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Key indicators

Single-crystal X-ray study

T = 150 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.018

wR factor = 0.038

Data-to-parameter ratio = 31.2

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.(1,4,7,10,13,16-Hexaoxacyclooctadecane)-
potassium dithiocyanatoaurate(I)

In the title compound, $[\text{K}(\text{C}_{12}\text{H}_{24}\text{O}_6)][\text{Au}(\text{SCN})_2]$, the Au^{I} atom is in a linear configuration with respect to the coordinating S atoms. The encapsulation of the K^+ ion by the 18-crown-6 ligand produces a large cation and prevents $\text{Au} \cdots \text{Au}$ interactions within the extended structure. Both Au and K occupy inversion centers.

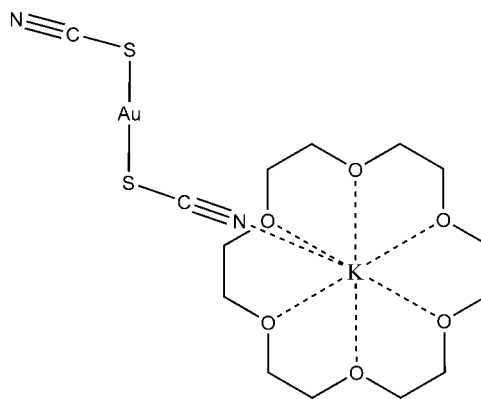
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Comment

We have reported the crystal structures of the alkali (K^+ , Rb^+ and Cs^+), NMe_4^+ , NBU_4^+ and PPh_4^+ salts of bis(thiocyanato)aurate(I) (Coker *et al.*, 2004). Recently, we have isolated and structurally characterized the NH_4^+ salt of this anion (Bedel *et al.*, 2004). It has been established that these compounds form monomers, dimers or polymeric chains of Au atoms. The formation and polymer propagation are related to the size of the counter-ion in the system. In the present work, the structure of the title compound, (I), is reported.



(I)

The geometry of the $\text{Au}(\text{SCN})_2^-$ (Fig. 1) anion in (I) is similar to that of the same species in tetraphenylphosphonium bis(thiocyanato)aurate(I) (Coker *et al.*, 2004) and tetraphenylarsonium bis(thiocyanato)aurate(I) (Schwerdferger *et al.*, 1990), which have larger counter-ions. The Au and K atoms of (I) lie on inversion centers, at $(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(0, 0, 0)$, respectively. The angles and distances that apply to the bis(thiocyanato)aurate(I) anion compare reasonably with the referenced complexes. Because of the symmetry of the $P\bar{1}$ space group, the $\text{C}-\text{S} \cdots \text{S}-\text{C}$ torsion angle is 180° . Tetraphenylarsonium bis(thiocyanato)aurate(I) has an $\text{Au}-\text{S}$ distance of 2.295 (5) \AA and $\text{Au}-\text{S}-\text{C}$, $\text{S}-\text{Au}-\text{S}$ and $\text{S}-\text{C}-\text{N}$ angles of 100.9 (4), 180.0 (10) and 175.9 (12) $^\circ$, respectively. Tetraphenylphosphonium bis(thiocyanato)aurate(I) has corresponding distances and angles of 2.294 (2) \AA , and 101.2 (2), 180.0 and 175.6 (7) $^\circ$.

The extended structure of (I) contains a zigzag polymeric chain of anions and cations (Fig. 2). This polymeric chain is formed by the coordination of the N atom of the thiocyanate to the vacant coordination sites on the K atom, making the K atom eight-coordinate. A similar type of configuration is seen for various crown-ether compounds with alkali cations (Steed, 2001) and, in particular, [K(18-crown-6)][Ag(CN)₂] (Schlueter & Geiser, 2003). The distances of the K···N interactions for the Ag complex are 2.860 (2) and 2.856 (2) Å, while for (I) the distance is 2.8699 (19) Å.

Experimental

Potassium bis(thiocyanato)aurate(I) was prepared following the method described by Coker *et al.* (2004). The complex was prepared by mixing 10 mM acetonitrile solutions of potassium bis(thiocyanato)aurate(I) (2 ml) and 1,4,7,10,13,16 hexaoxacyclooctadecane (18-crown-6 ether) (2 ml). The mixed solution was stirred for 30 min and filtered. Crystals were obtained as colorless plates by slow diffusion of diethyl ether into an acetonitrile solution at 277 K.

Crystal data

[K(C ₁₂ H ₂₄ O ₆)] [Au(SCN) ₂]	$Z = 1$
$M_r = 616.54$	$D_x = 1.911 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.2401 (2) \text{ \AA}$	Cell parameters from 4565 reflections
$b = 8.0946 (2) \text{ \AA}$	$\theta = 2.1\text{--}32.2^\circ$
$c = 10.2386 (3) \text{ \AA}$	$\mu = 7.29 \text{ mm}^{-1}$
$\alpha = 75.814 (1)^\circ$	$T = 150 (2) \text{ K}$
$\beta = 70.486 (1)^\circ$	Plate, colorless
$\gamma = 73.894 (1)^\circ$	$0.12 \times 0.12 \times 0.08 \text{ mm}$
$V = 535.63 (3) \text{ \AA}^3$	

Data collection

Bruker SMART 6000 CCD diffractometer	3771 independent reflections
ω scans	3768 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$R_{\text{int}} = 0.021$
$T_{\text{min}} = 0.447$, $T_{\text{max}} = 0.558$	$\theta_{\text{max}} = 32.2^\circ$
9875 measured reflections	$h = -10 \rightarrow 10$
	$k = -12 \rightarrow 11$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0096P)^2 + 0.467P]$
$R[F^2 > 2\sigma(F^2)] = 0.018$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.039$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.82 \text{ e \AA}^{-3}$
3771 reflections	$\Delta\rho_{\text{min}} = -0.53 \text{ e \AA}^{-3}$
121 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Au1—S1	2.2965 (5)	K1—O8	2.7829 (14)
S1—C1	1.684 (2)	K1—O5	2.7966 (14)
C1—N1	1.150 (3)	K1—O2	2.8419 (14)
N1—K1	2.8699 (19)		
S1—Au1—S1 ⁱ	180	N1—C1—S1	176.23 (19)
C1—S1—Au1	99.79 (7)		
Au1—S1—C1—N1	−170 (3)		

Symmetry code: (i) $-1 - x, 1 - y, 1 - z$.

H atoms were either located directly or positioned geometrically (C—H = 0.99 Å) and treated with a riding model. The $U_{\text{iso}}(\text{H})$ values were constrained as $1.2U_{\text{eq}}$ of the carrier atom.

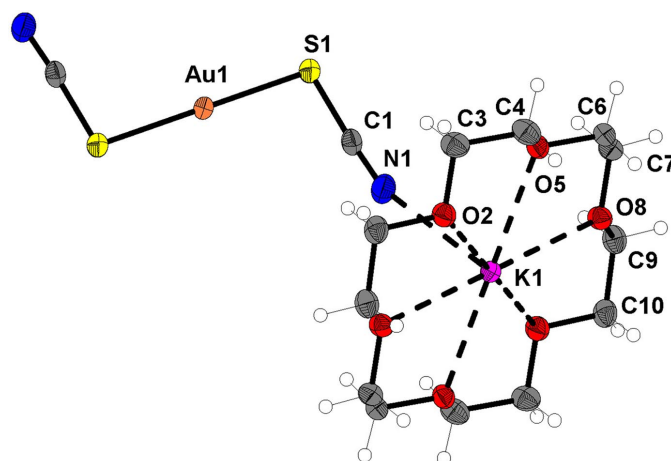


Figure 1

A view of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme for the contents of the asymmetric unit. Dashed lines show the interactions with the potassium cation.

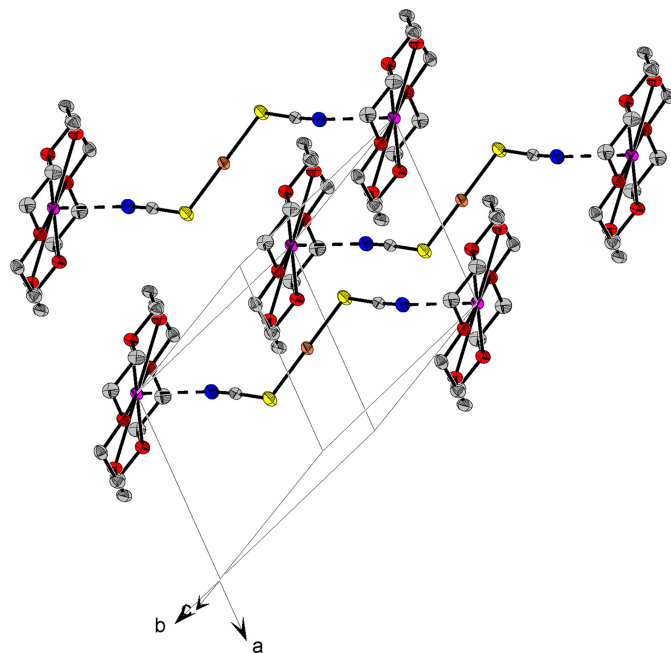


Figure 2

Fragments of the infinite chains (I).

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2002); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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