metal-organic compounds

Acta Crystallographica Section C Crystal Structure Communications

ISSN 0108-2701

Bis(acridine-N)(nitrato-O,O')silver(I)

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Received 4 April 2000 Accepted 15 August 2000

The title complex, $[Ag(NO_3)(C_{13}H_9N)_2]$, is the first complex of silver and acridine to be reported. The silver coordination is distorted trigonal. The N-Ag-N angle involving the N atoms of the acridine ligands is 145.84 (6)°. The nitrate ion coordinates to silver as an asymmetrically chelating bidentate ligand. The crystal structure consists of neutral complex molecules linked into chains by means of attractive π - π interactions among the parallel acridine ligands.

Comment

Elucidation of the exact structure of adsorbate molecules on a metal surface is a crucial step in some applications of surfaceenhanced Raman scattering (SERS) (Moskovits, 1993). Comparison of the vibrational spectra of a metal-adsorbate synthetic complex and the SERS spectra of a molecule adsorbed on a metal surface yields useful information about the orientation of the adsorbate in the SERS system (Vlckova *et al.*, 1993). In our studies, we are dealing with the incorporation of acridine (acr) into Ag-colloid–acridine systems (Michl & Sloufova, 2000). As no structure data for acridine-silver complexes were available, the novel complex [Ag(acr)₂-(NO₃)], (I), was prepared and characterized by X-ray diffraction analysis.



The silver coordination is distorted trigonal. The nitrate ion coordinates to silver as an asymmetrically chelating bidentate ligand; the Ag-O2D and Ag-O3D distances are 2.627 and 2.558 Å, respectively. Defining dummy atom D3 as situated at the centre of gravity of O2D and O3D, the coordination sphere may be defined by D3 and the acridine N1A and N1B atoms. The N1A-Ag-N1B angle is increased from an ideal value of 120° to 145.84 (6)°; angles N1A-Ag-D3 and

N1*B*-Ag-*D*3 are decreased to 101.01 and 111.07°, respectively.

Neutral molecules of complex (I) are linked into chains running parallel to [101]. The chains are generated by the



Figure 1

The asymmetric unit of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

action of inversion centres. Linkage is realised by attractive π - π interactions (Desiraju, 1995) among the planar acridine ligands. These interactions are similar to those found between the layers of graphite (Wyckoff, 1965). Acridine molecule A (atoms N1A to C14A) interacts with another acridine molecule A generated by (-x + 1, -y, -z + 2), as shown in Fig. 2. As the two molecules are related by translations and inversion only, the two interacting planar molecules are parallel, the distance between the planes being 3.326 (2) Å.





Acridine molecule *B* (atoms N1*B* to C14*B*) interacts with another acridine molecule *B* generated by (-x, -y, -z + 1). The two molecules are exactly parallel, for the same reasons as discussed above, and the distance between them is 3.343 (3) Å. There are two such [101] chains in the unit cell, which corresponds to two molecules per unit cell.

Examination of the structure with *PLATON* (Spek, 1990) showed that there are no solvent-accessible voids in the crystal lattice.

The structure of the analogous complex with the same ligands and Cu as the central metal atom has been reported (Kuroda-Sowa *et al.*, 1995).

Experimental

Yellow-brown crystals of (I) were obtained by mixing a water solution of AgNO₃ ($4.2 \times 10^{-2} M$) and a dioxane solution of acridine ($4.2 \times 10^{-2} M$) in an equimolar ratio. Crystals of (I) suitable for X-ray analysis appeared over a period of two days. No recrystallization was necessary.

Crystal data

$[Ag(NO_3)(C_{13}H_9N)_2]$
$M_r = 528.30$
Triclinic, P1
a = 9.128 (3) Å
b = 10.096 (2) Å
c = 11.763 (2) Å
$\alpha = 108.19 \ (1)^{\circ}$
$\beta = 91.93 \ (2)^{\circ}$
$\gamma = 94.23 \ (2)^{\circ}$
V = 1025.2 (4) Å ³
Z = 2

Data collection

Enraf-Nonius CAD-4 diffract-
ometer
Background-peak-background
scans
Absorption correction: spherical
(JANA2000; Petricek & Dusek,
2000)
$T_{\min} = 0.793, T_{\max} = 0.797$
3593 measured reflections

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.020$ $wR(F^2) = 0.056$ S = 1.1923593 reflections 335 parameters H atoms treated by a mixture of independent and constrained refinement $D_x = 1.711 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation Cell parameters from 25 reflections $\theta = 12-13^{\circ}$ $\mu = 1.020 \text{ mm}^{-1}$ T = 150 (2) KPrism with strongly rounded edges, translucent intense brown $0.20 \times 0.15 \times 0.15 \text{ mm}$

3593 independent reflections 3466 reflections with $I > 2\sigma(I)$ $\theta_{\text{max}} = 24.98^{\circ}$ $h = 0 \rightarrow 10$ $k = -11 \rightarrow 11$ $l = -13 \rightarrow 13$ 3 standard reflections frequency: 60 min intensity decay: none $w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.7513P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.002$ $\Delta\rho_{\text{max}} = 0.58 \text{ e} \text{ Å}^{-3}$ $\Delta\rho_{\text{min}} = -0.72 \text{ e} \text{ Å}^{-3}$

Extinction correction: *SHELXL*97 (Sheldrick, 1997)

Extinction coefficient: 0.0035 (7)

Data collection was carried out at 150 K, as the crystals decay rapidly under X-rays at room temperature. The H atoms were clearly

Table 1

Selected geometric parameters (Å, °).

Ag-N1B	2.216 (2)	Ag-O2D	2.627 (2)
Ag-N1A	2.226 (2)	Ag-O3D	2.558 (2)
N1B-Ag-N1A	145.84 (6)	N1B - Ag - O2D	101.09 (6)
N1B - Ag - O3D	117.72 (6)	N1A - Ag - O2D	103.64 (6)
N1A - Ag - O3D	96.31 (6)		

visible in the difference Fourier maps; they were set to calculated positions and their X-H distances (where X is the relevant heavy atom) and isotropic displacement parameters were refined.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *JANA*2000 (Petricek & Dusek, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1990).

Financial support through GACR 203/97/0242, GACR 203/ 1999/0242 and grant 1830/2000 awarded by GA of the Board of Universities (FRVS) is gratefully ackowledged.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1049). Services for accessing these data are described at the back of the journal.

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