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Bis[μ-1,2-bis(1*H*-imidazol-1-ylmethyl)benzene-κ^2N:N']disilver(I) bis(4-aminobenzenesulfonate) hexahydrate

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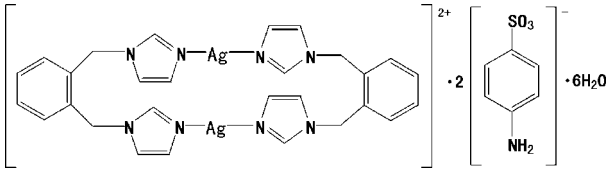
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.091; data-to-parameter ratio = 16.1.

In the binuclear cation of the title compound, $[Ag_2(C_{14}H_{14}N_4)_2](C_6H_6NO_3S)_2\cdot 6H_2O$, two Ag^I atoms are bridged by two 1,2-bis[(1*H*-imidazol-1-yl)methyl]benzene (IBI) ligands to form a 22-membered ring with crystallographic twofold rotation symmetry. Each Ag^I atom is two-coordinate, with a slightly distorted linear coordination geometry. The sulfonate anion does not coordinate to the silver ion but acts as a counteranion.

Related literature

For studies on silver sulfonates, see: Liu *et al.* (2007); Li *et al.* (2006). For related literature, see: Aakeröy & Beatty (1998); Cote & Shimizu (2004); Shimizu *et al.* (1998); Smith *et al.* (1996).



Experimental

Crystal data

$[Ag_2(C_{14}H_{14}N_4)_2](C_6H_6NO_3S)_2\cdot 6H_2O$
M_r = 1144.78
Monoclinic, $C2/c$
a = 14.842 (3) Å
b = 16.283 (3) Å
c = 19.527 (4) Å
β = 104.76 (3)°
V = 4563.6 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 293 (2) K
0.27 × 0.26 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.698, T_{max} = 0.811
22007 measured reflections
5221 independent reflections
4333 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.091
S = 1.06
5221 reflections
324 parameters
11 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N5	2.102 (2)	Ag1—N4	2.103 (2)
N5—Ag1—N4	176.46 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···$OW1^{i}$	0.85 (3)	2.16 (3)	3.003 (4)	173 (4)
$OW1$—H1A···$OW2^{ii}$	0.85 (4)	1.95 (4)	2.800 (5)	175 (5)
$OW3$—H3A···O3	0.85 (5)	2.35 (9)	2.815 (4)	115 (8)
$OW1$—H1B···O1	0.86 (5)	2.12 (5)	2.963 (4)	171 (5)
$OW2$—H2A···O2	0.84 (5)	1.95 (5)	2.775 (4)	169 (7)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; 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: GW2032).

References

Aakeröy, C. B. & Beatty, A. M. (1998). *Chem. Commun.* pp. 1067–1068.
Cote, A. P. & Shimizu, G. K. H. (2004). *Inorg. Chem.* **43**, 6663–6673.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Li, F.-F., Ma, J.-F., Song, S.-Y., Yang, J., Jia, H.-Q. & Hu, N.-H. (2006). *Cryst. Growth Des.* **6**, 209–215.
Liu, H.-Y., Wu, H., Ma, J.-F., Song, S.-Y., Yang, J., Liu, Y.-Y. & Su, Z.-M. (2007). *Inorg. Chem.* **46**, 7299–7311.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shimizu, G. K. H., Enright, G. D., Ratcliffe, C. I., Rego, G. S., Ried, J. L. & Ripmeester, J. A. (1998). *Chem. Mater.* **10**, 3282–3283.
Smith, G., Lynch, D. E. & Kennard, C. H. L. (1996). *Inorg. Chem.* **35**, 2711–2712.

supplementary materials

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Bis[μ-1,2-bis(1*H*-imidazol-1-ylmethyl)benzene-κ^2N:*N*']disilver(I) bis(4-aminobenzenesulfonate) hexahydrate

H.-Y. Liu, H.-M. Sun and J.-F. Ma

Comment

Over the past decades, the design and synthesis of Ag(I) compounds have attracted great attention because of the versatility of their coordination geometries (Aakeröy & Beatty, 1998; Smith *et al.*, 1996). In particular, silver-sulfonate complexes have attracted great attention by reason of their abilities to form inorganic-organic lamellar structures and intercalate guest molecules (Shimizu *et al.*, 1998; Cote & Shimizu, 2004; Liu *et al.*, 2007). In this paper, the synthesis and the crystal structure of a novel silver-sulfonate complex (I) $[Ag_2(IBI)_2]L_2 \cdot 6H_2O$ (IBI = 1,2-bis ((1*H*-imidazol-1-yl)methyl)benzene and *L* = *p*-aminobenzenesulfonic acid) is presented.

The molecular structure of (I) is shown in Fig.1. Selected bond distances and angles are listed in Table 1. The compound (I) shows a binuclear structure, where each of Ag(I) atoms has a slightly distorted linear geometry and is coordinated by two N atoms from the IBI ligands. The Ag—N (IBI) distances in (I) are near to that in the related compounds (Li *et al.*, 2006). Notably, the *L* ligand does not coordinate to the Ag(I) center, acting as a counter-anion. Finally, N—H···O and O—H···O hydrogen bonds between water molecules and the *L* ligands result in the formation of a three-dimensional network (Table 2).

Experimental

An aqueous solution (10 ml) of *p*-aminobenzenesulfonic acid (0.5 mmol) was added to solid Ag_2CO_3 (0.25 mmol) and stirred for several minutes until no further CO_2 was given off. The 1-(3-(1*H*-imidazol-1-yl)methyl)benzyl)-1*H*-imidazole (0.5 mmol) was then added and a precipitate was formed. The precipitate was dissolved by ammonium hydroxide. Crystals of (I) were obtained by evaporation of the solution for several days at room temperature.

Refinement

H atoms bonded to N atom were located in a difference map and refined with distance restraints of N—H = 0.85±0.01 Å. H atoms bonded to C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier). H atoms bonded to O atoms of water molecules were located in a difference Fourier map and refined isotropically with distance restraints of O—H = 0.85±0.01 Å and H···H = 1.3±0.01 Å, with U_{iso}(H) = 1.5 U_{eq}(N).

Figures

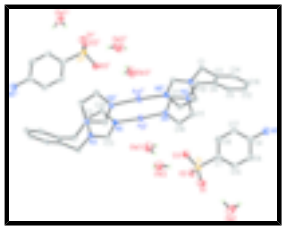


Fig. 1. The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.

Bis[μ-1,2-bis(1*H*-imidazol-1-ylmethyl)benzene- κ^2N,N']disilver(I)] bis(4-aminobenzenesulfonate) hexahydrate

Crystal data

$[Ag_2(C_{14}H_{14}N_4)_2](C_6H_6NO_3S)_2{\cdot}6H_2O$	$F_{000} = 2336$
$M_r = 1144.78$	$D_x = 1.666$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 5221 reflections
$a = 14.842$ (3) Å	$\theta = 3.1$–27.5º
$b = 16.283$ (3) Å	$\mu = 1.02$ mm^{-1}
$c = 19.527$ (4) Å	$T = 293$ (2) K
$\beta = 104.76$ (3)º	Block, colorless
$V = 4563.6$ (16) Å^3	0.27 × 0.26 × 0.19 mm
$Z = 4$	

Data collection

Rigaku RAXIS-RAPID diffractometer	5221 independent reflections
Radiation source: fine-focus sealed tube	4333 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 293(2)$ K	$\theta_{min} = 3.1$º
ω scans	$h = -19\rightarrow15$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -20\rightarrow21$
$T_{min} = 0.698$, $T_{max} = 0.811$	$l = -25\rightarrow25$
22007 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 5.1924P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.004$
5221 reflections	$\Delta\rho_{max} = 0.91$ e Å^{-3}
324 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
11 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.449998 (13)	1.092109 (13)	0.518907 (12)	0.04061 (9)
C1	0.18894 (16)	0.84749 (15)	0.31821 (13)	0.0290 (5)
H1AA	0.1922	0.7939	0.2973	0.035*
H2AA	0.1956	0.8887	0.2840	0.035*
C2	0.73559 (17)	1.15989 (15)	0.54897 (13)	0.0319 (5)
H2	0.7865	1.1780	0.5335	0.038*
C3	0.09499 (15)	0.85728 (14)	0.33396 (12)	0.0256 (5)
C4	0.26422 (17)	1.05237 (15)	0.41358 (14)	0.0321 (5)
H4	0.2926	1.0561	0.3764	0.039*
C5	−0.03160 (17)	0.93772 (16)	0.35446 (13)	0.0329 (5)
H5	−0.0578	0.9886	0.3593	0.040*
C6	0.05636 (15)	0.93418 (14)	0.34222 (12)	0.0257 (5)
C7	0.16588 (19)	0.85770 (15)	0.66231 (14)	0.0347 (6)
C8	0.0204 (2)	0.78904 (17)	0.65491 (16)	0.0422 (6)
H8	−0.0197	0.7628	0.6775	0.051*
C9	−0.0061 (2)	0.79756 (15)	0.58140 (16)	0.0387 (6)
C10	0.10692 (17)	1.01380 (14)	0.33853 (13)	0.0312 (5)
H10A	0.1393	1.0100	0.3013	0.037*
H10B	0.0618	1.0580	0.3264	0.037*
C11	0.15902 (17)	1.03440 (16)	0.47255 (14)	0.0343 (5)
H11	0.1030	1.0236	0.4840	0.041*
C12	−0.08107 (17)	0.86696 (18)	0.35968 (14)	0.0362 (6)
H12	−0.1400	0.8703	0.3679	0.043*
C13	0.64699 (16)	1.12020 (16)	0.61609 (14)	0.0310 (5)
H13	0.6271	1.1062	0.6560	0.037*

C14	0.04452 (17)	0.78665 (15)	0.33941 (14)	0.0324 (5)
H14	0.0698	0.7355	0.3341	0.039*
C15	0.1045 (2)	0.81852 (16)	0.69489 (15)	0.0402 (6)
H15	0.1202	0.8122	0.7438	0.048*
C16	−0.04243 (18)	0.79123 (17)	0.35252 (14)	0.0372 (6)
H16	−0.0750	0.7434	0.3565	0.045*
C17	0.0561 (2)	0.83721 (17)	0.54977 (15)	0.0422 (6)
H17	0.0405	0.8438	0.5009	0.051*
C18	0.24085 (17)	1.05413 (17)	0.51802 (14)	0.0358 (6)
H18	0.2508	1.0594	0.5668	0.043*
C19	0.1406 (2)	0.86694 (17)	0.58966 (15)	0.0389 (6)
H19	0.1807	0.8934	0.5673	0.047*
C20	0.64898 (17)	1.14382 (16)	0.50806 (14)	0.0344 (5)
H20	0.6303	1.1489	0.4590	0.041*
N1	−0.0886 (2)	0.76439 (16)	0.54189 (17)	0.0481 (6)
H1N	−0.132 (2)	0.760 (3)	0.563 (2)	0.084 (15)*
H2N	−0.109 (3)	0.783 (3)	0.4999 (10)	0.080 (14)*
N2	0.17443 (13)	1.03327 (11)	0.40591 (11)	0.0268 (4)
N3	0.73354 (13)	1.14420 (11)	0.61745 (10)	0.0244 (4)
N4	0.30739 (14)	1.06528 (13)	0.48088 (12)	0.0339 (5)
N5	0.59315 (14)	1.11888 (13)	0.55039 (12)	0.0313 (4)
O1	0.29951 (17)	0.85170 (14)	0.77672 (12)	0.0566 (6)
O2	0.25394 (14)	0.98490 (12)	0.72646 (12)	0.0474 (5)
O3	0.33681 (15)	0.89252 (13)	0.66753 (12)	0.0497 (5)
S1	0.27191 (5)	0.89939 (4)	0.71192 (4)	0.03645 (15)
OW1	0.2289 (2)	0.74243 (17)	0.87271 (17)	0.0708 (7)
H1B	0.243 (4)	0.774 (3)	0.842 (2)	0.106*
H1A	0.202 (3)	0.701 (2)	0.850 (3)	0.106*
OW2	0.3692 (4)	1.10983 (19)	0.7022 (2)	0.1041 (13)
H2A	0.331 (3)	1.072 (3)	0.703 (4)	0.156*
H2B	0.421 (2)	1.085 (3)	0.712 (4)	0.156*
OW3	0.5016 (4)	0.9682 (4)	0.6533 (2)	0.167 (3)
H3A	0.445 (2)	0.983 (5)	0.638 (4)	0.250*
H3B	0.496 (7)	0.929 (4)	0.680 (4)	0.250*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02279 (11)	0.04981 (14)	0.04500 (14)	−0.00688 (7)	0.00086 (8)	−0.00582 (9)
C1	0.0220 (11)	0.0381 (12)	0.0248 (12)	0.0044 (8)	0.0022 (9)	−0.0043 (9)
C2	0.0251 (12)	0.0412 (13)	0.0291 (12)	−0.0012 (9)	0.0062 (10)	0.0036 (10)
C3	0.0201 (11)	0.0311 (11)	0.0220 (11)	0.0015 (8)	−0.0010 (8)	−0.0034 (9)
C4	0.0282 (12)	0.0318 (12)	0.0370 (14)	−0.0042 (9)	0.0094 (10)	−0.0011 (10)
C5	0.0251 (12)	0.0416 (13)	0.0283 (12)	0.0083 (9)	−0.0002 (9)	−0.0088 (10)
C6	0.0213 (11)	0.0304 (11)	0.0214 (11)	0.0017 (8)	−0.0019 (8)	−0.0040 (9)
C7	0.0453 (15)	0.0265 (11)	0.0358 (14)	0.0102 (10)	0.0165 (12)	0.0000 (10)
C8	0.0500 (17)	0.0365 (14)	0.0460 (16)	−0.0001 (11)	0.0227 (14)	0.0025 (12)
C9	0.0464 (16)	0.0290 (12)	0.0427 (15)	0.0064 (10)	0.0151 (12)	−0.0049 (11)

C10	0.0315 (12)	0.0298 (11)	0.0276 (12)	0.0018 (9)	−0.0010 (10)	0.0011 (9)
C11	0.0272 (12)	0.0429 (13)	0.0336 (13)	0.0003 (10)	0.0092 (10)	−0.0071 (11)
C12	0.0199 (11)	0.0568 (16)	0.0309 (13)	−0.0026 (10)	0.0048 (10)	−0.0062 (12)
C13	0.0232 (11)	0.0395 (12)	0.0310 (12)	−0.0010 (9)	0.0080 (10)	−0.0025 (10)
C14	0.0289 (12)	0.0311 (12)	0.0335 (13)	−0.0007 (9)	0.0014 (10)	−0.0070 (10)
C15	0.0535 (17)	0.0386 (14)	0.0329 (14)	0.0074 (11)	0.0192 (12)	0.0033 (11)
C16	0.0279 (13)	0.0459 (14)	0.0341 (14)	−0.0114 (10)	0.0010 (10)	−0.0030 (11)
C17	0.0531 (17)	0.0447 (15)	0.0313 (14)	0.0009 (12)	0.0152 (13)	0.0001 (11)
C18	0.0291 (13)	0.0448 (14)	0.0322 (13)	−0.0001 (10)	0.0053 (10)	−0.0109 (11)
C19	0.0465 (16)	0.0397 (14)	0.0358 (14)	0.0012 (11)	0.0200 (12)	0.0004 (11)
C20	0.0292 (13)	0.0431 (14)	0.0281 (12)	0.0003 (10)	0.0024 (10)	0.0015 (10)
N1	0.0451 (15)	0.0444 (14)	0.0557 (17)	0.0000 (11)	0.0141 (13)	−0.0051 (13)
N2	0.0242 (9)	0.0254 (9)	0.0289 (10)	−0.0003 (7)	0.0032 (8)	−0.0026 (8)
N3	0.0194 (9)	0.0280 (9)	0.0250 (10)	0.0024 (7)	0.0043 (7)	−0.0013 (7)
N4	0.0272 (11)	0.0335 (10)	0.0393 (12)	−0.0019 (8)	0.0051 (9)	−0.0037 (9)
N5	0.0238 (10)	0.0352 (10)	0.0334 (11)	0.0020 (8)	0.0044 (8)	−0.0024 (9)
O1	0.0655 (15)	0.0591 (13)	0.0405 (12)	0.0144 (11)	0.0052 (11)	0.0087 (10)
O2	0.0445 (11)	0.0367 (10)	0.0614 (14)	0.0059 (8)	0.0144 (10)	−0.0101 (9)
O3	0.0419 (12)	0.0608 (13)	0.0496 (13)	0.0099 (9)	0.0177 (10)	−0.0103 (10)
S1	0.0411 (4)	0.0358 (3)	0.0335 (3)	0.0124 (2)	0.0114 (3)	−0.0012 (3)
OW1	0.0701 (18)	0.0705 (17)	0.083 (2)	0.0168 (13)	0.0392 (16)	0.0159 (15)
OW2	0.160 (4)	0.0675 (19)	0.082 (2)	−0.043 (2)	0.024 (3)	−0.0034 (17)
OW3	0.179 (4)	0.240 (6)	0.075 (3)	−0.151 (4)	0.020 (3)	0.016 (3)

Geometric parameters (Å, °)

Ag1—N5	2.102 (2)	C11—N2	1.378 (3)
Ag1—N4	2.103 (2)	C11—H11	0.9300
C1—N3^{i}	1.478 (3)	C12—C16	1.382 (4)
C1—C3	1.511 (3)	C12—H12	0.9300
C1—H1AA	0.9700	C13—N5	1.328 (3)
C1—H2AA	0.9700	C13—N3	1.336 (3)
C2—C20	1.355 (4)	C13—H13	0.9300
C2—N3	1.369 (3)	C14—C16	1.380 (4)
C2—H2	0.9300	C14—H14	0.9300
C3—C14	1.391 (3)	C15—H15	0.9300
C3—C6	1.404 (3)	C16—H16	0.9300
C4—N4	1.324 (3)	C17—C19	1.384 (4)
C4—N2	1.339 (3)	C17—H17	0.9300
C4—H4	0.9300	C18—N4	1.378 (3)
C5—C12	1.384 (4)	C18—H18	0.9300
C5—C6	1.387 (3)	C19—H19	0.9300
C5—H5	0.9300	C20—N5	1.373 (3)
C6—C10	1.509 (3)	C20—H20	0.9300
C7—C19	1.380 (4)	N1—H1N	0.85 (3)
C7—C15	1.392 (4)	N1—H2N	0.85 (3)
C7—S1	1.761 (3)	N3—C1^{i}	1.478 (3)
C8—C15	1.379 (4)	O1—S1	1.452 (2)
C8—C9	1.395 (4)	O2—S1	1.459 (2)

C8—H8	0.9300	O3—S1	1.455 (2)
C9—N1	1.380 (4)	OW1—H1B	0.86 (5)
C9—C17	1.393 (4)	OW1—H1A	0.85 (4)
C10—N2	1.471 (3)	OW2—H2A	0.84 (5)
C10—H10A	0.9700	OW2—H2B	0.85 (4)
C10—H10B	0.9700	OW3—H3A	0.85 (5)
C11—C18	1.348 (4)	OW3—H3B	0.84 (7)
N5—Ag1—N4	176.46 (9)	C16—C14—C3	121.1 (2)
$N3^{i}$—C1—C3	112.11 (19)	C16—C14—H14	119.4
$N3^{i}$—C1—H1AA	109.2	C3—C14—H14	119.4
C3—C1—H1AA	109.2	C8—C15—C7	120.3 (3)
$N3^{i}$—C1—H2AA	109.2	C8—C15—H15	119.9
C3—C1—H2AA	109.2	C7—C15—H15	119.9
H1AA—C1—H2AA	107.9	C14—C16—C12	119.9 (2)
C20—C2—N3	106.6 (2)	C14—C16—H16	120.0
C20—C2—H2	126.7	C12—C16—H16	120.0
N3—C2—H2	126.7	C19—C17—C9	121.3 (3)
C14—C3—C6	119.0 (2)	C19—C17—H17	119.3
C14—C3—C1	118.1 (2)	C9—C17—H17	119.3
C6—C3—C1	122.9 (2)	C11—C18—N4	109.3 (2)
N4—C4—N2	111.4 (2)	C11—C18—H18	125.3
N4—C4—H4	124.3	N4—C18—H18	125.3
N2—C4—H4	124.3	C7—C19—C17	120.7 (3)
C12—C5—C6	121.2 (2)	C7—C19—H19	119.7
C12—C5—H5	119.4	C17—C19—H19	119.7
C6—C5—H5	119.4	C2—C20—N5	109.3 (2)
C5—C6—C3	119.1 (2)	C2—C20—H20	125.4
C5—C6—C10	118.3 (2)	N5—C20—H20	125.4
C3—C6—C10	122.6 (2)	C9—N1—H1N	115 (3)
C19—C7—C15	118.8 (3)	C9—N1—H2N	117 (3)
C19—C7—S1	119.6 (2)	H1N—N1—H2N	111 (4)
C15—C7—S1	121.5 (2)	C4—N2—C11	106.9 (2)
C15—C8—C9	121.7 (3)	C4—N2—C10	125.6 (2)
C15—C8—H8	119.2	C11—N2—C10	127.5 (2)
C9—C8—H8	119.2	C13—N3—C2	107.2 (2)
N1—C9—C17	121.8 (3)	C13—N3—$C1^{i}$	125.4 (2)
N1—C9—C8	120.9 (3)	C2—N3—$C1^{i}$	127.4 (2)
C17—C9—C8	117.2 (3)	C4—N4—C18	105.7 (2)
N2—C10—C6	112.10 (19)	C4—N4—Ag1	124.93 (18)
N2—C10—H10A	109.2	C18—N4—Ag1	129.30 (18)
C6—C10—H10A	109.2	C13—N5—C20	105.7 (2)
N2—C10—H10B	109.2	C13—N5—Ag1	126.94 (18)
C6—C10—H10B	109.2	C20—N5—Ag1	127.27 (17)
H10A—C10—H10B	107.9	O1—S1—O3	113.29 (14)
C18—C11—N2	106.7 (2)	O1—S1—O2	111.45 (14)
C18—C11—H11	126.7	O3—S1—O2	111.77 (13)
N2—C11—H11	126.7	O1—S1—C7	106.71 (14)
C16—C12—C5	119.6 (2)	O3—S1—C7	106.10 (13)

C16—C12—H12	120.2	O2—S1—C7	107.04 (12)
C5—C12—H12	120.2	H1B—OW1—H1A	106 (5)
N5—C13—N3	111.3 (2)	H2A—OW2—H2B	103 (5)
N5—C13—H13	124.4	H3A—OW3—H3B	101 (9)
N3—C13—H13	124.4		
N3^{i}—C1—C3—C14	−100.7 (2)	N3—C2—C20—N5	0.4 (3)
N3^{i}—C1—C3—C6	80.3 (3)	N4—C4—N2—C11	0.3 (3)
C12—C5—C6—C3	1.0 (4)	N4—C4—N2—C10	−178.9 (2)
C12—C5—C6—C10	−178.9 (2)	C18—C11—N2—C4	−0.1 (3)
C14—C3—C6—C5	−1.0 (3)	C18—C11—N2—C10	179.0 (2)
C1—C3—C6—C5	178.0 (2)	C6—C10—N2—C4	128.4 (2)
C14—C3—C6—C10	178.8 (2)	C6—C10—N2—C11	−50.6 (3)
C1—C3—C6—C10	−2.1 (3)	N5—C13—N3—C2	0.5 (3)
C15—C8—C9—N1	177.0 (3)	N5—C13—N3—C1^{i}	180.0 (2)
C15—C8—C9—C17	0.0 (4)	C20—C2—N3—C13	−0.5 (3)
C5—C6—C10—N2	98.1 (2)	C20—C2—N3—C1^{i}	−180.0 (2)
C3—C6—C10—N2	−81.7 (3)	N2—C4—N4—C18	−0.3 (3)
C6—C5—C12—C16	−0.1 (4)	N2—C4—N4—Ag1	177.37 (15)
C6—C3—C14—C16	0.2 (4)	C11—C18—N4—C4	0.3 (3)
C1—C3—C14—C16	−178.9 (2)	C11—C18—N4—Ag1	−177.31 (18)
C9—C8—C15—C7	−0.3 (4)	N3—C13—N5—C20	−0.3 (3)
C19—C7—C15—C8	0.5 (4)	N3—C13—N5—Ag1	−176.41 (15)
S1—C7—C15—C8	177.7 (2)	C2—C20—N5—C13	−0.1 (3)
C3—C14—C16—C12	0.7 (4)	C2—C20—N5—Ag1	176.04 (17)
C5—C12—C16—C14	−0.8 (4)	C19—C7—S1—O1	−155.0 (2)
N1—C9—C17—C19	−177.0 (3)	C15—C7—S1—O1	27.9 (2)
C8—C9—C17—C19	−0.1 (4)	C19—C7—S1—O3	−33.9 (2)
N2—C11—C18—N4	−0.1 (3)	C15—C7—S1—O3	149.0 (2)
C15—C7—C19—C17	−0.6 (4)	C19—C7—S1—O2	85.6 (2)
S1—C7—C19—C17	−177.7 (2)	C15—C7—S1—O2	−91.5 (2)
C9—C17—C19—C7	0.3 (4)		

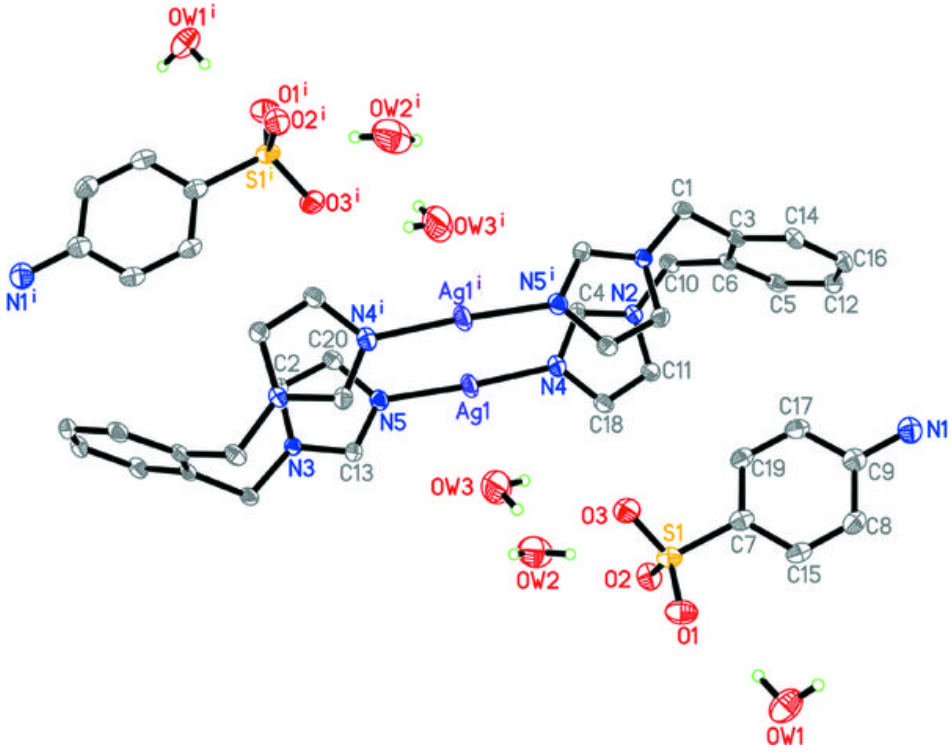
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···OW1^{ii}	0.85 (3)	2.16 (3)	3.003 (4)	173 (4)
OW1—H1A···OW2^{iii}	0.85 (4)	1.95 (4)	2.800 (5)	175 (5)
OW3—H3A···O3	0.85 (5)	2.35 (9)	2.815 (4)	115 (8)
OW1—H1B···O1	0.86 (5)	2.12 (5)	2.963 (4)	171 (5)
OW2—H2A···O2	0.84 (5)	1.95 (5)	2.775 (4)	169 (7)

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

Fig. 1


OW1i
O1i
O2i
OW2i
S1i
O3i
OW3i
N1i
N4i
Ag1i
N5i
C1
C3
C14
C16
C10
C6
C5
C12
C4
N2
C20
C2
C11
N5
Ag1
N4
C18
N3
C13
OW3
O3
S1
C7
C17
N1
C19
C9
C8
C15
OW2
O2
O1
OW1