

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

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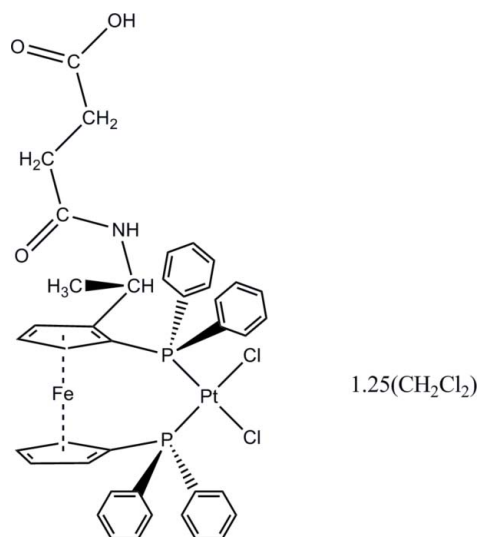
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.004$ Å; some non-H atoms missing; disorder in solvent or counterion; R factor = 0.025; wR factor = 0.065; data-to-parameter ratio = 23.9.

The dinuclear title compound, $[FePtCl_2(C_{17}H_{14}P)(C_{23}H_{23}NO_3P)] \cdot 1.25CH_2Cl_2$, 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 $29.4(2)^\circ$ 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).



Experimental

Crystal data

$[FePtCl_2(C_{17}H_{14}P)(C_{23}H_{23}NO_3P)] \cdot 1.25CH_2Cl_2$
 $M_r = 1069.64$
 Monoclinic, $P2_1/n$
 $a = 13.0154(8)$ Å
 $b = 15.7866(10)$ Å
 $c = 19.3403(12)$ Å

$\beta = 100.916(1)^\circ$
 $V = 3901.9(4)$ Å³
 $Z = 4$
 Mo- $K\alpha$ radiation
 $\mu = 4.39$ mm⁻¹
 $T = 100(2)$ K
 $0.35 \times 0.33 \times 0.30$ 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, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|-------------------------|-------|--------------|--------------|----------------|
| 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) $-x + 2, -y, -z$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE*; 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).

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

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supplementary materials

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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 PtCl₂(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 PtCl₂[1,1'-bis(diphenylphosphino)ferrocene] (Clemente *et al.*, 1986) and 4.32 (18)° for PtCl₂(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 interactions (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 2.69 Å 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 parameters 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 R²₂(8) (Bernstein *et al.*, 1995).

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%). ^1H NMR (400 MHz, CD_2Cl_2 , p.p.m.): δ 1.93 (d, 3H, $J = 6.8$ Hz, $-\text{CHCH}_3$), 1.95–2.45 (m, 4H, $-\text{CH}_2\text{CH}_2-$), 3.40–5.10 (m, 7H, ferrocene), 6.90–8.33 (m, 22H, PPh, $-\text{CHCH}_3$ and $-\text{CHNHCO}-$), 11.50–12.55 (br s, 1H, $-\text{COOH}$). ^{31}P NMR (202 MHz, CD_2Cl_2 , p.p.m. relative to H_3PO_4): δ 14.41 (d, $J_{\text{PP}'}$ = 8.3 Hz, ^{195}Pt satellites $J_{\text{PtP}} = 3778$ Hz), 8.91 (d, $J_{\text{PP}'}$ = 8.3 Hz, ^{195}Pt satellites $J_{\text{PtP}} = 3761$ Hz). HRMS (FAB+) m/z calculated for $\text{C}_{40}\text{H}_{37}\text{Cl}_2\text{FeNO}_3\text{P}_2\text{Pt}$: 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 \AA^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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

The highest difference peak is 0.xxÅ from Pt1.

Figures

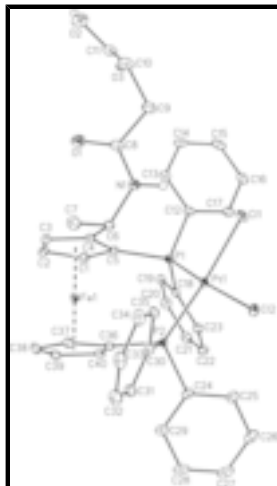


Fig. 1. : The molecular structure of (I) drawn with 30% probability ellipsoids. All hydrogen atoms attached to carbon atoms are omitted for clarity.

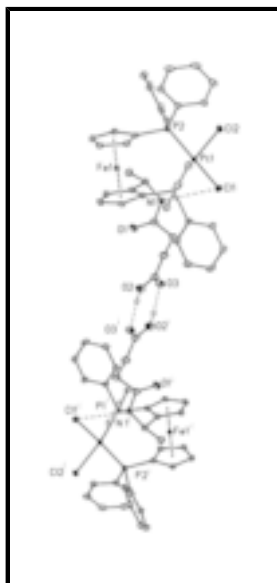


Fig. 2. : A centrosymmetric dimer of compound (I) formed due to the intermolecular hydrogen bonding interaction. The intermolecular hydrogen bond and intramolecular hydrogen bond are shown with the thinner dashed lines. [Symmetry transformation: $i: -x + 2, -y, -z.$]

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Crystal data

$[\text{FePtCl}_2(\text{C}_{17}\text{H}_{14}\text{P})(\text{C}_{23}\text{H}_{23}\text{NO}_3\text{P})] \cdot 1.25\text{CH}_2\text{Cl}_2$

$M_r = 1069.64$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 13.0154\ (8)\ \text{\AA}$

$b = 15.7866\ (10)\ \text{\AA}$

$c = 19.3403\ (12)\ \text{\AA}$

$F_{000} = 2114$

$D_x = 1.821\ \text{Mg m}^{-3}$

Mo- $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 21973 reflections

$\theta = 2.2\text{--}29.6^\circ$

$\mu = 4.39\ \text{mm}^{-1}$

$T = 100\ (2)\ \text{K}$

supplementary materials

$\beta = 100.916 (1)^\circ$ Block, yellow
 $V = 3901.9 (4) \text{ \AA}^3$ $0.35 \times 0.33 \times 0.30 \text{ mm}$
 $Z = 4$

Data collection

| | |
|--|--|
| Bruker SMART1000 CCD diffractometer | 10833 independent reflections |
| Radiation source: fine-focus sealed tube | 9395 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.036$ |
| $T = 100(2) \text{ K}$ | $\theta_{\text{max}} = 29.6^\circ$ |
| ω scans | $\theta_{\text{min}} = 1.7^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2003) | $h = -18 \rightarrow 18$ |
| $T_{\text{min}} = 0.309$, $T_{\text{max}} = 0.353$ | $k = -21 \rightarrow 21$ |
| 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 |
| $wR(F^2) = 0.065$ | $w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.9654P]$ |
| $S = 1.08$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 10833 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 453 parameters | $\Delta\rho_{\text{max}} = 1.45 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.48 \text{ e \AA}^{-3}$ |
| | 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

$F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is

not relevant to the choice of reflections for refinement. R -factors based

on F^2 are statistically about twice as large as those based on F , and R -

factors based on ALL data will be even larger.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|---------------|----------------------------------|
| 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* |

supplementary materials

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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) |

H40 0.2421 0.2008 0.0627 0.020*

Atomic displacement parameters (Å²)

| | 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) |

supplementary materials

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| 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—C11 | 2.3588 (6) | C14—H14 | 0.9500 |
| Pt1—C12 | 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) |

| | | | |
|-------------|-------------|---------------|-------------|
| 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—C11 | 165.62 (2) | C10—C9—H9B | 109.3 |
| P1—Pt1—C11 | 90.50 (2) | H9A—C9—H9B | 107.9 |
| P2—Pt1—C12 | 86.98 (2) | C11—C10—C9 | 113.2 (2) |
| P1—Pt1—C12 | 170.47 (2) | C11—C10—H10A | 108.9 |
| C11—Pt1—C12 | 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) |

supplementary materials

| | | | |
|-------------|-------------|-------------|-------------|
| 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) |

| | | | |
|----------------|--------------|-----------------|--------------|
| 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) |
| C11—Pt1—P1—C5 | -112.39 (9) | C17—C12—C13—C14 | 1.4 (4) |
| C12—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) |
| C11—Pt1—P1—C12 | 10.38 (9) | C13—C14—C15—C16 | -2.0 (4) |
| C12—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) |
| C11—Pt1—P1—C18 | 124.06 (9) | C13—C12—C17—C16 | -1.3 (4) |
| C12—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) |
| C11—Pt1—P2—C36 | 102.85 (13) | C12—P1—C18—C23 | 124.6 (2) |
| C12—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) |
| C11—Pt1—P2—C24 | -131.39 (12) | C12—P1—C18—C19 | -50.4 (2) |
| C12—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) |
| C11—Pt1—P2—C30 | -12.14 (13) | P1—C18—C19—C20 | 179.4 (2) |
| C12—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) |

supplementary materials

| | | | |
|---------------|--------------|-----------------|--------------|
| 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) |

| | | | |
|---------------|--------------|-----------------|--------------|
| 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) |

supplementary materials

| | | | |
|----------------|--------------|-----------------|--------------|
| 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) |

| | | | |
|----------------|------------|----------------|-------------|
| 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, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O2—H2 \cdots O3 ⁱ | 0.84 | 1.82 | 2.656 (3) | 177 |
| N1—H1 \cdots Cl1 | 0.88 | 2.69 | 3.477 (2) | 150 |

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

Fig. 1

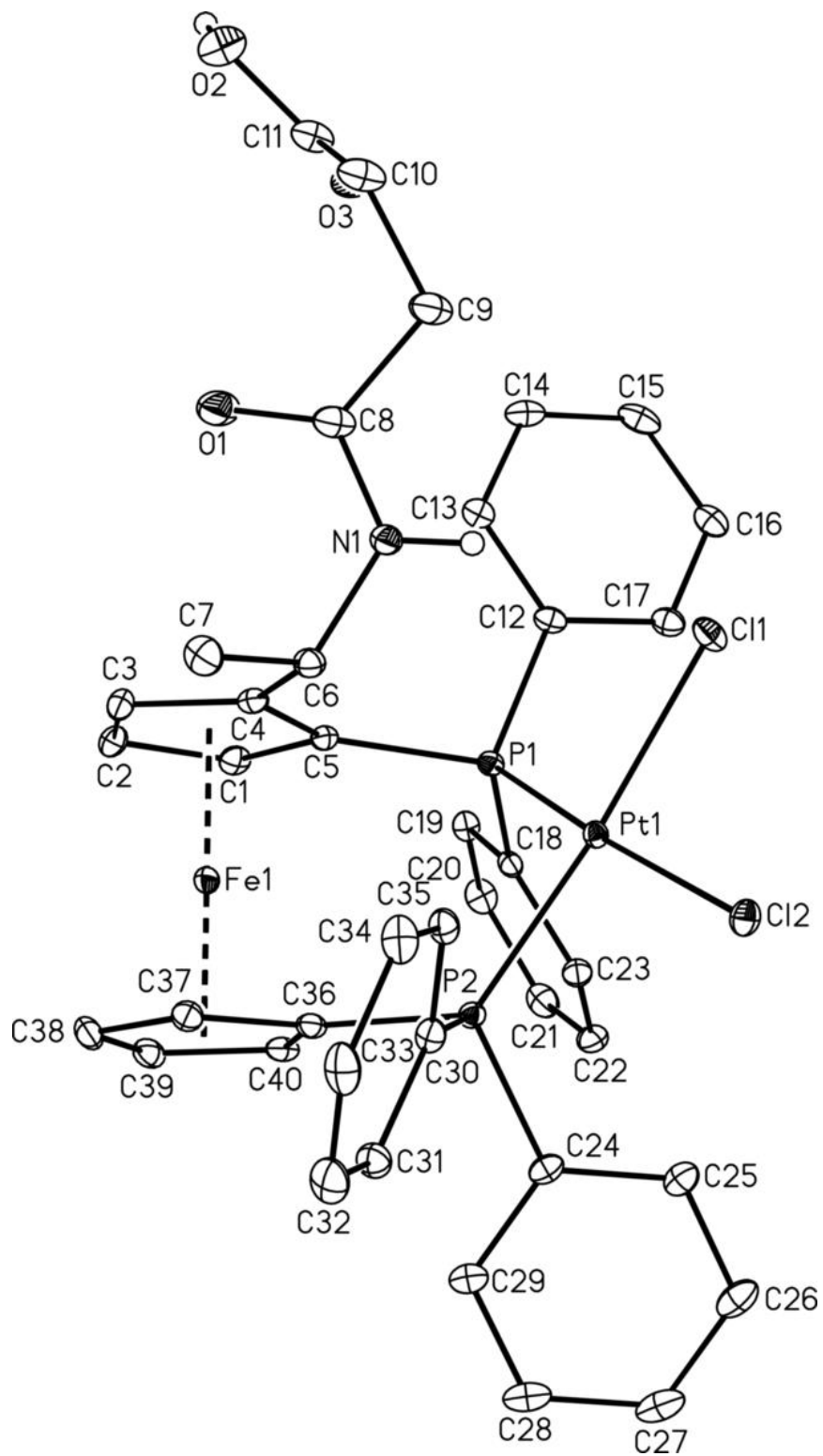


Fig. 2

