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[μ-Ferrocene-1,1′-diylbis(diphenylphosphine)-κ^2P:P']bis[chloridogold(I)]

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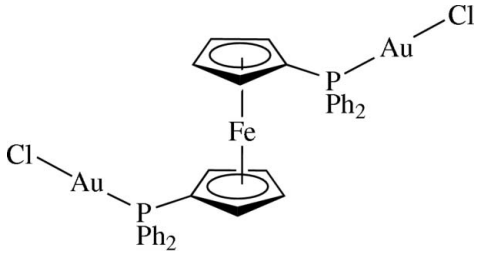
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.023; wR factor = 0.060; data-to-parameter ratio = 24.4.

A triclinic polymorph of the title compound, $[Au_2Cl_2\{Fe(C_{17}H_{14}P)_2\}]$ or $C_{34}H_{28}Au_2Cl_2FeP_2$, for which a monoclinic structure has already been found, is reported. It contains two linear gold(I) centres bridged by a 1,1′-bis(diphenylphosphine)ferrocenyl ligand. Molecules assemble into a three-dimensional network through weak Cl···HC$_{phenyl}$ hydrogen bonds.

Related literature

For related literature, see: Allen (2002); Bruno *et al.* (2002); Canales *et al.* (1997); Constable *et al.* (2007); Crespo *et al.* (2000); Desiraju & Steiner (1999); Gimeno *et al.* (1993); Hill *et al.* (1989).



Experimental

Crystal data

$[Au_2Cl_2\{Fe(C_{17}H_{14}P)_2\}]$
M_r = 1019.23
Triclinic, $P\overline{1}$
a = 8.6273 (1) Å
b = 9.0401 (1) Å
c = 10.3715 (1) Å
α = 80.9701 (7)°
β = 86.0279 (7)°
γ = 81.6056 (7)°
V = 789.42 (1) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 10.02 mm^{-1}
T = 173 K
0.15 × 0.08 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.41, T_{max} = 0.74
9181 measured reflections
4616 independent reflections
4217 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 0.97
4592 reflections
188 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.50 e Å^{-3}
$\Delta\rho_{min}$ = −1.28 e Å^{-3}

Table 1
Intermolecular contacts (Å, °).

*Cg*1 and *Cg*2 are the centroids of the cyclopentadienyl and C6–C11 phenyl rings, respectively.

D—H···A	H···A	D···A	D—H···A
C8—H6···Cl1^{i}	2.73	3.703 (4)	166
C13—H10···Cl1^{ii}	2.80	3.653 (4)	144
C14—H11···Cl1^{iii}	2.86	3.796 (4)	156
*Cg*1···H14—C17^{iv}	3.31	3.71	137
*Cg*2···H4—C5^{iv}	2.84	3.67	141

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

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CRYSTALS*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2366).

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supplementary materials

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[μ-Ferrocene-1,1'-diylbis(diphenylphosphine)-κ^2*P*:*P*']bis[chloridogold(I)]

E. C. Constable, C. E. Housecroft, M. Neuburger, S. Schaffner and E. Shardlow

Comment

The structure of unsolvated **I** has previously been reported (Crespo *et al.*, 2000) as has the structure of **I**·2CH_2Cl_2 (Canales *et al.*, 1997). During the course of our investigations of 2,2':6',2''-terpyridine ligands functionalized in the 4'-position with alkyl gold(I) phosphine moieties (Constable *et al.*, 2007), we have prepared a number of gold(I) phosphine derivatives including compound **I**. Crystals grown from CH_3CN proved to be a polymorph, **Ia**, (triclinic, $P\bar{1}$) of those grown by Crespo *et al.* from CH_2Cl_2/*n*-heptane, **Ib**, (monoclinic, $P2_1/n$, refcode XEGGEV) (CSD, Version 5.2.7; Allen, 2002; Bruno *et al.*, 2002). The molecular structure of **Ia** is shown in Fig. 1. In both this and **Ib**, the Fe atom lies on an inversion centre. Bond distances are angles are unexceptional and show little variation between polymorphs. The difference in the structures is in the orientation of the phenyl rings and the effect that this has on the molecular packing. The hydrogen bond acceptor strength of an M—Cl chlorine atom is greater than that of a CCl group, and examples of CH···ClM interactions in the solid state have been recognized for some time (Desiraju & Steiner, 1999). Fig. 2 compares the CH···Cl close contacts that exist in polymorphs **Ia** and **Ib**, and details of those in **Ia** are given in Table 1. In **Ia**, CH···Cl interactions involving H6 connect molecules into chains running parallel to the crystallographic *b* axis. These chains are interconnected by interactions involving H10 such that the lattice is extended in the *c* direction, while contacts involving H11 extend the lattice in the *a* direction. In addition to these non-classical hydrogen bonds, the molecular packing in **Ia** involves $CH_{phenyl}\cdots\pi_{cyclopentadienyl}$ and $CH_{cyclopentadienyl}\cdots\pi_{phenyl}$ interactions (Table 1). The differences between the molecular structures of **Ia** and **Ib** are relatively small, but are sufficient to cause significant differences in assembly of molecules in the crystal lattice.

Experimental

Crystals of compound **I** (Hill *et al.*, 1989; Gimeno *et al.*, 1993) were grown from a CH_3CN solution by slow evaporation at room temperature.

Refinement

All H atoms were treated as riding models, with C—H = 1.00 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

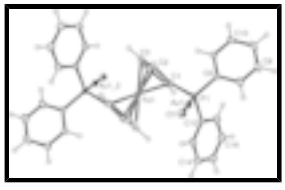
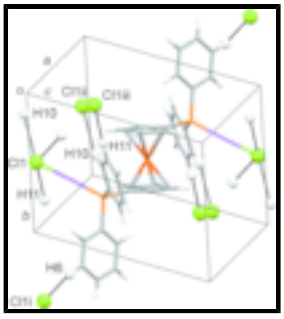
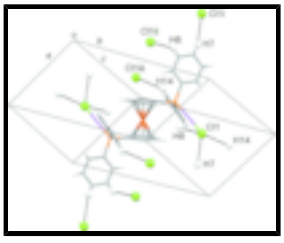


Fig. 1. The molecular structure of **Ia** with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitary radius.
Fig. 2 Close Cl···HC contacts in (*a*) **Ia** (symmetry codes: i = *x*, −1 + *y*, *z*; ii = 1 – *x*, 1 – *y*, 2 – *z*; iii = – 1 + *x*, *y*, *z*) and (*b*) **Ib** (CSD refcode XEGGEV) (symmetry codes: i = −1 + *x*, *y*, −1 + *z*; ii = –*x*, 1 –*y*, 1 – *z*; iii = *x*, *y*, −1 + *z*).





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Crystal data

$[Au_2Cl_2\{Fe(C_{17}H_{14}P)_2\}]$	$Z = 1$
$M_r = 1019.23$	$F_{000} = 480$
Triclinic, $P\overline{1}$	$D_x = 2.144$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.62730$ (10) Å	Cell parameters from 4616 reflections
$b = 9.04010$ (10) Å	$\theta = 1$–30º
$c = 10.37150$ (10) Å	$\mu = 10.02$ mm^{-1}
$\alpha = 80.9701$ (7)º	$T = 173$ K
$\beta = 86.0279$ (7)º	Plate, colourless
$\gamma = 81.6056$ (7)º	0.15 × 0.08 × 0.03 mm
$V = 789.417$ (14) Å^3	

Data collection

Nonius KappaCCD diffractometer	4217 reflections with $I > 2.0\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 173$ K	$\theta_{max} = 30.0$º
φ & ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (DENZO/SCALEPACK; Otwinowski & Minor, 1997)	$h = -11\rightarrow12$
$T_{min} = 0.41$, $T_{max} = 0.74$	$k = -12\rightarrow12$
9181 measured reflections	$l = -14\rightarrow14$
4616 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.023$	Method = Modified Sheldrick (1997) $w = 1/[\sigma^2(F^2) + (0.04P)^2 + 0.29P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$wR(F^2) = 0.060$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.97$	$\Delta\rho_{max} = 1.50$ e Å^{-3}
4592 reflections	$\Delta\rho_{min} = -1.28$ e Å^{-3}
188 parameters	Extinction correction: Larson (1970), Equation 22
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 17.7 (19)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.676196 (12)	0.288418 (11)	0.887313 (10)	0.0239
Fe1	0.5000	0.5000	0.5000	0.0196
P1	0.58777 (9)	0.18016 (8)	0.73340 (7)	0.0200
Cl1	0.77243 (11)	0.39466 (9)	1.04541 (8)	0.0322
C1	0.5978 (3)	0.2875 (3)	0.5729 (3)	0.0217
C2	0.7182 (3)	0.3798 (3)	0.5271 (3)	0.0270
C3	0.6988 (4)	0.4300 (4)	0.3915 (3)	0.0330
C4	0.5690 (4)	0.3719 (4)	0.3530 (3)	0.0317
C5	0.5056 (4)	0.2828 (3)	0.4649 (3)	0.0257
C6	0.7023 (3)	−0.0012 (3)	0.7130 (3)	0.0230
C7	0.7062 (4)	−0.1191 (4)	0.8177 (3)	0.0379
C8	0.7948 (5)	−0.2580 (4)	0.8063 (4)	0.0435
C9	0.8807 (4)	−0.2802 (4)	0.6918 (4)	0.0387
C10	0.8771 (4)	−0.1646 (4)	0.5876 (4)	0.0373
C11	0.7883 (4)	−0.0242 (3)	0.5984 (3)	0.0277
C12	0.3878 (3)	0.1418 (3)	0.7685 (3)	0.0214
C13	0.2850 (4)	0.2409 (4)	0.8355 (3)	0.0281
C14	0.1308 (4)	0.2151 (4)	0.8643 (4)	0.0366
C15	0.0793 (4)	0.0893 (5)	0.8311 (4)	0.0396
C16	0.1833 (4)	−0.0119 (4)	0.7659 (4)	0.0380
C17	0.3355 (4)	0.0154 (4)	0.7331 (3)	0.0324
H1	0.8008	0.4037	0.5807	0.0323*
H2	0.7659	0.4961	0.3329	0.0374*
H3	0.5282	0.3898	0.2631	0.0375*
H4	0.4134	0.2269	0.4672	0.0307*
H5	0.6443	−0.1032	0.9008	0.0445*
H6	0.7974	−0.3419	0.8818	0.0507*
H7	0.9440	−0.3805	0.6840	0.0466*
H8	0.9394	−0.1805	0.5047	0.0444*

H9	0.7862	0.0598	0.5230	0.0341*
H10	0.3232	0.3299	0.8631	0.0347*
H11	0.0564	0.2879	0.9097	0.0446*
H12	−0.0314	0.0699	0.8530	0.0481*
H13	0.1466	−0.1040	0.7429	0.0483*
H14	0.4083	−0.0558	0.6848	0.0409*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.02774 (8)	0.02168 (7)	0.02296 (8)	−0.00291 (4)	−0.00047 (4)	−0.00619 (4)
Fe1	0.0205 (3)	0.0160 (2)	0.0210 (3)	0.0003 (2)	0.0025 (2)	−0.0029 (2)
P1	0.0228 (3)	0.0166 (3)	0.0203 (3)	−0.0005 (3)	0.0000 (3)	−0.0041 (3)
Cl1	0.0438 (4)	0.0305 (4)	0.0254 (4)	−0.0080 (3)	−0.0015 (3)	−0.0108 (3)
C1	0.0243 (13)	0.0166 (12)	0.0226 (13)	0.0014 (10)	0.0014 (10)	−0.0026 (10)
C2	0.0174 (12)	0.0240 (14)	0.0363 (17)	0.0019 (10)	0.0026 (11)	0.0000 (12)
C3	0.0328 (16)	0.0239 (14)	0.0358 (17)	0.0050 (12)	0.0147 (14)	0.0005 (12)
C4	0.0422 (18)	0.0247 (15)	0.0245 (15)	0.0070 (13)	0.0050 (13)	−0.0060 (12)
C5	0.0335 (15)	0.0161 (12)	0.0271 (15)	0.0015 (11)	−0.0009 (12)	−0.0066 (11)
C6	0.0238 (13)	0.0168 (12)	0.0276 (14)	0.0007 (10)	−0.0033 (11)	−0.0035 (10)
C7	0.052 (2)	0.0260 (16)	0.0307 (17)	0.0057 (15)	−0.0018 (15)	0.0016 (13)
C8	0.056 (2)	0.0263 (17)	0.044 (2)	0.0059 (16)	−0.0097 (18)	0.0017 (15)
C9	0.0330 (17)	0.0246 (16)	0.058 (2)	0.0070 (13)	−0.0125 (16)	−0.0112 (15)
C10	0.0261 (15)	0.0291 (16)	0.057 (2)	0.0010 (13)	0.0061 (15)	−0.0164 (16)
C11	0.0277 (14)	0.0229 (14)	0.0318 (16)	−0.0015 (11)	0.0027 (12)	−0.0052 (12)
C12	0.0221 (12)	0.0210 (12)	0.0207 (13)	−0.0018 (10)	−0.0005 (10)	−0.0031 (10)
C13	0.0267 (14)	0.0277 (15)	0.0305 (16)	−0.0014 (12)	0.0007 (12)	−0.0088 (12)
C14	0.0269 (15)	0.044 (2)	0.0368 (18)	0.0015 (14)	0.0048 (13)	−0.0095 (15)
C15	0.0281 (16)	0.050 (2)	0.040 (2)	−0.0112 (15)	−0.0002 (14)	−0.0006 (16)
C16	0.0408 (19)	0.0343 (18)	0.042 (2)	−0.0169 (15)	−0.0013 (15)	−0.0038 (15)
C17	0.0346 (17)	0.0267 (15)	0.0372 (18)	−0.0059 (13)	0.0021 (14)	−0.0093 (13)

Geometric parameters (Å, °)

Au1—P1	2.2283 (7)	C5—H4	1.000
Au1—Cl1	2.2838 (8)	C6—C7	1.395 (4)
Fe1—C3^{i}	2.061 (3)	C6—C11	1.385 (4)
Fe1—C4^{i}	2.061 (3)	C7—C8	1.389 (5)
Fe1—C5^{i}	2.046 (3)	C7—H5	1.000
Fe1—C2^{i}	2.046 (3)	C8—C9	1.382 (6)
Fe1—C1^{i}	2.033 (3)	C8—H6	1.000
Fe1—C1	2.033 (3)	C9—C10	1.379 (5)
Fe1—C2	2.046 (3)	C9—H7	1.000
Fe1—C3	2.061 (3)	C10—C11	1.399 (4)
Fe1—C4	2.061 (3)	C10—H8	1.000
Fe1—C5	2.046 (3)	C11—H9	1.000
P1—C1	1.793 (3)	C12—C13	1.397 (4)
P1—C6	1.821 (3)	C12—C17	1.396 (4)

P1—C12	1.811 (3)	C13—C14	1.389 (5)
C1—C2	1.436 (4)	C13—H10	1.000
C1—C5	1.428 (4)	C14—C15	1.379 (5)
C2—C3	1.422 (5)	C14—H11	1.000
C2—H1	1.000	C15—C16	1.403 (5)
C3—C4	1.411 (5)	C15—H12	1.000
C3—H2	1.000	C16—C17	1.381 (5)
C4—C5	1.429 (4)	C16—H13	1.000
C4—H3	1.000	C17—H14	1.000
P1—Au1—Cl1	178.51 (2)	C1—C2—C3	107.3 (3)
$C3^{i}$—Fe1—$C4^{i}$	40.03 (14)	Fe1—C2—C3	70.32 (17)
$C3^{i}$—Fe1—$C5^{i}$	68.05 (13)	C1—C2—H1	126.2
$C4^{i}$—Fe1—$C5^{i}$	40.72 (12)	Fe1—C2—H1	126.2
$C3^{i}$—Fe1—$C2^{i}$	40.51 (13)	C3—C2—H1	126.4
$C4^{i}$—Fe1—$C2^{i}$	68.30 (14)	C2—C3—Fe1	69.16 (16)
$C5^{i}$—Fe1—$C2^{i}$	68.93 (13)	C2—C3—C4	108.9 (3)
$C3^{i}$—Fe1—$C1^{i}$	68.42 (12)	Fe1—C3—C4	69.99 (17)
$C4^{i}$—Fe1—$C1^{i}$	68.61 (12)	C2—C3—H2	125.6
$C5^{i}$—Fe1—$C1^{i}$	40.98 (12)	Fe1—C3—H2	126.7
$C2^{i}$—Fe1—$C1^{i}$	41.22 (11)	C4—C3—H2	125.4
$C3^{i}$—Fe1—C1	111.58 (12)	C3—C4—Fe1	69.99 (18)
$C4^{i}$—Fe1—C1	111.39 (12)	C3—C4—C5	108.1 (3)
$C5^{i}$—Fe1—C1	139.02 (12)	Fe1—C4—C5	69.07 (17)
$C2^{i}$—Fe1—C1	138.78 (11)	C3—C4—H3	126.1
$C1^{i}$—Fe1—C1	179.994	Fe1—C4—H3	126.6
$C3^{i}$—Fe1—C2	139.49 (13)	C5—C4—H3	125.9
$C4^{i}$—Fe1—C2	111.70 (14)	C4—C5—C1	107.8 (3)
$C5^{i}$—Fe1—C2	111.07 (13)	C4—C5—Fe1	70.21 (17)
$C2^{i}$—Fe1—C2	179.994	C1—C5—Fe1	69.04 (16)
$C1^{i}$—Fe1—C2	138.78 (11)	C4—C5—H4	126.2
$C3^{i}$—Fe1—C3	179.994	C1—C5—H4	126.1
$C4^{i}$—Fe1—C3	139.97 (14)	Fe1—C5—H4	126.3
$C5^{i}$—Fe1—C3	111.95 (13)	P1—C6—C7	118.7 (2)
$C2^{i}$—Fe1—C3	139.49 (13)	P1—C6—C11	122.1 (2)
$C1^{i}$—Fe1—C3	111.58 (12)	C7—C6—C11	119.2 (3)
$C3^{i}$—Fe1—C4	139.97 (14)	C6—C7—C8	120.1 (3)
$C4^{i}$—Fe1—C4	179.994	C6—C7—H5	119.6
$C5^{i}$—Fe1—C4	139.28 (12)	C8—C7—H5	120.2
$C2^{i}$—Fe1—C4	111.70 (14)	C7—C8—C9	120.3 (3)
$C1^{i}$—Fe1—C4	111.39 (12)	C7—C8—H6	119.8
$C3^{i}$—Fe1—C5	111.95 (13)	C9—C8—H6	119.9
$C4^{i}$—Fe1—C5	139.28 (12)	C8—C9—C10	120.0 (3)

C5^{i}—Fe1—C5	179.994	C8—C9—H7	120.0
C2^{i}—Fe1—C5	111.07 (13)	C10—C9—H7	120.1
C1^{i}—Fe1—C5	139.02 (12)	C9—C10—C11	120.0 (3)
C1—Fe1—C2	41.22 (11)	C9—C10—H8	120.0
C1—Fe1—C3	68.42 (12)	C11—C10—H8	120.0
C2—Fe1—C3	40.51 (13)	C10—C11—C6	120.3 (3)
C1—Fe1—C4	68.61 (12)	C10—C11—H9	120.0
C2—Fe1—C4	68.30 (14)	C6—C11—H9	119.7
C3—Fe1—C4	40.03 (14)	P1—C12—C13	118.3 (2)
C1—Fe1—C5	40.98 (12)	P1—C12—C17	122.0 (2)
C2—Fe1—C5	68.93 (13)	C13—C12—C17	119.7 (3)
C3—Fe1—C5	68.05 (13)	C12—C13—C14	119.9 (3)
C4—Fe1—C5	40.72 (12)	C12—C13—H10	119.8
Au1—P1—C1	113.78 (10)	C14—C13—H10	120.3
Au1—P1—C6	112.85 (10)	C13—C14—C15	120.5 (3)
C1—P1—C6	103.33 (13)	C13—C14—H11	119.9
Au1—P1—C12	112.80 (10)	C15—C14—H11	119.6
C1—P1—C12	107.81 (13)	C14—C15—C16	119.5 (3)
C6—P1—C12	105.49 (13)	C14—C15—H12	120.5
P1—C1—Fe1	131.79 (15)	C16—C15—H12	120.0
P1—C1—C2	123.9 (2)	C15—C16—C17	120.4 (3)
Fe1—C1—C2	69.86 (16)	C15—C16—H13	119.6
P1—C1—C5	127.7 (2)	C17—C16—H13	120.0
Fe1—C1—C5	69.98 (15)	C12—C17—C16	119.9 (3)
C2—C1—C5	107.9 (3)	C12—C17—H14	120.1
C1—C2—Fe1	68.93 (15)	C16—C17—H14	120.0

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Table 1 Intermolecular contacts (Å, °)

D—H···A	H···A	D···A	D-H···A	Symmetry code
C8—H6···Cl1^{i}	2.73	3.703 (4)	166	*x*, −1 + *y*, *z*
C13–H10···Cl1^{ii}	2.80	3.653 (4)	144	1 − *x*, 1 − *y*, 2 − *z*
C14—H11···Cl1^{iii}	2.86	3.796 (4)	156	-1 + *x*, *y*, *z*
Cyclopentadienyl(centroid)···H14—C17^{iv}	2.84	3.71	137	1 − *x*,-*y*,1 − *z*
Phenyl(C6–C11)(centroid)···H14—C5^{iv}	2.84	3.67	141	1 − *x*, −*y*, 1 − *z*

Fig. 1

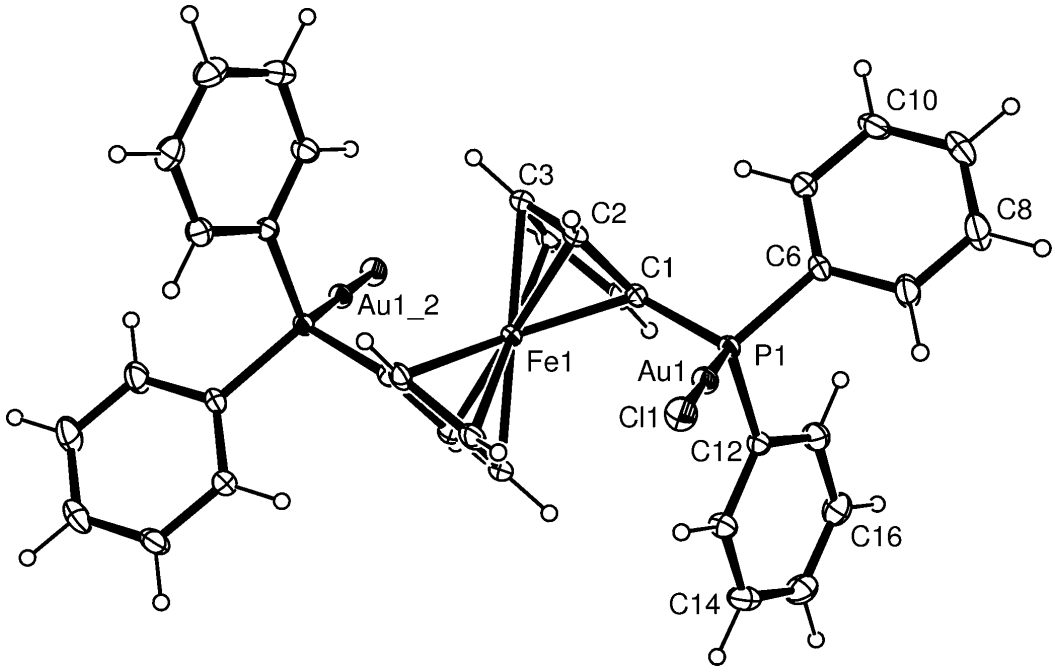

Fig. 2

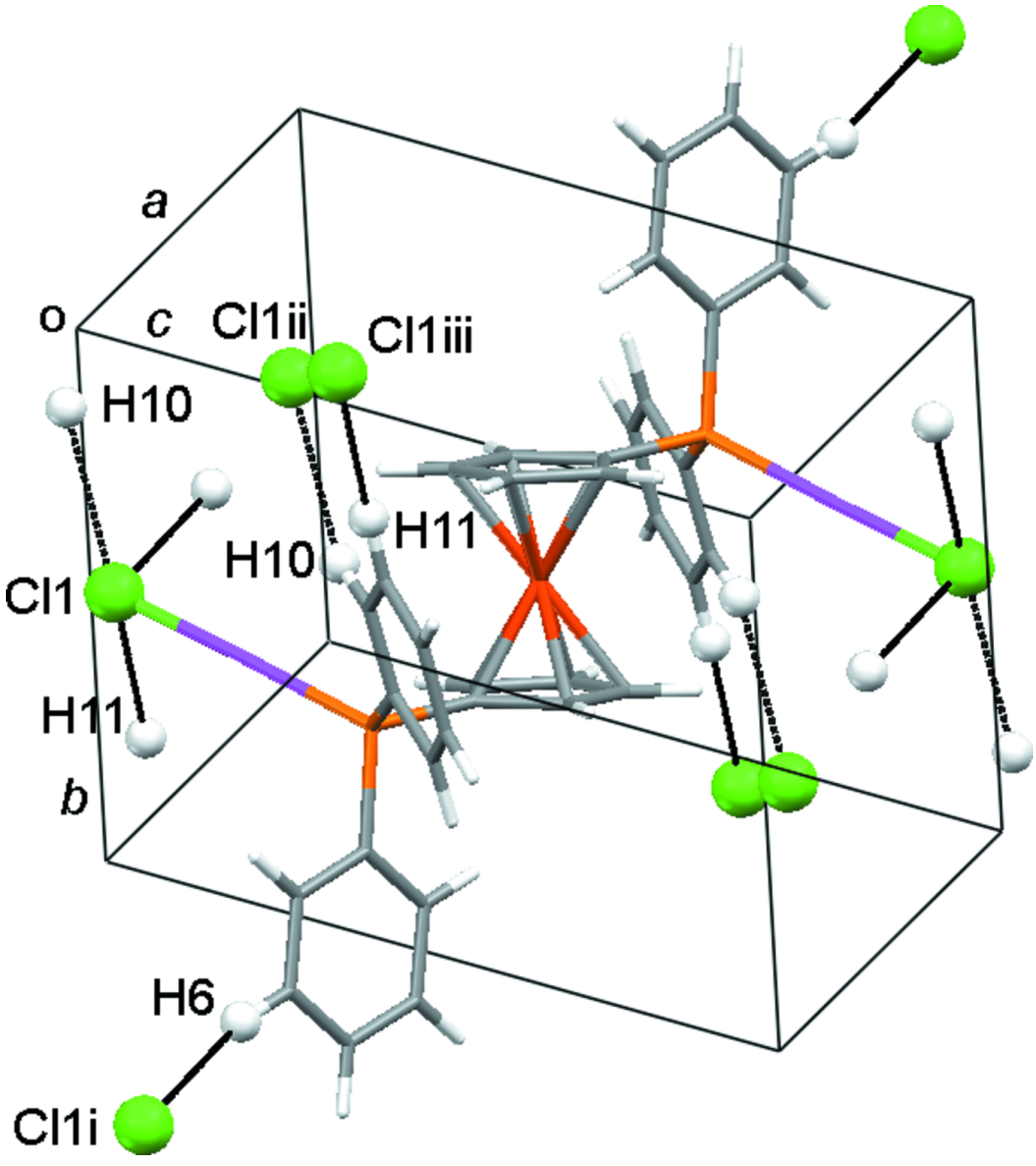

Fig. 3