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Molecular structures of the pentaphenylcyclopentadienyl iron complexes $[(C_5Ph_5)Fe(CO)_2R]$ (R = Me, Ph, iPr and Bu)

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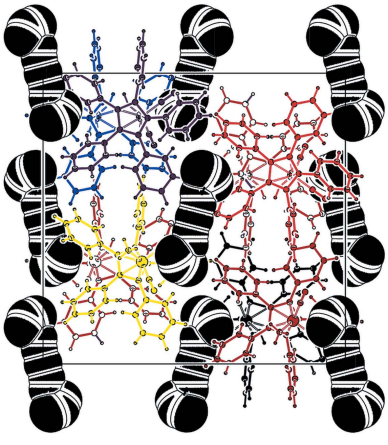
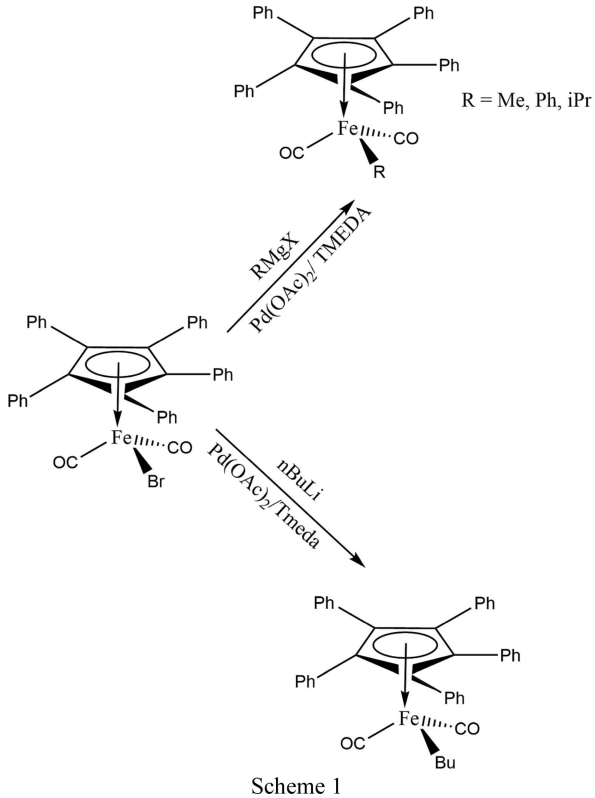
The Pd^{II}-catalysed reaction of $[(C_5Ph_5)Fe(CO)_2Br]$ with Grignard compounds $RMgX$ or butyl lithium gave the iron alkyl/aryl complexes $[(C_5Ph_5)Fe(CO)_2R]$ (R = Me, Ph, iPr and Bu) in 59–73% yield, namely, dicarbonylmethyl(η^5-pentaphenylcyclopentadienyl)iron, $[Fe(CH_3)(C_{35}H_{25})(CO)_2]$, dicarbonyl($\eta^5$-pentaphenylcyclopentadienyl)phenyliron, $[Fe(C_6H_5)(C_{35}H_{25})(CO)_2]$, dicarbonyl(isopropyl)($\eta^5$-pentaphenylcyclopentadienyl)iron, $[Fe(C_3H_7)(C_{35}H_{25})(CO)_2]$, and butyldicarbonyl($\eta^5$-pentaphenylcyclopentadienyl)iron, $[Fe(C_4H_9)(C_{35}H_{25})(CO)_2]$. The crystal structure determinations showed the usual 'paddle-wheel' orientation of the phenyl rings, with an average canting angle of *ca* 50°. The bond parameters are mainly dictated by the steric requirements of the alkyl/aryl groups and only the phenyl complex shows electronic effects.

1. Introduction

Pentaarylcyclopentadienyl complexes have been known for nearly 60 years. They were studied mainly because the bulky nature of these cyclopentadienyl derivatives gives their complexes high kinetic stability, including the formation of stable radicals (Field *et al.*, 2011) or unusual structures in main group or lanthanoid metallocenes (Schulte *et al.*, 2020). Also, several examples of their application as asymmetric catalysts (Ruble *et al.*, 1997; Field *et al.*, 2011) and as mimics for hydrogenase (Hemming *et al.*, 2018) were found. So far (*Scifinder*, accessed on 12th May 2021), 451 publications describing 723 substances have appeared, an increase of 80% during the last decade. On the other hand, a survey of the Cambridge Structural Database (CSD, Version 5.42, accessed on 5th June, 2021; Groom *et al.*, 2016) showed only 118 entries, of which roughly half (52) contained iron as the central metal atom. Of these, *ca* 80% (41) were ferrocene derivatives. The molecular structure of the very first pentaphenylcyclopentadienyl complex, *i.e.* $[(C_5Ph_5)Fe(CO)_2Br]$ (McVey & Pauson, 1965), was published only 25 years later (Field *et al.*, 1989) and there are only three other structure determinations of molecules containing the $[(C_5Ph_5)Fe(CO)_2]$ moiety in the CSD: MARFET and MARFIX (Hemming *et al.*, 2018), and PUYDES (Carter *et al.*, 2002). A very important subgroup of compounds containing the [CpFe(CO)] moiety contains the derived alkyl and aryl complexes $[CpFe(CO)_2R]$ (Pannell & Sharma, 2010). These compounds were shown to have catalytic properties, for example, in dehydrogenative couplings (Fukumoto *et al.*, 2015; Argouarch *et al.*, 2012) or, perhaps more importantly, as reagents in photoinduced DNA cleavage (Mohler *et al.*, 2002; Mohler & Shell, 2005). Therefore, it seemed worthwhile to study compounds of the type $[(C_5Ph_5)Fe(CO)_2R]$, which might combine the unique properties of the pentaphenylcyclo-



pentadienyl moiety with the reactivity of the iron–alkyl and iron–aryl groups. Such compounds have been reported before, but were usually only partially characterized (Connelly & Manners, 1989; Brégaint *et al.*, 1990, 1992; Kuksis & Baird, 1994; Kuksis *et al.*, 1996). In particular, no crystal structures have been published. During the course of our studies on the coordination chemistry of perhalogenated cyclopentadienyl complexes (Klein-Heßling *et al.*, 2021; Sünkel *et al.*, 2015) we also studied the $[(C_5X_5)Fe(CO)_2R]$ system. In the search for possible synthetic applications for these compounds and also for the sake of comparison, we chose to prepare the alkyl and aryl $[(C_5Ph_5)Fe(CO)_2R]$ derivatives (*R* = Me, **1**, Ph, **2**, iPr, **3**, and Bu, **4**) (Scheme 1). We report here the results of our crystal structure studies.



Scheme 1

2. Experimental

2.1. Synthesis and crystallization

The starting material $[(C_5Ph_5)Fe(CO)_2Br]$ was prepared according to the literature from $Fe(CO)_5$ and C_5Ph_5Br (McVey & Pauson, 1965). The reagents MeMgBr (3.0 *M* solution in Et_2O), PhMgCl [2.0 *M* solution in tetrahydrofuran (THF)], iPrMgCl (1.3 *M* solution with LiCl in THF) and BuLi (2.5 *M* solution in hexane), as well as *N*,*N*,*N*′,*N*′-tetramethylethylendiamine (TMEDA) and palladium acetate, were commercial products (Sigma–Aldrich) and were used as provided.

2.1.1. $[(C_5Ph_5)Fe(CO)_2Me]$, (1). A solution of $[(C_5Ph_5)Fe(CO)_2Br]$ (0.30 g, 0.47 mmol) in THF (12 ml), palladium(II) acetate (0.01 g, 0.05 mmol) and TMEDA (0.07 ml, 0.71 mmol) was treated at 0 °C with an MeMgBr solution (0.24 ml, 0.71 mmol) and stirred for 60 min. After evaporation of the solvent, the residue was redissolved in the minimum amount of petroleum ether and placed on top of a silica-gel chromatography column. Elution with petroleum ether/Et_2O (9:1 *v*/*v*) yielded, after evaporation, compound **1** as a yellow solid (yield: 0.17 g, 0.30 mmol, 63%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether solution in a refrigerator at 5 °C.

IR (ATR): ν (CO) 1993, 1941 cm^{-1}. UV–Vis (CH_2Cl_2): λ_{max} = 369 nm. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.20–6.90 (*m*, Ph), 0.62 (*s*, Me) ppm. ^{13}C NMR ($CDCl_3$, 100.5 MHz): δ 217.8 (CO), 132.2, 131.9, 127.7, 127.5 (4 × Ph), 102.1 (C5), −7.5 (Me) ppm.

2.1.2. $[(C_5Ph_5)Fe(CO)_2Ph]$, (2). A solution of $[(C_5Ph_5)Fe(CO)_2Br]$ (0.05 g, 0.08 mmol) in THF (10 ml), palladium(II) acetate (0.002 g, 0.01 mmol) and TMEDA (0.01 ml, 0.08 mmol) was treated at 0 °C with a PhMgCl solution (0.05 ml, 0.10 mmol) and stirred for 60 min. After evaporation of the solvent, the residue was redissolved in the minimum amount of petroleum ether and placed on top of a silica-gel chromatography column. Elution with petroleum ether/Et_2O (9:1 *v*/*v*) yielded, after evaporation, compound **2** as a yellow solid (yield: 0.03 g, 0.05 mmol, 59%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether solution in a refrigerator at 5 °C.

IR (ATR): ν (CO) 2009, 1968 cm^{-1}. UV–Vis (CH_2Cl_2): λ_{max} = 364 nm. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.23–6.81 (*m*,

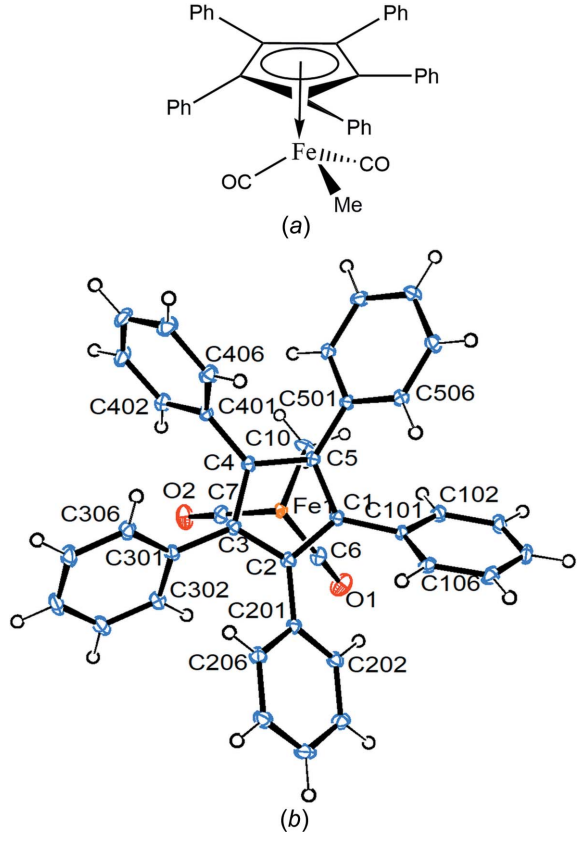


Figure 1
Displacement ellipsoid plot (top view) of compound **1**, with ellipsoids drawn at the 30% probability level.

Table 1
Experimental details.

Experiments were carried out with Mo $K\alpha$ radiation using a Bruker D8 Venture diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Krause *et al.*, 2015). H-atom parameters were constrained.

	1	**2**	**3**	**4**
Crystal data				
Chemical formula	$[Fe(CH_3)(C_{35}H_{25})(CO)_2]$	$[Fe(C_6H_5)(C_{35}H_{25})(CO)_2]$	$[Fe(C_3H_7)(C_{35}H_{25})(CO)_2]$	$[Fe(C_4H_9)(C_{35}H_{25})(CO)_2]$
M_r	572.45	634.52	600.50	614.53
Crystal system, space group	Orthorhombic, *Pbca*	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
Temperature (K)	105	105	110	108
a, b, c (Å)	13.6393 (3), 20.4360 (5), 21.1978 (5)	12.1860 (4), 16.9411 (6), 15.0691 (6)	12.5488 (7), 13.5046 (7), 18.0119 (11)	12.1141 (4), 16.0945 (5), 16.1650 (5)
α, β, γ (°)	90, 90, 90	90, 93.320 (1), 90	90, 93.208 (2), 90	90, 95.706 (1), 90
V (Å^3)	5908.5 (2)	3105.71 (19)	3047.6 (3)	3136.08 (17)
Z	8	4	4	4
μ (mm^{-1})	0.54	0.52	0.53	0.52
Crystal size (mm)	0.06 × 0.05 × 0.04	0.08 × 0.02 × 0.02	0.06 × 0.04 × 0.03	0.08 × 0.05 × 0.04
Data collection				
T_{min}, T_{max}	0.718, 0.746	0.669, 0.745	0.719, 0.746	0.832, 0.862
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	61228, 6765, 5439	31592, 6352, 5025	52953, 6732, 5995	55494, 7202, 6246
R_{int}	0.053	0.050	0.031	0.041
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.649	0.625	0.641	0.650
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.090, 1.06	0.041, 0.088, 1.04	0.032, 0.088, 1.06	0.033, 0.090, 1.05
No. of reflections	6765	6352	6732	7202
No. of parameters	371	415	390	398
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.49	0.32, −0.41	0.36, −0.36	0.37, −0.47

Computer programs: *APEX2* (Bruker, 2011), *SAINT* (Bruker, 2011), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *WinGX* (Farrugia, 2012).

Ph) ppm. ^{13}C NMR ($CDCl_3$, 100.5 MHz): δ 216.5 (CO), 147–123 (35 × Ph), 102.8 (C5) ppm.

2.1.3. [(C_5Ph_5)Fe(CO)$_2$iPr], (3). A solution of [(C_5Ph_5)Fe(CO)$_2$Br] (0.10 g, 0.16 mmol) in THF (10 ml), palladium(II) acetate (0.004 g, 0.02 mmol) and TMEDA (0.02 ml, 0.16 mmol) was treated at 0°C with an iPrMgCl solution (0.18 ml, 0.24 mmol) and stirred for 60 min. After evaporation of the solvent, the residue was redissolved in the minimum amount of petroleum ether and placed on top of a silica-gel chromatography column. Elution with petroleum ether/Et_2O (9:1 *v*/*v*) yielded, after evaporation, compound **3** as a yellow solid (yield: 0.07 g, 0.12 mmol, 73%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether solution in a refrigerator at 5 °C.

IR (ATR): ν (CO) 1991, 1939 cm^{-1}. UV–Vis (CH_2Cl_2): λ_{max} = 367 nm. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32–6.85 (*m*, Ph), 3.07 (*m*, $CHMe_2$), 1.46 (*m*, $CHMe_2$) ppm.

2.1.4. [(C_5Ph_5)Fe(CO)$_2$Bu], (4). A solution of [(C_5Ph_5)Fe(CO)$_2$Br] (0.05 g, 0.08 mmol) in THF (10 ml), palladium(II) acetate (0.002 g, 0.01 mmol) and TMEDA (0.01 ml, 0.08 mmol) was treated at −30 °C with a BuLi solution (0.04 ml, 0.10 mmol) and stirred for 60 min. After evaporation of the solvent, the residue was redissolved in the minimum amount of petroleum ether and placed on top of a silica-gel chromatography column. Elution with petroleum ether/Et_2O (9:1 *v*/*v*) yielded after evaporation compound **4** as a yellow solid (yield: 0.03 g, 0.05 mmol, 63%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether solution in a refrigerator at 5 °C.

IR (ATR): ν (CO) 1993, 1939 cm^{-1}. UV–Vis (CH_2Cl_2): λ_{max} = 378 nm. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.22–6.84 (*m*, Ph), 1.95–0.80 (4 *m*, Bu) ppm. ^{13}C NMR ($CDCl_3$, 100.5 MHz): δ 218.7 (CO), 132.2, 132.0, 127.7, 127.4 (4 × Ph), 102.3 (C5), 38.5, 28.2, 17.7, 14.1 (4 × Bu) ppm.

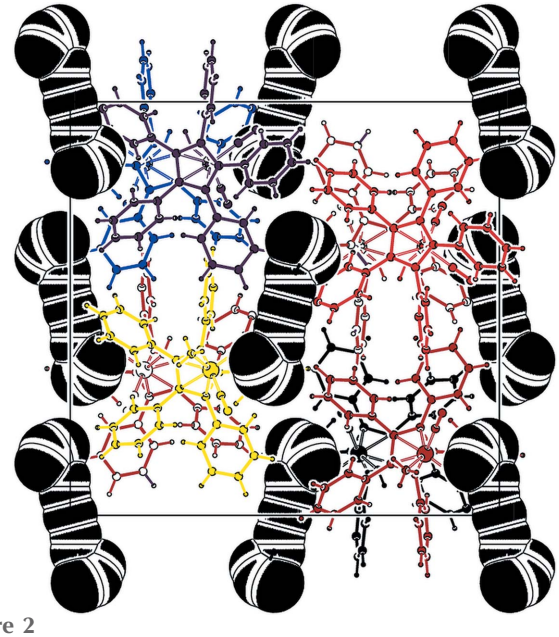


Figure 2
PLATON (Spek, 2020) cavity plot of compound **1**.

Table 2
Comparison of important bond parameters (Å, °) of compounds **1**–**4** and some related structures from the CSD.

	1	**2**	**3**	**4**	SIRMIP	MARFET	MARFIX	PUYDES	HOZWIC	CECKUS01
Fe—Ct (Å)	1.7403 (8)	1.7625 (10)	1.7586 (7)	1.7603 (7)	1.738 (5)	1.7464 (10)	1.7360 (12)/ 1.7306 (12)	1.715 (3)	1.730	1.730
Fe—C_α(*R*) (Å)	2.073 (2)	2.022 (2)	2.1188 (17)	2.0810 (16)	n.a.	n.a.	n.a.	n.a.	2.069 (10)	2.002 (2)
Fe—C(CO) (Å)	1.751 (2) 1.754 (2)	1.755 (2) 1.760 (2)	1.745 (2) 1.756 (2)	1.755 (2) 1.755 (2)	1.812 (5) 1.786 (5)		1.803 (3) 1.813 (3)	1.714 (6) 1.715 (6)	1.739 (11) 1.751 (11)	1.756 (1)
C—O (Å)	1.149 (2) 1.136 (2)	1.152 (3) 1.148 (3)	1.145 (3) 1.148 (2)	1.150 (1) 1.148 (2)	1.052 (6) 1.097 (6)	1.133 (3) 1.137 (4)	1.131 (4)/ 1.126 (4) 1.137 (3)/ 1.132 (4)	1.182 (7) 1.187 (7)	1.153 (13) 1.139 (14)	1.151 (2) 1.151 (2)
IR (ν_{CO}, cm^{-1})	1993, 1941	2009, 1968	1991, 1939	1993, 1939	2033, 1993*			1872, 1806*	1987, 1933*	1994, 1937*
$(C_{i,Ph}—Cp)_{av}$ (Å)	0.122	0.188	0.144	0.160	0.15	0.147	0.144/0.145		n.a.	n.a.
$(Cp–Ph)_{av}$ (°)	50.3	48.5	50.6	50.2	58.7	52.3	51.8/51.4	53.4	n.a.	n.a.
$[C_\alpha—Fe—Ct—C_{Cp}]_{min}$	9.35	26.46	5.13	32.19	n.a.	n.a.	n.a.	n.a.	1.44	0.0
Ct—Fe—C_α—C_β (°)	n.a.	95.8 79.8	141.1 91.8	167.4	n.a.	n.a.	n.a.	n.a.	179.9	87.5

CSD refcodes: SIRMIP is $[(C_5Ph_5)Fe(CO)_2Br]$ (Field *et al.*, 1989), MARFET is $[(C_5Ph_5)Fe(CO)_2FBF_3]$ (Hemming *et al.*, 2018), MARFIX is $[(C_5Ph_5)Fe(CO)_2(H_2O)]BF_4$ (Hemming *et al.*, 2018), PUYDES is $[PPN][(C_5Ph_5)Fe(CO)_2]$ (Carter *et al.*, 2002), HOZWIC is $[(C_5Me_5)Fe(CO)_2C_5H_{11}]$ (Hill *et al.*, 1999) and CECKUS01 is $[(C_5Me_5)Fe(CO)_2Ph]$ (Kalman *et al.*, 2013). Notes: Ct is the centroid of the cyclopentadienyl ring. $(C_{i,Ph}—Cp)_{av}$ is the average distance of the phenyl *ipso*-C atoms from the plane of the Cp ring. $(Cp–Ph)_{av}$ is the average dihedral angle of the five phenyl rings with respect to the plane of the Cp ring, $[C_\alpha—Fe—Ct—C_{Cp}]_{min}$ is the smallest torsion angle between the α-alkyl/aryl C atom, the Fe atom, the centroid of the cyclopentadienyl ring and a Cp-ring C atom. 'n.a.' denotes not applicable. The asterisk (*) denotes solution spectra.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms on C atoms were calculated in ideal positions riding on their parent atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms. The methyl groups were allowed to rotate along the C—C bonds to best fit the experimental electron density.

3. Results and discussion

The title compounds were prepared in medium to good yields from $[(C_5Ph_5)Fe(CO)_2Br]$ and either Grignard reagents *R*Mg*X* or butyl lithium in the presence of catalytic amounts of $Pd(OAc)_2$ and TMEDA (Scheme 1).

The synthesis is based on a procedure that was described for the preparation of aryl iron complexes $[(C_5H_5)Fe(CO)_2Ar]$ (Yasuda *et al.*, 2008). Compounds **1** and **3** had been prepared before by reaction of $[(C_5Ph_5)Fe(CO)_2]_2$ with the corresponding alkyl iodides (no yields given; Kuksis *et al.*, 1996) or of $[(C_5Ph_5)Fe(CO)_2Br]$ and MeMgBr (55% yield; Connelly & Manners, 1989).

All four compounds, particularly phenyl compound **2**, showed a pale-blue fluorescence when irradiated at 365 nm.

3.1. Crystal structures

3.1.1. $[(C_5Ph_5)Fe(CO)_2Me]$, 1. Compound **1** crystallizes in the orthorhombic space group *Pbca* with one molecule in the asymmetric unit (Fig. 1).

The Fe—C(methyl) bond eclipses the cyclopentadienyl (Cp) C5—C501 bond, while the Fe1—C6 bond bisects the

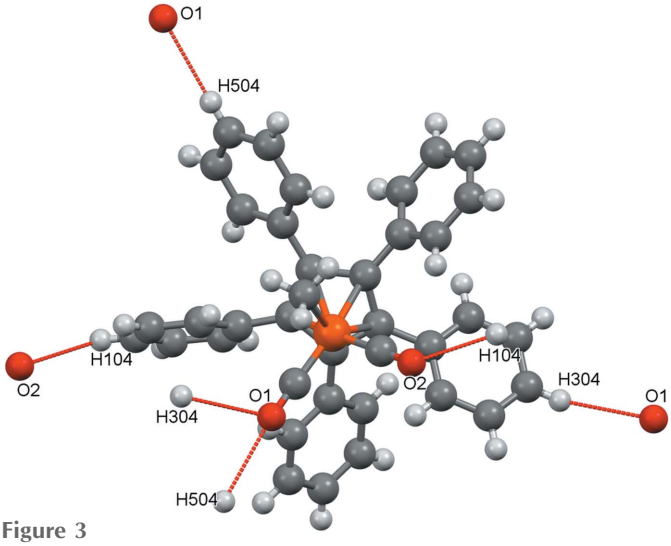


Figure 3
The nonclassical C—H···O contacts in compound **1**.

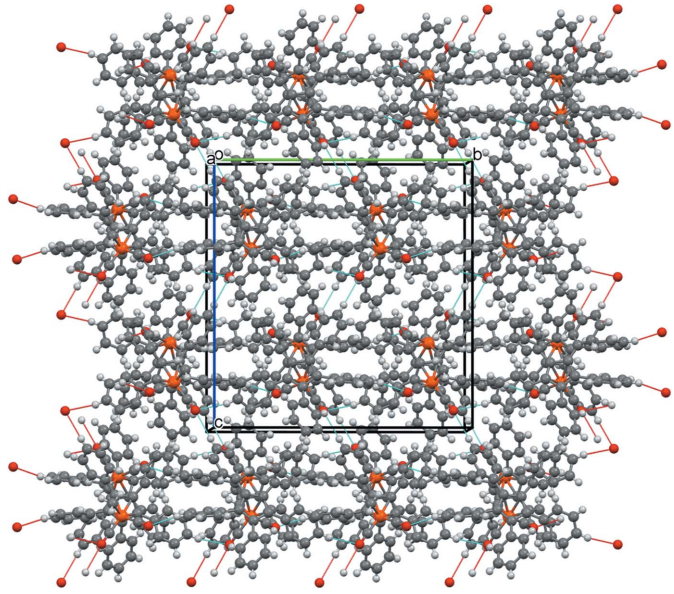


Figure 4
Packing diagram of compound **1**, viewed along the crystallographic *a* axis.

Table 3
Nonclassical C—H···O contacts in **1**–**4**.

Compound	Atom pair	Distance (Å)	Symmetry code
1	H504···O1	2.597	$-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$
	H104···O2	2.611	$-x+\frac{1}{2}, y-\frac{1}{2}, z$
	O1···H304	2.703	$-x+\frac{1}{2}, y-\frac{1}{2}, z$
2	O1···H404	2.475	$-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$
3	H14···O2	2.694	$-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$
	H56···O1	2.430	$-x+1, -y+2, -z+1$
4	O2···H504	2.589	$-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$

cyclopentadienyl C1—C2 bond. All the phenyl rings are canted in the same way, as usual, with angles between the planes of the cyclopentadienyl and phenyl rings ranging from 37.80 (9) to 58.66 (9)°. The Cp ring is essentially planar, with a sigpln parameter of *PLATON*, defined as:

$$\sqrt{\sum_{j=1}^{N} \frac{D_j^2}{(N-3)}},$$

of 0.023 (Spek, 2020). Table 2 collects some important bond parameters for compounds **1**–**4**, together with the corresponding data from the other four published structures containing the $[(C_5Ph_5)Fe(CO)_2]$ moiety. *PLATON* analysis of the crystal structure showed that 6.3% of the volume contained solvent-accessible voids. A *PLATON* cavity plot (see Fig. 2) shows that the dumbbell-shaped voids are arranged in an fcc-type (fcc is face-centred cubic) lattice.

When looking at intermolecular interactions in mercury, some 'nonclassical' C—H···O contacts [for the concept of C—H···O contacts, see Desiraju (2005)] appear (Fig. 3). Atom O1 accepts hydrogen bonds from H304 and H305, while atom O2 accepts a hydrogen bond from H104 (see Table 3 for the hydrogen-bond distances).

These contacts 'join' individual molecules in all directions, leading to the packing shown in Fig. 4.

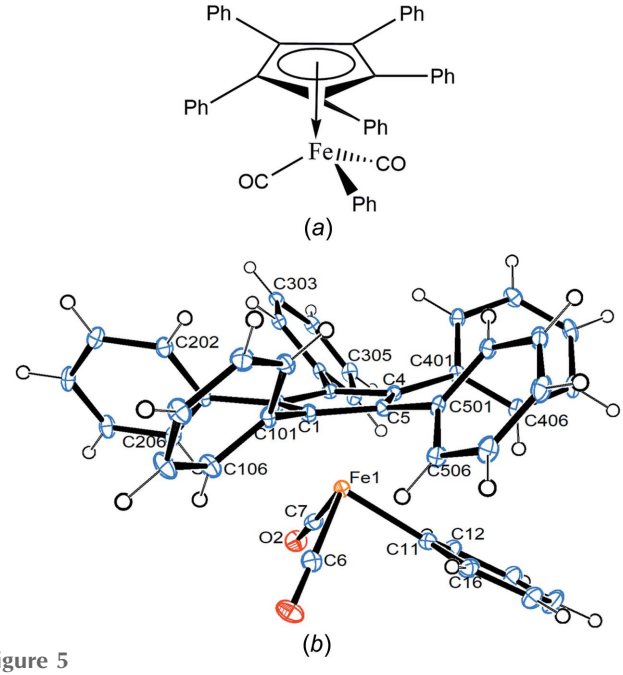


Figure 5
Displacement ellipsoid plot (side view) of compound **2**, with ellipsoids drawn at the 30% probability level.

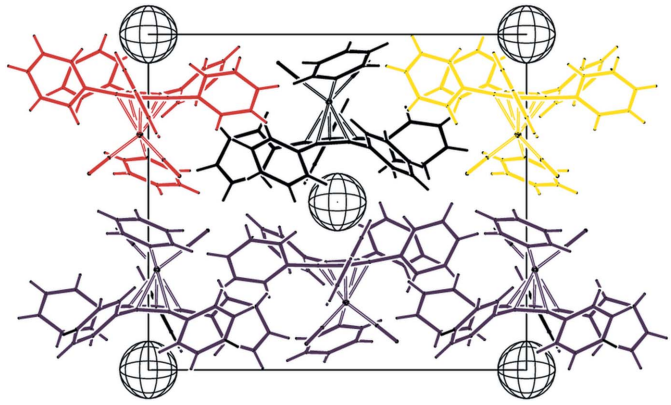


Figure 6
PLATON (Spek, 2020) cavity plot of compound **2**.

3.1.2. $[(C_5Ph_5)Fe(CO)_2Ph]$, **2**. Compound **2** crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit (Fig. 5 shows a side view).

The iron–phenyl bond Fe1—C11 nearly bisects the cyclopentadienyl C4—C5 bond. As usual, the phenyl rings exhibit a chiral propeller arrangement (but, of course, in a centrosymmetric space group like $P2_1/n$, both enantiomers are present), with interplanar Cp–Ph angles ranging from 30.41 (12) to 59.17 (12)°. The Cp ring is essentially planar, with sigpln = 0.008. The five *ipso*-C atoms of the phenyl rings are all situated on the distal side of the Cp ring, with distances from the ring plane ranging from 0.147 (2) to 0.224 (2) Å. The σ-phenyl ring lies approximately perpendicular to the plane containing the Cp ring centroid, the Fe atom and the α-phenyl C atom, with light 'bending' at the α-phenyl C atom [Fe1—C11···C14 = 174.3 (2)°].

The closest structural 'relative' to **2** that can be found in the literature is CECKUS01 $[(C_5Me_5)Fe(CO)_2Ph]$ (Kalman *et al.*, 2013). There, the iron–phenyl bond length is 2.002 (2) Å. As in **2**, the σ-phenyl ring is oriented perpendicular to the plane defined by the Cp centroid, the Fe atom and the α-phenyl C atom, with a slight bend at the α-phenyl C atom.

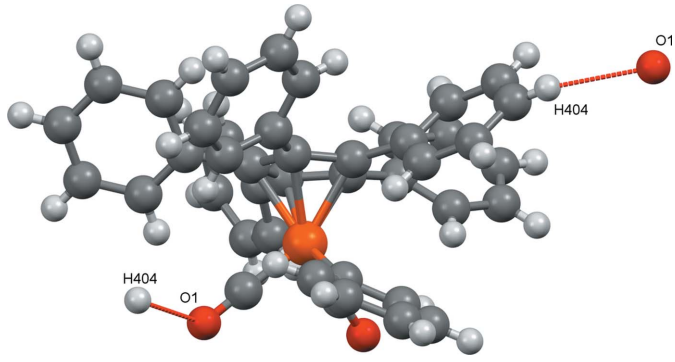


Figure 7
The nonclassical C—H···O contacts in compound **2**.

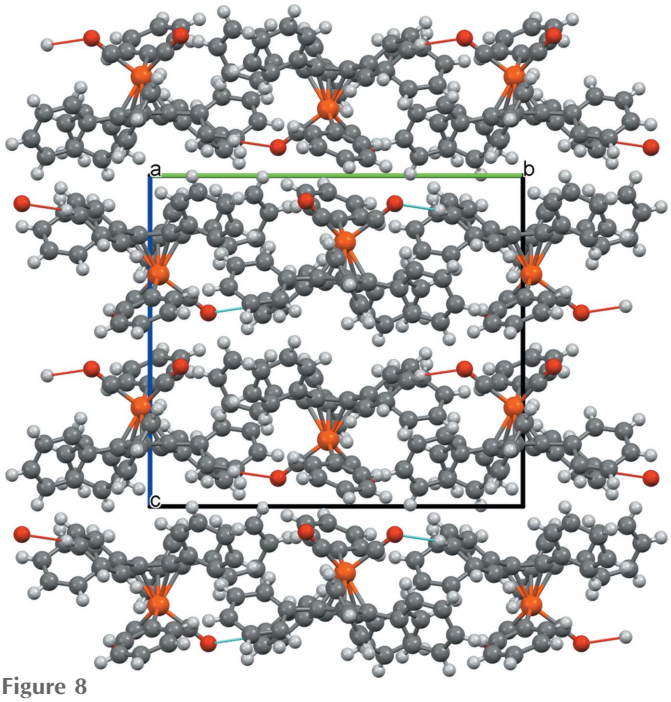


Figure 8
Packing diagram of compound **2**, viewed along the crystallographic *a* direction.

A *PLATON* (Spek, 2020) analysis of the crystal structure shows solvent-accessible voids of only 22 Å^3 (0.7%). A cavity plot (Fig. 6) shows a 'body-centred' arrangement of these small spherical voids (radius 1.28 Å each), that appear to be 'sandwiched' by two cyclopentadienyl rings.

As observed for compound **1**, there are also C—H···O contacts in compound **2** (Fig. 7). However, here only atom O1 is involved in a contact with H404. The individual molecules are 'aligned' by these contacts in the *a* and *b* directions (Fig. 8).

3.1.3. [(C$_5$Ph$_5$)Fe(CO)$_2$iPr], 3. Compound **3** also crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit (Fig. 9 shows a top view).

The iron–isopropyl bond Fe—C8 eclipses the exocyclic cyclopentadienyl C2—C21 bond, while the Fe—C6O1 bond bisects the cyclopentadienyl C3—C4 bond. Again, all the phenyl rings show a paddle-wheel orientation, with interplanar angles ranging from 43.72 (8) and 60.94 (8)°. The cyclopentadienyl ring deviates slightly from planarity, with a sigpln parameter of 0.030. All the phenyl-ring *ipso*-C atoms are located on the distal side of the Cp ring, with distances from the plane ranging from 0.056 (1) to 0.279 (1) Å. *PLATON* (Spek, 2020) analysis of the crystal structure shows solvent-accessible voids of only 18 Å^3 (0.6%). A cavity plot (Fig. 10) again shows a body-centred arrangement of the small spherical voids (radius 1.26 Å).

There are intra- and intermolecular C—H···O contacts involving both carbonyl O atoms (Fig. 11). By means of these contacts, the individual molecules are connected in all directions (Fig. 12).

3.1.4. [(C$_5$Ph$_5$)Fe(CO)$_2$Bu], 4. Compound **4** also crystallizes in the monoclinic space group $P2_1/n$, with one molecule in the asymmetric unit (Fig. 13 shows a side view).

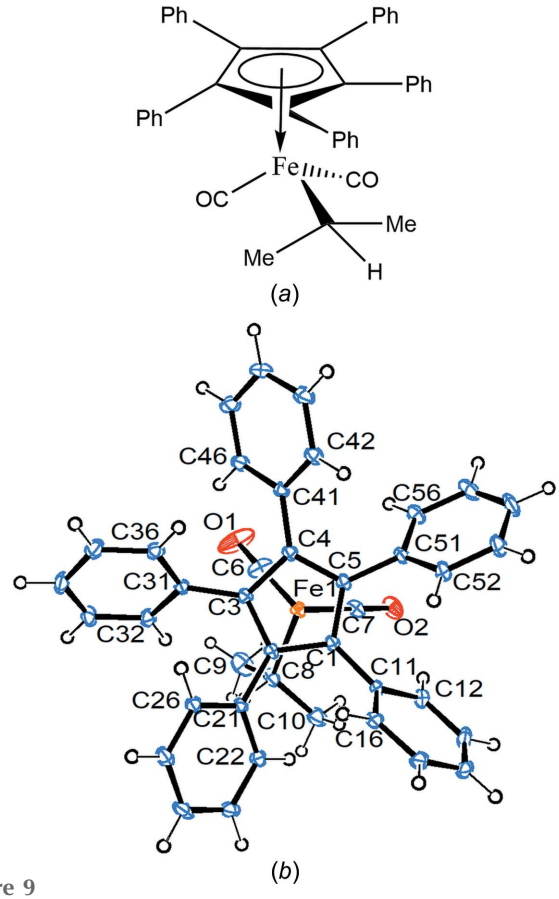


Figure 9
Displacement ellipsoid plot (top view) of compound **3**, with ellipsoids drawn at the 30% probability level.

The iron–butyl bond bisects the cyclopentadienyl C4—C5 bond, while both iron–carbonyl bonds, Fe—C6 and Fe—C7, eclipse the exocyclic cyclopentadienyl C1—C101 and C3—C301 bonds, respectively. The C_α—C_β bond of the butyl group only deviates slightly from the plane bisecting the Fe(CO)$_2$ unit. All the phenyl rings adopt a paddle-wheel orientation, with interplanar angles ranging from 42.85 (8) to 59.68 (7)°. The Cp ring is planar, with a sigpln parameter of 0.017. All

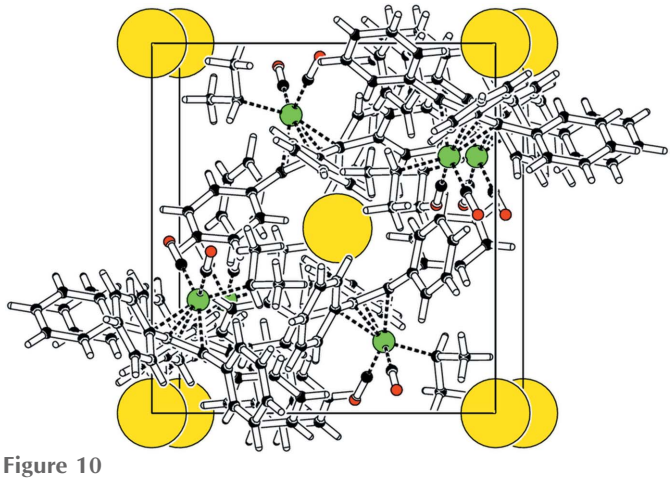


Figure 10
PLATON (Spek, 2020) cavity plot of compound **3**.

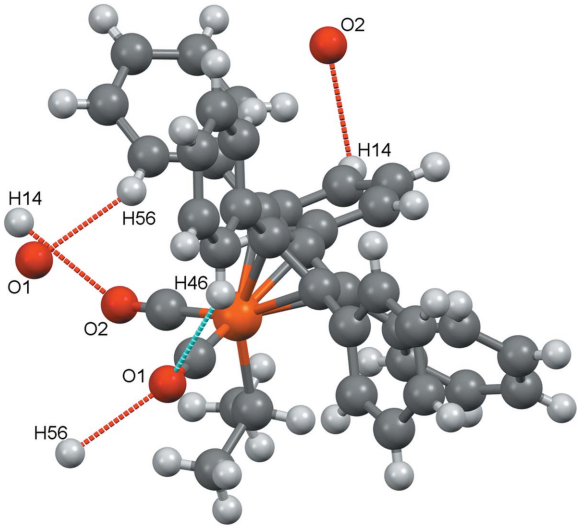


Figure 11
The nonclassical C—H···O contacts in compound **3**.

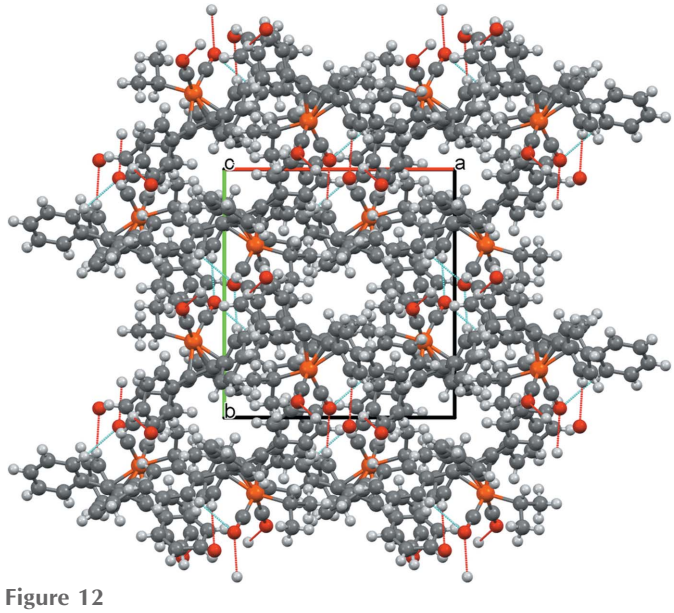


Figure 12
Packing diagram of compound **3**, viewed along the crystallographic *c* direction.

phenyl *ipso*-C atoms are located on the distal side of the Cp ring, with distances from the plane ranging from 0.098 (1) to 0.237 (1) Å. A *PLATON* analysis (Spek, 2020) of the crystal structure shows essentially no solvent-accessible voids.

The closest structural 'relative' of **4** that can be found in the literature is $[(C_5Me_5)Fe(CO)_2(n\text{-}C_5H_{11})]$ (CSD refcode HOZWIC; Hill *et al.*, 1999). There, the Fe—C_α(alkyl) bond has a length of 2.069 (10) Å. Similar to **4**, the C_α—C_β bond of the pentyl moiety bisects the $Fe(CO)_2$ moiety, but in contrast to **4**, all the C—C bonds of the alkyl group are in a *transoid* orientation.

As with the other structures reported here, there are also C—H···O contacts in compound **4**, but only atom O2 is involved (see Fig. 14). The individual molecules are connected in the *a* and *b* directions *via* these contacts (Fig. 15).

3.2. Comparison of the structures of 1–4 with each other and with some other $[C_5Ph_5]$ complexes

Table 2 collects some important bond parameters of pentaphenylcyclopentadienyl complexes, including the IR carbonyl stretching frequencies. The Fe—centroid distances (Fe—Ct) fall into three groups. The shortest bond can be found in anionic $[(C_5Ph_5)Fe(CO)_2][PPN]$ (CSD refcode PUYDES; Carter *et al.*, 2002), with a value of 1.715 Å; a medium bond length of *ca* 1.74 Å is formed by **1** and the cationoid $[(C_5Ph_5)Fe(CO)_2Br]$ (SIRMIP; Field *et al.*, 1989), $[(C_5Ph_5)Fe(CO)_2(FBF_3)]$ (MARFET; Hemming *et al.*, 2018) and $[(C_5Ph_5)Fe(CO)_2(H_2O)]BF_4$ (MARFIX; Hemming *et al.*, 2018); and the longest bond of *ca* 1.76 Å is found for **2**–**4**. The C—O bond lengths of the metal carbonyls can also be divided in three groups. The shortest C—O bonds are found for the bromide complex, with a value of 1.07 (3) Å, an intermediate bond of 1.14 (1) Å is found for **1**–**4** and the tetrafluoroborate and aqua complexes, and the longest bond of 1.185 (3) Å is found for the anionic complex. This parallels the information obtained from the IR carbonyl frequencies: the highest ν(CO) value is observed for the bromide complex and the lowest frequencies are obtained for the anionic complex. Considering bond strengths, apparently the strongest metal–Cp bond and the strongest back donation to the carbonyl ligands is found for the anionic complex, which is not unexpected. In addition, the relative order of the C—O bond lengths (shorter/stronger for the cationoid complexes in comparison with the more 'neutral' complexes) is in agreement with generally accepted

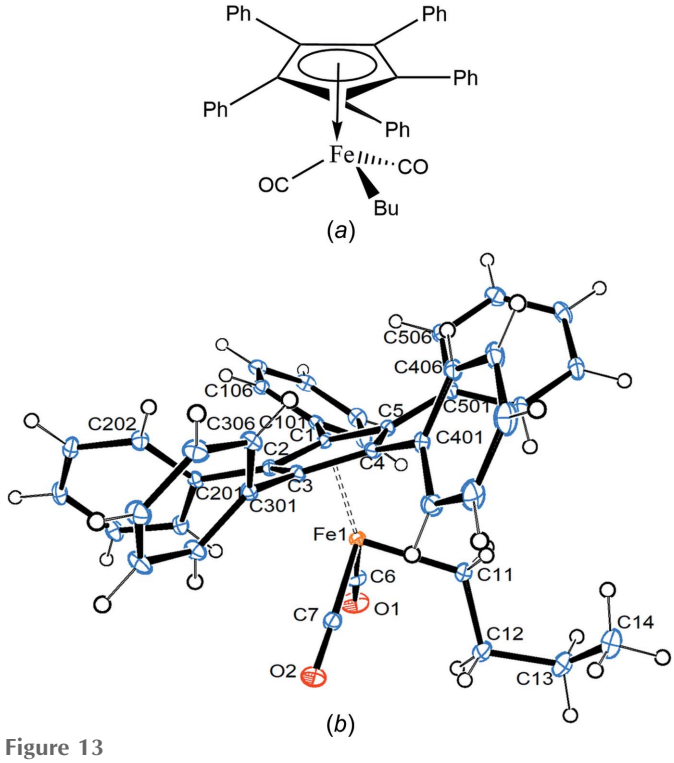


Figure 13
Displacement ellipsoid plot (side view) of compound **1**, with ellipsoids drawn at the 30% probability level.

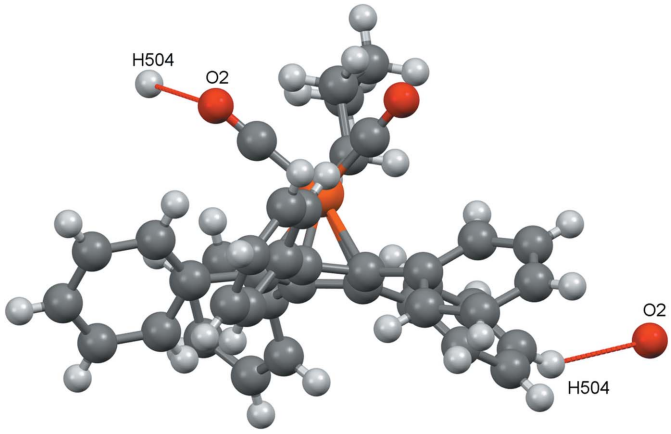


Figure 14
The nonclassical C—H···O contacts in compound **4**.

bonding concepts. The only deviation from this trend is apparently the rather high ν(CO) frequency observed for phenyl compound **2**, which is not paralleled in the crystal structure C—O bond length. However, the relative order of the Fe—Ct distances is less dictated by electronic than by steric requirements. This is also reflected in the metal–carbon bond lengths (Fe—C_R) to the alkyl or aryl residues. While the relatively short Fe—C(phenyl) bond might indicate some back donation into the aromatic ring system [compare the same tendency in the pair Cp*Fe(CO)$_2$C$_5$H$_{11}$/C$_6$H$_5$], the other Fe—C_R bonds are ordered according to the increasing steric demand of the alkyl moiety. The deviation of the phenyl *ipso*-C atoms from the cyclopentadienyl ring plane is smallest for methyl complex **1**, largest for phenyl complex **2** and intermediate for all the other compounds of Table 2. The average 'canting' angle is smallest for phenyl compound **2** and largest for the bromide compound. The other compounds can be divided into two groups: an angle of 50.4 (2)° is found for **1**, **3** and **4**, and an angle of 52.4 (10)° is found for the rest. The extrema might be explained by the large size of bromine, forcing the phenyl rings into a more perpendicular orientation with respect to the cyclopentadienyl ring, and on the near perpendicular orientation of the σ-phenyl ring with respect to the plane defined by Ct—Fe—C$_\alpha$, which forces the other phenyl rings into a 'flatter' orientation.

When comparing the 'nonclassical' C—H···O interactions, it appears that nearly always the *para* H atom of one phenyl group is involved. The only exception to this 'rule' occurs in compound **3**, where two *ortho* H atoms are also involved. The observed distances are in the range 2.43–2.70 Å (Table 3). For comparison, such contacts are also observed in [(C$_5$Ph$_5$)Fe(CO)$_2$Br] (2.69 Å) and in [(C$_5$Ph$_5$)Fe(CO)$_2$(H$_2$O)]BF$_4$ (2.534 Å). In the anionic complex [PPN][(C$_5$Ph$_5$)Fe(CO)$_2$], only C—H···O contacts occur with the phenyl rings of the PPN$^+$ cation.

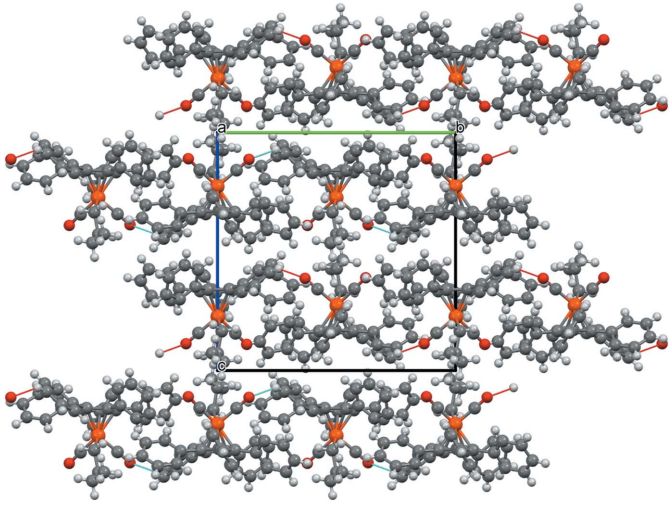


Figure 15
Packing diagram of compound **4**, viewed along the crystallographic *a* direction.

4. Conclusion

Four pentaphenylcyclopentadienyl iron alkyl and aryl complexes were prepared *via* a new route and characterized by IR, NMR and UV spectroscopy, and by X-ray crystallography. The molecular structures show the longest distances between the Fe atom and the cyclopentadienyl ring reported so far. The Fe—C(alkyl and aryl) bonds and the C—O bonds are in the same ranges as found for other compounds of this type. All compounds show a pale-blue solid-state fluorescence, which has not been described before for this type of compound. The fact that the phenyl compound shows a much stronger solid-state fluorescence than the others cannot be derived from the bond parameters. Despite this, all the compounds obviously interact with light and might be of use for DNA cleavage reactions. This is, however, beyond the scope of this study.

Acknowledgements

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supporting information

Acta Cryst. (2021). C**77**, 374-382 [https://doi.org/10.1107/S2053229621006057]

Molecular structures of the pentaphenylcyclopentadienyl iron complexes $[(C_5Ph_5)Fe(CO)_2R]$ (*R* = Me, Ph, iPr and Bu)

Karlheinz Sünkel and Christian Klein-Hessling

Computing details

For all structures, data collection: *APEX2* (Bruker, 2011); cell refinement: *APEX2* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2011); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2020) and *WinGX* (Farrugia, 2012).

Dicarbonylmethyl(η^5-pentaphenylcyclopentadienyl)iron (compd-1)

Crystal data

$[Fe(CH_3)(C_{35}H_{25})(CO)_2]$
M_r = 572.45
Orthorhombic, *Pbca*
a = 13.6393 (3) Å
b = 20.4360 (5) Å
c = 21.1978 (5) Å
V = 5908.5 (2) Å^3
Z = 8
F(000) = 2384
D_x = 1.287 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 9987 reflections
θ = 2.6–27.5°
μ = 0.54 mm^{-1}
T = 105 K
Block, brown
0.06 × 0.05 × 0.04 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.391 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.718, T_{max} = 0.746
61228 measured reflections
6765 independent reflections
5439 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −17→17
k = −26→26
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.06
6765 reflections
371 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 4.2957P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.37682 (12)	0.59963 (8)	0.30454 (8)	0.0147 (3)
C2	0.39675 (12)	0.65428 (8)	0.34615 (8)	0.0155 (3)
C3	0.36342 (12)	0.71238 (8)	0.31556 (8)	0.0150 (3)
C4	0.32506 (12)	0.69423 (8)	0.25424 (8)	0.0151 (3)
C5	0.33648 (12)	0.62477 (8)	0.24718 (8)	0.0142 (3)
C6	0.20994 (14)	0.59950 (9)	0.39146 (9)	0.0230 (4)
C7	0.16177 (13)	0.70981 (9)	0.35113 (9)	0.0223 (4)
C10	0.12282 (14)	0.60934 (10)	0.28236 (9)	0.0271 (4)
H10A	0.140202	0.566911	0.263946	0.041*
H10B	0.101259	0.639108	0.248876	0.041*
H10C	0.069641	0.603426	0.312926	0.041*
C101	0.40372 (12)	0.53019 (8)	0.31622 (7)	0.0152 (3)
C102	0.33482 (13)	0.47999 (8)	0.31259 (8)	0.0191 (4)
H102	0.267726	0.490162	0.305614	0.023*
C103	0.36376 (14)	0.41499 (9)	0.31915 (8)	0.0224 (4)
H103	0.316409	0.380977	0.316894	0.027*
C104	0.46177 (15)	0.39992 (9)	0.32897 (8)	0.0229 (4)
H104	0.481612	0.355530	0.332721	0.027*
C105	0.53075 (14)	0.44948 (9)	0.33332 (8)	0.0216 (4)
H105	0.597809	0.439086	0.340131	0.026*
C106	0.50173 (13)	0.51446 (8)	0.32770 (8)	0.0173 (3)
H106	0.548930	0.548388	0.331696	0.021*
C201	0.45262 (12)	0.65138 (8)	0.40618 (8)	0.0162 (3)
C202	0.43646 (13)	0.60253 (9)	0.45131 (8)	0.0195 (4)
H202	0.386610	0.570823	0.444600	0.023*
C203	0.49288 (14)	0.60012 (9)	0.50587 (8)	0.0227 (4)
H203	0.481837	0.566528	0.536023	0.027*
C204	0.56530 (14)	0.64658 (10)	0.51650 (9)	0.0242 (4)
H204	0.603014	0.645203	0.554155	0.029*
C205	0.58241 (13)	0.69495 (9)	0.47204 (9)	0.0233 (4)
H205	0.631990	0.726757	0.479155	0.028*
C206	0.52692 (13)	0.69692 (9)	0.41694 (8)	0.0195 (4)
H206	0.539841	0.729706	0.386281	0.023*
C301	0.36893 (12)	0.77994 (8)	0.34182 (8)	0.0164 (3)
C302	0.34005 (13)	0.79307 (9)	0.40373 (8)	0.0210 (4)
H302	0.314161	0.758830	0.429060	0.025*
C303	0.34877 (14)	0.85577 (9)	0.42876 (9)	0.0258 (4)
H303	0.329104	0.864096	0.470996	0.031*
C304	0.38610 (14)	0.90603 (9)	0.39210 (10)	0.0279 (4)

H304	0.391811	0.948876	0.409092	0.034*
C305	0.41507 (14)	0.89371 (9)	0.33065 (10)	0.0259 (4)
H305	0.440747	0.928148	0.305481	0.031*
C306	0.40665 (13)	0.83090 (9)	0.30562 (9)	0.0208 (4)
H306	0.426855	0.822782	0.263450	0.025*
C401	0.29641 (12)	0.74027 (8)	0.20307 (8)	0.0167 (3)
C402	0.21648 (14)	0.78238 (9)	0.20753 (9)	0.0226 (4)
H402	0.175744	0.781049	0.243862	0.027*
C403	0.19573 (16)	0.82634 (9)	0.15933 (10)	0.0298 (4)
H403	0.141215	0.855020	0.163018	0.036*
C404	0.25409 (16)	0.82852 (10)	0.10599 (9)	0.0302 (4)
H404	0.239837	0.858689	0.073144	0.036*
C405	0.33345 (15)	0.78651 (9)	0.10067 (9)	0.0279 (4)
H405	0.373477	0.787702	0.064005	0.033*
C406	0.35456 (13)	0.74261 (9)	0.14894 (9)	0.0216 (4)
H406	0.409069	0.713954	0.145027	0.026*
C501	0.31740 (12)	0.58676 (8)	0.18883 (8)	0.0150 (3)
C502	0.23958 (13)	0.60131 (8)	0.14830 (8)	0.0180 (3)
H502	0.195688	0.635739	0.158762	0.022*
C503	0.22546 (14)	0.56613 (9)	0.09292 (8)	0.0221 (4)
H503	0.171512	0.576187	0.066277	0.026*
C504	0.28959 (15)	0.51655 (9)	0.07640 (8)	0.0235 (4)
H504	0.279675	0.492483	0.038595	0.028*
C505	0.36850 (14)	0.50215 (9)	0.11537 (8)	0.0216 (4)
H505	0.413369	0.468667	0.103844	0.026*
C506	0.38194 (13)	0.53655 (8)	0.17107 (8)	0.0178 (3)
H506	0.435715	0.525960	0.197659	0.021*
O1	0.18451 (11)	0.56829 (7)	0.43347 (7)	0.0378 (4)
O2	0.10615 (11)	0.74773 (7)	0.36704 (7)	0.0346 (3)
Fe1	0.24425 (2)	0.64866 (2)	0.32754 (2)	0.01420 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0143 (7)	0.0142 (8)	0.0155 (7)	−0.0008 (6)	0.0003 (6)	0.0004 (6)
C2	0.0148 (8)	0.0157 (8)	0.0160 (8)	−0.0024 (6)	0.0015 (6)	0.0005 (6)
C3	0.0141 (8)	0.0141 (8)	0.0168 (8)	−0.0026 (6)	0.0006 (6)	0.0011 (6)
C4	0.0146 (8)	0.0140 (8)	0.0167 (8)	−0.0005 (6)	0.0009 (6)	−0.0002 (6)
C5	0.0131 (7)	0.0143 (7)	0.0153 (8)	−0.0012 (6)	0.0011 (6)	0.0007 (6)
C6	0.0207 (9)	0.0210 (9)	0.0272 (9)	0.0000 (7)	0.0027 (7)	0.0019 (8)
C7	0.0199 (9)	0.0203 (9)	0.0266 (9)	−0.0033 (7)	0.0010 (7)	0.0034 (7)
C10	0.0196 (9)	0.0398 (12)	0.0221 (9)	−0.0078 (8)	0.0002 (7)	−0.0119 (8)
C101	0.0196 (8)	0.0134 (8)	0.0124 (7)	0.0015 (6)	0.0010 (6)	0.0006 (6)
C102	0.0207 (9)	0.0176 (8)	0.0190 (8)	−0.0007 (7)	0.0001 (7)	−0.0008 (7)
C103	0.0310 (10)	0.0140 (8)	0.0221 (9)	−0.0035 (7)	0.0036 (8)	−0.0003 (7)
C104	0.0363 (10)	0.0146 (8)	0.0178 (8)	0.0071 (7)	0.0078 (8)	0.0025 (7)
C105	0.0234 (9)	0.0246 (9)	0.0167 (8)	0.0073 (7)	0.0030 (7)	0.0045 (7)
C106	0.0193 (8)	0.0197 (8)	0.0130 (7)	−0.0006 (7)	0.0010 (7)	0.0019 (7)

C201	0.0160 (8)	0.0160 (8)	0.0165 (8)	0.0027 (7)	−0.0004 (6)	−0.0027 (6)
C202	0.0223 (9)	0.0194 (9)	0.0168 (8)	−0.0010 (7)	0.0014 (7)	−0.0018 (7)
C203	0.0281 (10)	0.0253 (9)	0.0147 (8)	0.0042 (8)	0.0018 (7)	0.0012 (7)
C204	0.0228 (9)	0.0329 (10)	0.0169 (8)	0.0059 (8)	−0.0047 (7)	−0.0050 (8)
C205	0.0205 (9)	0.0243 (9)	0.0250 (9)	0.0008 (7)	−0.0045 (7)	−0.0065 (8)
C206	0.0189 (8)	0.0187 (8)	0.0210 (8)	0.0003 (7)	−0.0022 (7)	−0.0005 (7)
C301	0.0128 (8)	0.0159 (8)	0.0205 (8)	−0.0002 (6)	−0.0034 (6)	−0.0014 (7)
C302	0.0213 (9)	0.0189 (8)	0.0228 (9)	−0.0015 (7)	0.0005 (7)	−0.0022 (7)
C303	0.0249 (9)	0.0241 (9)	0.0284 (10)	0.0016 (8)	−0.0012 (8)	−0.0092 (8)
C304	0.0250 (10)	0.0173 (9)	0.0415 (11)	0.0013 (8)	−0.0071 (9)	−0.0101 (8)
C305	0.0259 (10)	0.0160 (9)	0.0359 (11)	−0.0042 (7)	−0.0044 (8)	0.0016 (8)
C306	0.0199 (9)	0.0182 (8)	0.0243 (9)	−0.0030 (7)	−0.0026 (7)	0.0011 (7)
C401	0.0190 (8)	0.0130 (8)	0.0181 (8)	−0.0031 (7)	−0.0037 (7)	−0.0004 (6)
C402	0.0262 (9)	0.0180 (9)	0.0235 (9)	0.0031 (7)	−0.0006 (7)	0.0005 (7)
C403	0.0343 (11)	0.0197 (9)	0.0355 (11)	0.0068 (8)	−0.0071 (9)	0.0047 (8)
C404	0.0412 (12)	0.0203 (9)	0.0290 (10)	−0.0049 (9)	−0.0111 (9)	0.0113 (8)
C405	0.0335 (11)	0.0267 (10)	0.0234 (9)	−0.0088 (8)	0.0001 (8)	0.0078 (8)
C406	0.0202 (8)	0.0202 (9)	0.0243 (9)	−0.0019 (7)	−0.0005 (7)	0.0026 (7)
C501	0.0163 (8)	0.0138 (7)	0.0149 (8)	−0.0020 (6)	−0.0002 (6)	0.0009 (6)
C502	0.0193 (8)	0.0157 (8)	0.0190 (8)	0.0006 (7)	−0.0013 (7)	0.0004 (6)
C503	0.0238 (9)	0.0241 (9)	0.0183 (8)	−0.0010 (7)	−0.0057 (7)	0.0017 (7)
C504	0.0322 (10)	0.0222 (9)	0.0160 (8)	−0.0011 (8)	−0.0022 (7)	−0.0044 (7)
C505	0.0269 (9)	0.0180 (9)	0.0199 (9)	0.0037 (7)	0.0031 (7)	−0.0032 (7)
C506	0.0189 (8)	0.0173 (8)	0.0172 (8)	0.0007 (7)	−0.0019 (7)	0.0004 (7)
O1	0.0389 (9)	0.0389 (9)	0.0357 (8)	−0.0018 (7)	0.0091 (7)	0.0162 (7)
O2	0.0290 (8)	0.0257 (7)	0.0490 (9)	0.0044 (6)	0.0115 (7)	−0.0048 (7)
Fe1	0.01451 (12)	0.01253 (12)	0.01557 (12)	−0.00121 (9)	0.00088 (9)	−0.00036 (9)

Geometric parameters (Å, º)

C1—C5	1.430 (2)	C203—H203	0.9500
C1—C2	1.449 (2)	C204—C205	1.386 (3)
C1—C101	1.486 (2)	C204—H204	0.9500
C1—Fe1	2.1240 (16)	C205—C206	1.392 (2)
C2—C3	1.427 (2)	C205—H205	0.9500
C2—C201	1.484 (2)	C206—H206	0.9500
C2—Fe1	2.1202 (16)	C301—C306	1.392 (2)
C3—C4	1.450 (2)	C301—C302	1.396 (2)
C3—C301	1.490 (2)	C302—C303	1.392 (2)
C3—Fe1	2.0981 (16)	C302—H302	0.9500
C4—C5	1.436 (2)	C303—C304	1.385 (3)
C4—C401	1.488 (2)	C303—H303	0.9500
C4—Fe1	2.1205 (16)	C304—C305	1.384 (3)
C5—C501	1.484 (2)	C304—H304	0.9500
C5—Fe1	2.1731 (16)	C305—C306	1.394 (2)
C6—O1	1.149 (2)	C305—H305	0.9500
C6—Fe1	1.7506 (19)	C306—H306	0.9500
C7—O2	1.136 (2)	C401—C402	1.392 (2)

C7—Fe1	1.7542 (19)	C401—C406	1.396 (2)
C10—Fe1	2.0751 (18)	C402—C403	1.390 (3)
C10—H10A	0.9800	C402—H402	0.9500
C10—H10B	0.9800	C403—C404	1.384 (3)
C10—H10C	0.9800	C403—H403	0.9500
C101—C102	1.393 (2)	C404—C405	1.386 (3)
C101—C106	1.396 (2)	C404—H404	0.9500
C102—C103	1.393 (2)	C405—C406	1.391 (3)
C102—H102	0.9500	C405—H405	0.9500
C103—C104	1.387 (3)	C406—H406	0.9500
C103—H103	0.9500	C501—C502	1.397 (2)
C104—C105	1.385 (3)	C501—C506	1.403 (2)
C104—H104	0.9500	C502—C503	1.390 (2)
C105—C106	1.391 (2)	C502—H502	0.9500
C105—H105	0.9500	C503—C504	1.384 (3)
C106—H106	0.9500	C503—H503	0.9500
C201—C206	1.395 (2)	C504—C505	1.388 (3)
C201—C202	1.400 (2)	C504—H504	0.9500
C202—C203	1.390 (2)	C505—C506	1.386 (2)
C202—H202	0.9500	C505—H505	0.9500
C203—C204	1.388 (3)	C506—H506	0.9500

C5—C1—C2	108.23 (14)	C303—C302—H302	119.6
C5—C1—C101	125.42 (15)	C301—C302—H302	119.6
C2—C1—C101	126.03 (14)	C304—C303—C302	120.02 (18)
C5—C1—Fe1	72.43 (9)	C304—C303—H303	120.0
C2—C1—Fe1	69.90 (9)	C302—C303—H303	120.0
C101—C1—Fe1	128.48 (12)	C305—C304—C303	119.87 (17)
C3—C2—C1	107.76 (14)	C305—C304—H304	120.1
C3—C2—C201	125.89 (15)	C303—C304—H304	120.1
C1—C2—C201	125.97 (15)	C304—C305—C306	120.14 (18)
C3—C2—Fe1	69.39 (9)	C304—C305—H305	119.9
C1—C2—Fe1	70.18 (9)	C306—C305—H305	119.9
C201—C2—Fe1	131.37 (12)	C301—C306—C305	120.64 (18)
C2—C3—C4	108.03 (14)	C301—C306—H306	119.7
C2—C3—C301	125.80 (15)	C305—C306—H306	119.7
C4—C3—C301	126.16 (14)	C402—C401—C406	118.66 (16)
C2—C3—Fe1	71.06 (9)	C402—C401—C4	123.16 (15)
C4—C3—Fe1	70.74 (9)	C406—C401—C4	118.15 (15)
C301—C3—Fe1	124.67 (12)	C403—C402—C401	120.61 (18)
C5—C4—C3	107.89 (14)	C403—C402—H402	119.7
C5—C4—C401	125.28 (15)	C401—C402—H402	119.7
C3—C4—C401	125.93 (14)	C404—C403—C402	120.30 (19)
C5—C4—Fe1	72.45 (9)	C404—C403—H403	119.8
C3—C4—Fe1	69.07 (9)	C402—C403—H403	119.8
C401—C4—Fe1	132.48 (12)	C403—C404—C405	119.72 (17)
C1—C5—C4	107.96 (14)	C403—C404—H404	120.1
C1—C5—C501	126.04 (14)	C405—C404—H404	120.1

C4—C5—C501	125.83 (15)	C404—C405—C406	120.08 (18)
C1—C5—Fe1	68.72 (9)	C404—C405—H405	120.0
C4—C5—Fe1	68.50 (9)	C406—C405—H405	120.0
C501—C5—Fe1	132.04 (11)	C405—C406—C401	120.62 (17)
O1—C6—Fe1	177.75 (18)	C405—C406—H406	119.7
O2—C7—Fe1	177.60 (17)	C401—C406—H406	119.7
Fe1—C10—H10A	109.5	C502—C501—C506	117.85 (15)
Fe1—C10—H10B	109.5	C502—C501—C5	122.30 (15)
H10A—C10—H10B	109.5	C506—C501—C5	119.76 (15)
Fe1—C10—H10C	109.5	C503—C502—C501	120.96 (16)
H10A—C10—H10C	109.5	C503—C502—H502	119.5
H10B—C10—H10C	109.5	C501—C502—H502	119.5
C102—C101—C106	119.07 (15)	C504—C503—C502	120.32 (16)
C102—C101—C1	121.81 (15)	C504—C503—H503	119.8
C106—C101—C1	119.02 (15)	C502—C503—H503	119.8
C103—C102—C101	120.37 (17)	C503—C504—C505	119.66 (16)
C103—C102—H102	119.8	C503—C504—H504	120.2
C101—C102—H102	119.8	C505—C504—H504	120.2
C104—C103—C102	119.98 (17)	C506—C505—C504	120.12 (16)
C104—C103—H103	120.0	C506—C505—H505	119.9
C102—C103—H103	120.0	C504—C505—H505	119.9
C105—C104—C103	120.13 (16)	C505—C506—C501	121.08 (16)
C105—C104—H104	119.9	C505—C506—H506	119.5
C103—C104—H104	119.9	C501—C506—H506	119.5
C104—C105—C106	119.93 (17)	C6—Fe1—C7	90.96 (9)
C104—C105—H105	120.0	C6—Fe1—C10	85.51 (9)
C106—C105—H105	120.0	C7—Fe1—C10	84.00 (8)
C105—C106—C101	120.48 (16)	C6—Fe1—C3	131.07 (8)
C105—C106—H106	119.8	C7—Fe1—C3	95.11 (7)
C101—C106—H106	119.8	C10—Fe1—C3	143.40 (7)
C206—C201—C202	118.57 (15)	C6—Fe1—C2	98.59 (8)
C206—C201—C2	119.12 (15)	C7—Fe1—C2	122.51 (8)
C202—C201—C2	122.24 (15)	C10—Fe1—C2	152.86 (7)
C203—C202—C201	120.44 (17)	C3—Fe1—C2	39.54 (6)
C203—C202—H202	119.8	C6—Fe1—C4	163.38 (8)
C201—C202—H202	119.8	C7—Fe1—C4	103.26 (7)
C204—C203—C202	120.31 (17)	C10—Fe1—C4	104.29 (7)
C204—C203—H203	119.8	C3—Fe1—C4	40.19 (6)
C202—C203—H203	119.8	C2—Fe1—C4	66.59 (6)
C205—C204—C203	119.82 (17)	C6—Fe1—C1	97.73 (7)
C205—C204—H204	120.1	C7—Fe1—C1	161.34 (7)
C203—C204—H204	120.1	C10—Fe1—C1	113.01 (7)
C204—C205—C206	119.97 (17)	C3—Fe1—C1	66.77 (6)
C204—C205—H205	120.0	C2—Fe1—C1	39.92 (6)
C206—C205—H205	120.0	C4—Fe1—C1	66.20 (6)
C205—C206—C201	120.86 (17)	C6—Fe1—C5	129.24 (7)
C205—C206—H206	119.6	C7—Fe1—C5	139.00 (7)
C201—C206—H206	119.6	C10—Fe1—C5	90.76 (7)

C306—C301—C302	118.59 (16)	C3—Fe1—C5	66.18 (6)
C306—C301—C3	120.39 (15)	C2—Fe1—C5	65.80 (6)
C302—C301—C3	120.98 (15)	C4—Fe1—C5	39.05 (6)
C303—C302—C301	120.73 (17)	C1—Fe1—C5	38.86 (6)
C5—C1—C2—C3	3.22 (18)	C1—C2—C201—C206	131.06 (18)
C101—C1—C2—C3	176.97 (15)	Fe1—C2—C201—C206	−134.30 (15)
Fe1—C1—C2—C3	−59.45 (11)	C3—C2—C201—C202	142.10 (17)
C5—C1—C2—C201	−169.99 (15)	C1—C2—C201—C202	−45.9 (2)
C101—C1—C2—C201	3.8 (3)	Fe1—C2—C201—C202	48.8 (2)
Fe1—C1—C2—C201	127.34 (16)	C206—C201—C202—C203	0.6 (2)
C5—C1—C2—Fe1	62.67 (11)	C2—C201—C202—C203	177.59 (16)
C101—C1—C2—Fe1	−123.58 (17)	C201—C202—C203—C204	0.6 (3)
C1—C2—C3—C4	−1.47 (18)	C202—C203—C204—C205	−1.0 (3)
C201—C2—C3—C4	171.75 (15)	C203—C204—C205—C206	0.1 (3)
Fe1—C2—C3—C4	−61.41 (11)	C204—C205—C206—C201	1.2 (3)
C1—C2—C3—C301	179.55 (15)	C202—C201—C206—C205	−1.5 (3)
C201—C2—C3—C301	−7.2 (3)	C2—C201—C206—C205	−178.60 (16)
Fe1—C2—C3—C301	119.60 (16)	C2—C3—C301—C306	131.01 (18)
C1—C2—C3—Fe1	59.95 (11)	C4—C3—C301—C306	−47.8 (2)
C201—C2—C3—Fe1	−126.83 (16)	Fe1—C3—C301—C306	−138.28 (14)
C2—C3—C4—C5	−0.82 (18)	C2—C3—C301—C302	−46.5 (2)
C301—C3—C4—C5	178.16 (15)	C4—C3—C301—C302	134.67 (18)
Fe1—C3—C4—C5	−62.44 (11)	Fe1—C3—C301—C302	44.2 (2)
C2—C3—C4—C401	−170.37 (15)	C306—C301—C302—C303	0.0 (3)
C301—C3—C4—C401	8.6 (3)	C3—C301—C302—C303	177.59 (16)
Fe1—C3—C4—C401	128.00 (16)	C301—C302—C303—C304	0.2 (3)
C2—C3—C4—Fe1	61.62 (11)	C302—C303—C304—C305	−0.3 (3)
C301—C3—C4—Fe1	−119.40 (17)	C303—C304—C305—C306	0.1 (3)
C2—C1—C5—C4	−3.73 (18)	C302—C301—C306—C305	−0.2 (3)
C101—C1—C5—C4	−177.52 (15)	C3—C301—C306—C305	−177.81 (16)
Fe1—C1—C5—C4	57.33 (11)	C304—C305—C306—C301	0.2 (3)
C2—C1—C5—C501	171.69 (15)	C5—C4—C401—C402	124.51 (19)
C101—C1—C5—C501	−2.1 (3)	C3—C4—C401—C402	−67.7 (2)
Fe1—C1—C5—C501	−127.26 (16)	Fe1—C4—C401—C402	26.1 (2)
C2—C1—C5—Fe1	−61.06 (11)	C5—C4—C401—C406	−57.6 (2)
C101—C1—C5—Fe1	125.15 (17)	C3—C4—C401—C406	110.21 (19)
C3—C4—C5—C1	2.82 (18)	Fe1—C4—C401—C406	−156.05 (13)
C401—C4—C5—C1	172.45 (15)	C406—C401—C402—C403	−0.7 (3)
Fe1—C4—C5—C1	−57.46 (11)	C4—C401—C402—C403	177.19 (17)
C3—C4—C5—C501	−172.61 (15)	C401—C402—C403—C404	0.4 (3)
C401—C4—C5—C501	−3.0 (3)	C402—C403—C404—C405	0.1 (3)
Fe1—C4—C5—C501	127.11 (16)	C403—C404—C405—C406	−0.4 (3)
C3—C4—C5—Fe1	60.28 (11)	C404—C405—C406—C401	0.0 (3)
C401—C4—C5—Fe1	−130.08 (16)	C402—C401—C406—C405	0.5 (3)
C5—C1—C101—C102	−59.9 (2)	C4—C401—C406—C405	−177.50 (16)
C2—C1—C101—C102	127.41 (18)	C1—C5—C501—C502	147.57 (17)
Fe1—C1—C101—C102	35.4 (2)	C4—C5—C501—C502	−37.8 (2)

C5—C1—C101—C106	116.52 (19)	Fe1—C5—C501—C502	54.6 (2)
C2—C1—C101—C106	−56.2 (2)	C1—C5—C501—C506	−36.0 (2)
Fe1—C1—C101—C106	−148.20 (13)	C4—C5—C501—C506	138.64 (17)
C106—C101—C102—C103	−1.2 (2)	Fe1—C5—C501—C506	−128.94 (15)
C1—C101—C102—C103	175.19 (16)	C506—C501—C502—C503	1.4 (2)
C101—C102—C103—C104	−0.4 (3)	C5—C501—C502—C503	177.91 (16)
C102—C103—C104—C105	1.1 (3)	C501—C502—C503—C504	−1.1 (3)
C103—C104—C105—C106	−0.1 (3)	C502—C503—C504—C505	−0.2 (3)
C104—C105—C106—C101	−1.5 (2)	C503—C504—C505—C506	1.1 (3)
C102—C101—C106—C105	2.2 (2)	C504—C505—C506—C501	−0.8 (3)
C1—C101—C106—C105	−174.35 (15)	C502—C501—C506—C505	−0.5 (2)
C3—C2—C201—C206	−40.9 (2)	C5—C501—C506—C505	−177.09 (16)

Dicarbonyl(η^5-pentaphenylcyclopentadienyl)phenyliron (compd-2)

Crystal data

$[Fe(C_6H_5)(C_{35}H_{25})(CO)_2]$
$M_r = 634.52$
Monoclinic, $P2_1/n$
$a = 12.1860$ (4) Å
$b = 16.9411$ (6) Å
$c = 15.0691$ (6) Å
$\beta = 93.320$ (1)°
$V = 3105.71$ (19) Å^3
$Z = 4$
$F(000) = 1320$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9920 reflections
$\theta = 2.7$–$26.4°$
$\mu = 0.52$ mm^{-1}
$T = 105$ K
Rod, yellow
0.08 × 0.02 × 0.02 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.391 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.669$, $T_{max} = 0.745$
31592 measured reflections
6352 independent reflections
5025 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.9°$
$h = -15\rightarrow14$
$k = -21\rightarrow21$
$l = -18\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.088$
$S = 1.04$
6352 reflections
415 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 3.2346P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.51430 (17)	0.41526 (12)	0.67825 (14)	0.0151 (4)
C2	0.58867 (16)	0.47964 (12)	0.68908 (14)	0.0146 (4)
C3	0.52471 (17)	0.55089 (12)	0.68962 (14)	0.0141 (4)
C4	0.41025 (16)	0.53041 (12)	0.67969 (13)	0.0136 (4)
C5	0.40380 (16)	0.44551 (12)	0.67353 (14)	0.0137 (4)
C6	0.51341 (19)	0.39573 (14)	0.86803 (16)	0.0219 (5)
C7	0.55900 (19)	0.54035 (13)	0.87419 (15)	0.0217 (5)
C11	0.35145 (18)	0.49501 (13)	0.86829 (15)	0.0198 (5)
C12	0.32867 (19)	0.56776 (14)	0.90712 (16)	0.0234 (5)
H12	0.381951	0.608656	0.906319	0.028*
C13	0.2305 (2)	0.58204 (16)	0.94684 (18)	0.0320 (6)
H13	0.217626	0.632230	0.972376	0.038*
C14	0.1516 (2)	0.52401 (17)	0.94948 (18)	0.0348 (6)
H14	0.083720	0.534105	0.975309	0.042*
C15	0.1732 (2)	0.45034 (15)	0.91363 (17)	0.0294 (6)
H15	0.120005	0.409429	0.915421	0.035*
C16	0.27212 (18)	0.43651 (14)	0.87527 (15)	0.0220 (5)
H16	0.286297	0.385286	0.852966	0.026*
C101	0.54613 (17)	0.33194 (12)	0.65979 (14)	0.0147 (4)
C102	0.50261 (17)	0.29643 (12)	0.58201 (14)	0.0167 (5)
H102	0.449561	0.323825	0.545005	0.020*
C103	0.53606 (18)	0.22142 (13)	0.55815 (15)	0.0200 (5)
H103	0.505680	0.197761	0.505098	0.024*
C104	0.61335 (19)	0.18106 (13)	0.61124 (16)	0.0216 (5)
H104	0.636721	0.129927	0.594607	0.026*
C105	0.6565 (2)	0.21561 (13)	0.68886 (16)	0.0249 (5)
H105	0.708980	0.187730	0.725954	0.030*
C106	0.62367 (18)	0.29089 (13)	0.71289 (15)	0.0206 (5)
H106	0.654432	0.314356	0.765923	0.025*
C201	0.71062 (17)	0.47448 (12)	0.68737 (14)	0.0151 (4)
C202	0.75535 (18)	0.44018 (13)	0.61354 (15)	0.0193 (5)
H202	0.707813	0.418926	0.567380	0.023*
C203	0.86791 (18)	0.43661 (13)	0.60647 (16)	0.0222 (5)
H203	0.897094	0.413373	0.555526	0.027*
C204	0.93826 (18)	0.46697 (13)	0.67376 (16)	0.0228 (5)
H204	1.015591	0.464829	0.668957	0.027*
C205	0.89509 (18)	0.50025 (13)	0.74760 (17)	0.0238 (5)
H205	0.943020	0.520498	0.794103	0.029*
C206	0.78185 (18)	0.50441 (13)	0.75454 (16)	0.0200 (5)

H206	0.753021	0.527848	0.805522	0.024*
C301	0.56873 (17)	0.63255 (12)	0.68749 (14)	0.0146 (4)
C302	0.64470 (17)	0.65157 (13)	0.62483 (14)	0.0165 (5)
H302	0.674713	0.610995	0.590090	0.020*
C303	0.67661 (18)	0.72939 (13)	0.61302 (15)	0.0188 (5)
H303	0.728402	0.741751	0.570357	0.023*
C304	0.63314 (18)	0.78920 (13)	0.66329 (16)	0.0216 (5)
H304	0.653611	0.842563	0.654154	0.026*
C305	0.55957 (18)	0.77044 (13)	0.72698 (16)	0.0222 (5)
H305	0.530776	0.811029	0.762393	0.027*
C306	0.52785 (18)	0.69276 (13)	0.73921 (15)	0.0190 (5)
H306	0.477810	0.680502	0.783259	0.023*
C401	0.31727 (17)	0.58652 (12)	0.66370 (14)	0.0153 (4)
C402	0.32838 (18)	0.64702 (13)	0.60196 (15)	0.0186 (5)
H402	0.396049	0.653287	0.574471	0.022*
C403	0.24202 (19)	0.69811 (13)	0.58019 (16)	0.0231 (5)
H403	0.250745	0.738910	0.537921	0.028*
C404	0.14308 (19)	0.68966 (13)	0.62004 (16)	0.0239 (5)
H404	0.083685	0.724398	0.605023	0.029*
C405	0.13130 (18)	0.63036 (13)	0.68181 (16)	0.0230 (5)
H405	0.063940	0.625152	0.710010	0.028*
C406	0.21712 (17)	0.57817 (13)	0.70314 (15)	0.0185 (5)
H406	0.207461	0.536846	0.744578	0.022*
C501	0.30530 (17)	0.39683 (12)	0.64965 (14)	0.0146 (4)
C502	0.23184 (17)	0.42020 (13)	0.57996 (15)	0.0169 (5)
H502	0.240297	0.470264	0.552794	0.020*
C503	0.14665 (17)	0.37086 (13)	0.55012 (15)	0.0197 (5)
H503	0.097295	0.387236	0.502553	0.024*
C504	0.13320 (18)	0.29777 (14)	0.58938 (16)	0.0230 (5)
H504	0.074776	0.264046	0.568986	0.028*
C505	0.20563 (18)	0.27431 (13)	0.65860 (16)	0.0215 (5)
H505	0.196882	0.224220	0.685638	0.026*
C506	0.29075 (18)	0.32343 (12)	0.68865 (15)	0.0174 (5)
H506	0.339693	0.306823	0.736378	0.021*
O1	0.53289 (15)	0.34343 (10)	0.91514 (12)	0.0311 (4)
O2	0.60742 (14)	0.58192 (10)	0.92221 (11)	0.0295 (4)
Fe1	0.48631 (2)	0.47746 (2)	0.79864 (2)	0.01477 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0144 (10)	0.0148 (10)	0.0161 (11)	0.0000 (9)	0.0009 (9)	0.0003 (8)
C2	0.0136 (10)	0.0135 (10)	0.0165 (11)	−0.0012 (9)	0.0003 (8)	−0.0017 (9)
C3	0.0152 (10)	0.0127 (10)	0.0143 (11)	−0.0010 (8)	0.0013 (8)	0.0003 (8)
C4	0.0147 (10)	0.0124 (10)	0.0139 (10)	−0.0006 (8)	0.0016 (8)	0.0006 (8)
C5	0.0135 (10)	0.0131 (10)	0.0144 (11)	−0.0006 (8)	0.0000 (8)	0.0001 (8)
C6	0.0208 (12)	0.0213 (12)	0.0232 (13)	−0.0036 (10)	−0.0020 (10)	−0.0034 (10)
C7	0.0242 (12)	0.0217 (12)	0.0197 (12)	−0.0001 (10)	0.0047 (10)	0.0023 (10)

C11	0.0205 (11)	0.0217 (12)	0.0171 (11)	−0.0001 (9)	0.0008 (9)	0.0024 (9)
C12	0.0237 (12)	0.0220 (12)	0.0248 (13)	−0.0025 (10)	0.0044 (10)	0.0009 (10)
C13	0.0317 (14)	0.0295 (14)	0.0357 (15)	0.0046 (12)	0.0104 (12)	−0.0049 (12)
C14	0.0288 (13)	0.0394 (15)	0.0379 (15)	0.0009 (12)	0.0169 (12)	0.0025 (13)
C15	0.0246 (13)	0.0322 (14)	0.0318 (14)	−0.0079 (11)	0.0048 (11)	0.0067 (11)
C16	0.0233 (12)	0.0216 (12)	0.0215 (12)	−0.0015 (10)	0.0036 (10)	0.0034 (10)
C101	0.0115 (10)	0.0114 (10)	0.0210 (12)	−0.0015 (8)	0.0007 (9)	0.0005 (9)
C102	0.0155 (10)	0.0158 (11)	0.0187 (11)	0.0004 (9)	−0.0005 (9)	0.0018 (9)
C103	0.0218 (11)	0.0195 (11)	0.0186 (12)	−0.0015 (10)	−0.0004 (9)	−0.0041 (9)
C104	0.0252 (12)	0.0124 (11)	0.0270 (13)	0.0041 (9)	−0.0008 (10)	−0.0014 (9)
C105	0.0269 (13)	0.0164 (11)	0.0301 (14)	0.0063 (10)	−0.0081 (10)	−0.0001 (10)
C106	0.0225 (12)	0.0167 (11)	0.0217 (12)	0.0016 (9)	−0.0054 (10)	−0.0035 (9)
C201	0.0155 (10)	0.0085 (9)	0.0213 (11)	0.0005 (9)	0.0005 (8)	0.0023 (9)
C202	0.0170 (11)	0.0178 (11)	0.0230 (12)	−0.0007 (9)	−0.0006 (9)	−0.0010 (9)
C203	0.0197 (11)	0.0205 (12)	0.0271 (13)	0.0016 (10)	0.0061 (10)	−0.0030 (10)
C204	0.0121 (10)	0.0180 (11)	0.0384 (14)	0.0000 (9)	0.0036 (10)	−0.0012 (10)
C205	0.0152 (11)	0.0219 (12)	0.0339 (14)	−0.0014 (9)	−0.0033 (10)	−0.0052 (10)
C206	0.0177 (11)	0.0172 (11)	0.0250 (12)	−0.0008 (9)	0.0021 (9)	−0.0044 (9)
C301	0.0119 (10)	0.0119 (10)	0.0195 (11)	0.0005 (8)	−0.0028 (8)	0.0001 (8)
C302	0.0143 (10)	0.0167 (11)	0.0182 (11)	0.0013 (9)	−0.0019 (9)	0.0001 (9)
C303	0.0163 (11)	0.0205 (11)	0.0192 (12)	−0.0028 (9)	−0.0022 (9)	0.0047 (9)
C304	0.0216 (12)	0.0117 (11)	0.0304 (13)	−0.0032 (9)	−0.0070 (10)	0.0020 (9)
C305	0.0219 (12)	0.0144 (11)	0.0300 (13)	0.0014 (9)	−0.0002 (10)	−0.0063 (10)
C306	0.0166 (11)	0.0178 (11)	0.0228 (12)	−0.0010 (9)	0.0035 (9)	−0.0017 (9)
C401	0.0147 (10)	0.0104 (10)	0.0205 (11)	−0.0004 (8)	−0.0009 (9)	−0.0039 (9)
C402	0.0153 (11)	0.0166 (11)	0.0240 (12)	−0.0017 (9)	0.0013 (9)	−0.0008 (9)
C403	0.0258 (12)	0.0155 (11)	0.0274 (13)	0.0017 (10)	−0.0035 (10)	0.0031 (10)
C404	0.0188 (11)	0.0173 (11)	0.0345 (14)	0.0062 (9)	−0.0062 (10)	−0.0045 (10)
C405	0.0141 (11)	0.0205 (12)	0.0344 (14)	0.0015 (9)	0.0018 (10)	−0.0063 (10)
C406	0.0164 (11)	0.0162 (11)	0.0231 (12)	−0.0002 (9)	0.0023 (9)	−0.0011 (9)
C501	0.0117 (10)	0.0137 (10)	0.0187 (11)	−0.0006 (8)	0.0044 (8)	−0.0030 (9)
C502	0.0148 (10)	0.0150 (10)	0.0212 (12)	0.0020 (9)	0.0028 (9)	−0.0016 (9)
C503	0.0127 (10)	0.0264 (12)	0.0200 (12)	0.0013 (9)	0.0006 (9)	−0.0055 (10)
C504	0.0157 (11)	0.0238 (12)	0.0295 (13)	−0.0062 (10)	0.0030 (10)	−0.0081 (10)
C505	0.0192 (11)	0.0149 (11)	0.0307 (13)	−0.0037 (9)	0.0052 (10)	−0.0017 (10)
C506	0.0165 (11)	0.0147 (11)	0.0213 (12)	−0.0004 (9)	0.0019 (9)	−0.0001 (9)
O1	0.0411 (11)	0.0209 (9)	0.0303 (10)	0.0000 (8)	−0.0069 (8)	0.0063 (8)
O2	0.0310 (10)	0.0299 (10)	0.0271 (10)	−0.0079 (8)	−0.0020 (8)	−0.0064 (8)
Fe1	0.01461 (15)	0.01271 (15)	0.01687 (16)	−0.00087 (13)	0.00001 (12)	0.00030 (13)

Geometric parameters (Å, º)

C1—C2	1.421 (3)	C201—C202	1.394 (3)
C1—C5	1.439 (3)	C202—C203	1.383 (3)
C1—C101	1.494 (3)	C202—H202	0.9500
C1—Fe1	2.142 (2)	C203—C204	1.388 (3)
C2—C3	1.437 (3)	C203—H203	0.9500
C2—C201	1.490 (3)	C204—C205	1.379 (3)

C2—Fe1	2.126 (2)	C204—H204	0.9500
C3—C4	1.437 (3)	C205—C206	1.392 (3)
C3—C301	1.485 (3)	C205—H205	0.9500
C3—Fe1	2.134 (2)	C206—H206	0.9500
C4—C5	1.443 (3)	C301—C306	1.393 (3)
C4—C401	1.488 (3)	C301—C302	1.398 (3)
C4—Fe1	2.164 (2)	C302—C303	1.389 (3)
C5—C501	1.483 (3)	C302—H302	0.9500
C5—Fe1	2.154 (2)	C303—C304	1.388 (3)
C6—O1	1.151 (3)	C303—H303	0.9500
C6—Fe1	1.755 (2)	C304—C305	1.388 (3)
C7—O2	1.148 (3)	C304—H304	0.9500
C7—Fe1	1.761 (2)	C305—C306	1.387 (3)
C11—C16	1.393 (3)	C305—H305	0.9500
C11—C12	1.399 (3)	C306—H306	0.9500
C11—Fe1	2.023 (2)	C401—C406	1.395 (3)
C12—C13	1.390 (3)	C401—C402	1.396 (3)
C12—H12	0.9500	C402—C403	1.387 (3)
C13—C14	1.377 (4)	C402—H402	0.9500
C13—H13	0.9500	C403—C404	1.385 (3)
C14—C15	1.391 (4)	C403—H403	0.9500
C14—H14	0.9500	C404—C405	1.383 (3)
C15—C16	1.387 (3)	C404—H404	0.9500
C15—H15	0.9500	C405—C406	1.393 (3)
C16—H16	0.9500	C405—H405	0.9500
C101—C106	1.389 (3)	C406—H406	0.9500
C101—C102	1.395 (3)	C501—C506	1.391 (3)
C102—C103	1.388 (3)	C501—C502	1.397 (3)
C102—H102	0.9500	C502—C503	1.387 (3)
C103—C104	1.381 (3)	C502—H502	0.9500
C103—H103	0.9500	C503—C504	1.386 (3)
C104—C105	1.384 (3)	C503—H503	0.9500
C104—H104	0.9500	C504—C505	1.385 (3)
C105—C106	1.391 (3)	C504—H504	0.9500
C105—H105	0.9500	C505—C506	1.385 (3)
C106—H106	0.9500	C505—H505	0.9500
C201—C206	1.390 (3)	C506—H506	0.9500

C2—C1—C5	108.73 (18)	C201—C206—H206	119.8
C2—C1—C101	125.15 (18)	C205—C206—H206	119.8
C5—C1—C101	125.42 (19)	C306—C301—C302	118.78 (19)
C2—C1—Fe1	69.94 (12)	C306—C301—C3	121.92 (19)
C5—C1—Fe1	70.86 (12)	C302—C301—C3	118.92 (19)
C101—C1—Fe1	132.69 (15)	C303—C302—C301	120.4 (2)
C1—C2—C3	107.62 (17)	C303—C302—H302	119.8
C1—C2—C201	125.64 (19)	C301—C302—H302	119.8
C3—C2—C201	126.23 (19)	C304—C303—C302	120.3 (2)
C1—C2—Fe1	71.16 (12)	C304—C303—H303	119.9

C3—C2—Fe1	70.58 (12)	C302—C303—H303	119.9
C201—C2—Fe1	130.00 (15)	C305—C304—C303	119.5 (2)
C4—C3—C2	108.68 (18)	C305—C304—H304	120.2
C4—C3—C301	124.93 (18)	C303—C304—H304	120.2
C2—C3—C301	125.85 (18)	C306—C305—C304	120.4 (2)
C4—C3—Fe1	71.61 (12)	C306—C305—H305	119.8
C2—C3—Fe1	70.00 (12)	C304—C305—H305	119.8
C301—C3—Fe1	130.95 (15)	C305—C306—C301	120.6 (2)
C3—C4—C5	107.23 (17)	C305—C306—H306	119.7
C3—C4—C401	126.03 (18)	C301—C306—H306	119.7
C5—C4—C401	126.03 (18)	C406—C401—C402	118.64 (19)
C3—C4—Fe1	69.34 (12)	C406—C401—C4	122.89 (19)
C5—C4—Fe1	70.08 (12)	C402—C401—C4	118.33 (19)
C401—C4—Fe1	133.19 (15)	C403—C402—C401	120.9 (2)
C1—C5—C4	107.73 (18)	C403—C402—H402	119.5
C1—C5—C501	123.77 (18)	C401—C402—H402	119.5
C4—C5—C501	127.59 (18)	C404—C403—C402	120.0 (2)
C1—C5—Fe1	70.01 (12)	C404—C403—H403	120.0
C4—C5—Fe1	70.87 (12)	C402—C403—H403	120.0
C501—C5—Fe1	133.02 (15)	C405—C404—C403	119.6 (2)
O1—C6—Fe1	178.1 (2)	C405—C404—H404	120.2
O2—C7—Fe1	178.7 (2)	C403—C404—H404	120.2
C16—C11—C12	116.1 (2)	C404—C405—C406	120.7 (2)
C16—C11—Fe1	121.54 (17)	C404—C405—H405	119.6
C12—C11—Fe1	122.23 (17)	C406—C405—H405	119.6
C13—C12—C11	122.0 (2)	C405—C406—C401	120.1 (2)
C13—C12—H12	119.0	C405—C406—H406	120.0
C11—C12—H12	119.0	C401—C406—H406	120.0
C14—C13—C12	120.5 (2)	C506—C501—C502	118.62 (19)
C14—C13—H13	119.7	C506—C501—C5	121.04 (19)
C12—C13—H13	119.7	C502—C501—C5	119.93 (19)
C13—C14—C15	118.8 (2)	C503—C502—C501	120.5 (2)
C13—C14—H14	120.6	C503—C502—H502	119.7
C15—C14—H14	120.6	C501—C502—H502	119.7
C16—C15—C14	120.1 (2)	C504—C503—C502	120.3 (2)
C16—C15—H15	119.9	C504—C503—H503	119.8
C14—C15—H15	119.9	C502—C503—H503	119.8
C15—C16—C11	122.4 (2)	C505—C504—C503	119.5 (2)
C15—C16—H16	118.8	C505—C504—H504	120.3
C11—C16—H16	118.8	C503—C504—H504	120.3
C106—C101—C102	118.76 (19)	C504—C505—C506	120.4 (2)
C106—C101—C1	122.75 (19)	C504—C505—H505	119.8
C102—C101—C1	118.28 (19)	C506—C505—H505	119.8
C103—C102—C101	120.6 (2)	C505—C506—C501	120.7 (2)
C103—C102—H102	119.7	C505—C506—H506	119.7
C101—C102—H102	119.7	C501—C506—H506	119.7
C104—C103—C102	120.3 (2)	C6—Fe1—C7	91.25 (10)
C104—C103—H103	119.9	C6—Fe1—C11	86.40 (10)

C102—C103—H103	119.9	C7—Fe1—C11	88.22 (10)
C103—C104—C105	119.6 (2)	C6—Fe1—C2	112.19 (10)
C103—C104—H104	120.2	C7—Fe1—C2	101.29 (9)
C105—C104—H104	120.2	C11—Fe1—C2	158.62 (8)
C104—C105—C106	120.4 (2)	C6—Fe1—C3	151.22 (10)
C104—C105—H105	119.8	C7—Fe1—C3	91.18 (9)
C106—C105—H105	119.8	C11—Fe1—C3	122.33 (8)
C101—C106—C105	120.4 (2)	C2—Fe1—C3	39.42 (8)
C101—C106—H106	119.8	C6—Fe1—C1	94.75 (9)
C105—C106—H106	119.8	C7—Fe1—C1	138.28 (9)
C206—C201—C202	118.5 (2)	C11—Fe1—C1	133.30 (9)
C206—C201—C2	123.17 (19)	C2—Fe1—C1	38.90 (8)
C202—C201—C2	118.34 (19)	C3—Fe1—C1	65.29 (8)
C203—C202—C201	121.0 (2)	C6—Fe1—C5	112.68 (9)
C203—C202—H202	119.5	C7—Fe1—C5	155.52 (9)
C201—C202—H202	119.5	C11—Fe1—C5	97.99 (8)
C202—C203—C204	120.1 (2)	C2—Fe1—C5	65.78 (8)
C202—C203—H203	120.0	C3—Fe1—C5	65.46 (8)
C204—C203—H203	120.0	C1—Fe1—C5	39.13 (8)
C205—C204—C203	119.5 (2)	C6—Fe1—C4	151.32 (9)
C205—C204—H204	120.2	C7—Fe1—C4	117.39 (9)
C203—C204—H204	120.2	C11—Fe1—C4	92.70 (8)
C204—C205—C206	120.5 (2)	C2—Fe1—C4	65.93 (8)
C204—C205—H205	119.7	C3—Fe1—C4	39.04 (8)
C206—C205—H205	119.7	C1—Fe1—C4	65.42 (8)
C201—C206—C205	120.4 (2)	C5—Fe1—C4	39.05 (8)

C5—C1—C2—C3	−1.0 (2)	C102—C101—C106—C105	−0.3 (3)
C101—C1—C2—C3	169.8 (2)	C1—C101—C106—C105	−175.0 (2)
Fe1—C1—C2—C3	−61.51 (14)	C104—C105—C106—C101	0.7 (4)
C5—C1—C2—C201	−173.3 (2)	C1—C2—C201—C206	−127.2 (2)
C101—C1—C2—C201	−2.5 (3)	C3—C2—C201—C206	61.9 (3)
Fe1—C1—C2—C201	126.2 (2)	Fe1—C2—C201—C206	−32.5 (3)
C5—C1—C2—Fe1	60.51 (15)	C1—C2—C201—C202	54.8 (3)
C101—C1—C2—Fe1	−128.7 (2)	C3—C2—C201—C202	−116.0 (2)
C1—C2—C3—C4	0.4 (2)	Fe1—C2—C201—C202	149.59 (17)
C201—C2—C3—C4	172.6 (2)	C206—C201—C202—C203	−0.7 (3)
Fe1—C2—C3—C4	−61.49 (14)	C2—C201—C202—C203	177.3 (2)
C1—C2—C3—C301	−171.4 (2)	C201—C202—C203—C204	0.4 (3)
C201—C2—C3—C301	0.8 (3)	C202—C203—C204—C205	0.3 (3)
Fe1—C2—C3—C301	126.7 (2)	C203—C204—C205—C206	−0.8 (4)
C1—C2—C3—Fe1	61.88 (14)	C202—C201—C206—C205	0.2 (3)
C201—C2—C3—Fe1	−125.9 (2)	C2—C201—C206—C205	−177.7 (2)
C2—C3—C4—C5	0.4 (2)	C204—C205—C206—C201	0.5 (3)
C301—C3—C4—C5	172.3 (2)	C4—C3—C301—C306	50.4 (3)
Fe1—C3—C4—C5	−60.12 (14)	C2—C3—C301—C306	−139.1 (2)
C2—C3—C4—C401	−170.5 (2)	Fe1—C3—C301—C306	−45.2 (3)
C301—C3—C4—C401	1.5 (3)	C4—C3—C301—C302	−122.5 (2)

Fe1—C3—C4—C401	129.1 (2)	C2—C3—C301—C302	48.1 (3)
C2—C3—C4—Fe1	60.47 (14)	Fe1—C3—C301—C302	141.97 (18)
C301—C3—C4—Fe1	−127.6 (2)	C306—C301—C302—C303	−1.6 (3)
C2—C1—C5—C4	1.2 (2)	C3—C301—C302—C303	171.51 (19)
C101—C1—C5—C4	−169.5 (2)	C301—C302—C303—C304	−0.1 (3)
Fe1—C1—C5—C4	61.16 (14)	C302—C303—C304—C305	1.6 (3)
C2—C1—C5—C501	171.01 (19)	C303—C304—C305—C306	−1.3 (3)
C101—C1—C5—C501	0.3 (3)	C304—C305—C306—C301	−0.4 (3)
Fe1—C1—C5—C501	−129.1 (2)	C302—C301—C306—C305	1.8 (3)
C2—C1—C5—Fe1	−59.94 (15)	C3—C301—C306—C305	−171.0 (2)
C101—C1—C5—Fe1	129.3 (2)	C3—C4—C401—C406	−141.1 (2)
C3—C4—C5—C1	−1.0 (2)	C5—C4—C401—C406	49.8 (3)
C401—C4—C5—C1	169.8 (2)	Fe1—C4—C401—C406	−46.3 (3)
Fe1—C4—C5—C1	−60.61 (14)	C3—C4—C401—C402	43.3 (3)
C3—C4—C5—C501	−170.2 (2)	C5—C4—C401—C402	−125.8 (2)
C401—C4—C5—C501	0.6 (4)	Fe1—C4—C401—C402	138.14 (19)
Fe1—C4—C5—C501	130.1 (2)	C406—C401—C402—C403	0.2 (3)
C3—C4—C5—Fe1	59.65 (14)	C4—C401—C402—C403	176.0 (2)
C401—C4—C5—Fe1	−129.5 (2)	C401—C402—C403—C404	0.2 (3)
C16—C11—C12—C13	−2.8 (3)	C402—C403—C404—C405	0.3 (3)
Fe1—C11—C12—C13	173.10 (19)	C403—C404—C405—C406	−1.2 (3)
C11—C12—C13—C14	0.2 (4)	C404—C405—C406—C401	1.6 (3)
C12—C13—C14—C15	1.5 (4)	C402—C401—C406—C405	−1.0 (3)
C13—C14—C15—C16	−0.7 (4)	C4—C401—C406—C405	−176.6 (2)
C14—C15—C16—C11	−2.1 (4)	C1—C5—C501—C506	47.2 (3)
C12—C11—C16—C15	3.7 (3)	C4—C5—C501—C506	−145.1 (2)
Fe1—C11—C16—C15	−172.21 (18)	Fe1—C5—C501—C506	−46.3 (3)
C2—C1—C101—C106	54.3 (3)	C1—C5—C501—C502	−125.4 (2)
C5—C1—C101—C106	−136.5 (2)	C4—C5—C501—C502	42.2 (3)
Fe1—C1—C101—C106	−40.2 (3)	Fe1—C5—C501—C502	141.03 (18)
C2—C1—C101—C102	−120.3 (2)	C506—C501—C502—C503	−0.4 (3)
C5—C1—C101—C102	48.9 (3)	C5—C501—C502—C503	172.4 (2)
Fe1—C1—C101—C102	145.14 (18)	C501—C502—C503—C504	0.2 (3)
C106—C101—C102—C103	0.1 (3)	C502—C503—C504—C505	−0.1 (3)
C1—C101—C102—C103	174.9 (2)	C503—C504—C505—C506	0.2 (3)
C101—C102—C103—C104	−0.2 (3)	C504—C505—C506—C501	−0.3 (3)
C102—C103—C104—C105	0.6 (3)	C502—C501—C506—C505	0.4 (3)
C103—C104—C105—C106	−0.9 (4)	C5—C501—C506—C505	−172.3 (2)

Dicarbonyl(isopropyl)(η^5-pentaphenylcyclopentadienyl)iron (compd-3)

Crystal data

$[Fe(C_3H_7)(C_{35}H_{25})(CO)_2]$	V = 3047.6 (3) Å^3
M_r = 600.50	Z = 4
Monoclinic, $P2_1/n$	$F(000)$ = 1256
a = 12.5488 (7) Å	D_x = 1.309 Mg m^{-3}
b = 13.5046 (7) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
c = 18.0119 (11) Å	Cell parameters from 9881 reflections
β = 93.208 (2)°	θ = 2.7–27.1°

μ = 0.53 mm^{-1}
T = 110 K

Block, brown
0.06 × 0.04 × 0.03 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.391 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.719, T_{max} = 0.746

52953 measured reflections
6732 independent reflections
5995 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.1°, θ_{min} = 3.1°
h = −15→16
k = −17→17
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.088
S = 1.06
6732 reflections
390 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 2.212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.34805 (12)	0.66256 (11)	0.45764 (8)	0.0172 (3)
C2	0.34016 (12)	0.65122 (11)	0.53606 (8)	0.0168 (3)
C3	0.43556 (11)	0.69012 (10)	0.57258 (8)	0.0164 (3)
C4	0.50756 (12)	0.71857 (11)	0.51583 (8)	0.0177 (3)
C5	0.45259 (12)	0.70276 (11)	0.44536 (8)	0.0175 (3)
C6	0.41931 (15)	0.90205 (14)	0.56241 (12)	0.0371 (4)
C7	0.33642 (13)	0.88526 (12)	0.43146 (10)	0.0264 (3)
C8	0.21376 (13)	0.84627 (13)	0.54392 (9)	0.0271 (3)
H8	0.193058	0.792073	0.578096	0.032*
C9	0.20660 (18)	0.94269 (16)	0.58861 (13)	0.0450 (5)
H9A	0.226676	0.998732	0.557772	0.067*
H9B	0.255237	0.939047	0.633026	0.067*
H9C	0.133334	0.951793	0.603527	0.067*
C10	0.12829 (15)	0.84813 (17)	0.48138 (11)	0.0395 (5)
H10A	0.057777	0.847803	0.502168	0.059*
H10B	0.135574	0.789650	0.449843	0.059*
H10C	0.136121	0.908130	0.451571	0.059*
C11	0.27332 (11)	0.62098 (11)	0.39884 (8)	0.0177 (3)

C12	0.22872 (13)	0.67774 (13)	0.34035 (8)	0.0240 (3)
H12	0.242070	0.746944	0.338923	0.029*
C13	0.16478 (14)	0.63360 (14)	0.28406 (9)	0.0292 (4)
H13	0.133882	0.673149	0.244902	0.035*
C14	0.14581 (13)	0.53313 (14)	0.28453 (9)	0.0286 (4)
H14	0.103324	0.503327	0.245339	0.034*
C15	0.18898 (13)	0.47583 (13)	0.34239 (9)	0.0259 (3)
H15	0.175767	0.406582	0.343127	0.031*
C16	0.25169 (12)	0.51956 (12)	0.39949 (8)	0.0213 (3)
H16	0.280166	0.479930	0.439413	0.026*
C21	0.25569 (12)	0.59558 (11)	0.57294 (8)	0.0176 (3)
C22	0.14750 (12)	0.60281 (12)	0.55034 (9)	0.0220 (3)
H22	0.125195	0.647807	0.512013	0.026*
C23	0.07219 (13)	0.54420 (13)	0.58384 (9)	0.0265 (3)
H23	−0.001265	0.550464	0.568781	0.032*
C24	0.10369 (14)	0.47687 (13)	0.63893 (9)	0.0278 (4)
H24	0.052165	0.436772	0.661279	0.033*
C25	0.21085 (14)	0.46850 (12)	0.66117 (9)	0.0254 (3)
H25	0.232871	0.422406	0.698804	0.030*
C26	0.28625 (12)	0.52736 (11)	0.62856 (8)	0.0205 (3)
H26	0.359477	0.521144	0.644268	0.025*
C31	0.45797 (12)	0.68718 (11)	0.65463 (8)	0.0178 (3)
C32	0.38537 (13)	0.72724 (12)	0.70234 (9)	0.0229 (3)
H32	0.327198	0.765913	0.682656	0.028*
C33	0.39780 (14)	0.71079 (13)	0.77856 (9)	0.0281 (4)
H33	0.347589	0.737510	0.810663	0.034*
C34	0.48309 (15)	0.65562 (14)	0.80774 (9)	0.0309 (4)
H34	0.490388	0.643078	0.859670	0.037*
C35	0.55793 (14)	0.61865 (13)	0.76118 (9)	0.0277 (4)
H35	0.617740	0.582616	0.781438	0.033*
C36	0.54550 (12)	0.63428 (12)	0.68473 (9)	0.0214 (3)
H36	0.596882	0.608801	0.652977	0.026*
C41	0.62197 (12)	0.74559 (11)	0.52894 (8)	0.0188 (3)
C42	0.69780 (13)	0.69979 (12)	0.48608 (9)	0.0229 (3)
H42	0.674755	0.656376	0.446901	0.027*
C43	0.80646 (14)	0.71711 (14)	0.50019 (10)	0.0306 (4)
H43	0.856918	0.685881	0.470501	0.037*
C44	0.84104 (14)	0.77976 (15)	0.55740 (11)	0.0330 (4)
H44	0.915201	0.790803	0.567513	0.040*
C45	0.76703 (14)	0.82637 (14)	0.59993 (10)	0.0304 (4)
H45	0.790518	0.869962	0.638878	0.036*
C46	0.65853 (13)	0.80939 (12)	0.58562 (9)	0.0242 (3)
H46	0.608495	0.841806	0.614963	0.029*
C51	0.49636 (12)	0.71843 (11)	0.37098 (8)	0.0195 (3)
C52	0.48776 (13)	0.64331 (13)	0.31800 (9)	0.0235 (3)
H52	0.453240	0.582965	0.329230	0.028*
C53	0.52961 (14)	0.65629 (15)	0.24850 (9)	0.0327 (4)
H53	0.524011	0.604592	0.212725	0.039*

C54	0.57922 (15)	0.74423 (16)	0.23160 (10)	0.0373 (4)
H54	0.606519	0.753514	0.183951	0.045*
C55	0.58896 (15)	0.81866 (14)	0.28434 (11)	0.0355 (4)
H55	0.623971	0.878727	0.273037	0.043*
C56	0.54789 (14)	0.80606 (12)	0.35364 (10)	0.0263 (3)
H56	0.554969	0.857566	0.389496	0.032*
O1	0.45705 (14)	0.96355 (12)	0.59890 (13)	0.0716 (6)
O2	0.31839 (11)	0.93700 (10)	0.38174 (8)	0.0387 (3)
Fe1	0.36538 (2)	0.80613 (2)	0.50730 (2)	0.01815 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0199 (7)	0.0161 (7)	0.0159 (7)	−0.0005 (5)	0.0035 (5)	0.0007 (5)
C2	0.0188 (7)	0.0159 (7)	0.0160 (7)	0.0000 (5)	0.0027 (5)	0.0005 (5)
C3	0.0175 (7)	0.0147 (6)	0.0173 (7)	−0.0003 (5)	0.0029 (5)	−0.0011 (5)
C4	0.0196 (7)	0.0156 (7)	0.0181 (7)	−0.0013 (5)	0.0034 (5)	−0.0007 (5)
C5	0.0211 (7)	0.0146 (6)	0.0170 (7)	−0.0010 (5)	0.0037 (5)	−0.0002 (5)
C6	0.0310 (9)	0.0236 (9)	0.0554 (12)	0.0072 (7)	−0.0081 (8)	−0.0090 (8)
C7	0.0264 (8)	0.0225 (8)	0.0314 (9)	0.0008 (6)	0.0095 (7)	0.0025 (7)
C8	0.0271 (8)	0.0293 (8)	0.0258 (8)	0.0048 (7)	0.0096 (6)	0.0038 (7)
C9	0.0496 (12)	0.0383 (11)	0.0489 (12)	0.0103 (9)	0.0192 (10)	−0.0055 (9)
C10	0.0269 (9)	0.0538 (12)	0.0383 (10)	0.0042 (8)	0.0068 (8)	0.0116 (9)
C11	0.0166 (7)	0.0232 (7)	0.0138 (6)	−0.0008 (6)	0.0043 (5)	−0.0010 (6)
C12	0.0285 (8)	0.0266 (8)	0.0170 (7)	0.0010 (6)	0.0017 (6)	0.0008 (6)
C13	0.0301 (9)	0.0409 (10)	0.0162 (7)	0.0057 (7)	−0.0014 (6)	−0.0011 (7)
C14	0.0210 (8)	0.0444 (10)	0.0204 (8)	−0.0014 (7)	0.0017 (6)	−0.0124 (7)
C15	0.0228 (8)	0.0289 (8)	0.0264 (8)	−0.0054 (6)	0.0060 (6)	−0.0094 (7)
C16	0.0205 (7)	0.0241 (8)	0.0195 (7)	−0.0016 (6)	0.0042 (6)	−0.0012 (6)
C21	0.0192 (7)	0.0199 (7)	0.0141 (6)	−0.0040 (6)	0.0050 (5)	−0.0039 (5)
C22	0.0211 (7)	0.0253 (8)	0.0198 (7)	−0.0005 (6)	0.0029 (6)	−0.0028 (6)
C23	0.0186 (7)	0.0323 (9)	0.0293 (8)	−0.0050 (6)	0.0068 (6)	−0.0082 (7)
C24	0.0287 (8)	0.0271 (8)	0.0291 (8)	−0.0095 (7)	0.0145 (7)	−0.0046 (7)
C25	0.0326 (9)	0.0230 (8)	0.0212 (7)	−0.0050 (7)	0.0082 (6)	0.0002 (6)
C26	0.0226 (7)	0.0206 (7)	0.0186 (7)	−0.0034 (6)	0.0037 (6)	−0.0017 (6)
C31	0.0189 (7)	0.0176 (7)	0.0169 (7)	−0.0049 (5)	0.0009 (5)	−0.0018 (5)
C32	0.0243 (8)	0.0247 (8)	0.0199 (7)	0.0007 (6)	0.0016 (6)	−0.0039 (6)
C33	0.0335 (9)	0.0328 (9)	0.0185 (8)	−0.0022 (7)	0.0057 (6)	−0.0059 (7)
C34	0.0400 (10)	0.0355 (9)	0.0165 (7)	−0.0071 (8)	−0.0038 (7)	0.0001 (7)
C35	0.0278 (8)	0.0279 (8)	0.0266 (8)	−0.0024 (7)	−0.0070 (6)	0.0033 (7)
C36	0.0204 (7)	0.0207 (7)	0.0232 (7)	−0.0030 (6)	0.0011 (6)	−0.0020 (6)
C41	0.0197 (7)	0.0179 (7)	0.0189 (7)	−0.0029 (5)	0.0032 (5)	0.0025 (6)
C42	0.0232 (8)	0.0226 (8)	0.0232 (8)	−0.0002 (6)	0.0044 (6)	−0.0010 (6)
C43	0.0221 (8)	0.0376 (10)	0.0328 (9)	0.0006 (7)	0.0089 (7)	−0.0017 (8)
C44	0.0188 (8)	0.0408 (10)	0.0397 (10)	−0.0071 (7)	0.0032 (7)	0.0003 (8)
C45	0.0263 (8)	0.0325 (9)	0.0322 (9)	−0.0092 (7)	0.0003 (7)	−0.0064 (7)
C46	0.0220 (8)	0.0255 (8)	0.0253 (8)	−0.0037 (6)	0.0049 (6)	−0.0032 (6)
C51	0.0190 (7)	0.0221 (7)	0.0178 (7)	0.0014 (6)	0.0046 (5)	0.0032 (6)

C52	0.0245 (8)	0.0269 (8)	0.0194 (7)	0.0003 (6)	0.0049 (6)	−0.0008 (6)
C53	0.0314 (9)	0.0472 (11)	0.0204 (8)	0.0035 (8)	0.0081 (7)	−0.0047 (8)
C54	0.0354 (10)	0.0545 (12)	0.0233 (8)	0.0060 (9)	0.0147 (7)	0.0106 (8)
C55	0.0354 (10)	0.0346 (10)	0.0380 (10)	0.0002 (8)	0.0151 (8)	0.0161 (8)
C56	0.0292 (8)	0.0221 (8)	0.0286 (8)	0.0004 (6)	0.0090 (7)	0.0040 (6)
O1	0.0538 (10)	0.0353 (8)	0.1213 (16)	0.0098 (7)	−0.0354 (10)	−0.0420 (10)
O2	0.0446 (8)	0.0339 (7)	0.0383 (7)	0.0068 (6)	0.0100 (6)	0.0182 (6)
Fe1	0.01987 (12)	0.01597 (11)	0.01882 (12)	−0.00017 (8)	0.00301 (8)	0.00005 (8)

Geometric parameters (Å, º)

C1—C2	1.430 (2)	C22—C23	1.396 (2)
C1—C5	1.448 (2)	C22—H22	0.9500
C1—C11	1.485 (2)	C23—C24	1.387 (3)
C1—Fe1	2.1411 (15)	C23—H23	0.9500
C2—C3	1.433 (2)	C24—C25	1.386 (2)
C2—C21	1.486 (2)	C24—H24	0.9500
C2—Fe1	2.1824 (14)	C25—C26	1.391 (2)
C3—C4	1.453 (2)	C25—H25	0.9500
C3—C31	1.489 (2)	C26—H26	0.9500
C3—Fe1	2.1205 (15)	C31—C36	1.394 (2)
C4—C5	1.426 (2)	C31—C32	1.396 (2)
C4—C41	1.487 (2)	C32—C33	1.391 (2)
C4—Fe1	2.1387 (15)	C32—H32	0.9500
C5—C51	1.491 (2)	C33—C34	1.383 (3)
C5—Fe1	2.1278 (15)	C33—H33	0.9500
C6—O1	1.145 (2)	C34—C35	1.387 (3)
C6—Fe1	1.7453 (19)	C34—H34	0.9500
C7—O2	1.148 (2)	C35—C36	1.393 (2)
C7—Fe1	1.7564 (17)	C35—H35	0.9500
C8—C10	1.511 (3)	C36—H36	0.9500
C8—C9	1.536 (3)	C41—C46	1.394 (2)
C8—Fe1	2.1189 (16)	C41—C42	1.402 (2)
C8—H8	1.0000	C42—C43	1.393 (2)
C9—H9A	0.9800	C42—H42	0.9500
C9—H9B	0.9800	C43—C44	1.384 (3)
C9—H9C	0.9800	C43—H43	0.9500
C10—H10A	0.9800	C44—C45	1.388 (3)
C10—H10B	0.9800	C44—H44	0.9500
C10—H10C	0.9800	C45—C46	1.390 (2)
C11—C12	1.395 (2)	C45—H45	0.9500
C11—C16	1.397 (2)	C46—H46	0.9500
C12—C13	1.391 (2)	C51—C56	1.392 (2)
C12—H12	0.9500	C51—C52	1.393 (2)
C13—C14	1.378 (3)	C52—C53	1.395 (2)
C13—H13	0.9500	C52—H52	0.9500
C14—C15	1.384 (3)	C53—C54	1.383 (3)
C14—H14	0.9500	C53—H53	0.9500

C15—C16	1.391 (2)	C54—C55	1.384 (3)
C15—H15	0.9500	C54—H54	0.9500
C16—H16	0.9500	C55—C56	1.387 (2)
C21—C26	1.399 (2)	C55—H55	0.9500
C21—C22	1.399 (2)	C56—H56	0.9500
C2—C1—C5	107.73 (12)	C25—C26—H26	119.6
C2—C1—C11	126.03 (13)	C21—C26—H26	119.6
C5—C1—C11	125.04 (13)	C36—C31—C32	119.09 (14)
C2—C1—Fe1	72.26 (8)	C36—C31—C3	120.02 (13)
C5—C1—Fe1	69.68 (8)	C32—C31—C3	120.47 (14)
C11—C1—Fe1	133.29 (11)	C33—C32—C31	120.32 (15)
C1—C2—C3	108.18 (12)	C33—C32—H32	119.8
C1—C2—C21	125.90 (13)	C31—C32—H32	119.8
C3—C2—C21	125.36 (13)	C34—C33—C32	120.18 (16)
C1—C2—Fe1	69.13 (8)	C34—C33—H33	119.9
C3—C2—Fe1	68.23 (8)	C32—C33—H33	119.9
C21—C2—Fe1	135.02 (10)	C33—C34—C35	120.00 (15)
C2—C3—C4	108.08 (12)	C33—C34—H34	120.0
C2—C3—C31	123.52 (13)	C35—C34—H34	120.0
C4—C3—C31	127.93 (13)	C34—C35—C36	120.07 (16)
C2—C3—Fe1	72.90 (8)	C34—C35—H35	120.0
C4—C3—Fe1	70.72 (8)	C36—C35—H35	120.0
C31—C3—Fe1	128.27 (10)	C35—C36—C31	120.27 (15)
C5—C4—C3	107.31 (12)	C35—C36—H36	119.9
C5—C4—C41	126.33 (13)	C31—C36—H36	119.9
C3—C4—C41	125.86 (13)	C46—C41—C42	118.05 (14)
C5—C4—Fe1	70.06 (8)	C46—C41—C4	122.90 (14)
C3—C4—Fe1	69.38 (8)	C42—C41—C4	118.90 (13)
C41—C4—Fe1	132.05 (10)	C43—C42—C41	120.87 (15)
C4—C5—C1	108.50 (12)	C43—C42—H42	119.6
C4—C5—C51	126.45 (13)	C41—C42—H42	119.6
C1—C5—C51	124.95 (13)	C44—C43—C42	120.09 (16)
C4—C5—Fe1	70.88 (8)	C44—C43—H43	120.0
C1—C5—Fe1	70.67 (8)	C42—C43—H43	120.0
C51—C5—Fe1	127.17 (10)	C43—C44—C45	119.78 (16)
O1—C6—Fe1	178.22 (17)	C43—C44—H44	120.1
O2—C7—Fe1	179.42 (15)	C45—C44—H44	120.1
C10—C8—C9	108.46 (16)	C44—C45—C46	120.10 (16)
C10—C8—Fe1	112.60 (12)	C44—C45—H45	119.9
C9—C8—Fe1	117.38 (13)	C46—C45—H45	119.9
C10—C8—H8	105.8	C45—C46—C41	121.10 (15)
C9—C8—H8	105.8	C45—C46—H46	119.5
Fe1—C8—H8	105.8	C41—C46—H46	119.5
C8—C9—H9A	109.5	C56—C51—C52	118.97 (14)
C8—C9—H9B	109.5	C56—C51—C5	121.41 (14)
H9A—C9—H9B	109.5	C52—C51—C5	119.60 (14)
C8—C9—H9C	109.5	C51—C52—C53	120.30 (16)

H9A—C9—H9C	109.5	C51—C52—H52	119.8
H9B—C9—H9C	109.5	C53—C52—H52	119.8
C8—C10—H10A	109.5	C54—C53—C52	120.14 (17)
C8—C10—H10B	109.5	C54—C53—H53	119.9
H10A—C10—H10B	109.5	C52—C53—H53	119.9
C8—C10—H10C	109.5	C53—C54—C55	119.75 (16)
H10A—C10—H10C	109.5	C53—C54—H54	120.1
H10B—C10—H10C	109.5	C55—C54—H54	120.1
C12—C11—C16	118.38 (14)	C54—C55—C56	120.37 (17)
C12—C11—C1	122.80 (14)	C54—C55—H55	119.8
C16—C11—C1	118.70 (13)	C56—C55—H55	119.8
C13—C12—C11	120.38 (16)	C55—C56—C51	120.45 (16)
C13—C12—H12	119.8	C55—C56—H56	119.8
C11—C12—H12	119.8	C51—C56—H56	119.8
C14—C13—C12	120.68 (16)	C6—Fe1—C7	92.72 (9)
C14—C13—H13	119.7	C6—Fe1—C8	87.68 (8)
C12—C13—H13	119.7	C7—Fe1—C8	86.34 (7)
C13—C14—C15	119.66 (15)	C6—Fe1—C3	95.58 (8)
C13—C14—H14	120.2	C7—Fe1—C3	160.43 (7)
C15—C14—H14	120.2	C8—Fe1—C3	111.64 (6)
C14—C15—C16	120.05 (16)	C6—Fe1—C5	126.20 (8)
C14—C15—H15	120.0	C7—Fe1—C5	94.67 (7)
C16—C15—H15	120.0	C8—Fe1—C5	145.91 (6)
C15—C16—C11	120.83 (15)	C3—Fe1—C5	66.19 (5)
C15—C16—H16	119.6	C6—Fe1—C4	94.25 (7)
C11—C16—H16	119.6	C7—Fe1—C4	121.85 (7)
C26—C21—C22	118.49 (14)	C8—Fe1—C4	151.54 (6)
C26—C21—C2	118.65 (13)	C3—Fe1—C4	39.90 (5)
C22—C21—C2	122.66 (14)	C5—Fe1—C4	39.06 (5)
C23—C22—C21	120.29 (15)	C6—Fe1—C1	159.51 (7)
C23—C22—H22	119.9	C7—Fe1—C1	102.37 (7)
C21—C22—H22	119.9	C8—Fe1—C1	106.84 (6)
C24—C23—C22	120.56 (15)	C3—Fe1—C1	65.92 (5)
C24—C23—H23	119.7	C5—Fe1—C1	39.65 (5)
C22—C23—H23	119.7	C4—Fe1—C1	66.06 (6)
C25—C24—C23	119.55 (15)	C6—Fe1—C2	129.29 (8)
C25—C24—H24	120.2	C7—Fe1—C2	137.85 (7)
C23—C24—H24	120.2	C8—Fe1—C2	91.53 (6)
C24—C25—C26	120.22 (16)	C3—Fe1—C2	38.87 (5)
C24—C25—H25	119.9	C5—Fe1—C2	65.25 (5)
C26—C25—H25	119.9	C4—Fe1—C2	65.45 (5)
C25—C26—C21	120.88 (15)	C1—Fe1—C2	38.61 (5)

C5—C1—C2—C3	3.86 (16)	C3—C2—C21—C26	−39.4 (2)
C11—C1—C2—C3	171.77 (14)	Fe1—C2—C21—C26	−133.21 (14)
Fe1—C1—C2—C3	−57.12 (10)	C1—C2—C21—C22	−43.9 (2)
C5—C1—C2—C21	−167.83 (14)	C3—C2—C21—C22	145.82 (15)
C11—C1—C2—C21	0.1 (2)	Fe1—C2—C21—C22	52.0 (2)

Fe1—C1—C2—C21	131.19 (15)	C26—C21—C22—C23	1.1 (2)
C5—C1—C2—Fe1	60.98 (10)	C2—C21—C22—C23	175.94 (14)
C11—C1—C2—Fe1	−131.11 (15)	C21—C22—C23—C24	−1.2 (2)
C1—C2—C3—C4	−4.70 (16)	C22—C23—C24—C25	0.5 (2)
C21—C2—C3—C4	167.05 (14)	C23—C24—C25—C26	0.1 (2)
Fe1—C2—C3—C4	−62.37 (10)	C24—C25—C26—C21	−0.1 (2)
C1—C2—C3—C31	−177.34 (13)	C22—C21—C26—C25	−0.5 (2)
C21—C2—C3—C31	−5.6 (2)	C2—C21—C26—C25	−175.52 (14)
Fe1—C2—C3—C31	124.99 (14)	C2—C3—C31—C36	117.57 (16)
C1—C2—C3—Fe1	57.67 (10)	C4—C3—C31—C36	−53.5 (2)
C21—C2—C3—Fe1	−130.58 (14)	Fe1—C3—C31—C36	−148.23 (12)
C2—C3—C4—C5	3.71 (16)	C2—C3—C31—C32	−55.0 (2)
C31—C3—C4—C5	175.93 (14)	C4—C3—C31—C32	133.93 (16)
Fe1—C3—C4—C5	−60.06 (10)	Fe1—C3—C31—C32	39.2 (2)
C2—C3—C4—C41	−168.56 (14)	C36—C31—C32—C33	−2.8 (2)
C31—C3—C4—C41	3.7 (2)	C3—C31—C32—C33	169.79 (14)
Fe1—C3—C4—C41	127.66 (15)	C31—C32—C33—C34	0.8 (3)
C2—C3—C4—Fe1	63.77 (10)	C32—C33—C34—C35	1.6 (3)
C31—C3—C4—Fe1	−124.01 (15)	C33—C34—C35—C36	−2.1 (3)
C3—C4—C5—C1	−1.33 (16)	C34—C35—C36—C31	0.1 (2)
C41—C4—C5—C1	170.90 (14)	C32—C31—C36—C35	2.4 (2)
Fe1—C4—C5—C1	−60.96 (10)	C3—C31—C36—C35	−170.28 (14)
C3—C4—C5—C51	−177.76 (14)	C5—C4—C41—C46	143.76 (16)
C41—C4—C5—C51	−5.5 (2)	C3—C4—C41—C46	−45.4 (2)
Fe1—C4—C5—C51	122.61 (15)	Fe1—C4—C41—C46	48.4 (2)
C3—C4—C5—Fe1	59.63 (10)	C5—C4—C41—C42	−40.9 (2)
C41—C4—C5—Fe1	−128.14 (15)	C3—C4—C41—C42	129.91 (16)
C2—C1—C5—C4	−1.55 (16)	Fe1—C4—C41—C42	−136.26 (13)
C11—C1—C5—C4	−169.61 (14)	C46—C41—C42—C43	0.5 (2)
Fe1—C1—C5—C4	61.09 (10)	C4—C41—C42—C43	−175.09 (15)
C2—C1—C5—C51	174.95 (13)	C41—C42—C43—C44	0.4 (3)
C11—C1—C5—C51	6.9 (2)	C42—C43—C44—C45	−1.0 (3)
Fe1—C1—C5—C51	−122.40 (14)	C43—C44—C45—C46	0.7 (3)
C2—C1—C5—Fe1	−62.64 (10)	C44—C45—C46—C41	0.2 (3)
C11—C1—C5—Fe1	129.30 (15)	C42—C41—C46—C45	−0.7 (2)
C2—C1—C11—C12	130.29 (16)	C4—C41—C46—C45	174.62 (15)
C5—C1—C11—C12	−63.8 (2)	C4—C5—C51—C56	−49.6 (2)
Fe1—C1—C11—C12	30.7 (2)	C1—C5—C51—C56	134.50 (16)
C2—C1—C11—C16	−53.7 (2)	Fe1—C5—C51—C56	43.2 (2)
C5—C1—C11—C16	112.20 (17)	C4—C5—C51—C52	129.03 (17)
Fe1—C1—C11—C16	−153.34 (12)	C1—C5—C51—C52	−46.8 (2)
C16—C11—C12—C13	−0.3 (2)	Fe1—C5—C51—C52	−138.17 (13)
C1—C11—C12—C13	175.70 (14)	C56—C51—C52—C53	−0.4 (2)
C11—C12—C13—C14	−1.0 (3)	C5—C51—C52—C53	−179.12 (15)
C12—C13—C14—C15	1.4 (3)	C51—C52—C53—C54	−0.5 (3)
C13—C14—C15—C16	−0.4 (2)	C52—C53—C54—C55	1.2 (3)
C14—C15—C16—C11	−1.0 (2)	C53—C54—C55—C56	−0.9 (3)
C12—C11—C16—C15	1.3 (2)	C54—C55—C56—C51	0.0 (3)

C1—C11—C16—C15	−174.90 (14)	C52—C51—C56—C55	0.7 (2)
C1—C2—C21—C26	130.93 (16)	C5—C51—C56—C55	179.35 (16)

Butyldicarbonyl(η^5-pentaphenylcyclopentadienyl)iron (compd-4)

Crystal data

$[Fe(C_4H_9)(C_{35}H_{25})(CO)_2]$
M_r = 614.53
Monoclinic, $P2_1/n$
a = 12.1141 (4) Å
b = 16.0945 (5) Å
c = 16.1650 (5) Å
β = 95.706 (1)°
V = 3136.08 (17) Å^3
Z = 4
$F(000)$ = 1288
D_x = 1.302 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9964 reflections
θ = 2.5–27.5°
μ = 0.52 mm^{-1}
T = 108 K
Block, yellow
0.08 × 0.05 × 0.04 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.391 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.832, T_{max} = 0.862
55494 measured reflections
7202 independent reflections
6246 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −15→15
k = −20→20
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.05
7202 reflections
398 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 1.832P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.47579 (11)	0.57025 (8)	0.83402 (8)	0.0131 (3)
C2	0.41324 (11)	0.49455 (8)	0.82891 (8)	0.0131 (3)
C3	0.49011 (11)	0.42693 (8)	0.83398 (8)	0.0131 (3)
C4	0.60059 (11)	0.46044 (8)	0.83961 (8)	0.0133 (3)
C5	0.59232 (11)	0.54974 (8)	0.84196 (8)	0.0136 (3)
C6	0.44862 (13)	0.57507 (10)	0.65645 (9)	0.0213 (3)

C7	0.47165 (12)	0.41992 (9)	0.65795 (9)	0.0188 (3)
C11	0.65229 (12)	0.51767 (10)	0.66507 (9)	0.0205 (3)
H11A	0.676910	0.575884	0.674250	0.025*
H11B	0.710971	0.481877	0.693225	0.025*
C12	0.64900 (15)	0.50065 (12)	0.57212 (10)	0.0308 (4)
H12A	0.586520	0.531874	0.542698	0.037*
H12B	0.635147	0.440720	0.561952	0.037*
C13	0.75680 (16)	0.52532 (15)	0.53626 (12)	0.0402 (5)
H13A	0.747528	0.516468	0.475359	0.048*
H13B	0.770138	0.585331	0.546278	0.048*
C14	0.85757 (17)	0.47728 (17)	0.57283 (14)	0.0495 (6)
H14A	0.872427	0.490479	0.632076	0.074*
H14B	0.921949	0.492711	0.543938	0.074*
H14C	0.843551	0.417572	0.566143	0.074*
C101	0.42810 (11)	0.65501 (8)	0.83848 (8)	0.0140 (3)
C102	0.46705 (12)	0.72134 (9)	0.79390 (9)	0.0188 (3)
H102	0.520362	0.711426	0.755731	0.023*
C103	0.42899 (13)	0.80141 (9)	0.80458 (10)	0.0229 (3)
H103	0.457138	0.846062	0.774470	0.028*
C104	0.34974 (13)	0.81655 (9)	0.85922 (10)	0.0225 (3)
H104	0.324338	0.871556	0.867102	0.027*
C105	0.30788 (12)	0.75098 (9)	0.90220 (9)	0.0202 (3)
H105	0.252455	0.760918	0.938669	0.024*
C106	0.34690 (11)	0.67068 (9)	0.89203 (8)	0.0156 (3)
H106	0.318025	0.626088	0.921799	0.019*
C201	0.29087 (11)	0.48686 (8)	0.82957 (9)	0.0137 (3)
C202	0.24907 (12)	0.44568 (9)	0.89560 (9)	0.0177 (3)
H202	0.298868	0.420759	0.937519	0.021*
C203	0.13555 (12)	0.44061 (9)	0.90089 (10)	0.0211 (3)
H203	0.108167	0.412026	0.946042	0.025*
C204	0.06197 (12)	0.47728 (10)	0.84024 (10)	0.0216 (3)
H204	−0.015679	0.474690	0.844189	0.026*
C205	0.10277 (13)	0.51768 (9)	0.77390 (10)	0.0212 (3)
H205	0.052807	0.542609	0.732101	0.025*
C206	0.21648 (12)	0.52190 (9)	0.76820 (9)	0.0174 (3)
H206	0.243564	0.548932	0.722038	0.021*
C301	0.45953 (11)	0.33829 (8)	0.84401 (8)	0.0140 (3)
C302	0.36941 (12)	0.30272 (9)	0.79632 (9)	0.0180 (3)
H302	0.331793	0.333313	0.751808	0.022*
C303	0.33424 (13)	0.22299 (9)	0.81338 (10)	0.0221 (3)
H303	0.272590	0.199448	0.780661	0.027*
C304	0.38875 (13)	0.17752 (9)	0.87802 (10)	0.0219 (3)
H304	0.364249	0.123118	0.889850	0.026*
C305	0.47916 (13)	0.21192 (9)	0.92524 (9)	0.0202 (3)
H305	0.517052	0.180811	0.969250	0.024*
C306	0.51457 (12)	0.29177 (9)	0.90842 (9)	0.0165 (3)
H306	0.576673	0.314872	0.940976	0.020*
C401	0.70126 (11)	0.40786 (9)	0.85278 (9)	0.0149 (3)

C402	0.71651 (12)	0.34096 (9)	0.80006 (10)	0.0206 (3)
H402	0.668327	0.334006	0.750481	0.025*
C403	0.80175 (13)	0.28462 (10)	0.81983 (11)	0.0270 (4)
H403	0.810627	0.238641	0.784232	0.032*
C404	0.87416 (13)	0.29490 (10)	0.89119 (11)	0.0279 (4)
H404	0.932333	0.256099	0.904443	0.034*
C405	0.86122 (12)	0.36198 (10)	0.94299 (10)	0.0224 (3)
H405	0.911031	0.369512	0.991622	0.027*
C406	0.77527 (11)	0.41846 (9)	0.92390 (9)	0.0165 (3)
H406	0.766971	0.464510	0.959530	0.020*
C501	0.68523 (11)	0.60888 (8)	0.86256 (8)	0.0144 (3)
C502	0.78843 (12)	0.60097 (9)	0.83100 (9)	0.0183 (3)
H502	0.799867	0.557541	0.792982	0.022*
C503	0.87442 (12)	0.65617 (10)	0.85483 (10)	0.0229 (3)
H503	0.943372	0.650880	0.831988	0.027*
C504	0.85986 (13)	0.71883 (10)	0.91175 (10)	0.0241 (3)
H504	0.918531	0.756447	0.927828	0.029*
C505	0.75916 (13)	0.72612 (10)	0.94494 (10)	0.0229 (3)
H505	0.749171	0.768297	0.984633	0.028*
C506	0.67288 (12)	0.67205 (9)	0.92041 (9)	0.0177 (3)
H506	0.604078	0.678017	0.943325	0.021*
O1	0.40743 (11)	0.62256 (8)	0.60997 (7)	0.0335 (3)
O2	0.44211 (10)	0.36770 (7)	0.61268 (7)	0.0286 (3)
Fe1	0.51082 (2)	0.50163 (2)	0.72658 (2)	0.01342 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0131 (6)	0.0145 (6)	0.0120 (6)	0.0004 (5)	0.0021 (5)	0.0011 (5)
C2	0.0133 (6)	0.0136 (6)	0.0124 (6)	0.0002 (5)	0.0008 (5)	0.0013 (5)
C3	0.0129 (6)	0.0141 (6)	0.0121 (6)	0.0000 (5)	−0.0004 (5)	0.0000 (5)
C4	0.0133 (6)	0.0144 (6)	0.0120 (6)	0.0006 (5)	0.0003 (5)	−0.0008 (5)
C5	0.0131 (6)	0.0147 (6)	0.0132 (6)	0.0004 (5)	0.0025 (5)	−0.0005 (5)
C6	0.0244 (8)	0.0227 (7)	0.0170 (7)	0.0030 (6)	0.0028 (6)	−0.0020 (6)
C7	0.0170 (7)	0.0221 (7)	0.0178 (7)	0.0006 (6)	0.0036 (5)	0.0002 (6)
C11	0.0166 (7)	0.0277 (8)	0.0175 (7)	−0.0031 (6)	0.0035 (6)	0.0000 (6)
C12	0.0232 (8)	0.0527 (12)	0.0172 (8)	−0.0049 (7)	0.0055 (6)	0.0000 (7)
C13	0.0342 (10)	0.0622 (13)	0.0266 (9)	−0.0120 (9)	0.0151 (8)	0.0001 (9)
C14	0.0269 (10)	0.0788 (16)	0.0453 (12)	−0.0054 (10)	0.0153 (9)	−0.0118 (11)
C101	0.0122 (6)	0.0137 (6)	0.0153 (6)	0.0007 (5)	−0.0024 (5)	−0.0004 (5)
C102	0.0176 (7)	0.0180 (7)	0.0207 (7)	−0.0002 (6)	0.0020 (6)	0.0030 (6)
C103	0.0265 (8)	0.0146 (7)	0.0268 (8)	−0.0013 (6)	−0.0021 (6)	0.0060 (6)
C104	0.0253 (8)	0.0156 (7)	0.0250 (8)	0.0054 (6)	−0.0063 (6)	−0.0034 (6)
C105	0.0188 (7)	0.0215 (7)	0.0197 (7)	0.0046 (6)	−0.0015 (6)	−0.0048 (6)
C106	0.0146 (6)	0.0166 (7)	0.0151 (6)	0.0007 (5)	−0.0004 (5)	−0.0001 (5)
C201	0.0126 (6)	0.0110 (6)	0.0177 (7)	−0.0001 (5)	0.0017 (5)	−0.0025 (5)
C202	0.0163 (7)	0.0177 (7)	0.0191 (7)	0.0008 (5)	0.0009 (5)	0.0020 (5)
C203	0.0189 (7)	0.0214 (7)	0.0241 (8)	−0.0029 (6)	0.0077 (6)	0.0017 (6)

C204	0.0127 (7)	0.0201 (7)	0.0326 (8)	−0.0004 (6)	0.0050 (6)	−0.0015 (6)
C205	0.0143 (7)	0.0204 (7)	0.0279 (8)	0.0018 (6)	−0.0026 (6)	0.0028 (6)
C206	0.0165 (7)	0.0141 (6)	0.0214 (7)	−0.0002 (5)	0.0014 (6)	0.0020 (5)
C301	0.0130 (6)	0.0136 (6)	0.0155 (6)	0.0004 (5)	0.0022 (5)	−0.0015 (5)
C302	0.0182 (7)	0.0157 (7)	0.0190 (7)	−0.0004 (5)	−0.0032 (5)	0.0002 (5)
C303	0.0221 (8)	0.0184 (7)	0.0244 (8)	−0.0056 (6)	−0.0051 (6)	−0.0018 (6)
C304	0.0273 (8)	0.0132 (7)	0.0247 (8)	−0.0041 (6)	0.0009 (6)	0.0007 (6)
C305	0.0244 (8)	0.0170 (7)	0.0184 (7)	0.0019 (6)	−0.0017 (6)	0.0021 (5)
C306	0.0158 (7)	0.0163 (7)	0.0168 (7)	−0.0005 (5)	−0.0012 (5)	−0.0015 (5)
C401	0.0119 (6)	0.0153 (6)	0.0178 (7)	0.0003 (5)	0.0032 (5)	0.0011 (5)
C402	0.0168 (7)	0.0214 (7)	0.0238 (7)	0.0010 (6)	0.0026 (6)	−0.0050 (6)
C403	0.0203 (8)	0.0216 (8)	0.0402 (10)	0.0056 (6)	0.0084 (7)	−0.0066 (7)
C404	0.0164 (7)	0.0247 (8)	0.0431 (10)	0.0085 (6)	0.0053 (7)	0.0054 (7)
C405	0.0129 (7)	0.0286 (8)	0.0254 (8)	0.0000 (6)	0.0008 (6)	0.0080 (6)
C406	0.0134 (6)	0.0180 (7)	0.0184 (7)	−0.0009 (5)	0.0024 (5)	0.0019 (5)
C501	0.0133 (6)	0.0139 (6)	0.0158 (6)	−0.0007 (5)	−0.0002 (5)	0.0036 (5)
C502	0.0152 (7)	0.0195 (7)	0.0203 (7)	0.0005 (5)	0.0019 (5)	0.0015 (6)
C503	0.0146 (7)	0.0253 (8)	0.0287 (8)	−0.0030 (6)	0.0020 (6)	0.0050 (6)
C504	0.0200 (7)	0.0187 (7)	0.0324 (9)	−0.0067 (6)	−0.0037 (6)	0.0033 (6)
C505	0.0259 (8)	0.0169 (7)	0.0252 (8)	−0.0015 (6)	−0.0013 (6)	−0.0024 (6)
C506	0.0165 (7)	0.0170 (7)	0.0194 (7)	0.0003 (5)	0.0009 (5)	0.0007 (5)
O1	0.0447 (8)	0.0305 (6)	0.0238 (6)	0.0133 (6)	−0.0043 (5)	0.0050 (5)
O2	0.0319 (6)	0.0287 (6)	0.0254 (6)	−0.0058 (5)	0.0033 (5)	−0.0098 (5)
Fe1	0.01263 (11)	0.01467 (11)	0.01291 (11)	0.00076 (7)	0.00095 (7)	−0.00002 (7)

Geometric parameters (Å, º)

C1—C2	1.4328 (19)	C201—C202	1.394 (2)
C1—C5	1.4430 (19)	C202—C203	1.389 (2)
C1—C101	1.4859 (18)	C202—H202	0.9500
C1—Fe1	2.1360 (13)	C203—C204	1.389 (2)
C2—C3	1.4294 (18)	C203—H203	0.9500
C2—C201	1.4887 (19)	C204—C205	1.387 (2)
C2—Fe1	2.1295 (14)	C204—H204	0.9500
C3—C4	1.4373 (18)	C205—C206	1.391 (2)
C3—C301	1.4868 (19)	C205—H205	0.9500
C3—Fe1	2.1467 (13)	C206—H206	0.9500
C4—C5	1.4415 (19)	C301—C302	1.3952 (19)
C4—C401	1.4822 (19)	C301—C306	1.3968 (19)
C4—Fe1	2.1366 (13)	C302—C303	1.388 (2)
C5—C501	1.4863 (19)	C302—H302	0.9500
C5—Fe1	2.1649 (14)	C303—C304	1.388 (2)
C6—O1	1.1502 (19)	C303—H303	0.9500
C6—Fe1	1.7552 (16)	C304—C305	1.387 (2)
C7—O2	1.1480 (19)	C304—H304	0.9500
C7—Fe1	1.7552 (15)	C305—C306	1.390 (2)
C11—C12	1.524 (2)	C305—H305	0.9500
C11—Fe1	2.0812 (15)	C306—H306	0.9500

C11—H11A	0.9900	C401—C406	1.396 (2)
C11—H11B	0.9900	C401—C402	1.397 (2)
C12—C13	1.533 (2)	C402—C403	1.387 (2)
C12—H12A	0.9900	C402—H402	0.9500
C12—H12B	0.9900	C403—C404	1.388 (2)
C13—C14	1.515 (3)	C403—H403	0.9500
C13—H13A	0.9900	C404—C405	1.385 (2)
C13—H13B	0.9900	C404—H404	0.9500
C14—H14A	0.9800	C405—C406	1.394 (2)
C14—H14B	0.9800	C405—H405	0.9500
C14—H14C	0.9800	C406—H406	0.9500
C101—C102	1.396 (2)	C501—C506	1.399 (2)
C101—C106	1.3963 (19)	C501—C502	1.4022 (19)
C102—C103	1.385 (2)	C502—C503	1.394 (2)
C102—H102	0.9500	C502—H502	0.9500
C103—C104	1.389 (2)	C503—C504	1.388 (2)
C103—H103	0.9500	C503—H503	0.9500
C104—C105	1.387 (2)	C504—C505	1.386 (2)
C104—H104	0.9500	C504—H504	0.9500
C105—C106	1.392 (2)	C505—C506	1.387 (2)
C105—H105	0.9500	C505—H505	0.9500
C106—H106	0.9500	C506—H506	0.9500
C201—C206	1.392 (2)		

C2—C1—C5	108.52 (12)	C204—C205—H205	119.8
C2—C1—C101	125.27 (12)	C206—C205—H205	119.8
C5—C1—C101	125.97 (12)	C205—C206—C201	120.55 (14)
C2—C1—Fe1	70.13 (8)	C205—C206—H206	119.7
C5—C1—Fe1	71.48 (8)	C201—C206—H206	119.7
C101—C1—Fe1	128.59 (9)	C302—C301—C306	118.76 (13)
C3—C2—C1	107.84 (12)	C302—C301—C3	121.54 (12)
C3—C2—C201	125.44 (12)	C306—C301—C3	119.34 (12)
C1—C2—C201	126.27 (12)	C303—C302—C301	120.54 (13)
C3—C2—Fe1	71.12 (8)	C303—C302—H302	119.7
C1—C2—Fe1	70.62 (8)	C301—C302—H302	119.7
C201—C2—Fe1	129.80 (10)	C304—C303—C302	120.30 (14)
C2—C3—C4	108.37 (12)	C304—C303—H303	119.9
C2—C3—C301	124.66 (12)	C302—C303—H303	119.9
C4—C3—C301	126.42 (12)	C305—C304—C303	119.64 (14)
C2—C3—Fe1	69.82 (8)	C305—C304—H304	120.2
C4—C3—Fe1	70.01 (8)	C303—C304—H304	120.2
C301—C3—Fe1	132.53 (9)	C304—C305—C306	120.24 (14)
C3—C4—C5	108.00 (11)	C304—C305—H305	119.9
C3—C4—C401	122.86 (12)	C306—C305—H305	119.9
C5—C4—C401	128.59 (12)	C305—C306—C301	120.51 (13)
C3—C4—Fe1	70.78 (8)	C305—C306—H306	119.7
C5—C4—Fe1	71.49 (7)	C301—C306—H306	119.7
C401—C4—Fe1	129.91 (10)	C406—C401—C402	118.91 (13)

C4—C5—C1	107.20 (11)	C406—C401—C4	120.03 (12)
C4—C5—C501	126.25 (12)	C402—C401—C4	120.61 (13)
C1—C5—C501	125.86 (12)	C403—C402—C401	120.25 (14)
C4—C5—Fe1	69.36 (7)	C403—C402—H402	119.9
C1—C5—Fe1	69.32 (8)	C401—C402—H402	119.9
C501—C5—Fe1	133.81 (10)	C402—C403—C404	120.52 (15)
O1—C6—Fe1	179.31 (15)	C402—C403—H403	119.7
O2—C7—Fe1	177.45 (14)	C404—C403—H403	119.7
C12—C11—Fe1	120.45 (11)	C405—C404—C403	119.70 (14)
C12—C11—H11A	107.2	C405—C404—H404	120.2
Fe1—C11—H11A	107.2	C403—C404—H404	120.2
C12—C11—H11B	107.2	C404—C405—C406	120.12 (15)
Fe1—C11—H11B	107.2	C404—C405—H405	119.9
H11A—C11—H11B	106.8	C406—C405—H405	119.9
C11—C12—C13	112.75 (15)	C405—C406—C401	120.47 (14)
C11—C12—H12A	109.0	C405—C406—H406	119.8
C13—C12—H12A	109.0	C401—C406—H406	119.8
C11—C12—H12B	109.0	C506—C501—C502	117.87 (13)
C13—C12—H12B	109.0	C506—C501—C5	119.08 (12)
H12A—C12—H12B	107.8	C502—C501—C5	122.90 (13)
C14—C13—C12	113.84 (17)	C503—C502—C501	120.70 (14)
C14—C13—H13A	108.8	C503—C502—H502	119.6
C12—C13—H13A	108.8	C501—C502—H502	119.6
C14—C13—H13B	108.8	C504—C503—C502	120.36 (14)
C12—C13—H13B	108.8	C504—C503—H503	119.8
H13A—C13—H13B	107.7	C502—C503—H503	119.8
C13—C14—H14A	109.5	C505—C504—C503	119.54 (14)
C13—C14—H14B	109.5	C505—C504—H504	120.2
H14A—C14—H14B	109.5	C503—C504—H504	120.2
C13—C14—H14C	109.5	C504—C505—C506	120.23 (14)
H14A—C14—H14C	109.5	C504—C505—H505	119.9
H14B—C14—H14C	109.5	C506—C505—H505	119.9
C102—C101—C106	118.48 (13)	C505—C506—C501	121.28 (14)
C102—C101—C1	121.60 (13)	C505—C506—H506	119.4
C106—C101—C1	119.81 (12)	C501—C506—H506	119.4
C103—C102—C101	120.89 (14)	C6—Fe1—C7	91.40 (7)
C103—C102—H102	119.6	C6—Fe1—C11	85.92 (7)
C101—C102—H102	119.6	C7—Fe1—C11	88.54 (6)
C102—C103—C104	120.13 (14)	C6—Fe1—C2	107.57 (6)
C102—C103—H103	119.9	C7—Fe1—C2	108.35 (6)
C104—C103—H103	119.9	C11—Fe1—C2	157.64 (6)
C105—C104—C103	119.69 (14)	C6—Fe1—C1	94.00 (6)
C105—C104—H104	120.2	C7—Fe1—C1	146.96 (6)
C103—C104—H104	120.2	C11—Fe1—C1	124.33 (6)
C104—C105—C106	120.13 (14)	C2—Fe1—C1	39.25 (5)
C104—C105—H105	119.9	C6—Fe1—C4	155.60 (6)
C106—C105—H105	119.9	C7—Fe1—C4	113.00 (6)
C105—C106—C101	120.64 (13)	C11—Fe1—C4	94.23 (6)

C105—C106—H106	119.7	C2—Fe1—C4	66.04 (5)
C101—C106—H106	119.7	C1—Fe1—C4	65.83 (5)
C206—C201—C202	118.68 (13)	C6—Fe1—C3	145.32 (6)
C206—C201—C2	122.40 (13)	C7—Fe1—C3	92.62 (6)
C202—C201—C2	118.87 (13)	C11—Fe1—C3	128.60 (6)
C203—C202—C201	120.82 (14)	C2—Fe1—C3	39.05 (5)
C203—C202—H202	119.6	C1—Fe1—C3	65.38 (5)
C201—C202—H202	119.6	C4—Fe1—C3	39.21 (5)
C202—C203—C204	120.09 (14)	C6—Fe1—C5	116.45 (6)
C202—C203—H203	120.0	C7—Fe1—C5	152.13 (6)
C204—C203—H203	120.0	C11—Fe1—C5	92.33 (6)
C205—C204—C203	119.47 (14)	C2—Fe1—C5	65.84 (5)
C205—C204—H204	120.3	C1—Fe1—C5	39.20 (5)
C203—C204—H204	120.3	C4—Fe1—C5	39.15 (5)
C204—C205—C206	120.36 (14)	C3—Fe1—C5	65.39 (5)

C5—C1—C2—C3	0.24 (15)	C3—C2—C201—C206	−126.66 (15)
C101—C1—C2—C3	−174.43 (12)	C1—C2—C201—C206	62.0 (2)
Fe1—C1—C2—C3	61.74 (9)	Fe1—C2—C201—C206	−32.30 (19)
C5—C1—C2—C201	172.81 (13)	C3—C2—C201—C202	55.7 (2)
C101—C1—C2—C201	−1.9 (2)	C1—C2—C201—C202	−115.59 (16)
Fe1—C1—C2—C201	−125.70 (14)	Fe1—C2—C201—C202	150.09 (11)
C5—C1—C2—Fe1	−61.50 (9)	C206—C201—C202—C203	−0.9 (2)
C101—C1—C2—Fe1	123.83 (13)	C2—C201—C202—C203	176.79 (13)
C1—C2—C3—C4	−1.79 (15)	C201—C202—C203—C204	−0.4 (2)
C201—C2—C3—C4	−174.44 (13)	C202—C203—C204—C205	1.0 (2)
Fe1—C2—C3—C4	59.62 (9)	C203—C204—C205—C206	−0.3 (2)
C1—C2—C3—C301	170.16 (12)	C204—C205—C206—C201	−1.0 (2)
C201—C2—C3—C301	−2.5 (2)	C202—C201—C206—C205	1.6 (2)
Fe1—C2—C3—C301	−128.42 (13)	C2—C201—C206—C205	−175.99 (13)
C1—C2—C3—Fe1	−61.41 (9)	C2—C3—C301—C302	46.1 (2)
C201—C2—C3—Fe1	125.94 (14)	C4—C3—C301—C302	−143.44 (14)
C2—C3—C4—C5	2.66 (15)	Fe1—C3—C301—C302	−47.69 (19)
C301—C3—C4—C5	−169.11 (12)	C2—C3—C301—C306	−127.07 (15)
Fe1—C3—C4—C5	62.17 (9)	C4—C3—C301—C306	43.4 (2)
C2—C3—C4—C401	174.79 (12)	Fe1—C3—C301—C306	139.19 (12)
C301—C3—C4—C401	3.0 (2)	C306—C301—C302—C303	0.9 (2)
Fe1—C3—C4—C401	−125.71 (13)	C3—C301—C302—C303	−172.28 (14)
C2—C3—C4—Fe1	−59.50 (9)	C301—C302—C303—C304	−0.3 (2)
C301—C3—C4—Fe1	128.72 (14)	C302—C303—C304—C305	−0.4 (2)
C3—C4—C5—C1	−2.48 (15)	C303—C304—C305—C306	0.5 (2)
C401—C4—C5—C1	−174.02 (13)	C304—C305—C306—C301	0.1 (2)
Fe1—C4—C5—C1	59.23 (9)	C302—C301—C306—C305	−0.8 (2)
C3—C4—C5—C501	168.41 (13)	C3—C301—C306—C305	172.50 (13)
C401—C4—C5—C501	−3.1 (2)	C3—C4—C401—C406	−118.24 (15)
Fe1—C4—C5—C501	−129.88 (13)	C5—C4—C401—C406	52.2 (2)
C3—C4—C5—Fe1	−61.71 (9)	Fe1—C4—C401—C406	150.09 (11)
C401—C4—C5—Fe1	126.76 (14)	C3—C4—C401—C402	53.96 (19)

C2—C1—C5—C4	1.39 (15)	C5—C4—C401—C402	−135.63 (15)
C101—C1—C5—C4	176.02 (12)	Fe1—C4—C401—C402	−37.71 (19)
Fe1—C1—C5—C4	−59.25 (9)	C406—C401—C402—C403	2.1 (2)
C2—C1—C5—C501	−169.55 (13)	C4—C401—C402—C403	−170.18 (14)
C101—C1—C5—C501	5.1 (2)	C401—C402—C403—C404	−1.3 (2)
Fe1—C1—C5—C501	129.81 (13)	C402—C403—C404—C405	−0.1 (3)
C2—C1—C5—Fe1	60.64 (9)	C403—C404—C405—C406	0.6 (2)
C101—C1—C5—Fe1	−124.73 (13)	C404—C405—C406—C401	0.3 (2)
Fe1—C11—C12—C13	173.47 (13)	C402—C401—C406—C405	−1.6 (2)
C11—C12—C13—C14	62.4 (2)	C4—C401—C406—C405	170.73 (13)
C2—C1—C101—C102	−138.63 (14)	C4—C5—C501—C506	−131.50 (14)
C5—C1—C101—C102	47.6 (2)	C1—C5—C501—C506	37.7 (2)
Fe1—C1—C101—C102	−46.80 (18)	Fe1—C5—C501—C506	132.89 (13)
C2—C1—C101—C106	45.2 (2)	C4—C5—C501—C502	43.9 (2)
C5—C1—C101—C106	−128.52 (15)	C1—C5—C501—C502	−146.88 (14)
Fe1—C1—C101—C106	137.06 (12)	Fe1—C5—C501—C502	−51.7 (2)
C106—C101—C102—C103	2.2 (2)	C506—C501—C502—C503	−2.0 (2)
C1—C101—C102—C103	−173.98 (13)	C5—C501—C502—C503	−177.41 (13)
C101—C102—C103—C104	−1.0 (2)	C501—C502—C503—C504	1.4 (2)
C102—C103—C104—C105	−0.8 (2)	C502—C503—C504—C505	0.1 (2)
C103—C104—C105—C106	1.4 (2)	C503—C504—C505—C506	−1.1 (2)
C104—C105—C106—C101	−0.2 (2)	C504—C505—C506—C501	0.5 (2)
C102—C101—C106—C105	−1.6 (2)	C502—C501—C506—C505	1.0 (2)
C1—C101—C106—C105	174.65 (13)	C5—C501—C506—C505	176.63 (13)