Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(1*H*-imidazolium-κN^3)silver(I) nitrate

Feng Sun, Zheng-Yuan Zhou, Mao-Sheng Liu, Xiu-Xia Zhou and Yue-Peng Cai*

School of Chemistry and the Environment, South China Normal University, Guangzhou 510631, People's Republic of China
Correspondence e-mail: ypcai8@yahoo.com

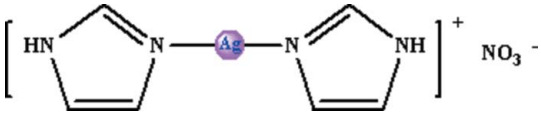
Received 23 July 2007; accepted 24 July 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.023; wR factor = 0.054; data-to-parameter ratio = 16.5.

In the title compound, $[Ag(C_3H_4N_2)_2)]NO_3$, the Ag^I atom exhibits an approximately linear coordination geometry formed by two N atoms of imidazolium cations. The uncoordinated nitrate anion is linked to the Ag^I complex *via* N—H···O hydrogen bonding, generating a one-dimensional supramolecular chain.

Related literature

For general background, see: Cai *et al.* (2003). For related literature, see: Xu *et al.* (2002).



Experimental

Crystal data

$[Ag(C_3H_4N_2)_2)]NO_3$
M_r = 306.04
Orthorhombic, $P2_12_12_1$
a = 4.9941 (4) Å
b = 10.9250 (8) Å
c = 18.0729 (12) Å
V = 986.07 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.04 mm^{-1}
T = 298 (2) K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.630, T_{max} = 0.720
5440 measured reflections
2266 independent reflections
2175 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.054
S = 1.06
2266 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), with 896 Friedel pairs
Flack parameter: 0.01 (4)

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.112 (2)	Ag1—N3	2.116 (2)
N1—Ag1—N3	172.62 (10)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.86	2.03	2.879 (4)	171
N4—H4···O3	0.86	2.00	2.853 (5)	174

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

Data collection: *SMART* (Bruker, 1998); 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*.

The work was supported by the National Natural Science Foundation of China and the NSF of Guangdong Province, China (grant No. 06025033).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2302).

References

Bruker (1998). *SMART* (Version 5.0) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Cai, Y.-P., Chen, C.-L., Zhang, L., Shi, J.-L., Xu, A.-W., Su, C.-Y. & Kang, B.-S. (2003). *Inorg. Chim. Acta*, **342**, 107–113.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
Xu, A.-W., Cai, Y.-P., Zhang, L.-Z., Su, C.-Y. & Kang, B.-S. (2002). *Acta Cryst.* E**58**, m770–m771.

 doi:10.1107/S1600536807036215

supplementary materials

Acta Cryst. (2007). E**63**, m2227 [**doi:10.1107/S1600536807036215**]

Bis(1*H*-imidazolium-κN^3)silver(I) nitrate

F. Sun, Z.-Y. Zhou, M.-S. Liu, X.-X. Zhou and Y.-P. Cai

Comment

As part of the structural studies of Ag^I compounds involving the N-heterocycle ligand (Cai *et al.*, 2003; Xu *et al.*, 2002), we report here the synthesis and structure of the title compound.

The crystal of the compound consists of $[Ag(C_3N_2H_4)_2)]^+$ cations and $(NO_3)^-$ anions. Fig. 1 shows the structure of the cation. The Ag^I atom exhibits a AgN_2 linear coordination geometry arising from two N atoms of imidazole molecules (Table 1). The uncoordinated nitrate anion interacts with imidazole by hydrogen bonding (Table 2), generating a one-dimensional supramolecular chain (Fig. 2).

Experimental

A solution of $AgNO_3$ (17 mg, 0.10 mmol) in CH_3OH (10 ml) was slowly added to a solution of imidazole (14 mg, 0.20 mmol) in CH_3OH (10 ml). The resultant solution was stirred for 10 min at room temperature and then filtered. After addition of diethyl ether (10 ml), the filtrate was cooled to 253 K. Microcrystalline material was collected after 24 h and dried under vacuum (yield: 20.8 mg, 68%). Colorless crystals suitable for X-ray diffraction were obtained in 2 d by slow diffusion of diethyl ether into a dilute solution of the title complex in methanol. The elemental analysis: calculated for $C_6H_8N_5AgO_3$ C 23.53, H 2.61, N 22.88%; found: C 23.48, H 2.68, N 22.75%.

Refinement

H atoms were placed in idealized positions with C—H = 0.93 and N—H = 0.86 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

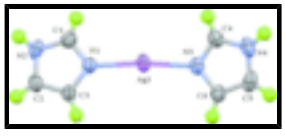


Fig. 1. The structure of the cation of the title compound. The atom-numbering scheme is shown at the 50% probability level.

Fig. 2. One-dimensional chain constructed by N—H···O hydrogen bonds.

Bis(1*H*-imidazolium-κN^3)silver(I) nitrate

Crystal data

$[Ag(C_3H_4N_2)_2)]NO_3$	F_{000} = 600
M_r = 306.04	D_x = 2.062 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 4145 reflections
a = 4.9941 (4) Å	θ = 2.9–27.6º
b = 10.9250 (8) Å	μ = 2.04 mm^{-1}
c = 18.0729 (12) Å	T = 298 (2) K
V = 986.07 (13) Å^3	Block, colourless
Z = 4	0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2266 independent reflections
Radiation source: fine-focus sealed tube	2175 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 298(2) K	θ_{max} = 27.6º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	h = −6→4
T_{min} = 0.630, T_{max} = 0.720	k = −14→9
5440 measured reflections	l = −22→23

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.019P)^2 + 0.36P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.023	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.054	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
S = 1.06	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
2266 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
137 parameters	Extinction coefficient: 0.0093 (6)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 896 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.01 (4)
Hydrogen site location: inferred from neighbouring sites	

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}
Ag1	0.05263 (5)	0.56829 (2)	0.394887 (14)	0.04765 (9)
O1	1.0937 (6)	−0.0388 (3)	0.25932 (16)	0.0760 (9)
O2	1.1043 (5)	0.0848 (2)	0.35189 (14)	0.0635 (7)
O3	0.8259 (7)	0.1125 (3)	0.26385 (16)	0.0848 (10)
N1	−0.2176 (4)	0.7170 (2)	0.39330 (15)	0.0402 (5)
N2	−0.5210 (5)	0.8442 (2)	0.35437 (16)	0.0509 (7)
H2	−0.6496	0.8741	0.3284	0.061*
N3	0.3587 (5)	0.4350 (2)	0.40299 (14)	0.0432 (5)
N4	0.6233 (6)	0.2898 (3)	0.36536 (18)	0.0565 (7)
H4	0.6916	0.2342	0.3375	0.068*
N5	1.0102 (5)	0.0531 (2)	0.29229 (14)	0.0464 (6)
C1	−0.4085 (7)	0.7350 (3)	0.34523 (19)	0.0484 (8)
H1	−0.4593	0.6788	0.3092	0.058*
C2	−0.3967 (7)	0.8998 (3)	0.4119 (2)	0.0526 (8)
H2A	−0.4331	0.9772	0.4308	0.063*
C3	−0.2096 (7)	0.8205 (3)	0.43611 (19)	0.0473 (7)
H3	−0.0937	0.8338	0.4756	0.057*
C4	0.4128 (8)	0.3589 (3)	0.3494 (2)	0.0549 (9)
H4A	0.3160	0.3537	0.3055	0.066*
C5	0.7112 (7)	0.3224 (3)	0.4332 (2)	0.0532 (9)
H5	0.8571	0.2898	0.4584	0.064*
C6	0.5441 (7)	0.4125 (3)	0.45737 (18)	0.0479 (7)
H6	0.5540	0.4519	0.5029	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.04804 (13)	0.03896 (13)	0.05596 (14)	0.01227 (10)	−0.00079 (11)	0.00013 (11)
O1	0.0810 (18)	0.0742 (18)	0.0727 (17)	0.0439 (16)	−0.0231 (15)	−0.0295 (14)
O2	0.0756 (18)	0.0613 (15)	0.0537 (14)	0.0062 (14)	−0.0167 (12)	−0.0076 (13)
O3	0.097 (2)	0.093 (2)	0.0643 (17)	0.0642 (18)	−0.0247 (16)	−0.0118 (15)
N1	0.0386 (11)	0.0367 (12)	0.0453 (13)	0.0026 (9)	−0.0026 (12)	0.0025 (12)

N2	0.0406 (15)	0.0531 (15)	0.0592 (16)	0.0129 (12)	−0.0048 (13)	0.0106 (13)
N3	0.0435 (11)	0.0367 (12)	0.0494 (13)	0.0065 (10)	0.0037 (11)	0.0005 (14)
N4	0.0585 (18)	0.0440 (15)	0.0671 (18)	0.0162 (13)	0.0129 (15)	−0.0032 (15)
N5	0.0491 (15)	0.0461 (14)	0.0441 (13)	0.0118 (12)	−0.0015 (11)	0.0010 (12)
C1	0.0458 (19)	0.0465 (17)	0.0529 (17)	0.0003 (14)	−0.0083 (14)	0.0007 (14)
C2	0.0551 (19)	0.0413 (16)	0.061 (2)	0.0132 (14)	0.0013 (15)	−0.0004 (14)
C3	0.0483 (17)	0.0399 (17)	0.0536 (18)	0.0074 (14)	−0.0072 (14)	−0.0026 (14)
C4	0.060 (2)	0.0515 (19)	0.0530 (18)	0.0147 (17)	−0.0017 (16)	−0.0076 (15)
C5	0.0415 (17)	0.0454 (19)	0.073 (2)	0.0072 (14)	−0.0014 (16)	0.0157 (18)
C6	0.0528 (16)	0.0402 (16)	0.0508 (17)	0.0020 (15)	−0.0040 (15)	0.0039 (13)

Geometric parameters (Å, °)

Ag1—N1	2.112 (2)	N4—C4	1.326 (4)
Ag1—N3	2.116 (2)	N4—C5	1.350 (5)
O1—N5	1.240 (3)	N4—H4	0.8600
O2—N5	1.225 (3)	C1—H1	0.9300
O3—N5	1.238 (3)	C2—C3	1.348 (4)
N1—C1	1.305 (4)	C2—H2A	0.9300
N1—C3	1.371 (4)	C3—H3	0.9300
N2—C1	1.328 (4)	C4—H4A	0.9300
N2—C2	1.355 (4)	C5—C6	1.362 (5)
N2—H2	0.8600	C5—H5	0.9300
N3—C4	1.305 (4)	C6—H6	0.9300
N3—C6	1.373 (4)		
N1—Ag1—N3	172.62 (10)	N1—C1—H1	124.4
C1—N1—C3	105.8 (3)	N2—C1—H1	124.4
C1—N1—Ag1	126.3 (2)	C3—C2—N2	106.1 (3)
C3—N1—Ag1	127.5 (2)	C3—C2—H2A	126.9
C1—N2—C2	107.7 (3)	N2—C2—H2A	126.9
C1—N2—H2	126.1	C2—C3—N1	109.1 (3)
C2—N2—H2	126.1	C2—C3—H3	125.4
C4—N3—C6	106.1 (3)	N1—C3—H3	125.4
C4—N3—Ag1	122.4 (2)	N3—C4—N4	111.4 (3)
C6—N3—Ag1	131.3 (2)	N3—C4—H4A	124.3
C4—N4—C5	107.8 (3)	N4—C4—H4A	124.3
C4—N4—H4	126.1	N4—C5—C6	106.4 (3)
C5—N4—H4	126.1	N4—C5—H5	126.8
O2—N5—O3	120.1 (3)	C6—C5—H5	126.8
O2—N5—O1	121.5 (3)	C5—C6—N3	108.2 (3)
O3—N5—O1	118.4 (3)	C5—C6—H6	125.9
N1—C1—N2	111.2 (3)	N3—C6—H6	125.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.03	2.879 (4)	171
N4—H4···O3	0.86	2.00	2.853 (5)	174

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

Fig. 1

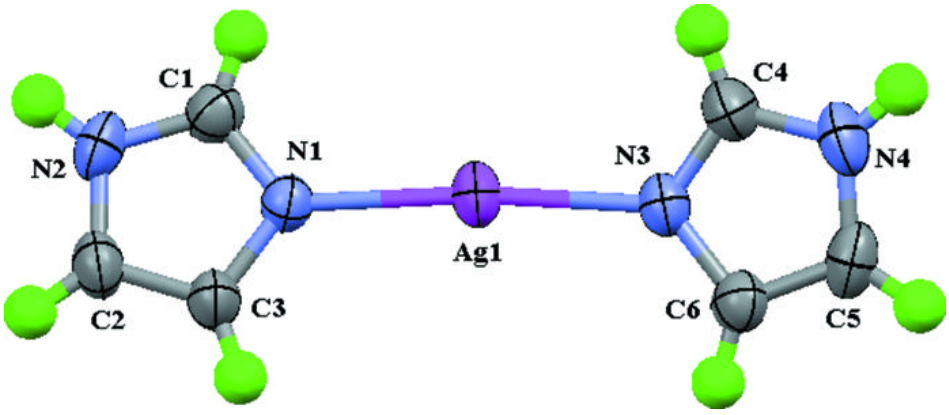


Fig. 2