

(6-Aminonaphthalene-1-sulfonato- κ O)-bis(3-methylisoquinoline- κ N)silver(I)

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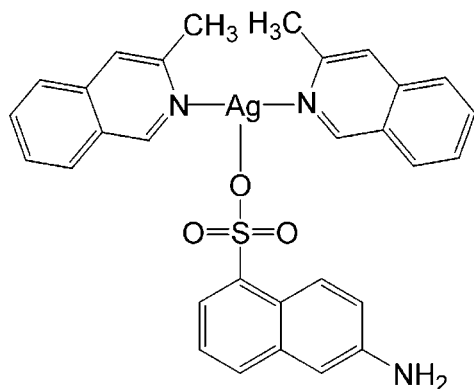
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Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.048; wR factor = 0.074; data-to-parameter ratio = 16.9.

The title compound, $[\text{Ag}(\text{C}_{10}\text{H}_8\text{NO}_3\text{S})(\text{C}_{10}\text{H}_9\text{N})_2]$, has a mononuclear structure in which the Ag^+ cation is three-coordinated by two N atoms from two different 3-methylisoquinoline molecules and one O atom from a 6-amino-naphthalene-1-sulfonate anion in a distorted trigonal-planar AgN_2O arrangement. A network of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds consolidates the structure.

Related literature

For the related compound, $\text{Ag}(\text{L1})(3\text{-iso})$ ($\text{L1} = 2\text{-amino-3,5-dimethylbenzenesulfonate}$, $3\text{-iso} = 3\text{-methylisoquinoline}$), containing a trigonal-planar AgN_3 arrangement, see: Li *et al.* (2007).

**Experimental***Crystal data* $[\text{Ag}(\text{C}_{10}\text{H}_8\text{NO}_3\text{S})(\text{C}_{10}\text{H}_9\text{N})_2]$ $M_r = 616.47$ Triclinic, $P\bar{1}$ $a = 9.8810$ (14) Å $b = 10.2220$ (17) Å $c = 13.256$ (2) Å $\alpha = 80.108$ (11)° $\beta = 86.653$ (11)° $\gamma = 84.143$ (10)° $V = 1311.0$ (4) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.89$ mm⁻¹ $T = 292$ (2) K $0.35 \times 0.33 \times 0.29$ mm*Data collection*

Bruker SMART APEX CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.709$, $T_{\max} = 0.766$

8844 measured reflections

5933 independent reflections

2404 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.064$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.048$ $wR(F^2) = 0.074$ $S = 0.76$

5933 reflections

351 parameters

3 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.38$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.35$ e Å⁻³**Table 1**

Selected geometric parameters (Å, °).

Ag1—N3	2.170 (4)	Ag1—O3	2.583 (3)
Ag1—N2	2.184 (4)		
N3—Ag1—N2	159.18 (13)	N2—Ag1—O3	98.76 (13)
N3—Ag1—O3	89.17 (12)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O2}^{\text{i}}$	0.90 (4)	2.51 (4)	3.365 (5)	160 (3)
$\text{N1}-\text{H2N}\cdots\text{O1}^{\text{ii}}$	0.81 (4)	2.30 (4)	3.008 (5)	146 (4)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2506).

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supplementary materials

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(6-Aminonaphthalene-1-sulfonato- κO)bis(3-methylisoquinoline- κN)silver(I)

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Comment

In this paper, the structure of the title compound, (I) (Fig. 1), containing two 3-methylisoquinoline molecules and one 6-amino-1-naphthalenesulfonate (*L*) anion is described.

In (I), two 3-methylisoquinoline molecules and one *L* anion are coordinated to the metal, resulting in a highly distorted trigonal planar coordination geometry for Ag (Table 1). Atoms Ag1, N2, N3 and O3 are close to coplanar and the bond-angle sum about Ag is 347.11°. The Ag—N distances in (I) are similar to the equivalent values in a related compound (Li *et al.*, 2007). The dihedral angle between the quinoline rings of the two coordinated 3-methylisoquinoline molecules is 22.2 (3)°.

The structure of (I) is completed by N—H···O hydrogen bonds (Table 2) to result in chains propagating in [100].

Experimental

An aqueous solution (10 ml) of 6-amino-1-naphthalenesulfonic acid (0.1115 g, 0.5 mmol) was added to solid Ag₂CO₃ (0.069 g, 0.25 mmol) and stirred for several minutes until no further CO₂ was given off; 3-methylisoquinoline (0.0715 g, 0.5 mmol) in methanol (5 ml) was then added and a white precipitate formed. The precipitate was dissolved by dropwise addition of an aqueous solution of NH₃ (14 *M*). Crystals of (I) were obtained by evaporation of the solution for several days at room temperature.

Refinement

The N-bound H atoms were located in a difference map and their positions were freely refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

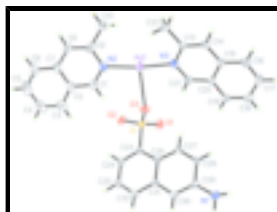


Fig. 1. The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

(6-Aminonaphthalene-1-sulfonato- κ O)bis(3-methylisoquinoline- κ N)silver(I)

Crystal data

[Ag(C ₁₀ H ₈ NO ₃ S)(C ₁₀ H ₉ N) ₂]	$Z = 2$
$M_r = 616.47$	$F_{000} = 628$
Triclinic, $P\bar{1}$	$D_x = 1.562 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 9.8810(14) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 10.2220(17) \text{ \AA}$	Cell parameters from 5933 reflections
$c = 13.256(2) \text{ \AA}$	$\theta = 2.0\text{--}28.3^\circ$
$\alpha = 80.108(11)^\circ$	$\mu = 0.89 \text{ mm}^{-1}$
$\beta = 86.653(11)^\circ$	$T = 292(2) \text{ K}$
$\gamma = 84.143(10)^\circ$	Block, colourless
$V = 1311.0(4) \text{ \AA}^3$	$0.35 \times 0.33 \times 0.29 \text{ mm}$

Data collection

Bruker SMART APEX CCD diffractometer	5933 independent reflections
Radiation source: fine-focus sealed tube	2404 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.064$
$T = 292(2) \text{ K}$	$\theta_{\text{max}} = 28.3^\circ$
ω scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.709$, $T_{\text{max}} = 0.766$	$k = -13 \rightarrow 10$
8844 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.074$	$w = 1/[\sigma^2(F_o^2)]$
$S = 0.76$	where $P = (F_o^2 + 2F_c^2)/3$
5933 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
351 parameters	$\Delta\rho_{\text{max}} = 0.38 \text{ e \AA}^{-3}$
3 restraints	$\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.45151 (4)	0.67693 (4)	0.24609 (3)	0.05828 (15)
C1	0.3993 (5)	0.4468 (5)	0.4152 (4)	0.0483 (13)
H1	0.4766	0.4132	0.3812	0.058*
C2	0.3389 (5)	0.3592 (5)	0.4960 (4)	0.0488 (14)
C3	0.3883 (6)	0.2245 (6)	0.5219 (5)	0.0706 (18)
H3	0.4644	0.1905	0.4868	0.085*
C4	0.3243 (7)	0.1436 (6)	0.5989 (5)	0.083 (2)
H4	0.3559	0.0539	0.6150	0.099*
C5	0.2106 (8)	0.1950 (7)	0.6541 (5)	0.089 (2)
H5	0.1692	0.1400	0.7078	0.107*
C6	0.1621 (6)	0.3237 (6)	0.6291 (4)	0.0735 (18)
H6	0.0869	0.3558	0.6662	0.088*
C7	0.2215 (5)	0.4123 (6)	0.5483 (4)	0.0534 (14)
C8	0.1762 (5)	0.5456 (5)	0.5152 (4)	0.0599 (15)
H8	0.1007	0.5837	0.5486	0.072*
C9	0.2389 (5)	0.6209 (5)	0.4359 (4)	0.0523 (14)
C10	0.1897 (5)	0.7653 (5)	0.3960 (4)	0.0753 (17)
H10A	0.1826	0.7775	0.3230	0.113*
H10B	0.2533	0.8227	0.4124	0.113*
H10C	0.1021	0.7870	0.4273	0.113*
C13	0.5358 (4)	0.9633 (4)	0.1512 (3)	0.0332 (11)
C14	0.6092 (4)	1.0543 (4)	0.0927 (3)	0.0397 (12)
H14	0.5902	1.1441	0.0973	0.048*
C15	0.7154 (4)	1.0151 (4)	0.0239 (3)	0.0359 (12)
C16	0.7952 (5)	1.1056 (5)	-0.0401 (4)	0.0494 (14)
H16	0.7775	1.1966	-0.0397	0.059*
C17	0.8978 (5)	1.0607 (5)	-0.1025 (4)	0.0533 (14)
H17	0.9502	1.1209	-0.1439	0.064*
C18	0.9241 (5)	0.9244 (5)	-0.1040 (4)	0.0497 (14)
H18	0.9947	0.8948	-0.1465	0.060*
C19	0.8488 (5)	0.8337 (5)	-0.0447 (3)	0.0445 (13)
H19	0.8675	0.7432	-0.0473	0.053*
C20	0.7421 (4)	0.8779 (4)	0.0207 (3)	0.0351 (11)

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C21	0.6583 (4)	0.7912 (4)	0.0831 (4)	0.0412 (13)
H21	0.6740	0.7007	0.0797	0.049*
C22	0.4221 (4)	1.0036 (4)	0.2248 (3)	0.0547 (14)
H22A	0.4298	0.9450	0.2895	0.082*
H22B	0.3358	0.9976	0.1970	0.082*
H22C	0.4288	1.0936	0.2344	0.082*
C23	0.8414 (4)	0.3038 (4)	0.2552 (3)	0.0328 (11)
C24	0.8408 (5)	0.1891 (4)	0.3251 (4)	0.0443 (13)
H24	0.7596	0.1508	0.3434	0.053*
C25	0.9623 (5)	0.1283 (4)	0.3697 (4)	0.0504 (14)
H25	0.9607	0.0495	0.4166	0.061*
C26	0.9638 (4)	0.3629 (4)	0.2255 (3)	0.0299 (11)
C27	0.9763 (4)	0.4796 (4)	0.1512 (3)	0.0349 (12)
H27	0.8980	0.5248	0.1217	0.042*
C28	1.0982 (4)	0.5274 (4)	0.1217 (3)	0.0383 (12)
H28	1.1019	0.6034	0.0720	0.046*
C29	1.2213 (4)	0.4623 (5)	0.1660 (4)	0.0383 (12)
C30	1.2132 (5)	0.3537 (4)	0.2412 (3)	0.0382 (12)
H30	1.2918	0.3133	0.2729	0.046*
C31	1.0875 (4)	0.3017 (4)	0.2714 (3)	0.0331 (11)
C32	1.0812 (5)	0.1832 (5)	0.3453 (4)	0.0496 (14)
H32	1.1599	0.1431	0.3772	0.060*
O1	0.7019 (3)	0.3847 (3)	0.0920 (2)	0.0576 (9)
O2	0.5813 (3)	0.2902 (3)	0.2478 (2)	0.0493 (9)
O3	0.6625 (3)	0.5087 (3)	0.2318 (2)	0.0513 (9)
S1	0.68386 (11)	0.37694 (12)	0.20242 (10)	0.0403 (3)
N1	1.3436 (4)	0.5164 (4)	0.1317 (3)	0.0478 (12)
N2	0.3539 (4)	0.5727 (4)	0.3847 (3)	0.0435 (10)
N3	0.5578 (4)	0.8287 (3)	0.1470 (3)	0.0403 (10)
H1N	1.419 (4)	0.461 (4)	0.147 (3)	0.060*
H2N	1.363 (5)	0.556 (4)	0.075 (3)	0.060*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0562 (3)	0.0463 (3)	0.0664 (3)	-0.0042 (2)	0.0173 (2)	0.0005 (2)
C1	0.051 (3)	0.056 (4)	0.042 (3)	-0.014 (3)	-0.004 (3)	-0.012 (3)
C2	0.057 (4)	0.050 (4)	0.043 (4)	-0.023 (3)	-0.013 (3)	-0.004 (3)
C3	0.071 (4)	0.061 (4)	0.081 (5)	-0.016 (4)	-0.017 (4)	-0.006 (4)
C4	0.100 (6)	0.061 (4)	0.087 (6)	-0.029 (4)	-0.046 (5)	0.012 (4)
C5	0.116 (6)	0.083 (5)	0.070 (5)	-0.056 (5)	-0.016 (5)	0.015 (4)
C6	0.097 (5)	0.088 (5)	0.037 (4)	-0.040 (4)	0.011 (3)	-0.001 (4)
C7	0.066 (4)	0.069 (4)	0.030 (3)	-0.029 (3)	0.005 (3)	-0.009 (3)
C8	0.068 (4)	0.070 (4)	0.045 (4)	-0.021 (3)	0.020 (3)	-0.019 (3)
C9	0.055 (4)	0.058 (4)	0.046 (4)	-0.011 (3)	0.015 (3)	-0.017 (3)
C10	0.076 (4)	0.064 (4)	0.077 (4)	0.004 (3)	0.029 (3)	-0.003 (4)
C13	0.033 (3)	0.030 (3)	0.036 (3)	-0.002 (2)	-0.005 (2)	-0.004 (2)
C14	0.046 (3)	0.028 (3)	0.048 (3)	-0.001 (2)	-0.006 (3)	-0.012 (3)

C15	0.035 (3)	0.034 (3)	0.039 (3)	-0.005 (2)	-0.009 (2)	-0.005 (2)
C16	0.055 (4)	0.040 (3)	0.056 (4)	-0.015 (3)	0.000 (3)	-0.010 (3)
C17	0.050 (3)	0.062 (4)	0.050 (4)	-0.022 (3)	0.000 (3)	-0.006 (3)
C18	0.046 (3)	0.060 (4)	0.048 (4)	-0.007 (3)	0.000 (3)	-0.024 (3)
C19	0.046 (3)	0.045 (3)	0.043 (3)	0.002 (3)	-0.001 (3)	-0.015 (3)
C20	0.035 (3)	0.032 (3)	0.041 (3)	-0.004 (2)	-0.006 (2)	-0.011 (3)
C21	0.043 (3)	0.032 (3)	0.051 (4)	-0.001 (2)	-0.005 (3)	-0.013 (3)
C22	0.048 (3)	0.054 (3)	0.063 (4)	-0.002 (3)	0.007 (3)	-0.017 (3)
C23	0.032 (3)	0.033 (3)	0.034 (3)	-0.003 (2)	0.001 (2)	-0.008 (2)
C24	0.050 (3)	0.036 (3)	0.048 (3)	-0.013 (3)	0.002 (3)	-0.005 (3)
C25	0.068 (4)	0.035 (3)	0.042 (3)	-0.003 (3)	-0.004 (3)	0.009 (3)
C26	0.034 (3)	0.026 (2)	0.029 (3)	0.001 (2)	-0.002 (2)	-0.006 (2)
C27	0.030 (3)	0.028 (3)	0.045 (3)	0.000 (2)	-0.006 (2)	-0.002 (2)
C28	0.040 (3)	0.031 (3)	0.043 (3)	-0.006 (2)	-0.007 (3)	0.000 (2)
C29	0.027 (3)	0.046 (3)	0.048 (3)	-0.005 (2)	-0.003 (3)	-0.021 (3)
C30	0.037 (3)	0.035 (3)	0.043 (3)	0.005 (2)	-0.012 (3)	-0.009 (3)
C31	0.037 (3)	0.035 (3)	0.028 (3)	0.000 (2)	-0.006 (2)	-0.007 (2)
C32	0.055 (4)	0.048 (3)	0.040 (3)	0.000 (3)	-0.004 (3)	0.010 (3)
O1	0.048 (2)	0.085 (3)	0.038 (2)	-0.0121 (19)	-0.0052 (18)	-0.002 (2)
O2	0.0342 (19)	0.048 (2)	0.068 (2)	-0.0149 (16)	0.0086 (18)	-0.0135 (18)
O3	0.0411 (19)	0.0293 (18)	0.084 (3)	0.0022 (15)	-0.0004 (18)	-0.0138 (18)
S1	0.0297 (7)	0.0384 (8)	0.0523 (9)	-0.0043 (6)	0.0004 (6)	-0.0065 (7)
N1	0.028 (2)	0.064 (3)	0.052 (3)	-0.010 (2)	0.000 (2)	-0.008 (3)
N2	0.051 (3)	0.044 (3)	0.037 (3)	-0.009 (2)	0.000 (2)	-0.011 (2)
N3	0.043 (2)	0.031 (2)	0.047 (3)	-0.0069 (19)	-0.006 (2)	-0.003 (2)

Geometric parameters (Å, °)

Ag1—N3	2.170 (4)	C18—C19	1.361 (6)
Ag1—N2	2.184 (4)	C18—H18	0.9300
Ag1—O3	2.583 (3)	C19—C20	1.414 (5)
C1—N2	1.321 (5)	C19—H19	0.9300
C1—C2	1.417 (6)	C20—C21	1.404 (6)
C1—H1	0.9300	C21—N3	1.337 (5)
C2—C3	1.404 (6)	C21—H21	0.9300
C2—C7	1.425 (6)	C22—H22A	0.9600
C3—C4	1.366 (7)	C22—H22B	0.9600
C3—H3	0.9300	C22—H22C	0.9600
C4—C5	1.411 (8)	C23—C24	1.364 (5)
C4—H4	0.9300	C23—C26	1.412 (5)
C5—C6	1.345 (7)	C23—S1	1.783 (4)
C5—H5	0.9300	C24—C25	1.407 (6)
C6—C7	1.419 (6)	C24—H24	0.9300
C6—H6	0.9300	C25—C32	1.351 (6)
C7—C8	1.393 (6)	C25—H25	0.9300
C8—C9	1.351 (6)	C26—C27	1.421 (5)
C8—H8	0.9300	C26—C31	1.434 (5)
C9—N2	1.380 (5)	C27—C28	1.358 (5)
C9—C10	1.520 (6)	C27—H27	0.9300

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C10—H10A	0.9600	C28—C29	1.432 (5)
C10—H10B	0.9600	C28—H28	0.9300
C10—H10C	0.9600	C29—C30	1.364 (6)
C13—C14	1.349 (5)	C29—N1	1.400 (5)
C13—N3	1.381 (5)	C30—C31	1.411 (5)
C13—C22	1.516 (5)	C30—H30	0.9300
C14—C15	1.422 (5)	C31—C32	1.425 (6)
C14—H14	0.9300	C32—H32	0.9300
C15—C20	1.408 (5)	O1—S1	1.453 (3)
C15—C16	1.414 (6)	O2—S1	1.450 (3)
C16—C17	1.364 (6)	O3—S1	1.457 (3)
C16—H16	0.9300	N1—H1N	0.90 (3)
C17—C18	1.394 (6)	N1—H2N	0.81 (3)
C17—H17	0.9300		
N3—Ag1—N2	159.18 (13)	C21—C20—C19	123.2 (4)
N3—Ag1—O3	89.17 (12)	C15—C20—C19	119.5 (5)
N2—Ag1—O3	98.76 (13)	N3—C21—C20	125.0 (4)
N2—C1—C2	124.9 (5)	N3—C21—H21	117.5
N2—C1—H1	117.5	C20—C21—H21	117.5
C2—C1—H1	117.5	C13—C22—H22A	109.5
C3—C2—C1	122.3 (6)	C13—C22—H22B	109.5
C3—C2—C7	120.7 (5)	H22A—C22—H22B	109.5
C1—C2—C7	117.0 (5)	C13—C22—H22C	109.5
C4—C3—C2	119.9 (6)	H22A—C22—H22C	109.5
C4—C3—H3	120.1	H22B—C22—H22C	109.5
C2—C3—H3	120.1	C24—C23—C26	120.7 (4)
C3—C4—C5	120.5 (6)	C24—C23—S1	118.3 (4)
C3—C4—H4	119.8	C26—C23—S1	121.0 (3)
C5—C4—H4	119.8	C23—C24—C25	120.5 (4)
C6—C5—C4	120.0 (7)	C23—C24—H24	119.8
C6—C5—H5	120.0	C25—C24—H24	119.8
C4—C5—H5	120.0	C32—C25—C24	120.8 (5)
C5—C6—C7	122.5 (6)	C32—C25—H25	119.6
C5—C6—H6	118.8	C24—C25—H25	119.6
C7—C6—H6	118.8	C23—C26—C27	125.2 (4)
C8—C7—C6	126.5 (6)	C23—C26—C31	118.9 (4)
C8—C7—C2	117.0 (5)	C27—C26—C31	115.9 (4)
C6—C7—C2	116.5 (5)	C28—C27—C26	122.4 (4)
C9—C8—C7	121.8 (5)	C28—C27—H27	118.8
C9—C8—H8	119.1	C26—C27—H27	118.8
C7—C8—H8	119.1	C27—C28—C29	120.8 (4)
C8—C9—N2	122.5 (5)	C27—C28—H28	119.6
C8—C9—C10	123.1 (5)	C29—C28—H28	119.6
N2—C9—C10	114.4 (5)	C30—C29—N1	123.4 (4)
C9—C10—H10A	109.5	C30—C29—C28	118.7 (4)
C9—C10—H10B	109.5	N1—C29—C28	117.9 (5)
H10A—C10—H10B	109.5	C29—C30—C31	121.0 (4)
C9—C10—H10C	109.5	C29—C30—H30	119.5
H10A—C10—H10C	109.5	C31—C30—H30	119.5

H10B—C10—H10C	109.5	C30—C31—C32	120.7 (4)
C14—C13—N3	122.4 (4)	C30—C31—C26	121.0 (4)
C14—C13—C22	121.6 (4)	C32—C31—C26	118.2 (4)
N3—C13—C22	116.0 (4)	C25—C32—C31	120.8 (4)
C13—C14—C15	121.0 (4)	C25—C32—H32	119.6
C13—C14—H14	119.5	C31—C32—H32	119.6
C15—C14—H14	119.5	S1—O3—Ag1	134.03 (16)
C20—C15—C16	118.8 (4)	O2—S1—O1	113.23 (19)
C20—C15—C14	117.5 (4)	O2—S1—O3	112.74 (17)
C16—C15—C14	123.7 (4)	O1—S1—O3	111.9 (2)
C17—C16—C15	120.6 (5)	O2—S1—C23	106.3 (2)
C17—C16—H16	119.7	O1—S1—C23	106.46 (19)
C15—C16—H16	119.7	O3—S1—C23	105.52 (18)
C16—C17—C18	120.0 (5)	C29—N1—H1N	115 (3)
C16—C17—H17	120.0	C29—N1—H2N	128 (3)
C18—C17—H17	120.0	H1N—N1—H2N	103 (4)
C19—C18—C17	121.5 (5)	C1—N2—C9	116.8 (4)
C19—C18—H18	119.3	C1—N2—Ag1	116.9 (3)
C17—C18—H18	119.3	C9—N2—Ag1	125.9 (4)
C18—C19—C20	119.6 (4)	C21—N3—C13	116.8 (4)
C18—C19—H19	120.2	C21—N3—Ag1	119.1 (3)
C20—C19—H19	120.2	C13—N3—Ag1	123.9 (3)
C21—C20—C15	117.3 (4)		
N2—C1—C2—C3	177.0 (4)	C27—C28—C29—C30	-2.2 (6)
N2—C1—C2—C7	-0.7 (7)	C27—C28—C29—N1	179.7 (4)
C1—C2—C3—C4	-178.5 (5)	N1—C29—C30—C31	-178.8 (4)
C7—C2—C3—C4	-0.8 (8)	C28—C29—C30—C31	3.2 (6)
C2—C3—C4—C5	-1.4 (9)	C29—C30—C31—C32	176.0 (4)
C3—C4—C5—C6	1.9 (9)	C29—C30—C31—C26	-1.2 (6)
C4—C5—C6—C7	-0.2 (9)	C23—C26—C31—C30	177.3 (4)
C5—C6—C7—C8	178.1 (6)	C27—C26—C31—C30	-1.9 (6)
C5—C6—C7—C2	-1.9 (8)	C23—C26—C31—C32	0.1 (6)
C3—C2—C7—C8	-177.6 (5)	C27—C26—C31—C32	-179.1 (4)
C1—C2—C7—C8	0.2 (7)	C24—C25—C32—C31	-2.0 (7)
C3—C2—C7—C6	2.4 (7)	C30—C31—C32—C25	-175.8 (4)
C1—C2—C7—C6	-179.8 (4)	C26—C31—C32—C25	1.5 (6)
C6—C7—C8—C9	-178.8 (5)	N3—Ag1—O3—S1	-126.1 (3)
C2—C7—C8—C9	1.1 (7)	N2—Ag1—O3—S1	73.2 (3)
C7—C8—C9—N2	-2.1 (8)	Ag1—O3—S1—O2	-44.1 (3)
C7—C8—C9—C10	178.2 (5)	Ag1—O3—S1—O1	84.9 (3)
N3—C13—C14—C15	-0.9 (7)	Ag1—O3—S1—C23	-159.8 (2)
C22—C13—C14—C15	-179.9 (4)	C24—C23—S1—O2	-1.0 (4)
C13—C14—C15—C20	-1.1 (6)	C26—C23—S1—O2	179.0 (3)
C13—C14—C15—C16	179.4 (4)	C24—C23—S1—O1	-122.0 (4)
C20—C15—C16—C17	-1.2 (6)	C26—C23—S1—O1	58.0 (4)
C14—C15—C16—C17	178.3 (4)	C24—C23—S1—O3	118.9 (4)
C15—C16—C17—C18	0.5 (7)	C26—C23—S1—O3	-61.0 (4)
C16—C17—C18—C19	0.4 (7)	C2—C1—N2—C9	-0.1 (7)
C17—C18—C19—C20	-0.5 (7)	C2—C1—N2—Ag1	-172.5 (3)

supplementary materials

C16—C15—C20—C21	-178.2 (4)	C8—C9—N2—C1	1.5 (7)
C14—C15—C20—C21	2.3 (6)	C10—C9—N2—C1	-178.7 (4)
C16—C15—C20—C19	1.0 (6)	C8—C9—N2—Ag1	173.1 (4)
C14—C15—C20—C19	-178.5 (4)	C10—C9—N2—Ag1	-7.1 (6)
C18—C19—C20—C21	179.0 (4)	N3—Ag1—N2—C1	-125.3 (4)
C18—C19—C20—C15	-0.2 (6)	O3—Ag1—N2—C1	-13.9 (3)
C15—C20—C21—N3	-1.8 (7)	N3—Ag1—N2—C9	63.1 (6)
C19—C20—C21—N3	179.0 (4)	O3—Ag1—N2—C9	174.5 (3)
C26—C23—C24—C25	0.7 (7)	C20—C21—N3—C13	0.0 (6)
S1—C23—C24—C25	-179.3 (3)	C20—C21—N3—Ag1	-174.9 (3)
C23—C24—C25—C32	0.9 (7)	C14—C13—N3—C21	1.4 (6)
C24—C23—C26—C27	178.0 (4)	C22—C13—N3—C21	-179.5 (4)
S1—C23—C26—C27	-2.1 (6)	C14—C13—N3—Ag1	176.0 (3)
C24—C23—C26—C31	-1.1 (6)	C22—C13—N3—Ag1	-4.9 (5)
S1—C23—C26—C31	178.9 (3)	N2—Ag1—N3—C21	136.8 (4)
C23—C26—C27—C28	-176.2 (4)	O3—Ag1—N3—C21	23.9 (3)
C31—C26—C27—C28	2.9 (6)	N2—Ag1—N3—C13	-37.6 (6)
C26—C27—C28—C29	-0.9 (6)	O3—Ag1—N3—C13	-150.6 (3)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N \cdots O2 ⁱ	0.90 (4)	2.51 (4)	3.365 (5)	160 (3)
N1—H2N \cdots O1 ⁱⁱ	0.81 (4)	2.30 (4)	3.008 (5)	146 (4)

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

Fig. 1

