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Hexakis(μ_3-*N*,*N*-diisopropyldithiocarbamato)hexasilver(I)(6 *Ag*—*Ag*)

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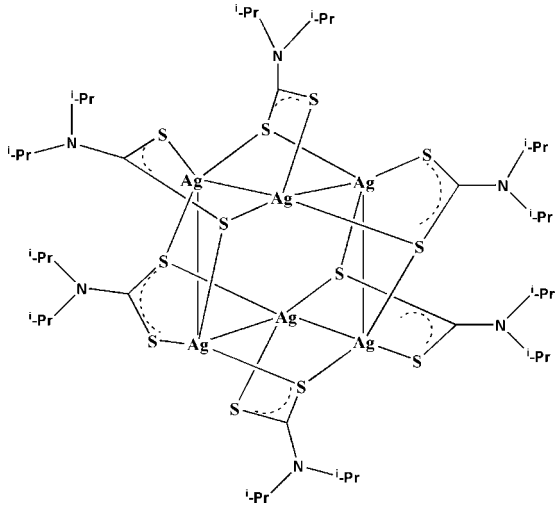
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; disorder in main residue; R factor = 0.037; wR factor = 0.088; data-to-parameter ratio = 17.4.

The title Ag^I complex, $[Ag_6(C_7H_{14}NS_2)_6]$, was obtained by the reaction of $Ag(NO_3)$ with Na(^{i}PrDTC) in a 1:1 molar ratio in methanol (^{i}PrDTC = *N*,*N*-diisopropyldithiocarbamate). The centrosymmetric hexanuclear structure comprises two Ag_3S_3 units which are held together by the S atoms of the thiocarbamate groups. The Ag···Ag distances range from 3.0382 (5) to 3.0985 (5) Å. One of the diisopropylamino groups is disordered over two positions, with site occupancy factors of *ca* 0.6 and 0.4.

Related literature

For related literature, see: Akerström (1959); Anacker-Eickhoff *et al.* (1982); Ebihara *et al.* (1994); Fan *et al.* (2004); Liu *et al.* (2006); Song *et al.* (2006); Tang *et al.* (2004); Zhang *et al.* (2002); Greenwood & Earnshaw (1989).



Experimental

Crystal data

$[Ag_6(C_7H_{14}NS_2)_6]$
M_r = 1705.21
Triclinic, $P\overline{1}$
a = 11.5958 (2) Å
b = 12.4826 (3) Å
c = 12.7543 (2) Å
α = 84.0830 (10)°
β = 78.8250 (10)°
γ = 62.8740 (10)°
V = 1611.69 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.21 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.666, T_{max} = 0.733
16354 measured reflections
5779 independent reflections
4071 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.088
S = 1.05
5779 reflections
333 parameters
60 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—Ag2	3.0755 (5)	Ag2—Ag3^i	3.0382 (5)
Ag1—Ag3	3.0985 (5)	Ag3—Ag2^i	3.0382 (5)

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2002); 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* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2019).

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supplementary materials

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Hexakis(μ_3-*N*,*N*-diisopropyldithiocarbamato)hexasilver(I)(6 *Ag*-*Ag*)

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Comment

Since their first description by Akerström (1959) Ag^I complexes with dialkyldithiocarbamates have been widely studied owing to their variable coordination modes and, for complexes containing the Ag—Ag metal bonds, also due to their potential photoluminescent properties. Differently substituted alkyl groups and reaction conditions may play crucial roles in the formation of a variety of complexes with unprecedented structures (Ebihara *et al.*, 1994; Liu *et al.*, 2006; Song *et al.*, 2006).

Early crystallographic studies revealed the hexameric nature of Ag_S_2CNR_2 (*R* = Et, Pr and n-Bu) complexes in the solid state (Anacker-Eickhoff *et al.*, 1963; Zhang *et al.*, 2002). Recently we synthesized the title ^{i}PrDTC complex, (I), (^{i}PrDTC = *N*,*N*-diisopropyldithiocarbamate).

In the solid state the title complex (I) has a hexameric structure similar to those described earlier with a core formed by two cyclohexane-like Ag_3S_3 rings stacked atop of each other (Fig.1). There are two types of S atoms: S2, S4 and S5 and their symmetry equivalents are coordinated to only one Ag atom each with Ag—S distances of 2.4798 (15), 2.5034 (13) and 2.4879 (15) Å. The remaining three crystallographically independent S atoms (S1, S3 and S6), on the other hand, are acting as bridges between each two Ag atoms with Ag—S distances between 2.4626 (13) and 2.6123 (12) Å. Each three Ag and three of these S atoms are forming the cyclohexane-like rings, which are bridged to each other *via* six Ag—Ag bonds (3.0382 (5)–3.0985 (5) Å). These distances are longer than those in metallic Ag (2.886 Å, Greenwood & Earnshaw, 1989), but still shorter than the sum of the Van der Waals radii of two Ag atoms (3.44 Å, Tang *et al.*, 1997). This thus may suggest to classify these interactions as weakly argentophilic. The thiocarbamato groups are, on the other hand, acting as clamps holding the two six-membered rings together with the mono-coordinated sulfur atoms S2, S4 and S5 (and their symmetry equivalents) bridging over to the other half of the molecule. This seems to be the more likely cause for the close contacts between the two six-membered rings, and the close Ag—Ag contacts may just be a side effect of the stronger forces exerted by the chelating ligands. The thiocarbamato groups themselves exhibit the expected planar geometry with basically sp^2 hybridized N atoms.

Experimental

Synthesis of sodium *N*,*N*-diisopropyldithiocarbamate, Na(^{i}PrDTC) was carried out according to the literature procedure (Fan *et al.*, 2004), with *N*,*N*'-diisopropylamine substituted for *N*,*N*'-dibenzylamine. Silver nitrate (0.17 g, 1.0 mmol) was added slowly to Na(^{i}PrDTC) (0.20 g, 1.0 mmol) in methanol solution (15 ml) with stirring. Then, a pale yellow solution was formed after 24 h. Some pale yellow crystals of the title complex (I) suitable for structure determination were obtained in 40% yield by slow evaporation for the filtrate of silver complex after some weeks.

Refinement

One of the diisopropylamine groups has both isopropylamines disordered over two positions with a site occupancy ratio of 0.57 (2):0.43 (2). The C—C distances within each isopropyl group were restrained to be the same within a standard deviation of 0.02 Å, rigid bond restraints were applied (DELU commands, standard deviation 0.01), and the atoms within the isopropyl groups were restrained to have the same U^{ij} components (SIMU commands, standard deviation 0.01). The central N-bonded C (C17 and C20) were restrained to be isotropic within a standard deviation of 0.01, and equivalent disordered C atoms were set to have identical anisotropic displacement parameters.

All H atoms were placed in calculated positions with C—H = 0.96(methyl) and 0.98 Å (C—H) and refined with U_{iso}(H) = 1.2U_{eq} (C). Methyl H atoms were allowed to rotate to best fit the experimental electron density.

Figures

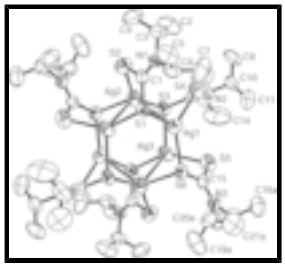


Fig. 1. The molecular structure of the title compound (I), with 50% probability displacement ellipsoids (H atoms are omitted for clarity).

Hexa-μ$_3$-*N*,*N*-diisopropyldithiocarbamato-hexasilver(I)(6 A g—Ag)

Crystal data

$[Ag_6(C_7H_{14}N_1S_2)_6]$	Z = 1
M_r = 1705.21	F_{000} = 852
Triclinic, $P\overline{1}$	D_x = 1.757 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.5958 (2) Å	Cell parameters from 1000 reflections
b = 12.4826 (3) Å	θ = 2.0–25.0º
c = 12.7543 (2) Å	μ = 2.21 mm^{-1}
α = 84.0830 (10)º	T = 293 (2) K
β = 78.8250 (10)º	Block, pale-yellow
γ = 62.8740 (10)º	0.20 × 0.20 × 0.15 mm
V = 1611.69 (6) Å^3	

Data collection

Bruker SMART APEXII diffractometer	5779 independent reflections
Radiation source: fine-focus sealed tube	4071 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033

T = 293(2) K

φ and ω scans

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

T_{min} = 0.666, T_{max} = 0.733

16354 measured reflections

θ_{max} = 25.2º

θ_{min} = 1.8º

h = −12→13

k = −14→13

l = −15→15

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.037

$wR(F^2)$ = 0.088

S = 1.05

5779 reflections

333 parameters

60 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.1926P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.56 e Å^{-3}

$\Delta\rho_{min}$ = −0.52 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C2	0.3470 (7)	0.6466 (6)	0.0839 (4)	0.111 (2)	
H2A	0.3687	0.5625	0.0909	0.167*	
H2B	0.3883	0.6622	0.0153	0.167*	
H2C	0.2535	0.6931	0.0904	0.167*	
C3	0.3950 (5)	0.6810 (5)	0.1704 (4)	0.0669 (14)	
H3	0.4905	0.6467	0.1483	0.080*	
C4	0.3496 (6)	0.8151 (5)	0.1763 (5)	0.098 (2)	
H4A	0.3900	0.8300	0.2285	0.147*	
H4B	0.2558	0.8552	0.1966	0.147*	
H4C	0.3744	0.8451	0.1077	0.147*	
C5	0.5925 (5)	0.5950 (6)	0.3133 (4)	0.0918 (19)	

H5A	0.5443	0.6713	0.3482	0.138*	
H5B	0.6272	0.6069	0.2408	0.138*	
H5C	0.6634	0.5431	0.3504	0.138*	
C6	0.5018 (5)	0.5380 (5)	0.3142 (4)	0.0693 (15)	
H6	0.4787	0.5162	0.3886	0.083*	
C7	0.5673 (6)	0.4230 (6)	0.2504 (7)	0.132 (3)	
H7A	0.5084	0.3871	0.2575	0.198*	
H7B	0.6461	0.3677	0.2769	0.198*	
H7C	0.5889	0.4413	0.1764	0.198*	
C9	0.2875 (6)	0.2859 (6)	−0.0444 (5)	0.106 (2)	
H9A	0.2194	0.3458	−0.0801	0.159*	
H9B	0.3538	0.2292	−0.0955	0.159*	
H9C	0.3259	0.3240	−0.0105	0.159*	
C10	0.2308 (5)	0.2222 (5)	0.0375 (4)	0.0740 (15)	
H10	0.1972	0.1839	−0.0039	0.089*	
C11	0.3296 (7)	0.1179 (5)	0.0940 (6)	0.117 (2)	
H11A	0.2840	0.0922	0.1544	0.176*	
H11B	0.3870	0.1429	0.1178	0.176*	
H11C	0.3803	0.0523	0.0455	0.176*	
C12	−0.0466 (7)	0.3541 (7)	−0.0128 (6)	0.131 (3)	
H12A	−0.0416	0.4292	−0.0246	0.197*	
H12B	−0.1343	0.3673	−0.0153	0.197*	
H12C	0.0137	0.2987	−0.0674	0.197*	
C13	−0.0119 (6)	0.3030 (6)	0.0942 (4)	0.0889 (19)	
H13	−0.0819	0.3583	0.1469	0.107*	
C14	−0.0086 (9)	0.1823 (9)	0.1203 (7)	0.168 (4)	
H14A	−0.0052	0.1644	0.1950	0.252*	
H14B	0.0677	0.1221	0.0788	0.252*	
H14C	−0.0863	0.1829	0.1038	0.252*	
C16A	0.364 (2)	−0.171 (3)	0.503 (2)	0.099 (5)	0.567 (17)
H16A	0.4493	−0.1853	0.5150	0.149*	0.567 (17)
H16B	0.3496	−0.1337	0.4343	0.149*	0.567 (17)
H16C	0.3599	−0.2465	0.5061	0.149*	0.567 (17)
C17A	0.2593 (12)	−0.0890 (10)	0.5893 (13)	0.081 (3)	0.567 (17)
H17A	0.2843	−0.1294	0.6572	0.098*	0.567 (17)
C18A	0.1173 (14)	−0.0634 (19)	0.5966 (18)	0.097 (4)	0.567 (17)
H18A	0.0680	−0.0256	0.6633	0.146*	0.567 (17)
H18B	0.1124	−0.1375	0.5925	0.146*	0.567 (17)
H18C	0.0814	−0.0107	0.5386	0.146*	0.567 (17)
C16B	0.327 (3)	−0.149 (4)	0.489 (3)	0.099 (5)	0.433 (17)
H16D	0.3614	−0.1106	0.4308	0.149*	0.433 (17)
H16E	0.2903	−0.1931	0.4612	0.149*	0.433 (17)
H16F	0.3960	−0.2026	0.5267	0.149*	0.433 (17)
C17B	0.2370 (15)	−0.0685 (14)	0.5524 (16)	0.081 (3)	0.433 (17)
H17B	0.1787	−0.0200	0.5015	0.098*	0.433 (17)
C18B	0.142 (2)	−0.101 (3)	0.631 (2)	0.097 (4)	0.433 (17)
H18D	0.0569	−0.0323	0.6409	0.146*	0.433 (17)
H18E	0.1726	−0.1243	0.6983	0.146*	0.433 (17)
H18F	0.1351	−0.1664	0.6039	0.146*	0.433 (17)

C19A	0.240 (4)	0.020 (4)	0.787 (2)	0.121 (8)	0.567 (17)
H19A	0.1506	0.0779	0.7838	0.181*	0.567 (17)
H19B	0.2680	0.0383	0.8462	0.181*	0.567 (17)
H19C	0.2447	−0.0591	0.7976	0.181*	0.567 (17)
C20A	0.3259 (14)	0.025 (3)	0.6862 (11)	0.084 (4)	0.567 (17)
H20A	0.3274	0.1029	0.6857	0.101*	0.567 (17)
C21A	0.4650 (14)	−0.068 (2)	0.682 (2)	0.115 (6)	0.567 (17)
H21A	0.5153	−0.0628	0.6143	0.172*	0.567 (17)
H21B	0.4683	−0.1463	0.6918	0.172*	0.567 (17)
H21C	0.5010	−0.0537	0.7382	0.172*	0.567 (17)
C19B	0.243 (6)	0.067 (5)	0.785 (3)	0.121 (8)	0.433 (17)
H19D	0.1765	0.0410	0.8080	0.181*	0.433 (17)
H19E	0.2032	0.1526	0.7714	0.181*	0.433 (17)
H19F	0.2965	0.0489	0.8395	0.181*	0.433 (17)
C20B	0.3260 (19)	0.005 (5)	0.6870 (14)	0.084 (4)	0.433 (17)
H20B	0.3428	−0.0781	0.7049	0.101*	0.433 (17)
C21B	0.4590 (19)	−0.007 (3)	0.651 (3)	0.115 (6)	0.433 (17)
H21D	0.4922	−0.0415	0.5815	0.172*	0.433 (17)
H21E	0.5150	−0.0578	0.7004	0.172*	0.433 (17)
H21F	0.4572	0.0712	0.6480	0.172*	0.433 (17)
N1	0.3763 (3)	0.6231 (3)	0.2760 (3)	0.0501 (9)	
N2	0.1125 (4)	0.3024 (3)	0.1115 (3)	0.0544 (10)	
N3	0.2622 (4)	0.0295 (3)	0.5920 (3)	0.0601 (10)	
C1	0.2593 (4)	0.6399 (4)	0.3313 (3)	0.0496 (11)	
C8	0.1157 (4)	0.3679 (4)	0.1861 (3)	0.0473 (11)	
C15	0.2239 (4)	0.1282 (4)	0.5297 (3)	0.0490 (11)	
S1	0.25423 (12)	0.55930 (11)	0.45194 (9)	0.0539 (3)	
S2	0.11601 (13)	0.74066 (13)	0.29098 (12)	0.0763 (4)	
S3	−0.03418 (12)	0.45673 (11)	0.26684 (9)	0.0567 (3)	
S4	0.25532 (13)	0.37190 (14)	0.20131 (10)	0.0700 (4)	
S5	0.16170 (14)	0.13468 (14)	0.41742 (11)	0.0767 (4)	
S6	0.24215 (11)	0.25148 (11)	0.56300 (10)	0.0548 (3)	
Ag1	0.21579 (4)	0.38209 (4)	0.40089 (3)	0.06482 (14)	
Ag2	−0.00718 (4)	0.61920 (4)	0.33669 (3)	0.06672 (14)	
Ag3	−0.03051 (4)	0.33627 (4)	0.44546 (3)	0.06702 (14)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.114 (5)	0.169 (7)	0.064 (4)	−0.075 (5)	−0.017 (3)	0.003 (4)
C3	0.062 (3)	0.086 (4)	0.051 (3)	−0.036 (3)	−0.004 (2)	0.013 (3)
C4	0.091 (5)	0.081 (5)	0.121 (5)	−0.047 (4)	−0.013 (4)	0.034 (4)
C5	0.051 (3)	0.137 (6)	0.088 (4)	−0.043 (4)	−0.016 (3)	0.005 (4)
C6	0.039 (3)	0.086 (4)	0.073 (3)	−0.025 (3)	−0.006 (2)	0.021 (3)
C7	0.071 (5)	0.076 (5)	0.219 (9)	−0.004 (4)	−0.027 (5)	−0.010 (5)
C9	0.094 (5)	0.130 (6)	0.080 (4)	−0.057 (4)	0.036 (3)	−0.013 (4)
C10	0.070 (4)	0.073 (4)	0.064 (3)	−0.025 (3)	0.015 (3)	−0.021 (3)
C11	0.105 (6)	0.071 (4)	0.127 (6)	−0.004 (4)	0.003 (4)	−0.016 (4)

C12	0.137 (7)	0.151 (7)	0.141 (6)	−0.076 (6)	−0.082 (5)	0.012 (5)
C13	0.074 (4)	0.137 (6)	0.077 (4)	−0.065 (4)	0.005 (3)	−0.038 (4)
C14	0.205 (10)	0.239 (11)	0.156 (8)	−0.191 (10)	−0.024 (7)	0.029 (7)
C16A	0.098 (11)	0.082 (9)	0.114 (8)	−0.037 (8)	−0.002 (8)	−0.032 (7)
C17A	0.090 (5)	0.063 (5)	0.099 (7)	−0.043 (4)	−0.011 (5)	−0.001 (5)
C18A	0.095 (7)	0.085 (11)	0.128 (12)	−0.060 (7)	−0.013 (6)	0.011 (7)
C16B	0.098 (11)	0.082 (9)	0.114 (8)	−0.037 (8)	−0.002 (8)	−0.032 (7)
C17B	0.090 (5)	0.063 (5)	0.099 (7)	−0.043 (4)	−0.011 (5)	−0.001 (5)
C18B	0.095 (7)	0.085 (11)	0.128 (12)	−0.060 (7)	−0.013 (6)	0.011 (7)
C19A	0.113 (6)	0.17 (3)	0.096 (5)	−0.067 (18)	−0.003 (4)	−0.064 (13)
C20A	0.076 (4)	0.075 (10)	0.085 (4)	−0.019 (4)	−0.026 (3)	0.021 (3)
C21A	0.068 (4)	0.15 (2)	0.123 (14)	−0.038 (8)	−0.038 (5)	0.004 (12)
C19B	0.113 (6)	0.17 (3)	0.096 (5)	−0.067 (18)	−0.003 (4)	−0.064 (13)
C20B	0.076 (4)	0.075 (10)	0.085 (4)	−0.019 (4)	−0.026 (3)	0.021 (3)
C21B	0.068 (4)	0.15 (2)	0.123 (14)	−0.038 (8)	−0.038 (5)	0.004 (12)
N1	0.041 (2)	0.059 (2)	0.049 (2)	−0.024 (2)	−0.0029 (17)	0.0038 (17)
N2	0.051 (2)	0.060 (2)	0.049 (2)	−0.024 (2)	0.0031 (17)	−0.0124 (19)
N3	0.054 (3)	0.049 (3)	0.075 (3)	−0.024 (2)	0.002 (2)	−0.008 (2)
C1	0.044 (3)	0.050 (3)	0.059 (3)	−0.026 (2)	−0.002 (2)	−0.008 (2)
C8	0.050 (3)	0.044 (3)	0.042 (2)	−0.019 (2)	−0.003 (2)	0.002 (2)
C15	0.031 (2)	0.048 (3)	0.062 (3)	−0.014 (2)	−0.001 (2)	−0.006 (2)
S1	0.0520 (7)	0.0636 (8)	0.0502 (6)	−0.0318 (6)	−0.0016 (5)	−0.0014 (6)
S2	0.0441 (8)	0.0757 (10)	0.0974 (10)	−0.0191 (7)	−0.0148 (7)	0.0167 (8)
S3	0.0424 (7)	0.0658 (8)	0.0525 (6)	−0.0173 (6)	0.0001 (5)	−0.0101 (6)
S4	0.0477 (8)	0.0978 (11)	0.0695 (8)	−0.0370 (8)	−0.0050 (6)	−0.0098 (7)
S5	0.0630 (9)	0.0913 (11)	0.0757 (9)	−0.0287 (8)	−0.0170 (7)	−0.0200 (8)
S6	0.0459 (7)	0.0489 (7)	0.0698 (7)	−0.0218 (6)	−0.0055 (6)	−0.0071 (6)
Ag1	0.0569 (3)	0.0674 (3)	0.0746 (3)	−0.0306 (2)	−0.01761 (19)	0.0068 (2)
Ag2	0.0528 (3)	0.0668 (3)	0.0729 (3)	−0.0160 (2)	−0.01406 (19)	−0.0149 (2)
Ag3	0.0492 (2)	0.0961 (3)	0.0570 (2)	−0.0345 (2)	−0.00242 (17)	−0.0089 (2)

Geometric parameters (Å, °)

C2—C3	1.504 (7)	C16B—H16E	0.9600
C2—H2A	0.9600	C16B—H16F	0.9600
C2—H2B	0.9600	C17B—C18B	1.512 (15)
C2—H2C	0.9600	C17B—N3	1.532 (12)
C3—N1	1.487 (5)	C17B—H17B	0.9800
C3—C4	1.515 (7)	C18B—H18D	0.9600
C3—H3	0.9800	C18B—H18E	0.9600
C4—H4A	0.9600	C18B—H18F	0.9600
C4—H4B	0.9600	C19A—C20A	1.486 (19)
C4—H4C	0.9600	C19A—H19A	0.9600
C5—C6	1.513 (7)	C19A—H19B	0.9600
C5—H5A	0.9600	C19A—H19C	0.9600
C5—H5B	0.9600	C20A—C21A	1.491 (19)
C5—H5C	0.9600	C20A—N3	1.511 (11)
C6—N1	1.498 (6)	C20A—H20A	0.9800
C6—C7	1.519 (8)	C21A—H21A	0.9600

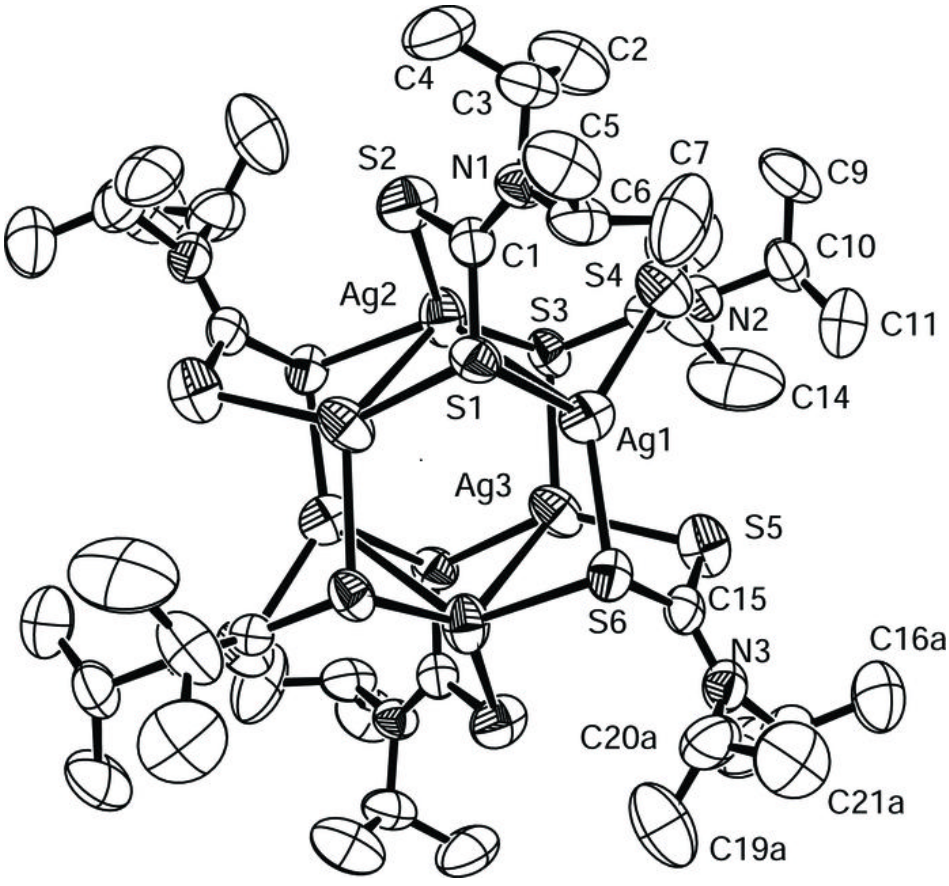
C6—H6	0.9800	C21A—H21B	0.9600
C7—H7A	0.9600	C21A—H21C	0.9600
C7—H7B	0.9600	C19B—C20B	1.46 (2)
C7—H7C	0.9600	C19B—H19D	0.9600
C9—C10	1.481 (7)	C19B—H19E	0.9600
C9—H9A	0.9600	C19B—H19F	0.9600
C9—H9B	0.9600	C20B—C21B	1.46 (2)
C9—H9C	0.9600	C20B—N3	1.475 (13)
C10—N2	1.489 (6)	C20B—H20B	0.9800
C10—C11	1.514 (7)	C21B—H21D	0.9600
C10—H10	0.9800	C21B—H21E	0.9600
C11—H11A	0.9600	C21B—H21F	0.9600
C11—H11B	0.9600	N1—C1	1.335 (5)
C11—H11C	0.9600	N2—C8	1.333 (5)
C12—C13	1.494 (8)	N3—C15	1.334 (5)
C12—H12A	0.9600	C1—S2	1.703 (5)
C12—H12B	0.9600	C1—S1	1.756 (4)
C12—H12C	0.9600	C8—S4	1.690 (5)
C13—C14	1.494 (9)	C8—S3	1.759 (4)
C13—N2	1.497 (6)	C15—S5	1.703 (4)
C13—H13	0.9800	C15—S6	1.750 (5)
C14—H14A	0.9600	S1—Ag3^{i}	2.4686 (12)
C14—H14B	0.9600	S1—Ag1	2.6123 (12)
C14—H14C	0.9600	S2—Ag2	2.4798 (15)
C16A—C17A	1.522 (18)	S3—Ag2	2.4626 (13)
C16A—H16A	0.9600	S3—Ag3	2.5934 (13)
C16A—H16B	0.9600	S4—Ag1	2.5034 (13)
C16A—H16C	0.9600	S5—Ag3	2.4879 (15)
C17A—N3	1.499 (10)	S6—Ag1	2.4742 (13)
C17A—C18A	1.512 (14)	S6—Ag2^{i}	2.5943 (12)
C17A—H17A	0.9800	Ag2—S6^{i}	2.5943 (12)
C18A—H18A	0.9600	Ag3—S1^{i}	2.4686 (12)
C18A—H18B	0.9600	Ag1—Ag2	3.0755 (5)
C18A—H18C	0.9600	Ag1—Ag3	3.0985 (5)
C16B—C17B	1.28 (3)	Ag2—Ag3^{i}	3.0382 (5)
C16B—H16D	0.9600	Ag3—Ag2^{i}	3.0382 (5)
C3—C2—H2A	109.5	H18D—C18B—H18E	109.5
C3—C2—H2B	109.5	C17B—C18B—H18F	109.5
H2A—C2—H2B	109.5	H18D—C18B—H18F	109.5
C3—C2—H2C	109.5	H18E—C18B—H18F	109.5
H2A—C2—H2C	109.5	C19A—C20A—C21A	113 (3)
H2B—C2—H2C	109.5	C19A—C20A—N3	110 (2)
N1—C3—C2	113.9 (4)	C21A—C20A—N3	116.1 (17)
N1—C3—C4	113.5 (4)	C19A—C20A—H20A	105.7
C2—C3—C4	113.9 (5)	C21A—C20A—H20A	105.7
N1—C3—H3	104.8	N3—C20A—H20A	105.7
C2—C3—H3	104.8	C20B—C19B—H19D	109.5

C4—C3—H3	104.8	C20B—C19B—H19E	109.5
C3—C4—H4A	109.5	H19D—C19B—H19E	109.5
C3—C4—H4B	109.5	C20B—C19B—H19F	109.5
H4A—C4—H4B	109.5	H19D—C19B—H19F	109.5
C3—C4—H4C	109.5	H19E—C19B—H19F	109.5
H4A—C4—H4C	109.5	C19B—C20B—C21B	123 (3)
H4B—C4—H4C	109.5	C19B—C20B—N3	117 (3)
C6—C5—H5A	109.5	C21B—C20B—N3	108 (2)
C6—C5—H5B	109.5	C19B—C20B—H20B	101.9
H5A—C5—H5B	109.5	C21B—C20B—H20B	101.9
C6—C5—H5C	109.5	N3—C20B—H20B	101.9
H5A—C5—H5C	109.5	C20B—C21B—H21D	109.5
H5B—C5—H5C	109.5	C20B—C21B—H21E	109.5
N1—C6—C5	112.4 (4)	H21D—C21B—H21E	109.5
N1—C6—C7	109.9 (5)	C20B—C21B—H21F	109.5
C5—C6—C7	112.6 (5)	H21D—C21B—H21F	109.5
N1—C6—H6	107.2	H21E—C21B—H21F	109.5
C5—C6—H6	107.2	C1—N1—C3	124.1 (4)
C7—C6—H6	107.2	C1—N1—C6	121.8 (4)
C6—C7—H7A	109.5	C3—N1—C6	114.1 (4)
C6—C7—H7B	109.5	C8—N2—C10	123.8 (4)
H7A—C7—H7B	109.5	C8—N2—C13	122.8 (4)
C6—C7—H7C	109.5	C10—N2—C13	113.5 (4)
H7A—C7—H7C	109.5	C15—N3—C20B	128 (2)
H7B—C7—H7C	109.5	C15—N3—C17A	133.4 (8)
C10—C9—H9A	109.5	C15—N3—C20A	119.3 (16)
C10—C9—H9B	109.5	C17A—N3—C20A	107.3 (17)
H9A—C9—H9B	109.5	C15—N3—C17B	112.1 (9)
C10—C9—H9C	109.5	C20B—N3—C17B	119 (2)
H9A—C9—H9C	109.5	N1—C1—S2	122.1 (3)
H9B—C9—H9C	109.5	N1—C1—S1	118.5 (3)
C9—C10—N2	114.7 (5)	S2—C1—S1	119.4 (3)
C9—C10—C11	115.1 (5)	N2—C8—S4	122.5 (3)
N2—C10—C11	113.3 (4)	N2—C8—S3	117.3 (3)
C9—C10—H10	104.0	S4—C8—S3	120.2 (2)
N2—C10—H10	104.0	N3—C15—S5	121.3 (3)
C11—C10—H10	104.0	N3—C15—S6	119.0 (3)
C10—C11—H11A	109.5	S5—C15—S6	119.7 (3)
C10—C11—H11B	109.5	C1—S1—$Ag3^{i}$	107.33 (15)
H11A—C11—H11B	109.5	C1—S1—Ag1	103.96 (14)
C10—C11—H11C	109.5	$Ag3^{i}$—S1—Ag1	93.55 (4)
H11A—C11—H11C	109.5	C1—S2—Ag2	98.28 (16)
H11B—C11—H11C	109.5	C8—S3—Ag2	106.79 (15)
C13—C12—H12A	109.5	C8—S3—Ag3	104.74 (14)
C13—C12—H12B	109.5	Ag2—S3—Ag3	96.28 (4)
H12A—C12—H12B	109.5	C8—S4—Ag1	98.69 (14)
C13—C12—H12C	109.5	C15—S5—Ag3	97.99 (15)
H12A—C12—H12C	109.5	C15—S6—Ag1	105.32 (16)

H12B—C12—H12C	109.5	C15—S6—Ag2^{i}	100.09 (14)
C12—C13—C14	115.0 (5)	Ag1—S6—Ag2^{i}	94.86 (4)
C12—C13—N2	112.4 (5)	S6—Ag1—S4	141.39 (5)
C14—C13—N2	110.7 (6)	S6—Ag1—S1	104.04 (4)
C12—C13—H13	106.0	S4—Ag1—S1	108.26 (4)
C14—C13—H13	106.0	S6—Ag1—Ag2	134.05 (3)
N2—C13—H13	106.0	S4—Ag1—Ag2	77.03 (4)
C13—C14—H14A	109.5	S1—Ag1—Ag2	72.09 (3)
C13—C14—H14B	109.5	S6—Ag1—Ag3	75.26 (3)
H14A—C14—H14B	109.5	S4—Ag1—Ag3	97.67 (3)
C13—C14—H14C	109.5	S1—Ag1—Ag3	131.70 (3)
H14A—C14—H14C	109.5	Ag2—Ag1—Ag3	75.187 (14)
H14B—C14—H14C	109.5	S3—Ag2—S2	141.34 (5)
N3—C17A—C18A	107.4 (13)	S3—Ag2—S6^{i}	101.69 (4)
N3—C17A—C16A	112.7 (17)	S2—Ag2—S6^{i}	110.55 (4)
C18A—C17A—C16A	120.2 (18)	S3—Ag2—Ag3^{i}	132.96 (3)
N3—C17A—H17A	105.1	S2—Ag2—Ag3^{i}	77.49 (4)
C18A—C17A—H17A	105.1	S6^{i}—Ag2—Ag3^{i}	74.78 (3)
C16A—C17A—H17A	105.1	S3—Ag2—Ag1	73.90 (3)
C17B—C16B—H16D	109.5	S2—Ag2—Ag1	98.83 (3)
C17B—C16B—H16E	109.5	S6^{i}—Ag2—Ag1	131.06 (3)
H16D—C16B—H16E	109.5	Ag3^{i}—Ag2—Ag1	74.569 (13)
C17B—C16B—H16F	109.5	S1^{i}—Ag3—S5	142.49 (5)
H16D—C16B—H16F	109.5	S1^{i}—Ag3—S3	105.24 (4)
H16E—C16B—H16F	109.5	S5—Ag3—S3	107.43 (5)
C16B—C17B—C18B	119 (3)	S1^{i}—Ag3—Ag2^{i}	74.60 (3)
C16B—C17B—N3	120 (3)	S5—Ag3—Ag2^{i}	97.04 (3)
C18B—C17B—N3	113.6 (17)	S3—Ag3—Ag2^{i}	130.71 (3)
C16B—C17B—H17B	99.0	S1^{i}—Ag3—Ag1	134.65 (3)
C18B—C17B—H17B	99.0	S5—Ag3—Ag1	74.06 (4)
N3—C17B—H17B	99.0	S3—Ag3—Ag1	71.86 (3)
C17B—C18B—H18D	109.5	Ag2^{i}—Ag3—Ag1	74.942 (13)
C17B—C18B—H18E	109.5		

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

Fig. 1


C4
C2
C3
C5
S2
N1
C7
C9
C6
C1
C10
S4
Ag2
S3
N2
C11
S1
C14
Ag1
Ag3
S5
C15
S6
N3
C16a
C20a
C21a
C19a