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$[\{(H_3C)_3NB(H)_2NC\}_2Au][AuI_2]$: a linear chain polymer of gold(I) iodide with an unusual isocyanoborane ligand showing aurophilic behaviour

William C. Kaska,[a] Hermann A. Mayer,[b] Mark R. J. Elsegood,[c] Peter N. Horton,[d] Michael B. Hursthouse,[d] Carl Redshaw[e] and Simon M. Humphrey[f]*

[a]Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106-9510, USA, [b]Universität Tübingen, Institut für Anorganische Chemie, Auf der Morgenstelle 18, D-72076 Tübingen, Germany, [c]Chemistry Department, Loughborough University, Loughborough, Leicestershire LE11 3TU, England, [d]School of Chemistry, University of Southampton, Southampton SO17 1BJ, England, [e]Wolfson Materials and Catalysis Centre, School of Chemical Sciences and Pharmacy, University of East Anglia, Norwich NR4 7TJ, England, and [f]University Chemical Laboratory, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

Correspondence e-mail: smh49@cam.ac.uk

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Treatment of the (isocyanoborane)gold(I) chloride adduct [*L*AuCl] [$L = (H_3C)_3NB(H)_2NC$] with KI at room temperature yields the unusal title compound, bis[isocyano(trimethylamino)borane]gold(I) diiodoaurate(I), $[Au(C_4H_{11}BN_2)_2][AuI_2]$, which forms *via* an *in situ* rearrangement of isocyanoborane and halide ligands. The structure consists of alternating $[L_2Au]^+$ and $[AuI_2]^-$ ions, which form an infinite linear one-dimensional chain due to aurophilic Au$\cdots$Au interactions. Both Au atoms occupy inversion centres.

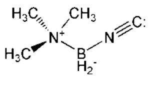
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(Au–I) = 0.001 Å
R factor = 0.049
wR factor = 0.125
Data-to-parameter ratio = 24.7

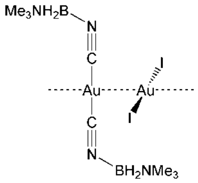
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

We have recently been interested in the formation of (isocyanide)gold(I) halide adducts, because of their propensity to interact aurophilically. The term aurophilicity is used to describe observed Au$\cdots$Au interactions. These intermolecular contacts have been shown to have bond energies and distances similar to those observed for classical hydrogen-bonding interactions (7.5–12.5 kcal mol^{-1} and 2.7–3.5 Å, respectively) (Schmidbaur, 1990, 2000; Mathieson *et al.*, 2000). Hence, aurophilic behaviour is considered to be a major factor in determining the particular supramolecular motif which a series of monomers is observed to adopt. Our recent synthetic studies have involved the use of an unusual zwitterionic isocyanoborane species (*L*) (Andersen *et al.*, 2001) (see scheme). The substitution reaction of [*L*AuCl], whereby chloride is replaced with iodide, has yielded (I), whose structure shows clear evidence for aurophilic effects directing the appearance of its extended structure.



(*L*)



(I)

Compound (I) crystallizes in the triclinic space group $P\overline{1}$ (Z = 2). The asymmetric unit comprises one equivalent of the isocyanoborane donor species and a single iodide, each coordinated to crystallographically distinct gold cations Au1 and Au2, both of which are located on inversion centres (Fig. 1). Both Au1 and Au2 exhibit pseudo-square-planar coordination geometry, with bonding angles of 91.443 (11) (I1—Au1$\cdots$Au2) and 97.1 (2)° (C1—Au2$\cdots$Au1^{i}; symmetry code as in Table 1). Au1 is *trans*-coordinated by two equivalents of iodide; Au2 is also *trans*-coordinated, by isocyanide moieties. The coordination of each gold ion is

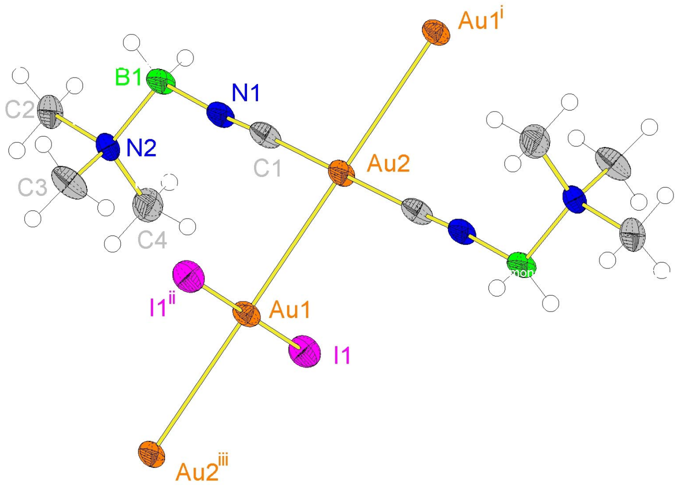


Figure 1
Part of the polymeric structure of (I), showing two asymmetric units and two additional Au atoms, with displacement ellipsoids drawn at the 50% probability level. Coordination environments of all unique atoms are drawn completed. [Symmetry codes: (i) $-x, -y, 1 - z$; (ii) $1 + x, y, z$; (iii) $-1 - x, -y, 1 - z$.]

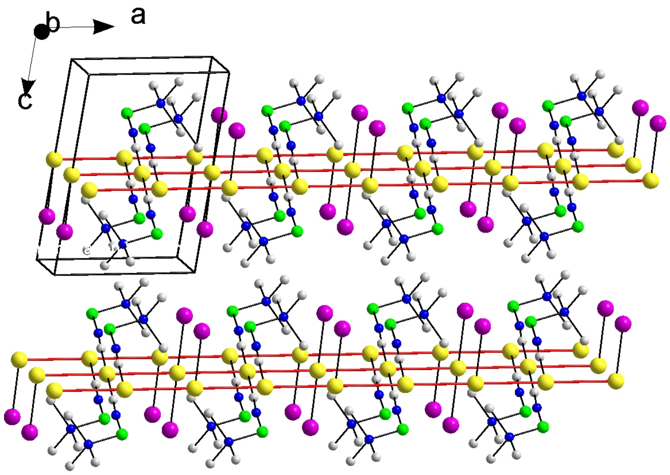


Figure 2
View of (I), showing the chains of aurophilically bound gold centres running parallel to the crystallographic *a* axis. Aurophilic type bonds are drawn in red.

completed by Au···Au contacts with adjacent Au centres, where Au1···Au2 is a mere 3.0438 (7) Å, suggesting that significant aurophilic character is present in (I). Literature values for observed Au···Au contact distances suggest an approximate range of 4.1 Å (as often associated with the inter–dimer bonding in chains of dimers) to 2.9 Å for complexes similar in topology to (I).

A perfectly linear infinite chain of gold atoms is thus formed, aligned parallel to the crystallographic *a* axis (Fig. 2). It can be seen that adjacent chains are displaced from each other along the *b* axis, thus forming a two-dimensional grid-like array of sheets. The B1—N1—C1 angle is 175.7 (7)°, this portion of the coordinated isocyanoborane being almost linear. Adjacent iodide and isocyanide substituents are aligned approximately orthogonally to one another (Fig. 3). A network of classical (van der Waals) intermolecular interactions is formed primarily between methyl H atoms and adjacent I$^-$ atoms (Fig. 3).

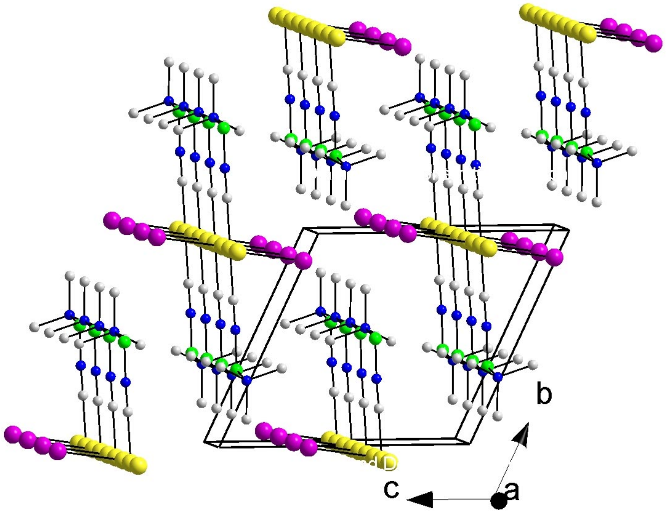


Figure 3
Projection of (I) on the *bc* plane, detailing the approximately orthogonal arrangement of the iodide and isocyanoborane substituents.

Experimental

A solution of [*L*AuCl] (42 mg, 0.202 mmol) in dichloromethane (10 ml) was stirred vigorously with KI (51 mg, 0.307 mmol) in H_2O (10 ml) over a period of 18 h. After removal of all solvent, the yellow–green residual solid was dissolved in dichloromethane (5 ml). Small light green shard-like crystals of (I) were grown from the solution by layering with heptane (1:1) and allowing slow evaporation of the solvent. For full experimental details and characterization data, see Humphrey *et al.* (2004).

Crystal data

$[Au(C_4H_{11}BN_2)_2][AuI_2]$
$M_r = 421.82$
Triclinic, $P\bar{1}$
$a = 6.0875$ (1) Å
$b = 9.3080$ (2) Å
$c = 9.6876$ (2) Å
$\alpha = 115.970$ (1)°
$\beta = 91.039$ (1)°
$\gamma = 102.127$ (2)°
$V = 478.680$ (16) Å^3

$Z = 2$
$D_x = 2.927$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 2009 reflections
$\theta = 2.9$–$27.5°$
$\mu = 18.52$ mm^{-1}
$T = 120$ (2) K
Shard, light green
0.10 × 0.06 × 0.02 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.267$, $T_{max} = 0.689$
7106 measured reflections

2174 independent reflections
2033 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 27.5°$
$h = -7 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.125$
$S = 1.06$
2174 reflections
88 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0926P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 6.24$ e Å^{-3}
$\Delta\rho_{min} = -4.28$ e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

Au1—I1	2.5604 (5)	C1—N1	1.156 (10)
Au1···Au2	3.0438 (1)	N1—B1	1.550 (9)
Au2—C1	1.977 (8)		
I1—Au1—I1^{i}	180	C1—Au2···Au1	82.9 (2)
I1—Au1···Au2	91.443 (11)	C1^{iii}—Au2···Au1	97.1 (2)
I1^{i}—Au1···Au2	88.557 (11)	N1—C1—Au2	178.1 (7)
Au2···Au1···Au2^{ii}	180	C1—N1—B1	175.7 (7)
C1—Au2—C1^{iii}	180	N1—B1—N2	108.2 (6)

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

Methyl H (C—H distance = 0.98 Å) and BH_2 (B—H distance = 0.99 Å) atoms were placed in calculated positions using a riding model. U_{iso} values were set to $1.2U_{eq}$ of the parent atom for BH ($1.5U_{eq}$ for methyl H). The maximum and minimum difference map features were located 0.94 Å from Au1 and 0.81 Å from Au2, respectively.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Crystal Impact, 2001); software used to prepare material for publication: *PLATON* (Spek, 2003).

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