

## $\mu$ -Bis(diphenylarsino)methane- $\kappa^2$ As:As'-bis[chloridogold(I)]

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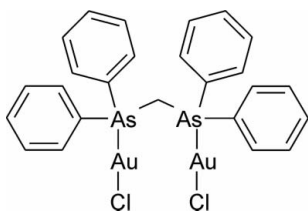
Received 30 January 2009; accepted 10 February 2009

Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.023;  $wR$  factor = 0.055; data-to-parameter ratio = 19.6.

The title structure,  $[\text{Au}_2\text{Cl}_2(\text{C}_{25}\text{H}_{22}\text{As}_2)]$ , consists of discrete molecules disposed about a crystallographic twofold axis. The Au atom exhibits a nearly linear coordination by As and Cl atoms.  $\text{Au}\cdots\text{Au}$  interactions [ $3.4285$ Å(4) Å] and a weak intermolecular  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bond are present.

### Related literature

For related structures, see: Healy (2003); Schmidbaur *et al.* (1977*a,b*). For the synthesis of related complexes, see: Monkowius *et al.* (2003*a,b*).



### Experimental

#### Crystal data

$[\text{Au}_2\text{Cl}_2(\text{C}_{25}\text{H}_{22}\text{As}_2)]$   
 $M_r = 937.11$   
 Monoclinic,  $C2/c$   
 $a = 22.7171$  (18) Å  
 $b = 7.3151$  (6) Å  
 $c = 18.2047$  (15) Å  
 $\beta = 120.342$  (8)°

$V = 2610.8$  (4) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 13.96$  mm<sup>-1</sup>  
 $T = 173$  K  
 $0.24 \times 0.20 \times 0.18$  mm

#### Data collection

Stoe IPDS diffractometer  
 Absorption correction: analytical  
 [from crystal shape; *X-SHAPE*  
 and *X-RED* in *IPDS Software*  
 (Stoe & Cie, 1998)]  
 $T_{\min} = 0.051$ ,  $T_{\max} = 0.083$

12353 measured reflections  
 2790 independent reflections  
 2431 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.062$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$   
 $wR(F^2) = 0.055$   
 $S = 0.96$   
 2790 reflections

142 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.65$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.70$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

|  |            |         |             |
|--|------------|---------|-------------|
| Au1—As1                                      | 2.3426 (5) | Au1—Cl1 | 2.2887 (16) |
| As1—Au1—Cl1                                  | 174.82 (4) |         |             |
| Symmetry code: (i) $-x, y, -z + \frac{1}{2}$ |            |         |             |

**Table 2**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                                      | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C1}-\text{H1A}\cdots\text{Cl1}^{\text{ii}}$ | 0.99  | 2.70        | 3.658 (4)   | 163           |

 Symmetry code: (ii)  $-x, y + 1, -z + \frac{1}{2}$ 

Data collection: *IPDS Software* (Stoe & Cie, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

This work was supported by the Bundesministerium für Bildung und Forschung (BMBF).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2133).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m281 [ doi:10.1107/S1600536809004802 ]

## $\mu$ -Bis(diphenylarsino)methane- $\kappa^2$ As:As'-bis[chloridogold(I)]

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### Comment

The title compound was prepared from dpam [dpam = bis(diphenylarsino)methane] and (tht)AuCl (tht = tetrahydrothiophene) in methylene chloride in nearly quantitative yields. It is isomorphous to the crystal structure of the phosphorus congener [dppm(AuCl)<sub>2</sub>], which was determined by Schmidbaur *et al.* (1977b) [ $a = 22.31(1) \text{ \AA}$ ,  $b = 7.215(7) \text{ \AA}$ ,  $c = 18.12(1) \text{ \AA}$  and  $\beta = 120.43(8)^\circ$ ]. The structure consists of discrete molecules of [dpam(AuCl)<sub>2</sub>] disposed about a crystallographic twofold axis, which passes through the Cl atom. The Au atom is in a standard linear coordination [As—Au—Cl 174.82(4)°] with As—Au and Au—Cl bond lengths of 2.3426(5) and 2.289(2) Å, respectively. The Au—As⋯As—Au torsion angle is 66.78(2)°, yielding a staggered conformation of both Ph<sub>2</sub>AsAuCl moieties and an intramolecular Au⋯Au distance of 3.4285(4) Å, indicative of attractive aurophilic interactions. The shortest intermolecular Au⋯Au distance is 5.863 Å. In its crystal, the complexes are linked to infinite chains *via* weak C—H⋯Cl intermolecular hydrogen bonds with C⋯Cl distance of 3.658(4) Å and a C1—H1a⋯Cl1<sup>ii</sup> angle of 163° (symmetry code: (ii)  $-x, y + 1, -z + 1/2$ ).

For comparison, the geometrical data of the phosphorus compound are: Au—P 2.238(5), Au—Cl 2.288(7), Au⋯Au 3.351(2) Å, P—Au—Cl 175(2), Au—P⋯P—Au 67(1)°. It should be noted, that a second polymorph of the phosphorus complex exists: Unlike the herein presented structure, there are no aurophilic bonds between the gold(I) atoms (Healy, 2003).

All attempts to prepare the 1:1 complex [(dpamAuCl)<sub>2</sub>] starting from the title compound analogous to the published synthesis of phosphorus complex [(dppmAuCl)<sub>2</sub>] (Schmidbaur *et al.*, 1977a) failed.

### Experimental

The title compound was prepared analogously to a previously published procedure (Monkowius *et al.*, 2003a,b): dpam (0.22 g, 0.47 mmol) and (tht)AuCl (0.30 g, 0.94 mmol, tht = tetrahydrothiophene) were stirred in methylene chloride (20 ml) at room temperature for 2 h. The product was precipitated with *n*-pentane and isolated by filtration. Recrystallization from methylene chloride/diethyl ether yields colourless crystals suitable for X-ray crystallography. Yield: 0.40 g (0.43 mmol, 91%); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): 7.55–7.60 (m, Ph—H, 8 H), 7.37–7.51 (m, Ph—H, 12 H), 3.48 p.p.m. (s, CH<sub>2</sub>, 2 H); <sup>13</sup>C NMR (75.5 MHz, CDCl<sub>3</sub>): 134.63, 132.93, 130.44, 129.23, 25.08 p.p.m.; MS (ESI):  $m/z$  (%) = 1605.3 [L<sub>2</sub>Au<sub>3</sub>Cl<sub>2</sub>]<sup>+</sup> (5), 1373.3 [L<sub>2</sub>Au<sub>3</sub>Cl]<sup>+</sup> (47), 1141.3 [L<sub>2</sub>Au]<sup>+</sup> (76), 901.1 [M—Cl]<sup>+</sup> (25), 669.2 [LAu]<sup>+</sup> (100); EA (C<sub>25</sub>H<sub>22</sub>As<sub>2</sub>Au<sub>2</sub>Cl<sub>2</sub>) calc.: C 32.04, H 2.37, found: C 32.01, H 2.37.

### Refinement

The H atoms were positioned with idealized geometry and were refined isotropic using a riding model with C—H = 0.95 and 0.99 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Figures

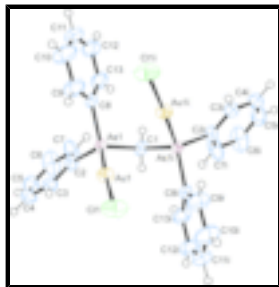


Fig. 1. View of the title compound with the atom numbering scheme (symmetry code: (i)  $-x, y, -z + 1/2$ ). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

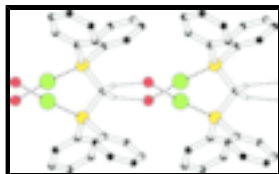


Fig. 2. Crystal structure of the title compound depicting the intermolecular hydrogen bonds between H1A and Cl1<sup>ii</sup> (symmetry code: (ii)  $-x, y + 1, -z + 1/2$ ). The H atoms not involved in hydrogen bonding have been omitted.

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### Crystal data

[Au<sub>2</sub>Cl<sub>2</sub>(C<sub>25</sub>H<sub>22</sub>As<sub>2</sub>)]

$M_r = 937.11$

Monoclinic,  $C2/c$

Hall symbol:  $-C\ 2yc$

$a = 22.7171$  (18) Å

$b = 7.3151$  (6) Å

$c = 18.2047$  (15) Å

$\beta = 120.342$  (8)°

$V = 2610.8$  (4) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1720$

Cell parameters were determined by indexing 8000 reflections with  $I/\sigma$  limit 6.0.

$D_x = 2.384$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 8000 reflections

$\theta = 2.1$ – $26.9$ °

$\mu = 13.96$  mm<sup>-1</sup>

$T = 173$  K

Prism, colourless

$0.24 \times 0.20 \times 0.18$  mm

### Data collection

Stoe IPDS diffractometer

2790 independent reflections

Radiation source: fine-focus sealed tube

2431 reflections with  $I > 2\sigma(I)$

Monochromator: graphite

$R_{int} = 0.062$

$T = 173$  K

$\theta_{max} = 26.9$ °

rotation scans

$\theta_{min} = 2.1$ °

Absorption correction: analytical

[from crystal shape; *X-SHAPE* and *X-RED* in *IPDS Software* (Stoe & Cie, 1998)]  $h = -28 \rightarrow 28$

$T_{min} = 0.051, T_{max} = 0.083$

$k = -9 \rightarrow 9$

12353 measured reflections

$l = -22 \rightarrow 22$

Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Hydrogen site location: inferred from neighbouring sites   |
| Least-squares matrix: full                                     | H-atom parameters constrained  |
| $R[F^2 > 2\sigma(F^2)] = 0.023$                                | $w = 1/[\sigma^2(F_o^2) + (0.0315P)^2]$  |
| $wR(F^2) = 0.055$  | where $P = (F_o^2 + 2F_c^2)/3$   |
| $S = 0.96$   | $(\Delta/\sigma)_{\max} = 0.001$   |
| 2790 reflections   | $\Delta\rho_{\max} = 1.65 \text{ e } \text{\AA}^{-3}$  |
| 142 parameters   | $\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$   |
| Primary atom site location: structure-invariant direct methods | Extinction correction: SHELXL97 (Sheldrick, 2008),<br>$F_c^* = kF_c[1+0.001F_c^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Secondary atom site location: difference Fourier map           | Extinction coefficient: 0.00085 (4)  |

Special details

**Experimental.** Data were collected applying an imaging plate system (Stoe) with the following measurement parameters:

Detector distance [mm] 65 Phi movement mode Oscillation Phi incr. [degrees] 1.2 Number of exposures 200 Irradiation / exposure [min] 2.00

For a detailed description of the method see: Sheldrick, G. M., Paulus, E., Vertesy, L. & Hahn, F. (1995). Acta Cryst. B51, 89–98.

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 ( $\text{\AA}^2$ )

|     | $x$           | $y$          | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| Au1 | 0.00458 (1)   | 0.59917 (2)  | 0.15885 (1)  | 0.0364 (1)                       |
| As1 | -0.05684 (2)  | 0.86199 (5)  | 0.15224 (2)  | 0.0286 (1)                       |
| Cl1 | 0.07339 (7)   | 0.35726 (17) | 0.17281 (11) | 0.0617 (5)                       |
| C1  | 0.00000       | 1.0152 (8)   | 0.25000      | 0.0335 (16)                      |
| C2  | -0.08392 (19) | 1.0208 (6)   | 0.0560 (3)   | 0.0345 (11)                      |
| C3  | -0.0783 (2)   | 0.9600 (7)   | -0.0115 (3)  | 0.0430 (14)                      |
| C4  | -0.0981 (2)   | 1.0716 (9)   | -0.0818 (3)  | 0.0553 (18)                      |
| C5  | -0.1228 (2)   | 1.2445 (8)   | -0.0834 (3)  | 0.0583 (17)                      |
| C6  | -0.1289 (3)   | 1.3050 (8)   | -0.0165 (4)  | 0.074 (2)                        |
| C7  | -0.1091 (3)   | 1.1941 (7)   | 0.0543 (3)   | 0.0640 (19)                      |
| C8  | -0.13949 (18) | 0.8231 (6)   | 0.1565 (2)   | 0.0330 (10)                      |

## supplementary materials

|      |             |             |            |             |
|------|-------------|-------------|------------|-------------|
| C9   | -0.1733 (3) | 0.6586 (8)  | 0.1285 (4) | 0.0591 (19) |
| C10  | -0.2351 (3) | 0.6299 (9)  | 0.1269 (5) | 0.078 (2)   |
| C11  | -0.2608 (2) | 0.7632 (10) | 0.1543 (4) | 0.0641 (18) |
| C12  | -0.2273 (3) | 0.9248 (9)  | 0.1831 (4) | 0.064 (2)   |
| C13  | -0.1665 (2) | 0.9580 (8)  | 0.1839 (3) | 0.0515 (16) |
| H1A  | -0.02910    | 1.09450     | 0.26260    | 0.0400*     |
| H3A  | -0.06070    | 0.84140     | -0.01000   | 0.0520*     |
| H4A  | -0.09480    | 1.02880     | -0.12880   | 0.0660*     |
| H5A  | -0.13560    | 1.32180     | -0.13100   | 0.0700*     |
| H6A  | -0.14670    | 1.42340     | -0.01840   | 0.0890*     |
| H7A  | -0.11280    | 1.23700     | 0.10110    | 0.0770*     |
| H9A  | -0.15470    | 0.56450     | 0.11040    | 0.0720*     |
| H10A | -0.25880    | 0.51740     | 0.10660    | 0.0930*     |
| H11A | -0.30250    | 0.74360     | 0.15340    | 0.0760*     |
| H12A | -0.24560    | 1.01640     | 0.20300    | 0.0770*     |
| H13A | -0.14390    | 1.07230     | 0.20310    | 0.0620*     |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$    | $U^{22}$   | $U^{33}$    | $U^{12}$     | $U^{13}$    | $U^{23}$     |
|-----|-------------|------------|-------------|--------------|-------------|--------------|
| Au1 | 0.0406 (1)  | 0.0289 (1) | 0.0443 (1)  | 0.0048 (1)   | 0.0248 (1)  | 0.0023 (1)   |
| As1 | 0.0285 (2)  | 0.0273 (2) | 0.0273 (2)  | 0.0012 (1)   | 0.0121 (1)  | -0.0007 (2)  |
| Cl1 | 0.0723 (8)  | 0.0355 (6) | 0.1015 (11) | 0.0191 (6)   | 0.0618 (8)  | 0.0183 (7)   |
| C1  | 0.026 (2)   | 0.032 (3)  | 0.034 (3)   | 0.0000       | 0.009 (2)   | 0.0000       |
| C2  | 0.0340 (18) | 0.032 (2)  | 0.0292 (19) | -0.0015 (16) | 0.0098 (15) | 0.0020 (16)  |
| C3  | 0.0330 (19) | 0.057 (3)  | 0.037 (2)   | 0.0046 (19)  | 0.0163 (17) | 0.004 (2)    |
| C4  | 0.041 (2)   | 0.087 (4)  | 0.041 (3)   | 0.004 (2)    | 0.023 (2)   | 0.014 (3)    |
| C5  | 0.054 (3)   | 0.065 (3)  | 0.044 (3)   | -0.007 (3)   | 0.016 (2)   | 0.017 (3)    |
| C6  | 0.107 (5)   | 0.036 (3)  | 0.058 (3)   | 0.010 (3)    | 0.026 (3)   | 0.011 (3)    |
| C7  | 0.106 (4)   | 0.038 (3)  | 0.038 (3)   | 0.010 (3)    | 0.029 (3)   | 0.001 (2)    |
| C8  | 0.0248 (16) | 0.041 (2)  | 0.0267 (18) | -0.0002 (16) | 0.0082 (14) | -0.0010 (17) |
| C9  | 0.051 (3)   | 0.049 (3)  | 0.084 (4)   | -0.013 (2)   | 0.039 (3)   | -0.021 (3)   |
| C10 | 0.058 (3)   | 0.071 (4)  | 0.108 (5)   | -0.028 (3)   | 0.045 (4)   | -0.019 (4)   |
| C11 | 0.035 (2)   | 0.092 (4)  | 0.065 (3)   | -0.008 (3)   | 0.025 (2)   | 0.001 (3)    |
| C12 | 0.043 (3)   | 0.087 (4)  | 0.065 (4)   | 0.006 (3)    | 0.029 (2)   | -0.015 (3)   |
| C13 | 0.040 (2)   | 0.054 (3)  | 0.057 (3)   | -0.006 (2)   | 0.022 (2)   | -0.017 (2)   |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|         |             |                     |            |
|---------|-------------|---------------------|------------|
| Au1—As1 | 2.3426 (5)  | C11—C12             | 1.360 (10) |
| Au1—Cl1 | 2.2887 (16) | C12—C13             | 1.395 (9)  |
| As1—C1  | 1.941 (3)   | C1—H1A              | 0.9900     |
| As1—C2  | 1.926 (5)   | C1—H1A <sup>i</sup> | 0.9900     |
| As1—C8  | 1.939 (5)   | C3—H3A              | 0.9500     |
| C2—C3   | 1.372 (7)   | C4—H4A              | 0.9500     |
| C2—C7   | 1.385 (7)   | C5—H5A              | 0.9500     |
| C3—C4   | 1.388 (7)   | C6—H6A              | 0.9500     |
| C4—C5   | 1.378 (9)   | C7—H7A              | 0.9500     |

|                         |             |                                       |        |
|-------------------------|-------------|---------------------------------------|--------|
| C5—C6                   | 1.367 (8)   | C9—H9A                                | 0.9500 |
| C6—C7                   | 1.391 (8)   | C10—H10A                              | 0.9500 |
| C8—C9                   | 1.379 (8)   | C11—H11A                              | 0.9500 |
| C8—C13                  | 1.381 (7)   | C12—H12A                              | 0.9500 |
| C9—C10                  | 1.405 (11)  | C13—H13A                              | 0.9500 |
| C10—C11                 | 1.355 (10)  |                                       |        |
| Au1…C6 <sup>ii</sup>    | 3.773 (6)   | C1…H13A <sup>i</sup>                  | 2.9600 |
| Au1…C7 <sup>ii</sup>    | 3.756 (6)   | C1…H13A                               | 2.9600 |
| Au1…C4 <sup>iii</sup>   | 3.910 (6)   | C1…H7A                                | 3.0900 |
| Au1…C5 <sup>iii</sup>   | 3.759 (5)   | C3…H11A <sup>viii</sup>               | 3.0300 |
| Au1…C8 <sup>i</sup>     | 3.601 (4)   | C4…H11A <sup>viii</sup>               | 3.0200 |
| Au1…C9 <sup>i</sup>     | 3.857 (7)   | C13…H1A                               | 2.8800 |
| Au1…Au1 <sup>i</sup>    | 3.4286 (4)  | C13…H4A <sup>ix</sup>                 | 2.9500 |
| Au1…H7A <sup>ii</sup>   | 3.5200      | H1A…C13                               | 2.8800 |
| Au1…H9A                 | 3.2700      | H1A…H13A                              | 2.2700 |
| Au1…H3A                 | 3.1900      | H1A…C11 <sup>x</sup>                  | 2.7000 |
| Au1…H6A <sup>ii</sup>   | 3.5600      | H3A…Au1                               | 3.1900 |
| Au1…H4A <sup>iii</sup>  | 3.6100      | H4A…Au1 <sup>iii</sup>                | 3.6100 |
| Au1…H5A <sup>iii</sup>  | 3.3100      | H4A…C11 <sup>v</sup>                  | 3.0400 |
| C11…H1A <sup>iv</sup>   | 2.7000      | H4A…C13 <sup>xi</sup>                 | 2.9500 |
| C11…H13A <sup>iv</sup>  | 2.8900      | H5A…Au1 <sup>iii</sup>                | 3.3100 |
| C11…H4A <sup>v</sup>    | 3.0400      | H5A…C11 <sup>iii</sup>                | 3.0300 |
| C11…H5A <sup>iii</sup>  | 3.0300      | H6A…Au1 <sup>vii</sup>                | 3.5600 |
| C11…H11A <sup>vi</sup>  | 3.1300      | H7A…Au1 <sup>vii</sup>                | 3.5200 |
| C3…C3 <sup>iii</sup>    | 3.416 (8)   | H7A…C1                                | 3.0900 |
| C3…C4 <sup>iii</sup>    | 3.481 (7)   | H7A…H13A                              | 2.5900 |
| C4…Au1 <sup>iii</sup>   | 3.910 (6)   | H9A…Au1                               | 3.2700 |
| C4…C3 <sup>iii</sup>    | 3.481 (7)   | H11A…C11 <sup>xii</sup>               | 3.1300 |
| C5…Au1 <sup>iii</sup>   | 3.759 (5)   | H11A…C3 <sup>viii</sup>               | 3.0300 |
| C6…Au1 <sup>vii</sup>   | 3.773 (6)   | H11A…C4 <sup>viii</sup>               | 3.0200 |
| C7…Au1 <sup>vii</sup>   | 3.756 (6)   | H13A…C1                               | 2.9600 |
| C8…Au1 <sup>i</sup>     | 3.601 (4)   | H13A…H1A                              | 2.2700 |
| C9…Au1 <sup>i</sup>     | 3.857 (7)   | H13A…H7A                              | 2.5900 |
| C1…H7A <sup>i</sup>     | 3.0900      | H13A…C11 <sup>x</sup>                 | 2.8900 |
| As1—Au1—C11             | 174.82 (4)  | As1—C1—H1A <sup>i</sup>               | 110.00 |
| Au1—As1—C1              | 108.88 (12) | As1 <sup>i</sup> —C1—H1A              | 110.00 |
| Au1—As1—C2              | 116.75 (14) | H1A—C1—H1A <sup>i</sup>               | 108.00 |
| Au1—As1—C8              | 116.18 (13) | As1 <sup>i</sup> —C1—H1A <sup>i</sup> | 110.00 |
| C1—As1—C2               | 104.16 (19) | C2—C3—H3A                             | 120.00 |
| C1—As1—C8               | 104.90 (11) | C4—C3—H3A                             | 120.00 |
| C2—As1—C8               | 104.72 (19) | C3—C4—H4A                             | 120.00 |
| As1—C1—As1 <sup>i</sup> | 109.5 (3)   | C5—C4—H4A                             | 120.00 |

## supplementary materials

|                             |              |                 |            |
|-----------------------------|--------------|-----------------|------------|
| As1—C2—C3                   | 119.2 (3)    | C4—C5—H5A       | 120.00     |
| As1—C2—C7                   | 120.7 (4)    | C6—C5—H5A       | 120.00     |
| C3—C2—C7                    | 120.1 (4)    | C5—C6—H6A       | 120.00     |
| C2—C3—C4                    | 120.1 (5)    | C7—C6—H6A       | 120.00     |
| C3—C4—C5                    | 119.9 (5)    | C2—C7—H7A       | 120.00     |
| C4—C5—C6                    | 120.1 (5)    | C6—C7—H7A       | 120.00     |
| C5—C6—C7                    | 120.4 (6)    | C8—C9—H9A       | 120.00     |
| C2—C7—C6                    | 119.4 (5)    | C10—C9—H9A      | 120.00     |
| As1—C8—C9                   | 118.9 (4)    | C9—C10—H10A     | 120.00     |
| As1—C8—C13                  | 121.7 (4)    | C11—C10—H10A    | 120.00     |
| C9—C8—C13                   | 119.4 (5)    | C10—C11—H11A    | 120.00     |
| C8—C9—C10                   | 120.1 (6)    | C12—C11—H11A    | 120.00     |
| C9—C10—C11                  | 119.8 (6)    | C11—C12—H12A    | 119.00     |
| C10—C11—C12                 | 120.4 (6)    | C13—C12—H12A    | 120.00     |
| C11—C12—C13                 | 120.9 (6)    | C8—C13—H13A     | 120.00     |
| C8—C13—C12                  | 119.3 (5)    | C12—C13—H13A    | 120.00     |
| As1—C1—H1A                  | 110.00       |                 |            |
| Au1—As1—C1—As1 <sup>i</sup> | -34.87 (4)   | C3—C2—C7—C6     | 0.4 (9)    |
| C2—As1—C1—As1 <sup>i</sup>  | -160.10 (16) | C7—C2—C3—C4     | -0.3 (8)   |
| C8—As1—C1—As1 <sup>i</sup>  | 90.12 (13)   | As1—C2—C7—C6    | -179.4 (5) |
| Au1—As1—C2—C3               | 12.2 (5)     | C2—C3—C4—C5     | 0.7 (8)    |
| C1—As1—C2—C3                | 132.3 (4)    | C3—C4—C5—C6     | -1.1 (8)   |
| C8—As1—C2—C3                | -117.9 (4)   | C4—C5—C6—C7     | 1.2 (10)   |
| Au1—As1—C2—C7               | -168.1 (4)   | C5—C6—C7—C2     | -0.8 (10)  |
| C1—As1—C2—C7                | -48.1 (5)    | As1—C8—C9—C10   | -176.9 (5) |
| C8—As1—C2—C7                | 61.9 (5)     | C13—C8—C9—C10   | 0.8 (8)    |
| C2—As1—C8—C9                | 104.0 (4)    | As1—C8—C13—C12  | 177.9 (4)  |
| Au1—As1—C8—C9               | -26.4 (4)    | C9—C8—C13—C12   | 0.3 (7)    |
| C1—As1—C8—C9                | -146.6 (4)   | C8—C9—C10—C11   | -1.1 (10)  |
| C2—As1—C8—C13               | -73.6 (4)    | C9—C10—C11—C12  | 0.2 (11)   |
| Au1—As1—C8—C13              | 156.0 (3)    | C10—C11—C12—C13 | 1.0 (10)   |
| C1—As1—C8—C13               | 35.7 (4)     | C11—C12—C13—C8  | -1.2 (8)   |
| As1—C2—C3—C4                | 179.4 (4)    |                 |            |

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

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

| $D-H\cdots A$                    | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C1—H1A $\cdots$ C11 <sup>x</sup> | 0.99  | 2.70        | 3.658 (4)   | 163           |

Symmetry codes: (x)  $-x, y+1, -z+1/2$ .

Fig. 1

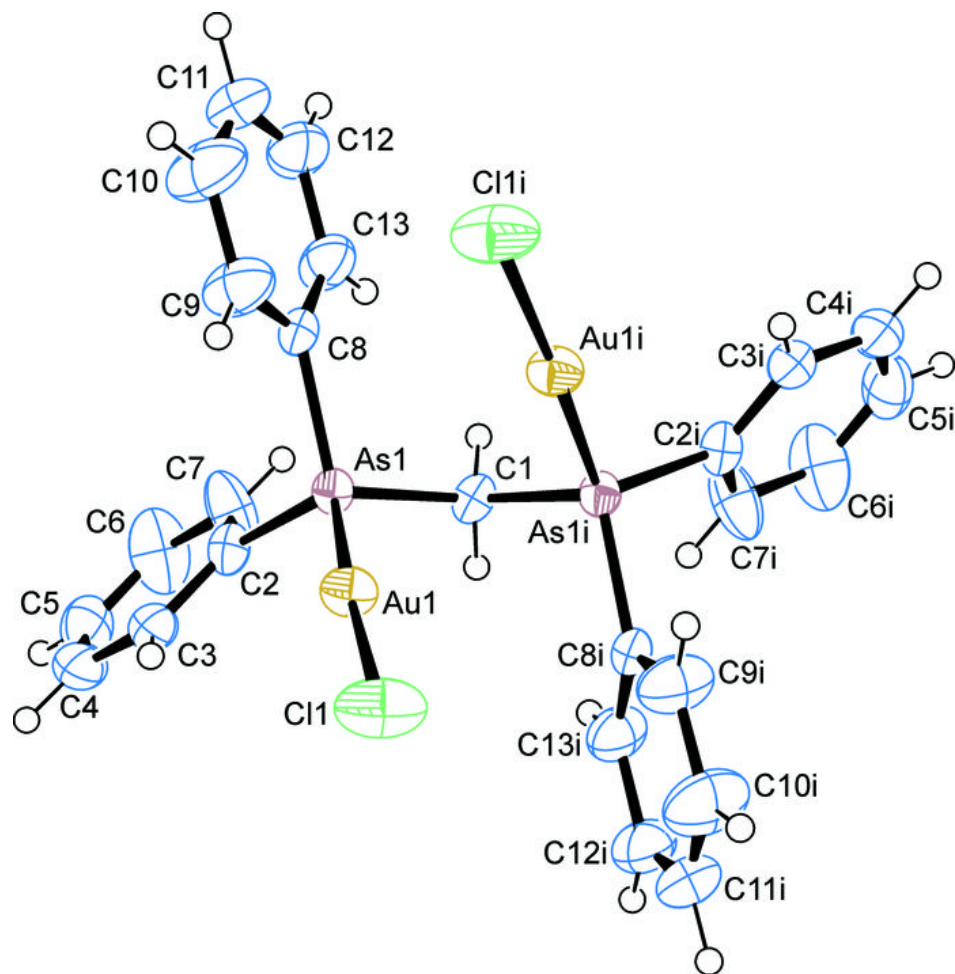


Fig. 2

