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Crystal structure of {μ_2-1,2-bis[(4-methylphenylsulfanyl]-3-oxoprop-1-ene-1,3-diyl-1:2κ^2C^3:C^1}-dicarbonyl-1κ^2C-[μ_2-methylenebis(diphenylphosphane)-1:2κ^2P:P'](triphenylphosphane-2κP)-ironplatinum(*Fe*—*Pt*), $[(OC)_2Fe(\mu\text{-dppm})\{\mu\text{-C}(=O)\text{-}C(4\text{-}MeC_6H_4SCH_2)=CCH_2SC_6H_4Me\text{-}4\}Pt(PPh_3)]$

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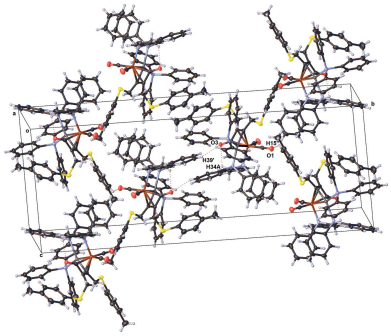
The title compound, $[FePt(C_{19}H_{18}OS_2)(C_{18}H_{15}P)(C_{25}H_{22}P_2)(CO)_2]$, **1**, $[(OC)_2Fe(\mu\text{-dppm})(\mu\text{-C}(=O)C(CH_2SC_6H_4Me\text{-}4)=CCH_2SC_6H_4Me\text{-}4)Pt(PPh_3)]$, represents the first example of a diphosphane-bridged heterobimetallic Fe—Pt dimetallacyclopentenone complex resulting from a bimetallic activation of metal-coordinated carbonyl ligand with an internal alkyne, namely 1,4-bis(*p*-tolylthio)but-2-yne. The bridging μ_2-C(=O)C($CH_2SC_6H_4Me$-4)=$CCH_2SC_6H_4$-Me-4 unit (stemming from a carbon–carbon coupling reaction between CO and the triple bond of the alkyne dithioether) forms a five-membered dimetallacyclopentenone ring, in which the C=C bond is π-coordinated to the Fe center. The latter is connected to the Pt center through a short metal–metal bond of 2.5697 (6) Å.

1. Chemical context

Acetylenic dithioether ligands of type $RSCH_2C{\equiv}CCH_2SR$ (*R* = aryl, alkyl) have in recent years not only attracted attention as reactive building blocks for further organic transformations (Pourcelot & Cadiot, 1966; Everhardus & Brandsma; 1978; Levanova *et al.*, 2015) but also as promising ligands for coordination chemistry because of their dytopic character, allowing both coordination to soft metal centers through dative *M*←S bonding and π-bonding *via* the acetylenic triple bond. In this context, we have explored in a series of several papers the coordination of this ligand family to Cu*X* salts in a self-assembly process to discrete molecular compounds, mono- and bidimensional coordination polymers and three-dimensional MOFs. For example, treatment of CuI with $PhSCH_2C{\equiv}CCH_2SPh$ afforded a three-dimensional network incorporating $Cu_6(\mu_3\text{-I})$ hexagonal prisms as connection nodes (Knorr *et al.*, 2009; Bai *et al.*, 2018). In contrast, reaction of $BzSCH_2C{\equiv}CCH_2SBz$ (Bz = benzyl) with both CuI and CuBr provided simple isostructural dinuclear zero-dimensional complexes $[\{Cu(\mu_2\text{-}X)_2Cu\}(\mu\text{-}BzSCH_2C{\equiv}CCH_2SBz)_2]$ (*X* = I, Br). A far more original material resulted from coordination to CuCl, yielding a luminescent 2D material $[\{Cu_2(\mu_2\text{-Cl})(\mu_3\text{-Cl})\}(\mu\text{-}BzSCH_2C{\equiv}CCH_2SBz)]_n$, in which



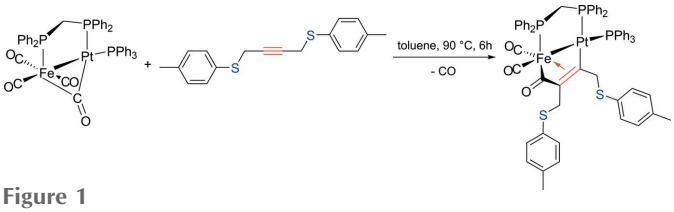
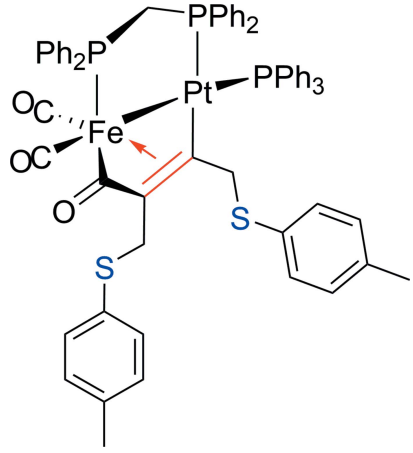


Figure 1
The reaction scheme for the synthesis of **1**.

the layers are assembled both by dative Cu—S thioether bonds and organometallic Cu-π–acetylenic interactions *via* the triple bond of the ligand. Furthermore, the Cu^{I} centers are interconnected through μ_2- and μ_3-bound chloro ligands. Treatment of CuI with the isomeric *p*-TolSCH$_2$C≡CCH$_2$STol-*p* (Tol = C$_6$H$_4$-*p*-Me) ligand led to the formation of a 2D network [{Cu$_4$(μ_3-I)$_4$}(μ-TolSCH$_2$C≡CCH$_2$STol)$_2$]$_n$ with closed cubane-type clusters as SBUs (Secondary Building Units), whilst with CuBr the 1D [{Cu(μ_2-Br)$_2$Cu}(μ-TolSCH$_2$C≡CCH$_2$STol)$_2$]$_n$ coordination polymer was generated (Aly *et al.*, 2014; Bonnot *et al.*, 2015). An alternative approach to combining a metallic scaffold with *R*SCH$_2$C≡CCH$_2$S*R*-type ligands has been developed by Went and coworkers, who post-functionalized dicobaltatetrahedrane complexes [Co$_2$(μ-HOCH$_2$C≡CCH$_2$OH)(CO)$_6$] in the presence of HBF$_4$·OEt$_2$ and various thiols *R*SH to obtain [Co$_2$(μ-*R*SCH$_2$C≡CCH$_2$S*R*)(CO)$_6$] and [Co$_2$(μ-*R*SCH$_2$C≡CCH$_2$S*R*)(μ-dppm)(CO)$_4$] [dppm = bis(diphenylphosphino)methane], respectively. Similar treatment of [Mo$_2$(μ-HOCH$_2$C≡CCH$_2$OH)(CO)$_4$Cp$_2$] with EtSH yielded [Mo$_2$(μ-EtSCH$_2$C≡CCH$_2$SEt)(CO)$_4$Cp$_2$]. These former Co–Co thioether complexes were then employed as metalloligands to coordinate further metal fragments such as [Cu(MeCN)$_4$]PF$_6$, AgBF$_4$ and [Mo(CO)$_4$(norbornadiene)] (Bennett, *et al.*, 1992; Gelling *et al.*, 1993). Related dicationic salts such as [(Co$_2$(CO)$_6$)$_2$-μ,η^2,η^2-(Me$_2$S—CH$_2$C≡CCH$_2$S-Me$_2$)][BF$_4$]$_2$ have also been described (Amouri *et al.*, 2000). We and Shaw's group have demonstrated that upon treatment of the μ-carbonyl complex [(OC)$_3$Fe(μ-dppm)(μ-CO)Pt-(PPh$_3$)] with ArC≡CH (Ar = Ph, *p*-Tol, 2,4,5-trimethylphenyl, *p*-C$_6$H$_4$F, 2,4-C$_6$H$_3$F$_2$, *p*-C$_6$H$_4$CF$_3$), dimetallacyclopentone complexes are formed, stemming from carbon–carbon coupling reactions between CO and the terminal alkyne (Fontaine *et al.*, 1988; Jourdain *et al.*, 2013; Knorr & Jourdain, 2017; Brieger *et al.*, 2019). The first step involves the formation of a kinetic isomer [(OC)$_2$Fe(μ-dppm){μ-C(=O)C(H)=C(Ar)}Pt(PPh$_3$)], which then evolves to the thermodynamic one [(OC)$_2$Fe(μ-dppm){μ-C(=O)C(Ar)=C(H)}Pt(PPh$_3$)]. We were now intrigued as to whether this route may be extended to internal alkynes *R*C≡C*R*, which are in general less reactive than terminal ones. We therefore probed the possibility of coupling [(OC)$_3$Fe(μ-dppm)(μ-CO)Pt(PPh$_3$)] with *p*-TolSCH$_2$C≡CCH$_2$STol-*p* in hot toluene as solvent and succeeded in isolating the targeted dimetallacyclopentone [(OC)$_2$Fe(μ-dppm)(μ-C(=O)C(4-MeC$_6$H$_4$SCH$_2$)=CCH$_2$S-C$_6$H$_4$Me-4)Pt(PPh$_3$)] (**1**) as a stable crystalline product according to the reaction scheme shown in Fig. 1. With this title compound **1** in hand, we now have the possibility of coordinating other metal fragments in upcoming studies, for example [Mo(CO)$_4$(norbornadiene)] or ReBr(CO)$_5$ in a chelating manner using the two adjacent thioether arms or of constructing coordination networks incorporating complex **1** as an organometallic building block by coordination of Cu*X* or Ag^{I} salts on the *S*-donor sites (see above).



2. Structural commentary

The heterobimetallic compound **1** crystallizes in the monoclinic crystal system, space group $P2_1/c$. The molecular structure is depicted in Fig. 2 and selected bond lengths and angles are given in Table 1.

The Fe—Pt bond [2.5697 (6) Å] is spanned by a dppm ligand and bridged by the C(=O)C(*R*)=C(*R*) (*R* = 4-MeC$_6$H$_4$SCH$_2$) unit resulting from the carbon–carbon coupling reaction between CO and the alkyne. This value,

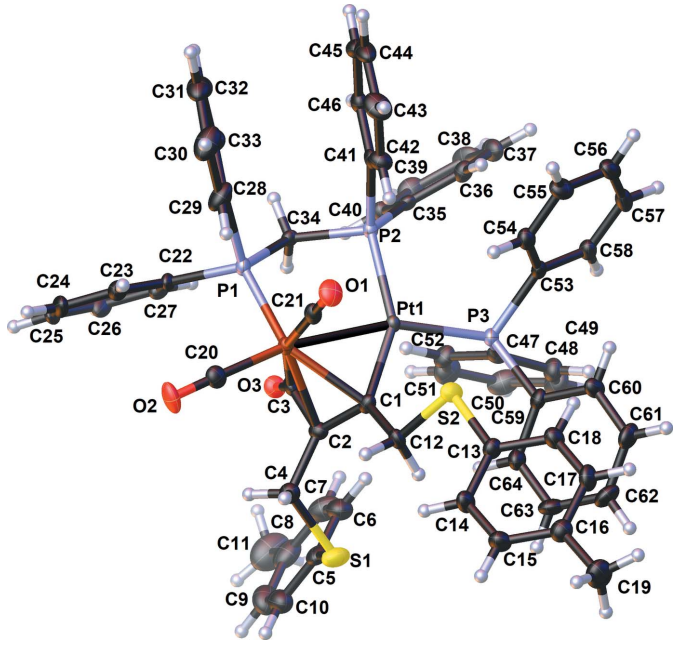


Figure 2
The molecular structure of the title complex **1**, with atom labeling. Displacement ellipsoids are drawn at the 30% probability level.

Table 1
Selected geometric parameters (Å, °).

Pt1—Fe1	2.5697 (6)	Fe1—C2	2.119 (4)
Pt1—P2	2.2850 (10)	Fe1—C3	1.932 (5)
Pt1—P3	2.2714 (12)	Fe1—C20	1.777 (5)
Pt1—C1	2.045 (4)	Fe1—C21	1.789 (5)
Fe1—P1	2.1966 (12)	O3—C3	1.216 (5)
Fe1—C1	2.162 (4)	C1—C2	1.407 (6)
P2—Pt1—Fe1	97.26 (3)	C1—Fe1—C2	38.35 (16)
P3—Pt1—Fe1	161.46 (3)	C20—Fe1—P1	95.66 (14)
P3—Pt1—P2	100.53 (4)	C21—Fe1—P1	102.63 (13)
C1—Pt1—Fe1	54.44 (12)	C3—Fe1—P1	88.88 (13)
C1—Pt1—P2	151.36 (12)	C1—Fe1—P1	141.85 (12)
C1—Pt1—P3	107.33 (12)	C2—Fe1—P1	130.91 (13)
Pt1—C1—Fe1	75.25 (13)	C20—Fe1—Pt1	168.78 (14)
C20—Fe1—C3	101.5 (2)	C21—Fe1—Pt1	87.76 (14)
C20—Fe1—C21	96.5 (2)	C2—Fe1—Pt1	73.72 (12)
C21—Fe1—C3	157.6 (2)	C1—Fe1—Pt1	50.30 (11)
C20—Fe1—C1	119.19 (18)	C3—Fe1—Pt1	72.18 (13)
C21—Fe1—C1	89.16 (18)	P1—Fe1—Pt1	93.50 (4)
C3—Fe1—C1	70.43 (18)	C2—C1—Pt1	109.1 (3)
C20—Fe1—C2	95.33 (18)	C2—C1—Fe1	69.2 (2)

which is less than 2.6 Å, is in the usual range for FePt(dppm)–dimetallacyclopentenone complexes. Note that extreme Fe—Pt distances are reported for the μ-carbene [$(OC)_3Fe\{\mu$-$C(Et)OSi(OMe)_3\}(\mu$-dppm$)Pt(PPh_3)$] [d(Fe—Pt) = 2.5062 (9) Å; YOTCIT; Braunstein *et al.*, 1995] and [$Fe(\eta^5$-$C_5H_4S)_2Pt(PPh_3)$] [d(Fe—Pt = 2.935 (2) Å; FENCUW; Akabori *et al.*, 1987]. Coupling of an internal alkyne does not affect the structural features of the [FeC(═*O*)C(*R*)═C(*R*)Pt] motif significantly with respect to carbon–carbon coupling with a terminal alkyne. The relevant bond lengths and angles are very similar to those of other Fe—Pt structures published by Fontaine *et al.* (1988) and our group (see above). The presence of a bulky substituent on the C1 atom bound to platinum implies a significant reduction of the P3—Pt—P2 angle [100.53 (4)°] concomitant with an increasing value of the angle P3—Pt—C1 of 107.33 (12)°. In related compounds described previously in the literature, these P3—Pt—P2 angles usually lie in the range 103.93 (8) to 106.63 (3)°, as exemplified by [$(OC)_2Fe(\mu$-dppm$)\{\mu$-C(═O)C$\{(CH_2)_3CCH\}$═C(H)$\}$Pt-(PPh_3)] (REDNEU) and [$(OC)_2Fe(\mu$-dppm$)\{\mu$-C(═O)C(*p*-$C_6H_4CF_3$)═C(H)$\}Pt(PPh_3)$] (PIXLAL), and 98.8 (3) to 104.95 (10)° for P3—Pt—C1 in [$(OC)_2Fe(\mu$-dppm$)\{\mu$-C(═O)C(H)═C(H)$\}Pt(PPh_3)$] (FEYBAM) and [$(OC)_2Fe(\mu$-dppm$)\{\mu$-C(═O)C(*o*,*p*-$C_6H_3F_2$)═C(H)$\}Pt(PPh_3)$] (PIX-KUE) (Fontaine *et al.*, 1988; Jourdain *et al.*, 2006, 2013). The crystal structure of the dithioether *p*-TolSCH$_2$C≡CCH$_2$STol-*p* (MULHUZ) was reported by Aly *et al.* (2014). After complexation and a coupling reaction with a CO ligand, the C1—C2 bond is considerably longer [1.407 (6) *vs* 1.266 (5) Å] as a result of the conversion to an olefinic moiety, σ-bound to Pt and η^2-coordinated to Fe. The alkyne bending angles are disparate [C1—C2—C4 = 126.2 (4), C2—C1—C12 = 119.6 (4)°] as well as the C1—C12 and C2—C4 distances [d(C1—C12) = 1.483 (6), d(C2—C4) = 1.511 (5) Å]. Compared to 1,4-bis(*p*-tolylthio)but-2-yne, the C—S bonds are also considerably elongated [d(C4—S1 = 1.830 (4), d(C12—S2) = 1.808 (4), d(C5—S1) = 1.782 (5), d(C13—S2) = 1.771 (4) *vs* 1.685 (2) and 1.714 (2) Å] but they fit well with those encountered in the dimetallatetrahedrane [$Co_2\{\mu$-$C_2(CH_2SMe)_2Mo(CO)_4\}(\mu$-dppm$)(CO)_4$] [$d$(C—S = 1.827 (4), 1.833 (4),1.790 (5) and 1.819 (5) Å; JIHMUI10; Gelling *et al.*, 1993].

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O1^{i}	0.93	2.67	3.316 (6)	128
C34—H34*A*···O3	0.97	2.62	3.271 (5)	125
C39—H39···O3^{ii}	0.93	2.49	3.239 (6)	138

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$.

3. Supramolecular features

In the crystal, the individual molecules are linked by weak intermolecular interactions; for example a contact between O3″···H39 [d = 2.49 Å and C3″—O3″···H39 = 138°; symmetry code: (″) $-x+1, -y+1, -z+1$] occurs (Fig. 3, Table 2. A second, yet still weaker intermolecular interaction of 2.67 Å is observed between the O1′···H15 [symmetry code: (′) $x, -y+\frac{3}{2}, z-\frac{1}{2}$] atoms of two adjacent molecules. In addition there is an intramolecular contact between O3···H34*A* (d = 2.62 Å and C3—O3···H34*A* = 125°). Furthermore, there are also several loose intermolecular C—H···π interactions present; for example a contact between C43—H43 and the midpoint of the C13═C14 double bond [d(H43···midpoint) = 2.73 Å and C—H···midpoint = 157°] of a tolyl ring attached to S2, as well as between C62—H62 and the C23—C24—C25 atoms of a phenyl ring [d(H62···centroid) = 2.64 Å and C—H···centroid = 148°] attached at P1. However, since all hydrogen atoms were not refined freely, a more accurate discussion of the bond lengths and angle is not appropriate.

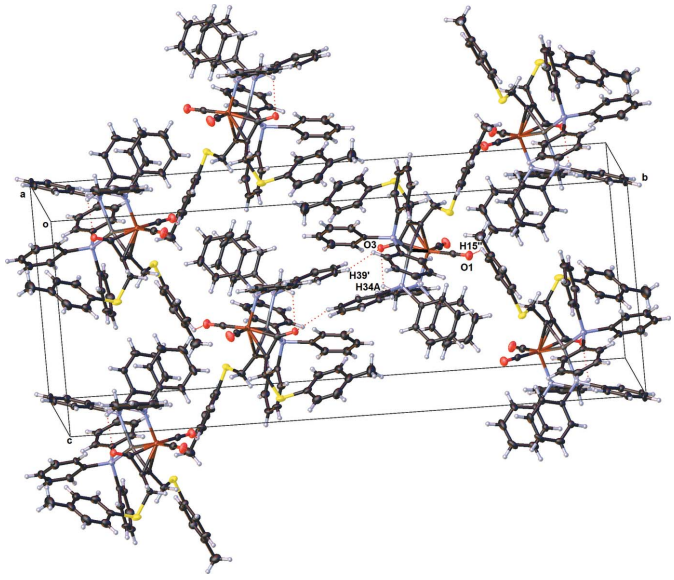


Figure 3
A partial view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds (Table 2) are shown as dashed lines.

4. Database survey

Other examples of crystallographically characterized dimetallacyclopentenone complexes are $Fe_2Cp_2(CO)(\mu$-CO)$\{\mu$-CH═C(Ph)C(═O)$\}$ (DAHTAJ; Boni *et al.*, 2011), $Fe_2Cp^*_2(CO)(\mu$-CO)$\{\mu$-C(C≡CH)═CHC(═O)$]$ (JUZHIV; Akita *et al.*, 1993), $Fe_2(CO)_5(\mu$-dppm$\{\mu$-C(═O)CH═CH$\}$ (GACWIQ10; Knox *et al.*, 1995), $Fe_2(CO)_5(\mu$-dppm$\{\mu$-C(═O)C(Ph)═CH$\}$ (PIHMOI; Hitchcock *et al.*, 1993), $Fe_2Cp_2(CO)(\mu$-CO)$\{\mu$-C(CO*R*)═C(Me)C(═O)$\}$ (*R* = Ph, Bu) (SIZNUK, SIZPAS; Wong *et al.*, 1991), $Fe_2\{(\eta$-$C_5H_4)_2$-$SiMe_2\}(CO)_2(\mu$-CO)$\{\mu$-C(Ph)═C(H)C(═O)$\}$ (ZUZGIK; McKee *et al.*, 1994), $Ru_2(CO)_4(\mu$-dppm$)_2\{\mu$-C(═O)C(CO_2Me)═C$(CO_2Me)\}$ (JITZAN; Johnson & Gladfelter, 1991), $Ru_2(CO)_4(\mu$-dppm$)_2\{\mu$-CH═CHC(═O)$\}$ (LIFYUU; Mirza *et al.*, 1994), $Ru_2(\eta$-$C_5HMe_4)_2(CO)(\mu$-CO$\{\mu$-C(═O)C(*R*)═C(*R*)$\}$ (*R* = Et, Me) (NEMVOS, NEMVUY; Horiuchi *et al.*, 2012), $Rh_2Cp_2(CO)_4\{\mu$-C(CF_3)═C(CF_3)-C(═O)$\}$ (TFPNRH; Dickson *et al.*, 1981), $Re_2Cp^*_2(CO)_2\{\mu$-CH═C$\{$C(═CH_2)$CH_3\}$C(═O)$\}$ (WEZKIV; Casey *et al.*, 1994). A rare example of a heterodinuclear combination is CpFe$\{\mu$-C(═O)C(CMe_2OH)═CH$\}(\mu$-CO)Ru(CO)Cp* (FEHGOP; Dennett *et al.*, 2005). We are also aware of $OsRu(CO)_8\{\mu$-HC═CHC(═O)$\}$ (Kiel *et al.*, 2000), but for the latter compound no structural data are available.

5. Synthesis and crystallization

$[(OC)_3Fe(\mu$-CO)$(\mu$-dppm)Pt$(PPh_3)]$ (200 mg, 0.2 mmol) was treated with an excess of 1,4-bis(*p*-tolylthio)but-2-yne (100 mg, 0.4 mmol) in toluene (5 mL). The solution was stirred at 363 K for 6h. The reaction mixture was filtered, and all volatiles removed under reduced pressure. The brown residue was redissolved in a minimum of toluene. Orange–yellow crystals were isolated by layering with heptane (152 mg, 76% yield).

Calculated for $C_{64}H_{55}FeO_3P_3PtS_2$ (1279.18 g mol^{-1}): C, 60.05; H, 4.36. Found: C, 59.80; H, 4.21. ^{1}H NMR: δ 2.21 (*s*, 3H, CH_3), 2.28 (*s*, 3H, CH_3), 3.67 (*br*, 2H, CH_2), 3.97(*br*, 2H, CH_2), 4.53 (*br*, 2H, PCH_2P, $^2J_{PtH}$ = 41), 6.45–7.85 (*m*, 43H, Ph). ^{31}P{1H} NMR: δ 6.8 (*d*, $P_{dppm\ Pt}$, $^2J_{PP}$ = 57, $^{2+3}J_{PP}$ = 5, $^1J_{PtP}$ = 2543), 32.7 (*d*, $P_{PPh3\ Pt}$, $^3J_{PP}$ = 32, $^{2+3}J_{PP}$ = 5, $^1J_{PtP}$ = 3506), 63.4 (*dd*, $P_{dppm\ Fe}$, $^2J_{PP}$ = 57, $^3J_{PP}$ = 32, $^1J_{PtP}$ = 135). IR(toluene): 1966, 1918s ν(CO), 1696m ν(C═O).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All of the hydrogen atoms were placed in geometrically calculated positions and each was assigned a fixed isotropic displacement parameter based on a riding model: C—H = 0.93–0.97 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[FePt(C_{19}H_{18}OS_2)(C_{18}H_{15}P)$-$(C_{25}H_{22}P_2)(CO)_2]$
M_r	1280.05
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	12.0071 (6), 36.1737 (15), 13.6980 (6)
β (°)	111.970 (5)
V (Å^3)	5517.5 (5)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	3.01
Crystal size (mm)	0.23 × 0.15 × 0.05
Data collection	
Diffractometer	Agilent Technologies Xcalibur, Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.837, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	47863, 10566, 8245
R_{int}	0.071
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.611
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.076, 1.03
No. of reflections	10566
No. of parameters	669
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.12, −0.64

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

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Crystal structure of {μ_2-1,2-bis[(4-methylphenylsulfanyl]-3-oxoprop-1-ene-1,3-diyl-1:2κ^2C^3:C^1}dicarbonyl-1κ^2C-[μ_2-methylenebis(diphenylphosphane)-1:2κ^2P:P'](triphenylphosphane-2κP)ironplatinum(*Fe—Pt*), [$(OC)_2$Fe(μ-dppm){μ-C(&z-dbnd;O)C(4-$MeC_6H_4SCH_2$)&z-dbnd;$CCH_2SC_6H_4$Me-4}Pt(PPh_3)]

Ahmed Said Mohamed, Isabelle Jourdain, Michael Knorr, Lukas Brieger and Carsten Strohmann

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

{μ_2-1,2-Bis[(4-methylphenylsulfanyl]-3-oxoprop-1-ene-1,3-diyl-1:2C^3:C^1}dicarbonyl-1κ^2C-[μ_2-methylenebis(diphenylphosphane)-1:2κ^2P:P'](triphenylphosphane-2κP)ironplatinum(*Fe—Pt*)

Crystal data

$[FePt(C_{19}H_{18}OS_2)(C_{18}H_{15}P)(C_{25}H_{22}P_2)(CO)_2]$
M_r = 1280.05
Monoclinic, $P2_1/c$
a = 12.0071 (6) Å
b = 36.1737 (15) Å
c = 13.6980 (6) Å
β = 111.970 (5)°
V = 5517.5 (5) Å^3
Z = 4
$F(000)$ = 2576
D_x = 1.541 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9511 reflections
θ = 2.7–28.7°
μ = 3.01 mm^{-1}
T = 293 K
Plate, yellow
0.23 × 0.15 × 0.05 mm

Data collection

Agilent Technologies Xcalibur, Sapphire3 diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0560 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Agilent, 2014)
T_{min} = 0.837, T_{max} = 1.000
47863 measured reflections
10566 independent reflections
8245 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 25.8°, θ_{min} = 2.2°
h = −11→14
k = −44→41
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.076$
$S = 1.03$
10566 reflections
669 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.5475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}

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. Crystal structure determination of compound 1 was accomplished on an Oxford diffraction Xcalibur S Diffractometer. Suitable crystals of 1 were covered with an inert oil (perfluoropolyalkylether and used for X-ray crystal structure determination. Graphite monochromated Mo-Kα radiation (λ = 0.71073?Å) was used. The processing and finalization of the crystal structure was done with the program Olex2 (Dolomanov, 2009). The crystal structures were solved by intrinsic phasing (SHELXT; Sheldrick, 2015a) and refined against F2 with the full-matrix least-squares method (SHELXL; Sheldrick, 2015b). A multi-scan absorption correction using the CrysAlis RED program (Oxford Diffraction, 2010) was employed. The non-hydrogen atoms were refined anisotropically.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.33424 (2)	0.62472 (2)	0.31155 (2)	0.01386 (6)
Fe1	0.52875 (5)	0.66228 (2)	0.35654 (4)	0.01541 (14)
S1	0.51458 (12)	0.61606 (4)	0.02018 (9)	0.0335 (3)
S2	0.19884 (11)	0.69548 (4)	0.12684 (8)	0.0242 (3)
P1	0.60180 (10)	0.64353 (3)	0.52099 (8)	0.0160 (3)
P2	0.36370 (10)	0.60649 (3)	0.47912 (8)	0.0136 (2)
P3	0.16428 (10)	0.59290 (3)	0.21914 (8)	0.0166 (3)
O1	0.3898 (3)	0.72834 (9)	0.3663 (2)	0.0305 (8)
O2	0.7452 (3)	0.70095 (9)	0.3644 (3)	0.0331 (8)
O3	0.6059 (3)	0.58365 (9)	0.3412 (2)	0.0226 (7)
C1	0.3927 (4)	0.64918 (12)	0.2048 (3)	0.0167 (10)
C2	0.5040 (4)	0.63378 (12)	0.2148 (3)	0.0184 (10)
C3	0.5576 (4)	0.61346 (14)	0.3138 (3)	0.0199 (11)
C4	0.5728 (4)	0.64158 (13)	0.1445 (3)	0.0214 (10)
H4A	0.656425	0.635059	0.181663	0.026*
H4B	0.569106	0.667854	0.129478	0.026*
C5	0.5750 (4)	0.57103 (14)	0.0594 (3)	0.0284 (12)
C6	0.5322 (5)	0.54791 (15)	0.1179 (4)	0.0356 (13)
H6	0.469522	0.555719	0.137208	0.043*
C7	0.5815 (5)	0.51369 (15)	0.1475 (4)	0.0413 (15)
H7	0.552057	0.498782	0.187748	0.050*
C8	0.6741 (5)	0.50038 (15)	0.1194 (4)	0.0398 (14)
C9	0.7145 (5)	0.52324 (16)	0.0597 (4)	0.0436 (15)
H9	0.775600	0.514984	0.038988	0.052*

C10	0.6673 (5)	0.55811 (16)	0.0295 (4)	0.0364 (14)
H10	0.696839	0.572966	−0.010742	0.044*
C11	0.7276 (6)	0.46250 (16)	0.1544 (5)	0.065 (2)
H11A	0.743383	0.459346	0.227930	0.097*
H11B	0.801292	0.460237	0.142632	0.097*
H11C	0.672116	0.443892	0.114692	0.097*
C12	0.3296 (4)	0.67416 (13)	0.1153 (3)	0.0208 (11)
H12A	0.305131	0.660195	0.050210	0.025*
H12B	0.384620	0.693322	0.112025	0.025*
C13	0.1237 (4)	0.71380 (13)	−0.0009 (3)	0.0213 (11)
C14	0.1814 (4)	0.72895 (13)	−0.0630 (3)	0.0256 (11)
H14	0.264781	0.728200	−0.039538	0.031*
C15	0.1159 (4)	0.74513 (14)	−0.1592 (3)	0.0299 (12)
H15	0.156559	0.755564	−0.198448	0.036*
C16	−0.0078 (4)	0.74615 (13)	−0.1983 (3)	0.0264 (11)
C17	−0.0649 (4)	0.73051 (14)	−0.1363 (3)	0.0286 (12)
H17	−0.148331	0.730799	−0.160551	0.034*
C18	−0.0010 (4)	0.71470 (13)	−0.0406 (3)	0.0252 (11)
H18	−0.041978	0.704399	−0.001440	0.030*
C19	−0.0794 (5)	0.76391 (16)	−0.3034 (4)	0.0428 (15)
H19A	−0.047412	0.787999	−0.306543	0.064*
H19B	−0.161883	0.766129	−0.310870	0.064*
H19C	−0.074281	0.748835	−0.359219	0.064*
C20	0.6604 (4)	0.68613 (13)	0.3621 (3)	0.0230 (11)
C21	0.4445 (4)	0.70239 (13)	0.3626 (3)	0.0199 (10)
C22	0.7607 (4)	0.62972 (13)	0.5705 (3)	0.0176 (10)
C23	0.8454 (4)	0.65829 (14)	0.5896 (3)	0.0246 (11)
H23	0.820210	0.682797	0.581983	0.030*
C24	0.9660 (4)	0.65016 (16)	0.6197 (3)	0.0326 (13)
H24	1.021532	0.669251	0.632344	0.039*
C25	1.0048 (4)	0.61401 (16)	0.6313 (3)	0.0324 (14)
H25	1.085863	0.608652	0.649885	0.039*
C26	0.9219 (4)	0.58565 (15)	0.6149 (3)	0.0315 (13)
H26	0.947659	0.561191	0.624560	0.038*
C27	0.8012 (4)	0.59378 (13)	0.5841 (3)	0.0234 (11)
H27	0.746189	0.574587	0.572385	0.028*
C28	0.6025 (4)	0.67405 (13)	0.6288 (3)	0.0198 (10)
C29	0.5891 (5)	0.71186 (14)	0.6141 (4)	0.0324 (13)
H29	0.581547	0.721995	0.549531	0.039*
C30	0.5869 (5)	0.73480 (15)	0.6941 (4)	0.0423 (15)
H30	0.577689	0.760181	0.683252	0.051*
C31	0.5983 (5)	0.71993 (16)	0.7901 (4)	0.0358 (13)
H31	0.595101	0.735182	0.843640	0.043*
C32	0.6144 (5)	0.68300 (15)	0.8061 (4)	0.0344 (13)
H32	0.623800	0.673087	0.871411	0.041*
C33	0.6168 (4)	0.65998 (13)	0.7268 (3)	0.0250 (11)
H33	0.628129	0.634720	0.739143	0.030*
C34	0.5268 (4)	0.60132 (12)	0.5404 (3)	0.0150 (10)

H34A	0.552067	0.580369	0.509554	0.018*
H34B	0.549824	0.596640	0.615122	0.018*
C35	0.3097 (4)	0.56202 (12)	0.5064 (3)	0.0160 (10)
C36	0.1925 (4)	0.55998 (13)	0.5041 (3)	0.0218 (11)
H36	0.144301	0.580982	0.488889	0.026*
C37	0.1481 (5)	0.52697 (14)	0.5244 (3)	0.0289 (12)
H37	0.069837	0.525755	0.522178	0.035*
C38	0.2195 (5)	0.49550 (14)	0.5482 (4)	0.0326 (13)
H38	0.189317	0.473274	0.561975	0.039*
C39	0.3353 (5)	0.49742 (13)	0.5512 (3)	0.0283 (12)
H39	0.383817	0.476506	0.567991	0.034*
C40	0.3792 (4)	0.53025 (13)	0.5296 (3)	0.0216 (11)
H40	0.457018	0.531125	0.530449	0.026*
C41	0.3264 (4)	0.63622 (12)	0.5696 (3)	0.0173 (10)
C42	0.2880 (4)	0.67210 (13)	0.5430 (3)	0.0237 (11)
H42	0.276531	0.680940	0.476120	0.028*
C43	0.2662 (5)	0.69537 (14)	0.6159 (4)	0.0348 (13)
H43	0.240436	0.719544	0.597655	0.042*
C44	0.2831 (4)	0.68214 (15)	0.7138 (4)	0.0334 (13)
H44	0.269937	0.697685	0.762477	0.040*
C45	0.3193 (4)	0.64629 (15)	0.7419 (3)	0.0295 (12)
H45	0.328276	0.637497	0.808180	0.035*
C46	0.3421 (4)	0.62350 (13)	0.6706 (3)	0.0203 (10)
H46	0.368134	0.599408	0.689833	0.024*
C47	0.1854 (4)	0.54327 (12)	0.2099 (3)	0.0190 (10)
C48	0.0931 (4)	0.52009 (13)	0.1484 (3)	0.0258 (11)
H48	0.018084	0.530064	0.109826	0.031*
C49	0.1112 (5)	0.48275 (14)	0.1440 (4)	0.0328 (13)
H49	0.047654	0.467587	0.104805	0.039*
C50	0.2232 (5)	0.46751 (15)	0.1974 (4)	0.0367 (14)
H50	0.234927	0.442181	0.194608	0.044*
C51	0.3172 (5)	0.49003 (15)	0.2546 (4)	0.0359 (13)
H51	0.393402	0.480116	0.288828	0.043*
C52	0.2979 (4)	0.52767 (13)	0.2611 (3)	0.0227 (11)
H52	0.361714	0.542713	0.300490	0.027*
C53	0.0484 (4)	0.60009 (13)	0.2734 (3)	0.0186 (10)
C54	0.0450 (4)	0.63486 (13)	0.3149 (3)	0.0231 (11)
H54	0.102310	0.652383	0.316344	0.028*
C55	−0.0423 (4)	0.64388 (14)	0.3541 (3)	0.0281 (12)
H55	−0.043485	0.667238	0.382068	0.034*
C56	−0.1277 (4)	0.61781 (14)	0.3515 (3)	0.0294 (12)
H56	−0.185895	0.623613	0.378580	0.035*
C57	−0.1272 (4)	0.58350 (14)	0.3091 (3)	0.0256 (12)
H57	−0.186297	0.566375	0.305649	0.031*
C58	−0.0381 (4)	0.57431 (14)	0.2713 (3)	0.0235 (11)
H58	−0.036596	0.550782	0.244489	0.028*
C59	0.0822 (4)	0.60429 (12)	0.0805 (3)	0.0188 (10)
C60	−0.0369 (4)	0.61515 (12)	0.0426 (3)	0.0223 (11)

H60	−0.077921	0.616660	0.088156	0.027*
C61	−0.0950 (4)	0.62378 (14)	−0.0626 (3)	0.0298 (12)
H61	−0.175186	0.630961	−0.087322	0.036*
C62	−0.0358 (5)	0.62189 (14)	−0.1314 (3)	0.0312 (12)
H62	−0.074977	0.628004	−0.201958	0.037*
C63	0.0821 (5)	0.61082 (14)	−0.0938 (3)	0.0299 (12)
H63	0.122595	0.609225	−0.139794	0.036*
C64	0.1415 (4)	0.60201 (13)	0.0108 (3)	0.0244 (11)
H64	0.221358	0.594538	0.034901	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01128 (9)	0.01589 (10)	0.01397 (8)	−0.00082 (8)	0.00420 (7)	0.00141 (7)
Fe1	0.0129 (3)	0.0159 (4)	0.0171 (3)	−0.0014 (3)	0.0053 (3)	0.0025 (3)
S1	0.0380 (8)	0.0434 (9)	0.0191 (6)	0.0099 (7)	0.0109 (6)	0.0031 (6)
S2	0.0228 (7)	0.0292 (7)	0.0210 (6)	0.0072 (6)	0.0087 (5)	0.0055 (5)
P1	0.0125 (6)	0.0177 (7)	0.0162 (5)	−0.0015 (5)	0.0035 (5)	0.0004 (5)
P2	0.0119 (6)	0.0134 (6)	0.0149 (5)	0.0001 (5)	0.0043 (5)	0.0015 (5)
P3	0.0129 (6)	0.0200 (7)	0.0159 (5)	−0.0013 (5)	0.0043 (5)	−0.0010 (5)
O1	0.026 (2)	0.026 (2)	0.038 (2)	0.0081 (17)	0.0105 (17)	−0.0009 (16)
O2	0.017 (2)	0.032 (2)	0.051 (2)	−0.0051 (17)	0.0128 (17)	0.0101 (17)
O3	0.0226 (19)	0.0190 (19)	0.0261 (17)	0.0048 (15)	0.0091 (15)	0.0030 (14)
C1	0.018 (3)	0.015 (3)	0.016 (2)	−0.004 (2)	0.0038 (19)	0.0017 (18)
C2	0.021 (3)	0.017 (3)	0.018 (2)	−0.003 (2)	0.009 (2)	−0.0023 (19)
C3	0.012 (2)	0.027 (3)	0.022 (2)	−0.003 (2)	0.008 (2)	−0.003 (2)
C4	0.023 (3)	0.019 (3)	0.022 (2)	−0.001 (2)	0.008 (2)	0.000 (2)
C5	0.028 (3)	0.036 (3)	0.018 (2)	−0.001 (2)	0.006 (2)	−0.009 (2)
C6	0.036 (3)	0.046 (4)	0.029 (3)	−0.002 (3)	0.016 (3)	−0.005 (3)
C7	0.063 (4)	0.029 (3)	0.030 (3)	−0.006 (3)	0.016 (3)	−0.002 (2)
C8	0.045 (4)	0.032 (4)	0.032 (3)	0.002 (3)	0.002 (3)	−0.010 (3)
C9	0.036 (4)	0.045 (4)	0.050 (3)	0.006 (3)	0.016 (3)	−0.013 (3)
C10	0.034 (3)	0.044 (4)	0.034 (3)	−0.007 (3)	0.017 (3)	−0.009 (3)
C11	0.082 (5)	0.040 (4)	0.062 (4)	0.020 (4)	0.015 (4)	−0.003 (3)
C12	0.014 (3)	0.026 (3)	0.023 (2)	−0.002 (2)	0.008 (2)	0.003 (2)
C13	0.019 (3)	0.024 (3)	0.019 (2)	0.001 (2)	0.004 (2)	0.002 (2)
C14	0.016 (3)	0.036 (3)	0.023 (2)	0.004 (2)	0.005 (2)	0.007 (2)
C15	0.026 (3)	0.042 (3)	0.023 (3)	0.001 (3)	0.011 (2)	0.005 (2)
C16	0.026 (3)	0.027 (3)	0.025 (3)	0.002 (2)	0.007 (2)	0.000 (2)
C17	0.015 (3)	0.033 (3)	0.032 (3)	0.003 (2)	0.004 (2)	0.001 (2)
C18	0.019 (3)	0.031 (3)	0.026 (3)	0.002 (2)	0.010 (2)	0.004 (2)
C19	0.035 (3)	0.054 (4)	0.034 (3)	0.004 (3)	0.006 (3)	0.011 (3)
C20	0.020 (3)	0.022 (3)	0.026 (2)	0.005 (2)	0.007 (2)	0.004 (2)
C21	0.016 (3)	0.021 (3)	0.021 (2)	−0.003 (2)	0.006 (2)	0.003 (2)
C22	0.009 (2)	0.027 (3)	0.015 (2)	0.002 (2)	0.0027 (18)	0.0000 (19)
C23	0.020 (3)	0.033 (3)	0.020 (2)	−0.001 (2)	0.006 (2)	0.000 (2)
C24	0.017 (3)	0.056 (4)	0.022 (3)	−0.014 (3)	0.006 (2)	−0.002 (3)
C25	0.010 (3)	0.066 (4)	0.021 (2)	0.002 (3)	0.005 (2)	−0.006 (3)

C26	0.020 (3)	0.040 (3)	0.030 (3)	0.011 (3)	0.005 (2)	−0.011 (2)
C27	0.021 (3)	0.028 (3)	0.019 (2)	0.005 (2)	0.005 (2)	−0.003 (2)
C28	0.013 (2)	0.019 (3)	0.023 (2)	0.000 (2)	0.002 (2)	−0.004 (2)
C29	0.035 (3)	0.024 (3)	0.026 (3)	−0.001 (2)	−0.003 (2)	−0.006 (2)
C30	0.041 (4)	0.025 (3)	0.046 (3)	0.006 (3)	0.001 (3)	−0.011 (3)
C31	0.027 (3)	0.042 (4)	0.038 (3)	0.000 (3)	0.012 (2)	−0.021 (3)
C32	0.032 (3)	0.043 (4)	0.031 (3)	−0.011 (3)	0.016 (2)	−0.010 (3)
C33	0.030 (3)	0.018 (3)	0.028 (3)	−0.001 (2)	0.011 (2)	−0.003 (2)
C34	0.015 (2)	0.016 (3)	0.012 (2)	0.002 (2)	0.0037 (18)	0.0012 (18)
C35	0.019 (3)	0.017 (3)	0.010 (2)	−0.002 (2)	0.0045 (19)	0.0010 (18)
C36	0.021 (3)	0.021 (3)	0.020 (2)	−0.002 (2)	0.004 (2)	0.000 (2)
C37	0.028 (3)	0.032 (3)	0.029 (3)	−0.013 (3)	0.013 (2)	−0.006 (2)
C38	0.048 (4)	0.019 (3)	0.034 (3)	−0.017 (3)	0.018 (3)	−0.001 (2)
C39	0.038 (3)	0.016 (3)	0.029 (3)	0.005 (2)	0.010 (2)	0.000 (2)
C40	0.021 (3)	0.022 (3)	0.022 (2)	0.000 (2)	0.008 (2)	0.003 (2)
C41	0.011 (2)	0.018 (3)	0.023 (2)	−0.005 (2)	0.0069 (19)	−0.0025 (19)
C42	0.027 (3)	0.021 (3)	0.027 (2)	0.000 (2)	0.015 (2)	−0.001 (2)
C43	0.039 (3)	0.020 (3)	0.052 (3)	0.003 (3)	0.025 (3)	−0.006 (3)
C44	0.026 (3)	0.044 (4)	0.036 (3)	−0.009 (3)	0.017 (2)	−0.022 (3)
C45	0.025 (3)	0.044 (4)	0.021 (2)	−0.003 (3)	0.010 (2)	−0.004 (2)
C46	0.015 (2)	0.022 (3)	0.023 (2)	−0.004 (2)	0.0062 (19)	−0.001 (2)
C47	0.022 (3)	0.019 (3)	0.019 (2)	0.000 (2)	0.010 (2)	0.0020 (19)
C48	0.021 (3)	0.027 (3)	0.027 (3)	−0.004 (2)	0.006 (2)	−0.004 (2)
C49	0.037 (3)	0.027 (3)	0.030 (3)	−0.012 (3)	0.008 (3)	−0.007 (2)
C50	0.057 (4)	0.021 (3)	0.031 (3)	0.001 (3)	0.016 (3)	0.000 (2)
C51	0.035 (3)	0.033 (3)	0.035 (3)	0.008 (3)	0.008 (3)	0.004 (3)
C52	0.026 (3)	0.017 (3)	0.022 (2)	−0.004 (2)	0.005 (2)	−0.005 (2)
C53	0.013 (3)	0.027 (3)	0.014 (2)	−0.002 (2)	0.0023 (19)	0.0020 (19)
C54	0.016 (3)	0.028 (3)	0.023 (2)	0.001 (2)	0.005 (2)	0.003 (2)
C55	0.026 (3)	0.032 (3)	0.029 (3)	0.009 (3)	0.014 (2)	0.001 (2)
C56	0.020 (3)	0.046 (4)	0.025 (2)	0.006 (3)	0.011 (2)	0.005 (2)
C57	0.014 (3)	0.036 (3)	0.025 (2)	0.000 (2)	0.006 (2)	0.010 (2)
C58	0.017 (3)	0.033 (3)	0.020 (2)	−0.004 (2)	0.005 (2)	0.002 (2)
C59	0.016 (3)	0.019 (3)	0.018 (2)	−0.003 (2)	0.0011 (19)	−0.0021 (19)
C60	0.018 (3)	0.027 (3)	0.022 (2)	0.006 (2)	0.008 (2)	0.007 (2)
C61	0.020 (3)	0.036 (3)	0.024 (2)	0.007 (2)	−0.002 (2)	−0.001 (2)
C62	0.034 (3)	0.037 (3)	0.015 (2)	0.001 (3)	0.001 (2)	0.001 (2)
C63	0.036 (3)	0.040 (3)	0.017 (2)	0.001 (3)	0.014 (2)	−0.001 (2)
C64	0.016 (3)	0.034 (3)	0.022 (2)	0.001 (2)	0.005 (2)	−0.002 (2)

Geometric parameters (Å, º)

Pt1—Fe1	2.5697 (6)	C26—C27	1.382 (6)
Pt1—P2	2.2850 (10)	C27—H27	0.9300
Pt1—P3	2.2714 (12)	C28—C29	1.383 (6)
Pt1—C1	2.045 (4)	C28—C33	1.385 (6)
Fe1—P1	2.1966 (12)	C29—H29	0.9300
Fe1—C1	2.162 (4)	C29—C30	1.383 (6)

Fe1—C2	2.119 (4)	C30—H30	0.9300
Fe1—C3	1.932 (5)	C30—C31	1.379 (7)
Fe1—C20	1.777 (5)	C31—H31	0.9300
Fe1—C21	1.789 (5)	C31—C32	1.356 (7)
S1—C4	1.830 (4)	C32—H32	0.9300
S1—C5	1.782 (5)	C32—C33	1.378 (6)
S2—C12	1.808 (4)	C33—H33	0.9300
S2—C13	1.771 (4)	C34—H34A	0.9700
P1—C22	1.839 (4)	C34—H34B	0.9700
P1—C28	1.841 (4)	C35—C36	1.399 (6)
P1—C34	1.842 (4)	C35—C40	1.385 (6)
P2—C34	1.829 (4)	C36—H36	0.9300
P2—C35	1.824 (4)	C36—C37	1.378 (6)
P2—C41	1.819 (4)	C37—H37	0.9300
P3—C47	1.824 (5)	C37—C38	1.388 (7)
P3—C53	1.824 (4)	C38—H38	0.9300
P3—C59	1.830 (4)	C38—C39	1.376 (7)
O1—C21	1.157 (5)	C39—H39	0.9300
O2—C20	1.141 (5)	C39—C40	1.377 (6)
O3—C3	1.216 (5)	C40—H40	0.9300
C1—C2	1.407 (6)	C41—C42	1.380 (6)
C1—C12	1.483 (6)	C41—C46	1.402 (6)
C2—C3	1.464 (6)	C42—H42	0.9300
C2—C4	1.511 (5)	C42—C43	1.404 (6)
C4—H4A	0.9700	C43—H43	0.9300
C4—H4B	0.9700	C43—C44	1.366 (6)
C5—C6	1.384 (6)	C44—H44	0.9300
C5—C10	1.397 (6)	C44—C45	1.376 (7)
C6—H6	0.9300	C45—H45	0.9300
C6—C7	1.367 (7)	C45—C46	1.381 (6)
C7—H7	0.9300	C46—H46	0.9300
C7—C8	1.392 (7)	C47—C48	1.394 (6)
C8—C9	1.373 (7)	C47—C52	1.388 (6)
C8—C11	1.513 (7)	C48—H48	0.9300
C9—H9	0.9300	C48—C49	1.373 (7)
C9—C10	1.381 (7)	C49—H49	0.9300
C10—H10	0.9300	C49—C50	1.382 (7)
C11—H11A	0.9600	C50—H50	0.9300
C11—H11B	0.9600	C50—C51	1.374 (7)
C11—H11C	0.9600	C51—H51	0.9300
C12—H12A	0.9700	C51—C52	1.389 (6)
C12—H12B	0.9700	C52—H52	0.9300
C13—C14	1.394 (6)	C53—C54	1.387 (6)
C13—C18	1.390 (6)	C53—C58	1.389 (6)
C14—H14	0.9300	C54—H54	0.9300
C14—C15	1.387 (6)	C54—C55	1.384 (6)
C15—H15	0.9300	C55—H55	0.9300
C15—C16	1.378 (6)	C55—C56	1.383 (7)

C16—C17	1.395 (6)	C56—H56	0.9300
C16—C19	1.516 (6)	C56—C57	1.371 (7)
C17—H17	0.9300	C57—H57	0.9300
C17—C18	1.373 (6)	C57—C58	1.391 (6)
C18—H18	0.9300	C58—H58	0.9300
C19—H19A	0.9600	C59—C60	1.383 (6)
C19—H19B	0.9600	C59—C64	1.390 (6)
C19—H19C	0.9600	C60—H60	0.9300
C22—C23	1.404 (6)	C60—C61	1.382 (6)
C22—C27	1.376 (6)	C61—H61	0.9300
C23—H23	0.9300	C61—C62	1.378 (6)
C23—C24	1.381 (6)	C62—H62	0.9300
C24—H24	0.9300	C62—C63	1.372 (7)
C24—C25	1.377 (7)	C63—H63	0.9300
C25—H25	0.9300	C63—C64	1.379 (6)
C25—C26	1.388 (7)	C64—H64	0.9300
C26—H26	0.9300		

P2—Pt1—Fe1	97.26 (3)	C24—C23—C22	120.3 (5)
P3—Pt1—Fe1	161.46 (3)	C24—C23—H23	119.9
P3—Pt1—P2	100.53 (4)	C23—C24—H24	119.7
C1—Pt1—Fe1	54.44 (12)	C25—C24—C23	120.5 (5)
C1—Pt1—P2	151.36 (12)	C25—C24—H24	119.7
C1—Pt1—P3	107.33 (12)	C24—C25—H25	120.2
P1—Fe1—Pt1	93.50 (4)	C24—C25—C26	119.5 (5)
C1—Fe1—Pt1	50.30 (11)	C26—C25—H25	120.2
C1—Fe1—P1	141.85 (12)	C25—C26—H26	120.0
C2—Fe1—Pt1	73.72 (12)	C27—C26—C25	119.9 (5)
C2—Fe1—P1	130.91 (13)	C27—C26—H26	120.0
C2—Fe1—C1	38.35 (16)	C22—C27—C26	121.3 (5)
C3—Fe1—Pt1	72.18 (13)	C22—C27—H27	119.3
C3—Fe1—P1	88.88 (13)	C26—C27—H27	119.3
C3—Fe1—C1	70.43 (18)	C29—C28—P1	120.7 (3)
C3—Fe1—C2	42.03 (17)	C29—C28—C33	118.0 (4)
C20—Fe1—Pt1	168.78 (14)	C33—C28—P1	121.2 (4)
C20—Fe1—P1	95.66 (14)	C28—C29—H29	119.5
C20—Fe1—C1	119.19 (18)	C28—C29—C30	120.9 (5)
C20—Fe1—C2	95.33 (18)	C30—C29—H29	119.5
C20—Fe1—C3	101.5 (2)	C29—C30—H30	120.1
C20—Fe1—C21	96.5 (2)	C31—C30—C29	119.8 (5)
C21—Fe1—Pt1	87.76 (14)	C31—C30—H30	120.1
C21—Fe1—P1	102.63 (13)	C30—C31—H31	120.1
C21—Fe1—C1	89.16 (18)	C32—C31—C30	119.8 (5)
C21—Fe1—C2	123.33 (18)	C32—C31—H31	120.1
C21—Fe1—C3	157.6 (2)	C31—C32—H32	119.6
C5—S1—C4	102.1 (2)	C31—C32—C33	120.7 (5)
C13—S2—C12	102.2 (2)	C33—C32—H32	119.6
C22—P1—Fe1	115.03 (13)	C28—C33—H33	119.6

C22—P1—C28	100.05 (19)	C32—C33—C28	120.7 (5)
C22—P1—C34	102.6 (2)	C32—C33—H33	119.6
C28—P1—Fe1	121.17 (15)	P1—C34—H34A	109.6
C28—P1—C34	103.71 (19)	P1—C34—H34B	109.6
C34—P1—Fe1	112.02 (13)	P2—C34—P1	110.3 (2)
C34—P2—Pt1	103.14 (13)	P2—C34—H34A	109.6
C35—P2—Pt1	121.79 (13)	P2—C34—H34B	109.6
C35—P2—C34	102.5 (2)	H34A—C34—H34B	108.1
C41—P2—Pt1	121.93 (15)	C36—C35—P2	118.3 (3)
C41—P2—C34	103.99 (19)	C40—C35—P2	123.3 (3)
C41—P2—C35	100.66 (19)	C40—C35—C36	118.5 (4)
C47—P3—Pt1	114.72 (15)	C35—C36—H36	119.9
C47—P3—C53	108.4 (2)	C37—C36—C35	120.2 (5)
C47—P3—C59	100.6 (2)	C37—C36—H36	119.9
C53—P3—Pt1	111.32 (15)	C36—C37—H37	119.8
C53—P3—C59	101.2 (2)	C36—C37—C38	120.4 (5)
C59—P3—Pt1	119.15 (15)	C38—C37—H37	119.8
Pt1—C1—Fe1	75.25 (13)	C37—C38—H38	120.2
C2—C1—Pt1	109.1 (3)	C39—C38—C37	119.6 (5)
C2—C1—Fe1	69.2 (2)	C39—C38—H38	120.2
C2—C1—C12	119.6 (4)	C38—C39—H39	120.0
C12—C1—Pt1	130.5 (3)	C38—C39—C40	120.1 (5)
C12—C1—Fe1	129.0 (3)	C40—C39—H39	120.0
C1—C2—Fe1	72.5 (2)	C35—C40—H40	119.4
C1—C2—C3	111.2 (4)	C39—C40—C35	121.2 (4)
C1—C2—C4	126.2 (4)	C39—C40—H40	119.4
C3—C2—Fe1	62.1 (2)	C42—C41—P2	121.3 (3)
C3—C2—C4	121.9 (4)	C42—C41—C46	118.5 (4)
C4—C2—Fe1	124.8 (3)	C46—C41—P2	120.1 (3)
O3—C3—Fe1	146.8 (3)	C41—C42—H42	119.7
O3—C3—C2	136.5 (4)	C41—C42—C43	120.6 (4)
C2—C3—Fe1	75.8 (3)	C43—C42—H42	119.7
S1—C4—H4A	109.0	C42—C43—H43	120.3
S1—C4—H4B	109.0	C44—C43—C42	119.3 (5)
C2—C4—S1	112.9 (3)	C44—C43—H43	120.3
C2—C4—H4A	109.0	C43—C44—H44	119.3
C2—C4—H4B	109.0	C43—C44—C45	121.3 (4)
H4A—C4—H4B	107.8	C45—C44—H44	119.3
C6—C5—S1	121.9 (4)	C44—C45—H45	120.3
C6—C5—C10	118.4 (5)	C44—C45—C46	119.4 (4)
C10—C5—S1	119.7 (4)	C46—C45—H45	120.3
C5—C6—H6	119.8	C41—C46—H46	119.6
C7—C6—C5	120.4 (5)	C45—C46—C41	120.8 (4)
C7—C6—H6	119.8	C45—C46—H46	119.6
C6—C7—H7	118.9	C48—C47—P3	122.3 (4)
C6—C7—C8	122.2 (5)	C52—C47—P3	120.0 (3)
C8—C7—H7	118.9	C52—C47—C48	117.7 (4)
C7—C8—C11	121.0 (5)	C47—C48—H48	119.5

C9—C8—C7	116.9 (5)	C49—C48—C47	121.0 (5)
C9—C8—C11	122.1 (5)	C49—C48—H48	119.5
C8—C9—H9	118.9	C48—C49—H49	119.8
C8—C9—C10	122.2 (5)	C48—C49—C50	120.5 (5)
C10—C9—H9	118.9	C50—C49—H49	119.8
C5—C10—H10	120.0	C49—C50—H50	120.2
C9—C10—C5	119.9 (5)	C51—C50—C49	119.6 (5)
C9—C10—H10	120.0	C51—C50—H50	120.2
C8—C11—H11A	109.5	C50—C51—H51	120.1
C8—C11—H11B	109.5	C50—C51—C52	119.8 (5)
C8—C11—H11C	109.5	C52—C51—H51	120.1
H11A—C11—H11B	109.5	C47—C52—C51	121.3 (4)
H11A—C11—H11C	109.5	C47—C52—H52	119.3
H11B—C11—H11C	109.5	C51—C52—H52	119.3
S2—C12—H12A	109.1	C54—C53—P3	116.1 (3)
S2—C12—H12B	109.1	C54—C53—C58	118.7 (4)
C1—C12—S2	112.3 (3)	C58—C53—P3	125.1 (4)
C1—C12—H12A	109.1	C53—C54—H54	119.5
C1—C12—H12B	109.1	C55—C54—C53	121.0 (5)
H12A—C12—H12B	107.9	C55—C54—H54	119.5
C14—C13—S2	124.4 (4)	C54—C55—H55	120.3
C18—C13—S2	118.1 (3)	C56—C55—C54	119.4 (5)
C18—C13—C14	117.5 (4)	C56—C55—H55	120.3
C13—C14—H14	119.6	C55—C56—H56	119.8
C15—C14—C13	120.7 (4)	C57—C56—C55	120.5 (4)
C15—C14—H14	119.6	C57—C56—H56	119.8
C14—C15—H15	119.1	C56—C57—H57	120.0
C16—C15—C14	121.7 (4)	C56—C57—C58	120.0 (5)
C16—C15—H15	119.1	C58—C57—H57	120.0
C15—C16—C17	117.2 (4)	C53—C58—C57	120.4 (5)
C15—C16—C19	121.7 (4)	C53—C58—H58	119.8
C17—C16—C19	121.1 (5)	C57—C58—H58	119.8
C16—C17—H17	119.2	C60—C59—P3	122.2 (3)
C18—C17—C16	121.6 (5)	C60—C59—C64	118.9 (4)
C18—C17—H17	119.2	C64—C59—P3	118.9 (3)
C13—C18—H18	119.4	C59—C60—H60	119.9
C17—C18—C13	121.2 (4)	C61—C60—C59	120.2 (4)
C17—C18—H18	119.4	C61—C60—H60	119.9
C16—C19—H19A	109.5	C60—C61—H61	119.6
C16—C19—H19B	109.5	C62—C61—C60	120.9 (5)
C16—C19—H19C	109.5	C62—C61—H61	119.6
H19A—C19—H19B	109.5	C61—C62—H62	120.6
H19A—C19—H19C	109.5	C63—C62—C61	118.8 (4)
H19B—C19—H19C	109.5	C63—C62—H62	120.6
O2—C20—Fe1	178.7 (4)	C62—C63—H63	119.4
O1—C21—Fe1	179.9 (5)	C62—C63—C64	121.1 (4)
C23—C22—P1	116.6 (4)	C64—C63—H63	119.4
C27—C22—P1	124.9 (4)	C59—C64—H64	119.9

C27—C22—C23	118.4 (4)	C63—C64—C59	120.1 (4)
C22—C23—H23	119.9	C63—C64—H64	119.9
Pt1—P2—C34—P1	52.0 (2)	C22—P1—C28—C29	109.4 (4)
Pt1—P2—C35—C36	−87.5 (3)	C22—P1—C28—C33	−70.4 (4)
Pt1—P2—C35—C40	92.7 (4)	C22—P1—C34—P2	−172.0 (2)
Pt1—P2—C41—C42	−5.3 (4)	C22—C23—C24—C25	0.1 (6)
Pt1—P2—C41—C46	177.8 (3)	C23—C22—C27—C26	−0.6 (6)
Pt1—P3—C47—C48	−174.1 (3)	C23—C24—C25—C26	−1.6 (7)
Pt1—P3—C47—C52	2.6 (4)	C24—C25—C26—C27	2.0 (7)
Pt1—P3—C53—C54	34.5 (4)	C25—C26—C27—C22	−0.9 (7)
Pt1—P3—C53—C58	−148.9 (3)	C27—C22—C23—C24	1.0 (6)
Pt1—P3—C59—C60	−122.1 (4)	C28—P1—C22—C23	−58.9 (3)
Pt1—P3—C59—C64	57.8 (4)	C28—P1—C22—C27	124.9 (4)
Pt1—C1—C2—Fe1	−65.2 (2)	C28—P1—C34—P2	84.2 (2)
Pt1—C1—C2—C3	−15.6 (4)	C28—C29—C30—C31	0.1 (8)
Pt1—C1—C2—C4	174.2 (3)	C29—C28—C33—C32	1.8 (7)
Pt1—C1—C12—S2	18.9 (5)	C29—C30—C31—C32	1.4 (8)
Fe1—P1—C22—C23	72.6 (3)	C30—C31—C32—C33	−1.4 (8)
Fe1—P1—C22—C27	−103.6 (3)	C31—C32—C33—C28	−0.2 (8)
Fe1—P1—C28—C29	−18.2 (5)	C33—C28—C29—C30	−1.7 (7)
Fe1—P1—C28—C33	162.1 (3)	C34—P1—C22—C23	−165.5 (3)
Fe1—P1—C34—P2	−48.1 (2)	C34—P1—C22—C27	18.3 (4)
Fe1—C1—C2—C3	49.6 (3)	C34—P1—C28—C29	−144.9 (4)
Fe1—C1—C2—C4	−120.6 (4)	C34—P1—C28—C33	35.3 (4)
Fe1—C1—C12—S2	−86.2 (4)	C34—P2—C35—C36	158.2 (3)
Fe1—C2—C3—O3	−170.8 (6)	C34—P2—C35—C40	−21.6 (4)
Fe1—C2—C4—S1	−172.3 (2)	C34—P2—C41—C42	110.2 (4)
S1—C5—C6—C7	−179.4 (4)	C34—P2—C41—C46	−66.6 (4)
S1—C5—C10—C9	180.0 (4)	C35—P2—C34—P1	179.29 (19)
S2—C13—C14—C15	−175.3 (4)	C35—P2—C41—C42	−143.8 (4)
S2—C13—C18—C17	176.1 (4)	C35—P2—C41—C46	39.3 (4)
P1—C22—C23—C24	−175.4 (3)	C35—C36—C37—C38	0.6 (6)
P1—C22—C27—C26	175.5 (3)	C36—C35—C40—C39	−0.8 (6)
P1—C28—C29—C30	178.5 (4)	C36—C37—C38—C39	−0.1 (7)
P1—C28—C33—C32	−178.5 (4)	C37—C38—C39—C40	−0.8 (7)
P2—C35—C36—C37	−179.9 (3)	C38—C39—C40—C35	1.3 (7)
P2—C35—C40—C39	179.0 (3)	C40—C35—C36—C37	−0.1 (6)
P2—C41—C42—C43	−176.3 (4)	C41—P2—C34—P1	−76.2 (2)
P2—C41—C46—C45	177.1 (3)	C41—P2—C35—C36	51.1 (3)
P3—C47—C48—C49	−179.2 (3)	C41—P2—C35—C40	−128.7 (4)
P3—C47—C52—C51	−179.3 (3)	C41—C42—C43—C44	−0.1 (7)
P3—C53—C54—C55	177.3 (3)	C42—C41—C46—C45	0.2 (7)
P3—C53—C58—C57	−175.9 (3)	C42—C43—C44—C45	−1.1 (8)
P3—C59—C60—C61	179.5 (4)	C43—C44—C45—C46	1.8 (7)
P3—C59—C64—C63	−179.3 (4)	C44—C45—C46—C41	−1.3 (7)
C1—C2—C3—Fe1	−55.2 (3)	C46—C41—C42—C43	0.5 (7)
C1—C2—C3—O3	134.0 (6)	C47—P3—C53—C54	161.5 (3)

C1—C2—C4—S1	−79.3 (5)	C47—P3—C53—C58	−21.8 (4)
C2—C1—C12—S2	−172.5 (3)	C47—P3—C59—C60	111.6 (4)
C3—C2—C4—S1	111.4 (4)	C47—P3—C59—C64	−68.5 (4)
C4—S1—C5—C6	72.5 (4)	C47—C48—C49—C50	−2.6 (7)
C4—S1—C5—C10	−108.5 (4)	C48—C47—C52—C51	−2.3 (6)
C4—C2—C3—Fe1	115.5 (4)	C48—C49—C50—C51	−0.5 (7)
C4—C2—C3—O3	−55.3 (8)	C49—C50—C51—C52	2.1 (7)
C5—S1—C4—C2	−78.1 (4)	C50—C51—C52—C47	−0.6 (7)
C5—C6—C7—C8	−1.0 (8)	C52—C47—C48—C49	3.9 (6)
C6—C5—C10—C9	−0.9 (7)	C53—P3—C47—C48	60.8 (4)
C6—C7—C8—C9	−0.2 (8)	C53—P3—C47—C52	−122.4 (3)
C6—C7—C8—C11	179.4 (5)	C53—P3—C59—C60	0.3 (4)
C7—C8—C9—C10	0.8 (8)	C53—P3—C59—C64	−179.9 (4)
C8—C9—C10—C5	−0.3 (8)	C53—C54—C55—C56	−0.3 (7)
C10—C5—C6—C7	1.6 (7)	C54—C53—C58—C57	0.7 (6)
C11—C8—C9—C10	−178.7 (5)	C54—C55—C56—C57	−0.9 (7)
C12—S2—C13—C14	−36.3 (5)	C55—C56—C57—C58	1.9 (7)
C12—S2—C13—C18	146.7 (4)	C56—C57—C58—C53	−1.9 (7)
C12—C1—C2—Fe1	124.0 (4)	C58—C53—C54—C55	0.4 (6)
C12—C1—C2—C3	173.6 (4)	C59—P3—C47—C48	−44.9 (4)
C12—C1—C2—C4	3.3 (7)	C59—P3—C47—C52	131.8 (3)
C13—S2—C12—C1	−166.4 (3)	C59—P3—C53—C54	−93.2 (3)
C13—C14—C15—C16	−1.5 (8)	C59—P3—C53—C58	83.5 (4)
C14—C13—C18—C17	−1.1 (7)	C59—C60—C61—C62	−0.3 (8)
C14—C15—C16—C17	0.6 (7)	C60—C59—C64—C63	0.6 (7)
C14—C15—C16—C19	179.8 (5)	C60—C61—C62—C63	0.8 (8)
C15—C16—C17—C18	−0.1 (7)	C61—C62—C63—C64	−0.6 (8)
C16—C17—C18—C13	0.4 (8)	C62—C63—C64—C59	−0.1 (8)
C18—C13—C14—C15	1.7 (7)	C64—C59—C60—C61	−0.4 (7)
C19—C16—C17—C18	−179.3 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O1^{i}	0.93	2.67	3.316 (6)	128
C34—H34*A*···O3	0.97	2.62	3.271 (5)	125
C39—H39···O3^{ii}	0.93	2.49	3.239 (6)	138

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+1, −*y*+1, −*z*+1.