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{1-[1-(3-Carboxypropanamido)ethyl]-1',2-bis(diphenylphosphino)ferrocene-kappa2P,P'}dichloridoplatinum(II) dichloromethane 1.25-solvate

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+46 46-222 00 00

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1-[1-(3-Carboxypropanamido)ethyl]-1′,2-bis(diphenylphosphino)ferrocene-κ^2*P,P′*dichloridoplatinum(II) dichloromethane 1.25-solvate

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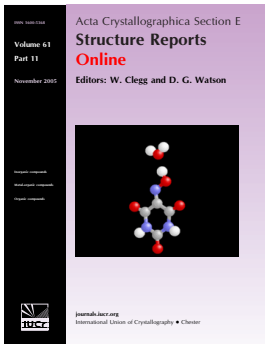

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{1-[1-(3-Carboxypropanamido)ethyl]-1′,2-bis(diphenylphosphino)ferrocene-κ^2P,P'}dichloridoplatinum(II) dichloromethane 1.25-solvate

Lara C. Spencer,[a]* Haris Bjelosevic,[b] James Darkwa,[c] Sofi K. C. Elmroth[d] and Tina Persson[b]

[a]Department of Chemistry, University of Wisconsin-Madison, 1101 University Ave, Madison, WI 53706, USA, [b]Organic Chemistry, Department of Chemistry, Lund University, PO Box 124, SE22100 Lund, Sweden, [c]Department of Chemistry, University of Johannesburg, Auckland Park Kingsway Campus, Johannesburg 2006, South Africa, and [d]Biochemistry, Department of Chemistry, Lund University, PO Box 124, SE22100 Lund, Sweden
Correspondence e-mail: laraharris@wisc.edu

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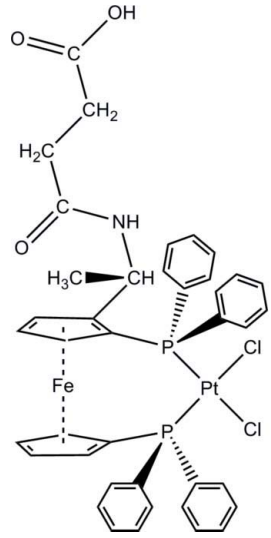
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; some non-H atoms missing; disorder in solvent or counterion; R factor = 0.025; wR factor = 0.065; data-to-parameter ratio = 23.9.

The dinuclear title compound, $[FePtCl_2(C_{17}H_{14}P)(C_{23}H_{23}NO_3P)]\cdot1.25CH_2Cl_2$, has a slightly distorted *cis*-$PtCl_2P_2$ square-planar geometry around the Pt atom, and the ferrocenylphosphine ligands are staggered at an angle of 29.4 (2)° about Pt. In the crystal structure, the complex forms centrosymmetric dimers *via* two strong intermolecular O—H···O bonds resulting in $R_2^2(8)$ rings. A weak intramolecular N—H···Cl bond leads to an $S(8)$ motif. The solvent is highly disordered and has not been modelled with discrete atoms.

Related literature

For background, see: Beagley *et al.* (2003); Bernstein *et al.* (1995); Bjelosevic *et al.* (2006); Clemente *et al.* (1986); Fouda *et al.* (2007); Spencer & Bjelosevic (2007); Top *et al.* (2003); Van Staveren & Metzler-Nolte (2004). For disordered solvent treatment, see: Spek (1983). Related structures were found from the Cambridge Structural Database (Allen, 2002).



1.25(CH_2Cl_2)

Experimental

Crystal data

$[FePtCl_2(C_{17}H_{14}P)(C_{23}H_{23}NO_3P)]\cdot1.25CH_2Cl_2$
M_r = 1069.64
Monoclinic, $P2_1/n$
a = 13.0154 (8) Å
b = 15.7866 (10) Å
c = 19.3403 (12) Å
β = 100.916 (1)°
V = 3901.9 (4) Å^3
Z = 4
Mo- $K\alpha$ radiation
μ = 4.39 mm^{-1}
T = 100 (2) K
0.35 × 0.33 × 0.30 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.309, T_{max} = 0.353
(expected range = 0.235–0.268)
56419 measured reflections
10833 independent reflections
9395 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.08
10833 reflections
453 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pt1—P2	2.2575 (6)	Pt1—Cl1	2.3588 (6)
Pt1—P1	2.2592 (6)	Pt1—Cl2	2.3592 (6)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3^{i}	0.84	1.82	2.656 (3)	177
N1—H1···Cl1	0.88	2.69	3.477 (2)	150

Symmetry code: (i) $-x+2, -y, -z$.

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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*, *PLATON* (Spek, 2003), *publCIF* (Westrip, 2007) and *modiCIFer* (Guzei, 2007).

Financial support from SIDA/NRF Swedish Research Links (to SKCE and JD: Platinum group metals: synthesis, catalytic and medicinal properties) is gratefully acknowledged. The authors thank Dr Ilia Guzei for his help and guidance in solving the structure and preparing the manuscript.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2623).

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{1-[1-(3-Carboxypropanamido)ethyl]-1',2-bis(diphenylphosphino)ferrocene-κ^2*P*,*P*'}dichloridoplatinum(II) dichloromethane 1.25-solvate

L. C. Spencer, H. Bjelosevic, J. Darkwa, S. K. C. Elmroth and T. Persson

Comment

Many ferrocenyl compounds have found interesting biological applications (Fouda *et al.*, 2007). With the rapid growth of bioorganometallic chemistry, the number of bioconjugates of ferrocene with proteins, DNA, RNA, carbohydrates, hormones *etc*. are increasing (Van Staveren & Metzler-Nolte, 2004). The electrochemical properties of ferrocene seem to improve the biological applications of already existing drugs (Beagley *et al.*, 2003, Top *et al.*, 2003).

Here we report the title compound, (I), a solvated platinum(II) complex with substituted 1,1'-bis(diphenylphosphino)ferrocene. The substituent is aimed to act as a linker arm with polar functionalities in order to increase the solubility of the compound in polar solvents. The carboxylic acid moiety is likely to facilitate further functionalization towards the synthesis of biologically active molecules.

The geometry around atom Pt1 in (I) is a slightly distorted square planar with the two phosphorous atoms *cis* to each other (Table 1). The P2—Pt1—P1 angle of 97.55 (2)° is significantly larger than 90° due to the geometry of the ferrocenyl moiety. The other bond angles about the Pt atom in (I) are consistent with those seen in related structures (Allen, 2002). Around Pt1, atoms P1 and Cl2 are slightly below and atoms P2 and Cl1 are slightly above the least squares plane defined by atoms Pt1, P1, P2, Cl1, and Cl2. This distorted square planar geometry is typical of this class of compounds with a *cis* substitution pattern around the central platinum(II) atom.

Atom Fe1 is almost equidistant from the centroids of the two five membered rings: Fe1···C_g(C1—C5) = 1.6404 (12) Å and Fe1···C_g(C36—C40) = 1.6512 (12) Å. The two five-membered rings are staggered about Pt1 with an angle of 29.4 (2)° calculated by taking the average and standard deviation of the dihedral angles C1-Centroid 1-Centroid 2-C40, C2-Centroid 1-Centroid 2-C39, C3-Centroid 1-Centroid 2 –C38, C4-Centroid 1-Centroid 2-C37, and C5-Centroid 1-Centroid 2-C36. This angle is slightly larger than the twist angle of 24.7 (2)° between the two five-membered rings in the complex $PtCl_2$(1-[1',2-bis(diphenylphosphino)ferrocenyl]ethylacetate) dichloromethane solvate (Spencer & Bjelosevic, 2007). A dihedral angle of 4.22 (17) ° is formed between the cyclopentadienyl rings. This angle is similar to the angles of 5.9° for the similar complexes $PtCl_2$[1,1'-bis(diphenylphosphino)ferrocene) (Clemente *et al.*, 1986) and 4.32 (18)° for $PtCl_2$(1-[1',2-bis(diphenylphosphino)ferrocenyl]ethylacetate) dichloromethane solvate (Spencer & Bjelosevic, 2007). The other geometrical parameters are typical.

Compound (I) participates in one intramolecular N—H···Cl and intermolecular O—H···O hydrogen bonding interations (Table 2). The intramolecular hydrogen-bonding interaction of the type N—H···Cl which leads to the motif S(8) (Bernstein *et al.*, 1995) may be regarded as weak, as its H···Cl separation of 2.69Å corresponds to a mean of 2.4 (1)Å for similar interactions in the Cambridge Structural Database (CSD; Version 5.28; August 2007 update; Allen, 2002). The prameters for the strong O—H···O interaction are comparable to those of similar hydrogen bonds. This interaction forms dimers of compound (I) and can be described using graph set notation by the motif $R^2_2(8)$ (Bernstein *et al.*, 1995).

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Experimental

(1,5-cyclooctadiene)platinum(II)chloride, (128 mg, 0.342 mmol), was added to a mixture of 1-[1-[(3-carboxy-1-oxopropyl)amino]ethyl]-1',2-bis(diphenylphosphino)ferrocene (Bjelosevic *et al.*, 2006), (241 mg, 0.346 mmol) in dry CH_2Cl_2 (20 ml). The resulting solution was stirred under N_2 atmosphere at room temperature for one hour and then reduced to about 5 ml. Dry Et_2O (35 ml) was added under stirring, resulting in precipitation of a yellow product. The product was collected, washed with dry Et_2O and evaporated under reduced pressure over night at room temperature to give the title compound as a yellow powder (293 mg, 88%). ^{1}H NMR (400 MHz, CD_2Cl_2, p.p.m.): δ 1.93 (d, 3H, J = 6.8 Hz, –CHCH_3), 1.95–2.45 (m, 4H, –CH_2CH_2-), 3.40–5.10 (m, 7H, ferrocene), 6.90–8.33 (m, 22H, PPh, –C*H*CH$_3$ and –CHN*H*CO–), 11.50–12.55 (br s, 1H, –COO*H*). ^{31}P NMR (202 MHz, CD_2Cl_2, p.p.m. relative to H_3PO_4): δ 14.41 (d, $J_{PP'}$ = 8.3 Hz, ^{195}Pt satellites J_{PtP} = 3778 Hz), 8.91 (d, $J_{PP'}$= 8.3 Hz, ^{195}Pt satellites J_{PtP} = 3761 Hz). HRMS (FAB+) *m/z* calculated for $C_{40}H_{37}Cl_2FeNO_3P_2Pt$: 962.0623, found 962.0626 $[M]^+$. El. anal: C 49.80, H 3.95, N 1.37. Crystallization from CH_2Cl_2/hexane solution, by slow evaporation at room temperature, resulted in yellow blocks of (I).

Refinement

Compound (I) co-crystallizes with approximately 1.25 solvent molecules of dichloromethane per platinum complex. A significant amount of time was invested in identifying and refining the disordered dichloromethane solvent molecules. Bond length restraints were applied to model the molecules but the resulting isotropic displacement coefficients suggested the molecules were mobile. In addition, the refinement was computationally unstable. Option SQUEEZE of program *PLATON* (Spek, 2003) was used to correct the diffraction data for diffuse scattering effects and to identify the solvate molecules. *PLATON* calculated the upper limit of volume that can be occupied by the solvent to be 476.2 Å^3, or 12.2% of the unit cell volume. The program calculated 216 electrons in the unit cell for the diffuse species. This approximately corresponds to 1.25 molecules of dichloromethane (52.5 electrons) per compound (I).

All H-atoms were placed in idealized locations (C—H = 0.95–1.00 Å, N—H = 0.86 Å, O—H = 0.84 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

The highest difference peak is 0.xxÅ from Pt1.

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Figures

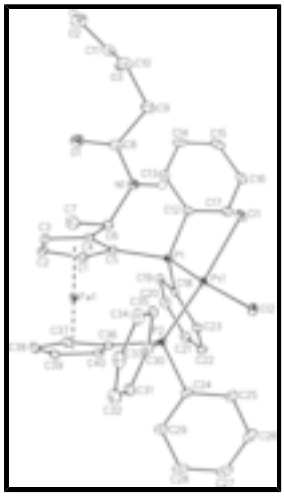

Fig. 1. : The molecular structure of (I) drawn with 30% probability ellipsoids. All hydrogen atoms attached to carbon atoms are omitted for clarity.

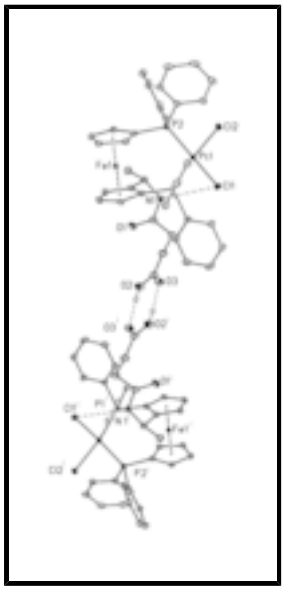

Fig. 2. : A centrosymmetric dimer of compound (I) formed due to the intermolecular hydrogen bonding interaction. The intermolecular hydrogen bond and intramolecular hydrogen bond are shown with the thinner dashed lines. [Symmetry transformation: i: $-x + 2, -y, -z$.]

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Crystal data

$[FePtCl_2(C_{17}H_{14}P)(C_{23}H_{23}NO_3P)]\cdot 1.25CH_2Cl_2$	F_{000} = 2114
M_r = 1069.64	D_x = 1.821 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo- $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 21973 reflections
a = 13.0154 (8) Å	θ = 2.2–29.6º
b = 15.7866 (10) Å	μ = 4.39 mm^{-1}
c = 19.3403 (12) Å	T = 100 (2) K

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β = 100.916 (1)º	Block, yellow
V = 3901.9 (4) Å^3	0.35 × 0.33 × 0.30 mm
Z = 4	

Data collection

Bruker SMART1000 CCD diffractometer	10833 independent reflections
Radiation source: fine-focus sealed tube	9395 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
T = 100(2) K	θ_{max} = 29.6º
ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$h = -18 \rightarrow 18$
T_{min} = 0.309, T_{max} = 0.353	$k = -21 \rightarrow 21$
56419 measured reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.025	H-atom parameters constrained
$wR(F^2)$ = 0.065	$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.9654P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001
10833 reflections	$\Delta\rho_{max}$ = 1.45 e Å^{-3}
453 parameters	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

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$F^2 > 2sigma(F^2)$ 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}
Pt1	0.517748 (7)	0.236711 (6)	0.227608 (5)	0.01205 (3)
Fe1	0.40957 (3)	0.25793 (2)	0.007455 (19)	0.01408 (7)
Cl1	0.67981 (5)	0.17995 (4)	0.28377 (3)	0.02068 (13)
Cl2	0.52630 (5)	0.32416 (4)	0.32745 (3)	0.01833 (12)
P1	0.50312 (5)	0.13556 (4)	0.14368 (3)	0.01277 (12)
P2	0.38650 (5)	0.32092 (4)	0.17376 (3)	0.01277 (12)
O1	0.79978 (17)	0.22592 (16)	0.02709 (11)	0.0341 (5)
O2	1.05274 (17)	0.10838 (14)	0.00910 (12)	0.0318 (5)
H2	1.0534	0.0631	−0.0136	0.048*
O3	0.93828 (15)	0.03658 (14)	0.05916 (11)	0.0305 (5)
N1	0.73423 (17)	0.25400 (14)	0.12523 (13)	0.0182 (4)
H1	0.7435	0.2469	0.1711	0.022*
C1	0.45365 (19)	0.13779 (16)	−0.00883 (13)	0.0174 (5)
H1A	0.4073	0.0868	−0.0140	0.021*
C2	0.4742 (2)	0.18988 (18)	−0.06440 (13)	0.0202 (5)
H2A	0.4430	0.1828	−0.1155	0.024*
C3	0.5439 (2)	0.25468 (17)	−0.03527 (14)	0.0187 (5)
H3	0.5692	0.3017	−0.0624	0.022*
C4	0.56845 (19)	0.24502 (15)	0.03934 (14)	0.0157 (5)
C5	0.51106 (18)	0.17171 (16)	0.05675 (13)	0.0142 (5)
C6	0.64074 (19)	0.30043 (17)	0.09061 (13)	0.0171 (5)
H6	0.6016	0.3165	0.1284	0.021*
C7	0.6698 (2)	0.38307 (18)	0.05800 (15)	0.0241 (6)
H7A	0.7097	0.4191	0.0949	0.036*
H7B	0.6059	0.4126	0.0356	0.036*
H7C	0.7125	0.3705	0.0226	0.036*
C8	0.8071 (2)	0.22138 (18)	0.09118 (16)	0.0239 (6)
C9	0.8993 (2)	0.1799 (2)	0.13841 (16)	0.0270 (6)
H9A	0.8792	0.1222	0.1509	0.032*
H9B	0.9180	0.2129	0.1825	0.032*
C10	0.9939 (2)	0.1743 (2)	0.10304 (17)	0.0284 (6)
H10A	0.9983	0.2268	0.0757	0.034*
H10B	1.0580	0.1707	0.1398	0.034*
C11	0.9903 (2)	0.09984 (19)	0.05495 (16)	0.0251 (6)
C12	0.59865 (18)	0.05016 (16)	0.16185 (13)	0.0157 (5)
C13	0.67153 (19)	0.03441 (16)	0.11885 (14)	0.0178 (5)
H13	0.6758	0.0711	0.0806	0.021*

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C14	0.7377 (2)	−0.03525 (17)	0.13238 (15)	0.0219 (6)
H14	0.7876	−0.0459	0.1033	0.026*
C15	0.7315 (2)	−0.08917 (17)	0.18795 (16)	0.0242 (6)
H15	0.7755	−0.1376	0.1960	0.029*
C16	0.66108 (19)	−0.07251 (17)	0.23194 (15)	0.0200 (5)
H16	0.6585	−0.1085	0.2709	0.024*
C17	0.59439 (19)	−0.00311 (16)	0.21893 (14)	0.0189 (5)
H17	0.5459	0.0081	0.2489	0.023*
C18	0.38247 (18)	0.07400 (16)	0.13510 (13)	0.0141 (5)
C19	0.36812 (19)	0.00308 (16)	0.09043 (13)	0.0166 (5)
H19	0.4207	−0.0121	0.0647	0.020*
C20	0.2775 (2)	−0.04485 (17)	0.08379 (14)	0.0219 (5)
H20	0.2667	−0.0911	0.0518	0.026*
C21	0.2025 (2)	−0.02546 (18)	0.12373 (15)	0.0237 (6)
H21	0.1403	−0.0582	0.1191	0.028*
C22	0.2191 (2)	0.04204 (18)	0.17043 (14)	0.0217 (5)
H22	0.1689	0.0541	0.1990	0.026*
C23	0.30772 (19)	0.09213 (17)	0.17606 (13)	0.0178 (5)
H23	0.3176	0.1387	0.2077	0.021*
C24	0.26636 (19)	0.31782 (16)	0.20920 (14)	0.0168 (5)
C25	0.2685 (2)	0.28888 (17)	0.27762 (14)	0.0197 (5)
H25	0.3311	0.2659	0.3043	0.024*
C26	0.1784 (2)	0.29372 (18)	0.30681 (16)	0.0259 (6)
H26	0.1801	0.2749	0.3537	0.031*
C27	0.0872 (2)	0.32574 (18)	0.26774 (17)	0.0283 (7)
H27	0.0262	0.3290	0.2879	0.034*
C28	0.0838 (2)	0.35315 (19)	0.19946 (17)	0.0277 (6)
H28	0.0205	0.3752	0.1729	0.033*
C29	0.17282 (19)	0.34854 (17)	0.16937 (15)	0.0215 (5)
H29	0.1700	0.3662	0.1221	0.026*
C30	0.4300 (2)	0.43184 (16)	0.18119 (13)	0.0161 (5)
C31	0.3561 (2)	0.49628 (17)	0.16439 (14)	0.0204 (5)
H31	0.2839	0.4825	0.1521	0.024*
C32	0.3874 (2)	0.57983 (18)	0.16548 (15)	0.0272 (6)
H32	0.3366	0.6233	0.1541	0.033*
C33	0.4933 (2)	0.60076 (18)	0.18318 (14)	0.0255 (6)
H33	0.5146	0.6584	0.1843	0.031*
C34	0.5667 (2)	0.53766 (18)	0.19900 (14)	0.0239 (6)
H34	0.6389	0.5516	0.2103	0.029*
C35	0.5351 (2)	0.45313 (17)	0.19849 (13)	0.0176 (5)
H35	0.5861	0.4098	0.2101	0.021*
C36	0.33884 (18)	0.31513 (16)	0.07995 (13)	0.0152 (5)
C37	0.35963 (19)	0.37625 (16)	0.02881 (13)	0.0176 (5)
H37	0.4048	0.4277	0.0392	0.021*
C38	0.3063 (2)	0.35052 (18)	−0.03852 (14)	0.0219 (5)
H38	0.3082	0.3801	−0.0840	0.026*
C39	0.2515 (2)	0.27440 (18)	−0.03070 (14)	0.0202 (5)
H39	0.2084	0.2413	−0.0698	0.024*
C40	0.2707 (2)	0.25155 (16)	0.04190 (15)	0.0168 (5)

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H40	0.2421	0.2008	0.0627	0.020*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01341 (5)	0.01136 (5)	0.01105 (5)	0.00026 (3)	0.00150 (3)	−0.00018 (3)
Fe1	0.01480 (16)	0.01564 (18)	0.01161 (17)	0.00201 (13)	0.00204 (13)	−0.00002 (13)
Cl1	0.0199 (3)	0.0201 (3)	0.0190 (3)	0.0042 (2)	−0.0041 (2)	−0.0016 (2)
Cl2	0.0228 (3)	0.0180 (3)	0.0140 (3)	−0.0016 (2)	0.0032 (2)	−0.0037 (2)
P1	0.0125 (3)	0.0119 (3)	0.0137 (3)	0.0011 (2)	0.0020 (2)	−0.0003 (2)
P2	0.0134 (3)	0.0122 (3)	0.0130 (3)	0.0009 (2)	0.0033 (2)	−0.0007 (2)
O1	0.0255 (11)	0.0534 (15)	0.0224 (11)	0.0109 (10)	0.0022 (9)	−0.0106 (10)
O2	0.0305 (11)	0.0261 (12)	0.0414 (13)	−0.0034 (9)	0.0135 (10)	−0.0064 (10)
O3	0.0255 (10)	0.0285 (12)	0.0391 (13)	−0.0023 (9)	0.0104 (9)	−0.0088 (10)
N1	0.0158 (10)	0.0208 (12)	0.0176 (11)	0.0015 (8)	0.0020 (9)	−0.0007 (8)
C1	0.0191 (11)	0.0160 (12)	0.0173 (12)	0.0012 (9)	0.0040 (10)	−0.0051 (10)
C2	0.0223 (12)	0.0258 (15)	0.0133 (12)	0.0031 (10)	0.0058 (10)	−0.0029 (10)
C3	0.0213 (12)	0.0211 (14)	0.0151 (12)	0.0024 (10)	0.0068 (10)	0.0024 (10)
C4	0.0135 (11)	0.0160 (12)	0.0182 (12)	0.0021 (9)	0.0048 (9)	−0.0006 (9)
C5	0.0131 (10)	0.0147 (12)	0.0152 (11)	0.0017 (9)	0.0041 (9)	0.0003 (9)
C6	0.0147 (11)	0.0177 (13)	0.0191 (12)	0.0001 (9)	0.0035 (9)	0.0009 (10)
C7	0.0240 (13)	0.0186 (14)	0.0293 (15)	−0.0036 (10)	0.0040 (11)	0.0040 (11)
C8	0.0175 (12)	0.0259 (15)	0.0270 (15)	0.0025 (10)	0.0009 (11)	−0.0081 (12)
C9	0.0190 (13)	0.0311 (16)	0.0294 (15)	0.0060 (11)	0.0012 (11)	−0.0057 (12)
C10	0.0180 (12)	0.0279 (16)	0.0369 (17)	0.0028 (11)	−0.0007 (12)	−0.0074 (13)
C11	0.0180 (12)	0.0235 (15)	0.0319 (16)	0.0034 (10)	0.0001 (11)	−0.0033 (12)
C12	0.0138 (11)	0.0121 (12)	0.0205 (13)	0.0009 (9)	0.0009 (9)	−0.0028 (9)
C13	0.0171 (11)	0.0153 (12)	0.0202 (13)	0.0001 (9)	0.0015 (10)	−0.0016 (10)
C14	0.0147 (11)	0.0207 (14)	0.0307 (15)	0.0009 (10)	0.0053 (11)	−0.0064 (11)
C15	0.0169 (12)	0.0152 (13)	0.0370 (16)	0.0025 (10)	−0.0037 (11)	−0.0022 (11)
C16	0.0163 (11)	0.0156 (13)	0.0258 (14)	−0.0029 (9)	−0.0021 (10)	0.0026 (10)
C17	0.0167 (11)	0.0150 (13)	0.0246 (14)	0.0005 (9)	0.0027 (10)	0.0017 (10)
C18	0.0135 (10)	0.0141 (12)	0.0139 (11)	0.0007 (9)	0.0009 (9)	0.0028 (9)
C19	0.0198 (12)	0.0141 (12)	0.0155 (12)	−0.0006 (9)	0.0021 (10)	−0.0006 (9)
C20	0.0241 (13)	0.0178 (13)	0.0219 (14)	−0.0041 (10)	−0.0004 (11)	−0.0023 (11)
C21	0.0200 (12)	0.0225 (14)	0.0274 (15)	−0.0035 (10)	0.0011 (11)	0.0070 (11)
C22	0.0176 (12)	0.0252 (14)	0.0241 (14)	0.0017 (10)	0.0085 (10)	0.0047 (11)
C23	0.0192 (12)	0.0169 (13)	0.0177 (12)	0.0029 (9)	0.0043 (10)	−0.0006 (10)
C24	0.0172 (11)	0.0144 (12)	0.0205 (13)	−0.0026 (9)	0.0078 (10)	−0.0042 (10)
C25	0.0232 (12)	0.0154 (12)	0.0228 (13)	−0.0017 (10)	0.0102 (11)	−0.0009 (10)
C26	0.0336 (15)	0.0171 (13)	0.0324 (16)	−0.0035 (11)	0.0202 (13)	−0.0031 (12)
C27	0.0271 (14)	0.0187 (14)	0.0449 (18)	−0.0018 (11)	0.0214 (13)	−0.0050 (13)
C28	0.0193 (13)	0.0246 (15)	0.0414 (18)	0.0022 (11)	0.0110 (12)	−0.0066 (13)
C29	0.0185 (12)	0.0201 (14)	0.0269 (14)	0.0016 (10)	0.0071 (11)	−0.0026 (11)
C30	0.0218 (12)	0.0117 (12)	0.0155 (12)	−0.0005 (9)	0.0049 (10)	0.0000 (9)
C31	0.0227 (12)	0.0182 (13)	0.0202 (13)	0.0029 (10)	0.0036 (10)	0.0003 (10)
C32	0.0405 (17)	0.0147 (14)	0.0269 (15)	0.0042 (12)	0.0082 (13)	0.0040 (11)
C33	0.0412 (16)	0.0141 (13)	0.0201 (13)	−0.0041 (11)	0.0031 (12)	0.0013 (10)

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C34	0.0293 (14)	0.0211 (14)	0.0201 (14)	−0.0084 (11)	0.0013 (11)	0.0005 (11)
C35	0.0209 (12)	0.0171 (13)	0.0144 (12)	0.0008 (10)	0.0019 (10)	0.0000 (10)
C36	0.0133 (10)	0.0162 (12)	0.0159 (12)	0.0037 (9)	0.0020 (9)	−0.0018 (9)
C37	0.0201 (12)	0.0142 (12)	0.0190 (12)	0.0029 (9)	0.0047 (10)	0.0008 (10)
C38	0.0253 (13)	0.0237 (14)	0.0155 (12)	0.0092 (11)	0.0009 (10)	0.0033 (10)
C39	0.0188 (12)	0.0239 (14)	0.0161 (12)	0.0055 (10)	−0.0012 (10)	−0.0037 (10)
C40	0.0125 (11)	0.0179 (13)	0.0197 (13)	0.0027 (9)	0.0023 (10)	−0.0036 (9)

Geometric parameters (Å, °)

Pt1—P2	2.2575 (6)	C13—H13	0.9500
Pt1—P1	2.2592 (6)	C14—C15	1.385 (4)
Pt1—Cl1	2.3588 (6)	C14—H14	0.9500
Pt1—Cl2	2.3592 (6)	C15—C16	1.389 (4)
Fe1—C5	2.007 (2)	C15—H15	0.9500
Fe1—C1	2.023 (3)	C16—C17	1.391 (4)
Fe1—C36	2.029 (2)	C16—H16	0.9500
Fe1—C40	2.044 (3)	C17—H17	0.9500
Fe1—C37	2.045 (3)	C18—C23	1.396 (3)
Fe1—C4	2.053 (3)	C18—C19	1.405 (3)
Fe1—C2	2.058 (2)	C19—C20	1.386 (3)
Fe1—C39	2.066 (3)	C19—H19	0.9500
Fe1—C38	2.069 (3)	C20—C21	1.389 (4)
Fe1—C3	2.071 (3)	C20—H20	0.9500
P1—C5	1.797 (2)	C21—C22	1.387 (4)
P1—C12	1.823 (2)	C21—H21	0.9500
P1—C18	1.827 (2)	C22—C23	1.386 (4)
P2—C36	1.805 (3)	C22—H22	0.9500
P2—C24	1.823 (2)	C23—H23	0.9500
P2—C30	1.837 (3)	C24—C25	1.395 (4)
O1—C8	1.227 (4)	C24—C29	1.398 (4)
O2—C11	1.318 (3)	C25—C26	1.396 (4)
O2—H2	0.8400	C25—H25	0.9500
O3—C11	1.218 (3)	C26—C27	1.377 (4)
N1—C8	1.354 (3)	C26—H26	0.9500
N1—C6	1.469 (3)	C27—C28	1.382 (4)
N1—H1	0.8800	C27—H27	0.9500
C1—C2	1.418 (4)	C28—C29	1.394 (4)
C1—C5	1.447 (3)	C28—H28	0.9500
C1—H1A	1.0000	C29—H29	0.9500
C2—C3	1.412 (4)	C30—C35	1.387 (3)
C2—H2A	1.0000	C30—C31	1.395 (4)
C3—C4	1.426 (4)	C31—C32	1.379 (4)
C3—H3	1.0000	C31—H31	0.9500
C4—C5	1.451 (3)	C32—C33	1.396 (4)
C4—C6	1.510 (4)	C32—H32	0.9500
C6—C7	1.527 (4)	C33—C34	1.374 (4)
C6—H6	1.0000	C33—H33	0.9500
C7—H7A	0.9800	C34—C35	1.395 (4)

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C7—H7B	0.9800	C34—H34	0.9500
C7—H7C	0.9800	C35—H35	0.9500
C8—C9	1.513 (4)	C36—C37	1.443 (3)
C9—C10	1.520 (4)	C36—C40	1.445 (3)
C9—H9A	0.9900	C37—C38	1.414 (4)
C9—H9B	0.9900	C37—H37	1.0000
C10—C11	1.494 (4)	C38—C39	1.420 (4)
C10—H10A	0.9900	C38—H38	1.0000
C10—H10B	0.9900	C39—C40	1.425 (4)
C12—C13	1.397 (3)	C39—H39	1.0000
C12—C17	1.397 (4)	C40—H40	1.0000
C13—C14	1.391 (4)		

P2—Pt1—P1	97.55 (2)	C8—C9—H9B	109.3
P2—Pt1—Cl1	165.62 (2)	C10—C9—H9B	109.3
P1—Pt1—Cl1	90.50 (2)	H9A—C9—H9B	107.9
P2—Pt1—Cl2	86.98 (2)	C11—C10—C9	113.2 (2)
P1—Pt1—Cl2	170.47 (2)	C11—C10—H10A	108.9
Cl1—Pt1—Cl2	86.90 (2)	C9—C10—H10A	108.9
C5—Fe1—C1	42.09 (10)	C11—C10—H10B	108.9
C5—Fe1—C36	108.51 (10)	C9—C10—H10B	108.9
C1—Fe1—C36	134.73 (10)	H10A—C10—H10B	107.8
C5—Fe1—C40	110.79 (10)	O3—C11—O2	123.4 (3)
C1—Fe1—C40	107.39 (10)	O3—C11—C10	123.7 (3)
C36—Fe1—C40	41.56 (10)	O2—C11—C10	112.8 (3)
C5—Fe1—C37	136.80 (10)	C13—C12—C17	119.8 (2)
C1—Fe1—C37	176.16 (10)	C13—C12—P1	122.2 (2)
C36—Fe1—C37	41.49 (10)	C17—C12—P1	118.02 (18)
C40—Fe1—C37	69.19 (10)	C14—C13—C12	119.7 (2)
C5—Fe1—C4	41.86 (9)	C14—C13—H13	120.2
C1—Fe1—C4	69.79 (10)	C12—C13—H13	120.2
C36—Fe1—C4	113.55 (10)	C15—C14—C13	120.4 (2)
C40—Fe1—C4	143.12 (11)	C15—C14—H14	119.8
C37—Fe1—C4	111.75 (10)	C13—C14—H14	119.8
C5—Fe1—C2	69.55 (10)	C14—C15—C16	120.1 (2)
C1—Fe1—C2	40.66 (10)	C14—C15—H15	120.0
C36—Fe1—C2	174.72 (11)	C16—C15—H15	120.0
C40—Fe1—C2	133.95 (11)	C15—C16—C17	120.0 (3)
C37—Fe1—C2	143.05 (11)	C15—C16—H16	120.0
C4—Fe1—C2	68.53 (10)	C17—C16—H16	120.0
C5—Fe1—C39	140.90 (11)	C16—C17—C12	120.0 (2)
C1—Fe1—C39	110.79 (11)	C16—C17—H17	120.0
C36—Fe1—C39	68.87 (10)	C12—C17—H17	120.0
C40—Fe1—C39	40.57 (10)	C23—C18—C19	119.1 (2)
C37—Fe1—C39	67.93 (10)	C23—C18—P1	121.26 (19)
C4—Fe1—C39	176.24 (11)	C19—C18—P1	119.44 (18)
C2—Fe1—C39	109.33 (11)	C20—C19—C18	120.2 (2)
C5—Fe1—C38	176.98 (11)	C20—C19—H19	119.9
C1—Fe1—C38	140.86 (11)	C18—C19—H19	119.9
C36—Fe1—C38	68.88 (10)	C19—C20—C21	120.2 (3)

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C40—Fe1—C38	68.42 (11)	C19—C20—H20	119.9
C37—Fe1—C38	40.20 (10)	C21—C20—H20	119.9
C4—Fe1—C38	137.27 (11)	C22—C21—C20	119.5 (2)
C2—Fe1—C38	113.19 (11)	C22—C21—H21	120.2
C39—Fe1—C38	40.16 (11)	C20—C21—H21	120.2
C5—Fe1—C3	69.11 (10)	C23—C22—C21	120.9 (2)
C1—Fe1—C3	68.23 (10)	C23—C22—H22	119.5
C36—Fe1—C3	144.53 (10)	C21—C22—H22	119.5
C40—Fe1—C3	173.90 (11)	C22—C23—C18	119.9 (2)
C37—Fe1—C3	115.32 (10)	C22—C23—H23	120.1
C4—Fe1—C3	40.45 (10)	C18—C23—H23	120.1
C2—Fe1—C3	40.00 (10)	C25—C24—C29	119.7 (2)
C39—Fe1—C3	135.99 (11)	C25—C24—P2	120.1 (2)
C38—Fe1—C3	112.01 (11)	C29—C24—P2	120.19 (19)
C5—P1—C12	104.91 (11)	C24—C25—C26	119.9 (3)
C5—P1—C18	106.54 (11)	C24—C25—H25	120.1
C12—P1—C18	99.63 (11)	C26—C25—H25	120.1
C5—P1—Pt1	115.84 (8)	C27—C26—C25	120.1 (3)
C12—P1—Pt1	115.01 (8)	C27—C26—H26	120.0
C18—P1—Pt1	113.28 (8)	C25—C26—H26	120.0
C36—P2—C24	102.74 (11)	C26—C27—C28	120.5 (3)
C36—P2—C30	99.73 (12)	C26—C27—H27	119.8
C24—P2—C30	105.64 (11)	C28—C27—H27	119.8
C36—P2—Pt1	121.32 (8)	C27—C28—C29	120.2 (3)
C24—P2—Pt1	116.02 (9)	C27—C28—H28	119.9
C30—P2—Pt1	109.28 (8)	C29—C28—H28	119.9
C11—O2—H2	109.5	C28—C29—C24	119.6 (3)
C8—N1—C6	124.3 (2)	C28—C29—H29	120.2
C8—N1—H1	117.8	C24—C29—H29	120.2
C6—N1—H1	117.8	C35—C30—C31	119.0 (2)
C2—C1—C5	108.0 (2)	C35—C30—P2	121.66 (19)
C2—C1—Fe1	70.98 (15)	C31—C30—P2	119.2 (2)
C5—C1—Fe1	68.37 (14)	C32—C31—C30	120.4 (3)
C2—C1—H1A	126.0	C32—C31—H31	119.8
C5—C1—H1A	126.0	C30—C31—H31	119.8
Fe1—C1—H1A	126.0	C31—C32—C33	120.3 (3)
C3—C2—C1	108.5 (2)	C31—C32—H32	119.8
C3—C2—Fe1	70.50 (15)	C33—C32—H32	119.8
C1—C2—Fe1	68.36 (14)	C34—C33—C32	119.7 (3)
C3—C2—H2A	125.8	C34—C33—H33	120.1
C1—C2—H2A	125.8	C32—C33—H33	120.1
Fe1—C2—H2A	125.8	C33—C34—C35	120.0 (3)
C2—C3—C4	109.3 (2)	C33—C34—H34	120.0
C2—C3—Fe1	69.50 (15)	C35—C34—H34	120.0
C4—C3—Fe1	69.10 (14)	C30—C35—C34	120.6 (2)
C2—C3—H3	125.3	C30—C35—H35	119.7
C4—C3—H3	125.3	C34—C35—H35	119.7
Fe1—C3—H3	125.3	C37—C36—C40	107.0 (2)
C3—C4—C5	107.1 (2)	C37—C36—P2	125.56 (19)

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C3—C4—C6	126.5 (2)	C40—C36—P2	127.4 (2)
C5—C4—C6	126.4 (2)	C37—C36—Fe1	69.86 (14)
C3—C4—Fe1	70.45 (15)	C40—C36—Fe1	69.76 (14)
C5—C4—Fe1	67.39 (13)	P2—C36—Fe1	127.05 (13)
C6—C4—Fe1	127.34 (17)	C38—C37—C36	108.4 (2)
C1—C5—C4	107.1 (2)	C38—C37—Fe1	70.81 (15)
C1—C5—P1	126.21 (19)	C36—C37—Fe1	68.65 (14)
C4—C5—P1	126.43 (19)	C38—C37—H37	125.8
C1—C5—Fe1	69.54 (14)	C36—C37—H37	125.8
C4—C5—Fe1	70.75 (14)	Fe1—C37—H37	125.8
P1—C5—Fe1	120.70 (12)	C37—C38—C39	108.3 (2)
N1—C6—C4	111.7 (2)	C37—C38—Fe1	68.99 (14)
N1—C6—C7	111.5 (2)	C39—C38—Fe1	69.80 (15)
C4—C6—C7	113.3 (2)	C37—C38—H38	125.8
N1—C6—H6	106.6	C39—C38—H38	125.8
C4—C6—H6	106.6	Fe1—C38—H38	125.8
C7—C6—H6	106.6	C38—C39—C40	108.7 (2)
C6—C7—H7A	109.5	C38—C39—Fe1	70.03 (15)
C6—C7—H7B	109.5	C40—C39—Fe1	68.86 (15)
H7A—C7—H7B	109.5	C38—C39—H39	125.6
C6—C7—H7C	109.5	C40—C39—H39	125.6
H7A—C7—H7C	109.5	Fe1—C39—H39	125.6
H7B—C7—H7C	109.5	C39—C40—C36	107.6 (2)
O1—C8—N1	122.8 (3)	C39—C40—Fe1	70.56 (15)
O1—C8—C9	122.4 (3)	C36—C40—Fe1	68.68 (14)
N1—C8—C9	114.8 (3)	C39—C40—H40	126.2
C8—C9—C10	111.8 (3)	C36—C40—H40	126.2
C8—C9—H9A	109.3	Fe1—C40—H40	126.2
C10—C9—H9A	109.3		

P2—Pt1—P1—C5	55.66 (9)	Pt1—P1—C12—C17	65.6 (2)
Cl1—Pt1—P1—C5	−112.39 (9)	C17—C12—C13—C14	1.4 (4)
Cl2—Pt1—P1—C5	173.58 (14)	P1—C12—C13—C14	−175.5 (2)
P2—Pt1—P1—C12	178.43 (9)	C12—C13—C14—C15	0.3 (4)
Cl1—Pt1—P1—C12	10.38 (9)	C13—C14—C15—C16	−2.0 (4)
Cl2—Pt1—P1—C12	−63.65 (16)	C14—C15—C16—C17	2.0 (4)
P2—Pt1—P1—C18	−67.88 (9)	C15—C16—C17—C12	−0.4 (4)
Cl1—Pt1—P1—C18	124.06 (9)	C13—C12—C17—C16	−1.3 (4)
Cl2—Pt1—P1—C18	50.04 (16)	P1—C12—C17—C16	175.7 (2)
P1—Pt1—P2—C36	−20.67 (10)	C5—P1—C18—C23	−126.6 (2)
Cl1—Pt1—P2—C36	102.85 (13)	C12—P1—C18—C23	124.6 (2)
Cl2—Pt1—P2—C36	167.75 (10)	Pt1—P1—C18—C23	2.0 (2)
P1—Pt1—P2—C24	105.09 (9)	C5—P1—C18—C19	58.4 (2)
Cl1—Pt1—P2—C24	−131.39 (12)	C12—P1—C18—C19	−50.4 (2)
Cl2—Pt1—P2—C24	−66.49 (9)	Pt1—P1—C18—C19	−173.11 (17)
P1—Pt1—P2—C30	−135.66 (8)	C23—C18—C19—C20	4.2 (4)
Cl1—Pt1—P2—C30	−12.14 (13)	P1—C18—C19—C20	179.4 (2)
Cl2—Pt1—P2—C30	52.76 (8)	C18—C19—C20—C21	−3.0 (4)
C5—Fe1—C1—C2	−119.3 (2)	C19—C20—C21—C22	−0.2 (4)
C36—Fe1—C1—C2	176.22 (15)	C20—C21—C22—C23	2.2 (4)

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C40—Fe1—C1—C2	138.72 (16)	C21—C22—C23—C18	−1.0 (4)
C37—Fe1—C1—C2	165.6 (15)	C19—C18—C23—C22	−2.2 (4)
C4—Fe1—C1—C2	−80.21 (16)	P1—C18—C23—C22	−177.3 (2)
C39—Fe1—C1—C2	95.82 (16)	C36—P2—C24—C25	155.4 (2)
C38—Fe1—C1—C2	61.8 (2)	C30—P2—C24—C25	−100.5 (2)
C3—Fe1—C1—C2	−36.78 (15)	Pt1—P2—C24—C25	20.7 (2)
C36—Fe1—C1—C5	−64.51 (19)	C36—P2—C24—C29	−28.0 (2)
C40—Fe1—C1—C5	−102.00 (15)	C30—P2—C24—C29	76.1 (2)
C37—Fe1—C1—C5	−75.2 (16)	Pt1—P2—C24—C29	−162.68 (18)
C4—Fe1—C1—C5	39.06 (14)	C29—C24—C25—C26	−2.4 (4)
C2—Fe1—C1—C5	119.3 (2)	P2—C24—C25—C26	174.2 (2)
C39—Fe1—C1—C5	−144.91 (14)	C24—C25—C26—C27	1.0 (4)
C38—Fe1—C1—C5	−178.95 (16)	C25—C26—C27—C28	0.1 (4)
C3—Fe1—C1—C5	82.50 (15)	C26—C27—C28—C29	0.1 (4)
C5—C1—C2—C3	0.8 (3)	C27—C28—C29—C24	−1.5 (4)
Fe1—C1—C2—C3	59.27 (18)	C25—C24—C29—C28	2.6 (4)
C5—C1—C2—Fe1	−58.51 (16)	P2—C24—C29—C28	−174.0 (2)
C5—Fe1—C2—C3	−81.51 (16)	C36—P2—C30—C35	−111.1 (2)
C1—Fe1—C2—C3	−120.1 (2)	C24—P2—C30—C35	142.7 (2)
C36—Fe1—C2—C3	−150.8 (11)	Pt1—P2—C30—C35	17.2 (2)
C40—Fe1—C2—C3	178.90 (16)	C36—P2—C30—C31	64.5 (2)
C37—Fe1—C2—C3	61.5 (2)	C24—P2—C30—C31	−41.8 (2)
C4—Fe1—C2—C3	−36.54 (15)	Pt1—P2—C30—C31	−167.27 (18)
C39—Fe1—C2—C3	140.16 (16)	C35—C30—C31—C32	−0.4 (4)
C38—Fe1—C2—C3	97.11 (17)	P2—C30—C31—C32	−176.1 (2)
C5—Fe1—C2—C1	38.61 (15)	C30—C31—C32—C33	0.2 (4)
C36—Fe1—C2—C1	−30.6 (12)	C31—C32—C33—C34	0.5 (4)
C40—Fe1—C2—C1	−61.0 (2)	C32—C33—C34—C35	−1.1 (4)
C37—Fe1—C2—C1	−178.41 (17)	C31—C30—C35—C34	−0.1 (4)
C4—Fe1—C2—C1	83.58 (16)	P2—C30—C35—C34	175.5 (2)
C39—Fe1—C2—C1	−99.72 (16)	C33—C34—C35—C30	0.8 (4)
C38—Fe1—C2—C1	−142.77 (15)	C24—P2—C36—C37	123.0 (2)
C3—Fe1—C2—C1	120.1 (2)	C30—P2—C36—C37	14.4 (2)
C1—C2—C3—C4	−0.3 (3)	Pt1—P2—C36—C37	−105.3 (2)
Fe1—C2—C3—C4	57.70 (18)	C24—P2—C36—C40	−54.6 (2)
C1—C2—C3—Fe1	−57.96 (17)	C30—P2—C36—C40	−163.2 (2)
C5—Fe1—C3—C2	82.70 (17)	Pt1—P2—C36—C40	77.0 (2)
C1—Fe1—C3—C2	37.37 (15)	C24—P2—C36—Fe1	−146.42 (16)
C36—Fe1—C3—C2	175.56 (17)	C30—P2—C36—Fe1	104.96 (17)
C40—Fe1—C3—C2	−7.5 (11)	Pt1—P2—C36—Fe1	−14.8 (2)
C37—Fe1—C3—C2	−144.25 (16)	C5—Fe1—C36—C37	141.43 (15)
C4—Fe1—C3—C2	121.3 (2)	C1—Fe1—C36—C37	−178.93 (15)
C39—Fe1—C3—C2	−60.5 (2)	C40—Fe1—C36—C37	−117.8 (2)
C38—Fe1—C3—C2	−100.31 (17)	C4—Fe1—C36—C37	96.73 (15)
C5—Fe1—C3—C4	−38.64 (14)	C2—Fe1—C36—C37	−151.1 (11)
C1—Fe1—C3—C4	−83.98 (16)	C39—Fe1—C36—C37	−80.15 (16)
C36—Fe1—C3—C4	54.2 (2)	C38—Fe1—C36—C37	−36.95 (15)
C40—Fe1—C3—C4	−128.8 (10)	C3—Fe1—C36—C37	61.7 (2)
C37—Fe1—C3—C4	94.40 (16)	C5—Fe1—C36—C40	−100.75 (16)

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C2—Fe1—C3—C4	−121.3 (2)	C1—Fe1—C36—C40	−61.1 (2)
C39—Fe1—C3—C4	178.17 (16)	C37—Fe1—C36—C40	117.8 (2)
C38—Fe1—C3—C4	138.34 (15)	C4—Fe1—C36—C40	−145.45 (15)
C2—C3—C4—C5	−0.3 (3)	C2—Fe1—C36—C40	−33.2 (12)
Fe1—C3—C4—C5	57.59 (16)	C39—Fe1—C36—C40	37.67 (15)
C2—C3—C4—C6	179.5 (2)	C38—Fe1—C36—C40	80.86 (16)
Fe1—C3—C4—C6	−122.6 (2)	C3—Fe1—C36—C40	179.51 (18)
C2—C3—C4—Fe1	−57.94 (19)	C5—Fe1—C36—P2	21.49 (19)
C5—Fe1—C4—C3	119.0 (2)	C1—Fe1—C36—P2	61.1 (2)
C1—Fe1—C4—C3	79.78 (16)	C40—Fe1—C36—P2	122.2 (2)
C36—Fe1—C4—C3	−149.10 (15)	C37—Fe1—C36—P2	−119.9 (2)
C40—Fe1—C4—C3	172.08 (17)	C4—Fe1—C36—P2	−23.2 (2)
C37—Fe1—C4—C3	−104.00 (16)	C2—Fe1—C36—P2	89.0 (11)
C2—Fe1—C4—C3	36.15 (15)	C39—Fe1—C36—P2	159.9 (2)
C39—Fe1—C4—C3	−19.7 (16)	C38—Fe1—C36—P2	−156.9 (2)
C38—Fe1—C4—C3	−65.3 (2)	C3—Fe1—C36—P2	−58.2 (3)
C1—Fe1—C4—C5	−39.27 (14)	C40—C36—C37—C38	−0.3 (3)
C36—Fe1—C4—C5	91.86 (16)	P2—C36—C37—C38	−178.37 (18)
C40—Fe1—C4—C5	53.0 (2)	Fe1—C36—C37—C38	59.85 (17)
C37—Fe1—C4—C5	136.96 (14)	C40—C36—C37—Fe1	−60.18 (16)
C2—Fe1—C4—C5	−82.89 (15)	P2—C36—C37—Fe1	121.78 (19)
C39—Fe1—C4—C5	−138.8 (16)	C5—Fe1—C37—C38	−179.41 (16)
C38—Fe1—C4—C5	175.69 (15)	C1—Fe1—C37—C38	−108.3 (16)
C3—Fe1—C4—C5	−119.0 (2)	C36—Fe1—C37—C38	−119.7 (2)
C5—Fe1—C4—C6	−119.4 (3)	C40—Fe1—C37—C38	−80.80 (17)
C1—Fe1—C4—C6	−158.7 (2)	C4—Fe1—C37—C38	138.88 (16)
C36—Fe1—C4—C6	−27.5 (3)	C2—Fe1—C37—C38	56.1 (2)
C40—Fe1—C4—C6	−66.4 (3)	C39—Fe1—C37—C38	−37.08 (16)
C37—Fe1—C4—C6	17.6 (3)	C3—Fe1—C37—C38	94.74 (17)
C2—Fe1—C4—C6	157.7 (3)	C5—Fe1—C37—C36	−59.7 (2)
C39—Fe1—C4—C6	101.8 (16)	C1—Fe1—C37—C36	11.4 (16)
C38—Fe1—C4—C6	56.3 (3)	C40—Fe1—C37—C36	38.88 (14)
C3—Fe1—C4—C6	121.6 (3)	C4—Fe1—C37—C36	−101.44 (15)
C2—C1—C5—C4	−1.0 (3)	C2—Fe1—C37—C36	175.76 (17)
Fe1—C1—C5—C4	−61.11 (16)	C39—Fe1—C37—C36	82.60 (16)
C2—C1—C5—P1	173.86 (18)	C38—Fe1—C37—C36	119.7 (2)
Fe1—C1—C5—P1	113.71 (19)	C3—Fe1—C37—C36	−145.58 (15)
C2—C1—C5—Fe1	60.14 (17)	C36—C37—C38—C39	0.4 (3)
C3—C4—C5—C1	0.8 (3)	Fe1—C37—C38—C39	58.91 (18)
C6—C4—C5—C1	−179.1 (2)	C36—C37—C38—Fe1	−58.52 (17)
Fe1—C4—C5—C1	60.33 (16)	C5—Fe1—C38—C37	8(2)
C3—C4—C5—P1	−174.00 (18)	C1—Fe1—C38—C37	174.21 (16)
C6—C4—C5—P1	6.1 (4)	C36—Fe1—C38—C37	38.10 (15)
Fe1—C4—C5—P1	−114.48 (19)	C40—Fe1—C38—C37	82.88 (16)
C3—C4—C5—Fe1	−59.53 (17)	C4—Fe1—C38—C37	−64.2 (2)
C6—C4—C5—Fe1	120.6 (2)	C2—Fe1—C38—C37	−147.14 (15)
C12—P1—C5—C1	87.3 (2)	C39—Fe1—C38—C37	120.0 (2)
C18—P1—C5—C1	−17.7 (2)	C3—Fe1—C38—C37	−103.67 (16)
Pt1—P1—C5—C1	−144.74 (18)	C5—Fe1—C38—C39	−112 (2)

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C12—P1—C5—C4	−98.8 (2)	C1—Fe1—C38—C39	54.3 (2)
C18—P1—C5—C4	156.1 (2)	C36—Fe1—C38—C39	−81.86 (16)
Pt1—P1—C5—C4	29.1 (2)	C40—Fe1—C38—C39	−37.08 (15)
C12—P1—C5—Fe1	173.35 (13)	C37—Fe1—C38—C39	−120.0 (2)
C18—P1—C5—Fe1	68.30 (16)	C4—Fe1—C38—C39	175.84 (16)
Pt1—P1—C5—Fe1	−58.70 (15)	C2—Fe1—C38—C39	92.90 (17)
C36—Fe1—C5—C1	137.46 (14)	C3—Fe1—C38—C39	136.37 (16)
C40—Fe1—C5—C1	93.26 (15)	C37—C38—C39—C40	−0.3 (3)
C37—Fe1—C5—C1	174.57 (15)	Fe1—C38—C39—C40	58.11 (18)
C4—Fe1—C5—C1	−117.6 (2)	C37—C38—C39—Fe1	−58.41 (17)
C2—Fe1—C5—C1	−37.34 (14)	C5—Fe1—C39—C38	175.56 (16)
C39—Fe1—C5—C1	58.5 (2)	C1—Fe1—C39—C38	−146.77 (15)
C38—Fe1—C5—C1	167.4 (19)	C36—Fe1—C39—C38	81.90 (16)
C3—Fe1—C5—C1	−80.22 (15)	C40—Fe1—C39—C38	120.5 (2)
C1—Fe1—C5—C4	117.6 (2)	C37—Fe1—C39—C38	37.12 (15)
C36—Fe1—C5—C4	−104.94 (15)	C4—Fe1—C39—C38	−48.7 (16)
C40—Fe1—C5—C4	−149.14 (15)	C2—Fe1—C39—C38	−103.39 (16)
C37—Fe1—C5—C4	−67.83 (19)	C3—Fe1—C39—C38	−67.0 (2)
C2—Fe1—C5—C4	80.26 (15)	C5—Fe1—C39—C40	55.1 (2)
C39—Fe1—C5—C4	176.07 (16)	C1—Fe1—C39—C40	92.77 (16)
C38—Fe1—C5—C4	−75 (2)	C36—Fe1—C39—C40	−38.56 (15)
C3—Fe1—C5—C4	37.38 (15)	C37—Fe1—C39—C40	−83.34 (16)
C1—Fe1—C5—P1	−120.8 (2)	C4—Fe1—C39—C40	−169.1 (15)
C36—Fe1—C5—P1	16.67 (17)	C2—Fe1—C39—C40	136.16 (15)
C40—Fe1—C5—P1	−27.53 (18)	C38—Fe1—C39—C40	−120.5 (2)
C37—Fe1—C5—P1	53.8 (2)	C3—Fe1—C39—C40	172.51 (15)
C4—Fe1—C5—P1	121.6 (2)	C38—C39—C40—C36	0.1 (3)
C2—Fe1—C5—P1	−158.13 (18)	Fe1—C39—C40—C36	58.92 (16)
C39—Fe1—C5—P1	−62.3 (2)	C38—C39—C40—Fe1	−58.82 (18)
C38—Fe1—C5—P1	47 (2)	C37—C36—C40—C39	0.1 (3)
C3—Fe1—C5—P1	158.99 (18)	P2—C36—C40—C39	178.13 (18)
C8—N1—C6—C4	63.6 (3)	Fe1—C36—C40—C39	−60.11 (17)
C8—N1—C6—C7	−64.3 (3)	C37—C36—C40—Fe1	60.24 (16)
C3—C4—C6—N1	−113.9 (3)	P2—C36—C40—Fe1	−121.8 (2)
C5—C4—C6—N1	65.9 (3)	C5—Fe1—C40—C39	−146.41 (15)
Fe1—C4—C6—N1	153.75 (18)	C1—Fe1—C40—C39	−101.88 (16)
C3—C4—C6—C7	13.0 (4)	C36—Fe1—C40—C39	118.8 (2)
C5—C4—C6—C7	−167.2 (2)	C37—Fe1—C40—C39	79.97 (16)
Fe1—C4—C6—C7	−79.4 (3)	C4—Fe1—C40—C39	178.82 (17)
C6—N1—C8—O1	−2.0 (4)	C2—Fe1—C40—C39	−65.2 (2)
C6—N1—C8—C9	177.1 (2)	C38—Fe1—C40—C39	36.72 (16)
O1—C8—C9—C10	20.2 (4)	C3—Fe1—C40—C39	−58.5 (11)
N1—C8—C9—C10	−158.9 (2)	C5—Fe1—C40—C36	94.80 (16)
C8—C9—C10—C11	−82.7 (3)	C1—Fe1—C40—C36	139.32 (15)
C9—C10—C11—O3	−21.9 (4)	C37—Fe1—C40—C36	−38.82 (14)
C9—C10—C11—O2	160.6 (3)	C4—Fe1—C40—C36	60.0 (2)
C5—P1—C12—C13	11.0 (2)	C2—Fe1—C40—C36	175.99 (15)
C18—P1—C12—C13	121.1 (2)	C39—Fe1—C40—C36	−118.8 (2)
Pt1—P1—C12—C13	−117.5 (2)	C38—Fe1—C40—C36	−82.07 (16)

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C5—P1—C12—C17	−165.9 (2)	C3—Fe1—C40—C36	−177.3 (10)
C18—P1—C12—C17	−55.8 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3^{i}	0.84	1.82	2.656 (3)	177
N1—H1···Cl1	0.88	2.69	3.477 (2)	150

Symmetry codes: (i) −*x*+2, −*y*, −*z*.

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Fig. 1

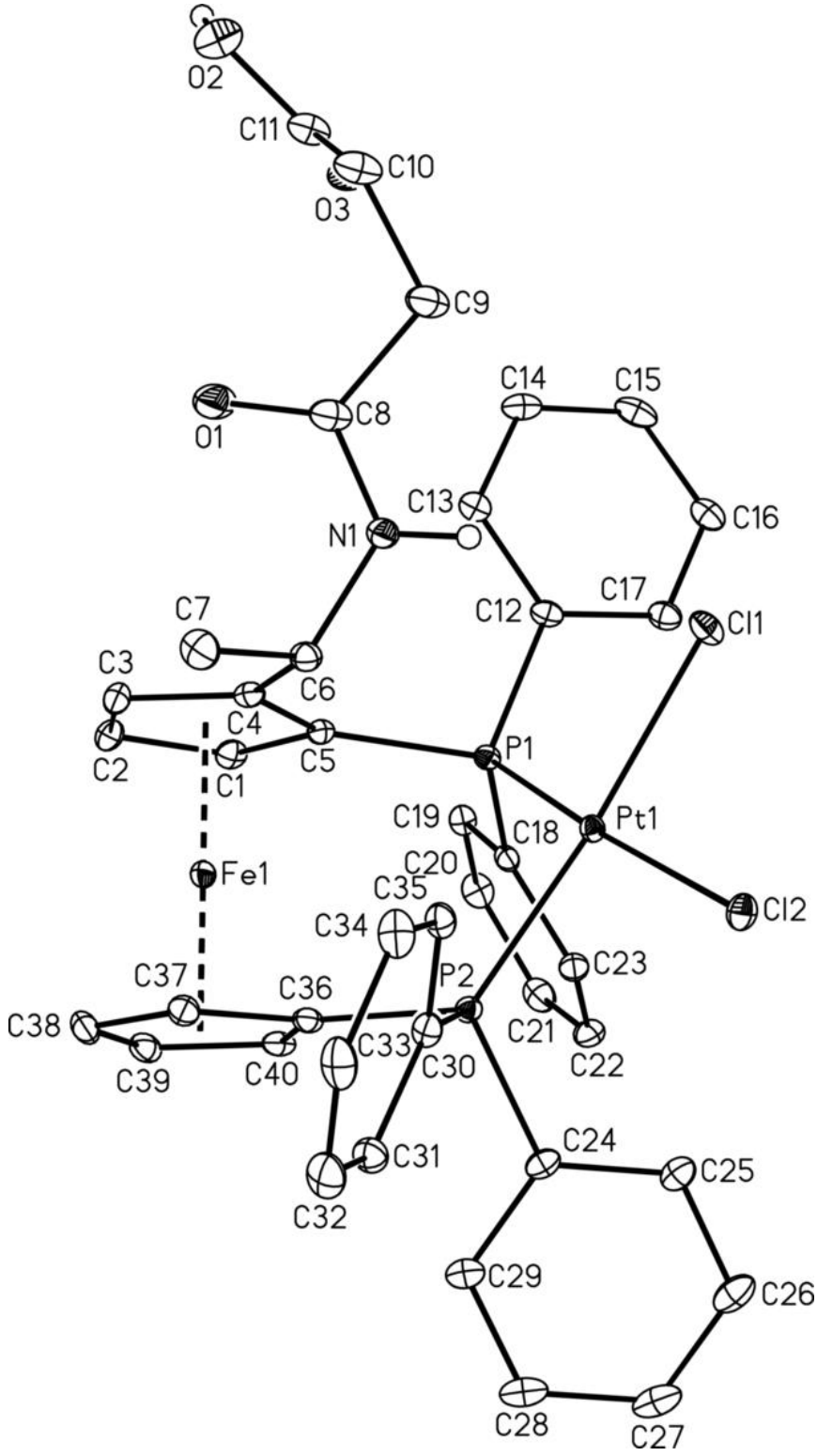

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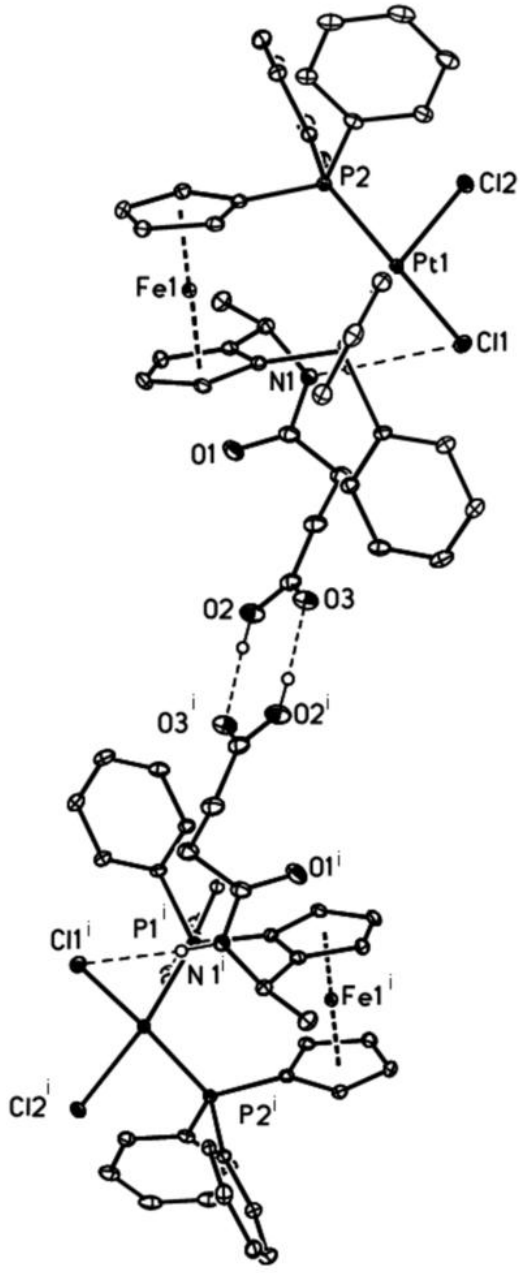
Fig. 2



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