Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis[μ-N-(1,3,4-thiadiazol-2-yl)pyridine-3-carboxamide-κ^2N^1,N^3]disilver(I) bis(perchlorate)

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Received 20 March 2007
Accepted 2 April 2007

In the title compound, $[Ag_2(C_8H_6N_4OS)_2](ClO_4)_2$, each Ag^I center in the centrosymmetric dinuclear complex cation is coordinated by one pyridine N and a thiadiazole N atom of two inversion-related *N*-(1,3,4-thiadiazol-2-yl)pyridine-3-carboxamide ligands in an almost linear geometry [Ag—N = 2.187 (3) and 2.172 (3) Å, and N—Ag—N = 171.8 (1)°]. Weak Ag···Ag and Ag–perchlorate interactions, together with π–π stacking interactions, link the complex cations along the *a* axis to form a ribbon.

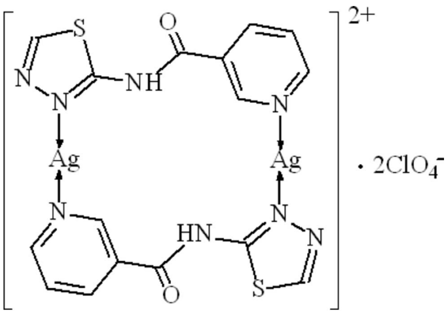
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.030
wR factor = 0.071
Data-to-parameter ratio = 13.3

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

Comment

1,3,4-Thiadiazole and its derivatives are versatile ligands that can bridge a variety of metal centers to form complexes with different structures and properties (Steel, 1990). In most cases, the ligand coordinates to the metal atom through the N—N azine group to form dinuclear complexes (Ferrer *et al.*, 1990; Tandon *et al.*, 1994; Sheppard *et al.*, 1996). The coordination properties may be changed by introducing substituent groups with donors. *N*-1,3,4-Thiadiazol-2-yl)pyridine-3-carboxamide (*L*) reacts with $AgClO_4$ to give a dinuclear complex, (I), without N—N azine coordination.



(I)

The asymmetric unit of (I) consists of one-half of the dimeric complex cation (Fig. 1), the other half being generated by an inversion center, and a perchlorate anion. Each Ag^I center is coordinated by one pyridine N and a thiadiazole N atom of two inversion-related *L* ligands in an almost linear geometry (Table 1). The Ag···Ag separation in the dimeric complex cation is 6.603 (2) Å.

The pyridine and thiadiazole rings of the *L* ligand are almost coplanar [dihedral angle is 9.6 (2)°], and thus the dimeric complex is approximately planar. The perchlorate anions lie on either side of the plane and weakly coordinate to Ag atoms, with Ag1···O3B and Ag1···O5 distances of 2.834 (3) and 2.923 (2) Å, respectively (Fig. 1). In addition, there are hydrogen-bonding interactions between O atoms of

doi:10.1107/S1600536807016066

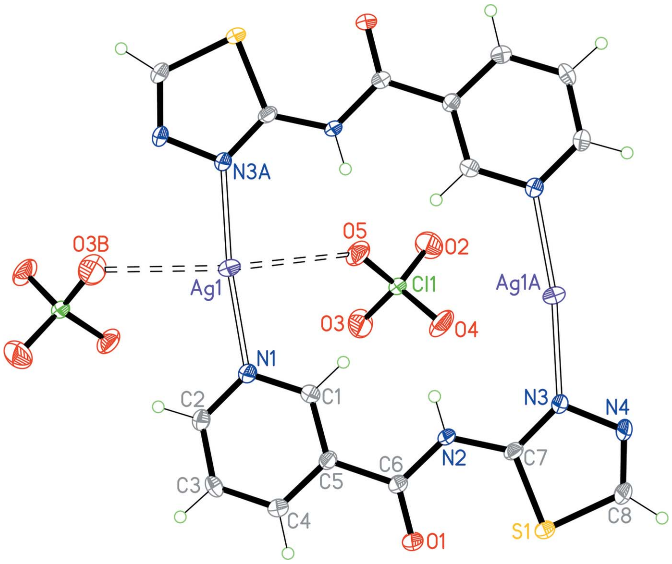


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level [symmetry codes: (A) $1 - x, 1 - y, 1 - z$; (B) $-x, 1 - y, 1 - z$].

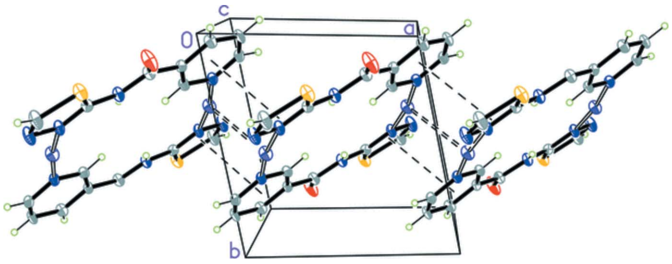


Figure 2
A view of the complex cations in (I), showing Ag···Ag weak interactions (dashed open lines) and π–π stacking interactions (dashed lines).

perchlorate anions and amido H atoms of the complex cations (Table 2).

In the crystal structure, dinuclear complex cations are held together by Ag···Ag($-x, 1 - y, 1 - z$) weak interactions (Table 1), π–π stacking interactions between the pyridine (centroid *Cg*1) and thiadiazole rings (centroid *Cg*2) [$Cg1\cdots Cg2(1 + x, y, z)$ = 3.650 (2) Å], and weak coordination of perchlorate anions (mentioned above) to form a ribbon along the *a* axis (Fig. 2).

Experimental

N-1,3,4-thiadiazol-2-yl)pyridine-3-carboxamid (*L*) was synthesized by the method of Hou *et al.* (2004). Single crystals of (I) suitable for X-ray analysis were obtained by diffusing a methanol solution (3 ml) of $AgClO_4$ (21 mg, 0.1 mmol) into a chloroform solution (3 ml) of *L* (21 mg, 0.1 mmol) using a methanol/chloroform mixed solution (4 ml, 1:1) as interlayer at room temperature. Colourless crystals were collected after one week (yield 50%). Analysis calculated for $C_8H_6AgClN_4O_5S$ (413.54): C 23.24, H 1.46, N 13.55%; found: C 23.01, H 1.55, N 13.48%.

Crystal data

$[Ag_2(C_8H_6N_4OS)_2](ClO_4)_2$
M_r = 827.10
Triclinic, $P\overline{1}$
a = 7.7234 (14) Å
b = 7.9089 (15) Å
c = 10.4790 (19) Å
α = 85.374 (3)°
β = 74.614 (3)°
γ = 76.403 (3)°
V = 599.74 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.10 mm^{-1}
T = 293 (2) K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.958, T_{max} = 1.000 (expected range = 0.656–0.685)
3416 measured reflections
2415 independent reflections
1994 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.071
S = 1.03
2415 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.187 (3)	O1—C6	1.204 (4)
Ag1—N3^i	2.172 (3)	N2—C6	1.376 (4)
Ag1···Ag1^{ii}	3.3170 (7)	N2—C7	1.368 (4)
N3^i—Ag1—N1	171.8 (1)		

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $-x, -y + 1, -z + 1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O5^i	0.86	2.14	2.910 (4)	149
N2—H2*B*···O4	0.86	2.52	2.981 (4)	114

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

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2 U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors thank Nankai University for supporting this work.

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