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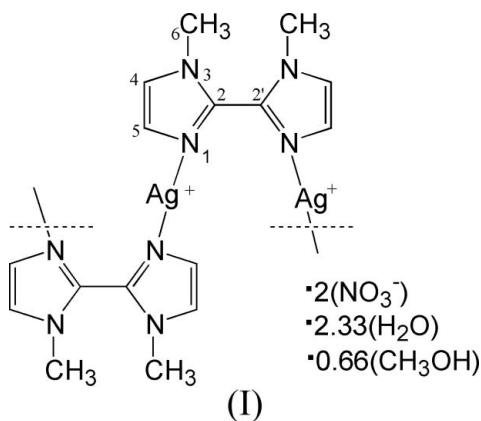
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å  
Disorder in main residue  
 $R$  factor = 0.047  
 $wR$  factor = 0.145  
Data-to-parameter ratio = 15.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[silver(I)- $\mu_2$ -1,1'-dimethyl-2,2'-biimidazole- $\kappa^3:N^3'$ ] nitrate 1.167-hydrate methanol 0.33-solvate]**

The title structure,  $\{[\text{Ag}(\text{C}_8\text{H}_{10}\text{N}_4)]\text{NO}_3 \cdot 1.167\text{H}_2\text{O} \cdot 0.33\text{CH}_4\text{O}\}_n$ , consists of helical chains in which approximately linearly coordinated Ag atoms alternate with bridging 1,1'-dimethyl-2,2'-biimidazole ligands in a *syn* conformation. The environment of each Ag atom is completed by weak Ag—O bonds to a bidentate nitrate ion.

## Comment

The crystal structure of the title compound, (I), contains single-stranded helices consisting of nearly linear two-coordinate Ag atoms bridged by 1,1'-dimethyl-2,2'-biimidazole ( $\text{Me}_2\text{biim}$ ) ligands in a *syn* conformation. The basic periodic pattern includes three Ag atoms and three ligands. A similar helix observed for the corresponding biimidazole complex possesses a crystallographic  $3_2$  axis (Hester *et al.*, 1997). In the present case, the three monomeric units are symmetry independent, but deviation from this higher symmetry is small. Since our  $\text{Me}_2\text{biim}$  complex crystallizes in a centrosymmetric space group, it contains both left- and right-handed helices.



The Ag—N distances [2.102 (4)–2.122 (4) Å; Table 1] are typical of two-coordinate complexes with *N*-heterocyclic ligands. Departure from linearity about the Ag atom [N—Ag—N = 163.7 (2)–170.8 (2)°] is significant but not unusual. The overall environment of each Ag atom is completed by two Ag—O ‘semi-bonds’ in the range 2.65–2.92 Å with bidentate nitrate ions, approximately perpendicular to the N—Ag—N direction (N1—Ag—O = 86–108°). Formation of a variable number of such weaker bonding interactions near the ‘equatorial’ plane is common in Ag chemistry.

The distances and angles in the ligand do not differ appreciably from those found for the free molecule (Therrien & Beauchamp, 1999), the most important structural modification being the conformational change from *anti* to *syn*.

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Distortions commonly noted when biimidazole is chelating are absent here; coordination takes place along the lone pair direction (difference between Ag–Ni1–Ci2 and Ag–Ni1–Ci5 < 6°) and the angles at the ring junction (C2'–Ci2–Ni1 and C2'–Ci2–Ni3) differ by < 4°. Although the two rings of Me<sub>2</sub>biim can be coplanar in the *anti* conformation, steric hindrance between the methyl groups forces a dihedral angle of 32.2 (2)–39.5 (2)° between the two rings in the *syn* orientation found here. No such steric effect is present in the non-methylated biimidazole–Ag compound, where the dihedral angle is smaller [23.2 (2)°] and probably controlled by the general structure of the helix. Our greater dihedral angle results in a longer periodic pattern (8.35 *versus* 7.76 Å) and slightly greater Ag···Ag distances (3.01–3.08 Å *versus* 3.00 Å) than in the biimidazole compound.

The –[Ag–Me<sub>2</sub>biim]<sub>n</sub>– helices are oriented along the *a* axis and their surface consists of an alternation of ligand methyl groups and free Oi2 atoms of weakly coordinated nitrates. Small channels (also oriented along *a*) at the junction of four helices are filled by water or methanol molecules acting as hydrogen-bond donors toward these O atoms. Details are provided in Table 2. In the channels at (*y*, *z*) = (0,  $\frac{1}{2}$ ) and ( $\frac{1}{2}$ , 0), water molecules O1, O2 and O3 and their symmetry-equivalent counterparts across the inversion centre define a closed loop of six water molecules hydrogen-bonded to one another and anchored to nitrate O atoms. In the other channels at (*y*, *z*) = (0, 0) and ( $\frac{1}{2}$ ,  $\frac{1}{2}$ ), one disordered methanol molecule is distributed statistically over two positions [C1X–O1X and C2X–O2X], forming hydrogen bonds to atoms O21b and O32, respectively. When the methanol (half) molecule present is C2X–O2X, an extra disordered (half) water molecule O4 is present as well, but it interacts only weakly with its surrounding. Solvent disorder in this region explains that nitrate ion N2/O21/O22/O23 is also disordered over two slightly different orientations.

## Experimental

Me<sub>2</sub>biim was prepared according to the method of Mohanty *et al.* (1994), by methylation of 2,2-biimidazole obtained by the method of Fieselmann *et al.* (1978). To synthesize the complex, AgNO<sub>3</sub> (34 mg, 0.20 mmol) was added to a stirred solution of Me<sub>2</sub>biim (32 mg, 0.20 mmol) in (undried) methanol (10 ml). The clear solution was refluxed for 1 h, the volume was reduced to 5 ml and the solution was cooled in a refrigerator. Colourless crystals of the water–methanol solvate were collected after 5 d.

### Crystal data

[Ag(C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>)]NO<sub>3</sub>·1.167H<sub>2</sub>O·0.33CH<sub>4</sub>O  
*M<sub>r</sub>* = 363.44  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 8.3497 (1) Å  
*b* = 23.0390 (2) Å  
*c* = 21.3683 (2) Å  
 $\beta$  = 93.342 (1)°  
*V* = 4103.60 (7) Å<sup>3</sup>  
*Z* = 12

*D<sub>x</sub>* = 1.765 Mg m<sup>−3</sup>  
 Cu *K*α radiation  
 Cell parameters from 24951 reflections  
 $\theta$  = 2.8–72.9°  
 $\mu$  = 12.05 mm<sup>−1</sup>  
*T* = 293 (2) K  
 Needle, colourless  
 0.59 × 0.11 × 0.05 mm

### Data collection

Bruker SMART 2000 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T*<sub>min</sub> = 0.25, *T*<sub>max</sub> = 0.55  
 49852 measured reflections

8069 independent reflections  
 5837 reflections with *I* > 2σ(*I*)  
*R*<sub>int</sub> = 0.053  
 $\theta$ <sub>max</sub> = 73.0°  
 $h$  = −9 → 8  
 $k$  = −28 → 28  
 $l$  = −26 → 26

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.047  
*wR* (*F*<sup>2</sup>) = 0.145  
*S* = 1.02  
 8069 reflections  
 527 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0883P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.94 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.58 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Ag1–N11	2.112 (4)	Ag2–O23A	2.84 (8)
Ag1–N21	2.118 (4)	Ag2–O21B	2.754 (16)
Ag1–O11	2.916 (5)	Ag2–O23B	2.91 (3)
Ag1–O13	2.873 (5)	Ag3–N51	2.102 (4)
Ag2–N31	2.117 (4)	Ag3–N61	2.108 (4)
Ag2–N41	2.122 (4)	Ag3–O31	2.834 (6)
Ag2–O21A	2.65 (4)	Ag3–O33	2.802 (6)
N11–Ag1–N21	170.77 (15)	C12–N11–Ag1	129.7 (3)
N11–Ag1–O11	87.38 (14)	C15–N11–Ag1	123.6 (3)
N11–Ag1–O13	102.75 (15)	N11–C12–C62 <sup>i</sup>	123.6 (4)
N21–Ag1–O11	100.64 (14)	N13–C12–C62 <sup>i</sup>	125.2 (4)
N21–Ag1–O13	86.34 (15)	C22–N21–Ag1	127.5 (3)
O11–Ag1–O13	42.59 (12)	C25–N21–Ag1	125.1 (3)
N31–Ag2–N41	163.72 (16)	N21–C22–C32	122.8 (4)
N31–Ag2–O21A	96.4 (6)	N23–C22–C32	126.9 (5)
N31–Ag2–O23A	88.6 (16)	C32–N31–Ag2	126.5 (3)
N41–Ag2–O21A	97.9 (6)	C35–N31–Ag2	127.4 (4)
N41–Ag2–O23A	107.1 (17)	N31–C32–C22	123.6 (4)
O21A–Ag2–O23A	44.5 (8)	N33–C32–C22	125.1 (5)
N31–Ag2–O21B	107.8 (2)	C42–N41–Ag2	128.8 (3)
N31–Ag2–O23B	88.4 (7)	C45–N41–Ag2	124.8 (3)
N41–Ag2–O21B	86.4 (2)	N41–C42–C52	124.1 (4)
N41–Ag2–O23B	107.7 (7)	N43–C42–C52	125.3 (4)
O21B–Ag2–O23B	43.5 (3)	N51–C52–C42	123.8 (4)
N51–Ag3–N61	164.75 (15)	N53–C52–C42	126.0 (4)
N51–Ag3–O31	106.24 (16)	C62–N61–Ag3	127.4 (3)
N51–Ag3–O33	86.62 (17)	C65–N61–Ag3	126.9 (4)
N61–Ag3–O31	88.51 (16)	N61–C62–C12 <sup>ii</sup>	123.3 (4)
N61–Ag3–O33	107.20 (18)	N63–C62–C12 <sup>ii</sup>	125.9 (4)
O31–Ag3–O33	43.87 (16)		

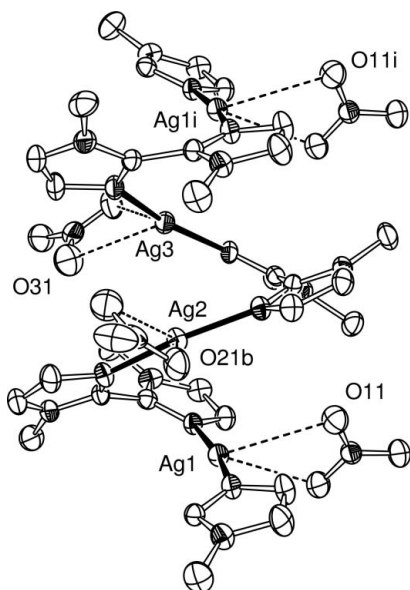
Symmetry codes: (i) *x* + 1, *y*, *z*; (ii) *x* − 1, *y*, *z*.

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1A···O2 <sup>iii</sup>	0.82	2.03	2.854 (3)	179
O1–H1B···O23B <sup>iv</sup>	0.82	2.15	2.974 (18)	178
O1–H1B···O23A <sup>iv</sup>	0.82	2.18	2.99 (4)	171
O2–H2A···O12 <sup>v</sup>	0.82	2.12	2.937 (5)	177
O2–H2B···O3	0.82	2.06	2.877 (4)	177
O3–H3A···O12	0.82	2.04	2.859 (4)	179
O3–H3B···O1	0.82	1.98	2.803 (2)	179
O1X–H1X···O21B	0.82	2.53	2.92 (2)	111
O2X–H2X···O32 <sup>vi</sup>	0.82	1.97	2.733 (19)	154

Symmetry codes: (iii) −*x*, −*y* + 2, −*z* + 1; (iv) *x*, −*y* +  $\frac{3}{2}$ , *z* +  $\frac{1}{2}$ ; (v) −*x* + 1, −*y* + 2, −*z* + 1; (vi) −*x*, *y* −  $\frac{1}{2}$ , −*z* +  $\frac{1}{2}$ .



**Figure 1**  
A view of a portion of the  $-\text{[Ag}^+ - \text{Me}_2\text{biim}]_n-$  helix. Dashed lines correspond to weak  $\text{Ag}i - \text{O}i1$  and  $\text{Ag}i - \text{O}i3$  bonds with nitrate ions. H atoms have been omitted for clarity. Displacement ellipsoids correspond to the 30% probability level. Only the major component, 'b', of the disordered nitrate anion is shown. [Symmetry code: (i)  $x - 1, y, z$ .]

Nitrate ion N2/O21/O22/O23 was found to be disordered over two slightly different orientations. The occupancies were first allowed to refine for a few cycles and then fixed to the normalized 0.70/0.30 values for the rest of the refinement. Restraints were applied to keep the geometry of these fractional nitrates close to that of the non-disordered ions. H atoms were positioned geometrically [C—

H(ring) = 0.93 Å, C—H(methyl) = 0.96 Å and O—H = 0.82 Å] and were included in the refinement in the riding-model approximation; their displacement parameters were set to 1.5 (methyl H atoms) or 1.2 (other H atoms) times  $U_{\text{eq}}$  of the parent site. For water molecule O4 (half occupancy), no peaks were visible in the electron density map for the two H atoms, and since no suitable hydrogen-bond acceptors could be identified, they were omitted.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *UdMX* (Maris, 2004).

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