

{Ba[Au(SCN)₂]₂]_n: a three-dimensional net comprised of monomeric and trimeric gold(I) units

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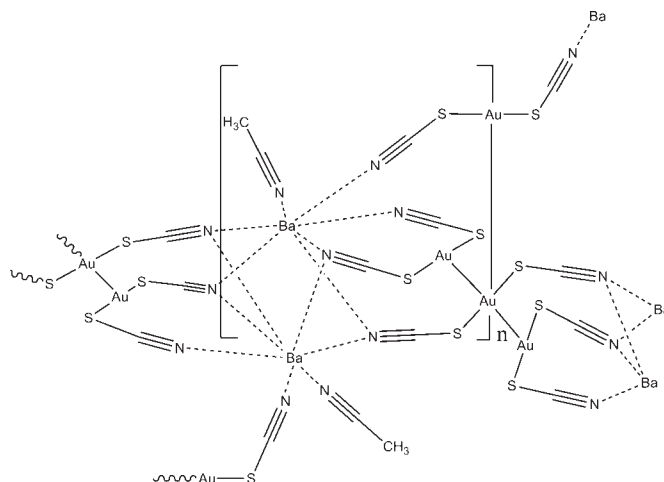
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.014$ Å; R factor = 0.031; wR factor = 0.079; data-to-parameter ratio = 16.4.

The noteworthy structural feature of the title complex, poly[acetoneitriletetra- μ_2 -thiocyanato-barium(II)digold(I)], {[Au₂Ba(SCN)₄(CH₃CN)]_n, is that the bis(thiocyanato)-aurate(I) anion adopts both monomeric and trimeric motifs. The trimer unit has an Au¹···Au distance of 3.1687 (3) Å. In both the monomeric and trimeric units, the Au¹ atoms are also bonded to two S atoms. Within the trimeric unit, the Au¹ atoms exist in differing environments; one Au atom has a T-shaped three-coordinate geometry while the other has a square-planar four-coordinate geometry. The Au¹ atom of the monomer adopts a linear two-coordinate geometry. The extended structure can be described as a three-dimensional coordination polymer consisting of chains of Ba atoms bridged by thiocyanate N atoms. These chains are cross-linked *via* the gold monomeric and trimeric units.

Related literature

For further information on gold chemistry, see: Anderson *et al.* (2007); Bondi (1964); Pathaneni & Desiraju (1993); Arvapally *et al.* (2007); Beavers *et al.* (2009); Coker (2003); Coker *et al.* (2004, 2006); Katz *et al.* (2008); Puddephatt (2008); Schmidbauer & Schier (2008); Schwerdtfeger *et al.* (1990); Stroud *et al.* (2009). For a description of the Cambridge Structural Database, see: Allen (2002)



Experimental

Crystal data

[Au₂Ba(NCS)₄(C₂H₃N)]
 $M_r = 804.65$
 Monoclinic, $P2_1/n$
 $a = 11.5586$ (3) Å
 $b = 7.4859$ (2) Å
 $c = 18.5798$ (4) Å
 $\beta = 106.450$ (1)°

$V = 1541.84$ (7) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 59.69$ mm⁻¹
 $T = 150$ K
 $0.15 \times 0.05 \times 0.02$ mm

Data collection

Bruker SMART6000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.060$, $T_{\max} = 0.302$

12455 measured reflections
 2743 independent reflections
 2559 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.053$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.079$
 $S = 1.04$
 2743 reflections

167 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 2.17$ e Å⁻³
 $\Delta\rho_{\min} = -1.27$ e Å⁻³

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL and DIAMOND (Brandenburg, 2009); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2340).

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supplementary materials

Acta Cryst. (2010). E66, m765-m766 [doi:10.1107/S1600536810021276]

{Ba[Au(SCN)₂]₂}_n: a three-dimensional net comprised of monomeric and trimeric gold(I) units

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Comment

The propensity for gold complexes to adopt fascinating structures, high stability and unexpected stoichiometries arising from various gold-gold interactions, termed *aurophilicity* or more generally *metalphilicity*, ultimately result in intriguing physical properties (Schmidbaur & Schier, 2008; Katz *et al.*, 2008; Puddephatt, 2008).

Over the course of our research on gold(I)-thiocyanate complexes we have observed a variety of interesting bonding motifs and luminescent properties (Coker *et al.*, 2004; Arvapally *et al.*, 2007) attributed to the [Au(SCN)₂]⁻ anion. The [Au(SCN)₂]⁻ anion has been observed as a monomer as well as adopting polymeric geometries. For example, in the tetraphenyl arsonium (Schwerdtfeger *et al.*, 1990) and phosphonium (Coker, 2003) salts, the [Au(SCN)₂]⁻ exists as a monomer. However, we have observed (Coker *et al.*, 2004) that the alkali (K⁺, Rb⁺ and Cs⁺) salts of this anion preferentially adopt a linear one-dimensional polymeric chain motif with Au—Au distances in the 3.0065 (5)-3.2654 (2) Å range. Ammonium or tetramethylammonium salts of bis(thiocyanato)aurate(I) exhibit a slight variation on this one-dimensional bonding theme; tending toward linear or nearly linear motifs with alternating sets of gold-gold distances; NH₄⁺ with distances of 3.1794 (2) and 3.2654 (2) Å (Coker *et al.*, 2006) and Me₄N⁺ with shorter distances of 3.1409 (3), 3.1723 (3) Å (Coker *et al.*, 2004). Alternatively, the [Au(SCN)₂]⁻ anion crystallizes as a dimer unit with a gold-gold bond distance of 3.0700 (8) Å in the tetrabutylammonium salt complex (Coker *et al.*, 2004).

More recently our investigations have turned to the alkaline earth salts of gold(I)-thiocyanate. Our motivation is to further explore the influence of the cation on the highly structurally-versatile behavior of the [Au(SCN)₂]⁻ anion. In the present work, the structure of the barium salt, (I), is presented.

The geometry of the anion in (I) (Fig. 1) is such that both monomeric and trimeric gold units are present with Au—Au and Au—S bond distances of 3.1687 (3) Å and 2.294 (2)-2.314 (2) Å, respectively. Within the trimer unit of (I), the gold atoms exist in differing environments; Au1 has a T-shaped three-coordinate geometry while Au2 has a square planar four-coordinate geometry. The monomeric gold, Au3, adopts a linear two-coordinate geometry. The S—Au1—Au2—S torsion angles, are intermediate between staggered and eclipsed (Table 1) geometries. As commented on by Pathaneni & Desiraju (1993) and further expanded by Anderson *et al.* (2007), complexes with larger Au—Au distances more frequently adopt an eclipsed conformation (L—Au—Au—L torsions ~ 0 or ±180°) presumably to lessen steric hindrance while the staggered conformation (L—Au—Au—L torsions ~ ±90°) is observed for smaller Au—Au distances. However it should be noted that there is a large spread of intermediates transitioning from eclipsed to staggered conformations with torsion angles in the ±50 to ±140° range.

The Au—Au bond distance observed in (I) is less than the sum of the van der Waals radii of 3.32 Å for a gold-gold interaction (Bondi, 1964). Furthermore, the recent literature (Schmidbaur & Schier, 2008; Katz *et al.*, 2008; Puddephatt, 2008; Anderson *et al.*, 2007) categorizes gold-gold distances in the range 2.5-3.5 Å as having significant Au—Au bonding

character. In the structure presented here, the Au—Au distance is comparable to those cited for the large variety of gold complexes discussed in the literature (see, for instance, the varied works in Chem. Soc. Rev. (2008), 37, 1745–2140, a dedicated issue summarizing gold chemistry). The distance also agrees well with our work on the metallocrown complexes (dbz-18-crown-6-Ba)[bis(thiocyanato)aurate(I)] (Au—Au = 3.1109 (10) Å, Au—S = 2.288 (4)–2.305 (4) Å) (Stroud *et al.*, 2009) and [CH₃CN-(dbz-18-crown-6-Na)]₂[Au(SCN)₂]₂.dbz-18-crown-6.CH₃CN (Au—Au = 3.0661 (4) Å, Au—S = 2.291 (2)–2.303 (2) Å) (Coker, 2003) where dbz-18-crown-6 = (6,7,9,10,17,18,20,21-octahydro- 5,8,11,16,19,22-hexaoxa-dibenzo[a,j]cyclooctadecene. The Au—S bond distances for (I) are consistent with other metal-thiocyanate complexes (average M—S distance of 2.39 Å where M = Pt, Pd, Ag or Au) reported in the literature (Cambridge Structural Database, Allen, 2002).

The extended structure of (I) (Fig. 2) can be described as a three-dimensional coordination polymer generated by Ba^{II}·N intermolecular interactions. As is common, a high coordination number about the barium atom in (I) is achieved. The nine-coordinate Ba atom is bound to the nitrogen atoms of the thiocyanate groups, a coordinated acetonitrile molecule (N7) and a long contact with a thiocyanate sulfur (S4) of the monomeric gold unit (Ba—N distances range: 2.777 (6)–3.0444 (7) Å; Ba··S4 = 3.422 (2) Å). The core barium bridged unit consists of a barium-barium pair (Ba··Ba = 4.4341 (5) Å) bridged by three μ-N(thiocyanate) groups arising from N2 and N3 of the trimer and N4 of the monomer gold units. Furthermore, these barium chains are propagated through the lattice parallel to the *b*-axis. The gold trimer units crosslink neighboring barium chains in a diagonal fashion along the [1 0 1] direction. The monomeric gold units crosslink the barium chains in a diagonal fashion along the [-2 0 2] direction completing the three-dimensional net.

A similar situation where a gold-cyanato anion, [Au(CN)₂]⁻, adopts multiple gold bonding motifs is observed for [poly[triaquatetra-μ-cyanido-tetracyanidobis(1,4,10,13-tetraoxa- 7,16-diazacyclo-octadecane) dibarium(II)tetragold(I)] (Beavers *et al.*, 2009). In that case, the coordination polymer consists of the [Au(CN)₂]⁻ anion in monomer, dimer and trimer environments (Au—Au = 3.2670 (2)–3.5655 (2) Å) while the barium atoms are bound to the diaza-18-crown-6 and solvent water molecules (Ba··N,O distances span the range 2.761 (2)–2.959 (3) Å).

To echo Katz *et al.* (2008) and Puddephatt (2008), taking advantage of Au^I *aurophilic* or other transition metal *metallophilic* interactions leads to a very useful design strategy to increase structural dimensionality of metal complexes. These complexes are highly prized due to their tunable physical properties, e.g. magnetic, vapochromic and optical properties.

Experimental

Reaction of barium hydroxide (1 equiv) with ammonium thiocyanate (2 equiv) in water results in the formation of barium thiocyanate with the release of ammonia gas. (I) was prepared following the method described by Coker *et al.* (2004). Crystals were obtained from slow diffusion of acetonitrile-diethyl ether solution at -4 °C.

Refinement

The H-atoms were placed in calculated positions (C—H = 0.98 Å) and treated with a riding model. The isotropic displacement parameters were defined as 1.5U_{eq} of the adjacent atom. The largest residual electron-density peaks are located near the gold trimer unit (approx. 1.6 Å from S2 and S3).

Figures

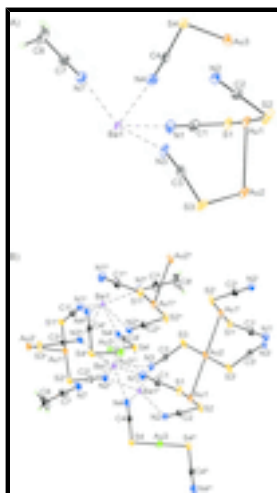


Fig. 1. : (a) Asymmetric unit of (I). (b) Partially extended structure of (I) showing the gold monomer (Au3, drawn in green) and trimer (Au1 and Au2, drawn in orange) units and the coordination about the barium atoms. Atomic labelling scheme and 50% probability ellipsoids are shown. [Symmetry codes: (i) $x-3/2, y-1/2, -z+1/2$; (ii) $x, y-1, z$; (iii) $-x+2, -y+2, -z+1$; (iv) $-x+1, -y+1, -z+1$].

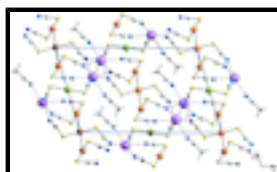


Fig. 2. : The three-dimensional polymeric network of (I) in the ac plane (Au atoms of the monomer and trimer units drawn in green and orange, respectively.)

poly[acetoneitriletetra- μ_2 -thiocyanato-barium(II)digold(I)]
Crystal data

[Au₂Ba(NCS)₄(C₂H₃N)]

$M_r = 804.65$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2yn$

$a = 11.5586\ (3)\ \text{\AA}$

$b = 7.4859\ (2)\ \text{\AA}$

$c = 18.5798\ (4)\ \text{\AA}$

$\beta = 106.450\ (1)^\circ$

$V = 1541.84\ (7)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1408$

$D_x = 3.466\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54178\ \text{\AA}$

Cell parameters from 7754 reflections

$\theta = 4.1\text{--}67.6^\circ$

$\mu = 59.69\ \text{mm}^{-1}$

$T = 150\ \text{K}$

Blade, colourless

$0.15 \times 0.05 \times 0.02\ \text{mm}$

Data collection

Bruker SMART6000 CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: $0.8\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2003)

2743 independent reflections

2559 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.053$

$\theta_{\text{max}} = 67.6^\circ, \theta_{\text{min}} = 5.0^\circ$

$h = -13 \rightarrow 13$

$k = -8 \rightarrow 8$

supplementary materials

$T_{\min} = 0.060$, $T_{\max} = 0.302$
12455 measured reflections

$l = -21 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.079$

$S = 1.04$

2743 reflections

167 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 5.0574P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 2.17 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.26 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. A suitable crystal was mounted in a loop with paratone-N and immediately transferred to the goniostat bathed in a cold stream.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.72117 (3)	0.76278 (4)	0.517412 (17)	0.02210 (12)
Au2	0.5000	0.5000	0.5000	0.02498 (14)
Au3	1.0000	1.0000	0.5000	0.02274 (14)
Ba1	0.84629 (4)	0.32246 (6)	0.29512 (2)	0.01596 (13)
S1	0.84496 (18)	0.5362 (3)	0.57927 (10)	0.0253 (4)
N1	0.8661 (6)	0.3726 (9)	0.4462 (4)	0.0262 (14)
C1	0.8583 (7)	0.4404 (11)	0.4997 (4)	0.0245 (17)
S2	0.60587 (19)	0.9988 (3)	0.45766 (12)	0.0306 (5)
N2	0.7123 (6)	1.0410 (9)	0.3392 (3)	0.0215 (13)
C2	0.6706 (7)	1.0228 (10)	0.3884 (4)	0.0218 (16)
S3	0.44661 (19)	0.4332 (3)	0.37321 (11)	0.0342 (5)
N3	0.6338 (6)	0.5268 (9)	0.3097 (3)	0.0210 (14)
C3	0.5617 (7)	0.4914 (10)	0.3398 (4)	0.0193 (16)
S4	1.03510 (17)	0.9889 (2)	0.38459 (11)	0.0226 (4)

N4	0.8861 (6)	0.6993 (9)	0.3176 (4)	0.0246 (14)
C4	0.9461 (7)	0.8143 (10)	0.3464 (4)	0.0213 (16)
N7	1.0607 (6)	0.3524 (10)	0.2496 (4)	0.0303 (16)
C7	1.1298 (8)	0.3672 (13)	0.2172 (4)	0.0303 (19)
C8	1.2207 (9)	0.3905 (18)	0.1769 (5)	0.053 (3)
H1	1.3014	0.3771	0.2120	0.079*
H2	1.2128	0.5099	0.1544	0.079*
H3	1.2089	0.3001	0.1373	0.079*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.02219 (19)	0.0297 (2)	0.01858 (19)	0.00115 (12)	0.01254 (14)	0.00146 (11)
Au2	0.0244 (3)	0.0357 (3)	0.0208 (3)	-0.00001 (18)	0.0161 (2)	0.00502 (17)
Au3	0.0219 (2)	0.0266 (3)	0.0183 (3)	0.00347 (17)	0.00345 (18)	-0.00422 (16)
Ba1	0.0183 (2)	0.0182 (2)	0.0161 (2)	0.00030 (16)	0.01252 (17)	0.00024 (15)
S1	0.0277 (10)	0.0341 (11)	0.0173 (9)	0.0060 (8)	0.0114 (8)	0.0013 (8)
N1	0.034 (4)	0.030 (4)	0.016 (3)	0.008 (3)	0.010 (3)	0.002 (3)
C1	0.024 (4)	0.030 (4)	0.022 (4)	0.007 (3)	0.009 (3)	0.009 (3)
S2	0.0326 (11)	0.0418 (12)	0.0264 (11)	0.0127 (9)	0.0229 (9)	0.0109 (8)
N2	0.026 (3)	0.023 (3)	0.018 (3)	-0.003 (3)	0.010 (3)	-0.001 (2)
C2	0.018 (4)	0.027 (4)	0.023 (4)	-0.003 (3)	0.008 (3)	-0.002 (3)
S3	0.0276 (10)	0.0560 (14)	0.0246 (10)	-0.0114 (10)	0.0165 (9)	0.0004 (9)
N3	0.023 (3)	0.029 (4)	0.015 (3)	0.006 (3)	0.011 (3)	0.002 (2)
C3	0.021 (4)	0.021 (4)	0.015 (4)	0.004 (3)	0.005 (3)	-0.001 (3)
S4	0.0199 (9)	0.0266 (10)	0.0226 (10)	-0.0036 (7)	0.0083 (7)	-0.0036 (7)
N4	0.024 (3)	0.024 (4)	0.028 (4)	0.002 (3)	0.012 (3)	0.000 (3)
C4	0.027 (4)	0.023 (4)	0.019 (4)	0.002 (3)	0.015 (3)	0.000 (3)
N7	0.025 (3)	0.045 (4)	0.024 (4)	-0.007 (3)	0.012 (3)	-0.006 (3)
C7	0.029 (4)	0.047 (5)	0.015 (4)	-0.011 (4)	0.006 (3)	0.000 (3)
C8	0.034 (5)	0.103 (9)	0.027 (5)	-0.014 (6)	0.019 (4)	-0.002 (5)

Geometric parameters (\AA , $^\circ$)

Au1—S2	2.301 (2)	Ba1—S4 ⁱⁱ	3.422 (2)
Au1—S1	2.305 (2)	S1—C1	1.689 (8)
Au1—Au2	3.1687 (3)	N1—C1	1.142 (10)
Au2—S3	2.314 (2)	S2—C2	1.671 (8)
Au2—S3 ⁱ	2.315 (2)	N2—C2	1.156 (10)
Au3—S4	2.2940 (19)	S3—C3	1.677 (8)
Ba1—N1	2.777 (6)	N3—C3	1.158 (10)
Ba1—N7	2.845 (7)	S4—C4	1.690 (8)
Ba1—N2 ⁱⁱ	2.868 (6)	N4—C4	1.140 (10)
Ba1—N4	2.869 (7)	N7—C7	1.134 (11)
Ba1—N2 ⁱⁱⁱ	2.899 (6)	C7—C8	1.463 (12)
Ba1—N3	2.971 (6)	C8—H1	0.9800
Ba1—N3 ⁱⁱⁱ	3.000 (6)	C8—H2	0.9800

supplementary materials

Ba1—N4 ⁱⁱⁱ	3.044 (7)	C8—H3	0.9800
S2—Au1—S1	177.06 (8)	N1—Ba1—S4 ⁱⁱ	75.45 (14)
S2—Au1—Au2	95.00 (6)	N7—Ba1—S4 ⁱⁱ	73.29 (16)
S1—Au1—Au2	87.88 (5)	N2 ⁱⁱ —Ba1—S4 ⁱⁱ	69.32 (14)
S3—Au2—S3 ⁱ	180.000 (1)	N4—Ba1—S4 ⁱⁱ	126.36 (14)
S3—Au2—Au1 ⁱ	77.71 (5)	N2 ⁱⁱⁱ —Ba1—S4 ⁱⁱ	142.31 (13)
S3—Au2—Au1	102.29 (5)	N3—Ba1—S4 ⁱⁱ	139.60 (12)
Au1 ⁱ —Au2—Au1	180.000 (11)	N3 ⁱⁱⁱ —Ba1—S4 ⁱⁱ	67.75 (13)
S4—Au3—S4 ^{iv}	180.00 (9)	N4 ⁱⁱⁱ —Ba1—S4 ⁱⁱ	115.49 (13)
N1—Ba1—N7	117.4 (2)	C1—S1—Au1	94.2 (3)
N1—Ba1—N2 ⁱⁱ	72.97 (19)	C1—N1—Ba1	159.3 (6)
N7—Ba1—N2 ⁱⁱ	136.8 (2)	N1—C1—S1	178.5 (8)
N1—Ba1—N4	75.90 (19)	C2—S2—Au1	97.4 (3)
N7—Ba1—N4	81.3 (2)	C2—N2—Ba1 ^v	133.8 (6)
N2 ⁱⁱ —Ba1—N4	139.29 (18)	C2—N2—Ba1 ^{vi}	124.5 (6)
N1—Ba1—N2 ⁱⁱⁱ	136.58 (19)	Ba1 ^v —N2—Ba1 ^{vi}	100.50 (19)
N7—Ba1—N2 ⁱⁱⁱ	73.17 (19)	N2—C2—S2	178.0 (7)
N2 ⁱⁱ —Ba1—N2 ⁱⁱⁱ	130.30 (9)	C3—S3—Au2	108.0 (3)
N4—Ba1—N2 ⁱⁱⁱ	63.85 (19)	C3—N3—Ba1	130.8 (5)
N1—Ba1—N3	70.83 (18)	C3—N3—Ba1 ^{vi}	132.9 (5)
N7—Ba1—N3	143.0 (2)	Ba1—N3—Ba1 ^{vi}	95.91 (17)
N2 ⁱⁱ —Ba1—N3	79.92 (18)	N3—C3—S3	173.1 (7)
N4—Ba1—N3	65.37 (18)	C4—S4—Au3	99.9 (2)
N2 ⁱⁱⁱ —Ba1—N3	77.90 (17)	C4—S4—Ba1 ^v	97.6 (3)
N1—Ba1—N3 ⁱⁱⁱ	139.16 (18)	Au3—S4—Ba1 ^v	99.81 (6)
N7—Ba1—N3 ⁱⁱⁱ	68.39 (19)	C4—N4—Ba1	149.5 (6)
N2 ⁱⁱ —Ba1—N3 ⁱⁱⁱ	77.89 (17)	C4—N4—Ba1 ^{vi}	113.3 (6)
N4—Ba1—N3 ⁱⁱⁱ	141.35 (18)	Ba1—N4—Ba1 ^{vi}	97.1 (2)
N2 ⁱⁱⁱ —Ba1—N3 ⁱⁱⁱ	84.24 (18)	N4—C4—S4	176.9 (7)
N3—Ba1—N3 ⁱⁱⁱ	131.05 (9)	C7—N7—Ba1	165.8 (7)
N1—Ba1—N4 ⁱⁱⁱ	122.71 (19)	N7—C7—C8	178.3 (10)
N7—Ba1—N4 ⁱⁱⁱ	119.52 (18)	C7—C8—H1	109.5
N2 ⁱⁱ —Ba1—N4 ⁱⁱⁱ	62.04 (18)	C7—C8—H2	109.5
N4—Ba1—N4 ⁱⁱⁱ	118.15 (17)	H1—C8—H2	109.5
N2 ⁱⁱⁱ —Ba1—N4 ⁱⁱⁱ	68.49 (18)	C7—C8—H3	109.5
N3—Ba1—N4 ⁱⁱⁱ	68.12 (18)	H1—C8—H3	109.5
N3 ⁱⁱⁱ —Ba1—N4 ⁱⁱⁱ	62.93 (18)	H2—C8—H3	109.5

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y-1, z$; (iii) $-x+3/2, y-1/2, -z+1/2$; (iv) $-x+2, -y+2, -z+1$; (v) $x, y+1, z$; (vi) $-x+3/2, y+1/2, -z+1/2$.

Fig. 1

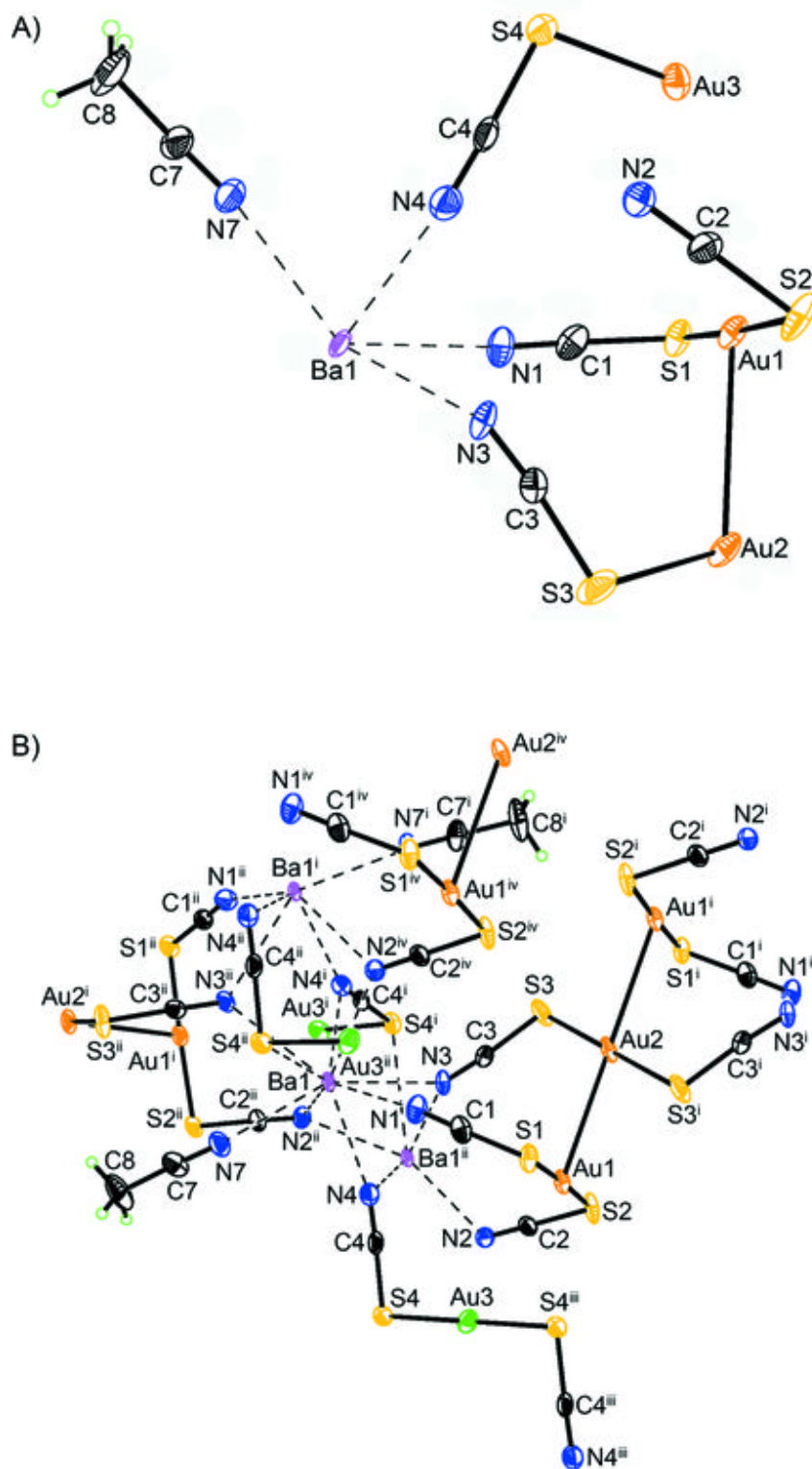


Fig. 2

