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Bis(acetonitrile-κN)hexakis(μ_2-4-amino-3,5-dimethyl-1,2,4-triazole-κ^2N^1:N^2)-tetrasilver(I) tetrakis(trifluoromethanesulfonate) acetonitrile disolvate

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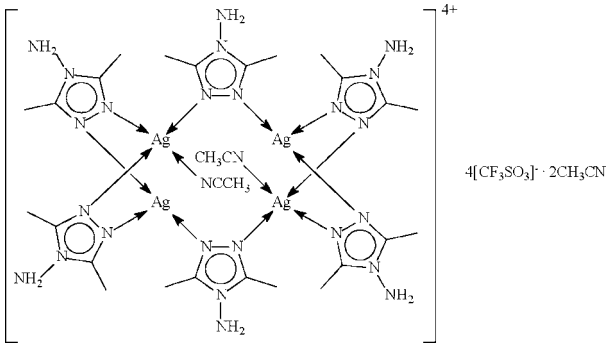
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.017 Å; R factor = 0.074; wR factor = 0.239; data-to-parameter ratio = 18.2.

The centrosymmetric tetranuclear cluster of the title compound, $[Ag_4(C_4H_8N_4)_6(C_2H_3N)_2](CF_3SO_3)_4{\cdot}2C_2H_3N$, has four 4-amino-3,5-dimethyl-1,2,4-triazole *N*-heterocycles, each functioning as a bridge between two Ag atoms. Two of the Ag atoms are additionally coordinated by acetonitrile molecules, so that there are three-coordinate Ag atoms in a trigonal–planar geometry and four-coordinate Ag atoms in a tetrahedral geometry. There are no short hydrogen bonds between cations and anions.

Related literature

For a study of the complex $[\mu_2\text{-}(C_4H_8N_4)_6Ag_4][\mu_2\text{-}(C_4H_8N_4)_6(C_2H_3N)_2Ag_4](ClO_4)_8{\cdot}2H_2O$, see Wang *et al.* (2006).



Experimental

Crystal data

$[Ag_4(C_4H_8N_4)_6(C_2H_3N)_2](CF_3O_3S)_4{\cdot}2C_2H_3N$
M_r = 1864.84
Triclinic, $P\overline{1}$
a = 12.110 (3) Å
b = 12.695 (3) Å
c = 13.001 (3) Å
α = 108.59 (2)°
β = 92.84 (2)°
γ = 108.68 (2)°
V = 1768.9 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.31 mm^{-1}
T = 295 (2) K
0.38 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.294, T_{max} = 0.790
17453 measured reflections
8026 independent reflections
5532 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.239
S = 1.07
8026 reflections
440 parameters
150 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.27 e Å^{-3}
$\Delta\rho_{min}$ = −1.07 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.232 (5)	Ag2—N7^{i}	2.241 (5)
Ag1—N5	2.238 (5)	Ag2—N9	2.371 (6)
Ag1—N10^{i}	2.290 (5)	Ag2—N13	2.395 (9)
Ag2—N2	2.267 (6)		
N1—Ag1—N5	131.8 (2)	N2—Ag2—N13	102.6 (3)
N1—Ag1—N10^{i}	109.7 (2)	N7^{i}—Ag2—N9	114.7 (2)
N5—Ag1—N10^{i}	117.2 (2)	N7^{i}—Ag2—N13	109.4 (3)
N2—Ag2—N9	97.9 (2)	N9—Ag2—N13	95.6 (3)
N2—Ag2—N7^{i}	130.8 (2)		

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2378).

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supplementary materials

Acta Cryst. (2007). E**63**, m1801 [**doi:10.1107/S1600536807026360**]

Bis(acetonitrile-κN)hexakis(μ_2-4-amino-3,5-dimethyl-1,2,4-triazole-$\kappa^2N^1:N^2$)tetrasilver(I) tetrakis(trifluoromethanesulfonate) acetonitrile disolvate

Y.-L. Wang, G. Yang and S. W. Ng

Comment

Silver perchlorate reacts with 4-amino-3,5-dimethyl-1,2,4-triazole in acetonitrile to form [μ_2-$(C_4H_8N_4)_6Ag_4$] [μ_2-$(C_4H_8N_4)_6(C_2H_3N)_2Ag_4$] 8[$ClO_4$]·2$H_2O$, which features two tetranuclear cluster ions. The N-heterocycles in both each bridges two silver atoms. In acetonitrile-coordinated cluster, there are three-coordinate trigonal planar and four-coordinate tetrahedral silver atoms, with the higher coordination arising from coordination by the water molecules. The solvent-free cluster has only trigonal-planar silver atoms (Wang *et al.*, 2006).

The synthesis when with silver trifluoromethylsulfonate in acetonitrile led to the isolation of the acetonitrile-coordinated tetranuclear cluster [μ_2-$(C_4H_8N_4)_6(C_2H_3N)_2Ag_4]^{4+}$, whose charge is balanced by four trifluoromethylsulfonate ions. The N-heterocycles bridge two silver atoms, and two of the silver atoms are also coordinated by acetonitrile. The salt crystallizes as an acetonitrile disolvate. The *N*-heterocycle each bridges to two silver atoms, and two of the silver atoms are also coordinated by acetonitrile.

Experimental

Silver trifluoromethylsulfonate (0.1 mmol, 26 mg) dissolved in water (2 ml) was mixed with 4-amino-3,5-dimethyl-1,2,4-triazole (0.1 mmol, 12 mg) dissolved in ethanol (2 ml) of ethanol). Ether was then diffused into the solution to yield prisms in about 50% yield.

Refinement

The two trifluoromethylsulfonate ions are not hydrogen bonded to the tetranuclear cluster. The six sulfur–oxygen bond distances were restrained to within 0.01 Å of each other, as were the six sulfur-oxygen and carbon-fluorine bond distances. The fluroine···fluorine distances were similarly restrained in each ion.

The anisotropic displacement parameters of the solvate acetonitrile molecule were restrained so that the atoms were nearly isotropic.

The carbon-bound H atoms were placed in calculated positions [C—H 0.93 to 0.96 Å; U(H) = 1.2 to 1.5 times U_{eq}(C)]. The nitrogen- and oxygen-bound H atoms were similarly treated. These were included in the refinement in the riding model approximation. The amino –NH_2 groups were assumed to be planar whereas the methyl groups were rotated to fit the electron density. The amino groups are probably not planar as there are short intermolecular H···H interactions; they are probably disordered as there are no strong N···O hydrogen bonds in the crystal structure.

The final difference Fourier map had a large peak at about 1 Å from Ag1 as well as a deep hole at a similar distance from this atom, and is probably a consequence of inadequate absorption. This is supported by the large difference between the expected and calculated transmission factors.

Figures

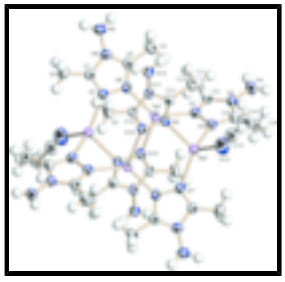


Fig. 1. Thermal ellipsoid plot of the tetranuclear $[(C_7H_8N_4)_6(C_2H_3N)_2Ag_4]^{4+}$ cation; ellipsoids are drawn at the 30% probability level. Symmetry code (i): $2-x$, $1-y$, $1-z$.

Bis(acetonitrile-κ*N*)hexakis(μ$_2$-4-amino-3,5-dimethyl-1,2,4-\ triazole-κ^2*N*^{1}:*N*^{2})tetrasilver(I) tetrakis(trifluoromethanesulfonate) acetonitrile disolvate

Crystal data

$[Ag_4(C_4H_8N_4)_6(C_2H_3N)_2](CF_3O_3S)_4\cdot 2C_2H_3N$	$Z = 1$
$M_r = 1864.84$	$F_{000} = 928$
Triclinic, $P\overline{1}$	$D_x = 1.751$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.110$ (3) Å	Cell parameters from 12901 reflections
$b = 12.695$ (3) Å	$\theta = 3.2$–27.5º
$c = 13.001$ (3) Å	$\mu = 1.31$ mm^{-1}
$\alpha = 108.59$ (2)º	$T = 295$ (2) K
$\beta = 92.84$ (2)º	Prism, colourless
$\gamma = 108.68$ (2)º	0.38 × 0.24 × 0.18 mm
$V = 1768.9$ (7) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	8026 independent reflections
Radiation source: fine-focus sealed tube	5532 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.046$
$T = 295$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.2$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -15\rightarrow15$
$T_{min} = 0.294$, $T_{max} = 0.790$	$k = -16\rightarrow16$
17453 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.074$	H-atom parameters constrained
$wR(F^2) = 0.239$	$w = 1/[\sigma^2(F_o^2) + (0.1356P)^2 + 1.8203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
8026 reflections	$\Delta\rho_{max} = 2.27$ e Å^{-3}
440 parameters	$\Delta\rho_{min} = -1.07$ e Å^{-3}
150 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.88000 (5)	0.37448 (5)	0.53930 (4)	0.0621 (2)
Ag2	0.88609 (5)	0.34115 (5)	0.27393 (5)	0.0638 (2)
S1	0.7324 (2)	−0.2778 (2)	0.18838 (19)	0.0805 (6)
S2	0.35409 (18)	0.13112 (19)	0.22789 (16)	0.0712 (5)
F1	0.9445 (7)	−0.1622 (9)	0.2985 (8)	0.170 (4)
F2	0.8266 (7)	−0.0761 (8)	0.3487 (7)	0.160 (3)
F3	0.8888 (11)	−0.0812 (11)	0.2008 (9)	0.217 (5)
F4	0.1809 (7)	−0.0452 (7)	0.2334 (7)	0.158 (3)
F5	0.1678 (7)	−0.0141 (7)	0.0858 (6)	0.160 (3)
F6	0.2856 (7)	−0.0934 (6)	0.1161 (7)	0.149 (3)
O1	0.6474 (7)	−0.2360 (8)	0.1530 (7)	0.132 (3)
O2	0.7789 (8)	−0.3403 (8)	0.0991 (6)	0.131 (3)
O3	0.7050 (9)	−0.3320 (9)	0.2672 (7)	0.159 (4)
O4	0.4239 (6)	0.1125 (7)	0.3072 (6)	0.110 (2)
O5	0.4112 (6)	0.1538 (7)	0.1402 (5)	0.111 (2)
O6	0.2899 (6)	0.2062 (6)	0.2726 (5)	0.0957 (19)
N1	0.7678 (5)	0.1969 (5)	0.4177 (4)	0.0578 (13)
N2	0.7624 (5)	0.1844 (5)	0.3087 (5)	0.0579 (13)
N3	0.6319 (5)	0.0297 (5)	0.3212 (5)	0.0582 (13)
N4	0.5376 (6)	−0.0794 (6)	0.2984 (6)	0.0746 (18)
H41	0.5009	−0.1217	0.2303	0.090*
H42	0.5155	−0.1049	0.3523	0.090*
N5	0.8361 (5)	0.5079 (5)	0.6744 (4)	0.0562 (13)
N6	0.7571 (5)	0.5996 (5)	0.8023 (5)	0.0561 (13)
N7	0.9223 (5)	0.6100 (5)	0.7420 (5)	0.0561 (13)
N8	0.6722 (5)	0.6246 (6)	0.8662 (6)	0.0739 (18)
H81	0.5984	0.5749	0.8477	0.089*
H82	0.6928	0.6899	0.9246	0.089*
N9	0.8379 (5)	0.4932 (5)	0.4025 (5)	0.0561 (13)

N10	0.9244 (4)	0.6030 (5)	0.4585 (5)	0.0541 (13)
N11	0.7536 (4)	0.6201 (5)	0.4680 (4)	0.0517 (12)
N12	0.6623 (5)	0.6652 (6)	0.4855 (5)	0.0665 (16)
H121	0.5886	0.6184	0.4565	0.080*
H112	0.6784	0.7404	0.5254	0.080*
N13	0.7755 (9)	0.3396 (10)	0.1152 (8)	0.114 (3)
N14	0.250 (3)	−0.308 (3)	0.189 (2)	0.264 (11)
C1	0.6685 (9)	0.0784 (10)	0.5277 (8)	0.097 (3)
H1A	0.7029	0.0213	0.5322	0.145*
H1B	0.5851	0.0474	0.5278	0.145*
H1C	0.7045	0.1508	0.5897	0.145*
C2	0.6887 (6)	0.1028 (7)	0.4236 (6)	0.0623 (17)
C3	0.6779 (6)	0.0828 (6)	0.2511 (6)	0.0569 (15)
C4	0.6397 (8)	0.0329 (8)	0.1312 (6)	0.075 (2)
H4A	0.6872	0.0858	0.0985	0.113*
H4B	0.5582	0.0233	0.1144	0.113*
H4C	0.6487	−0.0429	0.1022	0.113*
C5	0.6178 (7)	0.4084 (9)	0.6657 (9)	0.084 (3)
H5A	0.6170	0.3615	0.5911	0.126*
H5B	0.5589	0.4444	0.6671	0.126*
H5C	0.6010	0.3585	0.7092	0.126*
C6	0.7363 (6)	0.5028 (7)	0.7115 (6)	0.0579 (16)
C7	0.8760 (6)	0.6652 (7)	0.8194 (6)	0.0579 (16)
C8	0.9362 (8)	0.7778 (9)	0.9108 (8)	0.091 (3)
H8A	1.0201	0.8008	0.9125	0.136*
H8B	0.9178	0.7680	0.9789	0.136*
H8C	0.9100	0.8382	0.9008	0.136*
C9	0.9304 (7)	0.8075 (7)	0.5646 (8)	0.077 (2)
H9A	0.9333	0.8188	0.6415	0.116*
H9B	0.8855	0.8506	0.5454	0.116*
H9C	1.0093	0.8363	0.5499	0.116*
C10	0.8730 (5)	0.6783 (6)	0.4979 (5)	0.0538 (15)
C11	0.7364 (6)	0.5056 (6)	0.4077 (5)	0.0559 (15)
C12	0.6179 (6)	0.4146 (7)	0.3571 (7)	0.069 (2)
H12C	0.6038	0.4019	0.2800	0.104*
H12D	0.5589	0.4413	0.3922	0.104*
H12E	0.6141	0.3414	0.3662	0.104*
C13	0.6966 (9)	0.3471 (10)	0.0752 (8)	0.089 (3)
C14	0.5926 (9)	0.3532 (13)	0.0198 (10)	0.115 (4)
H14A	0.5555	0.2814	−0.0426	0.172*
H14B	0.6158	0.4199	−0.0045	0.172*
H14C	0.5379	0.3625	0.0699	0.172*
C15	0.8526 (9)	−0.1444 (10)	0.2621 (8)	0.116 (4)
C16	0.2423 (8)	−0.0117 (9)	0.1627 (7)	0.104 (3)
C17	0.148 (2)	−0.3490 (19)	0.1723 (19)	0.167 (7)
C18	0.021 (3)	−0.403 (3)	0.146 (3)	0.265 (13)
H18A	−0.0037	−0.4790	0.1551	0.398*
H18B	−0.0053	−0.4133	0.0717	0.398*
H18C	−0.0137	−0.3526	0.1952	0.398*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0531 (3)	0.0673 (4)	0.0490 (3)	0.0140 (2)	0.0020 (2)	0.0068 (2)
Ag2	0.0540 (3)	0.0680 (4)	0.0571 (3)	0.0103 (3)	0.0154 (2)	0.0165 (3)
S1	0.0831 (14)	0.0877 (14)	0.0694 (13)	0.0274 (12)	0.0081 (10)	0.0298 (11)
S2	0.0701 (11)	0.0772 (12)	0.0525 (10)	0.0166 (9)	0.0108 (8)	0.0146 (9)
F1	0.111 (5)	0.201 (7)	0.171 (7)	0.060 (5)	−0.003 (5)	0.032 (6)
F2	0.139 (5)	0.150 (6)	0.147 (6)	0.057 (5)	0.001 (5)	−0.007 (5)
F3	0.220 (8)	0.199 (8)	0.194 (8)	0.006 (6)	0.045 (7)	0.088 (7)
F4	0.138 (5)	0.147 (6)	0.165 (7)	0.002 (4)	0.055 (5)	0.067 (5)
F5	0.136 (5)	0.156 (6)	0.127 (6)	0.009 (5)	−0.038 (5)	0.023 (5)
F6	0.173 (6)	0.091 (4)	0.146 (6)	0.029 (4)	0.037 (5)	0.009 (4)
O1	0.126 (5)	0.131 (6)	0.123 (6)	0.054 (5)	−0.029 (4)	0.022 (5)
O2	0.137 (6)	0.129 (6)	0.112 (6)	0.050 (5)	0.019 (5)	0.022 (5)
O3	0.195 (8)	0.164 (7)	0.108 (6)	0.024 (6)	0.033 (6)	0.071 (6)
O4	0.095 (4)	0.120 (5)	0.113 (5)	0.039 (4)	−0.005 (4)	0.041 (4)
O5	0.113 (5)	0.122 (5)	0.089 (5)	0.023 (4)	0.036 (4)	0.039 (4)
O6	0.107 (4)	0.099 (4)	0.075 (4)	0.046 (4)	0.015 (3)	0.013 (3)
N1	0.052 (3)	0.064 (3)	0.042 (3)	0.007 (3)	0.010 (2)	0.012 (2)
N2	0.060 (3)	0.060 (3)	0.042 (3)	0.011 (3)	0.015 (2)	0.012 (2)
N3	0.049 (3)	0.062 (3)	0.050 (3)	0.008 (2)	0.011 (2)	0.012 (3)
N4	0.071 (4)	0.066 (4)	0.057 (4)	−0.010 (3)	0.007 (3)	0.018 (3)
N5	0.050 (3)	0.067 (3)	0.041 (3)	0.016 (3)	0.009 (2)	0.010 (2)
N6	0.051 (3)	0.070 (3)	0.054 (3)	0.026 (3)	0.017 (2)	0.025 (3)
N7	0.050 (3)	0.063 (3)	0.044 (3)	0.013 (2)	0.010 (2)	0.012 (2)
N8	0.058 (3)	0.086 (4)	0.073 (4)	0.023 (3)	0.028 (3)	0.023 (4)
N9	0.046 (3)	0.060 (3)	0.048 (3)	0.012 (2)	0.003 (2)	0.006 (2)
N10	0.044 (3)	0.060 (3)	0.049 (3)	0.014 (2)	0.004 (2)	0.014 (2)
N11	0.049 (3)	0.061 (3)	0.042 (3)	0.020 (2)	0.008 (2)	0.013 (2)
N12	0.046 (3)	0.073 (4)	0.065 (4)	0.023 (3)	0.008 (3)	0.003 (3)
N13	0.110 (7)	0.126 (8)	0.094 (6)	0.028 (6)	−0.019 (5)	0.043 (6)
N14	0.259 (14)	0.272 (14)	0.261 (15)	0.092 (10)	0.042 (10)	0.099 (10)
C1	0.088 (6)	0.121 (8)	0.057 (5)	0.001 (5)	0.013 (4)	0.036 (5)
C2	0.056 (4)	0.072 (4)	0.051 (4)	0.015 (3)	0.015 (3)	0.018 (3)
C3	0.056 (4)	0.050 (3)	0.048 (3)	0.008 (3)	0.004 (3)	0.006 (3)
C4	0.090 (6)	0.079 (5)	0.035 (3)	0.013 (4)	0.005 (3)	0.009 (3)
C5	0.045 (4)	0.091 (6)	0.092 (6)	0.007 (4)	0.005 (4)	0.021 (5)
C6	0.050 (3)	0.069 (4)	0.051 (4)	0.017 (3)	0.005 (3)	0.021 (3)
C7	0.054 (4)	0.068 (4)	0.048 (3)	0.019 (3)	0.013 (3)	0.018 (3)
C8	0.081 (6)	0.089 (6)	0.071 (5)	0.023 (5)	0.019 (4)	−0.006 (5)
C9	0.055 (4)	0.066 (4)	0.083 (6)	0.012 (3)	−0.003 (4)	0.002 (4)
C10	0.048 (3)	0.065 (4)	0.042 (3)	0.017 (3)	0.006 (2)	0.013 (3)
C11	0.053 (4)	0.065 (4)	0.041 (3)	0.013 (3)	0.005 (3)	0.017 (3)
C12	0.051 (4)	0.064 (4)	0.069 (5)	0.010 (3)	0.000 (3)	0.004 (4)
C13	0.088 (6)	0.103 (7)	0.060 (5)	0.019 (5)	−0.003 (4)	0.025 (5)
C14	0.081 (6)	0.158 (11)	0.099 (8)	0.037 (7)	−0.001 (6)	0.044 (8)

C15	0.095 (8)	0.135 (10)	0.098 (9)	0.035 (7)	−0.001 (6)	0.025 (8)
C16	0.110 (8)	0.090 (7)	0.095 (8)	0.017 (6)	0.024 (7)	0.030 (6)
C17	0.171 (10)	0.171 (10)	0.182 (11)	0.066 (8)	0.025 (8)	0.088 (8)
C18	0.256 (16)	0.269 (16)	0.278 (16)	0.092 (10)	0.023 (10)	0.109 (10)

Geometric parameters (Å, °)

Ag1—N1	2.232 (5)	N10—C10	1.291 (9)
Ag1—N5	2.238 (5)	N10—Ag1^{i}	2.290 (5)
Ag1—N10^{i}	2.290 (5)	N11—C11	1.354 (9)
Ag1—Ag2	3.3469 (11)	N11—C10	1.366 (8)
Ag2—N2	2.267 (6)	N11—N12	1.396 (7)
Ag2—N7^{i}	2.241 (5)	N12—H121	0.8800
Ag2—N9	2.371 (6)	N12—H112	0.8800
Ag2—N13	2.395 (9)	N13—C13	1.110 (13)
S1—O3	1.404 (6)	N14—C17	1.15 (3)
S1—O1	1.419 (6)	C1—C2	1.496 (11)
S1—O2	1.434 (6)	C1—H1A	0.9600
S1—C15	1.776 (12)	C1—H1B	0.9600
S2—O6	1.420 (5)	C1—H1C	0.9600
S2—O4	1.425 (5)	C3—C4	1.469 (9)
S2—O5	1.422 (5)	C4—H4A	0.9600
S2—C16	1.781 (11)	C4—H4B	0.9600
F1—C15	1.301 (7)	C4—H4C	0.9600
F2—C15	1.306 (8)	C5—C6	1.486 (10)
F3—C15	1.299 (8)	C5—H5A	0.9600
F4—C16	1.301 (7)	C5—H5B	0.9600
F5—C16	1.298 (7)	C5—H5C	0.9600
F6—C16	1.302 (7)	C7—C8	1.466 (11)
N1—C2	1.298 (9)	C8—H8A	0.9600
N1—N2	1.370 (8)	C8—H8B	0.9600
N2—C3	1.318 (8)	C8—H8C	0.9600
N3—C3	1.341 (9)	C9—C10	1.493 (10)
N3—C2	1.349 (9)	C9—H9A	0.9600
N3—N4	1.415 (8)	C9—H9B	0.9600
N4—H41	0.8800	C9—H9C	0.9600
N4—H42	0.8800	C11—C12	1.479 (9)
N5—C6	1.313 (9)	C12—H12C	0.9600
N5—N7	1.363 (8)	C12—H12D	0.9600
N6—C6	1.347 (9)	C12—H12E	0.9600
N6—C7	1.379 (9)	C13—C14	1.456 (14)
N6—N8	1.404 (8)	C14—H14A	0.9600
N7—C7	1.294 (9)	C14—H14B	0.9600
N7—Ag2^{i}	2.241 (5)	C14—H14C	0.9600
N8—H81	0.8800	C17—C18	1.44 (3)
N8—H82	0.8800	C18—H18A	0.9600
N9—C11	1.291 (9)	C18—H18B	0.9600
N9—N10	1.383 (7)	C18—H18C	0.9600

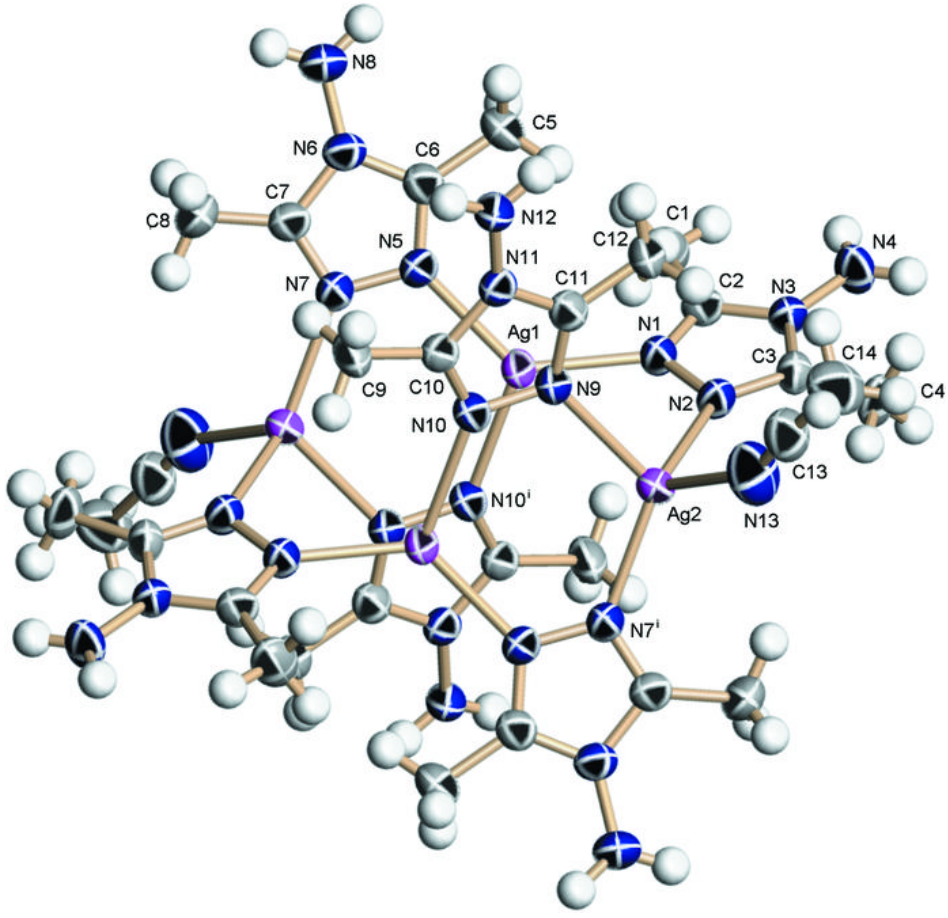
N1—Ag1—N5	131.8 (2)	N3—C2—C1	126.1 (7)
N1—Ag1—N10^{i}	109.7 (2)	N2—C3—N3	108.0 (6)
N5—Ag1—N10^{i}	117.2 (2)	N2—C3—C4	127.2 (7)
N1—Ag1—Ag2	64.14 (15)	N3—C3—C4	124.8 (6)
N5—Ag1—Ag2	131.10 (16)	C3—C4—H4A	109.5
N10^{i}—Ag1—Ag2	82.56 (14)	C3—C4—H4B	109.5
N2—Ag2—N9	97.9 (2)	H4A—C4—H4B	109.5
N2—Ag2—N7^{i}	130.8 (2)	C3—C4—H4C	109.5
N2—Ag2—N13	102.6 (3)	H4A—C4—H4C	109.5
N7^{i}—Ag2—N9	114.7 (2)	H4B—C4—H4C	109.5
N7^{i}—Ag2—N13	109.4 (3)	C6—C5—H5A	109.5
N9—Ag2—N13	95.6 (3)	C6—C5—H5B	109.5
N7^{i}—Ag2—Ag1	105.28 (15)	H5A—C5—H5B	109.5
N2—Ag2—Ag1	63.63 (14)	C6—C5—H5C	109.5
N9—Ag2—Ag1	55.38 (15)	H5A—C5—H5C	109.5
N13—Ag2—Ag1	142.1 (3)	H5B—C5—H5C	109.5
O3—S1—O1	116.7 (5)	N5—C6—N6	108.7 (6)
O3—S1—O2	114.5 (5)	N5—C6—C5	128.0 (7)
O1—S1—O2	112.9 (4)	N6—C6—C5	123.3 (7)
O3—S1—C15	103.2 (6)	N7—C7—N6	108.2 (6)
O1—S1—C15	102.8 (5)	N7—C7—C8	127.5 (7)
O2—S1—C15	104.7 (5)	N6—C7—C8	124.3 (6)
O6—S2—O4	115.0 (4)	C7—C8—H8A	109.5
O6—S2—O5	114.5 (4)	C7—C8—H8B	109.5
O4—S2—O5	114.9 (4)	H8A—C8—H8B	109.5
O6—S2—C16	103.9 (4)	C7—C8—H8C	109.5
O4—S2—C16	102.9 (4)	H8A—C8—H8C	109.5
O5—S2—C16	103.6 (4)	H8B—C8—H8C	109.5
C2—N1—N2	107.5 (5)	C10—C9—H9A	109.5
C2—N1—Ag1	134.9 (5)	C10—C9—H9B	109.5
N2—N1—Ag1	116.6 (4)	H9A—C9—H9B	109.5
C3—N2—N1	108.0 (6)	C10—C9—H9C	109.5
C3—N2—Ag2	136.6 (5)	H9A—C9—H9C	109.5
N1—N2—Ag2	115.2 (4)	H9B—C9—H9C	109.5
C3—N3—C2	107.4 (6)	N10—C10—N11	108.3 (6)
C3—N3—N4	128.8 (6)	N10—C10—C9	127.4 (6)
C2—N3—N4	123.8 (6)	N11—C10—C9	124.2 (6)
N3—N4—H41	120.0	N9—C11—N11	108.8 (6)
N3—N4—H42	120.0	N9—C11—C12	128.1 (7)
H41—N4—H42	120.0	N11—C11—C12	123.0 (6)
C6—N5—N7	107.9 (5)	C11—C12—H12C	109.5
C6—N5—Ag1	130.7 (5)	C11—C12—H12D	109.5
N7—N5—Ag1	121.0 (4)	H12C—C12—H12D	109.5
C6—N6—C7	106.5 (5)	C11—C12—H12E	109.5
C6—N6—N8	125.4 (6)	H12C—C12—H12E	109.5
C7—N6—N8	128.1 (6)	H12D—C12—H12E	109.5
C7—N7—N5	108.8 (5)	N13—C13—C14	178.1 (13)

C7—N7—Ag2^{i}	127.3 (5)	C13—C14—H14A	109.5
N5—N7—Ag2^{i}	123.7 (4)	C13—C14—H14B	109.5
N6—N8—H81	120.0	H14A—C14—H14B	109.5
N6—N8—H82	120.0	C13—C14—H14C	109.5
H81—N8—H82	120.0	H14A—C14—H14C	109.5
C11—N9—N10	107.9 (6)	H14B—C14—H14C	109.5
C11—N9—Ag2	128.4 (4)	F3—C15—F1	106.1 (8)
N10—N9—Ag2	120.3 (4)	F3—C15—F2	106.6 (8)
C10—N10—N9	108.2 (5)	F1—C15—F2	105.3 (7)
C10—N10—Ag1^{i}	131.8 (4)	F3—C15—S1	111.5 (8)
N9—N10—Ag1^{i}	119.9 (4)	F1—C15—S1	113.4 (8)
C11—N11—C10	106.7 (5)	F2—C15—S1	113.3 (8)
C11—N11—N12	123.7 (5)	F5—C16—F4	106.8 (7)
C10—N11—N12	129.4 (6)	F5—C16—F6	106.1 (7)
N11—N12—H121	120.0	F4—C16—F6	107.4 (7)
N11—N12—H112	120.0	F5—C16—S2	112.8 (7)
H121—N12—H112	120.0	F4—C16—S2	111.0 (7)
C13—N13—Ag2	150.4 (10)	F6—C16—S2	112.5 (7)
C2—C1—H1A	109.5	N14—C17—C18	178 (3)
C2—C1—H1B	109.5	C17—C18—H18A	109.5
H1A—C1—H1B	109.5	C17—C18—H18B	109.5
C2—C1—H1C	109.5	H18A—C18—H18B	109.5
H1A—C1—H1C	109.5	C17—C18—H18C	109.5
H1B—C1—H1C	109.5	H18A—C18—H18C	109.5
N1—C2—N3	109.1 (6)	H18B—C18—H18C	109.5
N1—C2—C1	124.8 (7)		
N1—Ag1—Ag2—N7^{i}	−125.5 (2)	N4—N3—C2—N1	−177.8 (7)
N5—Ag1—Ag2—N7^{i}	110.5 (2)	C3—N3—C2—C1	−178.3 (9)
N10^{i}—Ag1—Ag2—N7^{i}	−9.4 (2)	N4—N3—C2—C1	4.5 (13)
N1—Ag1—Ag2—N2	2.8 (2)	N1—N2—C3—N3	−1.5 (8)
N5—Ag1—Ag2—N2	−121.2 (3)	Ag2—N2—C3—N3	−176.5 (5)
N10^{i}—Ag1—Ag2—N2	119.0 (2)	N1—N2—C3—C4	179.3 (8)
N1—Ag1—Ag2—N9	124.7 (2)	Ag2—N2—C3—C4	4.3 (13)
N5—Ag1—Ag2—N9	0.7 (2)	C2—N3—C3—N2	1.4 (8)
N10^{i}—Ag1—Ag2—N9	−119.1 (2)	N4—N3—C3—N2	178.3 (7)
N1—Ag1—Ag2—N13	78.8 (5)	C2—N3—C3—C4	−179.4 (8)
N5—Ag1—Ag2—N13	−45.2 (5)	N4—N3—C3—C4	−2.5 (13)
N10^{i}—Ag1—Ag2—N13	−165.0 (4)	N7—N5—C6—N6	−0.4 (8)
N5—Ag1—N1—C2	−48.6 (8)	Ag1—N5—C6—N6	172.8 (5)
N10^{i}—Ag1—N1—C2	117.3 (7)	N7—N5—C6—C5	−179.8 (8)
Ag2—Ag1—N1—C2	−171.7 (8)	Ag1—N5—C6—C5	−6.6 (12)
N5—Ag1—N1—N2	118.5 (5)	C7—N6—C6—N5	0.1 (8)
N10^{i}—Ag1—N1—N2	−75.6 (5)	N8—N6—C6—N5	−179.0 (6)
Ag2—Ag1—N1—N2	−4.6 (4)	C7—N6—C6—C5	179.5 (8)
C2—N1—N2—C3	1.0 (8)	N8—N6—C6—C5	0.5 (12)
Ag1—N1—N2—C3	−169.4 (5)	N5—N7—C7—N6	−0.6 (8)

C2—N1—N2—Ag2	177.3 (5)	$Ag2^{i}$—N7—C7—N6	−174.9 (4)
Ag1—N1—N2—Ag2	6.8 (6)	N5—N7—C7—C8	179.2 (9)
$N7^{i}$—Ag2—N2—C3	−101.9 (7)	$Ag2^{i}$—N7—C7—C8	4.9 (12)
N9—Ag2—N2—C3	125.4 (7)	C6—N6—C7—N7	0.3 (8)
N13—Ag2—N2—C3	27.9 (8)	N8—N6—C7—N7	179.3 (7)
Ag1—Ag2—N2—C3	170.3 (8)	C6—N6—C7—C8	−179.5 (9)
$N7^{i}$—Ag2—N2—N1	83.2 (5)	N8—N6—C7—C8	−0.5 (12)
N9—Ag2—N2—N1	−49.4 (5)	N9—N10—C10—N11	−0.5 (7)
N13—Ag2—N2—N1	−146.9 (5)	$Ag1^{i}$—N10—C10—N11	176.2 (4)
Ag1—Ag2—N2—N1	−4.5 (4)	N9—N10—C10—C9	179.7 (8)
N1—Ag1—N5—C6	4.8 (8)	$Ag1^{i}$—N10—C10—C9	−3.5 (12)
$N10^{i}$—Ag1—N5—C6	−160.3 (6)	C11—N11—C10—N10	−0.4 (7)
Ag2—Ag1—N5—C6	94.9 (6)	N12—N11—C10—N10	−175.7 (6)
N1—Ag1—N5—N7	177.3 (4)	C11—N11—C10—C9	179.4 (8)
$N10^{i}$—Ag1—N5—N7	12.2 (6)	N12—N11—C10—C9	4.1 (11)
Ag2—Ag1—N5—N7	−92.6 (5)	N10—N9—C11—N11	−1.5 (8)
C6—N5—N7—C7	0.6 (8)	Ag2—N9—C11—N11	−160.3 (5)
Ag1—N5—N7—C7	−173.4 (5)	N10—N9—C11—C12	177.7 (7)
C6—N5—N7—$Ag2^{i}$	175.2 (5)	Ag2—N9—C11—C12	18.8 (11)
Ag1—N5—N7—$Ag2^{i}$	1.2 (7)	C10—N11—C11—N9	1.2 (7)
$N7^{i}$—Ag2—N9—C11	158.4 (6)	N12—N11—C11—N9	176.9 (6)
N2—Ag2—N9—C11	−59.5 (6)	C10—N11—C11—C12	−178.0 (7)
N13—Ag2—N9—C11	44.1 (7)	N12—N11—C11—C12	−2.4 (11)
Ag1—Ag2—N9—C11	−109.6 (6)	O3—S1—C15—F3	−179.1 (8)
$N7^{i}$—Ag2—N9—N10	1.8 (6)	O1—S1—C15—F3	−57.3 (8)
N2—Ag2—N9—N10	144.0 (5)	O2—S1—C15—F3	60.8 (8)
N13—Ag2—N9—N10	−112.5 (5)	O3—S1—C15—F1	61.2 (8)
Ag1—Ag2—N9—N10	93.8 (5)	O1—S1—C15—F1	−177.0 (7)
C11—N9—N10—C10	1.2 (8)	O2—S1—C15—F1	−58.9 (8)
Ag2—N9—N10—C10	162.1 (5)	O3—S1—C15—F2	−58.8 (8)
C11—N9—N10—$Ag1^{i}$	−175.9 (4)	O1—S1—C15—F2	63.0 (8)
Ag2—N9—N10—$Ag1^{i}$	−15.0 (6)	O2—S1—C15—F2	−178.9 (7)
$N7^{i}$—Ag2—N13—C13	−156 (2)	O6—S2—C16—F5	60.0 (7)
N2—Ag2—N13—C13	62 (2)	O4—S2—C16—F5	−179.9 (6)
N9—Ag2—N13—C13	−37 (2)	O5—S2—C16—F5	−59.9 (7)
Ag1—Ag2—N13—C13	0(2)	O6—S2—C16—F4	−59.8 (7)
N2—N1—C2—N3	−0.2 (8)	O4—S2—C16—F4	60.4 (7)
Ag1—N1—C2—N3	167.7 (5)	O5—S2—C16—F4	−179.7 (6)
N2—N1—C2—C1	177.5 (8)	O6—S2—C16—F6	179.9 (6)
Ag1—N1—C2—C1	−14.6 (13)	O4—S2—C16—F6	−60.0 (7)
C3—N3—C2—N1	−0.7 (8)	O5—S2—C16—F6	60.0 (7)

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

Fig. 1


N8
C5
N6
C6
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N7
Ag1
N1
C3
C14
C9
C10
N9
N2
C4
N10
C13
N10i
Ag2
N13
N7i