metal-organic compounds

(Acridine-*N*)trichlorogold(III)

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The title compound, $[AuCl_3(C_{13}H_9N)]$, is the first complex of gold and acridine to be reported. The coordination sphere of the Au atom is square planar. The crystal structure is built up of neutral complex molecules linked into chains by means of attractive π–π interactions between the parallel acridine ligands.

Comment

Single crystals of the title complex, (I), were prepared in order to obtain an insight into the vibrational spectra of the molecule and, subsequently, to compare these spectra of (I) with the SERS (surface-enhanced Raman scattering) spectra of the ligand adsorbed onto colloidal gold (Jeong *et al.*, 2000; Muniz-Miranda, 2000). This work is part of our project on the comparison of synthetic metal–ligand complexes (where the metal is Ag, Au, Pd or Pt and the ligand is an N-containing organic base) with analogous SERS systems (Srnova *et al.*, 1997, 1999). Having searched the Cambridge Structural Database (Allen & Kennard, 1993), we have found that (I) is the first complex of gold and acridine to be reported.

(I)
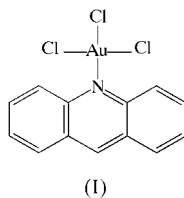
The coordination of the Au atom in (I) is square planar, formed by the three Cl atoms and the N1 atom of the acridine (acr) ligand (Fig. 1). The relevant distances and angles are summarized in Table 1.

The angle between the plane formed by the acr ligand and that given by the Au coordination sphere (Au/Cl1/Cl2/Cl3/N1) is 77.53 (8)°, which differs from the ideal value of 90°. This is due to π–π interactions between parallel acr ligands, which will be discussed below. If the angle were 90°, the Cl atoms of adjacent complex molecules would be too close to each other, and this would hinder the π–π interactions.
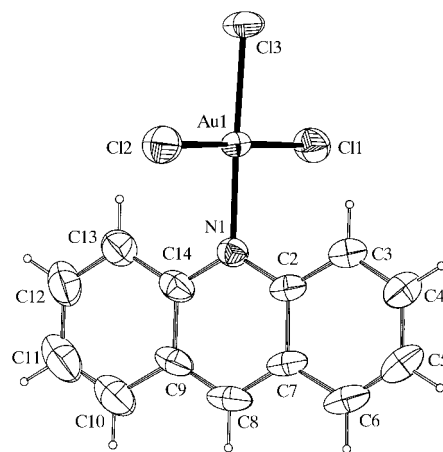
Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Neutral molecules of (I) are linked into chains running parallel to [100]. The linkage is realised by π–π interactions (Desiraju, 1995) between the planar acr ligands. As there is just one acr ligand per asymmetric unit and the space group $P\bar{1}$ is generated by inversions and translations only, all the planes defined by the planar acr ligands are exactly parallel, *i.e.* the π–π interacting acr molecules are always parallel due to the space-group symmetry. Two types of π–π interaction found in the crystal structure of (I) are shown in Fig. 2. In type (i), the interaction between the acr ligand at (x, y, z) and that
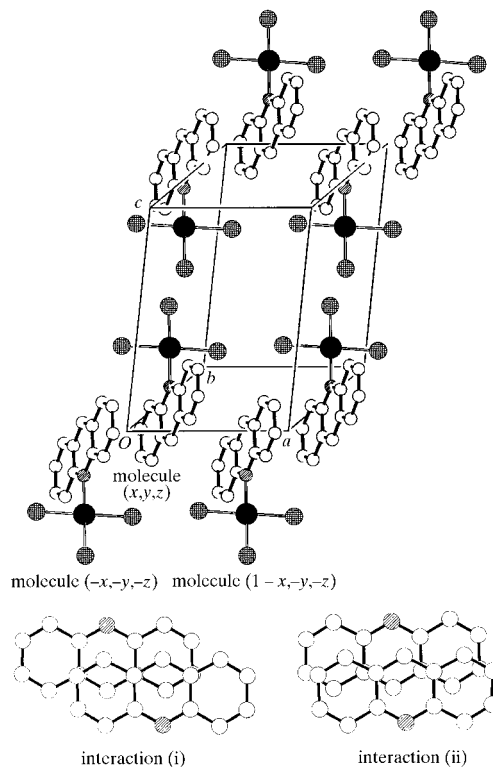
Figure 2
The scheme of attractive π–π interactions between acridine ligands in (I).

generated by $(-x, -y, -z)$ is, from the point of view of geometry, similar to the interaction found between the layers in graphite (Wyckoff, 1965). In type (ii), the interaction between the acr ligand at (x, y, z) and that generated by $(1 - x, -y, -z)$ is somewhat different, the molecules being mutually shifted, as shown in Fig. 2. In both cases, the interacting ligands exhibit a parallel-displaced geometry connected *via* a slightly attractive interaction (Hunter & Sanders, 1990; Hobza *et al.*, 1994). The distances between the parallel planes are 3.460 (7) Å for interaction (i) and 3.620 (7) Å for interaction (ii).

Examination of the structure with *PLATON* (Spek, 1990) showed that there are no solvent-accessible voids in the crystal lattice. The structure of an analogous complex, with the same ligands as (I) and with Cu as the central metal atom, has been reported by Healy *et al.* (1985).

Experimental

Orange crystals of (I) were obtained by mixing equimolar amounts of $HAuCl_4\cdot 3H_2O$ in water (0.04 *M*) and acridine in dioxane (0.04 *M*). Within 3 h, thin needle crystals appeared and these were filtered off. Prismatic crystals of (I) suitable for X-ray analysis grew from the mother liquor over a period of 2 d. No recrystallization was necessary.

Crystal data

$[AuCl_3(C_{13}H_9N)]$	$Z = 2$
$M_r = 482.53$	$D_x = 2.342$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.6207$ (4) Å	Cell parameters from 3668
$b = 9.5869$ (5) Å	reflections
$c = 10.6829$ (5) Å	$\theta = 1$–25°
$\alpha = 71.115$ (3)°	$\mu = 11.316$ mm^{-1}
$\beta = 84.066$ (3)°	$T = 293$ (2) K
$\gamma = 67.921$ (2)°	Prism, dark orange
$V = 684.16$ (6) Å^3	$0.21 \times 0.11 \times 0.06$ mm

Data collection

Nonius KappaCCD diffractometer	2229 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.032$
Absorption correction: Gaussian	$\theta_{max} = 25.06°$
(*NUMERIC*; Nonius, 1999)	$h = 0 \rightarrow 9$
$T_{min} = 0.102$, $T_{max} = 0.546$	$k = -10 \rightarrow 11$
5224 measured reflections	$l = -12 \rightarrow 12$
2413 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0142P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.025$	$+ 0.3962P]$
$wR(F^2) = 0.059$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.094$	$(\Delta/\sigma)_{max} = 0.034$
2413 reflections	$\Delta\rho_{max} = 0.99$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -1.20$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	(Sheldrick, 1997)
	Extinction coefficient: 0.0058 (5)

Because of the presence of the Au atom in (I), application of the proper absorption correction was the crucial step in the data reduction. Several types of absorption correction were tried. The best results were achieved with a numerical absorption correction based on indexed crystal faces. H atoms were clearly visible in the difference electron-density map. They were set at calculated positions, with a C—H distance of 0.93 Å, and their isotropic displacement parameters were set equal to $1.2U_{eq}$ of the parent atom. The deepest hole in the final difference electron-density map was found 0.98 Å from the Au1 atom.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; 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); software used to prepare material for publication: *SHELXL*97.

Table 1
Selected geometric parameters (Å, °).

Au1—N1	2.056 (4)	Au1—Cl1	2.2745 (13)
Au1—Cl3	2.2588 (13)	Au1—Cl2	2.2751 (14)
N1—Au1—Cl3	177.13 (13)	N1—Au1—Cl2	89.64 (12)
N1—Au1—Cl1	89.61 (12)	Cl3—Au1—Cl2	90.12 (6)
Cl3—Au1—Cl1	90.57 (5)	Cl1—Au1—Cl2	178.57 (6)

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