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catena-Poly[ammonium [bis(thiocyanato)-aurate(**I**)](*Au*—*Au*)]

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Key indicators

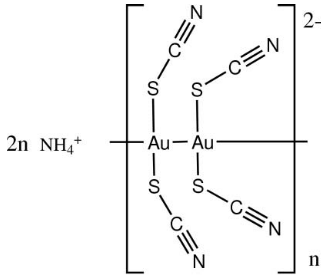
Single-crystal X-ray study
T = 150 K
Mean σ(N–C) = 0.007 Å
R factor = 0.022
wR factor = 0.059
Data-to-parameter ratio = 16.1

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

In the title compound, $\{NH_4[Au(SCN)_2]\}_n$, the Au^I atom is in a linear configuration with the coordinating S atoms. The extended structure can be described as a one-dimensional polymeric chain with alternating Au—Au bond distances of 3.1409 (3) and 3.1723 (3) Å.

Comment

Photophysical studies of Au^I complexes have gained widespread attention in recent years, focusing particularly on the relationship of emission and excitation energies and the type of gold–gold interaction (Rawashdeh-Omary *et al.*, 2001; Lee *et al.*, 2002; Chen *et al.*, 2005). We have reported the crystal structures and emission spectra of the alkali (K^+, Rb^+,Cs^+), NMe_4^+, NBu_4^+ and PPh_4^+ salts of bis(thiocyanato)aurate(I) (Coker *et al.*, 2004). These complexes were found to have monomer, dimer or polymeric chain structures with a range of Au—Au distances. Furthermore, it was discovered that, while the Au—Au distance does not correlate with the size of the cation, the inverse distance does correlate with the emission energy.



(I)

Here we report the preparation and structural characterization of $NH_4[Au(SCN)_2]$, (I) (Fig. 1). Compound (I) is considered to be approximately isostructural with the alkali salt complexes (Coker *et al.*, 2004). The space group and unit-cell parameters observed here are very similar to those observed previously. These complexes all have the same general features with only small differences in the overall structure.

The emission spectrum of (I) shows an emission band at 627 nm, which lies between the bands for the NBu_4^+ (539 nm) and NMe_4^+ (635 nm) complexes. Thus, based on the emission spectra, one would expect that the Au—Au distance for (I) would be in the range 3.07–3.18 Å. In (I), we observe the short Au—Au distance of 3.1409 (3) Å within the predicted range and relatively close to the NMe_4^+ distance of 3.1794 (2) Å. The extended structure of (I) (Fig. 2) adopts the same one-dimensional polymeric motif, with an antiparallel arrangement of the ribbons, as we found for the alkali metal salts.

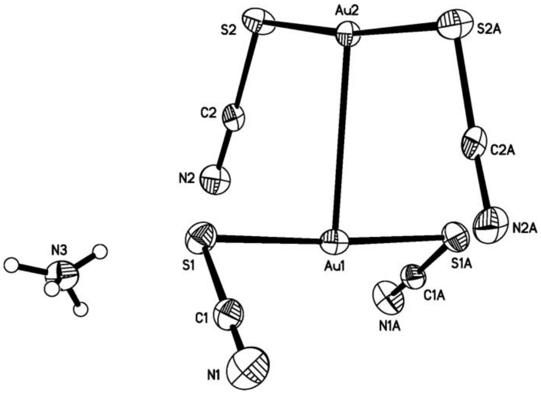


Figure 1
A segment of the polymeric chain structure of (I) with 50% probability displacement ellipsoids [symmetry code: (A) $1 - x, y, \frac{1}{2} - z$].

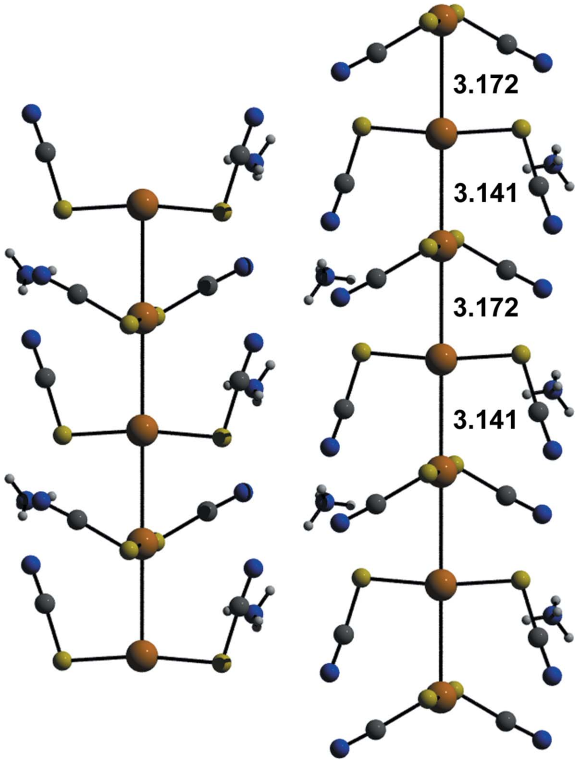


Figure 2
Antiparallel one-dimensional extended packing arrangement of (I) (the *c* axis runs horizontally and the *b* axis runs vertically).

Experimental

$ClAuSC_4H_8$ (1 equivalent) was dissolved in acetonitrile (30 ml). NH_4SCN (2 equivalents), dissolved in a minimal amount of acetonitrile, was added and the mixture stirred for 15 min. The solution was filtered and evaporated at room temperature to give a very pale-pink solid (95% yield). This solid was dissolved in a minimal amount of acetonitrile, to which was added a solvent mixture consisting of diethyl ether, dichloromethane and carbon tetrachloride (1:1:1 *v*/*v*/*v*), until the solution became cloudy. The resulting solution was placed in a freezer (253 K) until precipitation occurred. The solution was filtered and the resulting solid was washed with two portions of diethyl ether. The purified solid was recrystallized from slow diffusion of acetonitrile–diethyl ether at 253 K. IR: 3236 (*s*), 2820 (*w*), 2126 (*s*), 2063 (*w*) cm^{-1}. Raman: 2120 (*s*), 2110 (*s*), 720 (*w*), 306 (*m*) cm^{-1}. Negative ion MS: 313 (*s*), 249 (*w*) *m*/*z*.

Crystal data

$(NH_4)[Au(NCS)_2]$
$M_r = 331.17$
Monoclinic, $C2/c$
$a = 12.9665\ (2)$ Å
$b = 6.3132\ (1)$ Å
$c = 17.6643\ (3)$ Å
$\beta = 110.122\ (1)^\circ$
$V = 1357.74\ (4)$ Å^3
$Z = 8$
$D_x = 3.240$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 3756 reflections
$\theta = 5.3–67.7^\circ$
$\mu = 45.69\ mm^{-1}$
$T = 150\ (2)$ K
Rod, colorless
$0.11 \times 0.04 \times 0.03$ mm

Data collection

Bruker SMART6000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.061, T_{max} = 0.256$
5457 measured reflections
1209 independent reflections
1123 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 67.7^\circ$
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 7$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.059$
$S = 1.16$
1209 reflections
75 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 4.3348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -1.58$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.000284 (16)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1···N2^{i}	0.92	2.10	2.987 (6)	161
N3—H2···N2^{ii}	0.88	2.17	3.020 (6)	163
N3—H3···N1^{iii}	0.88	2.24	3.004 (6)	145

Symmetry codes: (i) $-x + 1, -y + 2, -z + 1$; (ii) $x, y - 1, z$; (iii) $-x + 1, -y + 1, -z + 1$.

H atoms were initially located in a difference Fourier map; the positions were then adjusted to give better H—N···H angles and held fixed in subsequent refinements; N—H = 0.86–0.92 Å and $U_{iso}(H) = 1.5U_{eq}(N)$. The maximum and minimum electron-density peaks are located 0.80 Å from atom Au1 and 0.86 Å from atom Au2, repsectively.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL*.

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