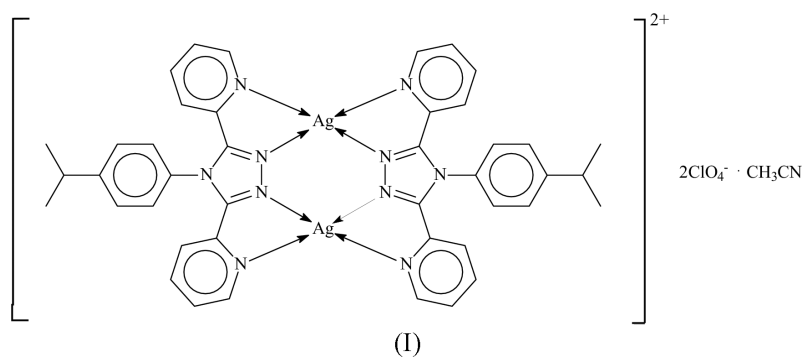


Bis[μ -3,5-bis(2-pyridyl)-4-(4-isopropylphenyl)-4H-1,2,4-triazole]disilver(I) diperchlorate acetonitrile solvate**Si-Chang Shao,^a Zhong-Lu You,^a
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Zhu^{a*} and Seik Weng Ng^b**^aDepartment of Chemistry, Fuyang Normal College, Fuyang, Anhui 236041, People's Republic of China, and ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, MalaysiaCorrespondence e-mail:
hailiang_zhu@163.com**Key indicators**Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
Disorder in solvent or counterion
 R factor = 0.053
 wR factor = 0.150
Data-to-parameter ratio = 15.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the centrosymmetric title compound, $[\text{Ag}_2(\text{C}_{21}\text{H}_{19}\text{N}_5)_2](\text{ClO}_4)_2 \cdot \text{CH}_3\text{CN}$, the N-heterocycle chelates to two Ag cations through its four Lewis basic atoms to confer a distorted square-planar environment for each metal atom. The perchlorate anion interacts weakly with the Ag atom at a distance exceeding 3.0 Å.

Comment

1,2,4-Triazoles having two *o*-pyridyl substituents in the 3,5-positions, as exemplified by 3,5-bis(2-pyridyl)-4-phenyl-1,2,4-triazole (Zhu *et al.*, 2000), represent a class of N-heterocycles that can function as a chelate to two metal atoms. A check of complexes in the Cambridge Structural Database (Version 5.25; Allen, 2002) gave eight examples, all of which, however, have the heterocycle chelating to only one metal atom. This feature is noted in the 4-tolyl derivative of bis(triphenylphosphine)silver perchlorate (Shao *et al.*, 1999). The Ag atom is sterically crowded, as it is coordinated by two bulky phosphine ligands. The ability of this class of triazoles to bind simultaneously to two metal atoms is now documented in the complex of the 4-isopropylphenyl derivative with silver perchlorate; the dinuclear compound crystallizes as an acetonitrile solvate, (I) (Fig. 1). The solvent molecule lies on a twofold axis and is thus disordered.



The dication lies on a centre of inversion. An examination of the twists of the pyridyl rings on the triazole ring relative to those in the parent heterocycle (Zhang *et al.*, 2005) shows that both pyridyl rings have been rotated in order to allow Lewis basic sites to interact. The ring that is involved in binding to atom Ag1 is twisted by 24.1 (3)° with respect to the five-membered ring and the twist is 33.4 (2)° for the other ring. The $\text{Ag}1/\text{N}2/\text{N}4/\text{Ag}1^i/\text{N}2^i/\text{N}4^i$ [symmetry code: (i) $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$] ring is buckled, and the disordered perchlorate group appears to fit into the folds of the buckled cation (Fig. 2) at a distance of > 3 Å.

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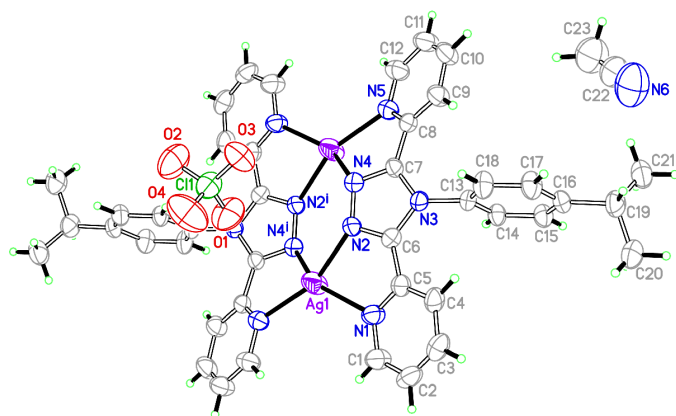


Figure 1
ORTEP (Johnson, 1976) plot, showing the numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii [symmetry code: (i) $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$]. Only one disorder component is shown for the perchlorate anion and for the acetonitrile molecule.

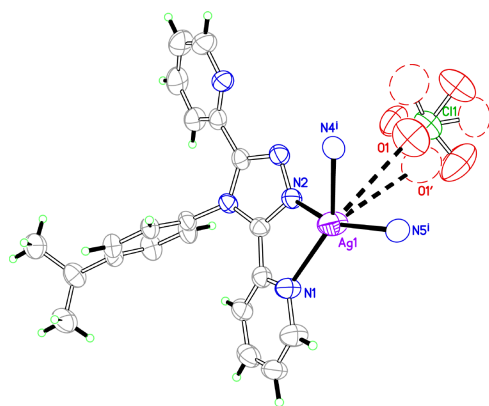


Figure 2
ORTEP (Johnson, 1976) plot, illustrating the distortion of the square-planar geometry of the Ag atom arising from the proximity of the disordered perchlorate anion.

Experimental

Silver perchlorate (0.10 mmol, 20.8 mg) and 3,5-bis(2-pyridyl)-4-isopropylphenyl-1,2,4-triazole (0.10 mmol, 34.1 mg) were dissolved in acetonitrile (10 ml) to give a colourless solution. The synthesis of the heterocycle has been reported elsewhere (Zhang *et al.*, 2005). Crystals separated from the solution, which was kept away from light, after 10 d. The compound was isolated in about 70% yield. Analysis calculated: C 46.4, H 3.6, N 13.5%; found: C 46.2, H 3.7, N 13.5%.

Crystal data

[Ag₂(C₂₁H₁₉N₅)₂](ClO₄)₂·C₂H₃N
M_r = 1138.52
 Monoclinic, C2/c
a = 15.830 (1) Å
b = 9.7850 (8) Å
c = 30.020 (2) Å
 β = 96.533 (2)°
V = 4619.7 (7) Å³
Z = 4

D_x = 1.637 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 2357 reflections
 θ = 2.5–21.6°
 μ = 1.03 mm⁻¹
T = 295 (2) K
 Block, colourless
 0.22 × 0.10 × 0.09 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
T_{min} = 0.313, *T_{max}* = 0.913
 13 366 measured reflections

5154 independent reflections
 3183 reflections with *I* > 2σ(*I*)
R_{int} = 0.048
 θ_{max} = 27.5°
h = −16 → 20
k = −12 → 12
l = −39 → 34

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.053
wR(*F*²) = 0.150
S = 1.00
 5154 reflections
 344 parameters

H-atom parameters constrained
w = 1/[σ²(*F_o*²) + (0.072*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.79 e Å⁻³
 Δρ_{min} = −0.58 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1–N1	2.371 (4)	Ag1–N4 ⁱ	2.396 (4)
Ag1–N2	2.300 (4)	Ag1–N5 ⁱ	2.284 (4)
N1–Ag1–N2	70.9 (1)	N2–Ag1–N4 ⁱ	100.6 (1)
N1–Ag1–N4 ⁱ	148.3 (1)	N2–Ag1–N5 ⁱ	159.2 (1)
N1–Ag1–N5 ⁱ	125.6 (1)	N4 ⁱ –Ag1–N5 ⁱ	71.9 (1)

Symmetry code: (i) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 1$.

In the heterocyclic ligand, the H atoms were placed in calculated positions [aromatic C–H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C); methine C–H = 0.98 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C); methyl C–H = 0.96 Å and *U*_{iso} = 1.5*U*_{eq}(C)], and were included in the riding-model approximation. Those on the acetonitrile molecule, which lies on a twofold axis, are disordered, and these were placed at calculated positions (C–H = 0.97 Å), with occupancies of 0.5 each and with *U*_{iso}(H) set at 1.5*U*_{eq}(C). The perchlorate anion is disordered, and this was refined as two partial anions whose occupancies refined to about 70 (1)/30 (1). The Cl–O distances were restrained to 1.44 (1) Å and the O···O distances were restrained to within 0.01 Å of each other. Additionally, the displacement parameters were restrained to be nearly isotropic. The anion had to be refined as two complete components, although atom Cl1 was only 0.3 Å from atom Cl1', as the attempt to force them to coincide led to a wide spread of Cl–O distances.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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