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

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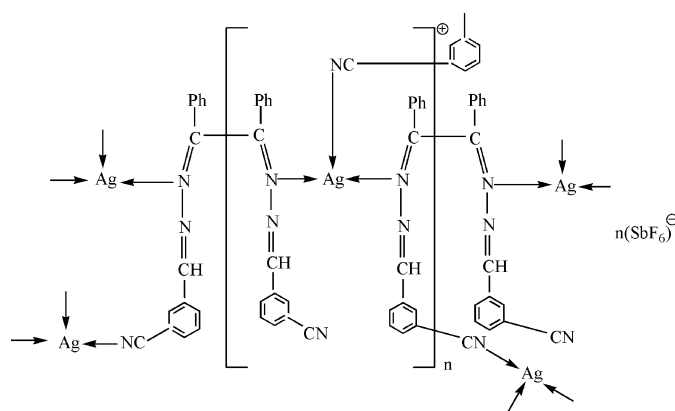
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.012$ Å; R factor = 0.072; wR factor = 0.223; data-to-parameter ratio = 16.0.

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: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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

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supplementary materials

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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

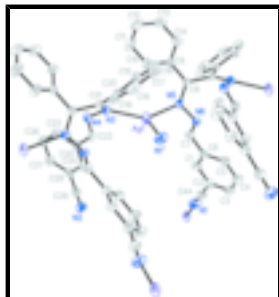


Fig. 1. Part of the polymeric structure and the atom-numbering scheme of the title compound. Displacement ellipsoids are shown at the 30% probability level and H atoms and SbF_6^- anion have been omitted for clarity. [Symmetry code: (i) $-x + 1, y - 1/2, -z + 3/2$]

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

