (13) | −0.0118 (14) | −0.0005 (14) |
| C7 | 0.054 (2) | 0.0309 (15) | 0.049 (2) | −0.0136 (15) | −0.0180 (17) | 0.0035 (15) |
| C8 | 0.057 (2) | 0.0329 (16) | 0.0454 (19) | −0.0040 (16) | −0.0121 (17) | −0.0037 (15) |
| C9 | 0.052 (2) | 0.0379 (17) | 0.0407 (18) | 0.0017 (16) | −0.0082 (17) | −0.0048 (15) |
| C10 | 0.055 (2) | 0.0391 (17) | 0.0422 (18) | −0.0104 (17) | −0.0107 (17) | 0.0027 (16) |
| C11 | 0.059 (3) | 0.0356 (16) | 0.0442 (19) | −0.0200 (17) | −0.0040 (17) | −0.0021 (15) |
| C12 | 0.046 (2) | 0.0318 (16) | 0.053 (2) | −0.0083 (15) | −0.0046 (17) | −0.0069 (16) |
| C13 | 0.042 (2) | 0.0469 (19) | 0.048 (2) | −0.0110 (16) | −0.0016 (17) | −0.0048 (17) |
| C14 | 0.064 (3) | 0.058 (2) | 0.048 (2) | −0.006 (2) | −0.017 (2) | 0.0007 (19) |
| C15 | 0.058 (3) | 0.049 (2) | 0.0436 (19) | −0.0066 (18) | −0.0071 (18) | −0.0067 (17) |
| C16 | 0.053 (3) | 0.080 (3) | 0.055 (2) | −0.019 (2) | −0.022 (2) | −0.017 (2) |
| C17 | 0.048 (2) | 0.076 (3) | 0.052 (2) | −0.018 (2) | −0.0129 (19) | −0.022 (2) |
| C18 | 0.056 (3) | 0.050 (2) | 0.057 (2) | −0.0168 (19) | −0.019 (2) | −0.0073 (19) |
| C19 | 0.088 (3) | 0.047 (2) | 0.060 (2) | −0.021 (2) | −0.043 (2) | 0.0001 (19) |
| C20 | 0.059 (3) | 0.057 (2) | 0.0376 (17) | −0.0276 (19) | −0.0206 (17) | 0.0026 (17) |
| C21 | 0.079 (3) | 0.100 (3) | 0.041 (2) | −0.059 (3) | −0.018 (2) | 0.011 (2) |
| C22 | 0.065 (3) | 0.144 (5) | 0.043 (2) | −0.049 (4) | −0.009 (2) | −0.001 (3) |
| C23 | 0.081 (4) | 0.110 (4) | 0.047 (2) | −0.012 (3) | −0.015 (2) | −0.030 (3) |
| C24 | 0.073 (3) | 0.060 (2) | 0.051 (2) | −0.020 (2) | −0.017 (2) | −0.013 (2) |
| C25 | 0.048 (2) | 0.0498 (19) | 0.0366 (16) | −0.0219 (17) | −0.0159 (16) | 0.0032 (16) |
| C26 | 0.051 (2) | 0.064 (2) | 0.0449 (19) | −0.026 (2) | −0.0159 (18) | 0.0026 (18) |
| C27 | 0.075 (3) | 0.061 (2) | 0.049 (2) | −0.020 (2) | −0.017 (2) | 0.004 (2) |
| C28 | 0.063 (3) | 0.064 (3) | 0.047 (2) | −0.020 (2) | −0.005 (2) | −0.001 (2) |
| C29 | 0.054 (3) | 0.058 (2) | 0.053 (2) | −0.020 (2) | −0.0076 (19) | −0.004 (2) |
| C30 | 0.056 (3) | 0.056 (2) | 0.055 (2) | −0.0096 (19) | −0.022 (2) | −0.0115 (19) |
| C31 | 0.051 (3) | 0.057 (2) | 0.053 (2) | −0.0085 (19) | −0.0183 (19) | −0.0155 (18) |
| C32 | 0.050 (3) | 0.062 (2) | 0.058 (2) | −0.017 (2) | −0.015 (2) | −0.013 (2) |
| C33 | 0.074 (3) | 0.057 (2) | 0.054 (2) | −0.021 (2) | −0.033 (2) | 0.0028 (19) |
| C34 | 0.049 (2) | 0.064 (2) | 0.0389 (17) | −0.0257 (19) | −0.0177 (17) | 0.0020 (17) |
| C35 | 0.064 (3) | 0.086 (3) | 0.047 (2) | −0.035 (3) | −0.016 (2) | 0.002 (2) |
| C36 | 0.071 (4) | 0.108 (4) | 0.047 (2) | −0.024 (3) | −0.010 (2) | −0.013 (3) |
| C37 | 0.102 (5) | 0.089 (4) | 0.058 (3) | −0.020 (3) | −0.031 (3) | −0.025 (3) |
| C38 | 0.089 (4) | 0.076 (3) | 0.060 (3) | −0.042 (3) | −0.034 (3) | 0.002 (2) |
| C39 | 0.060 (3) | 0.069 (2) | 0.0423 (19) | −0.031 (2) | −0.0258 (18) | 0.0057 (19) |
| C40 | 0.054 (3) | 0.096 (3) | 0.051 (2) | −0.039 (2) | −0.017 (2) | 0.006 (2) |
| N1 | 0.052 (2) | 0.0457 (16) | 0.0515 (17) | −0.0198 (15) | −0.0194 (15) | −0.0032 (14) |
| N2 | 0.062 (2) | 0.060 (2) | 0.0488 (18) | −0.0249 (18) | −0.0172 (17) | −0.0071 (16) |
| N3 | 0.070 (3) | 0.0564 (19) | 0.0496 (19) | −0.0232 (18) | −0.0090 (17) | −0.0071 (17) |
| N4 | 0.050 (2) | 0.0619 (19) | 0.0448 (17) | −0.0266 (17) | −0.0124 (15) | 0.0048 (16) |
| N5 | 0.071 (3) | 0.068 (2) | 0.0485 (19) | 0.001 (2) | −0.023 (2) | −0.0029 (19) |
| N6 | 0.100 (3) | 0.0504 (19) | 0.061 (2) | 0.016 (2) | −0.036 (2) | −0.0224 (18) |
| N7 | 0.0403 (18) | 0.0440 (15) | 0.0406 (15) | −0.0167 (13) | −0.0046 (13) | 0.0010 (13) |
| N8 | 0.058 (2) | 0.0554 (18) | 0.0439 (16) | −0.0223 (16) | −0.0093 (15) | −0.0044 (15) |
| N9 | 0.058 (2) | 0.0583 (19) | 0.0448 (17) | −0.0223 (17) | −0.0136 (16) | −0.0088 (15) |
| N10 | 0.055 (2) | 0.0435 (15) | 0.0468 (16) | −0.0206 (15) | −0.0211 (15) | −0.0006 (14) |
| O1 | 0.116 (3) | 0.0512 (16) | 0.099 (2) | −0.0303 (18) | −0.061 (2) | −0.0044 (17) |
| O2 | 0.059 (2) | 0.0723 (19) | 0.103 (3) | −0.0016 (17) | −0.033 (2) | −0.0103 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1W | 0.067 (3) | 0.118 (3) | 0.067 (2) | −0.034 (2) | 0.0094 (17) | −0.043 (2) |
| O3 | 0.098 (3) | 0.0560 (16) | 0.077 (2) | −0.0340 (17) | −0.046 (2) | 0.0235 (16) |
| O2W | 0.092 (3) | 0.108 (3) | 0.131 (4) | −0.050 (3) | −0.020 (3) | −0.010 (3) |
| O4 | 0.0386 (18) | 0.113 (3) | 0.0653 (18) | −0.0073 (17) | −0.0007 (14) | −0.0401 (18) |
| O3W | 0.069 (3) | 0.094 (3) | 0.165 (5) | −0.008 (2) | −0.041 (3) | −0.005 (3) |
| O5 | 0.067 (2) | 0.0644 (16) | 0.0407 (13) | −0.0052 (14) | −0.0208 (13) | −0.0158 (12) |
| O4W | 0.188 (6) | 0.085 (3) | 0.127 (4) | −0.043 (4) | −0.051 (4) | −0.010 (3) |
| O6 | 0.095 (2) | 0.0394 (13) | 0.0644 (17) | −0.0098 (14) | −0.0358 (17) | −0.0090 (13) |
| S1 | 0.0593 (7) | 0.0375 (4) | 0.0692 (6) | −0.0130 (4) | −0.0298 (5) | 0.0011 (4) |
| S2 | 0.0410 (5) | 0.0485 (5) | 0.0396 (4) | −0.0005 (4) | −0.0116 (4) | −0.0141 (4) |
| Ag1 | 0.0758 (3) | 0.0704 (2) | 0.04346 (17) | −0.03161 (18) | −0.00942 (15) | −0.01273 (15) |
| Ag2 | 0.0871 (3) | 0.0778 (2) | 0.04749 (19) | −0.0295 (2) | −0.01030 (17) | −0.01494 (17) |
| Cl1 | 0.0453 (5) | 0.0444 (4) | 0.0475 (5) | −0.0044 (4) | −0.0209 (4) | −0.0021 (4) |
| Cl2 | 0.0497 (6) | 0.0453 (5) | 0.0618 (6) | 0.0019 (4) | −0.0213 (5) | −0.0022 (4) |
| Cl3 | 0.0803 (8) | 0.0638 (6) | 0.0436 (5) | 0.0058 (5) | −0.0142 (5) | −0.0120 (5) |
| Cl4 | 0.0791 (8) | 0.0626 (6) | 0.0467 (5) | −0.0158 (6) | 0.0014 (5) | −0.0164 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.382 (4) | C26—H26B | 0.97 |
| C1—C6 | 1.401 (4) | C27—C28 | 1.345 (6) |
| C1—S2 | 1.756 (3) | C27—N3 | 1.357 (6) |
| C2—C3 | 1.377 (5) | C27—H27 | 0.93 |
| C2—H2 | 0.93 | C28—N4 | 1.358 (6) |
| C3—C4 | 1.402 (5) | C28—H28 | 0.93 |
| C3—Cl2 | 1.734 (3) | C29—N3 | 1.308 (5) |
| C4—N6 | 1.353 (5) | C29—N4 | 1.319 (5) |
| C4—C5 | 1.398 (5) | C29—H29 | 0.93 |
| C5—C6 | 1.364 (5) | C30—C31 | 1.346 (6) |
| C5—H5 | 0.93 | C30—N2 | 1.360 (6) |
| C6—Cl1 | 1.738 (3) | C30—H30 | 0.93 |
| C7—C8 | 1.369 (5) | C31—N1 | 1.363 (5) |
| C7—C12 | 1.387 (5) | C31—H31 | 0.93 |
| C7—S1 | 1.773 (4) | C32—N2 | 1.317 (5) |
| C8—C9 | 1.373 (5) | C32—N1 | 1.341 (5) |
| C8—Cl3 | 1.756 (4) | C32—H32 | 0.93 |
| C9—C10 | 1.388 (5) | C33—N1 | 1.468 (5) |
| C9—H9 | 0.93 | C33—C34$^{ii}$ | 1.499 (6) |
| C10—N5 | 1.371 (5) | C33—H33A | 0.97 |
| C10—C11 | 1.383 (6) | C33—H33B | 0.97 |
| C11—C12 | 1.385 (5) | C34—C39 | 1.390 (5) |
| C11—Cl4 | 1.748 (4) | C34—C35 | 1.393 (6) |
| C12—H12 | 0.93 | C34—C33$^{ii}$ | 1.499 (6) |
| C13—N8 | 1.313 (5) | C35—C36 | 1.355 (7) |
| C13—N7 | 1.331 (5) | C35—H35 | 0.93 |
| C13—H13 | 0.93 | C36—C37 | 1.362 (8) |
| C14—C15 | 1.350 (6) | C36—H36 | 0.93 |
| C14—N8 | 1.362 (6) | C37—C38 | 1.383 (8) |

| | | | |
|---|---|---|---|
| C14—H14 | 0.93 | C37—H37 | 0.93 |
| C15—N7 | 1.359 (5) | C38—C39 | 1.388 (7) |
| C15—H15 | 0.93 | C38—H38 | 0.93 |
| C16—C17 | 1.349 (6) | C39—C40 | 1.495 (6) |
| C16—N9 | 1.369 (6) | C40—N4 | 1.478 (5) |
| C16—H16 | 0.93 | C40—H40A | 0.97 |
| C17—N10 | 1.370 (5) | C40—H40B | 0.97 |
| C17—H17 | 0.93 | N2—Ag2 | 2.092 (3) |
| C18—N9 | 1.303 (5) | N3—Ag2 | 2.090 (4) |
| C18—N10 | 1.327 (5) | N5—H5A | 0.84 (3) |
| C18—H18 | 0.93 | N5—H5B | 0.81 (6) |
| C19—N10 | 1.475 (4) | N6—H6A | 0.83 (3) |
| C19—C20$^{i}$ | 1.508 (6) | N6—H6B | 0.80 (3) |
| C19—H19A | 0.97 | N8—Ag1 | 2.103 (3) |
| C19—H19B | 0.97 | N9—Ag1 | 2.100 (3) |
| C20—C21 | 1.387 (6) | O1—S1 | 1.430 (3) |
| C20—C25 | 1.394 (5) | O2—S1 | 1.443 (4) |
| C20—C19$^{i}$ | 1.508 (6) | O1W—H1A | 0.80 (6) |
| C21—C22 | 1.356 (8) | O1W—H1B | 0.83 (7) |
| C21—H21 | 0.93 | O3—S1 | 1.450 (3) |
| C22—C23 | 1.369 (8) | O2W—H2A | 0.81 (6) |
| C22—H22 | 0.93 | O2W—H2B | 0.83 (3) |
| C23—C24 | 1.395 (7) | O4—S2 | 1.443 (3) |
| C23—H23 | 0.93 | O3W—H3A | 0.82 (7) |
| C24—C25 | 1.381 (6) | O3W—H3B | 0.83 (3) |
| C24—H24 | 0.93 | O5—S2 | 1.451 (3) |
| C25—C26 | 1.502 (5) | O4W—H4A | 0.84 (10) |
| C26—N7 | 1.476 (4) | O4W—H4B | 0.87 (8) |
| C26—H26A | 0.97 | O6—S2 | 1.449 (3) |

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|---|---|---|---|
| C2—C1—C6 | 117.7 (3) | N3—C29—N4 | 111.7 (4) |
| C2—C1—S2 | 118.7 (2) | N3—C29—H29 | 124.1 |
| C6—C1—S2 | 123.6 (2) | N4—C29—H29 | 124.1 |
| C3—C2—C1 | 121.0 (3) | C31—C30—N2 | 110.0 (4) |
| C3—C2—H2 | 119.5 | C31—C30—H30 | 125.0 |
| C1—C2—H2 | 119.5 | N2—C30—H30 | 125.0 |
| C2—C3—C4 | 121.5 (3) | C30—C31—N1 | 105.9 (4) |
| C2—C3—Cl2 | 119.2 (3) | C30—C31—H31 | 127.1 |
| C4—C3—Cl2 | 119.3 (3) | N1—C31—H31 | 127.1 |
| N6—C4—C5 | 121.0 (3) | N2—C32—N1 | 110.6 (4) |
| N6—C4—C3 | 122.0 (3) | N2—C32—H32 | 124.7 |
| C5—C4—C3 | 117.1 (3) | N1—C32—H32 | 124.7 |
| C6—C5—C4 | 121.2 (3) | N1—C33—C34$^{ii}$ | 112.0 (3) |
| C6—C5—H5 | 119.4 | N1—C33—H33A | 109.2 |
| C4—C5—H5 | 119.4 | C34$^{ii}$—C33—H33A | 109.2 |
| C5—C6—C1 | 121.6 (3) | N1—C33—H33B | 109.2 |
| C5—C6—Cl1 | 117.6 (2) | C34$^{ii}$—C33—H33B | 109.2 |
| C1—C6—Cl1 | 120.8 (3) | H33A—C33—H33B | 107.9 |

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|---|---|---|---|
| C8—C7—C12 | 117.2 (3) | C39—C34—C35 | 118.6 (4) |
| C8—C7—S1 | 125.6 (3) | C39—C34—C33$^{ii}$ | 122.9 (4) |
| C12—C7—S1 | 117.1 (3) | C35—C34—C33$^{ii}$ | 118.5 (4) |
| C7—C8—C9 | 122.4 (4) | C36—C35—C34 | 121.9 (4) |
| C7—C8—Cl3 | 121.2 (3) | C36—C35—H35 | 119.1 |
| C9—C8—Cl3 | 116.4 (3) | C34—C35—H35 | 119.1 |
| C8—C9—C10 | 121.0 (4) | C35—C36—C37 | 119.5 (5) |
| C8—C9—H9 | 119.5 | C35—C36—H36 | 120.2 |
| C10—C9—H9 | 119.5 | C37—C36—H36 | 120.2 |
| N5—C10—C11 | 122.6 (4) | C36—C37—C38 | 120.5 (5) |
| N5—C10—C9 | 120.5 (4) | C36—C37—H37 | 119.7 |
| C11—C10—C9 | 116.9 (3) | C38—C37—H37 | 119.7 |
| C10—C11—C12 | 121.7 (4) | C37—C38—C39 | 120.3 (4) |
| C10—C11—Cl4 | 119.6 (3) | C37—C38—H38 | 119.8 |
| C12—C11—Cl4 | 118.6 (3) | C39—C38—H38 | 119.8 |
| C11—C12—C7 | 120.8 (4) | C38—C39—C34 | 119.1 (4) |
| C11—C12—H12 | 119.6 | C38—C39—C40 | 118.3 (4) |
| C7—C12—H12 | 119.6 | C34—C39—C40 | 122.6 (4) |
| N8—C13—N7 | 111.7 (3) | N4—C40—C39 | 112.6 (3) |
| N8—C13—H13 | 124.2 | N4—C40—H40A | 109.1 |
| N7—C13—H13 | 124.2 | C39—C40—H40A | 109.1 |
| C15—C14—N8 | 110.5 (4) | N4—C40—H40B | 109.1 |
| C15—C14—H14 | 124.8 | C39—C40—H40B | 109.1 |
| N8—C14—H14 | 124.8 | H40A—C40—H40B | 107.8 |
| C14—C15—N7 | 105.4 (4) | C32—N1—C31 | 107.6 (3) |
| C14—C15—H15 | 127.3 | C32—N1—C33 | 125.1 (4) |
| N7—C15—H15 | 127.3 | C31—N1—C33 | 127.3 (4) |
| C17—C16—N9 | 110.0 (4) | C32—N2—C30 | 105.9 (3) |
| C17—C16—H16 | 125.0 | C32—N2—Ag2 | 128.8 (3) |
| N9—C16—H16 | 125.0 | C30—N2—Ag2 | 125.3 (3) |
| C16—C17—N10 | 105.4 (4) | C29—N3—C27 | 104.9 (4) |
| C16—C17—H17 | 127.3 | C29—N3—Ag2 | 124.5 (3) |
| N10—C17—H17 | 127.3 | C27—N3—Ag2 | 130.6 (3) |
| N9—C18—N10 | 111.9 (4) | C29—N4—C28 | 107.8 (3) |
| N9—C18—H18 | 124.0 | C29—N4—C40 | 125.9 (4) |
| N10—C18—H18 | 124.0 | C28—N4—C40 | 126.2 (4) |
| N10—C19—C20$^{i}$ | 112.7 (3) | C10—N5—H5A | 112 (4) |
| N10—C19—H19A | 109.1 | C10—N5—H5B | 113 (4) |
| C20$^{i}$—C19—H19A | 109.1 | H5A—N5—H5B | 126 (5) |
| N10—C19—H19B | 109.1 | C4—N6—H6A | 124 (5) |
| C20$^{i}$—C19—H19B | 109.1 | C4—N6—H6B | 120 (5) |
| H19A—C19—H19B | 107.8 | H6A—N6—H6B | 113 (6) |
| C21—C20—C25 | 118.5 (4) | C13—N7—C15 | 107.5 (3) |
| C21—C20—C19$^{i}$ | 118.8 (4) | C13—N7—C26 | 126.3 (3) |
| C25—C20—C19$^{i}$ | 122.7 (4) | C15—N7—C26 | 126.1 (4) |
| C22—C21—C20 | 121.5 (4) | C13—N8—C14 | 104.8 (3) |
| C22—C21—H21 | 119.3 | C13—N8—Ag1 | 125.4 (3) |
| C20—C21—H21 | 119.3 | C14—N8—Ag1 | 129.8 (3) |

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|---|---|---|---|
| C21—C22—C23 | 120.5 (5) | C18—N9—C16 | 105.3 (3) |
| C21—C22—H22 | 119.7 | C18—N9—Ag1 | 128.8 (3) |
| C23—C22—H22 | 119.7 | C16—N9—Ag1 | 125.8 (3) |
| C22—C23—C24 | 119.5 (5) | C18—N10—C17 | 107.4 (3) |
| C22—C23—H23 | 120.3 | C18—N10—C19 | 125.5 (4) |
| C24—C23—H23 | 120.3 | C17—N10—C19 | 127.1 (4) |
| C25—C24—C23 | 120.2 (4) | H1A—O1W—H1B | 104 (5) |
| C25—C24—H24 | 119.9 | H2A—O2W—H2B | 104 (6) |
| C23—C24—H24 | 119.9 | H3A—O3W—H3B | 105 (4) |
| C24—C25—C20 | 119.9 (4) | H4A—O4W—H4B | 101 (4) |
| C24—C25—C26 | 118.0 (3) | O1—S1—O2 | 113.8 (2) |
| C20—C25—C26 | 122.1 (4) | O1—S1—O3 | 112.0 (2) |
| N7—C26—C25 | 112.3 (3) | O2—S1—O3 | 111.8 (2) |
| N7—C26—H26A | 109.1 | O1—S1—C7 | 108.49 (17) |
| C25—C26—H26A | 109.1 | O2—S1—C7 | 104.3 (2) |
| N7—C26—H26B | 109.1 | O3—S1—C7 | 105.73 (18) |
| C25—C26—H26B | 109.1 | O4—S2—O6 | 112.7 (2) |
| H26A—C26—H26B | 107.9 | O4—S2—O5 | 113.29 (19) |
| C28—C27—N3 | 110.4 (4) | O6—S2—O5 | 111.49 (18) |
| C28—C27—H27 | 124.8 | O4—S2—C1 | 105.88 (18) |
| N3—C27—H27 | 124.8 | O6—S2—C1 | 107.38 (17) |
| C27—C28—N4 | 105.2 (4) | O5—S2—C1 | 105.46 (16) |
| C27—C28—H28 | 127.4 | N9—Ag1—N8 | 175.91 (13) |
| N4—C28—H28 | 127.4 | N3—Ag2—N2 | 178.95 (15) |

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| C6—C1—C2—C3 | 1.0 (5) | C33$^{ii}$—C34—C39—C38 | −179.2 (3) |
| S2—C1—C2—C3 | −179.5 (3) | C35—C34—C39—C40 | 179.1 (4) |
| C1—C2—C3—C4 | −1.5 (5) | C33$^{ii}$—C34—C39—C40 | 0.5 (5) |
| C1—C2—C3—Cl2 | 179.6 (3) | C38—C39—C40—N4 | −95.9 (4) |
| C2—C3—C4—N6 | −179.4 (4) | C34—C39—C40—N4 | 84.4 (5) |
| Cl2—C3—C4—N6 | −0.5 (6) | N2—C32—N1—C31 | −0.5 (5) |
| C2—C3—C4—C5 | 0.9 (5) | N2—C32—N1—C33 | −178.8 (3) |
| Cl2—C3—C4—C5 | 179.8 (3) | C30—C31—N1—C32 | 0.6 (5) |
| N6—C4—C5—C6 | −179.6 (4) | C30—C31—N1—C33 | 178.9 (4) |
| C3—C4—C5—C6 | 0.1 (5) | C34$^{ii}$—C33—N1—C32 | −145.3 (4) |
| C4—C5—C6—C1 | −0.6 (5) | C34$^{ii}$—C33—N1—C31 | 36.7 (6) |
| C4—C5—C6—Cl1 | 178.6 (3) | N1—C32—N2—C30 | 0.2 (5) |
| C2—C1—C6—C5 | 0.0 (5) | N1—C32—N2—Ag2 | −177.8 (2) |
| S2—C1—C6—C5 | −179.4 (3) | C31—C30—N2—C32 | 0.2 (5) |
| C2—C1—C6—Cl1 | −179.1 (2) | C31—C30—N2—Ag2 | 178.3 (3) |
| S2—C1—C6—Cl1 | 1.5 (4) | N4—C29—N3—C27 | 0.6 (5) |
| C12—C7—C8—C9 | −1.1 (5) | N4—C29—N3—Ag2 | 178.8 (3) |
| S1—C7—C8—C9 | −176.0 (3) | C28—C27—N3—C29 | −0.6 (5) |
| C12—C7—C8—Cl3 | 179.4 (3) | C28—C27—N3—Ag2 | −178.6 (3) |
| S1—C7—C8—Cl3 | 4.5 (5) | N3—C29—N4—C28 | −0.4 (5) |
| C7—C8—C9—C10 | 1.6 (6) | N3—C29—N4—C40 | −176.5 (3) |
| Cl3—C8—C9—C10 | −178.9 (3) | C27—C28—N4—C29 | 0.0 (5) |
| C8—C9—C10—N5 | 176.3 (4) | C27—C28—N4—C40 | 176.1 (4) |

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| C8—C9—C10—C11 | −1.3 (6) | C39—C40—N4—C29 | −135.6 (4) |
| N5—C10—C11—C12 | −177.1 (4) | C39—C40—N4—C28 | 49.0 (6) |
| C9—C10—C11—C12 | 0.5 (5) | N8—C13—N7—C15 | 1.5 (4) |
| N5—C10—C11—Cl4 | 2.0 (5) | N8—C13—N7—C26 | 178.6 (3) |
| C9—C10—C11—Cl4 | 179.6 (3) | C14—C15—N7—C13 | −1.2 (4) |
| C10—C11—C12—C7 | 0.0 (5) | C14—C15—N7—C26 | −178.3 (4) |
| Cl4—C11—C12—C7 | −179.1 (3) | C25—C26—N7—C13 | 124.6 (4) |
| C8—C7—C12—C11 | 0.3 (5) | C25—C26—N7—C15 | −58.8 (5) |
| S1—C7—C12—C11 | 175.7 (3) | N7—C13—N8—C14 | −1.2 (5) |
| N8—C14—C15—N7 | 0.5 (5) | N7—C13—N8—Ag1 | 179.5 (2) |
| N9—C16—C17—N10 | 0.1 (5) | C15—C14—N8—C13 | 0.4 (5) |
| C25—C20—C21—C22 | −0.2 (6) | C15—C14—N8—Ag1 | 179.7 (3) |
| C19$^{i}$—C20—C21—C22 | −178.3 (4) | N10—C18—N9—C16 | −0.5 (4) |
| C20—C21—C22—C23 | 0.0 (7) | N10—C18—N9—Ag1 | 175.9 (2) |
| C21—C22—C23—C24 | 0.6 (8) | C17—C16—N9—C18 | 0.2 (5) |
| C22—C23—C24—C25 | −0.8 (7) | C17—C16—N9—Ag1 | −176.3 (3) |
| C23—C24—C25—C20 | 0.6 (6) | N9—C18—N10—C17 | 0.6 (5) |
| C23—C24—C25—C26 | 179.5 (4) | N9—C18—N10—C19 | 178.9 (3) |
| C21—C20—C25—C24 | −0.1 (5) | C16—C17—N10—C18 | −0.4 (5) |
| C19$^{i}$—C20—C25—C24 | 177.9 (3) | C16—C17—N10—C19 | −178.7 (4) |
| C21—C20—C25—C26 | −179.0 (3) | C20$^{i}$—C19—N10—C18 | 157.7 (4) |
| C19$^{i}$—C20—C25—C26 | −1.0 (5) | C20$^{i}$—C19—N10—C17 | −24.3 (6) |
| C24—C25—C26—N7 | 104.5 (4) | C8—C7—S1—O1 | −49.1 (4) |
| C20—C25—C26—N7 | −76.6 (4) | C12—C7—S1—O1 | 135.9 (3) |
| N3—C27—C28—N4 | 0.4 (5) | C8—C7—S1—O2 | −170.8 (3) |
| N2—C30—C31—N1 | −0.5 (5) | C12—C7—S1—O2 | 14.2 (3) |
| C39—C34—C35—C36 | −0.1 (6) | C8—C7—S1—O3 | 71.2 (4) |
| C33$^{ii}$—C34—C35—C36 | 178.5 (4) | C12—C7—S1—O3 | −103.8 (3) |
| C34—C35—C36—C37 | 1.0 (7) | C2—C1—S2—O4 | 115.0 (3) |
| C35—C36—C37—C38 | −1.0 (8) | C6—C1—S2—O4 | −65.6 (3) |
| C36—C37—C38—C39 | 0.3 (7) | C2—C1—S2—O6 | −124.4 (3) |
| C37—C38—C39—C34 | 0.5 (6) | C6—C1—S2—O6 | 55.1 (3) |
| C37—C38—C39—C40 | −179.2 (4) | C2—C1—S2—O5 | −5.4 (3) |
| C35—C34—C39—C38 | −0.6 (5) | C6—C1—S2—O5 | 174.1 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2*W*—H2*A*···O6 | 0.81 (6) | 2.15 (7) | 2.868 (5) | 148 (7) |
| O3*W*—H3*A*···O2 | 0.82 (7) | 2.00 (7) | 2.819 (6) | 172 (9) |
| O1*W*—H1*A*···O4$^{iii}$ | 0.80 (6) | 1.99 (6) | 2.762 (5) | 165 (7) |
| N6—H6*B*···O2$^{iv}$ | 0.80 (3) | 2.19 (4) | 2.928 (5) | 154 (6) |
| N5—H5*B*···O5$^{v}$ | 0.81 (6) | 2.28 (6) | 2.913 (5) | 136 (5) |

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