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Bis(4,4′-di-*tert*-butyl-2,2′-bipyridine-κ^2N,N')silver(I) trifluoromethanesulfonate

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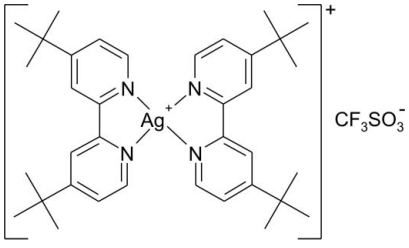
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.140; data-to-parameter ratio = 17.6.

In the crystal structure of the title compound, $[Ag(C_{18}H_{24}N_2)_2](CF_3SO_3)$, the Ag atoms are coordinated by four N atoms of two 4,4′-di-*tert*-butyl-2,2′-bipyridine (*tert*-bubpy) ligands within a strongly distorted tetrahedron.

Related literature

For related literature, see: Bowmaker *et al.* (2005) and references therein.



Experimental

Crystal data

$[Ag(C_{18}H_{24}N_2)_2](CF_3SO_3)$
M_r = 793.73
Triclinic, $P\overline{1}$
a = 9.9251 (17) Å
b = 13.3620 (18) Å
c = 15.9435 (19) Å
α = 78.435 (15)°
β = 84.990 (17)°
γ = 69.339 (18)°
V = 1937.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 295 K
0.23 × 0.17 × 0.12 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: analytical [from crystal shape; *X-SHAPE* and *X-RED* (Stoe & Cie, 1998)]
T_{min} = 0.859, T_{max} = 0.915
22997 measured reflections
7777 independent reflections
5433 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.140
S = 1.03
7777 reflections
442 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.306 (2)	Ag1—N3	2.328 (3)
Ag1—N2	2.305 (3)	Ag1—N4	2.333 (3)
N1—Ag1—N2	72.66 (9)	N2—Ag1—N3	152.82 (12)
N1—Ag1—N3	113.58 (9)	N2—Ag1—N4	115.29 (10)
N1—Ag1—N4	152.56 (11)	N3—Ag1—N4	72.16 (10)
N1—C5—C6—N2	−21.5 (6)	N3—C23—C24—N4	−25.2 (4)

Data collection: *IPDS* (Stoe & Cie, 1998); cell refinement: *IPDS*; data reduction: *X-RED* (Stoe & Cie, 1998); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2048).

References

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  doi:10.1107/S1600536807036835

supplementary materials

Acta Cryst. (2007). E**63**, m2364 [**doi:10.1107/S1600536807036835**]

Bis(4,4'-di-*tert*-butyl-2,2'-bipyridine-κ^2N,N')silver(I) trifluoromethanesulfonate

T. Fischer, M. Zabel, H. Yersin and U. Monkowius

Comment

Crystals of the title compound were obtained as a side-product in the preparation of [(*tert*.-bubpy)$_2$Pt]CF_3O_3S in acetonitrile solution. To identify this compound a single-crystal structure analysis was performed.

The asymmetric unit consists of one complex cation [(*tert*.-bubpy)$_2$Ag]$^+$ and one $[CF_3O_3S]^-$ anion, which are located in general positions. The Ag atom is coordinated by four nitrogen atoms of two *tert*.-bubpy ligands within a strongly distorted tetrahedron. The four Ag—N bonds are similar and are in the range of 2.305 (3)–2.333 (3) Å. The bite angles are 72.66 (9) and 72.16 (10) ° [(N1—Ag1—N2) and (N3—Ag1—N4), respectively]. These values are typical for bpy ligands in Ag(I) complexes (Bowmaker *et al.*, 2005). The *tert*.-bubpy ligands deviate from planarity significantly [(N1—C5—C6—N2) −21.5 (6) and (N3—C23—C24—N4) −25.2 (4) °].

Experimental

The title complex was isolated as a side-product in the preparation of [(*tert*.-bubpy)$_2$Pt]CF_3O_3S. For the synthesis of this Pt complex *via* [Pt(NCMe)$_4$]CF_3O_3S, K_2PtCl_4 and Ag(CF_3O_3S) were suspended in acetonitrile. After 2 h of stirring the reaction mixture was filtrated to remove the precipitating AgCl and the solvent was distilled off in vacuum. Without further purification the obtained white powder was stirred with an excess of 4,4'-di-*tert*.-butyl-2,2'-bipyridine in CH_2Cl_2 at r.t. The Pt complex was precipitated with hexanes and isolated by filtration. Obviously, the precursor complex [Pt(NCMe)$_4$]CF_3O_3S contained considerable amounts of a silver species, because the title complex [(*tert*.-bubpy)$_2$Ag]CF_3O_3S was obtained as yellow crystals after cooling of the filtrated solution in the refrigerator.

Refinement

All hydrogen atoms were positioned with idealized geometry and refined isotropic using a riding model with C—H = 0.96 Å] for methyl and C—H = 0.93 for aromatic H atoms. U_{iso}(H) values were set to 1.2 U_{eq} (1.5 U_{eq} for methyl) of the parent atom. Some of the carbon atoms of the *tert*-butyl groups shows unusual large anisotropic displacement parameters indicative for disordering. However, a refinement uisng a split model does not lead to a significant improvement of the structure model.

Figures

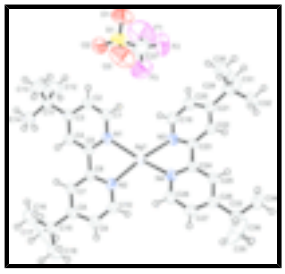


Fig. 1. View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

Bis(4,4'-di-*tert*-butyl-2,2'-bipyridine-κ^2N,N')silver(I) trifluoromethanesulfonate

Crystal data

$[Ag(C_{18}H_{24}N_2)_2](CF_3SO_3)$	$Z = 2$
$M_r = 793.73$	$F_{000} = 824$
Triclinic, $P\overline{1}$	Cell parameters were determined by indexing 8000 reflections with I/sigma limit 6.0.
Hall symbol: -P 1	$D_x = 1.360$ Mg m^{-3}
$a = 9.9251$ (17) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 13.3620$ (18) Å	Cell parameters from 8000 reflections
$c = 15.9435$ (19) Å	$\theta = 2.2$–27.0°
$\alpha = 78.435$ (15)°	$\mu = 0.63$ mm^{-1}
$\beta = 84.990$ (17)°	$T = 295$ K
$\gamma = 69.339$ (18)°	Prism, yellow
$V = 1937.9$ (5) Å^3	0.23 × 0.17 × 0.12 mm

Data collection

Stoe IPDS diffractometer	7777 independent reflections
Radiation source: fine-focus sealed tube	5433 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.037$
$T = 295$(1) K	$\theta_{max} = 27.0^\circ$
φ scans	$\theta_{min} = 2.2^\circ$
Absorption correction: analytical [from crystal shape; X-SHAPE and X-RED (Stoe & Cie, 1998)]	$h = -12 \rightarrow 12$
$T_{min} = 0.859$, $T_{max} = 0.915$	$k = -16 \rightarrow 17$
22997 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.140$	$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
7777 reflections	$\Delta\rho_{max} = 0.77$ e Å^{-3}
442 parameters	$\Delta\rho_{min} = -0.50$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Data were collected applying an imaging plate system (Stoe) with the following measurement parameters:

Detector distance [mm] 65 Phi movement mode Oscillation Phi incr. [degrees] 1.4 Number of exposures 194 Irradiation / exposure [min] 3.00

For a detailed description of the method see: Sheldrick, G·*M*., Paulus, E. Vertesy, *L*. & Hahn, F. (1995) Acta Cryst. B51, 89–98.

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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}
Ag1	0.76501 (4)	0.05607 (2)	0.25906 (1)	0.0653 (1)
N1	0.7378 (3)	0.1950 (2)	0.14261 (15)	0.0508 (9)
N2	0.8067 (4)	−0.0206 (2)	0.13780 (16)	0.0554 (9)
N3	0.8393 (3)	0.0903 (2)	0.38163 (15)	0.0503 (9)
N4	0.6759 (3)	−0.0370 (2)	0.37763 (15)	0.0493 (8)
C1	0.7275 (4)	0.2978 (3)	0.1460 (2)	0.0567 (10)
C2	0.7424 (4)	0.3718 (3)	0.0764 (2)	0.0537 (10)
C3	0.7691 (4)	0.3430 (3)	−0.00515 (19)	0.0466 (10)
C4	0.7826 (4)	0.2363 (3)	−0.00852 (18)	0.0484 (10)
C5	0.7654 (4)	0.1651 (3)	0.06562 (18)	0.0480 (10)
C6	0.7767 (4)	0.0513 (3)	0.06272 (18)	0.0485 (10)
C7	0.7522 (4)	0.0222 (3)	−0.01157 (19)	0.0532 (10)
C8	0.7550 (4)	−0.0834 (3)	−0.0123 (2)	0.0524 (10)
C9	0.7855 (5)	−0.1557 (3)	0.0657 (2)	0.0639 (13)
C10	0.8102 (5)	−0.1226 (3)	0.1369 (2)	0.0652 (13)
C11	0.7785 (4)	0.4266 (3)	−0.0848 (2)	0.0534 (10)
C12	0.8981 (6)	0.4703 (4)	−0.0732 (3)	0.0809 (17)
C13	0.6352 (5)	0.5197 (3)	−0.0945 (3)	0.0747 (14)
C14	0.8108 (6)	0.3776 (3)	−0.1666 (2)	0.0751 (16)

C15	0.7265 (5)	−0.1165 (3)	−0.0936 (2)	0.0625 (13)
C16	0.6101 (7)	−0.0220 (4)	−0.1481 (3)	0.097 (2)
C17	0.8640 (7)	−0.1465 (10)	−0.1432 (5)	0.187 (5)
C18	0.6651 (11)	−0.2095 (6)	−0.0730 (4)	0.141 (4)
C19	0.8914 (4)	0.1709 (3)	0.3809 (2)	0.0595 (13)
C20	0.8901 (4)	0.2158 (3)	0.4514 (2)	0.0583 (11)
C21	0.8338 (4)	0.1783 (3)	0.5295 (2)	0.0496 (10)
C22	0.7794 (4)	0.0951 (3)	0.53029 (18)	0.0467 (10)
C23	0.7828 (4)	0.0531 (2)	0.45618 (18)	0.0441 (9)
C24	0.7211 (4)	−0.0339 (2)	0.45442 (17)	0.0435 (9)
C25	0.7160 (4)	−0.1101 (3)	0.52774 (19)	0.0481 (10)
C26	0.6656 (4)	−0.1954 (3)	0.5235 (2)	0.0499 (10)
C27	0.6206 (4)	−0.1966 (3)	0.4431 (2)	0.0576 (13)
C28	0.6267 (4)	−0.1178 (3)	0.3738 (2)	0.0580 (11)
C29	0.8231 (4)	0.2319 (3)	0.6082 (2)	0.0563 (11)
C30	0.6958 (7)	0.3397 (4)	0.5946 (4)	0.0938 (19)
C31	0.9582 (6)	0.2577 (7)	0.6161 (4)	0.117 (3)
C32	0.7945 (10)	0.1617 (5)	0.6897 (3)	0.117 (3)
C33	0.6695 (5)	−0.2856 (3)	0.6013 (2)	0.0576 (13)
C34	0.6815 (18)	−0.2528 (7)	0.6824 (3)	0.260 (10)
C35	0.7979 (7)	−0.3834 (5)	0.5897 (5)	0.146 (3)
C36	0.5380 (8)	−0.3174 (7)	0.6059 (5)	0.155 (3)
S1	0.64907 (16)	0.61423 (11)	0.22335 (9)	0.0869 (5)
F1	0.8850 (6)	0.5950 (6)	0.2871 (5)	0.206 (4)
F2	0.7421 (8)	0.5286 (5)	0.3770 (2)	0.187 (3)
F3	0.8608 (6)	0.4380 (4)	0.2800 (4)	0.165 (2)
O1	0.5899 (6)	0.7159 (3)	0.2491 (3)	0.130 (2)
O2	0.7180 (5)	0.6117 (3)	0.1412 (2)	0.1054 (16)
O3	0.5594 (6)	0.5447 (5)	0.2418 (4)	0.153 (3)
C37	0.7952 (8)	0.5385 (5)	0.2913 (5)	0.110 (3)
H1	0.70900	0.31940	0.19900	0.0680*
H2	0.73500	0.44120	0.08290	0.0650*
H4	0.80330	0.21230	−0.06060	0.0580*
H7	0.73350	0.07360	−0.06190	0.0640*
H9	0.78890	−0.22690	0.06930	0.0770*
H10	0.83060	−0.17320	0.18770	0.0780*
H12A	0.98830	0.41120	−0.06520	0.0970*
H12B	0.87610	0.50480	−0.02390	0.0970*
H12C	0.90470	0.52230	−0.12310	0.0970*
H13A	0.61540	0.55270	−0.04450	0.0900*
H13B	0.56000	0.49240	−0.10110	0.0900*
H13C	0.63950	0.57300	−0.14400	0.0900*
H14A	0.73560	0.35120	−0.17510	0.0900*
H14B	0.90120	0.31860	−0.16130	0.0900*
H14C	0.81570	0.43250	−0.21480	0.0900*
H16A	0.64170	0.03950	−0.16400	0.1160*
H16B	0.52190	−0.00210	−0.11540	0.1160*
H16C	0.59450	−0.04470	−0.19880	0.1160*
H17A	0.93540	−0.20590	−0.10940	0.2250*

H17B	0.89600	−0.08520	−0.15770	0.2250*
H17C	0.84950	−0.16800	−0.19480	0.2250*
H18A	0.57570	−0.18660	−0.04180	0.1690*
H18B	0.73240	−0.27170	−0.03890	0.1690*
H18C	0.64900	−0.22830	−0.12530	0.1690*
H19	0.93030	0.19760	0.32990	0.0710*
H20	0.92720	0.27170	0.44690	0.0700*
H22	0.74040	0.06700	0.58080	0.0560*
H25	0.74600	−0.10460	0.57970	0.0580*
H27	0.58640	−0.25080	0.43630	0.0690*
H28	0.59500	−0.12060	0.32140	0.0700*
H30A	0.60910	0.32560	0.58860	0.1130*
H30B	0.71290	0.38620	0.54370	0.1130*
H30C	0.68580	0.37460	0.64300	0.1130*
H31A	0.97130	0.30630	0.56550	0.1410*
H31B	1.04000	0.19160	0.62280	0.1410*
H31C	0.94870	0.29150	0.66510	0.1410*
H32A	0.87110	0.09250	0.69810	0.1410*
H32B	0.70490	0.15090	0.68540	0.1410*
H32C	0.78930	0.19700	0.73730	0.1410*
H34A	0.60050	−0.18910	0.68930	0.3120*
H34B	0.76890	−0.23710	0.68160	0.3120*
H34C	0.68280	−0.31080	0.72930	0.3120*
H35A	0.88350	−0.36470	0.58500	0.1740*
H35B	0.78760	−0.40740	0.53850	0.1740*
H35C	0.80470	−0.44060	0.63810	0.1740*
H36A	0.53330	−0.34400	0.55500	0.1860*
H36B	0.45360	−0.25510	0.61060	0.1860*
H36C	0.54300	−0.37340	0.65500	0.1860*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.1025 (3)	0.0651 (2)	0.0316 (1)	−0.0345 (2)	−0.0021 (1)	−0.0052 (1)
N1	0.0720 (19)	0.0471 (14)	0.0333 (11)	−0.0201 (14)	−0.0024 (11)	−0.0075 (10)
N2	0.079 (2)	0.0468 (14)	0.0367 (12)	−0.0172 (15)	−0.0057 (12)	−0.0053 (11)
N3	0.0677 (18)	0.0551 (15)	0.0345 (11)	−0.0292 (14)	0.0002 (11)	−0.0082 (11)
N4	0.0688 (18)	0.0510 (14)	0.0355 (11)	−0.0292 (14)	−0.0078 (11)	−0.0056 (10)
C1	0.079 (2)	0.0523 (18)	0.0397 (14)	−0.0190 (18)	−0.0018 (15)	−0.0164 (13)
C2	0.071 (2)	0.0441 (16)	0.0492 (16)	−0.0202 (16)	−0.0056 (15)	−0.0129 (13)
C3	0.0539 (19)	0.0461 (16)	0.0437 (14)	−0.0212 (15)	−0.0031 (13)	−0.0083 (12)
C4	0.064 (2)	0.0479 (16)	0.0364 (13)	−0.0232 (16)	0.0006 (13)	−0.0083 (12)
C5	0.064 (2)	0.0450 (16)	0.0360 (13)	−0.0198 (15)	−0.0046 (13)	−0.0063 (12)
C6	0.064 (2)	0.0446 (16)	0.0359 (13)	−0.0184 (15)	−0.0013 (13)	−0.0053 (12)
C7	0.081 (2)	0.0444 (16)	0.0364 (13)	−0.0256 (17)	−0.0045 (14)	−0.0035 (12)
C8	0.067 (2)	0.0462 (17)	0.0436 (15)	−0.0178 (16)	0.0000 (14)	−0.0111 (13)
C9	0.098 (3)	0.0434 (17)	0.0512 (17)	−0.0259 (19)	−0.0042 (18)	−0.0063 (14)
C10	0.101 (3)	0.0447 (18)	0.0438 (16)	−0.0198 (19)	−0.0081 (17)	−0.0014 (13)

C11	0.068 (2)	0.0503 (17)	0.0464 (15)	−0.0275 (17)	−0.0020 (15)	−0.0053 (13)
C12	0.088 (3)	0.084 (3)	0.088 (3)	−0.051 (3)	0.005 (2)	−0.018 (2)
C13	0.083 (3)	0.062 (2)	0.068 (2)	−0.019 (2)	−0.002 (2)	0.0026 (19)
C14	0.114 (4)	0.066 (2)	0.0462 (17)	−0.037 (2)	0.010 (2)	−0.0057 (16)
C15	0.086 (3)	0.060 (2)	0.0479 (17)	−0.027 (2)	−0.0063 (17)	−0.0183 (15)
C16	0.126 (5)	0.084 (3)	0.082 (3)	−0.027 (3)	−0.037 (3)	−0.017 (3)
C17	0.089 (4)	0.353 (14)	0.132 (6)	−0.021 (6)	0.004 (4)	−0.175 (8)
C18	0.263 (10)	0.113 (5)	0.095 (4)	−0.120 (6)	−0.056 (5)	−0.002 (3)
C19	0.077 (3)	0.067 (2)	0.0447 (16)	−0.041 (2)	0.0076 (15)	−0.0070 (15)
C20	0.074 (2)	0.060 (2)	0.0538 (17)	−0.0390 (19)	0.0023 (16)	−0.0115 (15)
C21	0.059 (2)	0.0460 (16)	0.0469 (15)	−0.0203 (15)	0.0021 (14)	−0.0123 (13)
C22	0.060 (2)	0.0460 (16)	0.0376 (13)	−0.0230 (15)	0.0014 (13)	−0.0076 (12)
C23	0.0551 (19)	0.0420 (15)	0.0373 (13)	−0.0197 (14)	−0.0021 (12)	−0.0062 (11)
C24	0.0572 (19)	0.0436 (15)	0.0335 (12)	−0.0215 (14)	−0.0017 (12)	−0.0075 (11)
C25	0.064 (2)	0.0471 (16)	0.0381 (14)	−0.0242 (16)	−0.0034 (13)	−0.0082 (12)
C26	0.063 (2)	0.0437 (16)	0.0452 (15)	−0.0222 (16)	0.0002 (14)	−0.0062 (13)
C27	0.078 (3)	0.0555 (19)	0.0538 (17)	−0.0393 (19)	−0.0068 (16)	−0.0099 (15)
C28	0.076 (2)	0.066 (2)	0.0432 (15)	−0.036 (2)	−0.0133 (15)	−0.0086 (15)
C29	0.065 (2)	0.059 (2)	0.0559 (17)	−0.0278 (18)	0.0021 (16)	−0.0249 (16)
C30	0.104 (4)	0.087 (3)	0.095 (3)	−0.021 (3)	−0.003 (3)	−0.048 (3)
C31	0.089 (4)	0.199 (7)	0.108 (4)	−0.070 (5)	0.022 (3)	−0.100 (5)
C32	0.235 (8)	0.098 (4)	0.044 (2)	−0.084 (5)	0.000 (3)	−0.022 (2)
C33	0.080 (3)	0.0487 (18)	0.0501 (16)	−0.0335 (19)	−0.0091 (16)	0.0019 (14)
C34	0.67 (3)	0.161 (7)	0.039 (2)	−0.268 (12)	−0.014 (6)	0.013 (3)
C35	0.108 (5)	0.109 (5)	0.158 (6)	−0.012 (4)	0.002 (4)	0.066 (5)
C36	0.117 (5)	0.165 (7)	0.164 (6)	−0.087 (5)	−0.033 (4)	0.098 (6)
S1	0.0946 (9)	0.0808 (8)	0.0881 (8)	−0.0286 (7)	0.0153 (6)	−0.0319 (6)
F1	0.151 (4)	0.265 (7)	0.264 (7)	−0.123 (5)	−0.029 (4)	−0.082 (6)
F2	0.312 (8)	0.180 (5)	0.069 (2)	−0.088 (5)	−0.026 (3)	−0.004 (2)
F3	0.181 (5)	0.102 (3)	0.180 (4)	−0.009 (3)	−0.045 (4)	−0.011 (3)
O1	0.142 (4)	0.088 (3)	0.151 (4)	−0.012 (3)	0.013 (3)	−0.061 (3)
O2	0.161 (4)	0.087 (2)	0.0691 (19)	−0.045 (2)	0.016 (2)	−0.0198 (17)
O3	0.132 (4)	0.207 (6)	0.191 (5)	−0.124 (4)	0.035 (4)	−0.091 (5)
C37	0.128 (5)	0.085 (4)	0.122 (5)	−0.049 (4)	−0.010 (4)	−0.003 (3)

Geometric parameters (Å, °)

Ag1—N1	2.306 (2)	C33—C35	1.499 (8)
Ag1—N2	2.305 (3)	C33—C36	1.501 (10)
Ag1—N3	2.328 (3)	C1—H1	0.9300
Ag1—N4	2.333 (3)	C2—H2	0.9300
S1—C37	1.761 (8)	C4—H4	0.9300
S1—O3	1.473 (7)	C7—H7	0.9300
S1—O1	1.406 (4)	C9—H9	0.9300
S1—O2	1.425 (4)	C10—H10	0.9300
F1—C37	1.347 (10)	C12—H12C	0.9600
F2—C37	1.419 (9)	C12—H12A	0.9600
F3—C37	1.311 (8)	C12—H12B	0.9600
N1—C5	1.342 (4)	C13—H13A	0.9600

N1—C1	1.353 (5)	C13—H13B	0.9600
N2—C6	1.358 (4)	C13—H13C	0.9600
N2—C10	1.354 (5)	C14—H14A	0.9600
N3—C19	1.347 (5)	C14—H14B	0.9600
N3—C23	1.348 (4)	C14—H14C	0.9600
N4—C24	1.353 (4)	C16—H16A	0.9600
N4—C28	1.346 (5)	C16—H16B	0.9600
C1—C2	1.366 (5)	C16—H16C	0.9600
C2—C3	1.406 (5)	C17—H17A	0.9600
C3—C4	1.396 (5)	C17—H17B	0.9600
C3—C11	1.534 (5)	C17—H17C	0.9600
C4—C5	1.400 (5)	C18—H18C	0.9600
C5—C6	1.495 (5)	C18—H18B	0.9600
C6—C7	1.384 (5)	C18—H18A	0.9600
C7—C8	1.404 (5)	C19—H19	0.9300
C8—C15	1.529 (5)	C20—H20	0.9300
C8—C9	1.396 (5)	C22—H22	0.9300
C9—C10	1.368 (5)	C25—H25	0.9300
C11—C12	1.535 (7)	C27—H27	0.9300
C11—C13	1.519 (6)	C28—H28	0.9300
C11—C14	1.534 (5)	C30—H30A	0.9600
C15—C16	1.546 (7)	C30—H30B	0.9600
C15—C17	1.484 (10)	C30—H30C	0.9600
C15—C18	1.536 (10)	C31—H31C	0.9600
C19—C20	1.373 (5)	C31—H31A	0.9600
C20—C21	1.393 (5)	C31—H31B	0.9600
C21—C22	1.394 (6)	C32—H32C	0.9600
C21—C29	1.543 (5)	C32—H32A	0.9600
C22—C23	1.399 (4)	C32—H32B	0.9600
C23—C24	1.499 (5)	C34—H34B	0.9600
C24—C25	1.398 (4)	C34—H34A	0.9600
C25—C26	1.412 (6)	C34—H34C	0.9600
C26—C33	1.539 (5)	C35—H35A	0.9600
C26—C27	1.399 (5)	C35—H35B	0.9600
C27—C28	1.378 (5)	C35—H35C	0.9600
C29—C30	1.535 (7)	C36—H36A	0.9600
C29—C31	1.519 (8)	C36—H36B	0.9600
C29—C32	1.511 (7)	C36—H36C	0.9600
C33—C34	1.473 (8)		
Ag1···H17B^{i}	3.7200	H13B···H14A	2.4900
Ag1···H31B^{ii}	3.4400	H13C···H12C	2.5100
Ag1···H32A^{ii}	3.5000	H13C···H14C	2.4600
Ag1···H34A^{iii}	3.5400	H13C···H34C^{ix}	2.4000
Ag1···H36B^{iii}	3.6700	H14A···H4	2.2800
F1···O1	2.852 (9)	H14A···H13B	2.4900
F1···O2	2.900 (8)	H14A···H32C^{x}	2.5900
F2···O1	2.920 (7)	H14A···C4	2.7800

F2···O3	2.864 (9)	H14B···H12A	2.5200
F3···O2	2.909 (7)	H14B···C4	2.8000
F3···O3	2.883 (9)	H14B···H4	2.3100
F1···H31C^{iv}	2.8400	H14C···H13C	2.4600
O1···C28^{v}	3.390 (6)	H14C···H12C	2.4600
O1···F2	2.920 (7)	H14C···H35C^{ix}	2.5900
O1···F1	2.852 (9)	H16A···C7	2.6900
O2···F3	2.909 (7)	H16A···H7	2.1300
O2···C9^{v}	3.374 (6)	H16A···H17B	2.4800
O2···F1	2.900 (8)	H16B···H18A	2.4000
O3···F2	2.864 (9)	H16B···C7	3.0800
O3···F3	2.883 (9)	H16C···H17C	2.4800
O1···H28^{v}	2.6800	H16C···H18C	2.3900
O2···H2	2.5800	H17A···H18B	2.5600
O2···H9^{v}	2.5300	H17B···C7	2.9700
O3···H13B^{vi}	2.8300	H17B···Ag1^{i}	3.7200
N1···C6	2.415 (4)	H17B···H16A	2.4800
N1···N2	2.732 (4)	H17C···H16C	2.4800
N2···N1	2.732 (4)	H17C···H18C	2.5000
N2···C5	2.423 (4)	H18A···H16B	2.4000
N3···N4	2.745 (4)	H18A···C9	2.9900
N3···C24	2.417 (4)	H18B···H9	2.1100
N4···N3	2.745 (4)	H18B···H17A	2.5600
N4···C23	2.425 (4)	H18B···C9	2.6900
N4···H31B^{ii}	2.8500	H18C···H16C	2.3900
C2···C13^{vi}	3.518 (7)	H18C···H17C	2.5000
C9···O2^{vii}	3.374 (6)	H20···C31	2.7000
C12···C12^{viii}	3.588 (8)	H20···H35A^{ii}	2.5600
C13···C2^{vi}	3.518 (7)	H20···H31A	2.1500
C28···O1^{vii}	3.390 (6)	H22···C25	2.7600
C2···H13A	2.7500	H22···C32	2.5400
C2···H12B	2.7600	H22···H32B	2.1300
C2···H13B^{vi}	2.9500	H22···H32A	2.5100
C4···H14A	2.7800	H22···H25	2.2800
C4···H14B	2.8000	H25···C34	2.5300
C4···H7	2.6900	H25···C22	2.7500
C7···H16A	2.6900	H25···H34B	2.1100
C7···H16B	3.0800	H25···H22	2.2800
C7···H4	2.7100	H25···H34A	2.5200
C7···H17B	2.9700	H27···H30A^{iii}	2.5700
C9···H18A	2.9900	H27···C36	2.7300
C9···H18B	2.6900	H27···H36A	2.1800
C12···H12B^{viii}	2.9800	H28···O1^{vii}	2.6800
C12···H2	2.8800	H30A···H32B	2.4500
C13···H2	2.9400	H30A···H27^{iii}	2.5700

C14···H4	2.5200	H30B···C20	2.9200
C16···H7	2.6700	H30B···H31A	2.4300
C18···H9	2.6000	H30C···H31C	2.4700
C20···H31A	2.6900	H30C···H32C	2.4600
C20···H30B	2.9200	H31A···C20	2.6900
C22···H25	2.7500	H31A···H30B	2.4300
C22···H32A	2.8900	H31A···H20	2.1500
C22···H32B	2.6900	H31B···Ag1^{ii}	3.4400
C23···H36B^{iii}	2.9600	H31B···N4^{ii}	2.8500
C24···H31B^{ii}	2.9300	H31B···C24^{ii}	2.9300
C25···H34B	2.6600	H31B···H32A	2.5700
C25···H34A	2.8800	H31C···H30C	2.4700
C25···H22	2.7600	H31C···H32C	2.4400
C27···H36A	2.7100	H31C···F1^{iv}	2.8400
C27···H35B	2.9000	H32A···H22	2.5100
C31···H20	2.7000	H32A···H31B	2.5700
C32···H22	2.5400	H32A···Ag1^{ii}	3.5000
C34···H25	2.5300	H32A···C22	2.8900
C36···H27	2.7300	H32B···H30A	2.4500
H2···H13A	2.3900	H32B···C22	2.6900
H2···C13	2.9400	H32B···H22	2.1300
H2···H12B	2.3300	H32C···H30C	2.4600
H2···O2	2.5800	H32C···H14A^{xi}	2.5900
H2···C12	2.8800	H32C···H31C	2.4400
H4···C14	2.5200	H34A···C25	2.8800
H4···H7	2.2000	H34A···H25	2.5200
H4···H14A	2.2800	H34A···H36B	2.4800
H4···H14B	2.3100	H34A···Ag1^{iii}	3.5400
H4···C7	2.7100	H34B···H25	2.1100
H7···C16	2.6700	H34B···C25	2.6600
H7···H4	2.2000	H34B···H35A	2.4400
H7···C4	2.6900	H34C···H13C^{xii}	2.4000
H7···H16A	2.1300	H34C···H35C	2.4100
H9···C18	2.6000	H34C···H36C	2.3500
H9···H18B	2.1100	H35A···H20^{ii}	2.5600
H9···O2^{vii}	2.5300	H35A···H34B	2.4400
H12A···H14B	2.5200	H35B···C27	2.9000
H12B···C2	2.7600	H35B···H36A	2.3700
H12B···H2	2.3300	H35C···H34C	2.4100
H12B···H12B^{viii}	2.5900	H35C···H36C	2.4400
H12B···C12^{viii}	2.9800	H35C···H14C^{xii}	2.5900
H12B···H13A	2.4700	H36A···C27	2.7100
H12C···H14C	2.4600	H36A···H27	2.1800
H12C···H13C	2.5100	H36A···H35B	2.3700
H13A···H12B	2.4700	H36B···H34A	2.4800
H13A···H2	2.3900	H36B···C23^{iii}	2.9600

H13A···C2	2.7500	H36B···Ag1^{iii}	3.6700
H13B···O3^{vi}	2.8300	H36C···H34C	2.3500
H13B···C2^{vi}	2.9500	H36C···H35C	2.4400
N1—Ag1—N2	72.66 (9)	C10—C9—H9	120.00
N1—Ag1—N3	113.58 (9)	N2—C10—H10	118.00
N1—Ag1—N4	152.56 (11)	C9—C10—H10	118.00
N2—Ag1—N3	152.82 (12)	H12B—C12—H12C	109.00
N2—Ag1—N4	115.29 (10)	C11—C12—H12A	110.00
N3—Ag1—N4	72.16 (10)	C11—C12—H12B	109.00
O3—S1—C37	101.1 (4)	C11—C12—H12C	110.00
O1—S1—O3	115.6 (4)	H12A—C12—H12B	109.00
O1—S1—C37	105.7 (3)	H12A—C12—H12C	110.00
O1—S1—O2	117.3 (3)	H13B—C13—H13C	110.00
O2—S1—C37	101.4 (3)	C11—C13—H13C	110.00
O2—S1—O3	112.9 (3)	C11—C13—H13A	109.00
C1—N1—C5	117.1 (3)	C11—C13—H13B	110.00
Ag1—N1—C5	116.0 (2)	H13A—C13—H13B	109.00
Ag1—N1—C1	125.3 (2)	H13A—C13—H13C	109.00
C6—N2—C10	116.7 (3)	C11—C14—H14B	110.00
Ag1—N2—C6	115.3 (2)	C11—C14—H14A	110.00
Ag1—N2—C10	124.1 (2)	H14A—C14—H14C	109.00
C19—N3—C23	117.2 (3)	C11—C14—H14C	109.00
Ag1—N3—C19	123.3 (2)	H14A—C14—H14B	110.00
Ag1—N3—C23	115.6 (2)	H14B—C14—H14C	109.00
Ag1—N4—C24	115.2 (2)	C15—C16—H16C	109.00
Ag1—N4—C28	123.7 (2)	C15—C16—H16A	109.00
C24—N4—C28	117.4 (3)	C15—C16—H16B	110.00
N1—C1—C2	124.1 (3)	H16B—C16—H16C	109.00
C1—C2—C3	120.0 (3)	H16A—C16—H16B	109.00
C2—C3—C11	120.8 (3)	H16A—C16—H16C	109.00
C4—C3—C11	123.1 (3)	H17A—C17—H17B	110.00
C2—C3—C4	116.1 (3)	H17A—C17—H17C	109.00
C3—C4—C5	120.7 (3)	H17B—C17—H17C	109.00
N1—C5—C4	122.1 (3)	C15—C17—H17C	109.00
N1—C5—C6	116.6 (3)	C15—C17—H17A	109.00
C4—C5—C6	121.3 (3)	C15—C17—H17B	110.00
N2—C6—C5	116.2 (3)	C15—C18—H18A	109.00
N2—C6—C7	122.0 (3)	H18A—C18—H18B	109.00
C5—C6—C7	121.7 (3)	C15—C18—H18B	109.00
C6—C7—C8	121.2 (3)	C15—C18—H18C	109.00
C7—C8—C9	115.7 (3)	H18A—C18—H18C	109.00
C9—C8—C15	122.5 (3)	H18B—C18—H18C	110.00
C7—C8—C15	121.9 (3)	C20—C19—H19	118.00
C8—C9—C10	120.5 (4)	N3—C19—H19	118.00
N2—C10—C9	123.8 (3)	C21—C20—H20	120.00
C3—C11—C14	112.2 (3)	C19—C20—H20	120.00
C12—C11—C13	109.4 (4)	C21—C22—H22	120.00
C3—C11—C12	109.3 (3)	C23—C22—H22	119.00

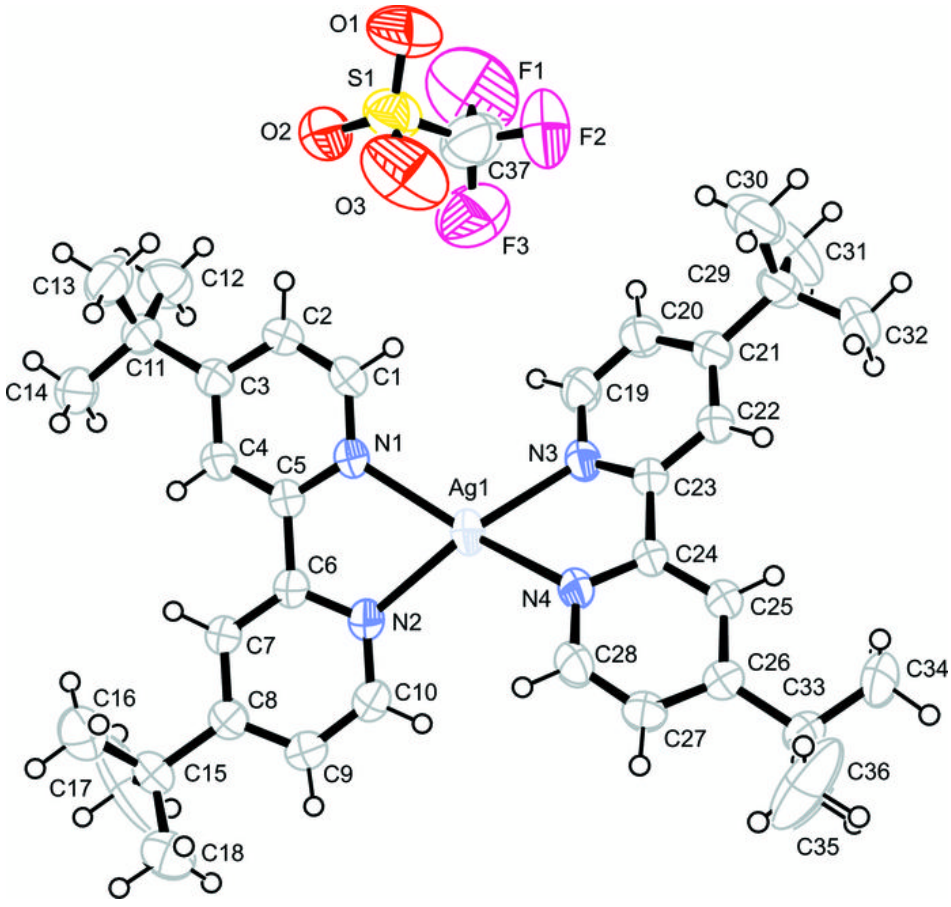
C3—C11—C13	108.5 (3)	C26—C25—H25	120.00
C12—C11—C14	108.8 (4)	C24—C25—H25	120.00
C13—C11—C14	108.7 (3)	C28—C27—H27	120.00
C16—C15—C18	104.7 (5)	C26—C27—H27	120.00
C8—C15—C16	111.1 (3)	N4—C28—H28	118.00
C8—C15—C17	107.5 (5)	C27—C28—H28	118.00
C8—C15—C18	111.7 (3)	H30A—C30—H30C	109.00
C16—C15—C17	109.8 (5)	C29—C30—H30A	109.00
C17—C15—C18	112.0 (6)	C29—C30—H30B	109.00
N3—C19—C20	123.6 (3)	C29—C30—H30C	109.00
C19—C20—C21	120.5 (4)	H30A—C30—H30B	109.00
C20—C21—C29	121.4 (3)	H30B—C30—H30C	110.00
C22—C21—C29	122.5 (3)	H31A—C31—H31C	109.00
C20—C21—C22	116.0 (3)	C29—C31—H31B	109.00
C21—C22—C23	120.9 (3)	H31B—C31—H31C	109.00
C22—C23—C24	122.1 (3)	C29—C31—H31A	110.00
N3—C23—C22	121.8 (3)	C29—C31—H31C	109.00
N3—C23—C24	116.1 (2)	H31A—C31—H31B	110.00
N4—C24—C23	116.4 (2)	C29—C32—H32B	109.00
N4—C24—C25	122.1 (3)	C29—C32—H32A	109.00
C23—C24—C25	121.5 (3)	H32A—C32—H32C	110.00
C24—C25—C26	120.5 (3)	C29—C32—H32C	109.00
C27—C26—C33	122.1 (3)	H32A—C32—H32B	109.00
C25—C26—C27	115.9 (3)	H32B—C32—H32C	109.00
C25—C26—C33	121.8 (3)	C33—C34—H34C	110.00
C26—C27—C28	120.4 (4)	C33—C34—H34A	109.00
N4—C28—C27	123.7 (3)	C33—C34—H34B	110.00
C31—C29—C32	110.5 (5)	H34A—C34—H34C	109.00
C21—C29—C31	111.0 (4)	H34B—C34—H34C	109.00
C21—C29—C30	107.6 (3)	H34A—C34—H34B	109.00
C30—C29—C32	108.1 (5)	H35A—C35—H35B	109.00
C21—C29—C32	111.6 (4)	H35A—C35—H35C	110.00
C30—C29—C31	107.9 (5)	C33—C35—H35A	109.00
C26—C33—C34	112.0 (5)	C33—C35—H35B	109.00
C34—C33—C35	109.3 (7)	C33—C35—H35C	109.00
C26—C33—C35	107.5 (4)	H35B—C35—H35C	110.00
C26—C33—C36	111.3 (4)	H36B—C36—H36C	109.00
C34—C33—C36	108.9 (8)	C33—C36—H36A	109.00
C35—C33—C36	107.7 (5)	C33—C36—H36B	109.00
C2—C1—H1	118.00	C33—C36—H36C	110.00
N1—C1—H1	118.00	H36A—C36—H36B	110.00
C1—C2—H2	120.00	H36A—C36—H36C	109.00
C3—C2—H2	120.00	S1—C37—F1	109.2 (5)
C3—C4—H4	120.00	S1—C37—F2	108.4 (6)
C5—C4—H4	120.00	S1—C37—F3	114.9 (6)
C6—C7—H7	119.00	F1—C37—F2	106.0 (7)
C8—C7—H7	119.00	F1—C37—F3	113.3 (7)
C8—C9—H9	120.00	F2—C37—F3	104.6 (6)
N2—Ag1—N1—C1	−168.3 (3)	C1—C2—C3—C4	−1.7 (6)

N3—Ag1—N1—C1	−16.6 (3)	C2—C3—C11—C13	−60.9 (5)
N4—Ag1—N1—C1	80.0 (4)	C11—C3—C4—C5	−176.5 (4)
N2—Ag1—N1—C5	−3.3 (3)	C2—C3—C4—C5	2.0 (6)
N3—Ag1—N1—C5	148.4 (3)	C2—C3—C11—C12	58.3 (5)
N4—Ag1—N1—C5	−115.0 (3)	C4—C3—C11—C12	−123.3 (4)
N1—Ag1—N2—C6	−8.3 (3)	C4—C3—C11—C13	117.5 (4)
N3—Ag1—N2—C6	−116.3 (3)	C2—C3—C11—C14	179.0 (4)
N4—Ag1—N2—C6	143.4 (3)	C4—C3—C11—C14	−2.5 (6)
N1—Ag1—N2—C10	−165.3 (4)	C3—C4—C5—C6	178.8 (4)
N3—Ag1—N2—C10	86.7 (5)	C3—C4—C5—N1	−1.1 (6)
N4—Ag1—N2—C10	−13.6 (4)	N1—C5—C6—C7	156.0 (4)
N1—Ag1—N3—C19	−13.7 (3)	C4—C5—C6—C7	−23.9 (6)
N2—Ag1—N3—C19	84.3 (3)	C4—C5—C6—N2	158.6 (4)
N4—Ag1—N3—C19	−164.9 (3)	N1—C5—C6—N2	−21.5 (6)
N1—Ag1—N3—C23	143.7 (2)	C5—C6—C7—C8	−176.3 (4)
N2—Ag1—N3—C23	−118.4 (3)	N2—C6—C7—C8	1.1 (6)
N4—Ag1—N3—C23	−7.6 (2)	C6—C7—C8—C15	179.3 (4)
N1—Ag1—N4—C24	−113.0 (3)	C6—C7—C8—C9	−0.8 (6)
N2—Ag1—N4—C24	145.8 (2)	C7—C8—C9—C10	0.1 (7)
N3—Ag1—N4—C24	−6.0 (2)	C7—C8—C15—C16	−36.3 (6)
N1—Ag1—N4—C28	89.5 (3)	C15—C8—C9—C10	−179.9 (4)
N2—Ag1—N4—C28	−11.7 (3)	C9—C8—C15—C17	−96.1 (6)
N3—Ag1—N4—C28	−163.5 (3)	C9—C8—C15—C16	143.7 (5)
O2—S1—C37—F1	68.0 (6)	C7—C8—C15—C17	83.9 (6)
O3—S1—C37—F1	−175.7 (6)	C7—C8—C15—C18	−152.8 (5)
O1—S1—C37—F2	60.1 (6)	C9—C8—C15—C18	27.2 (7)
O2—S1—C37—F2	−177.0 (5)	C8—C9—C10—N2	0.3 (8)
O3—S1—C37—F2	−60.7 (5)	N3—C19—C20—C21	0.4 (6)
O1—S1—C37—F3	176.7 (6)	C19—C20—C21—C22	−0.6 (6)
O1—S1—C37—F1	−54.8 (6)	C19—C20—C21—C29	−176.4 (4)
O3—S1—C37—F3	55.9 (7)	C20—C21—C29—C30	75.8 (5)
O2—S1—C37—F3	−60.4 (6)	C22—C21—C29—C32	18.7 (6)
C5—N1—C1—C2	0.5 (6)	C29—C21—C22—C23	175.9 (4)
Ag1—N1—C5—C6	13.6 (5)	C22—C21—C29—C31	142.4 (5)
Ag1—N1—C1—C2	165.3 (3)	C22—C21—C29—C30	−99.8 (5)
Ag1—N1—C5—C4	−166.5 (3)	C20—C21—C29—C31	−42.0 (6)
C1—N1—C5—C6	179.9 (4)	C20—C21—C22—C23	0.1 (6)
C1—N1—C5—C4	−0.2 (6)	C20—C21—C29—C32	−165.8 (5)
C6—N2—C10—C9	0.0 (7)	C21—C22—C23—C24	−178.1 (3)
C10—N2—C6—C5	176.9 (4)	C21—C22—C23—N3	0.5 (6)
Ag1—N2—C10—C9	156.7 (4)	C22—C23—C24—C25	−28.9 (5)
C10—N2—C6—C7	−0.6 (6)	N3—C23—C24—N4	−25.2 (4)
Ag1—N2—C6—C5	18.1 (5)	C22—C23—C24—N4	153.5 (3)
Ag1—N2—C6—C7	−159.4 (3)	N3—C23—C24—C25	152.4 (3)
Ag1—N3—C19—C20	157.2 (3)	C23—C24—C25—C26	−176.1 (3)
Ag1—N3—C23—C24	19.2 (4)	N4—C24—C25—C26	1.4 (6)
C19—N3—C23—C24	178.0 (3)	C24—C25—C26—C27	−0.9 (6)
C19—N3—C23—C22	−0.7 (5)	C24—C25—C26—C33	175.2 (4)
C23—N3—C19—C20	0.3 (6)	C25—C26—C27—C28	0.0 (6)

Ag1—N3—C23—C22	−159.5 (3)	C27—C26—C33—C34	−164.4 (8)
Ag1—N4—C24—C25	−159.8 (3)	C27—C26—C33—C35	75.5 (6)
C28—N4—C24—C23	176.8 (3)	C27—C26—C33—C36	−42.2 (6)
C28—N4—C24—C25	−0.8 (5)	C25—C26—C33—C35	−100.4 (5)
Ag1—N4—C24—C23	17.8 (4)	C33—C26—C27—C28	−176.1 (4)
C24—N4—C28—C27	−0.2 (6)	C25—C26—C33—C34	19.8 (9)
Ag1—N4—C28—C27	156.9 (3)	C25—C26—C33—C36	141.9 (5)
N1—C1—C2—C3	0.5 (7)	C26—C27—C28—N4	0.6 (6)
C1—C2—C3—C11	176.9 (4)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+2, −*y*, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*, *y*+1, *z*; (vi) −*x*+1, −*y*+1, −*z*; (vii) *x*, *y*−1, *z*; (viii) −*x*+2, −*y*+1, −*z*; (ix) *x*, *y*+1, *z*−1; (x) *x*, *y*, *z*−1; (xi) *x*, *y*, *z*+1; (xii) *x*, *y*−1, *z*+1.

Fig. 1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