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Bis{2-[(2-hydroxyethyl)iminomethyl]phenolato}gold(III) tetrachloroaurate(III)

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The title compound, $[Au^{III}(C_9H_{10}NO_2)_2][Au^{III}Cl_4]$, contains $[Au^{III}(C_9H_{10}NO_2)_2]^+$ cations and $[Au^{III}Cl_4]^-$ anions with each of the gold(III) ions in a typical four-coordinate square-planar geometry. Both gold(III) metal centers are located on inversion centers.

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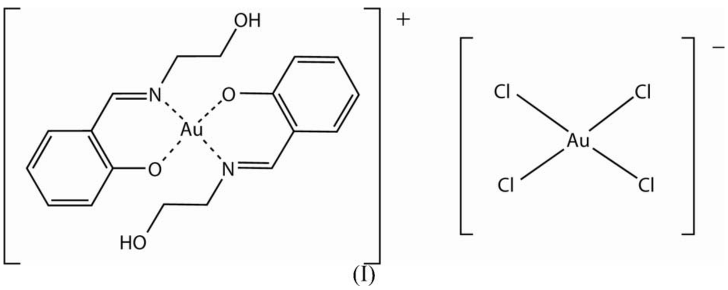
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.008 Å
R factor = 0.059
wR factor = 0.171
Data-to-parameter ratio = 14.8

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

Comment

The Schiff base ligand 2-[(2-hydroxyethyl)iminomethyl]phenol (H_2Sae, also called salicylidene-2-ethanolamine) has previously been incorporated into a number of polynuclear transition metal complexes, since this polydentate ligand has the ability to function both as a chelating and as a bridging ligand after deprotonation (Boskovic *et al.*, 2002, 2004; Gu *et al.*, 2004; Hecht *et al.*, 2004; Nihei *et al.*, 2003; Sieber *et al.*, 2005; Zhang *et al.*, 2005). Only a few Schiff base complexes of gold(III) have been reported in the literature, since gold(III) is rather unstable towards reduction and it can easily undergo hydrolysis (Barnholtz *et al.*, 2001; Dar *et al.*, 1992; Inazu, 1966). Nevertheless, soluble and kinetically stable Schiff base gold(III) complexes are of interest, *e.g.* for their potential use in radiotherapy and as active hydrogenation catalysts (Barnholtz *et al.*, 2001; Comas-Vives *et al.*, 2006). Because gold(III) and platinum(II) are isoelectronic, complexes of gold have also been evaluated as potential anticancer agents (Shaw, 1999).



(I)

The title compound, $[Au^{III}(C_9H_{10}NO_2)_2][Au^{III}Cl_4]$, (I), contains $[Au^{III}(C_9H_{10}NO_2)_2]^+$ cations and $[Au^{III}Cl_4]^-$ anions. Both Au^{III} ions are located on inversion centers [Wyckhoff positions 1c (Au1) and 1g (Au2)]. The molecular structure of (I) is shown in Fig. 1, and selected bond length and angles are given in Table 1. In the $[Au^{III}Cl_4]^-$ anion, four chloride ions are coordinated to gold(III). The gold(III)–chloride distances are 2.2798 (13) and 2.2829 (13) Å, giving a slightly distorted square-planar geometry. In the $[Au^{III}(HSae)_2]^+$ cation, two monodeprotonated salicylidene-2-ethanolamine ligands, $HSae^-$, are coordinated to gold(III) (see Fig. 1). The ligand acts as a bidentate ligand; the hydroxyethyl function is, in

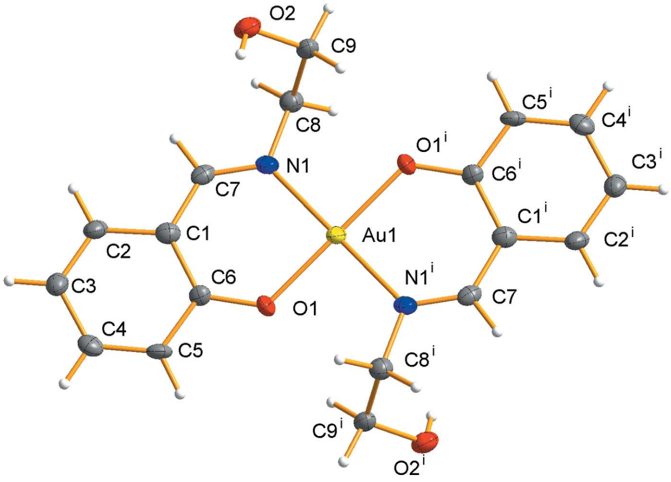


Figure 1
The cation $[Au^{III}(HSae)_2]^+$ of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-1+x, y, 1+z$.]

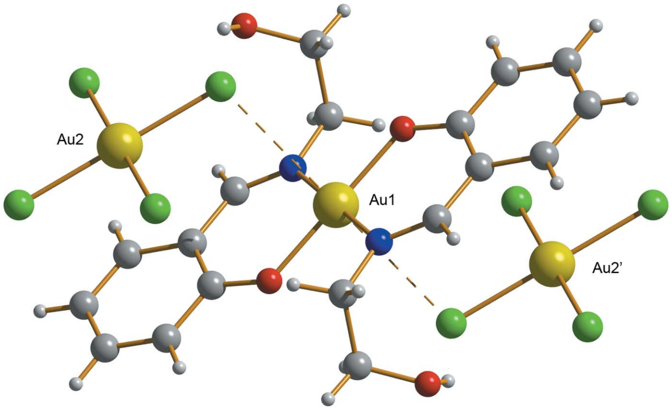


Figure 2
Weak Au···Cl interactions (dashed lines) between $[Au^{III}(HSae)_2]^+$ cations and $[AuCl_4]^-$ anions.

contrast to other reported complexes with transition metals, not involved in the coordination to the metal ion. The Au—N and Au—O distances are 2.051 (6) and 1.978 (4) Å, respectively. The AuN_2O_2 unit has a slightly distorted square-planar geometry. Perpendicular to this plane, weak contacts from the gold(III) metal center to chlorides of the tetrachloroaurate anion can be found at about 3.37 Å, which complete the coordination environment of Au11 as an elongated, distorted octahedron (Fig. 2). Considering these weak contacts, the stacking of cations and anions results in a two-dimensional chain along [001].

Experimental

The ligand H_2Sae was synthesized by reacting salicylaldehyde (12.2 g, 10 mmol) with ethanolamine (6.1 g, 10 mmol) in ethanol (50 ml) under reflux for 1 h. The solvent was evaporated under reduced pressure to give a yellow oil. $[Au^{III}(C_9H_{10}NO_2)_2][Au^{III}Cl_4]$ was synthesized by adding a solution of $NaAuCl_4\cdot 2H_2O$ (0.2 g, 0.503 mmol) in 20 ml of absolute ethanol to a stirred solution of H_2Sae (0.164 g, 1 mmol) in 20 ml of ethanol. The mixture was stirred at 323 K for 1 h. After the mixture was cooled to room temperature, it was placed overnight in a refrigerator at 277 K. Dark-red crystals were precipitated, collected by filtration, washed with cold ethanol and chloroform, and dried in a desiccator.

Crystal data

$[Au(C_9H_{10}NO_2)_2][AuCl_4]$
$M_r = 864.10$
Triclinic, $P\overline{1}$
$a = 8.2088$ (3) Å
$b = 8.7386$ (3) Å
$c = 8.9678$ (3) Å
$\alpha = 107.490$ (2)°
$\beta = 104.690$ (2)°
$\gamma = 107.429$ (2)°

$V = 542.05$ (4) Å^3
$Z = 1$
$D_x = 2.647$ Mg m^{-3}
Cu $K\alpha$ radiation
$\mu = 29.88$ mm^{-1}
$T = 100$ (2) K
Plate, red
0.3 × 0.3 × 0.1 mm

Data collection

Bruker SMART 6000 diffractometer
ω and φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
$T_{min} = 0.025$, $T_{max} = 0.416$

8454 measured reflections
2065 independent reflections
1806 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 71.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.171$
$S = 1.11$
2065 reflections
140 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1334P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 3.74$ e Å^{-3}
$\Delta\rho_{min} = -3.69$ e Å^{-3}

H atoms were refined in the riding mode with constrained X—H distances (C—H = 0.95 and 0.99 Å, and O—H = 0.84 Å) and isotropic displacement parameters fixed at 1.2 times U_{eq} of the parent C atoms and 1.5 times U_{eq}(O) for atom H2*A*. The highest peak and deepest hole in the final difference map are located 1.19 and 0.84 Å, respectively, from atom Au1.

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: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003).

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