Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-methyl-1*H*-imidazole)silver(I) nitrate methanol solvate

Jin Liu,[a] Xiao-Yu Su,[a] Wen-Hai Wang,[a] Zhi-Hua Mao[b]* and Ru-Gang Xie[a]*

[a]Department of Chemistry, Sichuan University, Chengdu 610064, People's Republic of China, and [b]Centre for Testing and Analysis, Sichuan University, Chengdu 610064, People's Republic of China

Correspondence e-mail: schemorg@mail.sc.cninfo.net

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.009 Å
R factor = 0.042
wR factor = 0.111
Data-to-parameter ratio = 14.3

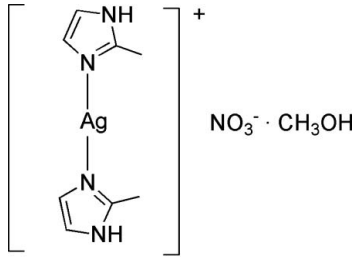
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 April 2006
Accepted 24 April 2006

The title complex, $[Ag(C_4H_6N_2)_2]NO_3\cdot CH_3OH$, features a mononuclear cation in which the Ag^I atom is coordinated in a linear fashion by two N atoms derived from the 2-methylimidazole ligands. The cations, anions and methanol molecules are linked by hydrogen bonds into a chain structure.

Comment

Imidazole and its derivatives have important biochemical functions, *e.g.* histidine as a metal ion-binding site plays an essential role in metalloenzymes (Sundberg *et al.*, 1977). Several supramolecular complexes containing 2-methylimidazole and metal salts have been prepared in recent years. Owing to their interesting architectures, they have potential applications in materials science (Huang *et al.*, 2004, 2006). In this paper, we report the crystal structure of the title compound, (I).



(I)

The Ag atom of the cation in (I) (Fig. 1) is coordinated by two 2-methylimidazole ligands. The Ag—N bond distances are 2.078 (4) and 2.084 (5) Å, values that agree well with those in related Ag complexes (Wang *et al.*, 2004). The Ag···O3 separation is 2.807 (6) Å, suggesting the existence of a weak interaction between these atoms. This Ag···O interaction could be responsible for the deviation of the N1—Ag—N3 angle of 174.7 (2)° from the ideal value of 180°.

The nitrate anion and methanol molecule play important roles in connecting the cations through hydrogen bonds, which are detailed in Table 1. These lead to the formation of a chain motif, as shown in Fig. 2.

Experimental

Siver(I) nitrate (0.5 mmol, 0.085 g) and 2-methylimidazole (1 mmol, 0.082 g) were dissolved in a mixed solvent of ethyl acetate (8 ml) and methanol (8 ml). After allowing the solution to stand in air for 2 d, colourless block-shaped single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent.

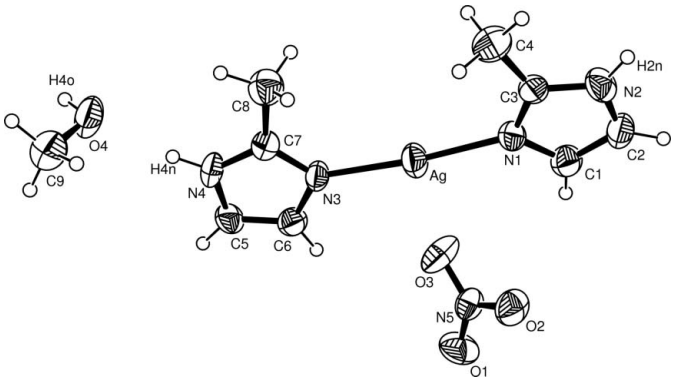


Figure 1
The asymmetric unit of (I), showing 40% probability displacement ellipsoids and the atomic numbering.

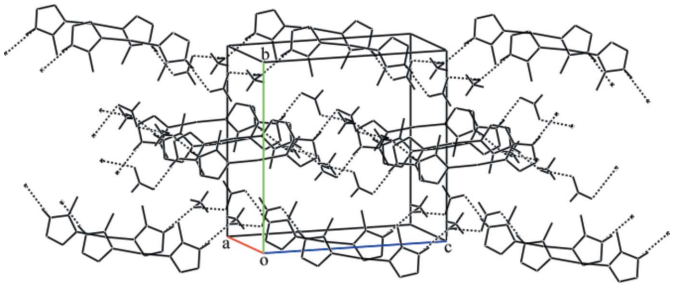


Figure 2
The crystal packing in (I), viewed approximately down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms have been omitted for clarity.

Crystal data

$[Ag(C_4H_6N_2)_2]NO_3\cdot CH_4O$
M_r = 366.14
Monoclinic, $P2_1/c$
a = 7.205 (5) Å
b = 13.857 (3) Å
c = 13.978 (4) Å
β = 90.74 (4)°
V = 1395.4 (11) Å^3
Z = 4
D_x = 1.743 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 294 (2) K
Block, colourless
0.20 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2937 measured reflections
2545 independent reflections
1380 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 25.4°
3 standard reflections
every 300 reflections
intensity decay: 1.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.111
S = 0.97
2545 reflections
178 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −1.11 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O2^{i}	0.86	2.02	2.879 (7)	172
N4—H4N···O4	0.86	1.95	2.795 (7)	169
O4—H4O···O1^{ii}	0.82	2.13	2.943 (7)	170

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

All H atoms were placed in idealized positions, with C—H = 0.93–0.96 Å, N—H = 0.86 Å and O—H = 0.82 Å, and with a common refined U_{iso}(H) = 0.124 (11) Å^2 for methyl H and 0.044 (6) Å^2 for the remaining H atoms. The deepest hole is loca\ted 0.07 Å from atom Ag1.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *MERCURY* (Version 1.2; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (grant No. 20472057) and the SRFDP of China (grant No. 20040610011).

References

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Gabe, E. J. & White, P. S. (1993). *DIFRAC*. American Crystallographic Association, Pittsburgh Meeting, 1193. Abstract PA 104.
Huang, X. C., Lin, Y. Y., Zhang, J. P. & Chen, X.-M. (2006). *Angew. Chem. Int. Ed.* **45**, 1557–1559.
Huang, X. C., Zhang, J. P. & Chen, X.-M. (2004). *J. Am. Chem. Soc.* **126**, 13218–13219.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sundberg, R. J., Yilmaz, I. & Mente, D. C. (1977). *Inorg. Chem.* **16**, 1470–1476.
Wang, L.-S., Zhang, J.-F. & Yang, S.-P. (2004). *Acta Cryst.* E**60**, m1484–m1486.