[2-(1-Acetoxyethyl)-1,1'-bis(diphenylphosphino)ferrocene-.kappa.2P,P']dichloridoplatinum(II) dichloromethane solvate

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[2-(1-Acetoxyethyl)-1,1′-bis(diphenylphosphino)ferrocene-κ^2P,P']dichloridoplatinum(II) dichloromethane solvate

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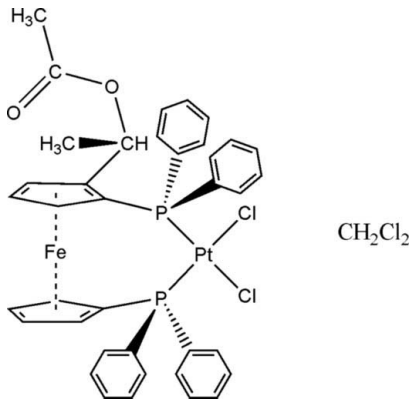
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.025; wR factor = 0.062; data-to-parameter ratio = 21.9.

In the dinuclear title compound $[FePtCl_2(C_{17}H_{14}P)(C_{21}H_{20}O_2P)]\cdot CH_2Cl_2$, the Pt^{II} atom has a square-planar geometry and the ferrocenyl–phosphine ligands are staggered at a 24.7 (2)° angle.

Related literature

For related literature, see: Bjelosevic *et al.* (2006); Clemente *et al.* (1986); Gan & Hor (1995); Mason *et al.* (1999); Puxty *et al.* (2005); Scarcia *et al.* (1988).



Experimental

Crystal data

$[FePtCl_2(C_{17}H_{14}P)(C_{21}H_{20}O_2P)]\cdot CH_2Cl_2$
M_r = 991.36
Monoclinic, $P2_1/n$
a = 10.512 (2) Å
b = 22.327 (5) Å
c = 15.734 (3) Å
β = 91.95 (3)°
V = 3690.6 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.59 mm^{-1}
T = 100 (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.296, T_{max} = 0.401
52878 measured reflections
10208 independent reflections
8965 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.03
10208 reflections
466 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Geometry (°) around atom Pt1.

	angle	average angle for relevant references in the CSD	number of relevant references in the CSD
P1—Pt1—Cl1	90.29 (3)	88 (3)	7
P2—Pt1—Cl2	85.33 (3)	88 (2)	7
Cl1—Pt1—Cl2	86.18 (3)	87 (1)	7
P2—Pt1—P1	98.27 (3)	99 (4)	7

Note: CSD (Cambridge Structural Database; Version 5.28, January 2007 release; Allen, 2002)

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *publCIF* (Westrip, 2007) and *modiCIFer* (Guzei, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2342).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bjelosevic, H., Spégel, C., Sykfont Snygg, Å., Gorton, L., Elmroth, S. K. C. & Persson, T. (2006). *Tetrahedron*, **62**, 4519–4527.
Bruker (2003). *SADABS* (Version 2.05), *SAINT* (Version 6.22), *SHELXTL* (Version 6.10) and *SMART* (Version 5.622). Bruker AXS Inc., Madison, Wisconsin, USA.
Clemente, D. A., Pilloni, G., Corain, B., Longato, B. & Tiripicchio-Camellini, M. (1986). *Inorg. Chim. Acta*, **115**, L9–L11.
Gan, K.-S. & Hor, T. S. A. (1995). *Ferrocenes – Homogeneous Catalysis, Organic Synthesis and Materials Science*, edited by Togni, A. & Hayashi, T., pp 4–104. Weinheim: VCH.
Guzei, I. A. (1995). *modiCIFer*. University of Wisconsin-Madison, USA.
Mason, R. W., McGrouther, K., Ranatunge-Bandarage, P. R. R., Robinson, B. H. & Simpson, J. (1999). *Appl. Organomet. Chem.* **13**, 163–173.
Puxty, G., Bjelosevic, H., Persson, T. & Elmroth, S. K. C. (2005). *Dalton Trans.* **18**, 3032–3038.
Scarcia, V., Furlani, A., Longato, B., Corain, B. & Pilloni, G. (1988). *Inorg. Chim. Acta*, **153**, 67–70.
Westrip, S. P. (2007). *publCIF*. In preparation.

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supplementary materials

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[2-(1-Acetoxyethyl)-1,1'-bis(diphenylphosphino)ferrocene-κ^2*P*,*P*']dichloridoplatinum(II) dichloromethane solvate

L. C. Spencer and H. Bjelosevic

Comment

The use of iron(II) ferrocenyl phosphine ligands in coordination chemistry has proven to be successful for various applications including catalysis where palladium, nickel and rhodium compounds are typically used and medical ones which use a platinum(II) metal center (Gan & Hor, 1995, Scarcia *et al.*, 1988, Mason *et al.*, 1999). One of the more commonly used ferrocenyl diphosphines is 1,1'-bis(diphenylphosphino)ferrocene (dppf).

The title compound was synthesized as one representative of a series of compounds for which a systematic kinetic analysis could be performed (Bjelosevic *et al.*, 2006). The study targeted the kinetics of the ligand exchange rate at the platinum center and its dependence on the choice of substituents on the cyclopentadienyl ring which significantly affected the reaction kinetics (Puxty *et al.*, 2005). The current crystal structure reveals that the acetate moiety is in a location close to the site of attack at the platinum atom for the entering ligand in support of the mechanistic model suggested earlier that included a hydrogen bonding interaction between the entering ligand and the acetate prior to ligand replacement (Puxty *et al.*, 2005)**.**

Compound (I) co-crystallizes in a 1:1 ratio with dichloromethane. The dichloromethane molecule is disordered over two positions in a 69.6 (2):30.4 (2) ratio. Compound (I) exhibits a distorted square planar geometry around atom Pt1 with the two phosphorous groups *cis* to each other. The P2—Pt1—P1 angle of 98.27 (3)° is significantly larger than 90° due to the geometry of the ferrocenyl moiety. Around the atom Pt1, atoms P1 and Cl1 are slightly below the least squares plane defined by atoms Pt1, P1, P2, Cl1, and Cl2 and atoms P2 and Cl2 are slightly above the plane. This distorted square planar geometry is typical for this class of compounds with *cis* substitution pattern (Table 1).

Atom Fe1 is almost equidistant from the centers of the two five-membered rings; Fe1-Centroid(C1—C5)=1.6392 (15)Å and Fe1-Centroid(C34—C38)=1.6496 (15)Å . The two five-membered rings are staggered with an angle of 24.7 (2)°. The cyclopentadienyl rings are not parallel to each other forming a dihedral angle of 4.32 (18)° between their least squares planes defined by the carbon atoms in the cyclopentadienyl rings. This angle is similar to the angle of 5.9° for a similar complex, $PtCl_2$(1-[1',2-bis(diphenylphosphino)ferrocenyl]), (Clemente *et al.*, 1986). The other geometrical parameters are typical.

Experimental

The synthetic procedure is described by (Bjelosevic *et al.*, 2006).

Refinement

All H-atoms were placed in idealized locations and refined as riding with appropriate displacement coefficients U_{iso}(H) = 1.5 times U_{eq}(bearing atom) for methyl H atoms and U_{iso}(H) = 1.2 times U_{eq}(bearing atom) for all other H atoms.

c—H distances were set to

C(sp^3)-H=1.00, C(sp^3)-2H=0.99, C(sp^3)-3H=0.98, C(sp^2)-H=0.95 Å.

The C—Cl distances were restrained so that they were the same within 0.02Å for all components of the disordered dichloromethane molecule. The distance between the two Cl atoms in both components of the disordered molecule were restrained to be the same distance within 0.02A%.

There was one large peak (c.a. 1.64 e $Å^{-3}$) observed near atom Pt1 in the final difference map and was considered noise.

Figures

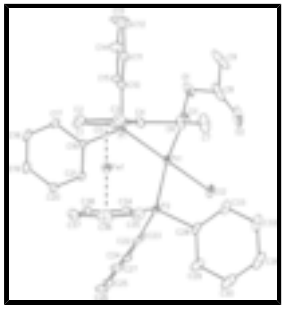

Fig. 1. Molecular Drawing of (I) shown with 30% probability ellipsoids. All hydrogen atoms and the solvent molecule are omitted for clarity.

[2-(1-Acetoxyethyl)-1,1'-bis(diphenylphosphino)ferrocene- κ^2P,P']dichloridoplatinum(II) dichloromethane solvate

Crystal data

$[FePtCl_2(C_{17}H_{14}P_1)(C_{21}H_{20}O_2P_1)]\cdot CH_2Cl_2$	F_{000} = 1952
M_r = 991.36	D_x = 1.784 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo- $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5453 reflections
a = 10.512 (2) Å	θ = 2.2–26.4º
b = 22.327 (5) Å	μ = 4.59 mm^{-1}
c = 15.734 (3) Å	T = 100 (2) K
β = 91.95 (3)º	Plate, yellow
V = 3690.6 (13) $Å^3$	0.30 × 0.30 × 0.20 mm
Z = 4	

Data collection

Bruker CCD-1000 area-detector diffractometer	10208 independent reflections
Radiation source: fine-focus sealed tube	8965 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 100(2) K	θ_{max} = 29.5º
0.30° ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	h = −14→14

T_{min} = 0.296, T_{max} = 0.401
52878 measured reflections

k = −30→30
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.04
10208 reflections
466 parameters
10 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
$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 6.0554P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}
Extinction correction: none

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1	0.140468 (8)	0.132603 (4)	0.758092 (6)	0.01436 (3)	

Fe1	0.54287 (3)	0.114340 (19)	0.80695 (3)	0.01972 (8)
Cl1	0.00138 (7)	0.10731 (3)	0.64455 (5)	0.02873 (15)
Cl2	−0.03911 (6)	0.12673 (3)	0.84410 (5)	0.02585 (15)
P1	0.30079 (6)	0.14445 (3)	0.66721 (4)	0.01477 (12)
P2	0.25011 (6)	0.15429 (3)	0.88039 (4)	0.01635 (12)
O1	0.2910 (2)	−0.01082 (9)	0.68141 (17)	0.0339 (5)
O2	0.1135 (2)	−0.02861 (12)	0.7561 (2)	0.0529 (8)
C1	0.5735 (3)	0.12949 (13)	0.68171 (19)	0.0230 (6)
H1	0.5937	0.1690	0.6556	0.028*
C2	0.6635 (3)	0.08684 (14)	0.7132 (2)	0.0282 (6)
H2	0.7581	0.0917	0.7146	0.034*
C3	0.5963 (3)	0.03736 (14)	0.7449 (2)	0.0268 (6)
H3	0.6361	0.0014	0.7728	0.032*
C4	0.4624 (3)	0.04795 (12)	0.73472 (19)	0.0217 (5)
C5	0.4477 (2)	0.10615 (12)	0.69515 (16)	0.0173 (5)
C6	0.3573 (3)	0.00707 (13)	0.7602 (2)	0.0265 (6)
H6	0.2973	0.0298	0.7962	0.032*
C7	0.4039 (3)	−0.04811 (15)	0.8084 (3)	0.0434 (9)
H7A	0.3306	−0.0712	0.8270	0.065*
H7B	0.4561	−0.0358	0.8582	0.065*
H7C	0.4549	−0.0729	0.7712	0.065*
C8	0.1648 (3)	−0.02605 (14)	0.6894 (3)	0.0441 (10)
C9	0.1061 (4)	−0.03844 (18)	0.6032 (4)	0.0662 (16)
H9A	0.0998	−0.0818	0.5945	0.099*
H9B	0.1592	−0.0209	0.5596	0.099*
H9C	0.0209	−0.0207	0.5991	0.099*
C10	0.2715 (3)	0.12169 (13)	0.55682 (18)	0.0247 (6)
C11	0.3360 (4)	0.07272 (14)	0.5227 (2)	0.0337 (7)
H11	0.3947	0.0504	0.5573	0.040*
C12	0.3135 (5)	0.05697 (18)	0.4381 (2)	0.0532 (11)
H12	0.3568	0.0238	0.4148	0.064*
C13	0.2292 (6)	0.0891 (2)	0.3881 (2)	0.0656 (15)
H13	0.2141	0.0779	0.3304	0.079*
C14	0.1652 (5)	0.13809 (19)	0.4209 (2)	0.0515 (11)
H14	0.1067	0.1601	0.3857	0.062*
C15	0.1867 (3)	0.15482 (15)	0.50520 (19)	0.0325 (7)
H15	0.1441	0.1885	0.5276	0.039*
C16	0.3434 (3)	0.22291 (11)	0.65452 (17)	0.0186 (5)
C17	0.4092 (3)	0.24223 (13)	0.58355 (19)	0.0287 (7)
H17	0.4325	0.2141	0.5415	0.034*
C18	0.4405 (4)	0.30218 (14)	0.5742 (2)	0.0391 (9)
H18	0.4841	0.3149	0.5254	0.047*
C19	0.4084 (4)	0.34376 (14)	0.6359 (3)	0.0406 (9)
H19	0.4315	0.3846	0.6299	0.049*
C20	0.3425 (3)	0.32510 (13)	0.7063 (2)	0.0313 (7)
H20	0.3209	0.3532	0.7488	0.038*
C21	0.3084 (3)	0.26527 (12)	0.71437 (18)	0.0222 (6)
H21	0.2604	0.2531	0.7614	0.027*
C22	0.2155 (3)	0.23025 (13)	0.91742 (16)	0.0200 (5)

C23	0.1044 (3)	0.25952 (13)	0.88866 (17)	0.0219 (5)	
H23	0.0444	0.2389	0.8528	0.026*	
C24	0.0811 (3)	0.31836 (13)	0.91199 (19)	0.0273 (6)	
H24	0.0059	0.3379	0.8915	0.033*	
C25	0.1668 (4)	0.34874 (16)	0.9650 (2)	0.0357 (7)	
H25	0.1498	0.3888	0.9816	0.043*	
C26	0.2771 (4)	0.32076 (17)	0.9936 (2)	0.0378 (8)	
H26	0.3365	0.3417	1.0294	0.045*	
C27	0.3018 (3)	0.26180 (15)	0.97022 (18)	0.0299 (7)	
H27	0.3779	0.2429	0.9903	0.036*	
C28	0.2114 (3)	0.10271 (13)	0.96601 (18)	0.0234 (6)	
C29	0.2326 (4)	0.11993 (16)	1.0500 (2)	0.0373 (8)	
H29	0.2623	0.1592	1.0627	0.045*	
C30	0.2107 (4)	0.07996 (19)	1.1159 (2)	0.0482 (10)	
H30	0.2246	0.0923	1.1733	0.058*	
C31	0.1692 (3)	0.02311 (18)	1.0985 (2)	0.0427 (9)	
H31	0.1538	−0.0039	1.1436	0.051*	
C32	0.1498 (3)	0.00492 (16)	1.0150 (2)	0.0356 (8)	
H32	0.1227	−0.0349	1.0029	0.043*	
C33	0.1696 (3)	0.04486 (14)	0.9482 (2)	0.0284 (7)	
H33	0.1547	0.0325	0.8910	0.034*	
C34	0.4223 (3)	0.15186 (13)	0.88959 (17)	0.0211 (5)	
C35	0.4938 (3)	0.10397 (15)	0.93073 (18)	0.0280 (6)	
H35	0.4574	0.0670	0.9563	0.034*	
C36	0.6248 (3)	0.11869 (17)	0.9281 (2)	0.0343 (7)	
H36	0.6968	0.0933	0.9504	0.041*	
C37	0.6368 (3)	0.17445 (16)	0.8869 (2)	0.0312 (7)	
H37	0.7188	0.1951	0.8750	0.037*	
C38	0.5133 (3)	0.19534 (14)	0.86199 (18)	0.0235 (6)	
H38	0.4931	0.2336	0.8315	0.028*	
C39	0.8601 (3)	0.24397 (18)	0.6923 (2)	0.0304 (9)	0.696 (2)
H39A	0.8000	0.2360	0.6438	0.037*	0.696 (2)
H39B	0.8837	0.2051	0.7187	0.037*	0.696 (2)
Cl3	0.78490 (15)	0.28920 (6)	0.76765 (8)	0.0470 (4)	0.696 (2)
Cl4	0.99801 (16)	0.27896 (7)	0.65465 (13)	0.0414 (4)	0.696 (2)
C39A	0.8471 (3)	0.2564 (4)	0.7340 (6)	0.0304 (9)	0.304 (2)
H39C	0.8535	0.2133	0.7200	0.037*	0.304 (2)
H39D	0.8622	0.2609	0.7961	0.037*	0.304 (2)
Cl3A	0.69277 (19)	0.28225 (10)	0.70574 (14)	0.0238 (6)	0.304 (2)
Cl4A	0.9650 (3)	0.29633 (19)	0.6802 (2)	0.0344 (8)	0.304 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.00934 (5)	0.01389 (5)	0.01969 (5)	−0.00178 (3)	−0.00177 (3)	0.00457 (3)
Fe1	0.01012 (16)	0.02461 (19)	0.02435 (19)	−0.00004 (14)	−0.00065 (14)	−0.00185 (15)
Cl1	0.0204 (3)	0.0288 (4)	0.0360 (4)	−0.0063 (3)	−0.0132 (3)	0.0016 (3)
Cl2	0.0103 (3)	0.0304 (4)	0.0370 (4)	0.0007 (2)	0.0040 (3)	0.0163 (3)

P1	0.0165 (3)	0.0132 (3)	0.0146 (3)	−0.0020 (2)	0.0008 (2)	−0.0004 (2)
P2	0.0125 (3)	0.0210 (3)	0.0156 (3)	0.0013 (2)	0.0010 (2)	0.0045 (2)
O1	0.0251 (11)	0.0188 (10)	0.0568 (15)	−0.0033 (8)	−0.0124 (10)	0.0002 (10)
O2	0.0263 (13)	0.0298 (14)	0.102 (3)	−0.0060 (10)	−0.0009 (15)	0.0286 (15)
C1	0.0158 (12)	0.0256 (14)	0.0282 (14)	−0.0023 (10)	0.0101 (11)	−0.0061 (11)
C2	0.0153 (13)	0.0317 (16)	0.0380 (16)	0.0015 (11)	0.0067 (12)	−0.0071 (13)
C3	0.0165 (13)	0.0265 (15)	0.0374 (16)	0.0045 (11)	0.0009 (12)	−0.0040 (12)
C4	0.0164 (12)	0.0186 (12)	0.0300 (14)	0.0002 (10)	−0.0009 (11)	−0.0016 (11)
C5	0.0142 (11)	0.0164 (12)	0.0214 (12)	−0.0014 (9)	0.0041 (9)	−0.0040 (10)
C6	0.0191 (13)	0.0201 (13)	0.0402 (17)	−0.0005 (10)	−0.0031 (12)	0.0084 (12)
C7	0.0315 (18)	0.0253 (16)	0.073 (3)	−0.0003 (13)	−0.0084 (17)	0.0212 (17)
C8	0.0275 (17)	0.0130 (14)	0.090 (3)	0.0004 (12)	−0.022 (2)	0.0055 (17)
C9	0.046 (2)	0.0266 (18)	0.123 (4)	−0.0008 (17)	−0.046 (3)	−0.018 (2)
C10	0.0342 (16)	0.0212 (13)	0.0184 (12)	−0.0010 (11)	−0.0039 (11)	−0.0030 (10)
C11	0.052 (2)	0.0248 (15)	0.0242 (14)	0.0048 (14)	−0.0014 (14)	−0.0081 (12)
C12	0.092 (3)	0.038 (2)	0.0300 (18)	0.013 (2)	−0.005 (2)	−0.0174 (16)
C13	0.116 (4)	0.058 (3)	0.0215 (17)	0.016 (3)	−0.015 (2)	−0.0196 (17)
C14	0.078 (3)	0.054 (2)	0.0217 (16)	0.010 (2)	−0.0167 (18)	−0.0029 (16)
C15	0.0456 (19)	0.0310 (16)	0.0203 (14)	0.0033 (14)	−0.0060 (13)	−0.0029 (12)
C16	0.0219 (13)	0.0130 (11)	0.0214 (12)	−0.0019 (10)	0.0060 (10)	0.0019 (10)
C17	0.0404 (17)	0.0190 (13)	0.0278 (15)	−0.0012 (12)	0.0187 (13)	−0.0010 (11)
C18	0.053 (2)	0.0224 (15)	0.0441 (19)	−0.0042 (14)	0.0318 (17)	0.0038 (14)
C19	0.051 (2)	0.0149 (14)	0.058 (2)	−0.0083 (14)	0.0297 (18)	−0.0017 (14)
C20	0.0409 (18)	0.0178 (13)	0.0364 (16)	−0.0050 (12)	0.0196 (14)	−0.0068 (12)
C21	0.0260 (14)	0.0192 (13)	0.0218 (13)	−0.0037 (11)	0.0089 (11)	0.0003 (10)
C22	0.0216 (13)	0.0267 (14)	0.0121 (11)	−0.0002 (11)	0.0049 (10)	0.0021 (10)
C23	0.0245 (14)	0.0234 (14)	0.0183 (12)	0.0013 (11)	0.0070 (10)	0.0031 (10)
C24	0.0326 (16)	0.0236 (14)	0.0264 (14)	0.0042 (12)	0.0113 (12)	0.0002 (11)
C25	0.044 (2)	0.0330 (17)	0.0312 (16)	−0.0003 (15)	0.0155 (15)	−0.0109 (14)
C26	0.0405 (19)	0.046 (2)	0.0272 (15)	−0.0040 (16)	0.0042 (14)	−0.0209 (15)
C27	0.0302 (16)	0.0414 (18)	0.0178 (13)	0.0018 (13)	−0.0004 (12)	−0.0087 (12)
C28	0.0187 (12)	0.0290 (15)	0.0229 (13)	0.0067 (11)	0.0050 (10)	0.0145 (11)
C29	0.052 (2)	0.0364 (18)	0.0235 (15)	0.0128 (16)	0.0060 (14)	0.0121 (13)
C30	0.069 (3)	0.050 (2)	0.0272 (16)	0.020 (2)	0.0116 (17)	0.0220 (16)
C31	0.0352 (18)	0.054 (2)	0.0397 (19)	0.0125 (16)	0.0086 (15)	0.0339 (17)
C32	0.0168 (13)	0.0384 (18)	0.052 (2)	0.0036 (12)	0.0017 (13)	0.0280 (16)
C33	0.0142 (12)	0.0350 (16)	0.0361 (16)	0.0033 (11)	0.0023 (11)	0.0170 (13)
C34	0.0159 (12)	0.0294 (14)	0.0177 (12)	0.0019 (11)	−0.0031 (10)	−0.0006 (11)
C35	0.0209 (14)	0.0400 (18)	0.0227 (13)	0.0071 (13)	−0.0058 (11)	0.0038 (12)
C36	0.0186 (14)	0.051 (2)	0.0321 (16)	0.0086 (13)	−0.0103 (12)	−0.0041 (15)
C37	0.0135 (13)	0.0427 (18)	0.0372 (17)	−0.0039 (12)	−0.0039 (12)	−0.0112 (14)
C38	0.0150 (12)	0.0300 (15)	0.0254 (13)	−0.0023 (11)	−0.0011 (10)	−0.0065 (11)
C39	0.041 (2)	0.024 (2)	0.026 (2)	0.0047 (17)	−0.008 (2)	−0.0019 (18)
Cl3	0.0678 (10)	0.0327 (7)	0.0404 (7)	0.0192 (6)	0.0008 (6)	−0.0052 (5)
Cl4	0.0288 (8)	0.0394 (8)	0.0549 (10)	0.0054 (6)	−0.0143 (7)	−0.0115 (7)
C39A	0.041 (2)	0.024 (2)	0.026 (2)	0.0047 (17)	−0.008 (2)	−0.0019 (18)
Cl3A	0.0242 (11)	0.0223 (11)	0.0249 (11)	0.0004 (8)	0.0022 (8)	0.0040 (8)
Cl4A	0.0214 (14)	0.045 (2)	0.0365 (17)	−0.0101 (13)	−0.0052 (12)	0.0154 (15)

Geometric parameters (Å, °)

Pt1—P2	2.2615 (9)	C14—H14	0.9500
Pt1—P1	2.2625 (9)	C15—H15	0.9500
Pt1—Cl1	2.3388 (10)	C16—C21	1.393 (4)
Pt1—Cl2	2.3635 (9)	C16—C17	1.401 (4)
Fe1—C5	2.002 (3)	C17—C18	1.388 (4)
Fe1—C34	2.028 (3)	C17—H17	0.9500
Fe1—C4	2.034 (3)	C18—C19	1.393 (5)
Fe1—C38	2.034 (3)	C18—H18	0.9500
Fe1—C1	2.036 (3)	C19—C20	1.391 (4)
Fe1—C35	2.045 (3)	C19—H19	0.9500
Fe1—C37	2.067 (3)	C20—C21	1.390 (4)
Fe1—C36	2.067 (3)	C20—H20	0.9500
Fe1—C3	2.064 (3)	C21—H21	0.9500
Fe1—C2	2.070 (3)	C22—C23	1.400 (4)
Fe1—Cent(C1-C5)	1.6392 (15)	C22—C27	1.399 (4)
Fe1—Cent(C34-C38)	1.6496 (15)	C23—C24	1.388 (4)
P1—C5	1.806 (3)	C23—H23	0.9500
P1—C16	1.821 (3)	C24—C25	1.384 (5)
P1—C10	1.826 (3)	C24—H24	0.9500
P2—C34	1.812 (3)	C25—C26	1.379 (5)
P2—C28	1.829 (3)	C25—H25	0.9500
P2—C22	1.834 (3)	C26—C27	1.394 (5)
O1—C8	1.379 (4)	C26—H26	0.9500
O1—C6	1.457 (4)	C27—H27	0.9500
O2—C8	1.198 (5)	C28—C33	1.390 (5)
C1—C2	1.419 (4)	C28—C29	1.387 (4)
C1—C5	1.444 (4)	C29—C30	1.393 (4)
C1—H1	1.0000	C29—H29	0.9500
C2—C3	1.411 (4)	C30—C31	1.367 (6)
C2—H2	1.0000	C30—H30	0.9500
C3—C4	1.431 (4)	C31—C32	1.384 (6)
C3—H3	1.0000	C31—H31	0.9500
C4—C5	1.447 (4)	C32—C33	1.399 (4)
C4—C6	1.498 (4)	C32—H32	0.9500
C6—C7	1.519 (4)	C33—H33	0.9500
C6—H6	1.0000	C34—C38	1.440 (4)
C7—H7A	0.9800	C34—C35	1.447 (4)
C7—H7B	0.9800	C35—C36	1.417 (4)
C7—H7C	0.9800	C35—H35	1.0000
C8—C9	1.496 (6)	C36—C37	1.412 (5)
C9—H9A	0.9800	C36—H36	1.0000
C9—H9B	0.9800	C37—C38	1.422 (4)
C9—H9C	0.9800	C37—H37	1.0000
C10—C15	1.397 (4)	C38—H38	1.0000
C10—C11	1.402 (4)	C39—Cl3	1.765 (3)
C11—C12	1.390 (4)	C39—Cl4	1.766 (3)

C11—H11	0.9500	C39—H39A	0.9900
C12—C13	1.368 (6)	C39—H39B	0.9900
C12—H12	0.9500	C39A—Cl3A	1.765 (3)
C13—C14	1.393 (6)	C39A—Cl4A	1.765 (3)
C13—H13	0.9500	C39A—H39C	0.9900
C14—C15	1.389 (4)	C39A—H39D	0.9900
P2—Pt1—P1	98.27 (3)	H9B—C9—H9C	109.5
P2—Pt1—Cl1	171.43 (3)	C15—C10—C11	119.8 (3)
P1—Pt1—Cl1	90.29 (3)	C15—C10—P1	119.3 (2)
P2—Pt1—Cl2	85.33 (3)	C11—C10—P1	120.8 (2)
P1—Pt1—Cl2	174.27 (2)	C12—C11—C10	119.7 (3)
Cl1—Pt1—Cl2	86.18 (3)	C12—C11—H11	120.2
Cent(C1-C5)—Fe1—Cent(C34-C38)	178.55 (8)	C10—C11—H11	120.2
C5—Fe1—C34	107.25 (11)	C13—C12—C11	120.3 (4)
C5—Fe1—C4	42.00 (11)	C13—C12—H12	119.9
C34—Fe1—C4	113.71 (11)	C11—C12—H12	119.9
C5—Fe1—C38	112.10 (11)	C12—C13—C14	120.7 (3)
C34—Fe1—C38	41.54 (11)	C12—C13—H13	119.7
C4—Fe1—C38	144.99 (11)	C14—C13—H13	119.7
C5—Fe1—C1	41.88 (10)	C13—C14—C15	120.0 (4)
C34—Fe1—C1	132.46 (11)	C13—C14—H14	120.0
C4—Fe1—C1	69.93 (12)	C15—C14—H14	120.0
C38—Fe1—C1	107.22 (12)	C14—C15—C10	119.5 (3)
C5—Fe1—C35	133.78 (11)	C14—C15—H15	120.2
C34—Fe1—C35	41.64 (12)	C10—C15—H15	120.2
C4—Fe1—C35	109.64 (13)	C21—C16—C17	118.6 (2)
C38—Fe1—C35	69.38 (13)	C21—C16—P1	120.5 (2)
C1—Fe1—C35	173.79 (12)	C17—C16—P1	120.9 (2)
C5—Fe1—C37	143.88 (13)	C18—C17—C16	120.5 (3)
C34—Fe1—C37	68.77 (12)	C18—C17—H17	119.8
C4—Fe1—C37	173.62 (13)	C16—C17—H17	119.8
C38—Fe1—C37	40.58 (12)	C17—C18—C19	120.3 (3)
C1—Fe1—C37	113.13 (13)	C17—C18—H18	119.8
C35—Fe1—C37	67.97 (14)	C19—C18—H18	119.8
C5—Fe1—C36	173.98 (12)	C20—C19—C18	119.7 (3)
C34—Fe1—C36	68.84 (12)	C20—C19—H19	120.2
C4—Fe1—C36	134.56 (14)	C18—C19—H19	120.2
C38—Fe1—C36	68.31 (13)	C19—C20—C21	119.8 (3)
C1—Fe1—C36	144.12 (13)	C19—C20—H20	120.1
C35—Fe1—C36	40.31 (13)	C21—C20—H20	120.1
C37—Fe1—C36	39.93 (14)	C20—C21—C16	121.1 (3)
C5—Fe1—C3	69.16 (12)	C20—C21—H21	119.5
C34—Fe1—C3	146.47 (12)	C16—C21—H21	119.5
C4—Fe1—C3	40.87 (11)	C23—C22—C27	118.3 (3)
C38—Fe1—C3	171.88 (12)	C23—C22—P2	120.1 (2)
C1—Fe1—C3	68.02 (12)	C27—C22—P2	121.5 (2)
C35—Fe1—C3	115.97 (13)	C24—C23—C22	120.6 (3)
C37—Fe1—C3	134.12 (12)	C24—C23—H23	119.7
C36—Fe1—C3	111.34 (13)	C22—C23—H23	119.7

C5—Fe1—C2	69.32 (11)	C25—C24—C23	120.4 (3)
C34—Fe1—C2	172.15 (13)	C25—C24—H24	119.8
C4—Fe1—C2	68.85 (12)	C23—C24—H24	119.8
C38—Fe1—C2	132.32 (12)	C26—C25—C24	119.8 (3)
C1—Fe1—C2	40.44 (12)	C26—C25—H25	120.1
C35—Fe1—C2	145.61 (13)	C24—C25—H25	120.1
C37—Fe1—C2	109.53 (12)	C25—C26—C27	120.2 (3)
C36—Fe1—C2	115.15 (13)	C25—C26—H26	119.9
C3—Fe1—C2	39.90 (12)	C27—C26—H26	119.9
C5—P1—C16	105.70 (12)	C26—C27—C22	120.7 (3)
C5—P1—C10	102.41 (13)	C26—C27—H27	119.7
C16—P1—C10	101.40 (13)	C22—C27—H27	119.7
C5—P1—Pt1	116.09 (9)	C33—C28—C29	119.3 (3)
C16—P1—Pt1	111.91 (9)	C33—C28—P2	120.9 (2)
C10—P1—Pt1	117.62 (11)	C29—C28—P2	119.7 (3)
C34—P2—C28	99.73 (13)	C30—C29—C28	120.4 (4)
C34—P2—C22	102.17 (13)	C30—C29—H29	119.8
C28—P2—C22	107.27 (13)	C28—C29—H29	119.8
C34—P2—Pt1	122.71 (9)	C31—C30—C29	120.3 (4)
C28—P2—Pt1	111.86 (11)	C31—C30—H30	119.8
C22—P2—Pt1	111.57 (9)	C29—C30—H30	119.8
C8—O1—C6	115.1 (3)	C30—C31—C32	120.0 (3)
C2—C1—C5	108.0 (3)	C30—C31—H31	120.0
C2—C1—Fe1	71.10 (18)	C32—C31—H31	120.0
C5—C1—Fe1	67.81 (15)	C31—C32—C33	120.3 (4)
C2—C1—H1	126.0	C31—C32—H32	119.8
C5—C1—H1	126.0	C33—C32—H32	119.8
Fe1—C1—H1	126.0	C28—C33—C32	119.7 (3)
C3—C2—C1	108.3 (3)	C28—C33—H33	120.1
C3—C2—Fe1	69.82 (17)	C32—C33—H33	120.1
C1—C2—Fe1	68.46 (16)	C38—C34—C35	107.0 (2)
C3—C2—H2	125.9	C38—C34—P2	128.9 (2)
C1—C2—H2	125.9	C35—C34—P2	124.1 (2)
Fe1—C2—H2	125.9	C38—C34—Fe1	69.46 (16)
C2—C3—C4	109.5 (3)	C35—C34—Fe1	69.81 (17)
C2—C3—Fe1	70.28 (17)	P2—C34—Fe1	127.29 (15)
C4—C3—Fe1	68.44 (16)	C36—C35—C34	107.8 (3)
C2—C3—H3	125.2	C36—C35—Fe1	70.70 (19)
C4—C3—H3	125.2	C34—C35—Fe1	68.55 (16)
Fe1—C3—H3	125.2	C36—C35—H35	126.1
C3—C4—C5	106.7 (2)	C34—C35—H35	126.1
C3—C4—C6	126.9 (3)	Fe1—C35—H35	126.1
C5—C4—C6	126.4 (2)	C37—C36—C35	108.7 (3)
C3—C4—Fe1	70.69 (17)	C37—C36—Fe1	70.02 (18)
C5—C4—Fe1	67.81 (15)	C35—C36—Fe1	68.99 (17)
C6—C4—Fe1	126.2 (2)	C37—C36—H36	125.6
C1—C5—C4	107.6 (2)	C35—C36—H36	125.6
C1—C5—P1	125.0 (2)	Fe1—C36—H36	125.6
C4—C5—P1	127.42 (19)	C36—C37—C38	108.7 (3)

C1—C5—Fe1	70.30 (16)	C36—C37—Fe1	70.04 (19)
C4—C5—Fe1	70.19 (16)	C38—C37—Fe1	68.45 (17)
P1—C5—Fe1	124.61 (14)	C36—C37—H37	125.6
O1—C6—C4	105.9 (2)	C38—C37—H37	125.6
O1—C6—C7	109.8 (3)	Fe1—C37—H37	125.6
C4—C6—C7	113.6 (3)	C37—C38—C34	107.8 (3)
O1—C6—H6	109.1	C37—C38—Fe1	70.97 (18)
C4—C6—H6	109.1	C34—C38—Fe1	69.00 (17)
C7—C6—H6	109.1	C37—C38—H38	126.1
C6—C7—H7A	109.5	C34—C38—H38	126.1
C6—C7—H7B	109.5	Fe1—C38—H38	126.1
H7A—C7—H7B	109.5	Cl3—C39—Cl4	111.3 (2)
C6—C7—H7C	109.5	Cl3—C39—H39A	109.4
H7A—C7—H7C	109.5	Cl4—C39—H39A	109.4
H7B—C7—H7C	109.5	Cl3—C39—H39B	109.4
O2—C8—O1	123.7 (4)	Cl4—C39—H39B	109.4
O2—C8—C9	126.9 (4)	H39A—C39—H39B	108.0
O1—C8—C9	109.4 (4)	Cl3A—C39A—Cl4A	111.6 (3)
C8—C9—H9A	109.5	Cl3A—C39A—H39C	109.3
C8—C9—H9B	109.5	Cl4A—C39A—H39C	109.3
H9A—C9—H9B	109.5	Cl3A—C39A—H39D	109.3
C8—C9—H9C	109.5	Cl4A—C39A—H39D	109.3
H9A—C9—H9C	109.5	H39C—C39A—H39D	108.0
P2—Pt1—P1—C5	49.63 (10)	C13—C14—C15—C10	−0.9 (7)
Cl1—Pt1—P1—C5	−129.92 (10)	C11—C10—C15—C14	1.3 (5)
P2—Pt1—P1—C16	−71.81 (10)	P1—C10—C15—C14	179.3 (3)
Cl1—Pt1—P1—C16	108.63 (10)	C5—P1—C16—C21	−108.5 (2)
P2—Pt1—P1—C10	171.38 (11)	C10—P1—C16—C21	145.0 (2)
Cl1—Pt1—P1—C10	−8.17 (11)	Pt1—P1—C16—C21	18.8 (3)
P1—Pt1—P2—C34	−19.00 (12)	C5—P1—C16—C17	73.1 (3)
Cl2—Pt1—P2—C34	165.49 (12)	C10—P1—C16—C17	−33.4 (3)
P1—Pt1—P2—C28	−137.29 (10)	Pt1—P1—C16—C17	−159.6 (2)
Cl2—Pt1—P2—C28	47.20 (10)	C21—C16—C17—C18	1.2 (5)
P1—Pt1—P2—C22	102.55 (9)	P1—C16—C17—C18	179.6 (3)
Cl2—Pt1—P2—C22	−72.96 (9)	C16—C17—C18—C19	0.9 (6)
C5—Fe1—C1—C2	−119.5 (2)	C17—C18—C19—C20	−1.2 (6)
C4—Fe1—C1—C2	−80.58 (18)	C18—C19—C20—C21	−0.4 (6)
C38—Fe1—C1—C2	136.32 (17)	C19—C20—C21—C16	2.5 (5)
C37—Fe1—C1—C2	93.40 (19)	C17—C16—C21—C20	−2.8 (5)
C36—Fe1—C1—C2	59.7 (3)	P1—C16—C21—C20	178.7 (3)
C3—Fe1—C1—C2	−36.69 (17)	C34—P2—C22—C23	153.1 (2)
C34—Fe1—C1—C5	−65.3 (2)	C28—P2—C22—C23	−102.5 (2)
C4—Fe1—C1—C5	38.95 (15)	Pt1—P2—C22—C23	20.3 (2)
C38—Fe1—C1—C5	−104.15 (16)	C34—P2—C22—C27	−22.8 (3)
C37—Fe1—C1—C5	−147.07 (16)	C28—P2—C22—C27	81.6 (3)
C36—Fe1—C1—C5	179.2 (2)	Pt1—P2—C22—C27	−155.6 (2)
C3—Fe1—C1—C5	82.84 (17)	C27—C22—C23—C24	0.1 (4)
C2—Fe1—C1—C5	119.5 (2)	P2—C22—C23—C24	−175.9 (2)
C5—C1—C2—C3	0.7 (3)	C22—C23—C24—C25	−0.8 (4)

Fe1—C1—C2—C3	58.6 (2)	C23—C24—C25—C26	1.1 (5)
C5—C1—C2—Fe1	−57.91 (19)	C24—C25—C26—C27	−0.8 (5)
C5—Fe1—C2—C3	−81.87 (19)	C25—C26—C27—C22	0.1 (5)
C4—Fe1—C2—C3	−36.76 (18)	C23—C22—C27—C26	0.2 (4)
C38—Fe1—C2—C3	176.58 (18)	P2—C22—C27—C26	176.2 (2)
C1—Fe1—C2—C3	−120.3 (3)	C34—P2—C28—C33	−104.3 (2)
C35—Fe1—C2—C3	57.4 (3)	C22—P2—C28—C33	149.6 (2)
C37—Fe1—C2—C3	136.66 (19)	Pt1—P2—C28—C33	26.9 (3)
C36—Fe1—C2—C3	93.7 (2)	C34—P2—C28—C29	71.0 (3)
C5—Fe1—C2—C1	38.38 (17)	C22—P2—C28—C29	−35.1 (3)
C4—Fe1—C2—C1	83.50 (18)	Pt1—P2—C28—C29	−157.8 (2)
C38—Fe1—C2—C1	−63.2 (2)	C33—C28—C29—C30	−0.8 (5)
C35—Fe1—C2—C1	177.7 (2)	P2—C28—C29—C30	−176.2 (3)
C37—Fe1—C2—C1	−103.08 (19)	C28—C29—C30—C31	0.7 (6)
C36—Fe1—C2—C1	−146.00 (19)	C29—C30—C31—C32	0.5 (6)
C3—Fe1—C2—C1	120.3 (3)	C30—C31—C32—C33	−1.4 (5)
C1—C2—C3—C4	−0.5 (4)	C29—C28—C33—C32	−0.1 (4)
Fe1—C2—C3—C4	57.3 (2)	P2—C28—C33—C32	175.3 (2)
C1—C2—C3—Fe1	−57.8 (2)	C31—C32—C33—C28	1.2 (4)
C5—Fe1—C3—C2	82.31 (19)	C28—P2—C34—C38	−157.2 (3)
C34—Fe1—C3—C2	172.3 (2)	C22—P2—C34—C38	−47.0 (3)
C4—Fe1—C3—C2	121.5 (3)	Pt1—P2—C34—C38	78.8 (3)
C1—Fe1—C3—C2	37.17 (18)	C28—P2—C34—C35	20.6 (3)
C35—Fe1—C3—C2	−148.04 (18)	C22—P2—C34—C35	130.8 (3)
C37—Fe1—C3—C2	−64.3 (3)	Pt1—P2—C34—C35	−103.4 (2)
C36—Fe1—C3—C2	−104.1 (2)	C28—P2—C34—Fe1	110.1 (2)
C5—Fe1—C3—C4	−39.17 (17)	C22—P2—C34—Fe1	−139.72 (18)
C34—Fe1—C3—C4	50.8 (3)	Pt1—P2—C34—Fe1	−13.9 (2)
C1—Fe1—C3—C4	−84.31 (19)	C5—Fe1—C34—C38	−104.10 (17)
C35—Fe1—C3—C4	90.5 (2)	C4—Fe1—C34—C38	−148.58 (17)
C37—Fe1—C3—C4	174.23 (19)	C1—Fe1—C34—C38	−64.7 (2)
C36—Fe1—C3—C4	134.40 (19)	C35—Fe1—C34—C38	118.1 (2)
C2—Fe1—C3—C4	−121.5 (3)	C37—Fe1—C34—C38	37.79 (18)
C2—C3—C4—C5	0.1 (3)	C36—Fe1—C34—C38	80.76 (19)
Fe1—C3—C4—C5	58.50 (19)	C3—Fe1—C34—C38	177.8 (2)
C2—C3—C4—C6	−179.7 (3)	C5—Fe1—C34—C35	137.83 (18)
Fe1—C3—C4—C6	−121.3 (3)	C4—Fe1—C34—C35	93.35 (19)
C2—C3—C4—Fe1	−58.4 (2)	C38—Fe1—C34—C35	−118.1 (2)
C5—Fe1—C4—C3	118.1 (2)	C1—Fe1—C34—C35	177.25 (18)
C34—Fe1—C4—C3	−152.12 (18)	C37—Fe1—C34—C35	−80.3 (2)
C38—Fe1—C4—C3	170.8 (2)	C36—Fe1—C34—C35	−37.32 (19)
C1—Fe1—C4—C3	79.24 (19)	C3—Fe1—C34—C35	59.7 (3)
C35—Fe1—C4—C3	−107.35 (19)	C5—Fe1—C34—P2	19.8 (2)
C36—Fe1—C4—C3	−69.1 (2)	C4—Fe1—C34—P2	−24.7 (2)
C2—Fe1—C4—C3	35.92 (18)	C38—Fe1—C34—P2	123.9 (3)
C34—Fe1—C4—C5	89.79 (17)	C1—Fe1—C34—P2	59.2 (3)
C38—Fe1—C4—C5	52.7 (3)	C35—Fe1—C34—P2	−118.1 (3)
C1—Fe1—C4—C5	−38.85 (15)	C37—Fe1—C34—P2	161.6 (2)
C35—Fe1—C4—C5	134.56 (15)	C36—Fe1—C34—P2	−155.4 (2)

C36—Fe1—C4—C5	172.85 (17)	C3—Fe1—C34—P2	−58.4 (3)
C3—Fe1—C4—C5	−118.1 (2)	C38—C34—C35—C36	0.3 (3)
C2—Fe1—C4—C5	−82.17 (17)	P2—C34—C35—C36	−177.9 (2)
C5—Fe1—C4—C6	−119.7 (3)	Fe1—C34—C35—C36	60.0 (2)
C34—Fe1—C4—C6	−30.0 (3)	C38—C34—C35—Fe1	−59.77 (19)
C38—Fe1—C4—C6	−67.0 (3)	P2—C34—C35—Fe1	122.0 (2)
C1—Fe1—C4—C6	−158.6 (3)	C5—Fe1—C35—C36	178.29 (19)
C35—Fe1—C4—C6	14.8 (3)	C34—Fe1—C35—C36	−119.1 (3)
C36—Fe1—C4—C6	53.1 (3)	C4—Fe1—C35—C36	137.0 (2)
C3—Fe1—C4—C6	122.2 (3)	C38—Fe1—C35—C36	−80.4 (2)
C2—Fe1—C4—C6	158.1 (3)	C37—Fe1—C35—C36	−36.7 (2)
C2—C1—C5—C4	−0.6 (3)	C3—Fe1—C35—C36	93.0 (2)
Fe1—C1—C5—C4	−60.58 (18)	C2—Fe1—C35—C36	56.0 (3)
C2—C1—C5—P1	179.0 (2)	C5—Fe1—C35—C34	−62.6 (2)
Fe1—C1—C5—P1	119.1 (2)	C4—Fe1—C35—C34	−103.96 (18)
C2—C1—C5—Fe1	60.0 (2)	C38—Fe1—C35—C34	38.69 (17)
C3—C4—C5—C1	0.3 (3)	C37—Fe1—C35—C34	82.37 (19)
C6—C4—C5—C1	−179.9 (3)	C36—Fe1—C35—C34	119.1 (3)
Fe1—C4—C5—C1	60.65 (18)	C3—Fe1—C35—C34	−147.97 (17)
C3—C4—C5—P1	−179.3 (2)	C2—Fe1—C35—C34	175.1 (2)
C6—C4—C5—P1	0.5 (4)	C34—C35—C36—C37	0.2 (4)
Fe1—C4—C5—P1	−119.0 (2)	Fe1—C35—C36—C37	58.9 (2)
C3—C4—C5—Fe1	−60.3 (2)	C34—C35—C36—Fe1	−58.7 (2)
C6—C4—C5—Fe1	119.5 (3)	C34—Fe1—C36—C37	−81.8 (2)
C16—P1—C5—C1	−18.4 (3)	C4—Fe1—C36—C37	175.25 (18)
C10—P1—C5—C1	87.4 (2)	C38—Fe1—C36—C37	−37.03 (18)
Pt1—P1—C5—C1	−143.1 (2)	C1—Fe1—C36—C37	52.6 (3)
C16—P1—C5—C4	161.2 (2)	C35—Fe1—C36—C37	−120.3 (3)
C10—P1—C5—C4	−93.0 (3)	C3—Fe1—C36—C37	134.25 (19)
Pt1—P1—C5—C4	36.5 (3)	C2—Fe1—C36—C37	90.8 (2)
C16—P1—C5—Fe1	70.64 (18)	C34—Fe1—C36—C35	38.51 (19)
C10—P1—C5—Fe1	176.43 (16)	C4—Fe1—C36—C35	−64.4 (3)
Pt1—P1—C5—Fe1	−54.06 (18)	C38—Fe1—C36—C35	83.3 (2)
C34—Fe1—C5—C1	135.43 (16)	C1—Fe1—C36—C35	172.9 (2)
C4—Fe1—C5—C1	−118.1 (2)	C37—Fe1—C36—C35	120.3 (3)
C38—Fe1—C5—C1	91.47 (17)	C3—Fe1—C36—C35	−105.4 (2)
C35—Fe1—C5—C1	173.59 (18)	C2—Fe1—C36—C35	−148.9 (2)
C37—Fe1—C5—C1	58.0 (2)	C35—C36—C37—C38	−0.6 (4)
C3—Fe1—C5—C1	−79.91 (17)	Fe1—C36—C37—C38	57.6 (2)
C2—Fe1—C5—C1	−37.10 (17)	C35—C36—C37—Fe1	−58.3 (2)
C34—Fe1—C5—C4	−106.52 (17)	C5—Fe1—C37—C36	172.42 (19)
C38—Fe1—C5—C4	−150.48 (16)	C34—Fe1—C37—C36	82.0 (2)
C1—Fe1—C5—C4	118.1 (2)	C38—Fe1—C37—C36	120.6 (3)
C35—Fe1—C5—C4	−68.4 (2)	C1—Fe1—C37—C36	−149.58 (18)
C37—Fe1—C5—C4	176.05 (19)	C35—Fe1—C37—C36	37.05 (18)
C3—Fe1—C5—C4	38.15 (16)	C3—Fe1—C37—C36	−68.4 (3)
C2—Fe1—C5—C4	80.96 (17)	C2—Fe1—C37—C36	−106.2 (2)
C34—Fe1—C5—P1	15.9 (2)	C5—Fe1—C37—C38	51.8 (3)
C4—Fe1—C5—P1	122.4 (2)	C34—Fe1—C37—C38	−38.65 (18)

C38—Fe1—C5—P1	−28.0 (2)	C1—Fe1—C37—C38	89.8 (2)
C1—Fe1—C5—P1	−119.5 (2)	C35—Fe1—C37—C38	−83.60 (19)
C35—Fe1—C5—P1	54.1 (2)	C36—Fe1—C37—C38	−120.6 (3)
C37—Fe1—C5—P1	−61.5 (3)	C3—Fe1—C37—C38	171.00 (18)
C3—Fe1—C5—P1	160.6 (2)	C2—Fe1—C37—C38	133.17 (19)
C2—Fe1—C5—P1	−156.6 (2)	C36—C37—C38—C34	0.8 (4)
C8—O1—C6—C4	−153.3 (2)	Fe1—C37—C38—C34	59.4 (2)
C8—O1—C6—C7	83.6 (3)	C36—C37—C38—Fe1	−58.6 (2)
C3—C4—C6—O1	−115.0 (3)	C35—C34—C38—C37	−0.7 (3)
C5—C4—C6—O1	65.2 (4)	P2—C34—C38—C37	177.4 (2)
Fe1—C4—C6—O1	152.9 (2)	Fe1—C34—C38—C37	−60.7 (2)
C3—C4—C6—C7	5.7 (5)	C35—C34—C38—Fe1	60.0 (2)
C5—C4—C6—C7	−174.1 (3)	P2—C34—C38—Fe1	−121.9 (2)
Fe1—C4—C6—C7	−86.5 (3)	C5—Fe1—C38—C37	−150.01 (19)
C6—O1—C8—O2	−4.8 (4)	C34—Fe1—C38—C37	118.6 (3)
C6—O1—C8—C9	175.3 (3)	C1—Fe1—C38—C37	−105.7 (2)
C5—P1—C10—C15	−162.0 (3)	C35—Fe1—C38—C37	79.8 (2)
C16—P1—C10—C15	−52.9 (3)	C36—Fe1—C38—C37	36.5 (2)
Pt1—P1—C10—C15	69.4 (3)	C2—Fe1—C38—C37	−68.4 (2)
C5—P1—C10—C11	15.9 (3)	C5—Fe1—C38—C34	91.40 (17)
C16—P1—C10—C11	125.0 (3)	C4—Fe1—C38—C34	56.3 (3)
Pt1—P1—C10—C11	−112.6 (3)	C1—Fe1—C38—C34	135.72 (16)
C15—C10—C11—C12	−1.0 (5)	C35—Fe1—C38—C34	−38.78 (16)
P1—C10—C11—C12	−178.9 (3)	C37—Fe1—C38—C34	−118.6 (3)
C10—C11—C12—C13	0.2 (7)	C36—Fe1—C38—C34	−82.13 (18)
C11—C12—C13—C14	0.3 (8)	C2—Fe1—C38—C34	173.01 (17)
C12—C13—C14—C15	0.1 (8)		

Geometry around atom Pt1

angle	angle, °	average angle, ° for relevant references in the CSD	number of relevant references in the CSD
P1—Pt1—Cl1	90.29 (3)	88 (3)	7
P2—Pt1—Cl2	85.33 (3)	88 (2)	7
Cl1—Pt1—Cl2	86.18 (3)	87 (1)	7
P2—Pt1—P1	98.27 (3)	99 (4)	7

CSD (Cambridge Structural Database; Version 5.28, January 2007 release; Allen, 2002)

Fig. 1