# metal-organic papers

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#### **Key indicators**

Single-crystal X-ray study T = 293 K Mean  $\sigma$ (C–C) = 0.005 Å R factor = 0.043 wR factor = 0.123 Data-to-parameter ratio = 13.5

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

# [8,8'-(Propane-1,3-diyldioxy)diquinoline- $\kappa^4 N, O, O', N'$ ]silver(I) trifluoromethane-sulfonate

Colourless prismatic crystals of the title compound,  $[Ag(C_{21}H_{18}N_2O_2)](CF_3O_3S)$ , form from ethanol solution of equivalent amounts of  $Ag(CF_3SO_3)$  and O,O'-bis(8-quinolyl)-1,5-dioxapentane [DPOQ; systematic name: 8,8'-(propane-1,3diyldioxy)diquinoline]. Building-block [Ag(DPOQ)] motifs and  $CF_3SO_3$  anions are connected *via* alternating weak C-H···O hydrogen-bond interactions into a three-dimensional network.

# Comment

Much interest has been shown during the last decade in the coordination chemistry of the lithium ion (Subramanian et al., 1995) since it has been successfully used in the treatment of manic depression, neurological and psychological disorder. O,O'-Bis(8-quinolyl)-1,5-dioxapentane (DPOQ) and its derivatives have been investigated for both transportation and quantitative estimation of lithium (Hiratani, 1987). In previous studies, we have used this highly flexible ligand with a long spacer,  $(CH_2)_6$ , O, O'-bis(8-quinolyl)-1,5-dioxaoctane (ODOQ; Cai et al., 2001). In those complexes, the high flexibility of ODOQ seemed to play an important role in the formation of single-strand double-helical structures. Very recently, we have obtained discrete single-strand helical complexes constructed by the ligand O, O'-bis(8-quinolyl)-1,8dioxaheptane (OHOQ), containing the non-restrained spacer (CH<sub>2</sub>)<sub>5</sub> (Cai et al., 2002). These findings prompted us to systematically investigate the influence of the spacers on fabricating new supramolecular structures. Herein we report the crystal structure of the title complex, (I).



The molecule of (I) consists of the  $CF_3SO_3^-$  anion and  $Ag(DPOQ)^+$  cation, which looks like a bat. Each silver(I) ion in the  $Ag(DPOQ)^+$  cation is coordinated by two imino N atoms and two O atoms of two 8-quinoline groups. The average Ag-N and Ag-O bond distances are 2.21 (3) and 2.56 (3) Å, respectively. The N-Ag-N and O-Ag-Oangles are 136.73 (8) and 72.09°, respectively. The environment of the silver(I) ion may be regarded as a tetrahedron. The  $CF_3SO_3^-$  anion does not bind to  $Ag^I$ , but is involved in the formation of intermolecular interactions through its O atoms. Each  $CF_3SO_3^-$  anion accepts weak  $C-H\cdots O$ hydrogen bonds from four neighboring  $Ag(DPOQ)^+$  cations, Received 14 October 2002 Accepted 21 November 2002 Online 30 November 2002

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 $D_r = 1.796 \text{ Mg m}^{-3}$ 

Cell parameters from 5699

Mo  $K\alpha$  radiation

reflections  $\theta = 4.8 - 55.0^{\circ}$ 

 $\mu=1.09~\mathrm{mm}^{-1}$ 

T = 293 (2) K

 $R_{\rm int}=0.065$ 

 $\theta_{\rm max} = 28.3^{\circ}$ 

 $h = -28 \rightarrow 29$ 

 $k = -17 \rightarrow 17$  $l = -13 \rightarrow 20$ 

Prism, pale yellow

 $0.28 \times 0.12 \times 0.10 \text{ mm}$ 

5118 independent reflections

3801 reflections with  $I > 2\sigma(I)$ 



# Figure 1

View of the title compound, with the atomic labelling. Displacement ellipsoids are drawn at the 30% probability level.



Figure 2

The three-dimensional coordination network in (I), viewed along the baxis.

with a mean C–O bond distance of 3.35 Å and C–H···O angle of 153° (Braga et al., 1998), thus forming a threedimensional network.

# Experimental

The title compound was prepared and characterized by a modification of the procedure of Cai et al. (2001). A solution of Ag(CF<sub>3</sub>SO<sub>3</sub>) (0.031 g, 0.12 mmol) in acetonitrile (10 ml) was added dropwise to a stirred solution of ligand DPOQ (0.04 g, 0.12 mmol) in MeOH (10 ml) at room temperature and the resulting mixture stirred for 30 min. Pale-yellow single crystals (0.06 g, 85%) were obtained from acetone by slow evaporation of the solvent. The assigned structure was substantiated by EA and MS data. Elemental analysis calculated for C<sub>22</sub>H<sub>18</sub>AgF<sub>3</sub>N<sub>2</sub>O<sub>5</sub>S: C 44.97, H 3.07, N 4.77%; found: C 44.85%, H 3.13, N 4.79% FAB-MS m/z (%): 588 (M<sup>+</sup> + 1, 68), 587 (M<sup>+</sup>, 56), 459  $(M^+ - C_9H_6N, 100), 330 (M^+ - Ag, 81).$ 

### Crystal data

[Ag(C21H18N2O2)](CF3O3S)  $M_{r} = 587.31$ Monoclinic, C2/c a = 21.9899 (11) Åb = 13.3576 (11) Å c = 15.2317 (10) Å $\beta = 103.828 (2)^{\circ}$  $V = 4344.4 (5) \text{ Å}^3$ Z = 8

### Data collection

Bruker SMART CCD area-detector diffractometer  $\varphi$  and  $\varphi$  scans Absorption correction: multi-scan (SADABS; Sheldrick, 1997)  $T_{\rm min}=0.664,\ T_{\rm max}=0.897$ 12912 measured reflections

# Refinement

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Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.068P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	+ 0.8339P]
$wR(F^2) = 0.123$	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{\rm max} = 0.001$
5118 reflections	$\Delta \rho_{\rm max} = 0.96 \ {\rm e} \ {\rm \AA}^{-3}$
380 parameters	$\Delta \rho_{\rm min} = -1.00 \text{ e} \text{ Å}^{-3}$
All H-atom parameters refined	Extinction correction: SHELXL97
	Extinction coefficient: 0.00076 (13)

All H atoms were located in a difference map and were refined isotropically. The range of C-H distances is 0.88 (4)-1.02 (4) Å.

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

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