metal-organic papers

Bis(3-methylisoquinoline-κN)silver(I) nitrate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
Disorder in solvent or counterion
R factor = 0.045
wR factor = 0.165
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, [Ag(C$_{10}$H$_9$N)$_2$]NO$_3$, the Ag^I cation, lying on a twofold rotation axis, is two-coordinated by two N atoms from two different 3-methylisoquinoline molecules in a linear coordination. The nitrate anions do not coordinate to the Ag^I cations, but rather act as counter-anions. The title compound forms a two-dimensional supramolecular structure through π–π interactions between the 3-methylisoquinoline ligands.

Comment

In recent years, there has been tremendous growth in the field of supramolecular coordination polymers prepared from nitrogen ligands and transition metals (Munakata *et al.*, 2001). In particular, polynuclear d^{10} metal complexes have attracted extensive attention owing to their appealing structures and photoluminescent properties. A series of d^{10} metal–organic structures has been reported recently (Ma *et al.*, 2005; Jung *et al.*, 2004). It is well known that silver is a soft metal centre with a good affinity for aromatic nitrogen ligands (Vranka & Amma, 1966; Carlucci *et al.*, 1994; Venkataraman *et al.*, 1995). The Ag^I cation displays various coordination modes, *viz.* linear, trigonal and tetrahedral, in compounds containing nitrogen ligands (Munakata *et al.*, 2001). In this paper, we report the preparation and crystal structure of [Ag(L)$_2$]NO$_3$ (L is 3-methylisoquinoline), (I).

(I)
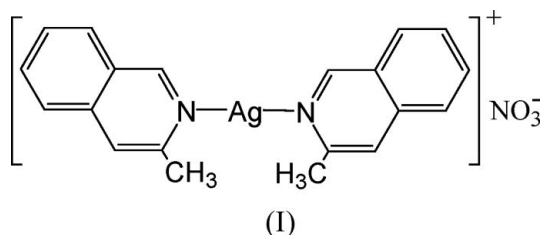
Selected bond lengths and angles for (I) are given in Table 1. As shown in Fig. 1, the Ag^I cation, lying on a twofold rotation axis, is two-coordinated by two N atoms from two different L molecules in a linear coordination. The nitrate anions do not coordinate to the Ag^I cations, but rather act as disordered counter-anions. The Ag—N distance of 2.143 (4) Å is similar to reported values (Makinen *et al.*, 2001).

There are weak π—π interactions between the L ligands. Adjacent ligand rings from different molecules are aligned in an offset fashion, being approximately parallel to each other at a distance of *ca* 3.5 Å, indicating the presence of π–π stacking interactions (Janiak, 2000), resulting in a two-dimensional supramolecular structure (Fig. 2).
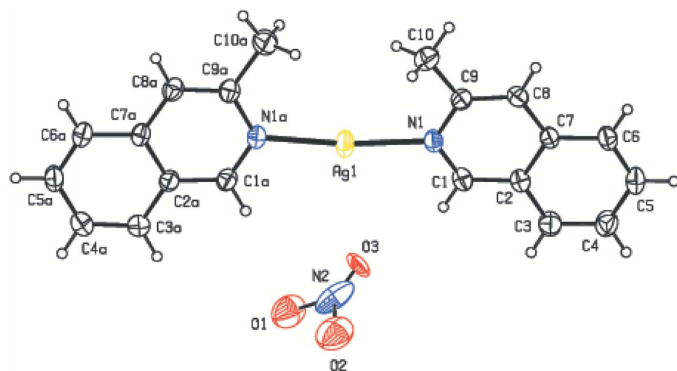
Figure 1
View of the coordination of Ag^I, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (a) $1 - x, y, \frac{3}{2} - z$.]

Experimental

After a mixture of $AgNO_3$ (0.085 g, 0.5 mmol) and L (0.0715 g, 0.5 mmol) in methanol (5 ml) had been stirred for 10 min, the white precipitate was dissolved by dropwise addition of dilute aqueous solution of NH_3. Crystals of (I) were obtained by evaporation of the solution for several days at room temperature.

Crystal data

$[Ag(C_{10}H_9N)_2]NO_3$	$D_x = 1.594$ Mg m^{-3}
$M_r = 456.24$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3040
$a = 10.418$ (5) Å	reflections
$b = 16.043$ (5) Å	$\theta = 2.2–28.3°$
$c = 11.484$ (5) Å	$\mu = 1.09$ mm^{-1}
$\beta = 98.031$ (5)°	$T = 292$ (2) K
$V = 1900.6$ (14) Å^3	Block, colourless
$Z = 4$	$0.46 \times 0.29 \times 0.25$ mm

Data collection

Bruker APEX CCD area-detector diffractometer	2213 independent reflections
φ and ω scans	1685 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.036$
	$\theta_{max} = 28.3°$
$T_{min} = 0.617$, $T_{max} = 0.764$	$h = -13 \rightarrow 11$
5724 measured reflections	$k = -21 \rightarrow 17$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.1128P)^2]$
$wR(F^2) = 0.165$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
2213 reflections	$\Delta\rho_{max} = 0.90$ e Å^{-3}
143 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.142 (4)		
N1^i—Ag1—N1	172.91 (11)	C9—N1—Ag1	122.6 (2)
C1—N1—Ag1	118.8 (2)		

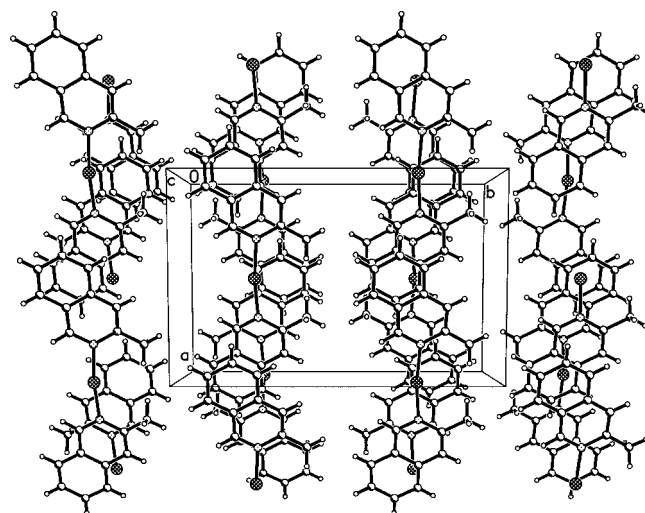Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

Figure 2
An edge view of the two-dimensional sheet of (I) generated by $\pi-\pi$ interactions of the L ligand. The nitrate anions have been omitted for clarity.

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.96 Å and $U_{iso}(H) = 1.2U_{eq}$(aromatic C) or $1.5U_{eq}$(methyl C). The atoms of nitrate group are refined with a fixed occupancy of 0.50 for the disorder.

Data collection: *SMART* (Bruker, 1997); 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-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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