metal-organic compounds

A new Ag^I complex based on 1-[(1*H*-benzimidazol-1-yl)methyl]-1*H*-1,2,4-triazole

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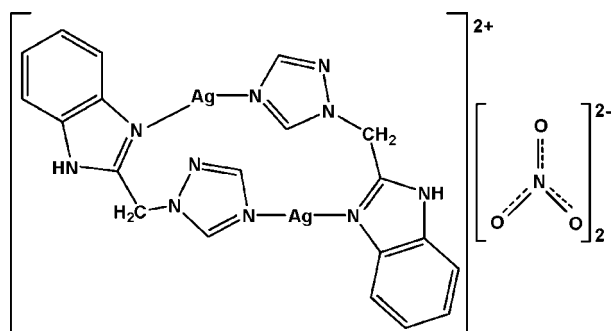Correspondence e-mail: mxr@zzu.edu.cn

In the title complex, bis{μ-1-[(1*H*-benzimidazol-1-yl)methyl]-1*H*-1,2,4-triazole}disilver(I) dinitrate, [Ag$_2$(C$_{10}$H$_9$N$_5$)$_2$](NO$_3$)$_2$, the Ag^I ion is nearly linearly coordinated [N—Ag—N angle is 155.72 (14)°] by two 1-[(1*H*-benzimidazole-1-yl)methyl]-1*H*-1,2,4-triazole (bmt) ligands. In addition, two bmt ligands link two Ag^I ions, forming a dinuclear unit with an Ag···Ag distance of 5.0179 (15) Å. The whole complex is generated by an inversion centre. The dinuclear units and the NO$_3^-$ counter-ions are connected by N—H···O hydrogen bonds and weak Ag···O interactions [2.831 (5), 2.887 (5) and 2.908 (5) Å], leading to a three-dimensional structure.

Related literature

For background to complexes based on benzimidazole or triazole and their derivatives, see: Yang *et al.* (2010); Li *et al.* (2010); Tian *et al.* (2011); Zhang *et al.* (2011).

Experimental

Crystal data

[Ag$_2$(C$_{10}$H$_9$N$_5$)$_2$](NO$_3$)$_2$	V = 1192.1 (4) Å^3
M_r = 738.20	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 9.4947 (19) Å	μ = 1.71 mm^{-1}
b = 13.569 (3) Å	T = 293 K
c = 10.174 (2) Å	0.19 × 0.17 × 0.14 mm
β = 114.56 (3)°	

Data collection

Rigaku Saturn diffractometer	9572 measured reflections
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2006)	2158 independent reflections
	1952 reflections with $I > 2\sigma(I)$
T_{min} = 0.737, T_{max} = 0.796	R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043	181 parameters
$wR(F^2)$ = 0.095	H-atom parameters constrained
S = 1.09	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
2158 reflections	$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O2	0.86	2.08	2.849 (6)	148

Data collection: *CrystalClear* (Rigaku/MSC, 2006); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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supporting information

A new Ag^I complex based on 1-[(1*H*-benzimidazol-1-yl)methyl]-1*H*-1,2,4-triazole

Yan-zhi Wang, Jun Zhang, Huai-xia Yang and Xiang-ru Meng

S1. Comment

Many complexes based on benzimidazole or triazole and their derivatives have been synthesized and characterized owing to the strong coordination abilities of these multidentate N-heterocyclic ligands and the interesting properties and potential applications of these complexes (Yang *et al.*, 2010; Li *et al.*, 2010; Tian *et al.*, 2011; Zhang *et al.*, 2011). We are engaged in the synthesis of unsymmetrical N-heterocyclic ligands and have synthesized the compound 1-[(1*H*-benzimidazole-1-yl)methyl]-1*H*-1,2,4-triazole (bmt). In this work, we selected this compound as ligand and generated a new complex [Ag$_2$(C$_{10}$H$_9$N$_5$)$_2$](NO$_3$)$_2$, (I), which is reported here.

In complex (I) each Ag^I ion is two-coordinated by two N atom from one triazole group and one benzimidazole group of two different 1-[(1*H*-benzimidazole-1-yl)methyl]-1*H*-1,2,4-triazole ligands and the nitrate anion does not coordinate to the Ag^I ion (Fig. 1). Two bmt ligands bridge two Ag^I ions leading to a dinuclear unit [Ag$_2$(C$_{10}$H$_9$N$_5$)$_2$] with Ag1—Ag1^i distance of 5.0179 (15) Å (symmetry code: (i) -*x*-1, -*y*+2, -*z*). [Ag$_2$(C$_{10}$H$_9$N$_5$)$_2$] units and NO$_3^-$ groups are linked through weak Ag···O interactions and N—H···O hydrogen bonds (Table 1) resulting in a three-dimensional packing in solid state.

S2. Experimental

The ligand 1-[(1*H*-benzimidazole-1-yl)methyl]-1*H*-1,2,4-triazole (0.1 mmol) in methanol (4 ml) was added dropwise to an aqueous solution (3 ml) of AgNO$_3$ (0.1 mmol). The resulting solution was allowed to stand at room temperature in the dark. After four weeks good quality colorless crystals were obtained from the filtrate and dried in air.

S3. Refinement

H atoms are positioned geometrically and refined as riding atoms, with C-H = 0.93 (aromatic) and 0.97 (CH$_2$) Å and N-H = 0.86 Å and with U$_{iso}$(H) = 1.2 U$_{eq}$(C,N).
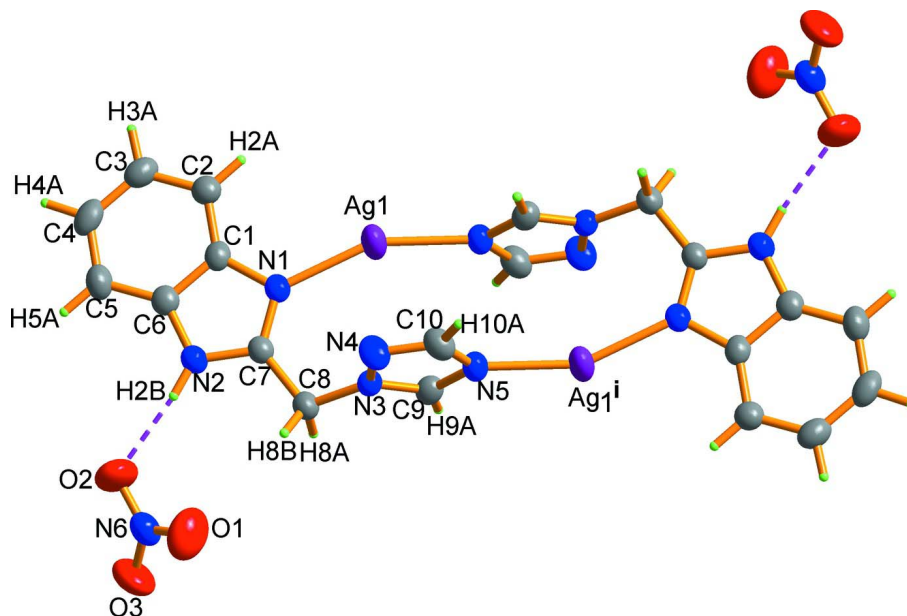
Figure 1

View of the title complex showing labeling and 30% probability displacement ellipsoids. Hydrogen bonds are indicated by dashed lines. Symmetry code: (*i*) -*x* - 1, -*y* + 2, -*z*.

bis{*µ*-1-[(1*H*-benzimidazol-1-yl)methyl]-1*H*-1,2,4- triazole}disilver(I) dinitrate

Crystal data

$[Ag_2(C_{10}H_9N_5)_2](NO_3)_2$	$F(000) = 728$
$M_r = 738.20$	$D_x = 2.057$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *Kα* radiation, $λ = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3140 reflections
$a = 9.4947$ (19) Å	$θ = 2.4–27.9°$
$b = 13.569$ (3) Å	$µ = 1.71$ mm^{-1}
$c = 10.174$ (2) Å	$T = 293$ K
$β = 114.56$ (3)°	Prism, colourless
$V = 1192.1$ (4) Å^3	$0.19 × 0.17 × 0.14$ mm
$Z = 2$	

Data collection

Rigaku Saturn diffractometer	9572 measured reflections
Radiation source: fine-focus sealed tube	2158 independent reflections
Graphite monochromator	1952 reflections with $I > 2σ(I)$
Detector resolution: 28.5714 pixels mm^{-1}	$R_{int} = 0.034$
ω scans	$θ_{max} = 25.3°, θ_{min} = 2.4°$
Absorption correction: multi-scan	$h = −11→10$
(*CrystalClear*; Rigaku/MSC, 2006)	$k = −16→16$
$T_{min} = 0.737, T_{max} = 0.796$	$l = −12→11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.043$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.095$	
$S = 1.09$	H-atom parameters constrained
2158 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 1.7006P]$ where $P = (F_o^2 + 2F_c^2)/3$
181 parameters	
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.70$ e Å^{-3}
	$\Delta\rho_{min} = -0.28$ e Å^{-3}

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	−0.34103 (4)	0.89095 (3)	0.20814 (4)	0.04938 (17)
N1	−0.0927 (4)	0.9097 (2)	0.3164 (4)	0.0326 (8)
N2	0.1479 (4)	0.9666 (3)	0.3996 (4)	0.0354 (8)
H2B	0.2248	1.0035	0.4080	0.043*
N3	−0.1878 (4)	1.0476 (2)	0.0747 (4)	0.0320 (8)
N4	−0.1943 (5)	0.9813 (3)	−0.0280 (4)	0.0449 (10)
N5	−0.4205 (4)	1.0613 (3)	−0.0931 (4)	0.0374 (8)
N6	0.3779 (5)	1.1840 (3)	0.4722 (5)	0.0470 (10)
O1	0.3112 (6)	1.1880 (4)	0.3398 (4)	0.0877 (14)
O2	0.3944 (6)	1.1033 (3)	0.5326 (5)	0.0818 (14)
O3	0.4245 (5)	1.2605 (3)	0.5397 (5)	0.0801 (13)
C1	0.0033 (5)	0.8484 (3)	0.4281 (4)	0.0320 (9)
C2	−0.0334 (6)	0.7641 (3)	0.4866 (5)	0.0387 (10)
H2A	−0.1339	0.7396	0.4515	0.046*
C3	0.0871 (6)	0.7193 (3)	0.5989 (5)	0.0446 (12)
H3A	0.0670	0.6633	0.6409	0.054*
C4	0.2383 (6)	0.7552 (3)	0.6518 (5)	0.0454 (12)
H4A	0.3158	0.7223	0.7277	0.055*
C5	0.2760 (5)	0.8380 (3)	0.5946 (5)	0.0415 (11)
H5A	0.3769	0.8618	0.6295	0.050*
C6	0.1542 (5)	0.8840 (3)	0.4813 (5)	0.0345 (10)
C7	−0.0011 (5)	0.9789 (3)	0.3042 (4)	0.0306 (9)
C8	−0.0451 (5)	1.0643 (3)	0.2027 (4)	0.0352 (10)
H8A	−0.0574	1.1222	0.2528	0.042*
H8B	0.0379	1.0774	0.1732	0.042*

C9	−0.3227 (5)	1.0931 (3)	0.0341 (5)	0.0353 (10)
H9A	−0.3452	1.1409	0.0881	0.042*
C10	−0.3371 (6)	0.9929 (4)	−0.1265 (5)	0.0450 (11)
H10A	−0.3772	0.9569	−0.2120	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0295 (2)	0.0625 (3)	0.0471 (3)	0.00013 (17)	0.00685 (17)	0.00857 (18)
N1	0.0290 (19)	0.0329 (19)	0.0328 (19)	0.0005 (16)	0.0098 (16)	−0.0039 (15)
N2	0.030 (2)	0.038 (2)	0.036 (2)	−0.0027 (16)	0.0114 (16)	−0.0009 (16)
N3	0.0292 (19)	0.0302 (17)	0.0335 (19)	0.0019 (15)	0.0100 (16)	0.0020 (15)
N4	0.040 (2)	0.046 (2)	0.047 (2)	0.0002 (19)	0.016 (2)	−0.0166 (19)
N5	0.030 (2)	0.041 (2)	0.036 (2)	0.0014 (17)	0.0097 (17)	0.0027 (17)
N6	0.036 (2)	0.056 (3)	0.047 (3)	−0.007 (2)	0.015 (2)	−0.004 (2)
O1	0.103 (4)	0.097 (3)	0.048 (2)	0.023 (3)	0.016 (2)	−0.003 (2)
O2	0.089 (3)	0.060 (3)	0.088 (3)	−0.008 (2)	0.029 (3)	0.028 (2)
O3	0.067 (3)	0.064 (3)	0.094 (3)	−0.025 (2)	0.019 (2)	−0.029 (2)
C1	0.033 (2)	0.032 (2)	0.028 (2)	0.0053 (18)	0.0098 (18)	−0.0064 (18)
C2	0.040 (3)	0.034 (2)	0.040 (2)	0.000 (2)	0.014 (2)	−0.0028 (19)
C3	0.060 (3)	0.033 (2)	0.037 (3)	0.004 (2)	0.018 (2)	0.000 (2)
C4	0.055 (3)	0.041 (3)	0.034 (2)	0.018 (2)	0.012 (2)	0.001 (2)
C5	0.034 (3)	0.049 (3)	0.035 (2)	0.005 (2)	0.008 (2)	−0.007 (2)
C6	0.036 (3)	0.035 (2)	0.031 (2)	0.0020 (19)	0.013 (2)	−0.0054 (18)
C7	0.030 (2)	0.031 (2)	0.028 (2)	−0.0005 (18)	0.0106 (18)	−0.0052 (17)
C8	0.031 (2)	0.034 (2)	0.036 (2)	−0.0011 (19)	0.0093 (19)	−0.0042 (19)
C9	0.037 (3)	0.037 (2)	0.032 (2)	0.003 (2)	0.015 (2)	0.0031 (19)
C10	0.040 (3)	0.049 (3)	0.043 (3)	−0.007 (2)	0.014 (2)	−0.010 (2)

Geometric parameters (Å, º)

Ag1—N1	2.163 (4)	N6—O2	1.233 (5)
Ag1—N5^i	2.171 (4)	C1—C6	1.390 (6)
N1—C7	1.321 (5)	C1—C2	1.399 (6)
N1—C1	1.397 (5)	C2—C3	1.377 (6)
N2—C7	1.353 (5)	C2—H2A	0.9300
N2—C6	1.382 (5)	C3—C4	1.395 (7)
N2—H2B	0.8600	C3—H3A	0.9300
N3—C9	1.325 (5)	C4—C5	1.380 (7)
N3—N4	1.361 (5)	C4—H4A	0.9300
N3—C8	1.454 (5)	C5—C6	1.396 (6)
N4—C10	1.318 (6)	C5—H5A	0.9300
N5—C9	1.313 (6)	C7—C8	1.492 (6)
N5—C10	1.352 (6)	C8—H8A	0.9700
N5—Ag1^i	2.171 (4)	C8—H8B	0.9700
N6—O3	1.222 (5)	C9—H9A	0.9300
N6—O1	1.229 (5)	C10—H10A	0.9300

N1—Ag1—N5[i]	155.72 (14)	C4—C3—H3A	118.9
C7—N1—C1	105.5 (4)	C5—C4—C3	121.9 (4)
C7—N1—Ag1	131.1 (3)	C5—C4—H4A	119.1
C1—N1—Ag1	123.3 (3)	C3—C4—H4A	119.1
C7—N2—C6	107.6 (4)	C4—C5—C6	116.2 (4)
C7—N2—H2B	126.2	C4—C5—H5A	121.9
C6—N2—H2B	126.2	C6—C5—H5A	121.9
C9—N3—N4	109.8 (4)	N2—C6—C1	105.5 (4)
C9—N3—C8	128.8 (4)	N2—C6—C5	132.3 (4)
N4—N3—C8	121.2 (3)	C1—C6—C5	122.2 (4)
C10—N4—N3	102.1 (4)	N1—C7—N2	112.2 (4)
C9—N5—C10	103.0 (4)	N1—C7—C8	127.7 (4)
C9—N5—Ag1[i]	125.8 (3)	N2—C7—C8	120.1 (4)
C10—N5—Ag1[i]	131.1 (3)	N3—C8—C7	112.8 (3)
O3—N6—O1	118.6 (5)	N3—C8—H8A	109.0
O3—N6—O2	122.2 (5)	C7—C8—H8A	109.0
O1—N6—O2	119.1 (5)	N3—C8—H8B	109.0
C6—C1—N1	109.2 (4)	C7—C8—H8B	109.0
C6—C1—C2	121.1 (4)	H8A—C8—H8B	107.8
N1—C1—C2	129.7 (4)	N5—C9—N3	110.5 (4)
C3—C2—C1	116.5 (4)	N5—C9—H9A	124.8
C3—C2—H2A	121.8	N3—C9—H9A	124.8
C1—C2—H2A	121.8	N4—C10—N5	114.6 (4)
C2—C3—C4	122.2 (4)	N4—C10—H10A	122.7
C2—C3—H3A	118.9	N5—C10—H10A	122.7

N5[i]—Ag1—N1—C7	−24.9 (5)	C4—C5—C6—N2	179.8 (4)
N5[i]—Ag1—N1—C1	149.8 (3)	C4—C5—C6—C1	−0.4 (6)
C9—N3—N4—C10	0.5 (5)	C1—N1—C7—N2	0.3 (4)
C8—N3—N4—C10	−176.4 (4)	Ag1—N1—C7—N2	175.7 (3)
C7—N1—C1—C6	0.1 (4)	C1—N1—C7—C8	−178.8 (4)
Ag1—N1—C1—C6	−175.7 (3)	Ag1—N1—C7—C8	−3.3 (6)
C7—N1—C1—C2	179.6 (4)	C6—N2—C7—N1	−0.7 (5)
Ag1—N1—C1—C2	3.7 (6)	C6—N2—C7—C8	178.5 (3)
C6—C1—C2—C3	0.2 (6)	C9—N3—C8—C7	114.0 (5)
N1—C1—C2—C3	−179.2 (4)	N4—N3—C8—C7	−69.8 (5)
C1—C2—C3—C4	−0.4 (6)	N1—C7—C8—N3	−23.6 (6)
C2—C3—C4—C5	0.1 (7)	N2—C7—C8—N3	157.4 (4)
C3—C4—C5—C6	0.3 (6)	C10—N5—C9—N3	0.7 (5)
C7—N2—C6—C1	0.7 (4)	Ag1[i]—N5—C9—N3	178.7 (3)
C7—N2—C6—C5	−179.5 (4)	N4—N3—C9—N5	−0.8 (5)
N1—C1—C6—N2	−0.5 (4)	C8—N3—C9—N5	175.8 (4)
C2—C1—C6—N2	180.0 (4)	N3—N4—C10—N5	0.0 (5)
N1—C1—C6—C5	179.6 (4)	C9—N5—C10—N4	−0.4 (5)
C2—C1—C6—C5	0.1 (6)	Ag1[i]—N5—C10—N4	−178.3 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O2	0.86	2.08	2.849 (6)	148