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Poly[[terachlorogold(III)potassium(I)(*Au*—*K*)]-μ-4,4′-bipyridine]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.040
wR factor = 0.099
Data-to-parameter ratio = 17.7

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

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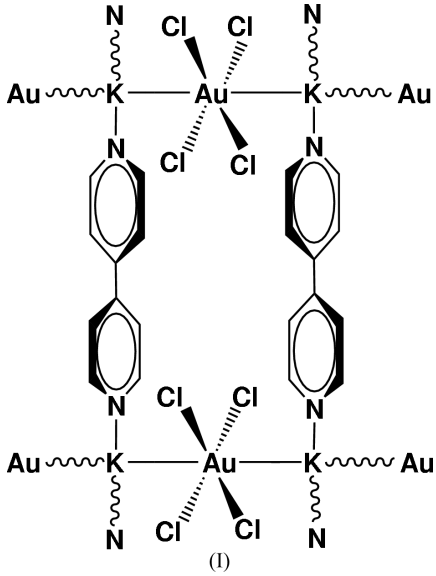
The title compound, $[KAuCl_4(C_{10}H_8N_2)]_n$, is a layer coordination polymer with an Au^{III}—K^{I} metal–metal bond. The Au and K atoms lie on positions of site symmetry 2/m and 222, respectively, and are arranged alternately to form Au—K—Au—K linear chains along the c axis. In addition, the Au atom is coordinated by four Cl atoms, and the K atom coordinated by two N atoms of bipyridine ligands.

Comment

Self-assembled coordination polymers with well defined channels or pores have attracted intense interest as microporous frameworks in which to carry out spatially confined reactions that are potentially catalyzed by functional appendages projecting to the inside of a framework structure (Pschirer *et al.*, 2002). Inorganic materials with inner cavities, such as zeolites, are known to bind many organic molecules in the cavity and often exhibit unique catalysis for organic reactions. Accordingly, non-interpenetrating rectangular grid polymers are an important class of network that have predictable openings and can accommodate guest molecules that meet size-exclusion criteria (Stang *et al.*, 1995; Dong *et al.*, 2000; Biradha & Fujita, 2001).



(I)

The title compound, (I), is a novel coordination layer polymer with an Au^{III}—K^{I} metal–metal bond (Fig. 1). A search of the Cambridge Structural Database (November 2003 update; Allen, 2002) indicated that tetrachloroaurate exists always as an isolated anion (Sakhawat & Elmer, 1982; Drew *et al.*, 1985; Yap *et al.*, 1995; Hussain, 1996). We report here the

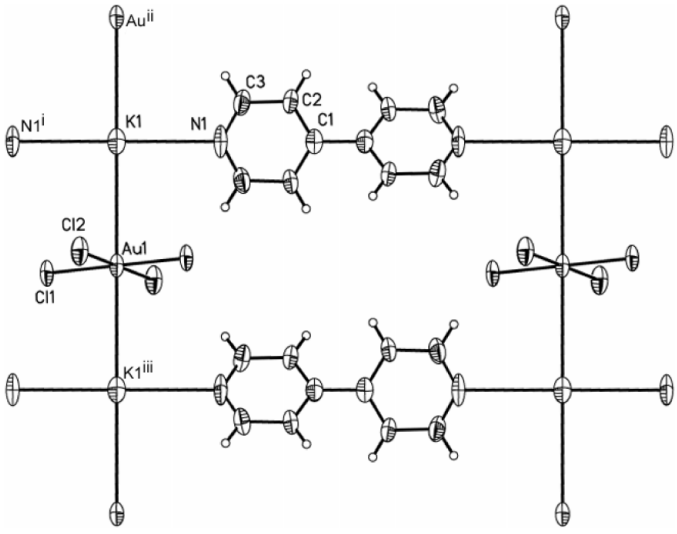


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. [Symmetry codes: (i) $2-x, -y, z$; (ii) $x, -y, \frac{1}{2}-z$; (iii) $2-x, -y, -z$.]

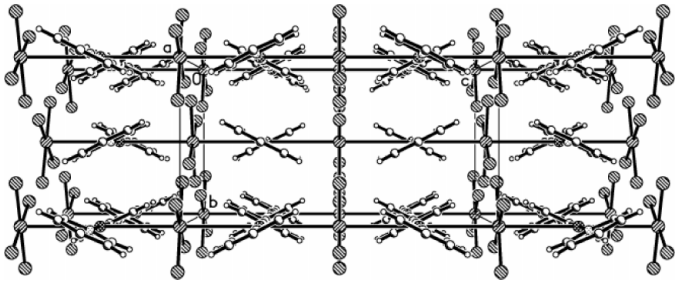


Figure 2
The crystal structure of (I).

first coordination polymer of tetrachloroaurate. The site symmetries of Au1 at (1,0,0) and K1 at (1,0,$\frac{1}{4}$) are 2/*m* and 222, respectively. The K atoms are bridged by 4,4′-bipyridine (4,4′-bipy) molecules, forming chains along the *a* axis. The K^+ cation is coordinated by two N atoms of 4,4′-bipy ligands and is bonded to two adjacent Au atoms. The K—N bond distance is 3.010 (9) Å, which is significantly longer than those of 2.800 (6)–2.893 (5) Å found in the $[K(phen)_3]^+$ complex (Bombieri *et al.*, 1984) and 2.74 (1)–2.81 (1) Å found in the macrocyclic K^+ complex of 7,16,21,26-tetraoxa-1,4,10,13-tetraazatricyclo[11.5.5.5]octacosane (Groth, 1984). The Au atom lies at the center of the square plane formed by four Cl atoms. The coordination geometry around the Au center can be described as as tetragonally elongated octahedral. The Au center binds to two adjacent K atoms, which are at the axial positions of the distorted octahedron. The Au—K distance is 3.6805 (10) Å and the Au—K—Au units are linear. The Au^{III}—K distance in (I) is close to the $Au^{I}\cdots K$ separations of 3.615 (5) and 3.575 (5) Å in $[Au_2K(C_{32}H_{24}N_2P_2)_3](ClO_4)_3\cdot 2HCl\cdot 2MeOH\cdot 0.5H_2O$ (Uang *et al.*, 1994). The dihedral angle in the 4,4′-bipy ligand is 52.8 (3)°. The coordination networks possess inner cavities of *ca* 7.36 (1) × 12.90 (1) $Å^2$. All the layers stack parallel to each other, with an interlayer separation of 3.916 (2) Å (corresponding to half of the *b* axis).

Experimental

The title complex, (I), was synthesized in air by the reaction of $KAuCl_4$ and 4,4′-bipyridine (molar ratio 1:2) in a mixture of ethanol and distilled water (50% *v*/*v*). After keeping the reaction mixture at room temperature for 45 d, yellow block crystals of (I) were obtained (yield 30%).

Crystal data

$[KAuCl_4(C_{10}H_8N_2)]$
M_r = 534.05
Orthorhombic, *Ibam*
a = 12.900 (3) Å
b = 7.8312 (19) Å
c = 14.722 (4) Å
V = 1487.3 (6) $Å^3$
Z = 4
D_x = 2.385 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 732 reflections
θ = 2.7–27.4°
μ = 10.87 mm^{-1}
T = 293 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.09, T_{max} = 0.11
4067 measured reflections
848 independent reflections
629 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.0°
h = −16 → 16
k = −9 → 10
l = −18 → 11

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.099
S = 1.09
848 reflections
48 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.19 e $Å^{-3}$
$\Delta\rho_{min}$ = −1.08 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

K1—N1	3.010 (9)	Au1—Cl1	2.281 (2)
K1—Au1	3.6805 (10)	Au1—Cl2	2.291 (3)
N1—K1—N1^{i}	180	Cl1—Au1—Cl2	89.84 (11)
N1—K1—Au1	90	K1—Au1—K1^{iii}	180
Au1—K1—Au1^{ii}	180		

Symmetry codes: (i) $2-x, -y, z$; (ii) $x, -y, \frac{1}{2}-z$; (iii) $2-x, -y, -z$.

A distance restraint was applied for C1—C1($1-x, -y, z$) of 1.450 (5) Å in order to avoid an unreasonable bond distance (1.56 Å). All H atoms bonded to C atoms were placed in calculated positions, with C—H distances of 0.93 Å, and were included in the refinement using the riding model, with $U_{iso} = 1.2U_{eq}$(C). The highest peak and deepest hole are 0.94 Å from Cl1 and 1.95 Å from Cl2, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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