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Bis(2-methyl-1*H*-imidazole-κN^3)silver(I) nitrate dihydrate

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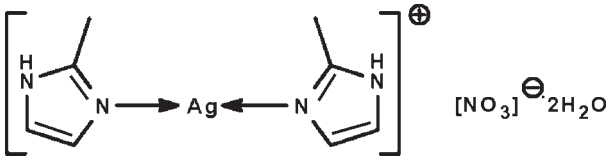
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.024; wR factor = 0.073; data-to-parameter ratio = 13.7.

The Ag^I atom in the salt, $[Ag(C_4H_6N_2)_2]NO_3{\cdot}2H_2O$, shows a nearly linear coordination [N—Ag—N = 178.26 (7)°]. The cation, anion and water molecules are linked by N—H···O and O—H···O hydrogen bonds into a layer motif extending parallel to (101).

Related literature

For the crystal structure of $[Ag(C_4H_6N_2)_2][NO_3]{\cdot}CH_3OH$, see: Liu *et al.* (2006).



Experimental

Crystal data

$[Ag(C_4H_6N_2)_2]NO_3{\cdot}2H_2O$
M_r = 370.13
Monoclinic, $P2_1/n$
a = 6.8001 (4) Å
b = 17.0196 (9) Å
c = 12.1453 (7) Å
β = 101.691 (1)°
V = 1376.48 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 295 K
0.21 × 0.19 × 0.17 mm

Data collection

Bruker APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.745, T_{max} = 0.786
7483 measured reflections
2721 independent reflections
2083 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.073
S = 0.99
2721 reflections
198 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1w	0.86 (1)	1.99 (1)	2.838 (3)	169 (3)
N4—H4···O1w^{i}	0.84 (1)	1.99 (1)	2.837 (3)	178 (3)
O1w—H11···O2w	0.85 (1)	1.89 (1)	2.726 (3)	170 (4)
O1w—H12···O1	0.85 (1)	1.99 (1)	2.826 (3)	171 (3)
O2w—H21···O1^{ii}	0.84 (1)	2.02 (1)	2.867 (3)	179 (4)
O2w—H22···O2^{iii}	0.84 (1)	2.15 (2)	2.955 (3)	159 (3)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5122).

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supporting information

Acta Cryst. (2009). E**65**, m1535 [doi:10.1107/S1600536809045838]

Bis(2-methyl-1*H*-imidazole-κN^3)silver(I) nitrate dihydrate

Fang-Di Cong, Feng-Yang Yu, Zhen Wei and Seik Weng Ng

S1. Experimental

Silver nitrate (0.5 mmol, 0.085 g) and 2-methyl-1*H*-imidazole (0.5 mmol, 0.041 g) in water (15 ml) were heated in a Parr bomb at 433 K for three days. Crystals of the adduct were isolated from the cool mixture in 30% yield.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C). The amino and water H atoms were located in a difference Fourier map, and were refined with a distance restraint of N–H = O–H = 0.85±0.01 Å; their displacement parameters were refined.

The final difference Fourier map had a peak that was displaced by 0.5 along *y* relative to Ag1. Thus, for the reflections with k odd a scale factor was refined to 1.035 (2) with respect to the reflections with k even. Although the refinement was not significantly improved, the final difference Fourier map now did not have any large peaks.

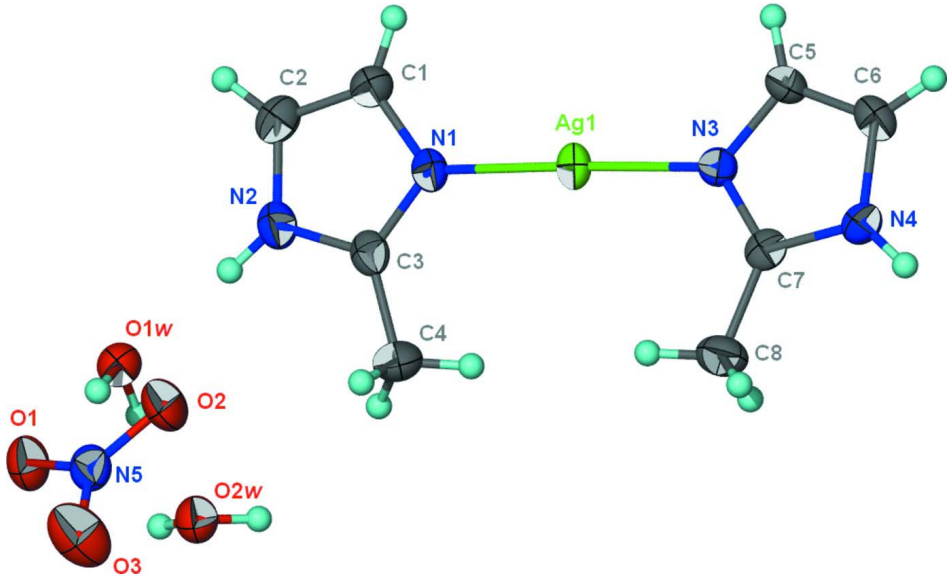

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $[Ag(C_4H_6N_2)_2][NO_3]\cdot 2H_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Bis(2-methyl-1*H*-imidazole-κN^3)silver(I) nitrate dihydrate

Crystal data

$[Ag(C4H6N_2)_2]NO_3 \cdot 2H_2O$
$M_r = 370.13$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 6.8001$ (4) Å
$b = 17.0196$ (9) Å
$c = 12.1453$ (7) Å
$\beta = 101.691$ (1)°
$V = 1376.48$ (13) Å^3
$Z = 4$
$F(000) = 744$
$D_x = 1.786$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3827 reflections
$\theta = 2.9$–$26.1°$
$\mu = 1.49$ mm^{-1}
$T = 295$ K
Block, colorless
0.21 × 0.19 × 0.17 mm

Data collection

Bruker APEX2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.745$, $T_{max} = 0.786$
7483 measured reflections
2721 independent reflections
2083 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 26.1°$, $\theta_{min} = 2.1°$
$h = -4 \rightarrow 8$
$k = -19 \rightarrow 21$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.073$
$S = 0.99$
2721 reflections
198 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.0379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.63346 (3)	0.501978 (10)	0.882866 (16)	0.02240 (9)
O1	−0.1909 (3)	0.26078 (11)	0.44924 (15)	0.0315 (5)
O2	−0.0592 (3)	0.30353 (12)	0.61645 (17)	0.0404 (5)
O3	−0.2399 (3)	0.19831 (13)	0.59642 (18)	0.0458 (6)
O1w	0.1172 (3)	0.35094 (12)	0.38606 (16)	0.0266 (4)
O2w	0.3941 (3)	0.24560 (11)	0.34310 (17)	0.0292 (4)
N1	0.4754 (4)	0.49985 (11)	0.7163 (2)	0.0217 (5)
N2	0.2877 (3)	0.45702 (14)	0.55959 (19)	0.0257 (5)
H2	0.228 (4)	0.4222 (13)	0.514 (2)	0.043 (9)*
N3	0.7904 (3)	0.50045 (10)	1.0498 (2)	0.0201 (5)
N4	0.9606 (3)	0.45734 (13)	1.21030 (19)	0.0219 (5)
H4	1.010 (4)	0.4257 (12)	1.2620 (16)	0.025 (8)*

N5	−0.1639 (3)	0.25410 (13)	0.55457 (19)	0.0275 (5)
C1	0.3998 (4)	0.56352 (16)	0.6500 (2)	0.0242 (6)
H1	0.4245	0.6160	0.6694	0.029*
C2	0.2853 (4)	0.53782 (17)	0.5535 (2)	0.0267 (6)
H2A	0.2177	0.5685	0.4944	0.032*
C3	0.4044 (4)	0.43623 (15)	0.6586 (2)	0.0230 (6)
C4	0.4422 (4)	0.35360 (15)	0.6951 (3)	0.0344 (7)
H4A	0.5512	0.3517	0.7592	0.052*
H4B	0.4764	0.3235	0.6349	0.052*
H4C	0.3236	0.3321	0.7150	0.052*
C5	0.8772 (4)	0.56384 (16)	1.1123 (2)	0.0232 (6)
H5	0.8652	0.6160	1.0893	0.028*
C6	0.9816 (4)	0.53821 (16)	1.2118 (2)	0.0243 (6)
H6	1.0535	0.5687	1.2698	0.029*
C7	0.8427 (3)	0.43705 (16)	1.1119 (2)	0.0206 (6)
C8	0.7814 (4)	0.35502 (14)	1.0811 (2)	0.0318 (7)
H8A	0.6674	0.3552	1.0198	0.048*
H8B	0.7466	0.3290	1.1447	0.048*
H8C	0.8906	0.3277	1.0589	0.048*
H11	0.192 (5)	0.3164 (18)	0.366 (3)	0.089 (16)*
H12	0.029 (4)	0.3258 (17)	0.412 (3)	0.052 (11)*
H21	0.517 (2)	0.2499 (19)	0.374 (3)	0.060 (11)*
H22	0.392 (5)	0.2426 (19)	0.2737 (10)	0.066 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.01779 (13)	0.02855 (14)	0.01956 (14)	−0.00075 (8)	0.00074 (9)	−0.00051 (8)
O1	0.0306 (10)	0.0386 (11)	0.0230 (11)	−0.0041 (9)	0.0001 (8)	−0.0002 (8)
O2	0.0438 (12)	0.0364 (12)	0.0350 (13)	−0.0013 (10)	−0.0064 (10)	−0.0126 (10)
O3	0.0549 (14)	0.0491 (13)	0.0362 (13)	−0.0194 (11)	0.0157 (11)	−0.0026 (10)
O1w	0.0270 (11)	0.0253 (11)	0.0268 (11)	0.0008 (9)	0.0038 (9)	0.0015 (8)
O2w	0.0280 (11)	0.0296 (11)	0.0276 (12)	0.0012 (9)	0.0001 (9)	−0.0027 (9)
N1	0.0174 (11)	0.0250 (12)	0.0218 (12)	−0.0016 (8)	0.0017 (9)	−0.0017 (9)
N2	0.0221 (12)	0.0310 (14)	0.0230 (13)	0.0004 (10)	0.0023 (10)	−0.0050 (11)
N3	0.0196 (12)	0.0203 (11)	0.0203 (12)	0.0006 (8)	0.0036 (9)	−0.0008 (8)
N4	0.0223 (12)	0.0226 (12)	0.0204 (12)	0.0018 (10)	0.0037 (10)	0.0034 (10)
N5	0.0212 (11)	0.0294 (12)	0.0305 (14)	0.0031 (10)	0.0019 (10)	−0.0050 (10)
C1	0.0249 (14)	0.0219 (14)	0.0254 (15)	0.0006 (11)	0.0038 (12)	0.0017 (11)
C2	0.0258 (15)	0.0308 (15)	0.0239 (15)	0.0043 (12)	0.0060 (12)	0.0043 (12)
C3	0.0171 (13)	0.0274 (14)	0.0251 (15)	−0.0001 (11)	0.0056 (11)	−0.0034 (11)
C4	0.0351 (16)	0.0227 (15)	0.0426 (18)	0.0058 (12)	0.0008 (14)	−0.0025 (12)
C5	0.0247 (15)	0.0183 (13)	0.0258 (16)	−0.0015 (10)	0.0033 (12)	−0.0043 (11)
C6	0.0223 (14)	0.0264 (15)	0.0247 (15)	−0.0048 (12)	0.0058 (11)	−0.0056 (12)
C7	0.0167 (13)	0.0229 (14)	0.0242 (15)	0.0025 (10)	0.0088 (11)	0.0005 (11)
C8	0.0326 (15)	0.0213 (14)	0.0416 (18)	−0.0033 (12)	0.0075 (13)	−0.0019 (12)

Geometric parameters (Å, º)

Ag1—N1	2.090 (2)	N4—C6	1.384 (4)
Ag1—N3	2.091 (2)	N4—H4	0.844 (10)
O1—N5	1.260 (3)	C1—C2	1.342 (4)
O2—N5	1.250 (3)	C1—H1	0.9300
O3—N5	1.238 (3)	C2—H2A	0.9300
O1w—H11	0.845 (10)	C3—C4	1.481 (4)
O1w—H12	0.848 (10)	C4—H4A	0.9600
O2w—H21	0.844 (10)	C4—H4B	0.9600
O2w—H22	0.842 (10)	C4—H4C	0.9600
N1—C3	1.326 (3)	C5—C6	1.344 (4)
N1—C1	1.385 (3)	C5—H5	0.9300
N2—C3	1.347 (4)	C6—H6	0.9300
N2—C2	1.377 (4)	C7—C8	1.483 (3)
N2—H2	0.856 (10)	C8—H8A	0.9600
N3—C7	1.323 (3)	C8—H8B	0.9600
N3—C5	1.381 (3)	C8—H8C	0.9600
N4—C7	1.342 (3)		
N1—Ag1—N3	178.27 (7)	N1—C3—N2	110.0 (2)
H11—O1w—H12	106 (4)	N1—C3—C4	126.5 (2)
H21—O2w—H22	105 (3)	N2—C3—C4	123.5 (2)
C3—N1—C1	106.2 (2)	C3—C4—H4A	109.5
C3—N1—Ag1	125.87 (18)	C3—C4—H4B	109.5
C1—N1—Ag1	127.32 (17)	H4A—C4—H4B	109.5
C3—N2—C2	108.0 (2)	C3—C4—H4C	109.5
C3—N2—H2	121 (2)	H4A—C4—H4C	109.5
C2—N2—H2	131 (2)	H4B—C4—H4C	109.5
C7—N3—C5	106.7 (2)	C6—C5—N3	109.3 (2)
C7—N3—Ag1	126.03 (17)	C6—C5—H5	125.4
C5—N3—Ag1	126.92 (16)	N3—C5—H5	125.4
C7—N4—C6	108.0 (2)	C5—C6—N4	106.1 (2)
C7—N4—H4	125.1 (18)	C5—C6—H6	127.0
C6—N4—H4	126.9 (19)	N4—C6—H6	127.0
O3—N5—O2	120.2 (2)	N3—C7—N4	109.9 (2)
O3—N5—O1	119.9 (2)	N3—C7—C8	126.5 (2)
O2—N5—O1	119.9 (2)	N4—C7—C8	123.6 (2)
C2—C1—N1	109.5 (2)	C7—C8—H8A	109.5
C2—C1—H1	125.3	C7—C8—H8B	109.5
N1—C1—H1	125.3	H8A—C8—H8B	109.5
C1—C2—N2	106.3 (2)	C7—C8—H8C	109.5
C1—C2—H2A	126.9	H8A—C8—H8C	109.5
N2—C2—H2A	126.9	H8B—C8—H8C	109.5
C3—N1—C1—C2	−0.2 (3)	C7—N3—C5—C6	0.1 (3)
Ag1—N1—C1—C2	−171.9 (2)	Ag1—N3—C5—C6	−173.71 (19)
N1—C1—C2—N2	0.4 (3)	N3—C5—C6—N4	0.5 (3)

C3—N2—C2—C1	−0.5 (3)	C7—N4—C6—C5	−1.0 (3)
C1—N1—C3—N2	−0.1 (3)	C5—N3—C7—N4	−0.8 (3)
Ag1—N1—C3—N2	171.74 (19)	Ag1—N3—C7—N4	173.13 (18)
C1—N1—C3—C4	−179.5 (3)	C5—N3—C7—C8	178.6 (2)
Ag1—N1—C3—C4	−7.7 (4)	Ag1—N3—C7—C8	−7.5 (4)
C2—N2—C3—N1	0.4 (3)	C6—N4—C7—N3	1.1 (3)
C2—N2—C3—C4	179.8 (2)	C6—N4—C7—C8	−178.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1*w*	0.86 (1)	1.99 (1)	2.838 (3)	169 (3)
N4—H4···O1*w*^{i}	0.84 (1)	1.99 (1)	2.837 (3)	178 (3)
O1*w*—H11···O2*w*	0.85 (1)	1.89 (1)	2.726 (3)	170 (4)
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Symmetry codes: (i) *x*+1, *y*, *z*+1; (ii) *x*+1, *y*, *z*; (iii) *x*+1/2, −*y*+1/2, *z*−1/2.