

Poly[[μ_3 -1,2-bis[(3-cyanobenzylidene)-hydrazono]-1,2-diphenylethane]silver(I)] hexafluoroantimonate]

Lian-Dong Liu

Department of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China

Correspondence e-mail: liandongliu1968@yahoo.com.cn

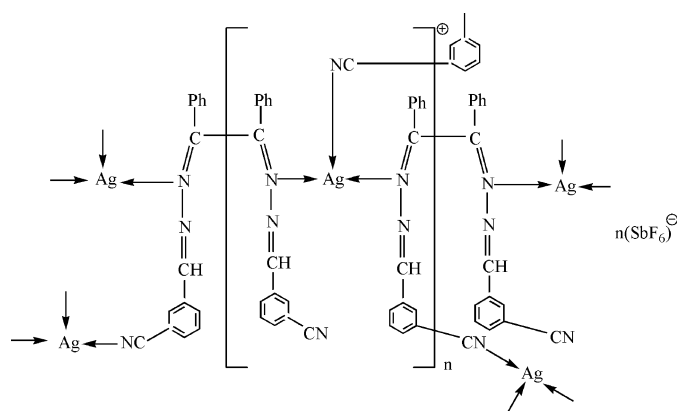
Received 22 November 2007; accepted 26 December 2007

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.012$ Å; R factor = 0.072; wR factor = 0.223; data-to-parameter ratio = 16.0.

In the title compound, $\{[\text{Ag}(\text{C}_{30}\text{H}_{20}\text{N}_6)][\text{SbF}_6]\}_n$, the Ag^+ cation has a three-coordinate environment completed by three N atoms of the 1,2-bis[(3-cyanobenzylidene)hydrazono]-1,2-diphenylethane ligand. The Ag^+ cation coordination geometry is best described as distorted T-shaped. The crystal structure forms a three-dimensional structural polymer.

Related literature

For a related structure, see: Wei *et al.* (2007).



Experimental

Crystal data

$[\text{Ag}(\text{C}_{30}\text{H}_{20}\text{N}_6)][\text{SbF}_6]$
 $M_r = 808.14$

Monoclinic, $P2_1/c$

$a = 15.1652$ (9) Å

$b = 14.6022$ (9) Å

$c = 14.0711$ (9) Å

$\beta = 94.2570$ (10)°

$V = 3107.4$ (3) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.57$ mm⁻¹

$T = 298$ (2) K

$0.35 \times 0.14 \times 0.08$ mm

Data collection

Bruker SMART APEX CCD diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.610$, $T_{\max} = 0.885$

15863 measured reflections

5885 independent reflections

4340 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.071$

$wR(F^2) = 0.223$

$S = 1.05$

5885 reflections

367 parameters

6 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 1.48$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.94$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------------------|-----------|------------------------|-----------|
| Ag1—N5 | 2.287 (6) | Ag1—N1 ⁱ | 2.354 (9) |
| Ag1—N3 | 2.334 (5) | | |
| N5—Ag1—N3 | 145.2 (2) | N3—Ag1—N1 ⁱ | 97.9 (3) |
| N5—Ag1—N1 ⁱ | 107.5 (3) | | |

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2129).

References

- Bruker (1997). SMART (Version 5.6) and SAINT (Version 5.06A), Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2001). SHELXTL. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1996). SADABS. Version 2.10. University of Göttingen, Germany.
- Wei, K.-J., Ni, J., Gao, J., Liu, Y.-Z. & Liu, Q.-L. (2007). *Eur. J. Inorg. Chem.* pp. 3868–3880.

supplementary materials

Acta Cryst. (2008). E64, m363 [doi:10.1107/S1600536807068432]

Poly[[μ_3 -1,2-bis[(3-cyanobenzylidene)hydrazono]-1,2-diphenylethane}silver(I)] hexafluoroantimonate]

L.-D. Liu

Comment

Silver complexes play a pivotal role in the area of self-assembly coordination chemistry (Wei *et al.*, 2007). Here I report a new Ag(I) coordination polymer, (I) using 1,2-bis(benzene)-1,2-bis((3-cyanobenzylidene)hydrazono)ethane as bridge ligand.

The asymmetric unit of (I) is shown in Fig. 1. It reveals that Ag1 atom is coordinated by three N atoms which come from three ligands, respectively. The Ag1 atom is in a distorted T shape coordination environment (Table 1). In the crystal structure each 1,2-bis(benzene)-1,2-bis((3-cyanobenzylidene)hydrazono)ethane molecule function as tridentate bridge ligand with its two N atoms from two hydrazone groups, respectively, and a N atom from one of two cyanato groups, which resulted in the connections of three Ag(I) ions with separations of 7.0839 (5) Å (between the two Ag⁺ ions which are coordinated by two hydrazone groups) and 10.7616 (9) Å (between the two Ag⁺ ions which are coordinated by a hydrazone group and a cyanato group, respectively). In the crystal structure exist a weak π - π stacking interreaction, [Cg1...Cg1ⁱ = 3.788 (5) Å and Cg1...Cg1ⁱ_{perp} = 3.479 Å, symmetry codes: (i) 1 - x, 2 - y, 2 - z, Cg1 is the centroid of the the C1—C6 ring; Cg1...Cg1ⁱ_{perp} is the perpendicular distance from ring Cg1 to ring Cg1ⁱ]. In addition to the weak π - π stacking interaction there also exists the weak interaction between C15—H15 bond and the conjugated π bond, and the relevant distances are H15...Cg2 = 2.86 Å and H15...Cg2_{perp} = 2.826 Å [Cg2 is the centroid of the C9—C14 ring; H15...Cg2_{perp} is the perpendicular distance from H15 to ring Cg2]. The counter hexafluoroantimonate anions are inserted in the micropores of the polymer by electrostatic force.

Experimental

8 ml benzene solution of AgSbF₆ (0.0171 g, 0.05 mmol) was added very slowly on the 8 ml tetrahydrofuran solution of 1,2-bis(benzene)-1,2-bis((3-cyanobenzylidene)hydrazono)ethane (0.0093 g, 0.02 mmol). The colorless single crystals were obtained after the solution had been allowed to stand at room temperature for one week.

Refinement

The H atoms were placed in calculated positions with C—H = 0.93 Å, and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The disordered F atoms were all refined isotropically.

Figures

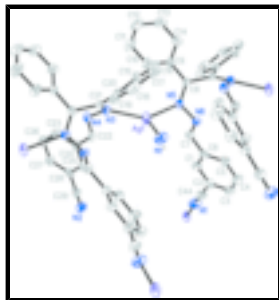


Fig. 1. Part of the polymeric structure and the atom-numbering scheme of the title compound. Displacement ellipsoids are shown at the 30% probability level and H atoms and SbF_6^- anion have been omitted for clarity. [Symmetry code: (i) $-x + 1, y - 1/2, -z + 3/2$]

Poly[[μ_3 -1,2-bis[(3-cyanobenzylidene)hydrazono]-1,2-diphenylethane]silver(I)] hexafluoroantimonate]

Crystal data

$[\text{Ag}(\text{C}_{30}\text{H}_{20}\text{N}_6)][\text{SbF}_6]$

$M_r = 808.14$

Monoclinic, $P2(1)/c$

Hall symbol: $-P\ 2ybc$

$a = 15.1652\ (9)\ \text{\AA}$

$b = 14.6022\ (9)\ \text{\AA}$

$c = 14.0711\ (9)\ \text{\AA}$

$\beta = 94.2570\ (10)^\circ$

$V = 3107.4\ (3)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1576$

$D_x = 1.727\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3506 reflections

$\theta = 2.4\text{--}21.8^\circ$

$\mu = 1.57\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, colorless

$0.35 \times 0.14 \times 0.08\ \text{mm}$

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ (2)\ \text{K}$

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.610, T_{\max} = 0.885$

15863 measured reflections

5885 independent reflections

4340 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 25.7^\circ$

$\theta_{\min} = 1.4^\circ$

$h = -18 \rightarrow 13$

$k = -17 \rightarrow 17$

$l = -17 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.071$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

| | |
|--|--|
| $wR(F^2) = 0.223$ | $w = 1/[\sigma^2(F_o^2) + (0.1282P)^2 + 7.595P]$ |
| $S = 1.05$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 5885 reflections | $(\Delta/\sigma)_{\max} = 0.001$ |
| 367 parameters | $\Delta\rho_{\max} = 1.48 \text{ e } \text{\AA}^{-3}$ |
| 6 restraints | $\Delta\rho_{\min} = -0.94 \text{ e } \text{\AA}^{-3}$ |
| 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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| Ag1 | 0.26219 (4) | 0.77830 (5) | 0.61460 (4) | 0.0554 (3) |
| C1 | 0.5013 (5) | 0.9755 (6) | 0.8609 (6) | 0.0471 (17) |
| H1 | 0.4774 | 1.0223 | 0.8222 | 0.056* |
| C2 | 0.5826 (5) | 0.9864 (6) | 0.9087 (6) | 0.0521 (19) |
| C3 | 0.6190 (6) | 0.9176 (8) | 0.9667 (7) | 0.068 (2) |
| H3 | 0.6742 | 0.9253 | 0.9990 | 0.082* |
| C4 | 0.5731 (6) | 0.8387 (7) | 0.9760 (7) | 0.069 (2) |
| H4 | 0.5970 | 0.7924 | 1.0152 | 0.082* |
| C5 | 0.4926 (5) | 0.8267 (6) | 0.9286 (6) | 0.0534 (19) |
| H5 | 0.4622 | 0.7720 | 0.9353 | 0.064* |
| C6 | 0.4551 (5) | 0.8952 (5) | 0.8701 (5) | 0.0447 (17) |
| C7 | 0.3681 (5) | 0.8834 (6) | 0.8173 (5) | 0.0483 (18) |
| H7 | 0.3486 | 0.9279 | 0.7733 | 0.058* |
| C8 | 0.1698 (4) | 0.8068 (4) | 0.8094 (5) | 0.0350 (14) |
| C9 | 0.0853 (4) | 0.8073 (5) | 0.7522 (5) | 0.0400 (15) |
| C10 | 0.0724 (6) | 0.8656 (6) | 0.6764 (6) | 0.056 (2) |
| H10 | 0.1173 | 0.9052 | 0.6613 | 0.067* |
| C11 | -0.0095 (7) | 0.8658 (8) | 0.6211 (7) | 0.081 (3) |
| H11 | -0.0183 | 0.9059 | 0.5700 | 0.098* |
| C12 | -0.0742 (7) | 0.8087 (9) | 0.6415 (8) | 0.089 (3) |
| H12 | -0.1278 | 0.8092 | 0.6048 | 0.107* |
| C13 | -0.0613 (6) | 0.7492 (9) | 0.7174 (8) | 0.083 (3) |
| H13 | -0.1056 | 0.7076 | 0.7294 | 0.100* |
| C14 | 0.0160 (5) | 0.7501 (7) | 0.7760 (6) | 0.061 (2) |

supplementary materials

| | | | | |
|-----|-------------|-------------|-------------|-------------|
| H14 | 0.0220 | 0.7136 | 0.8303 | 0.073* |
| C15 | 0.1073 (5) | 0.6282 (6) | 0.5563 (5) | 0.0505 (18) |
| H15 | 0.0979 | 0.6863 | 0.5806 | 0.061* |
| C16 | 0.0836 (6) | 0.5516 (7) | 0.6067 (6) | 0.065 (3) |
| H16 | 0.0582 | 0.5586 | 0.6645 | 0.078* |
| C17 | 0.0973 (6) | 0.4656 (7) | 0.5719 (7) | 0.068 (3) |
| H17 | 0.0823 | 0.4141 | 0.6060 | 0.082* |
| C18 | 0.1329 (6) | 0.4568 (6) | 0.4874 (9) | 0.071 (3) |
| H18 | 0.1418 | 0.3983 | 0.4639 | 0.085* |
| C19 | 0.1569 (5) | 0.5322 (5) | 0.4337 (6) | 0.0485 (18) |
| H19 | 0.1805 | 0.5244 | 0.3751 | 0.058* |
| C20 | 0.1444 (4) | 0.6192 (5) | 0.4706 (5) | 0.0383 (15) |
| C21 | 0.1707 (4) | 0.7000 (5) | 0.4178 (4) | 0.0348 (14) |
| C22 | 0.2843 (5) | 0.8878 (5) | 0.4167 (5) | 0.0446 (17) |
| H22 | 0.3236 | 0.8636 | 0.4640 | 0.054* |
| C23 | 0.2510 (5) | 1.0143 (6) | 0.3026 (6) | 0.0524 (19) |
| H23 | 0.1958 | 0.9887 | 0.2866 | 0.063* |
| C24 | 0.3115 (5) | 0.9698 (5) | 0.3671 (5) | 0.0447 (17) |
| C25 | 0.3932 (5) | 1.0076 (5) | 0.3876 (6) | 0.0499 (18) |
| H25 | 0.4338 | 0.9774 | 0.4294 | 0.060* |
| C26 | 0.2742 (6) | 1.0966 (6) | 0.2630 (7) | 0.062 (2) |
| H26 | 0.2337 | 1.1269 | 0.2211 | 0.074* |
| C27 | 0.3561 (5) | 1.1342 (5) | 0.2845 (6) | 0.0513 (18) |
| H27 | 0.3711 | 1.1894 | 0.2570 | 0.062* |
| C28 | 0.4167 (5) | 1.0895 (5) | 0.3478 (5) | 0.0442 (16) |
| C29 | 0.5013 (5) | 1.1297 (6) | 0.3716 (6) | 0.0519 (19) |
| C44 | 0.6304 (6) | 1.0721 (7) | 0.8957 (7) | 0.062 (2) |
| F1 | 0.7216 (7) | 0.8582 (8) | 0.4958 (8) | 0.166 (4)* |
| F2 | 0.6267 (14) | 0.8795 (14) | 0.3382 (15) | 0.287 (8)* |
| F3 | 0.8623 (11) | 0.9046 (13) | 0.3989 (13) | 0.249 (7)* |
| F4 | 0.7568 (6) | 0.7731 (7) | 0.3528 (7) | 0.146 (3)* |
| F5 | 0.7664 (9) | 0.9245 (9) | 0.2583 (10) | 0.200 (5)* |
| F6 | 0.7215 (7) | 1.0152 (8) | 0.3911 (7) | 0.150 (3)* |
| N1 | 0.6676 (5) | 1.1345 (6) | 0.8850 (7) | 0.076 (2) |
| N2 | 0.5688 (5) | 1.1629 (5) | 0.3896 (6) | 0.068 (2) |
| N3 | 0.1969 (4) | 0.7738 (4) | 0.4591 (4) | 0.0381 (13) |
| N4 | 0.2127 (4) | 0.8481 (4) | 0.4001 (4) | 0.0415 (13) |
| N5 | 0.2418 (4) | 0.8153 (4) | 0.7693 (4) | 0.0381 (13) |
| N6 | 0.3198 (4) | 0.8160 (4) | 0.8293 (4) | 0.0425 (14) |
| Sb1 | 0.73809 (5) | 0.89221 (4) | 0.37378 (4) | 0.0695 (3) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|-------------|-------------|-------------|
| Ag1 | 0.0756 (5) | 0.0607 (4) | 0.0291 (3) | -0.0012 (3) | -0.0009 (3) | -0.0029 (2) |
| C1 | 0.035 (4) | 0.058 (4) | 0.049 (4) | -0.004 (3) | 0.008 (3) | -0.004 (4) |
| C2 | 0.046 (4) | 0.054 (5) | 0.057 (5) | -0.003 (4) | 0.006 (4) | -0.012 (4) |
| C3 | 0.040 (5) | 0.095 (7) | 0.068 (6) | 0.002 (5) | -0.007 (4) | 0.006 (5) |

| | | | | | | |
|-----|------------|------------|------------|------------|------------|-------------|
| C4 | 0.048 (5) | 0.076 (6) | 0.080 (7) | 0.003 (5) | -0.009 (4) | 0.009 (5) |
| C5 | 0.045 (4) | 0.056 (5) | 0.058 (5) | -0.004 (4) | -0.001 (4) | 0.005 (4) |
| C6 | 0.039 (4) | 0.059 (5) | 0.036 (4) | -0.001 (3) | 0.005 (3) | -0.005 (3) |
| C7 | 0.039 (4) | 0.066 (5) | 0.040 (4) | 0.003 (4) | 0.004 (3) | 0.002 (4) |
| C8 | 0.035 (4) | 0.037 (3) | 0.032 (3) | 0.001 (3) | -0.001 (3) | 0.001 (3) |
| C9 | 0.039 (4) | 0.047 (4) | 0.033 (3) | 0.000 (3) | -0.002 (3) | -0.007 (3) |
| C10 | 0.057 (5) | 0.063 (5) | 0.047 (4) | 0.001 (4) | -0.015 (4) | 0.011 (4) |
| C11 | 0.070 (7) | 0.101 (8) | 0.069 (6) | 0.019 (6) | -0.024 (5) | 0.017 (6) |
| C12 | 0.047 (6) | 0.131 (10) | 0.087 (8) | 0.014 (6) | -0.017 (5) | 0.000 (7) |
| C13 | 0.035 (5) | 0.129 (9) | 0.085 (7) | -0.025 (5) | 0.002 (5) | -0.010 (7) |
| C14 | 0.048 (5) | 0.084 (6) | 0.049 (5) | -0.009 (4) | 0.002 (4) | 0.008 (4) |
| C15 | 0.049 (4) | 0.063 (5) | 0.039 (4) | -0.009 (4) | 0.002 (3) | 0.003 (3) |
| C16 | 0.055 (5) | 0.091 (8) | 0.048 (5) | -0.012 (5) | -0.002 (4) | 0.025 (5) |
| C17 | 0.054 (5) | 0.079 (7) | 0.068 (6) | -0.025 (5) | -0.016 (5) | 0.037 (5) |
| C18 | 0.055 (5) | 0.044 (5) | 0.108 (9) | -0.003 (4) | -0.029 (6) | 0.010 (5) |
| C19 | 0.046 (4) | 0.043 (4) | 0.055 (5) | -0.006 (3) | -0.007 (3) | 0.001 (3) |
| C20 | 0.031 (3) | 0.049 (4) | 0.034 (3) | -0.006 (3) | -0.004 (3) | 0.002 (3) |
| C21 | 0.028 (3) | 0.046 (4) | 0.030 (3) | -0.001 (3) | -0.001 (2) | 0.002 (3) |
| C22 | 0.042 (4) | 0.057 (5) | 0.034 (4) | 0.000 (3) | -0.008 (3) | 0.006 (3) |
| C23 | 0.055 (5) | 0.053 (4) | 0.047 (4) | -0.008 (4) | -0.010 (4) | 0.002 (4) |
| C24 | 0.056 (5) | 0.042 (4) | 0.036 (4) | -0.001 (3) | 0.001 (3) | 0.001 (3) |
| C25 | 0.050 (5) | 0.048 (4) | 0.050 (4) | 0.002 (4) | -0.011 (3) | -0.001 (3) |
| C26 | 0.063 (5) | 0.053 (5) | 0.069 (6) | 0.006 (4) | -0.001 (4) | 0.022 (4) |
| C27 | 0.061 (5) | 0.041 (4) | 0.052 (5) | -0.004 (4) | 0.006 (4) | 0.010 (3) |
| C28 | 0.041 (4) | 0.049 (4) | 0.044 (4) | -0.002 (3) | 0.004 (3) | -0.002 (3) |
| C29 | 0.051 (5) | 0.056 (5) | 0.047 (4) | -0.006 (4) | -0.003 (3) | -0.001 (4) |
| C44 | 0.041 (5) | 0.075 (6) | 0.071 (6) | -0.011 (4) | 0.002 (4) | -0.015 (5) |
| N1 | 0.049 (4) | 0.072 (5) | 0.105 (7) | -0.013 (4) | -0.006 (4) | -0.006 (5) |
| N2 | 0.059 (5) | 0.074 (5) | 0.068 (5) | -0.014 (4) | -0.010 (4) | 0.006 (4) |
| N3 | 0.038 (3) | 0.041 (3) | 0.035 (3) | 0.000 (2) | 0.000 (2) | 0.001 (2) |
| N4 | 0.050 (4) | 0.044 (3) | 0.030 (3) | -0.001 (3) | 0.002 (2) | 0.002 (2) |
| N5 | 0.035 (3) | 0.048 (3) | 0.031 (3) | 0.000 (2) | -0.002 (2) | 0.001 (2) |
| N6 | 0.031 (3) | 0.063 (4) | 0.033 (3) | -0.004 (3) | -0.001 (2) | 0.001 (3) |
| Sb1 | 0.1014 (6) | 0.0518 (4) | 0.0563 (4) | 0.0034 (3) | 0.0135 (3) | -0.0063 (3) |

Geometric parameters (Å, °)

| | | | |
|---------------------|------------|-----------------------|------------|
| Ag1—N5 | 2.287 (6) | C16—H16 | 0.9300 |
| Ag1—N3 | 2.334 (5) | C17—C18 | 1.347 (15) |
| Ag1—N1 ⁱ | 2.354 (9) | C17—H17 | 0.9300 |
| C1—C2 | 1.369 (11) | C18—C19 | 1.399 (12) |
| C1—C6 | 1.377 (11) | C18—H18 | 0.9300 |
| C1—H1 | 0.9300 | C19—C20 | 1.391 (10) |
| C2—C3 | 1.384 (13) | C19—H19 | 0.9300 |
| C2—C44 | 1.465 (13) | C20—C21 | 1.465 (9) |
| C3—C4 | 1.357 (13) | C21—N3 | 1.273 (8) |
| C3—H3 | 0.9300 | C21—C8 ⁱⁱⁱ | 1.527 (9) |
| C4—C5 | 1.359 (12) | C22—N4 | 1.238 (9) |
| C4—H4 | 0.9300 | C22—C24 | 1.460 (10) |

supplementary materials

| | | | |
|------------------------|------------|---------------------------|------------|
| C5—C6 | 1.390 (11) | C22—H22 | 0.9300 |
| C5—H5 | 0.9300 | C23—C26 | 1.380 (12) |
| C6—C7 | 1.476 (10) | C23—C24 | 1.402 (10) |
| C7—N6 | 1.246 (10) | C23—H23 | 0.9300 |
| C7—H7 | 0.9300 | C24—C25 | 1.367 (11) |
| C8—N5 | 1.270 (8) | C25—C28 | 1.379 (11) |
| C8—C9 | 1.463 (9) | C25—H25 | 0.9300 |
| C8—C21 ⁱⁱ | 1.527 (9) | C26—C27 | 1.371 (12) |
| C9—C10 | 1.367 (10) | C26—H26 | 0.9300 |
| C9—C14 | 1.403 (11) | C27—C28 | 1.394 (11) |
| C10—C11 | 1.416 (12) | C27—H27 | 0.9300 |
| C10—H10 | 0.9300 | C28—C29 | 1.428 (11) |
| C11—C12 | 1.335 (16) | C29—N2 | 1.144 (10) |
| C11—H11 | 0.9300 | C44—N1 | 1.088 (11) |
| C12—C13 | 1.379 (16) | F1—Sb1 | 1.822 (11) |
| C12—H12 | 0.9300 | F2—Sb1 | 1.74 (2) |
| C13—C14 | 1.383 (12) | F3—Sb1 | 1.899 (17) |
| C13—H13 | 0.9300 | F4—Sb1 | 1.791 (10) |
| C14—H14 | 0.9300 | F5—Sb1 | 1.775 (14) |
| C15—C20 | 1.374 (10) | F6—Sb1 | 1.833 (12) |
| C15—C16 | 1.387 (11) | N1—Ag1 ^{iv} | 2.354 (9) |
| C15—H15 | 0.9300 | N3—N4 | 1.398 (8) |
| C16—C17 | 1.369 (14) | N5—N6 | 1.402 (8) |
| N5—Ag1—N3 | 145.2 (2) | C20—C19—C18 | 118.0 (8) |
| N5—Ag1—N1 ⁱ | 107.5 (3) | C20—C19—H19 | 121.0 |
| N3—Ag1—N1 ⁱ | 97.9 (3) | C18—C19—H19 | 121.0 |
| C2—C1—C6 | 119.9 (8) | C15—C20—C19 | 119.4 (7) |
| C2—C1—H1 | 120.0 | C15—C20—C21 | 120.8 (7) |
| C6—C1—H1 | 120.0 | C19—C20—C21 | 119.8 (7) |
| C1—C2—C3 | 120.6 (8) | N3—C21—C20 | 122.5 (6) |
| C1—C2—C44 | 118.3 (8) | N3—C21—C8 ⁱⁱⁱ | 119.4 (6) |
| C3—C2—C44 | 121.0 (8) | C20—C21—C8 ⁱⁱⁱ | 118.1 (6) |
| C4—C3—C2 | 119.3 (8) | N4—C22—C24 | 124.7 (6) |
| C4—C3—H3 | 120.4 | N4—C22—H22 | 117.7 |
| C2—C3—H3 | 120.4 | C24—C22—H22 | 117.7 |
| C5—C4—C3 | 120.7 (9) | C26—C23—C24 | 119.5 (7) |
| C5—C4—H4 | 119.6 | C26—C23—H23 | 120.3 |
| C3—C4—H4 | 119.6 | C24—C23—H23 | 120.3 |
| C4—C5—C6 | 120.7 (8) | C25—C24—C23 | 119.2 (7) |
| C4—C5—H5 | 119.7 | C25—C24—C22 | 120.9 (7) |
| C6—C5—H5 | 119.7 | C23—C24—C22 | 119.7 (7) |
| C1—C6—C5 | 118.7 (7) | C24—C25—C28 | 121.5 (7) |
| C1—C6—C7 | 119.6 (7) | C24—C25—H25 | 119.3 |
| C5—C6—C7 | 121.7 (7) | C28—C25—H25 | 119.3 |
| N6—C7—C6 | 122.4 (7) | C27—C26—C23 | 120.8 (8) |
| N6—C7—H7 | 118.8 | C27—C26—H26 | 119.6 |
| C6—C7—H7 | 118.8 | C23—C26—H26 | 119.6 |

| | | | |
|------------------------------|------------|-----------------------------|------------|
| N5—C8—C9 | 120.1 (6) | C26—C27—C28 | 119.8 (7) |
| N5—C8—C21 ⁱⁱ | 120.4 (6) | C26—C27—H27 | 120.1 |
| C9—C8—C21 ⁱⁱ | 119.5 (6) | C28—C27—H27 | 120.1 |
| C10—C9—C14 | 119.4 (7) | C25—C28—C27 | 119.2 (7) |
| C10—C9—C8 | 120.1 (7) | C25—C28—C29 | 121.1 (7) |
| C14—C9—C8 | 120.4 (7) | C27—C28—C29 | 119.7 (7) |
| C9—C10—C11 | 119.9 (9) | N2—C29—C28 | 179.0 (9) |
| C9—C10—H10 | 120.0 | N1—C44—C2 | 178.1 (11) |
| C11—C10—H10 | 120.0 | C44—N1—Ag1 ^{iv} | 170.3 (9) |
| C12—C11—C10 | 120.6 (10) | C21—N3—N4 | 116.5 (5) |
| C12—C11—H11 | 119.7 | C21—N3—Ag1 | 123.2 (4) |
| C10—C11—H11 | 119.7 | N4—N3—Ag1 | 117.1 (4) |
| C11—C12—C13 | 119.7 (9) | C22—N4—N3 | 116.0 (6) |
| C11—C12—H12 | 120.1 | C8—N5—N6 | 116.6 (5) |
| C13—C12—H12 | 120.1 | C8—N5—Ag1 | 125.5 (4) |
| C12—C13—C14 | 121.4 (10) | N6—N5—Ag1 | 114.0 (4) |
| C12—C13—H13 | 119.3 | C7—N6—N5 | 113.7 (6) |
| C14—C13—H13 | 119.3 | F2—Sb1—F5 | 93.5 (8) |
| C13—C14—C9 | 118.7 (8) | F2—Sb1—F4 | 90.6 (7) |
| C13—C14—H14 | 120.6 | F5—Sb1—F4 | 93.1 (6) |
| C9—C14—H14 | 120.6 | F2—Sb1—F1 | 92.5 (8) |
| C20—C15—C16 | 120.7 (8) | F5—Sb1—F1 | 173.9 (6) |
| C20—C15—H15 | 119.6 | F4—Sb1—F1 | 85.7 (5) |
| C16—C15—H15 | 119.6 | F2—Sb1—F6 | 90.2 (7) |
| C17—C16—C15 | 120.3 (9) | F5—Sb1—F6 | 84.6 (5) |
| C17—C16—H16 | 119.9 | F4—Sb1—F6 | 177.7 (5) |
| C15—C16—H16 | 119.9 | F1—Sb1—F6 | 96.4 (5) |
| C18—C17—C16 | 119.0 (8) | F2—Sb1—F3 | 173.9 (8) |
| C18—C17—H17 | 120.5 | F5—Sb1—F3 | 80.9 (7) |
| C16—C17—H17 | 120.5 | F4—Sb1—F3 | 87.5 (6) |
| C17—C18—C19 | 122.6 (9) | F1—Sb1—F3 | 93.1 (6) |
| C17—C18—H18 | 118.7 | F6—Sb1—F3 | 91.5 (6) |
| C19—C18—H18 | 118.7 | | |
| C6—C1—C2—C3 | -0.3 (12) | N4—C22—C24—C25 | -177.8 (8) |
| C6—C1—C2—C44 | 178.9 (7) | N4—C22—C24—C23 | 6.8 (12) |
| C1—C2—C3—C4 | 0.0 (14) | C23—C24—C25—C28 | 1.4 (12) |
| C44—C2—C3—C4 | -179.2 (9) | C22—C24—C25—C28 | -174.0 (7) |
| C2—C3—C4—C5 | 0.4 (15) | C24—C23—C26—C27 | 1.3 (14) |
| C3—C4—C5—C6 | -0.5 (15) | C23—C26—C27—C28 | -0.6 (14) |
| C2—C1—C6—C5 | 0.2 (11) | C24—C25—C28—C27 | -0.6 (12) |
| C2—C1—C6—C7 | -179.1 (7) | C24—C25—C28—C29 | 178.3 (7) |
| C4—C5—C6—C1 | 0.2 (12) | C26—C27—C28—C25 | 0.2 (12) |
| C4—C5—C6—C7 | 179.5 (8) | C26—C27—C28—C29 | -178.8 (8) |
| C1—C6—C7—N6 | -173.4 (7) | C25—C28—C29—N2 | 178 (100) |
| C5—C6—C7—N6 | 7.4 (12) | C27—C28—C29—N2 | -3(59) |
| N5—C8—C9—C10 | -39.2 (10) | C1—C2—C44—N1 | -114 (34) |
| C21 ⁱⁱ —C8—C9—C10 | 138.3 (7) | C3—C2—C44—N1 | 65 (35) |
| N5—C8—C9—C14 | 142.7 (8) | C2—C44—N1—Ag1 ^{iv} | -150 (31) |

supplementary materials

| | | | |
|-------------------------------|------------|-------------------------------|------------|
| C21 ⁱⁱ —C8—C9—C14 | -39.8 (10) | C20—C21—N3—N4 | -174.7 (6) |
| C14—C9—C10—C11 | -2.0 (13) | C8 ⁱⁱⁱ —C21—N3—N4 | 7.9 (9) |
| C8—C9—C10—C11 | 179.9 (8) | C20—C21—N3—Ag1 | 26.0 (9) |
| C9—C10—C11—C12 | -0.6 (16) | C8 ⁱⁱⁱ —C21—N3—Ag1 | -151.5 (5) |
| C10—C11—C12—C13 | 0.1 (18) | N5—Ag1—N3—C21 | -105.2 (6) |
| C11—C12—C13—C14 | 3.2 (18) | N1 ⁱ —Ag1—N3—C21 | 31.9 (6) |
| C12—C13—C14—C9 | -5.8 (16) | N5—Ag1—N3—N4 | 95.6 (5) |
| C10—C9—C14—C13 | 5.1 (13) | N1 ⁱ —Ag1—N3—N4 | -127.2 (5) |
| C8—C9—C14—C13 | -176.8 (8) | C24—C22—N4—N3 | -176.3 (7) |
| C20—C15—C16—C17 | 0.3 (13) | C21—N3—N4—C22 | -130.8 (7) |
| C15—C16—C17—C18 | -1.0 (13) | Ag1—N3—N4—C22 | 29.8 (8) |
| C16—C17—C18—C19 | 0.4 (13) | C9—C8—N5—N6 | 178.7 (6) |
| C17—C18—C19—C20 | 1.0 (12) | C21 ⁱⁱ —C8—N5—N6 | 1.2 (9) |
| C16—C15—C20—C19 | 1.1 (11) | C9—C8—N5—Ag1 | -24.7 (9) |
| C16—C15—C20—C21 | -179.1 (7) | C21 ⁱⁱ —C8—N5—Ag1 | 157.7 (5) |
| C18—C19—C20—C15 | -1.7 (10) | N3—Ag1—N5—C8 | 34.6 (7) |
| C18—C19—C20—C21 | 178.5 (6) | N1 ⁱ —Ag1—N5—C8 | -100.4 (6) |
| C15—C20—C21—N3 | 30.8 (10) | N3—Ag1—N5—N6 | -168.3 (4) |
| C19—C20—C21—N3 | -149.4 (7) | N1 ⁱ —Ag1—N5—N6 | 56.6 (5) |
| C15—C20—C21—C8 ⁱⁱⁱ | -151.7 (6) | C6—C7—N6—N5 | -177.2 (6) |
| C19—C20—C21—C8 ⁱⁱⁱ | 28.1 (9) | C8—N5—N6—C7 | -126.7 (7) |
| C26—C23—C24—C25 | -1.7 (12) | Ag1—N5—N6—C7 | 74.1 (7) |
| C26—C23—C24—C22 | 173.8 (8) | | |

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

Fig. 1

