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Bis(μ-2,5-di-3-pyridyl-1,3,4-oxadiazole-κ^2N^2:N^5)-disilver(I) bis(trifluoromethanesulfonate)

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Key indicators

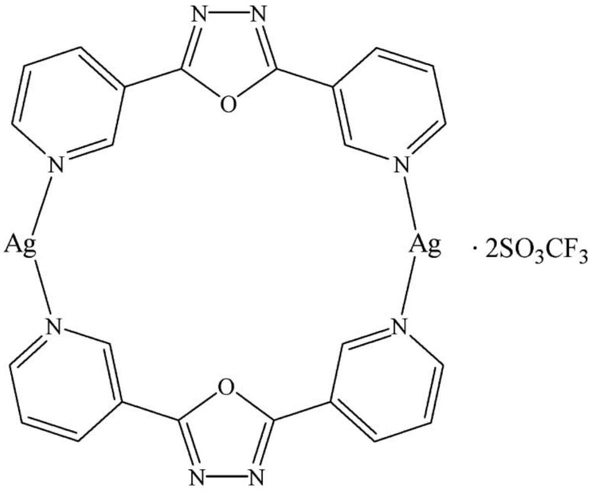
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.040
wR factor = 0.113
Data-to-parameter ratio = 11.6

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

The title centrosymmetric dinuclear macrocyclic complex, $[Ag_2(C_{12}H_8N_4O)_2](CF_3O_3S)_2$, has been synthesized from solution reactions of the new oxadiazole ligand 2,5-di-3-pyridyl-1,3,4-oxadiazole and $AgSO_3CF_3$. Weak O$\cdots$Ag and inter-macrocycle $Ag^I\cdots Ag^I$ interactions bind these macrocycles together into a one-dimensional structure.

Comment

Combining metal ions with oxadiazole ligands may result in coordination polymers with novel network connectivities (Dong *et al.*, 2003). Our interest in understanding the relationship between the metal coordination modes with such ligands led us to synthesize the title Ag^I complex shown in Fig.1.



(I)

The Ag^I center adopts a nearly linear $\{AgN_2\}$ coordination with two pyridyl N atoms. Two $SO_3CF_3{}^-$ anions are located above and below the centrosymmetric macrocycle plane and weakly coordinate to two Ag^I centers. These weak O$\cdots$Ag interactions bind these macrocycles together into a one-dimensional structure as shown in Fig. 2. The shortest inter-macrocycle $Ag^I\cdots Ag^I$ contact distance is 3.38 (8) Å.

Experimental

A solution of $AgSO_3CF_3$ (25.6 mg, 0.10 mmol) in MeOH (10 ml) was layered over a solution of 2,5-di-3-pyridyl-1,3,4-oxadiazole (25.2 mg, 0.10 mmol) in dichloromethane (10 ml). The solutions were left for about one week at room temperature, and colorless single crystals of (I) were obtained.

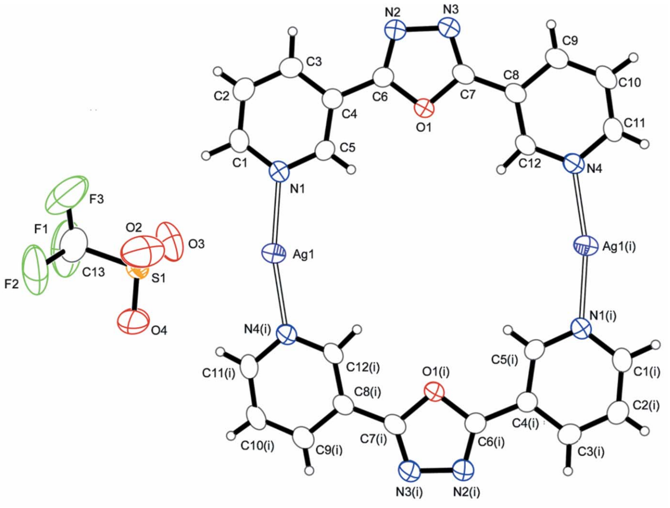


Figure 1
View of (I), showing 50% probability displacement ellipsoids. H atoms are shown as small circles of arbitrary radii. [Symmetry code: (i) $-x + 1$, $-y$, $-z + 2$.]

Crystal data

$[Ag_2(C_{12}H_8N_4O)_2](CF_3O_3S)_2$
$M_r = 962.35$
Triclinic, $P\overline{1}$
$a = 8.3112$ (14) Å
$b = 9.4620$ (16) Å
$c = 10.7660$ (18) Å
$\alpha = 75.293$ (2)°
$\beta = 79.256$ (2)°
$\gamma = 75.352$ (2)°
$V = 785.5$ (2) Å^3
$Z = 1$
$D_x = 2.034$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2803 reflections
$\theta = 2.6$–28.3°
$\mu = 1.48$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.38 × 0.22 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.603$, $T_{max} = 0.831$
4122 measured reflections
2725 independent reflections
2568 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0°$
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 11$
$l = -10 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.113$
$S = 1.00$
2725 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.5163P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.83$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

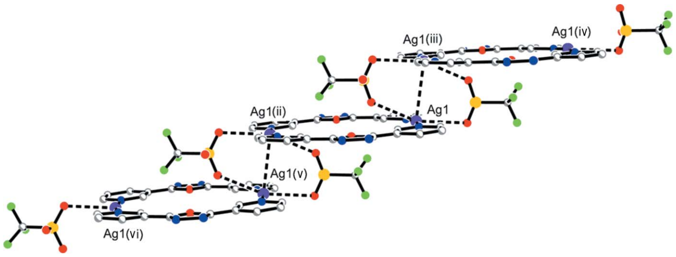


Figure 2
Packing diagram, showing weak O···Ag and $Ag^I\cdots Ag^I$ interactions in the one-dimensional structure. [Symmetry code: (ii) $-x + 1$, $-y$, $-z + 1$; (iii) $-x + 1$, $-y + 1$, $-z + 1$; (iv) x, $y + 1$, z; (v) x, $y - 1$, z; (vi) $-x + 1$, $-y - 1$, $-z + 1$.]

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.166 (3)	Ag1—Ag1^{ii}	3.3792 (8)
Ag1—N4^{iii}	2.167 (3)	Ag1—O3^{iii}	2.763 (6)
N1—Ag1—N4^{iii}	166.90 (12)	C1—N1—Ag1	123.9 (3)
N1—Ag1—Ag1^{ii}	90.05 (9)	C11—N4—Ag1^{iii}	121.8 (3)
N4^{iii}—Ag1—Ag1^{ii}	96.21 (10)	C12—N4—Ag1^{iii}	120.3 (3)
C5—N1—Ag1	118.4 (3)		

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

H atoms were included in calculated positions and refined as riding [C—H = 0.93 Å; $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5. A06). Bruker AXS Inc., Madison, Wisconsin, USA.
Dong, Y. B., Cheng, J. Y., Huang, R. Q., Smith, M. D. & zur Loye, H. C. (2003). *Inorg. Chem.* **42**, 5699–5706.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.

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