

Bis(μ -pyridine-1-carbaldehyde azine- $\kappa^2N,N':\kappa^2N'',N'''$)disilver(I) bis(methanesulfonate)

Grant A. Broker and Edward R. T. Tiekink*

Department of Chemistry, University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249-0698, USA

Correspondence e-mail: edward.tiekink@utsa.edu

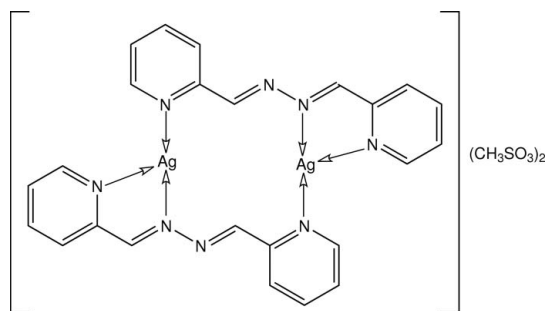
Received 11 August 2007; accepted 12 August 2007

 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.029; wR factor = 0.067; data-to-parameter ratio = 14.3.

The asymmetric unit of the title compound, $[Ag_2(C_{12}H_{10}N_4)_2](CH_3SO_3)_2$, comprises a dinuclear dication, with each Ag atom in an approximate T-shaped AgN_3 geometry, and two methylsulfonate anions. Weak connections between the ions are afforded by long (>2.6 Å) $Ag \cdots O$ contacts. The crystal structure comprises zigzag layers connected by π - π interactions [centroid-to-centroid separation = $3.667(3)$ Å]. The layers are stabilized by $C-H \cdots O$ interactions between the anions and cations as well as between anions.

Related literature

For related dinuclear structures, see: Hamblin *et al.* (2002); Kennedy *et al.* (2005). For a polymeric analogue, see Guo *et al.* (2002).



Experimental

Crystal data

 $[Ag_2(C_{12}H_{10}N_4)_2](CH_3SO_3)_2$
 $M_r = 826.40$

 Monoclinic, $P2_1/c$
 $a = 9.017(5)$ Å

 $b = 19.115(5)$ Å

 $c = 17.397(7)$ Å

 $\beta = 105.605(16)^\circ$
 $V = 2888(2)$ Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 1.56$ mm⁻¹
 $T = 120(2)$ K

 $0.18 \times 0.10 \times 0.08$ mm

Data collection

 Rigaku AFC12 κ /SATURN724

diffractometer

Absorption correction: multi-scan

 (*ABSCOR*; Higashi, 1995)

 $T_{\min} = 0.804$, $T_{\max} = 1.000$

(expected range = 0.710–0.883)

30221 measured reflections

5668 independent reflections

 5514 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.067$
 $S = 1.10$

5668 reflections

397 parameters

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.93$ e Å⁻³
 $\Delta\rho_{\min} = -0.67$ e Å⁻³
Table 1

Selected geometric parameters (Å, °).

Ag1–N1	2.237 (2)	Ag2–N3	2.295 (2)
Ag1–N7	2.269 (2)	Ag2–N5	2.248 (2)
Ag1–N8	2.489 (2)	Ag2–N4	2.472 (2)
N1–Ag1–N7	175.91 (8)	N3–Ag2–N4	71.00 (8)
N1–Ag1–N8	110.56 (8)	N3–Ag2–N5	172.76 (8)
N7–Ag1–N8	71.09 (8)	N4–Ag2–N5	115.64 (8)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C7–H7 \cdots O3 ⁱ	0.95	2.28	3.131 (4)	149
C21–H21 \cdots O5 ⁱⁱ	0.95	2.36	3.164 (4)	143
C24–H24 \cdots O4 ⁱⁱⁱ	0.95	2.35	3.258 (4)	161

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

Data collection: *CrystalClear* (Rigaku/MSK, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2507).

References

- Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
- Brandenburg, K. (2006). *DIAMOND*. Release 3.1. Crystal Impact GbR, Bonn, Germany.
- Guo, D., He, C., Duan, C.-Y., Qian, C.-Q. & Meng, Q.-J. (2002). *New J. Chem.* **26**, 796–802.
- Hamblin, J., Jackson, A., Alcock, N. W. & Hannon, M. J. (2002). *J. Chem. Soc. Dalton Trans.* pp. 1635–1641.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Kennedy, A. R., Brown, K. G., Graham, D., Kirkhouse, J. B., Kittner, M., Major, C., McHugh, C. J., Murdoch, P. & Smith, W. E. (2005). *New J. Chem.* **29**, 826–832.
- Rigaku/MSK (2005). *CrystalClear*. Rigaku/MSK Inc., The Woodlands, Texas, USA.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E63, m2368 [doi:10.1107/S1600536807039980]

Bis(μ -pyridine-1-carbaldehyde azine- $\kappa^2N,N':\kappa^2N'',N'''$)disilver(I) bis(methanesulfonate)

G. A. Broker and E. R. T. Tiekink

Comment

The dication in the title compound $[\text{Ag}(2\text{---PA})]_2[\text{MeSO}_3]_2$ (I), Fig. 1, (PA = 2-pyridinealdazine) adopts a ring structure in which the two Ag atoms are bridged by two 2-PA molecules. Each 2-PA ligand is tridentate, forming a single bond to one Ag atom and chelating the other. Within the chelate, the Ag—N_{azo} bond distance is significantly shorter than the Ag—N_{pyridine} bond (Table 1). The coordination geometry around each Ag atom is T-shaped.

Each of the $[\text{MeSO}_3]^-$ anions forms two close contacts with Ag, *i.e.* Ag1 \cdots O1, O4 = 2.620 (2) and 2.902 (2) Å and Ag2 \cdots O2, O5 = 2.635 (2) and 2.699 (3) Å.

The $[\text{Ag}(2\text{---PA})]_2$ chelate structure of (I) has two precedents in the literature, namely in the $[\text{CF}_3\text{SO}_3]^-$ (Hamblin *et al.*, 2002) and $[\text{NO}_3]^-$ salts (Kennedy *et al.*, 2005) for which similar ring structures have been reported. In a third structure, *i.e.* the $[\text{BF}_4]^-$ salt, characterized as an acetonitrile solvate, a polymeric structure is observed due to a rotation of one of the pyridine rings (Guo *et al.*, 2002); in this case, the 2-PA ligand is tetradentate forming two chelate rings.

The global crystal packing in (I) is based on the stacking of zigzag layers. A number of C—H \cdots O interactions cooperate to stabilize the layers (Fig. 2). All the sulfonate-O atoms accept one or more C—H \cdots O interactions (Table 2) arising from both cation \cdots anion and anion \cdots anion contacts. Connections between layers are of the type $\pi\cdots\pi$ with the shortest distance of 3.667 (3) Å occurring between the ring centroids of (N4, C8–C12) and (N5, C13–C17); symmetry operation: $-x, 1-y, 1-z$.

Experimental

Ag(MeSO₃) (Aldrich, 0.05 g, 0.25 mmol) was dissolved in CH₃CN (20 ml) and layered on top of a CH₂Cl₂ solution (20 ml) containing (0.05 g, 0.25 mmol) of 2-pyridinealdazine (Aldrich). After three days, colourless prisms of (I) were observed at the interface between the two layers; m.p. 491–493 K.

Refinement

All the H atoms were included in the riding-model approximation, with C—H = 0.95–0.98 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$.

Figures

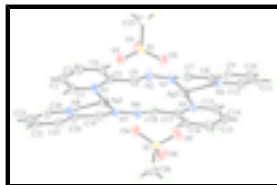


Fig. 1. The molecular structure of (I) showing displacement ellipsoids at the 70% probability level (arbitrary spheres for the H atoms).

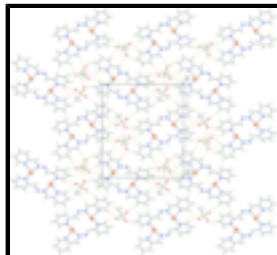


Fig. 2. View of a layer in (I) highlighting the C—H...O hydrogen bonds, shown as orange-dashed lines. Colour code: orange (silver), yellow (sulfur), red (oxygen), blue (nitrogen), grey (carbon) and green (hydrogen).

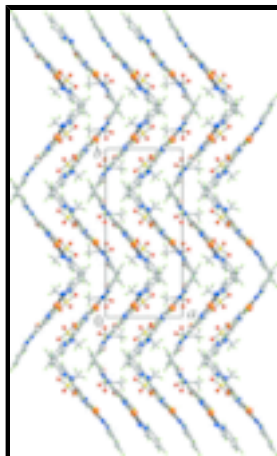


Fig. 3. View of the crystal packing in (I) down the *c* axis highlighting the layer arrangement. The N—H...O hydrogen bonds are shown as orange-dashed lines. Colour code as for Fig. 2.

Bis(μ -pyridine-1-carbaldehyde azine- κ^2N,N' : κ^2N'',N''')disilver(I) bis(methanesulfonate)

Crystal data

[Ag₂(C₁₂H₁₀N₄)₂](CH₃SO₃)₂

M_r = 826.40

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 9.017 (5) Å

b = 19.115 (5) Å

c = 17.397 (7) Å

β = 105.605 (16)°

V = 2888 (2) Å³

Z = 4

*F*₀₀₀ = 1648

D_x = 1.901 Mg m⁻³

Mo *K*α radiation

λ = 0.71070 Å

Cell parameters from 5950 reflections

θ = 1.6–30.2°

μ = 1.56 mm⁻¹

T = 120 (2) K

Prism, colourless

0.18 × 0.10 × 0.08 mm

Data collection

Rigaku AFC12κ/SATURN724 diffractometer	5668 independent reflections
Radiation source: fine-focus sealed tube	5514 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.030$
$T = 120(2)$ K	$\theta_{\text{max}} = 26.0^\circ$
ω scans	$\theta_{\text{min}} = 1.6^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.804$, $T_{\text{max}} = 1.000$	$k = -21 \rightarrow 23$
30221 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 5.0008P]$
$S = 1.10$	where $P = (F_o^2 + 2F_c^2)/3$
5668 reflections	$(\Delta/\sigma)_{\text{max}} = 0.003$
397 parameters	$\Delta\rho_{\text{max}} = 0.93 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.67 \text{ e } \text{\AA}^{-3}$
	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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.36970 (2)	0.431855 (10)	0.877448 (11)	0.01905 (7)
Ag2	0.12996 (2)	0.555838 (10)	0.637545 (12)	0.01861 (7)
S1	-0.00614 (7)	0.38534 (3)	0.72639 (4)	0.01684 (13)
S2	0.50982 (8)	0.59359 (3)	0.75240 (4)	0.01902 (14)
O1	0.0808 (2)	0.40311 (11)	0.80742 (11)	0.0250 (4)

supplementary materials

O2	0.0099 (2)	0.43659 (10)	0.66748 (12)	0.0254 (4)
O3	0.0223 (3)	0.31478 (10)	0.70343 (12)	0.0327 (5)
O4	0.4588 (2)	0.56243 (10)	0.81728 (11)	0.0234 (4)
O5	0.3881 (3)	0.63161 (12)	0.69664 (14)	0.0403 (6)
O6	0.5892 (3)	0.54368 (12)	0.71478 (14)	0.0391 (6)
N1	0.2639 (2)	0.50211 (11)	0.95097 (12)	0.0171 (4)
N2	0.0415 (3)	0.61510 (12)	0.80323 (12)	0.0201 (5)
N3	0.0258 (2)	0.62142 (11)	0.72049 (12)	0.0175 (4)
N4	-0.0242 (2)	0.65172 (11)	0.55969 (13)	0.0167 (4)
N5	0.2546 (2)	0.48734 (11)	0.57028 (12)	0.0162 (4)
N6	0.4392 (2)	0.36098 (11)	0.71502 (12)	0.0163 (4)
N7	0.4598 (2)	0.35786 (11)	0.79848 (12)	0.0159 (4)
N8	0.5297 (2)	0.34012 (11)	0.96246 (13)	0.0185 (4)
C1	0.3001 (3)	0.49111 (13)	1.03027 (15)	0.0187 (5)
H1	0.3772	0.4575	1.0526	0.022*
C2	0.2305 (3)	0.52640 (14)	1.08101 (15)	0.0212 (5)
H2	0.2591	0.5168	1.1366	0.025*
C3	0.1183 (3)	0.57609 (14)	1.04902 (16)	0.0212 (6)
H3	0.0670	0.6006	1.0819	0.025*
C4	0.0833 (3)	0.58891 (14)	0.96759 (15)	0.0196 (5)
H4	0.0092	0.6235	0.9442	0.024*
C5	0.1567 (3)	0.55113 (13)	0.92028 (15)	0.0154 (5)
C6	0.1246 (3)	0.56322 (13)	0.83390 (15)	0.0167 (5)
H6	0.1654	0.5327	0.8015	0.020*
C7	-0.0379 (3)	0.67938 (13)	0.69345 (15)	0.0176 (5)
H7	-0.0655	0.7115	0.7289	0.021*
C8	-0.0691 (3)	0.69731 (13)	0.60850 (15)	0.0168 (5)
C9	-0.1457 (3)	0.75943 (13)	0.58199 (15)	0.0189 (5)
H9	-0.1751	0.7902	0.6182	0.023*
C10	-0.1784 (3)	0.77554 (14)	0.50134 (16)	0.0210 (5)
H10	-0.2297	0.8179	0.4814	0.025*
C11	-0.1347 (3)	0.72881 (14)	0.45026 (16)	0.0195 (5)
H11	-0.1562	0.7383	0.3948	0.023*
C12	-0.0587 (3)	0.66767 (13)	0.48238 (15)	0.0173 (5)
H12	-0.0299	0.6356	0.4472	0.021*
C13	0.2301 (3)	0.50199 (13)	0.49181 (15)	0.0187 (5)
H13	0.1620	0.5392	0.4700	0.022*
C14	0.2983 (3)	0.46610 (14)	0.44149 (15)	0.0199 (5)
H14	0.2789	0.4791	0.3870	0.024*
C15	0.3956 (3)	0.41065 (14)	0.47201 (15)	0.0200 (5)
H15	0.4453	0.3853	0.4391	0.024*
C16	0.4185 (3)	0.39312 (14)	0.55176 (15)	0.0187 (5)
H16	0.4823	0.3546	0.5739	0.022*
C17	0.3474 (3)	0.43242 (13)	0.59903 (15)	0.0159 (5)
C18	0.3710 (3)	0.41726 (13)	0.68453 (15)	0.0156 (5)
H18	0.3354	0.4494	0.7172	0.019*
C19	0.5368 (3)	0.30401 (13)	0.83006 (15)	0.0167 (5)
H19	0.5670	0.2706	0.7968	0.020*
C20	0.5797 (3)	0.29291 (13)	0.91728 (15)	0.0168 (5)

C21	0.6740 (3)	0.23671 (13)	0.94907 (15)	0.0187 (5)
H21	0.7057	0.2041	0.9154	0.022*
C22	0.7208 (3)	0.22950 (14)	1.03204 (16)	0.0207 (5)
H22	0.7854	0.1918	1.0559	0.025*
C23	0.6721 (3)	0.27789 (14)	1.07885 (15)	0.0200 (5)
H23	0.7036	0.2743	1.1354	0.024*
C24	0.5766 (3)	0.33171 (14)	1.04198 (16)	0.0203 (5)
H24	0.5425	0.3644	1.0746	0.024*
C25	-0.2005 (3)	0.3882 (2)	0.72741 (18)	0.0348 (7)
H25A	-0.2253	0.4352	0.7427	0.052*
H25B	-0.2183	0.3541	0.7660	0.052*
H25C	-0.2661	0.3770	0.6741	0.052*
C26	0.6481 (3)	0.65761 (15)	0.79671 (18)	0.0273 (6)
H26A	0.7344	0.6352	0.8354	0.041*
H26B	0.6008	0.6925	0.8239	0.041*
H26C	0.6859	0.6806	0.7553	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02153 (12)	0.01992 (11)	0.01598 (11)	0.00613 (7)	0.00552 (8)	-0.00123 (7)
Ag2	0.02197 (12)	0.01738 (11)	0.01718 (11)	0.00465 (7)	0.00650 (8)	-0.00088 (7)
S1	0.0187 (3)	0.0178 (3)	0.0146 (3)	-0.0006 (2)	0.0054 (2)	0.0008 (2)
S2	0.0215 (3)	0.0219 (3)	0.0128 (3)	-0.0032 (3)	0.0033 (2)	-0.0005 (2)
O1	0.0225 (10)	0.0322 (11)	0.0174 (9)	-0.0018 (8)	0.0006 (8)	-0.0003 (8)
O2	0.0354 (11)	0.0214 (10)	0.0202 (10)	-0.0009 (8)	0.0088 (9)	0.0046 (8)
O3	0.0562 (14)	0.0183 (10)	0.0277 (11)	0.0062 (9)	0.0184 (10)	0.0025 (8)
O4	0.0290 (11)	0.0255 (10)	0.0174 (10)	-0.0016 (8)	0.0092 (8)	0.0003 (8)
O5	0.0351 (12)	0.0348 (12)	0.0377 (13)	-0.0094 (10)	-0.0132 (10)	0.0146 (10)
O6	0.0491 (14)	0.0396 (13)	0.0384 (13)	-0.0098 (11)	0.0286 (11)	-0.0169 (10)
N1	0.0217 (11)	0.0163 (10)	0.0135 (10)	-0.0004 (9)	0.0048 (9)	0.0000 (8)
N2	0.0261 (12)	0.0218 (11)	0.0118 (10)	0.0055 (9)	0.0039 (9)	0.0021 (9)
N3	0.0215 (11)	0.0185 (11)	0.0131 (10)	0.0038 (9)	0.0056 (8)	-0.0010 (8)
N4	0.0164 (10)	0.0166 (10)	0.0172 (11)	0.0003 (8)	0.0045 (9)	-0.0003 (8)
N5	0.0188 (11)	0.0147 (10)	0.0156 (10)	0.0010 (8)	0.0053 (8)	-0.0004 (8)
N6	0.0179 (11)	0.0189 (11)	0.0113 (10)	0.0013 (8)	0.0027 (8)	0.0014 (8)
N7	0.0171 (10)	0.0176 (10)	0.0135 (10)	-0.0001 (8)	0.0048 (8)	-0.0006 (8)
N8	0.0189 (11)	0.0208 (11)	0.0157 (11)	0.0011 (9)	0.0047 (9)	0.0003 (9)
C1	0.0229 (13)	0.0169 (12)	0.0159 (12)	0.0015 (10)	0.0045 (10)	0.0019 (10)
C2	0.0285 (14)	0.0217 (13)	0.0133 (12)	-0.0017 (11)	0.0058 (11)	0.0003 (10)
C3	0.0240 (14)	0.0221 (13)	0.0196 (13)	0.0008 (11)	0.0095 (11)	-0.0039 (11)
C4	0.0186 (13)	0.0207 (13)	0.0189 (13)	0.0038 (10)	0.0040 (10)	-0.0001 (10)
C5	0.0172 (12)	0.0144 (11)	0.0152 (12)	-0.0011 (9)	0.0051 (10)	0.0009 (9)
C6	0.0170 (12)	0.0189 (12)	0.0150 (12)	-0.0003 (10)	0.0053 (10)	-0.0021 (10)
C7	0.0191 (13)	0.0184 (13)	0.0152 (12)	0.0014 (10)	0.0041 (10)	-0.0023 (10)
C8	0.0169 (12)	0.0172 (12)	0.0160 (12)	-0.0003 (10)	0.0040 (10)	-0.0001 (10)
C9	0.0214 (13)	0.0161 (12)	0.0194 (13)	0.0016 (10)	0.0062 (10)	-0.0012 (10)
C10	0.0232 (13)	0.0172 (12)	0.0222 (14)	0.0024 (10)	0.0054 (11)	0.0035 (10)

supplementary materials

C11	0.0200 (13)	0.0214 (13)	0.0170 (13)	-0.0007 (10)	0.0044 (10)	0.0036 (10)
C12	0.0175 (12)	0.0183 (12)	0.0169 (12)	-0.0016 (10)	0.0060 (10)	-0.0012 (10)
C13	0.0210 (13)	0.0178 (12)	0.0171 (13)	0.0005 (10)	0.0048 (10)	0.0027 (10)
C14	0.0228 (13)	0.0230 (13)	0.0141 (12)	-0.0031 (11)	0.0050 (10)	-0.0004 (10)
C15	0.0206 (13)	0.0238 (13)	0.0166 (13)	-0.0005 (11)	0.0066 (10)	-0.0035 (10)
C16	0.0177 (12)	0.0200 (13)	0.0181 (13)	0.0004 (10)	0.0040 (10)	-0.0022 (10)
C17	0.0145 (12)	0.0160 (12)	0.0165 (12)	-0.0016 (9)	0.0028 (10)	-0.0008 (9)
C18	0.0145 (12)	0.0186 (12)	0.0149 (12)	-0.0016 (10)	0.0060 (10)	-0.0014 (10)
C19	0.0183 (12)	0.0155 (12)	0.0162 (12)	-0.0003 (10)	0.0042 (10)	-0.0026 (10)
C20	0.0152 (12)	0.0178 (12)	0.0175 (12)	-0.0014 (10)	0.0045 (10)	-0.0007 (10)
C21	0.0208 (13)	0.0181 (12)	0.0180 (13)	0.0008 (10)	0.0064 (10)	0.0008 (10)
C22	0.0200 (13)	0.0206 (13)	0.0211 (13)	0.0006 (10)	0.0048 (11)	0.0066 (10)
C23	0.0244 (14)	0.0224 (13)	0.0141 (12)	-0.0023 (11)	0.0068 (10)	0.0009 (10)
C24	0.0211 (13)	0.0198 (13)	0.0212 (13)	0.0000 (10)	0.0079 (11)	-0.0029 (10)
C25	0.0216 (15)	0.059 (2)	0.0235 (15)	-0.0058 (14)	0.0060 (12)	-0.0075 (14)
C26	0.0246 (14)	0.0261 (14)	0.0285 (15)	-0.0050 (12)	0.0022 (12)	-0.0032 (12)

Geometric parameters (Å, °)

Ag1—N1	2.237 (2)	C6—H6	0.9500
Ag1—N7	2.269 (2)	C7—C8	1.469 (3)
Ag1—N8	2.489 (2)	C7—H7	0.9500
Ag2—N3	2.295 (2)	C8—C9	1.389 (4)
Ag2—N5	2.248 (2)	C9—C10	1.388 (4)
Ag2—N4	2.472 (2)	C9—H9	0.9500
S1—O3	1.449 (2)	C10—C11	1.389 (4)
S1—O2	1.453 (2)	C10—H10	0.9500
S1—O1	1.457 (2)	C11—C12	1.394 (4)
S1—C25	1.758 (3)	C11—H11	0.9500
S2—O6	1.450 (2)	C12—H12	0.9500
S2—O5	1.450 (2)	C13—C14	1.380 (4)
S2—O4	1.456 (2)	C13—H13	0.9500
S2—C26	1.769 (3)	C14—C15	1.387 (4)
N1—C1	1.346 (3)	C14—H14	0.9500
N1—C5	1.349 (3)	C15—C16	1.387 (4)
N2—C6	1.271 (3)	C15—H15	0.9500
N2—N3	1.413 (3)	C16—C17	1.391 (4)
N3—C7	1.278 (3)	C16—H16	0.9500
N4—C12	1.332 (3)	C17—C18	1.474 (3)
N4—C8	1.352 (3)	C18—H18	0.9500
N5—C17	1.352 (3)	C19—C20	1.477 (3)
N5—C13	1.352 (3)	C19—H19	0.9500
N6—C18	1.281 (3)	C20—C21	1.389 (4)
N6—N7	1.414 (3)	C21—C22	1.397 (4)
N7—C19	1.280 (3)	C21—H21	0.9500
N8—C24	1.343 (3)	C22—C23	1.380 (4)
N8—C20	1.351 (3)	C22—H22	0.9500
C1—C2	1.388 (4)	C23—C24	1.383 (4)
C1—H1	0.9500	C23—H23	0.9500

C2—C3	1.390 (4)	C24—H24	0.9500
C2—H2	0.9500	C25—H25A	0.9800
C3—C4	1.388 (4)	C25—H25B	0.9800
C3—H3	0.9500	C25—H25C	0.9800
C4—C5	1.389 (4)	C26—H26A	0.9800
C4—H4	0.9500	C26—H26B	0.9800
C5—C6	1.470 (3)	C26—H26C	0.9800
N1—Ag1—N7	175.91 (8)	C9—C8—C7	118.5 (2)
N1—Ag1—N8	110.56 (8)	C8—C9—C10	118.5 (2)
N7—Ag1—N8	71.09 (8)	C8—C9—H9	120.8
N3—Ag2—N4	71.00 (8)	C10—C9—H9	120.8
N3—Ag2—N5	172.76 (8)	C11—C10—C9	119.0 (2)
N4—Ag2—N5	115.64 (8)	C11—C10—H10	120.5
O3—S1—O2	112.01 (12)	C9—C10—H10	120.5
O3—S1—O1	113.25 (12)	C10—C11—C12	118.4 (2)
O2—S1—O1	113.30 (12)	C10—C11—H11	120.8
O3—S1—C25	106.44 (16)	C12—C11—H11	120.8
O2—S1—C25	105.93 (15)	N4—C12—C11	123.6 (2)
O1—S1—C25	105.14 (13)	N4—C12—H12	118.2
O6—S2—O5	113.86 (15)	C11—C12—H12	118.2
O6—S2—O4	112.20 (13)	N5—C13—C14	123.9 (2)
O5—S2—O4	112.57 (14)	N5—C13—H13	118.0
O6—S2—C26	106.03 (15)	C14—C13—H13	118.0
O5—S2—C26	105.25 (14)	C13—C14—C15	118.7 (2)
O4—S2—C26	106.13 (13)	C13—C14—H14	120.6
C1—N1—C5	117.7 (2)	C15—C14—H14	120.6
C1—N1—Ag1	117.97 (17)	C16—C15—C14	118.4 (2)
C5—N1—Ag1	124.12 (17)	C16—C15—H15	120.8
C6—N2—N3	112.4 (2)	C14—C15—H15	120.8
C7—N3—N2	111.2 (2)	C15—C16—C17	119.5 (2)
C7—N3—Ag2	117.47 (17)	C15—C16—H16	120.3
N2—N3—Ag2	130.38 (16)	C17—C16—H16	120.3
C12—N4—C8	117.3 (2)	N5—C17—C16	122.6 (2)
C12—N4—Ag2	131.85 (17)	N5—C17—C18	115.6 (2)
C8—N4—Ag2	110.66 (16)	C16—C17—C18	121.8 (2)
C17—N5—C13	116.8 (2)	N6—C18—C17	120.4 (2)
C17—N5—Ag2	127.32 (17)	N6—C18—H18	119.8
C13—N5—Ag2	115.86 (17)	C17—C18—H18	119.8
C18—N6—N7	112.1 (2)	N7—C19—C20	121.2 (2)
C19—N7—N6	112.4 (2)	N7—C19—H19	119.4
C19—N7—Ag1	118.86 (17)	C20—C19—H19	119.4
N6—N7—Ag1	128.72 (15)	N8—C20—C21	123.3 (2)
C24—N8—C20	117.2 (2)	N8—C20—C19	117.7 (2)
C24—N8—Ag1	131.92 (18)	C21—C20—C19	118.9 (2)
C20—N8—Ag1	110.83 (16)	C20—C21—C22	118.0 (2)
N1—C1—C2	123.3 (2)	C20—C21—H21	121.0
N1—C1—H1	118.3	C22—C21—H21	121.0
C2—C1—H1	118.3	C23—C22—C21	119.2 (2)
C1—C2—C3	118.8 (2)	C23—C22—H22	120.4

supplementary materials

C1—C2—H2	120.6	C21—C22—H22	120.4
C3—C2—H2	120.6	C22—C23—C24	118.8 (2)
C4—C3—C2	118.1 (2)	C22—C23—H23	120.6
C4—C3—H3	121.0	C24—C23—H23	120.6
C2—C3—H3	121.0	N8—C24—C23	123.4 (2)
C3—C4—C5	119.9 (2)	N8—C24—H24	118.3
C3—C4—H4	120.0	C23—C24—H24	118.3
C5—C4—H4	120.0	S1—C25—H25A	109.5
N1—C5—C4	122.1 (2)	S1—C25—H25B	109.5
N1—C5—C6	115.9 (2)	H25A—C25—H25B	109.5
C4—C5—C6	122.0 (2)	S1—C25—H25C	109.5
N2—C6—C5	118.9 (2)	H25A—C25—H25C	109.5
N2—C6—H6	120.5	H25B—C25—H25C	109.5
C5—C6—H6	120.5	S2—C26—H26A	109.5
N3—C7—C8	121.2 (2)	S2—C26—H26B	109.5
N3—C7—H7	119.4	H26A—C26—H26B	109.5
C8—C7—H7	119.4	S2—C26—H26C	109.5
N4—C8—C9	123.3 (2)	H26A—C26—H26C	109.5
N4—C8—C7	118.2 (2)	H26B—C26—H26C	109.5
N8—Ag1—N1—C1	2.9 (2)	Ag2—N4—C8—C7	-7.1 (3)
N8—Ag1—N1—C5	-171.47 (19)	N3—C7—C8—N4	-2.1 (4)
C6—N2—N3—C7	-170.1 (2)	N3—C7—C8—C9	176.7 (2)
C6—N2—N3—Ag2	-1.8 (3)	N4—C8—C9—C10	0.2 (4)
N4—Ag2—N3—C7	-10.50 (18)	C7—C8—C9—C10	-178.5 (2)
N4—Ag2—N3—N2	-178.2 (2)	C8—C9—C10—C11	0.6 (4)
N5—Ag2—N4—C12	6.5 (2)	C9—C10—C11—C12	-0.5 (4)
N3—Ag2—N4—C12	-176.6 (2)	C8—N4—C12—C11	1.4 (4)
N5—Ag2—N4—C8	-168.07 (16)	Ag2—N4—C12—C11	-172.87 (18)
N3—Ag2—N4—C8	8.83 (16)	C10—C11—C12—N4	-0.6 (4)
N4—Ag2—N5—C17	179.03 (19)	C17—N5—C13—C14	-2.5 (4)
N4—Ag2—N5—C13	-2.8 (2)	Ag2—N5—C13—C14	179.2 (2)
C18—N6—N7—C19	-175.7 (2)	N5—C13—C14—C15	1.3 (4)
C18—N6—N7—Ag1	6.4 (3)	C13—C14—C15—C16	0.8 (4)
N8—Ag1—N7—C19	4.51 (18)	C14—C15—C16—C17	-1.7 (4)
N8—Ag1—N7—N6	-177.7 (2)	C13—N5—C17—C16	1.5 (4)
N1—Ag1—N8—C24	-9.6 (3)	Ag2—N5—C17—C16	179.64 (18)
N7—Ag1—N8—C24	174.4 (2)	C13—N5—C17—C18	-179.5 (2)
N1—Ag1—N8—C20	173.08 (16)	Ag2—N5—C17—C18	-1.3 (3)
N7—Ag1—N8—C20	-2.94 (16)	C15—C16—C17—N5	0.6 (4)
C5—N1—C1—C2	1.4 (4)	C15—C16—C17—C18	-178.4 (2)
Ag1—N1—C1—C2	-173.3 (2)	N7—N6—C18—C17	176.2 (2)
N1—C1—C2—C3	-0.4 (4)	N5—C17—C18—N6	170.4 (2)
C1—C2—C3—C4	-1.2 (4)	C16—C17—C18—N6	-10.6 (4)
C2—C3—C4—C5	1.8 (4)	N6—N7—C19—C20	176.2 (2)
C1—N1—C5—C4	-0.8 (4)	Ag1—N7—C19—C20	-5.6 (3)
Ag1—N1—C5—C4	173.60 (19)	C24—N8—C20—C21	0.9 (4)
C1—N1—C5—C6	177.9 (2)	Ag1—N8—C20—C21	178.6 (2)
Ag1—N1—C5—C6	-7.7 (3)	C24—N8—C20—C19	-176.3 (2)
C3—C4—C5—N1	-0.8 (4)	Ag1—N8—C20—C19	1.5 (3)

C3—C4—C5—C6	-179.4 (2)	N7—C19—C20—N8	2.5 (4)
N3—N2—C6—C5	177.8 (2)	N7—C19—C20—C21	-174.7 (2)
N1—C5—C6—N2	-170.2 (2)	N8—C20—C21—C22	-0.9 (4)
C4—C5—C6—N2	8.5 (4)	C19—C20—C21—C22	176.2 (2)
N2—N3—C7—C8	-178.9 (2)	C20—C21—C22—C23	0.1 (4)
Ag2—N3—C7—C8	11.2 (3)	C21—C22—C23—C24	0.8 (4)
C12—N4—C8—C9	-1.2 (4)	C20—N8—C24—C23	0.0 (4)
Ag2—N4—C8—C9	174.3 (2)	Ag1—N8—C24—C23	-177.15 (19)
C12—N4—C8—C7	177.5 (2)	C22—C23—C24—N8	-0.8 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C7—H7 \cdots O3 ⁱ	0.95	2.28	3.131 (4)	149
C21—H21 \cdots O5 ⁱⁱ	0.95	2.36	3.164 (4)	143
C24—H24 \cdots O4 ⁱⁱⁱ	0.95	2.35	3.258 (4)	161

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

Fig. 1

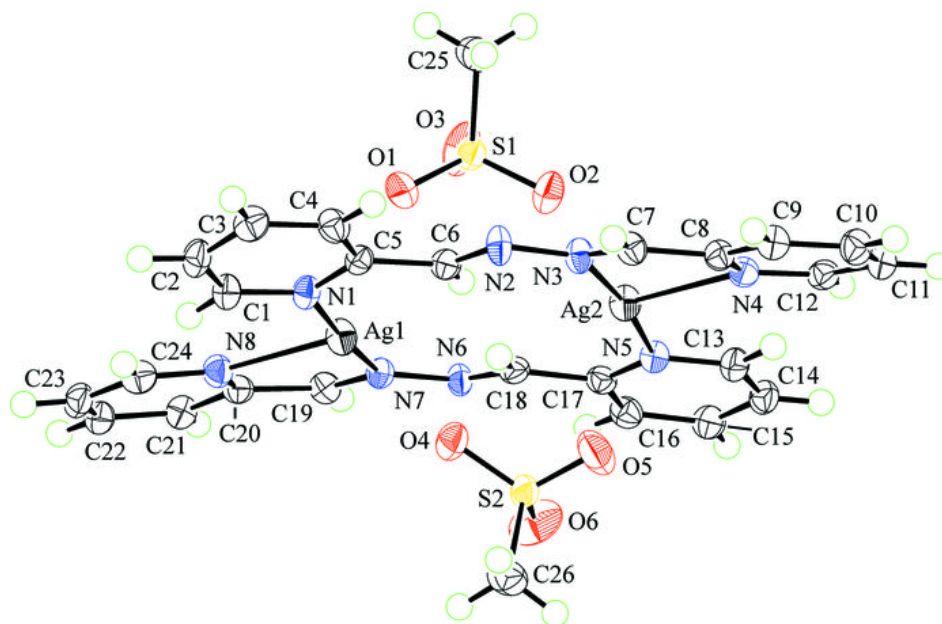


Fig. 2

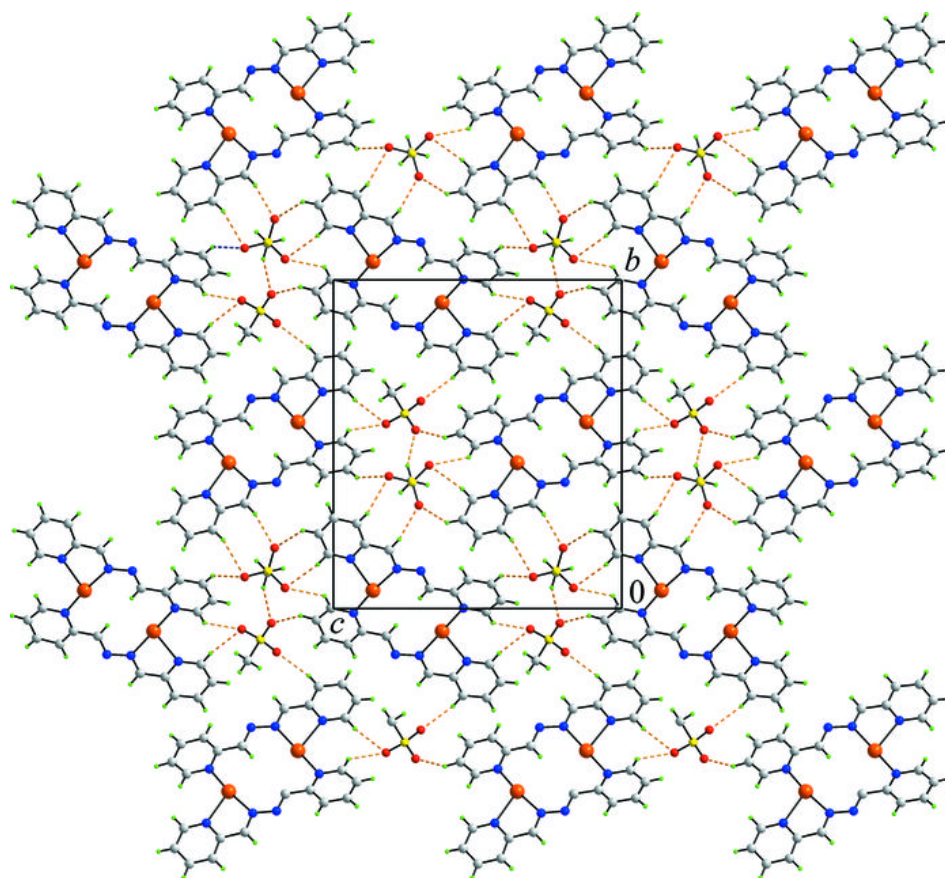


Fig. 3

