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A triclinic polymorph of bis[μ-1-(2-pyridylmethyl)-1*H*-benzotriazole]bis[nitratosilver(I)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.040
wR factor = 0.087
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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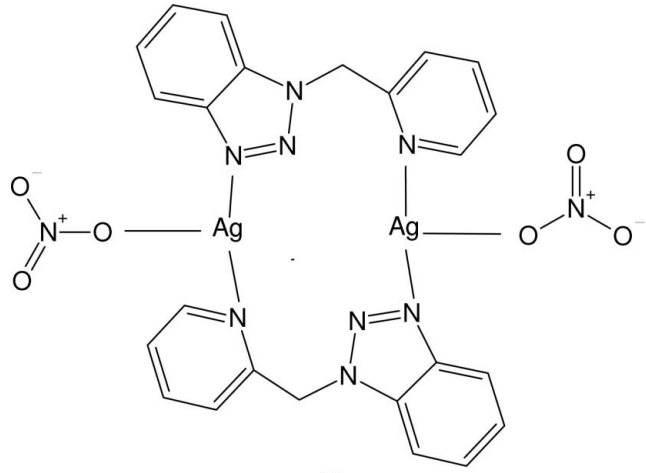
The title complex, $[Ag_2(NO_3)_2(C_{12}H_{10}N_4)_2]$, is a cyclic dimer containing a 14-membered centrosymmetric metallacyclic ring. The Ag atom is three-coordinated by two N atoms and one O atom. It complements the previously described monoclinic modification [Richardson & Steel (2003). *Dalton Trans*. pp. 992–1000] of the same phase.

Comment

In a search for new coordination polymers, our work has focused on the design and synthesis of some novel flexible hybrid ligands (Liu *et al.*, 2005). Recently, we obtained a heterocyclic ligand 1-(2-pyridylmethyl)benzotriazole (pybta) using benzotriazole and 2-picolyl chloride with the aid of polyethylene glycols (Evans & Lin, 2001). The reaction of pybta with silver nitrate then afforded the title compound, $[Ag(NO_3)(pybta)]_2$, (I).



(I)

Compound (I) is a cyclic dimer (Figs. 1 and 2) which is built up about a crystallographic centre of inversion, with a separation between the Ag atoms of 4.881 (3) Å. The Ag atom is three-coordinated by two ligand N atoms and one nitrate O atom in a distorted T-shape (Table 1). Due to the existence of the CH_2 spacer between the benzotriazole and pyridyl ring systems, there is sufficient flexibility for the pybta to be twisted to meet the silver coordination requirements; the resulting dihedral angle between the mean planes of these two ring systems is 64.02 (12)°. This means that the 14-membered dimetallocyclic ring in (I) is far from being planar. Such cyclic dinuclear complexes have been reported for a number of silver complexes of heterocyclic ligands in recent years, including a monoclinic polymorph of (I) (Richardson & Steel, 2003).

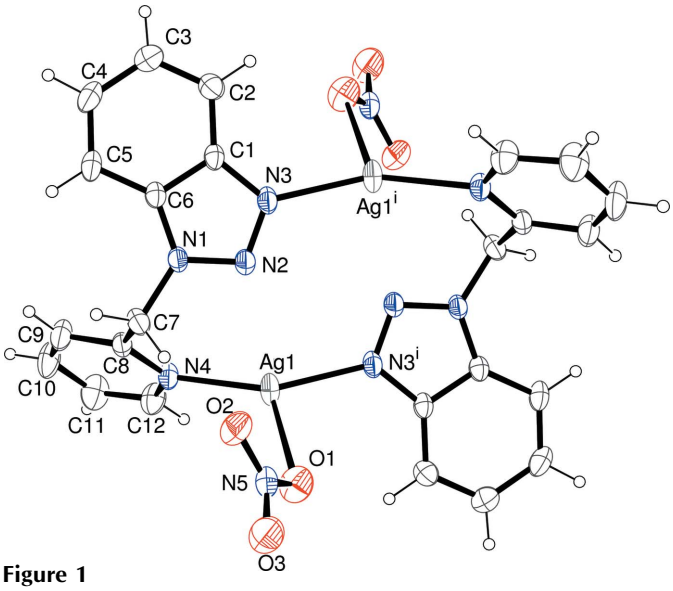


Figure 1
A view of the structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry code: (i) $1-x, 2-y, 2-z$.]

Experimental

A solution of pybta (0.021 g, 0.10 mmol) in MeOH (5 ml) was carefully layered on a solution of $AgNO_3$ (0.017 g, 0.10 mmol) in H_2O (5 ml). Diffusion between the two phases over a period of two weeks produced colourless block-shaped crystals, which were washed with water and ethanol several times and then dried in air.

Crystal data

$[Ag_2(NO_3)_2(C_{12}H_{10}N_4)_2]$
$M_r = 760.24$
Triclinic, $P\overline{1}$
$a = 8.914$ (5) Å
$b = 9.020$ (6) Å
$c = 9.505$ (6) Å
$\alpha = 109.898$ (8)°
$\beta = 101.234$ (3)°
$\gamma = 101.797$ (4)°
$V = 673.8$ (7) Å^3
$Z = 1$
$D_x = 1.873$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.51$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.808$, $T_{max} = 1.000$
(expected range = 0.694–0.860)
5247 measured reflections
3046 independent reflections
2412 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.087$
$S = 1.00$
3046 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 0.95P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}

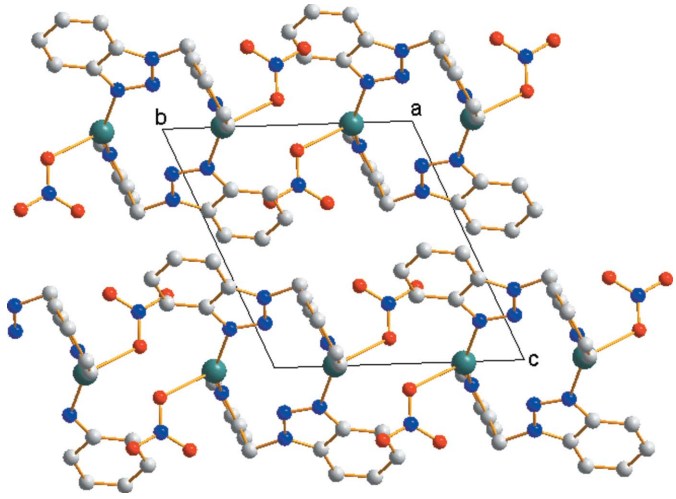


Figure 2
The packing of (I), viewed down [100]. H atoms have been omitted.

Table 1
Selected geometric parameters (Å, °).

Ag1—N3^i	2.199 (3)	Ag1—O1	2.558 (4)
Ag1—N4	2.218 (3)		
N3^i—Ag1—N4	148.45 (12)	N4—Ag1—O1	117.89 (11)
N3^i—Ag1—O1	93.29 (12)		

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

H-atom positions were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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