A potassium crown ether complex with dichloroaurate(I)

The title compound, (1,4,7,10,13,16-hexaoxacyclooctane)-potassium dichloroaurate(I), [K(C₁₂H₂₄O₆)][AuCl₂], consists of potassium ion encapsulated by the 18-membered crown ether 1,4,7,10,13,16-hexaoxacyclooctane and a linear dichloroaurate(I) monoanion. The potassium occupies a crystallographic center of symmetry with a ring coordination number of six, and two chlorides in axial sites at a distance of 3.2306 (5) Å. The linear anionic species sits on another crystallographic center of symmetry.

Comment

Although cations are the dominant species in the coordination chemistry of crown ethers, the counter-anions can also play an important role in the binding mode, cation–anion pairing, and the geometry of the structure (Bajaj & Poonia, 1988). Current interests of a number of researchers are thus also focused on the coordination chemistry of anions (Bianchi et al., 1997). Our interests in this area involve exploring dual host receptors (Kavallieratos et al., 2000; Qian et al., 2001), extending previous work to anionic metal complexes.

The formula unit of (I) is shown in Fig. 1. The linear dichloroaurate(I) and the 18-crown-6 potassium complex form infinite alternating cation/anion layers, separated by 3.9618 (2) Å, along the b axis (Fig. 2).

The crown ether adopts D₃d symmetry, as observed in most other complexes of 18-crown-6 (Dunitz et al., 1974). The potassium ion is located at the center of the crown and is coordinated to the six O atoms with an average K—O bond distance of 2.810 Å, which is consistent with previously reported results (2.801 Å; Seiler et al., 1974). The linear dichloroaurate anions sit above and below the plane of the crown ether, with one of the Cl atoms closer to the potassium [3.2306 (5) Å] than is the gold [3.9618 (2) Å]. The presence of two chlorides approximately above and below the potassium ion thus completes a pseudo-hexagonal bipyramidal coordination sphere for the alkali metal ion.
Equimolar amounts (0.065 mmol each) of 18-crown-6 and potassium tetrachloroaurate(III) were dissolved in methanol. Single crystals of the reduced gold complex with the potassium crown ether complex were grown by diffusion of diethyl ether into the methanolic solution of the mixture. $^1$H NMR (500 MHz, CDCl$_3$, TMS): $\delta$ 3.66 (t, CH$_2$). $^{13}$C NMR (125 MHz, CDCl$_3$, TMS): $\delta$ 70.4 (CH$_2$). MS (FAB): m/z 303 (18C6 + K)$^+$. 

Crystal data

$[\text{K(C}_{12}\text{H}_{24}\text{O}_6)][\text{AuCl}_2]$  

$M_r = 571.28$  

Monoclinic, $P 2_1/n$  

$a = 8.7583$ (4) Å  

$b = 7.9237$ (4) Å  

$c = 13.8393$ (6) Å  

$\beta = 103.785$ (2)°  

$V = 932.76$ (8) Å$^3$  

$Z = 2$  

$D_x = 2.034$ Mg m$^{-3}$  

Mo $K\alpha$ radiation  

Cell parameters from 4929 reflections  

$\theta$ range $= 3.0$–30.5°  

$\theta$ max = 8.42 mm$^{-1}$  

$T = 100$ (2) K  

Prism, colorless  

0.310 x 0.160 x 0.110 mm

Data collection

Bruker APEX diffractometer  

Absorption correction: multi-scan  

(SADABS; Sheldrick, 1996; Blessing, 1995)  

$T_{\text{min}} = 0.180$, $T_{\text{max}} = 0.458$  

7528 measured reflections

Refinement

Reﬁnement on $F^2$  

$R(F^2 > 2\sigma(F^2)) = 0.017$  

$wR(F^2) = 0.047$  

$S = 1.04$  

2470 reflections  

103 parameters  

H-atom parameters constrained

Crystal decay was determined by remeasuring the first 50 frames of data at the end of data collection and comparing the intensities from the first and last runs. All H atoms were constrained with a riding model. Residual peaks $> 0.5$ e Å$^{-3}$ and troughs $< 0.5$ e Å$^{-3}$ were near the Au and K atoms.

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

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References