Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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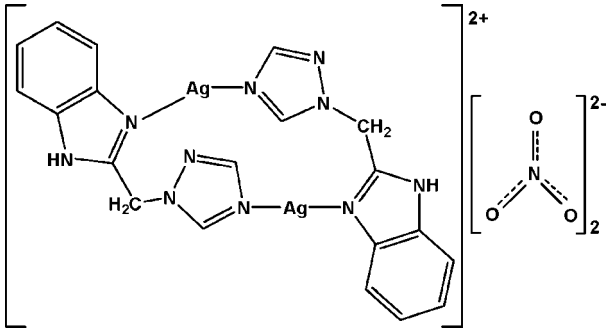
Received 8 November 2011; accepted 15 November 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.043; wR factor = 0.095; data-to-parameter ratio = 11.9.

In the title complex, bis{μ-1-[(1*H*-benzimidazol-1-yl)methyl]-1*H*-1,2,4-triazole}disilver(I) dinitrate, $[Ag_2(C_{10}H_9N_5)_2](NO_3)_2$, 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

$[Ag_2(C_{10}H_9N_5)_2](NO_3)_2$
M_r = 738.20
Monoclinic, $P2_1/c$
a = 9.4947 (19) Å
b = 13.569 (3) Å
c = 10.174 (2) Å
β = 114.56 (3)°
V = 1192.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.71 mm^{-1}
T = 293 K
0.19 × 0.17 × 0.14 mm

Data collection

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

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*B*···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*.

The authors thank the Science and Technology Department of Henan Province (082102330003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2136).

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supplementary materials

Acta Cryst. (2011). E**67**, m1788 [**doi:10.1107/S1600536811048501**]

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

Y. Wang, J. Zhang, H. Yang and X. Meng

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 $[Ag_2(C_{10}H_9N_5)_2](NO_3)_2$, (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 $[Ag_2(C_{10}H_9N_5)_2]$ with Ag1—$Ag1^{i}$ distance of 5.0179 (15) Å (symmetry code: (i) *-x*-1, *-y*+2, *-z*). $[Ag_2(C_{10}H_9N_5)_2]$ 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.

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.

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 $U_{iso}(H) = 1.2\ U_{eq}(C,N)$.

Figures

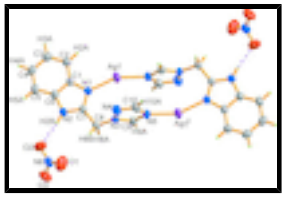


Fig. 1. View of the title complex showing labeling and 30% probability displacement ellipsoids. Hydrogen bonds are indicated by dashed lines. Symmetry code: *(i) -x* - 1, *-y* + 2, *-z*.

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 $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3140 reflections
$a = 9.4947$ (19) Å	$\theta = 2.4$–$27.9°$
$b = 13.569$ (3) Å	$\mu = 1.71$ mm^{-1}
$c = 10.174$ (2) Å	$T = 293$ K
$\beta = 114.56$ (3)°	Prism, colourless
$V = 1192.1$ (4) Å^3	0.19 × 0.17 × 0.14 mm
$Z = 2$	

Data collection

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

Refinement

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

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)

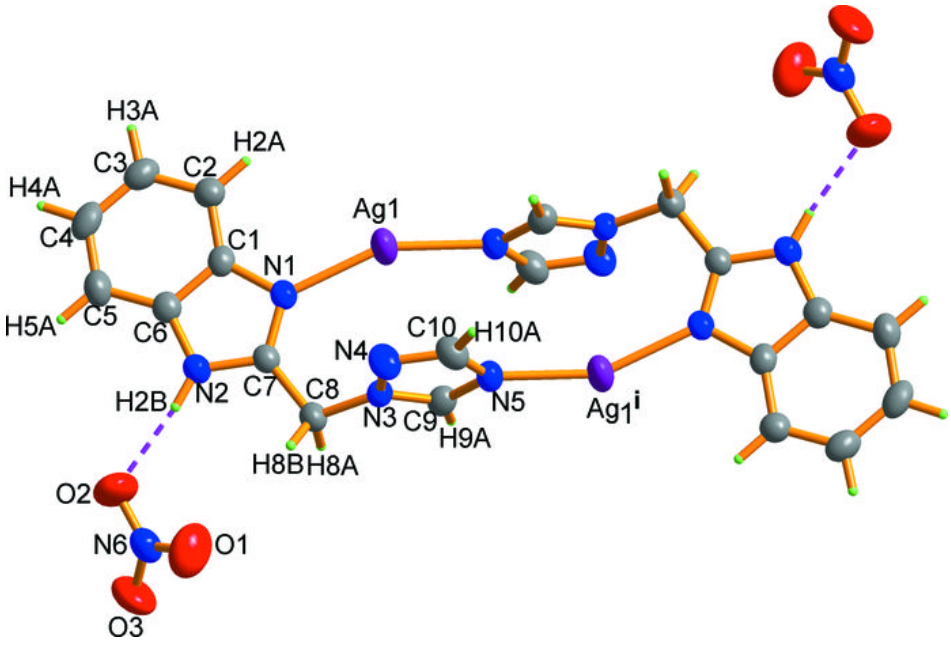
C10—N5—Ag1^{i}	131.1 (3)	N3—C8—C7	112.8 (3)
O3—N6—O1	118.6 (5)	N3—C8—H8A	109.0
O3—N6—O2	122.2 (5)	C7—C8—H8A	109.0
O1—N6—O2	119.1 (5)	N3—C8—H8B	109.0
C6—C1—N1	109.2 (4)	C7—C8—H8B	109.0
C6—C1—C2	121.1 (4)	H8A—C8—H8B	107.8
N1—C1—C2	129.7 (4)	N5—C9—N3	110.5 (4)
C3—C2—C1	116.5 (4)	N5—C9—H9A	124.8
C3—C2—H2A	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 codes: (i) −*x*−1, −*y*+2, −*z*.

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.

Fig. 1


H3A
H2A
C3
C2
H4A
Ag1
C4
C1
N1
H5A
C5
C6
C10
H10A
N4
H2B
N2
C7
C8
N3
C9
N5
Ag1i
H9A
H8B
H8A
O2
N6
O1
O3