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Dicarbonyl{[(*E,E*)-(2,3,4,5-**η**)-6-methoxy-6-oxo-2,4-hexadienyl]triphenylphosphonium}(triphenylphosphane-**κ***P*)iron(1+) hexafluoridophosphate

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Dicarbonyl{[(*E*,*E*)-(2,3,4,5-η)-6-methoxy-6-oxo-2,4-hexadienyl]triphenylphosphonium}(triphenylphosphane-κP)iron(1+) hexafluoridophosphate

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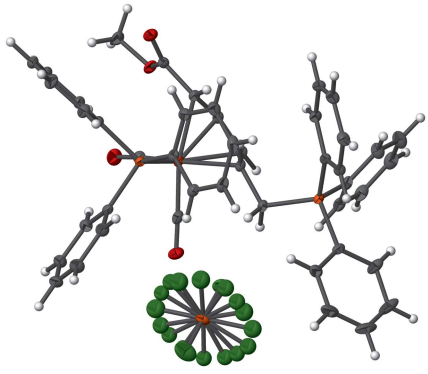
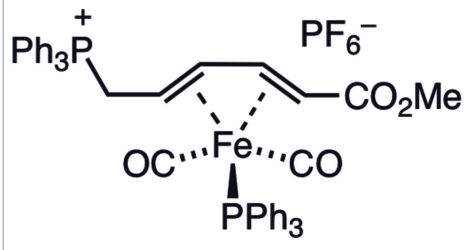
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Fe(C_{25}H_{24}O_2P)(C_{18}H_{15}P)(CO)_2]PF_6$, the Fe atom adopts a square-based pyramidal coordination geometry with the carbonyl groups and the two C=C bonds of the diene defining the basal sites and the phosphane ligand the apical position. The diene ligand has an *E*,*E* geometry, with the phosphonium fragment pointed away from the Fe atom. The crystal structure displays C—H···F and C—H···O hydrogen bonding. The PF_6^- anion is rotationally disordered over four orientations.

3D view



Chemical scheme



Structure description

Acyclic (dienyl)iron cations and acyclic (diene)iron complexes have been utilized in organic synthesis as the coordination to iron serves as a protecting group for the diene against oxidation, reduction and cycloaddition (Cox & Ley, 1998; Donaldson, 2000; Donaldson & Chaudhury, 2009; Grée, 1989; Iwata & Takemoto, 1996). The reaction of acyclic tricarbonyl(dienyl)iron cations with phosphines results in the formation of iron-complexed dienylphosphonium salts (McArdle & Sherlock, 1978; Salzer & Hafner, 1983). It was eventually demonstrated that this reaction proceeds *via* kinetic nucleophilic attack on the *cisoid* form of the cation, and that this C—P bond formation is reversible in certain cases (Donaldson *et al.*, 1994, 1995). These dienylphosphonium salts have been utilized in Wittig-type olefination reactions (Hafner *et al.* 1983). To our knowledge, there is only one report of the reaction of a dicarbonyl(triphenylphosphine)-ligated (pentadienyl)iron cation with triphenylphosphine (Chaudhury *et al.*, 2007). In a continuation of this work, we present here the synthesis and crystal structure of a 2*E*,4*E*-dienylphosphonium salt complexed to an $Fe(CO)_2PPh_3$ fragment with hexafluoridophosphate counter-ions.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C26—H26···F1	0.95	2.43	3.1353 (15)	131
C28—H28···F5B^{i}	0.95	2.49	3.322 (8)	146
C28—H28···F5C^{i}	0.95	2.55	3.320 (15)	139
C32—H32···O4^{ii}	0.95	2.56	3.3659 (16)	143
C34—H34···F1	0.95	2.41	3.1349 (16)	133
C40—H40···F2^{iii}	0.95	2.40	3.2586 (16)	150

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

The title compound (Fig. 1) consists of a (*trans*,*trans*-dienyl)phosphonium ligand coordinated to iron, with the phosphonium group orientated distal to the metal atom. The complex exhibits the typical square-based pyramidal structure of (diene)Fe(CO)2*L* complexes, with the triphenylphosphine ligand oriented in the axial position. Crystal structures of other acyclic (diene)Fe(CO)$_2$*L* complexes exhibit both axial (Howell *et al.*, 1994; Zutin *et al.*, 2001) and basal (Howell *et al.*, 1996) phosphine orientations. The crystal structure (Fig. 2) exhibits several interactions between phenyl hydrogen atoms and fluorine atoms of the PF_6^- anion which are within the range of C—H···F hydrogen bonds (2.40–2.56 Å). C—H···F and C—H···O hydrogen-bond geometries are summarized in Table 1.

Synthesis and crystallization

To a solution of dicarbonyl(1-methoxycarbonylpentadienyl)-(triphenylphosphine)iron(1+) hexafluorophosphate (100 mg, 0.155 mmol) in CH_2Cl_2 (20 ml) was added triphenylphosphine (61 mg, 0.23 mmol). The reaction mixture was stirred for 24 h,

Table 2
Experimental details.

Crystal data	
Chemical formula	[Fe($C_{25}H_{24}O_2P$)($C_{18}H_{15}P$)(CO)$_2$]-PF_6
M_r	906.52
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	9.10074 (14), 17.7897 (3), 24.9408 (3)
β (°)	97.7826 (14)
V (Å^3)	4000.72 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.57
Crystal size (mm)	0.23 × 0.12 × 0.1
Data collection	
Diffractometer	Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min}, T_{max}	0.830, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	79564, 14181, 11299
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.763
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.095, 1.10
No. of reflections	14181
No. of parameters	573
No. of restraints	60
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.00, −0.68

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL2018* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

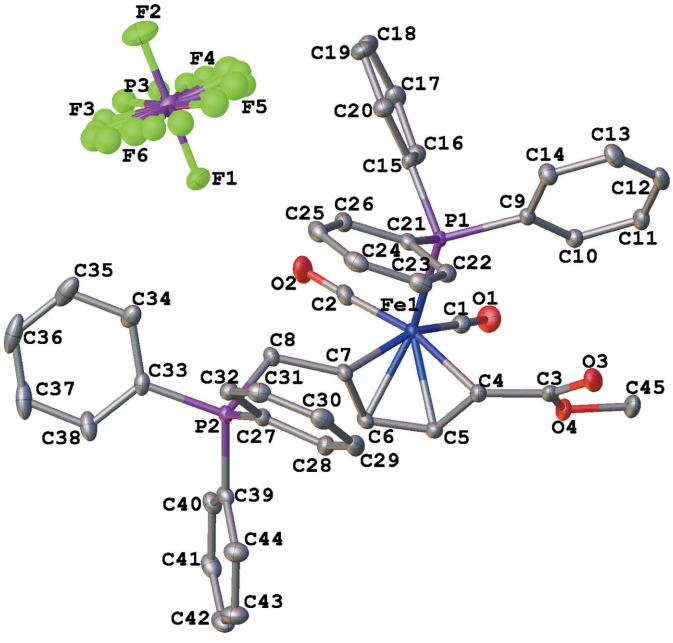


Figure 1
A view of title compound showing 50% displacement ellipsoids and H atoms omitted for clarity.

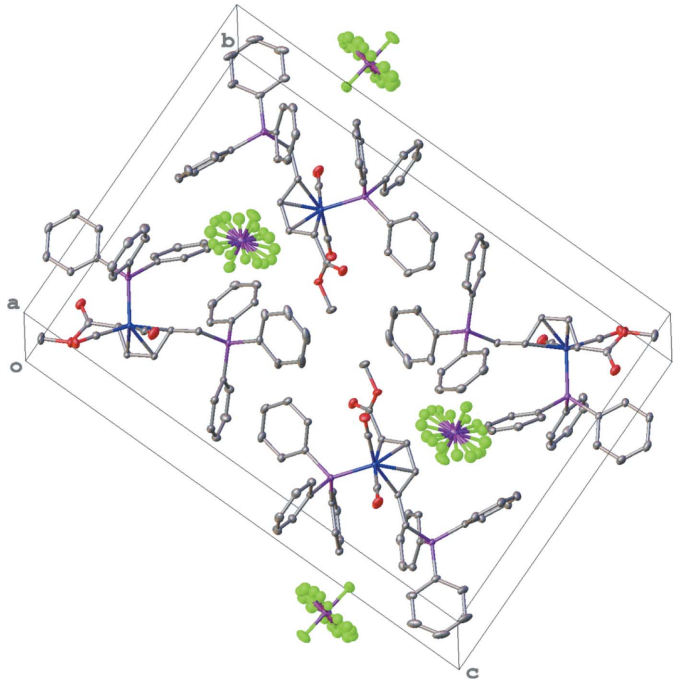


Figure 2
Packing diagram of the title compound.

and the solvent evaporated. The residue was taken up in a minimal amount of CH_2Cl_2 and diethyl ether was slowly added until the mixture became cloudy. After standing for 24 h, the yellow blocks of the title compound that had formed were collected (121 mg, 86%).

Refinement

The crystal data, data collection and structure refinement details are summarized in Table 2. The PF_6^- anion is rotationally disordered over four sets of sites (occupancy ratio 0.43/0.37/0.13/0.07).

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full crystallographic data

IUCrData (2018). **3**, x180902 [https://doi.org/10.1107/S2414314618009021]

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Crystal data

$[Fe(C_{25}H_{24}O_2P)(C_{18}H_{15}P)(CO)_2]PF_6$
M_r = 906.52
Monoclinic, $P2_1/n$
a = 9.10074 (14) Å
b = 17.7897 (3) Å
c = 24.9408 (3) Å
β = 97.7826 (14)°
V = 4000.72 (10) Å^3
Z = 4
$F(000)$ = 1864
D_x = 1.505 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 37568 reflections
θ = 3.3–32.8°
μ = 0.57 mm^{-1}
T = 100 K
Block, yellow
0.23 × 0.12 × 0.1 mm

Data collection

Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3756 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2010)
T_{min} = 0.830, T_{max} = 1.000
79564 measured reflections
14181 independent reflections
11299 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 32.8°, θ_{min} = 3.3°
h = −13→13
k = −26→27
l = −36→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
S = 1.10
14181 reflections
573 parameters
60 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.8274P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 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}	Occ. (<1)
Fe1	0.50960 (2)	0.18533 (2)	0.15093 (2)	0.01166 (4)	
P1	0.53777 (3)	0.28527 (2)	0.09909 (2)	0.01150 (6)	
P2	0.67576 (3)	0.28331 (2)	0.33137 (2)	0.01235 (6)	
O1	0.33714 (11)	0.08143 (6)	0.07598 (4)	0.0254 (2)	
O2	0.22620 (11)	0.23511 (7)	0.18090 (4)	0.0293 (2)	
O3	0.85441 (11)	0.12133 (6)	0.07077 (4)	0.0243 (2)	
O4	0.67251 (10)	0.04156 (5)	0.08681 (4)	0.02058 (18)	
C1	0.40987 (13)	0.12215 (7)	0.10423 (5)	0.0166 (2)	
C2	0.33740 (14)	0.21459 (8)	0.17000 (5)	0.0180 (2)	
C3	0.76111 (13)	0.10278 (7)	0.09825 (5)	0.0175 (2)	
C4	0.72672 (13)	0.14296 (7)	0.14662 (5)	0.0155 (2)	
H4	0.7993 (18)	0.1815 (9)	0.1577 (7)	0.019*	
C5	0.65260 (13)	0.10463 (7)	0.18571 (5)	0.0156 (2)	
H5	0.6340 (17)	0.0511 (10)	0.1824 (6)	0.019*	
C6	0.60214 (13)	0.14789 (7)	0.22669 (5)	0.0152 (2)	
H6	0.5415 (17)	0.1248 (9)	0.2520 (7)	0.018*	
C7	0.62429 (13)	0.22720 (7)	0.22568 (4)	0.0141 (2)	
H7	0.7171 (17)	0.2484 (9)	0.2157 (6)	0.017*	
C8	0.55786 (13)	0.27530 (7)	0.26610 (4)	0.0149 (2)	
H8A	0.461176	0.253617	0.272032	0.018*	
H8B	0.539080	0.326234	0.250704	0.018*	
C9	0.60530 (12)	0.27239 (7)	0.03350 (4)	0.0139 (2)	
C10	0.58330 (13)	0.20434 (7)	0.00597 (5)	0.0165 (2)	
H10	0.536751	0.163867	0.021954	0.020*	
C11	0.62896 (14)	0.19495 (8)	−0.04491 (5)	0.0198 (2)	
H11	0.613347	0.148260	−0.063292	0.024*	
C12	0.69673 (14)	0.25342 (8)	−0.06849 (5)	0.0213 (3)	
H12	0.729058	0.246773	−0.102839	0.026*	
C13	0.71752 (15)	0.32195 (9)	−0.04192 (5)	0.0225 (3)	
H13	0.763208	0.362345	−0.058308	0.027*	
C14	0.67164 (14)	0.33170 (8)	0.00870 (5)	0.0188 (2)	
H14	0.685451	0.378880	0.026511	0.023*	
C15	0.36613 (13)	0.33712 (7)	0.07575 (5)	0.0145 (2)	
C16	0.24015 (14)	0.29442 (8)	0.05757 (5)	0.0187 (2)	
H16	0.246233	0.241113	0.058428	0.022*	
C17	0.10591 (14)	0.32883 (8)	0.03823 (5)	0.0223 (3)	
H17	0.021498	0.299132	0.025636	0.027*	
C18	0.09603 (15)	0.40663 (9)	0.03743 (5)	0.0244 (3)	
H18	0.004221	0.430387	0.025019	0.029*	

C19	0.22024 (16)	0.44958 (8)	0.05477 (6)	0.0251 (3)
H19	0.213155	0.502859	0.054087	0.030*
C20	0.35557 (14)	0.41551 (7)	0.07322 (5)	0.0194 (2)
H20	0.440703	0.445552	0.084079	0.023*
C21	0.66857 (13)	0.35214 (7)	0.13420 (4)	0.0137 (2)
C22	0.82075 (13)	0.34249 (7)	0.13237 (5)	0.0169 (2)
H22	0.853714	0.305226	0.109456	0.020*
C23	0.92369 (14)	0.38739 (8)	0.16407 (5)	0.0199 (2)
H23	1.026643	0.380742	0.162608	0.024*
C24	0.87633 (15)	0.44197 (8)	0.19791 (5)	0.0208 (2)
H24	0.946840	0.472871	0.219150	0.025*
C25	0.72615 (15)	0.45121 (7)	0.20057 (5)	0.0193 (2)
H25	0.693907	0.488315	0.223766	0.023*
C26	0.62226 (14)	0.40605 (7)	0.16923 (5)	0.0162 (2)
H26	0.519633	0.411947	0.171685	0.019*
C27	0.85540 (12)	0.31824 (7)	0.32212 (5)	0.0135 (2)
C28	0.95012 (13)	0.27317 (7)	0.29597 (5)	0.0169 (2)
H28	0.921031	0.223813	0.284488	0.020*
C29	1.08716 (14)	0.30144 (8)	0.28702 (5)	0.0200 (2)
H29	1.151400	0.271516	0.268846	0.024*
C30	1.13055 (14)	0.37306 (8)	0.30446 (5)	0.0210 (2)
H30	1.223740	0.392179	0.297667	0.025*
C31	1.03898 (13)	0.41695 (8)	0.33172 (5)	0.0191 (2)
H31	1.070734	0.465372	0.344517	0.023*
C32	0.90055 (13)	0.39010 (7)	0.34036 (5)	0.0154 (2)
H32	0.836944	0.420400	0.358547	0.018*
C33	0.58470 (13)	0.34724 (7)	0.37171 (5)	0.0162 (2)
C34	0.53274 (14)	0.41623 (8)	0.34941 (5)	0.0214 (3)
H34	0.549894	0.429734	0.313930	0.026*
C35	0.45616 (15)	0.46475 (9)	0.37934 (7)	0.0306 (3)
H35	0.420563	0.511510	0.364434	0.037*
C36	0.43204 (16)	0.44459 (10)	0.43098 (7)	0.0351 (4)
H36	0.378966	0.477699	0.451270	0.042*
C37	0.48378 (17)	0.37715 (10)	0.45355 (6)	0.0325 (4)
H37	0.466493	0.364337	0.489145	0.039*
C38	0.56163 (15)	0.32762 (8)	0.42411 (5)	0.0233 (3)
H38	0.598222	0.281339	0.439562	0.028*
C39	0.69439 (13)	0.19343 (7)	0.36416 (5)	0.0155 (2)
C40	0.56826 (14)	0.14868 (8)	0.36508 (5)	0.0186 (2)
H40	0.474281	0.165616	0.348174	0.022*
C41	0.58142 (15)	0.07944 (8)	0.39086 (5)	0.0217 (3)
H41	0.496283	0.048708	0.391445	0.026*
C42	0.71826 (17)	0.05501 (8)	0.41571 (5)	0.0246 (3)
H42	0.726633	0.007179	0.432788	0.029*
C43	0.84305 (16)	0.09954 (8)	0.41593 (6)	0.0258 (3)
H43	0.936155	0.082706	0.433713	0.031*
C44	0.83189 (15)	0.16903 (8)	0.39007 (5)	0.0211 (2)
H44	0.917303	0.199724	0.390029	0.025*

C45	0.68939 (16)	0.00183 (9)	0.03779 (5)	0.0250 (3)	
H45A	0.665296	0.035475	0.006737	0.038*	
H45B	0.622336	−0.041520	0.033938	0.038*	
H45C	0.792058	−0.015554	0.039308	0.038*	
F1	0.39357 (10)	0.47983 (5)	0.23666 (4)	0.0312 (2)	
F2	0.25298 (11)	0.64373 (5)	0.21053 (5)	0.0403 (2)	
P3	0.32448 (4)	0.56186 (2)	0.22344 (2)	0.02096 (7)	0.37
F3	0.2106 (4)	0.54962 (16)	0.26530 (16)	0.0271 (7)*	0.37
F4	0.2034 (4)	0.52417 (17)	0.17613 (14)	0.0287 (8)*	0.37
F5	0.4294 (4)	0.5771 (2)	0.17871 (16)	0.0364 (9)*	0.37
F6	0.4418 (4)	0.5997 (2)	0.26859 (16)	0.0354 (9)*	0.37
P3A	0.32448 (4)	0.56186 (2)	0.22344 (2)	0.02096 (7)	0.43
F3A	0.1811 (3)	0.52250 (14)	0.19014 (15)	0.0259 (6)*	0.43
F4A	0.4034 (4)	0.56212 (17)	0.16926 (12)	0.0268 (6)*	0.43
F5A	0.4666 (3)	0.59915 (16)	0.25598 (15)	0.0280 (6)*	0.43
F6A	0.2465 (4)	0.55559 (16)	0.27815 (12)	0.0266 (6)*	0.43
P3B	0.32448 (4)	0.56186 (2)	0.22344 (2)	0.02096 (7)	0.13
F3B	0.1640 (6)	0.5296 (4)	0.2111 (4)	0.0215 (14)*	0.13
F4B	0.3488 (11)	0.5597 (4)	0.1627 (3)	0.0243 (16)*	0.13
F5B	0.4940 (8)	0.5955 (4)	0.2370 (4)	0.0305 (18)*	0.13
F6B	0.3016 (11)	0.5704 (5)	0.2882 (3)	0.0288 (16)*	0.13
P3C	0.32448 (4)	0.56186 (2)	0.22344 (2)	0.02096 (7)	0.07
F3C	0.1707 (12)	0.5445 (8)	0.2403 (7)	0.026 (3)*	0.07
F4C	0.268 (2)	0.5397 (9)	0.1629 (5)	0.038 (3)*	0.07
F5C	0.4811 (14)	0.5899 (9)	0.2041 (7)	0.036 (3)*	0.07
F6C	0.3860 (18)	0.5892 (9)	0.2862 (5)	0.034 (3)*	0.07

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01364 (8)	0.01179 (8)	0.00994 (7)	−0.00023 (6)	0.00305 (5)	−0.00066 (6)
P1	0.01232 (12)	0.01155 (13)	0.01090 (12)	0.00070 (10)	0.00255 (9)	−0.00062 (10)
P2	0.01393 (13)	0.01307 (13)	0.01041 (12)	−0.00088 (10)	0.00300 (9)	−0.00133 (10)
O1	0.0278 (5)	0.0223 (5)	0.0254 (5)	−0.0058 (4)	0.0005 (4)	−0.0071 (4)
O2	0.0223 (5)	0.0447 (7)	0.0230 (5)	0.0070 (4)	0.0110 (4)	0.0005 (5)
O3	0.0229 (4)	0.0329 (6)	0.0189 (4)	0.0057 (4)	0.0089 (3)	0.0021 (4)
O4	0.0282 (5)	0.0190 (4)	0.0153 (4)	0.0051 (4)	0.0055 (3)	−0.0044 (3)
C1	0.0186 (5)	0.0152 (5)	0.0161 (5)	0.0007 (4)	0.0033 (4)	0.0005 (4)
C2	0.0216 (6)	0.0206 (6)	0.0121 (5)	−0.0015 (5)	0.0035 (4)	−0.0003 (4)
C3	0.0183 (5)	0.0205 (6)	0.0135 (5)	0.0077 (4)	0.0017 (4)	0.0016 (4)
C4	0.0172 (5)	0.0167 (5)	0.0129 (5)	0.0031 (4)	0.0028 (4)	−0.0004 (4)
C5	0.0203 (5)	0.0140 (5)	0.0125 (5)	0.0028 (4)	0.0021 (4)	0.0008 (4)
C6	0.0203 (5)	0.0151 (5)	0.0105 (5)	−0.0003 (4)	0.0025 (4)	0.0009 (4)
C7	0.0165 (5)	0.0153 (5)	0.0105 (4)	−0.0005 (4)	0.0024 (4)	−0.0004 (4)
C8	0.0172 (5)	0.0169 (5)	0.0107 (5)	−0.0005 (4)	0.0019 (4)	−0.0011 (4)
C9	0.0134 (5)	0.0167 (5)	0.0116 (5)	0.0024 (4)	0.0017 (4)	0.0000 (4)
C10	0.0192 (5)	0.0164 (5)	0.0136 (5)	0.0022 (4)	0.0017 (4)	−0.0010 (4)
C11	0.0217 (6)	0.0235 (6)	0.0139 (5)	0.0047 (5)	0.0013 (4)	−0.0040 (5)

C12	0.0190 (6)	0.0329 (7)	0.0124 (5)	0.0052 (5)	0.0033 (4)	−0.0008 (5)
C13	0.0229 (6)	0.0291 (7)	0.0166 (5)	−0.0029 (5)	0.0067 (4)	0.0028 (5)
C14	0.0219 (6)	0.0194 (6)	0.0160 (5)	−0.0024 (5)	0.0050 (4)	−0.0001 (4)
C15	0.0157 (5)	0.0163 (5)	0.0120 (5)	0.0036 (4)	0.0035 (4)	0.0000 (4)
C16	0.0174 (5)	0.0198 (6)	0.0187 (5)	0.0020 (4)	0.0015 (4)	−0.0010 (5)
C17	0.0163 (5)	0.0308 (7)	0.0195 (6)	0.0035 (5)	0.0014 (4)	−0.0004 (5)
C18	0.0210 (6)	0.0317 (7)	0.0209 (6)	0.0129 (5)	0.0038 (5)	0.0025 (5)
C19	0.0301 (7)	0.0205 (6)	0.0246 (6)	0.0106 (5)	0.0035 (5)	0.0026 (5)
C20	0.0220 (6)	0.0168 (6)	0.0196 (5)	0.0025 (5)	0.0032 (4)	0.0012 (5)
C21	0.0164 (5)	0.0131 (5)	0.0118 (5)	−0.0014 (4)	0.0022 (4)	0.0011 (4)
C22	0.0177 (5)	0.0170 (5)	0.0163 (5)	0.0007 (4)	0.0034 (4)	0.0022 (4)
C23	0.0167 (5)	0.0230 (6)	0.0196 (6)	−0.0030 (5)	0.0006 (4)	0.0043 (5)
C24	0.0248 (6)	0.0192 (6)	0.0167 (5)	−0.0065 (5)	−0.0029 (4)	0.0024 (5)
C25	0.0280 (6)	0.0157 (6)	0.0140 (5)	−0.0031 (5)	0.0025 (4)	−0.0016 (4)
C26	0.0197 (5)	0.0153 (5)	0.0141 (5)	−0.0007 (4)	0.0037 (4)	−0.0006 (4)
C27	0.0138 (5)	0.0145 (5)	0.0126 (5)	0.0002 (4)	0.0029 (4)	0.0003 (4)
C28	0.0184 (5)	0.0173 (6)	0.0152 (5)	0.0019 (4)	0.0031 (4)	−0.0018 (4)
C29	0.0167 (5)	0.0267 (7)	0.0176 (5)	0.0046 (5)	0.0058 (4)	0.0017 (5)
C30	0.0143 (5)	0.0273 (7)	0.0214 (6)	−0.0014 (5)	0.0026 (4)	0.0054 (5)
C31	0.0170 (5)	0.0183 (6)	0.0212 (6)	−0.0029 (4)	−0.0003 (4)	0.0020 (5)
C32	0.0163 (5)	0.0145 (5)	0.0154 (5)	0.0005 (4)	0.0023 (4)	−0.0001 (4)
C33	0.0139 (5)	0.0196 (6)	0.0158 (5)	−0.0024 (4)	0.0044 (4)	−0.0059 (4)
C34	0.0179 (5)	0.0241 (7)	0.0208 (6)	0.0042 (5)	−0.0024 (4)	−0.0074 (5)
C35	0.0180 (6)	0.0317 (8)	0.0400 (8)	0.0076 (5)	−0.0044 (5)	−0.0180 (7)
C36	0.0181 (6)	0.0430 (9)	0.0462 (9)	−0.0043 (6)	0.0117 (6)	−0.0294 (8)
C37	0.0319 (7)	0.0406 (9)	0.0296 (7)	−0.0169 (7)	0.0209 (6)	−0.0185 (7)
C38	0.0276 (7)	0.0249 (7)	0.0202 (6)	−0.0103 (5)	0.0127 (5)	−0.0074 (5)
C39	0.0212 (5)	0.0138 (5)	0.0115 (5)	−0.0025 (4)	0.0025 (4)	−0.0011 (4)
C40	0.0212 (6)	0.0205 (6)	0.0149 (5)	−0.0040 (5)	0.0049 (4)	−0.0002 (4)
C41	0.0297 (6)	0.0192 (6)	0.0175 (5)	−0.0080 (5)	0.0077 (5)	−0.0011 (5)
C42	0.0383 (7)	0.0154 (6)	0.0203 (6)	−0.0021 (5)	0.0054 (5)	0.0023 (5)
C43	0.0295 (7)	0.0198 (6)	0.0264 (7)	0.0012 (5)	−0.0024 (5)	0.0056 (5)
C44	0.0222 (6)	0.0176 (6)	0.0223 (6)	−0.0031 (5)	−0.0013 (5)	0.0021 (5)
C45	0.0307 (7)	0.0279 (7)	0.0161 (5)	0.0105 (6)	0.0018 (5)	−0.0071 (5)
F1	0.0343 (5)	0.0298 (5)	0.0312 (5)	0.0138 (4)	0.0105 (4)	0.0049 (4)
F2	0.0383 (5)	0.0219 (5)	0.0584 (7)	0.0049 (4)	−0.0022 (5)	0.0023 (4)
P3	0.01575 (14)	0.02113 (17)	0.02609 (17)	0.00089 (12)	0.00322 (12)	0.00016 (13)
P3A	0.01575 (14)	0.02113 (17)	0.02609 (17)	0.00089 (12)	0.00322 (12)	0.00016 (13)
P3B	0.01575 (14)	0.02113 (17)	0.02609 (17)	0.00089 (12)	0.00322 (12)	0.00016 (13)
P3C	0.01575 (14)	0.02113 (17)	0.02609 (17)	0.00089 (12)	0.00322 (12)	0.00016 (13)

Geometric parameters (Å, º)

Fe1—P1	2.2334 (3)	C26—H26	0.9500
Fe1—C1	1.7769 (12)	C27—C28	1.4013 (16)
Fe1—C2	1.7762 (13)	C27—C32	1.3998 (17)
Fe1—C4	2.1312 (12)	C28—H28	0.9500
Fe1—C5	2.0497 (12)	C28—C29	1.3906 (18)

Fe1—C6	2.0717 (11)	C29—H29	0.9500
Fe1—C7	2.1431 (11)	C29—C30	1.386 (2)
P1—C9	1.8379 (11)	C30—H30	0.9500
P1—C15	1.8394 (12)	C30—C31	1.3857 (19)
P1—C21	1.8212 (12)	C31—H31	0.9500
P2—C8	1.8298 (12)	C31—C32	1.3911 (17)
P2—C27	1.7929 (12)	C32—H32	0.9500
P2—C33	1.7939 (12)	C33—C34	1.4030 (19)
P2—C39	1.7936 (13)	C33—C38	1.3959 (18)
O1—C1	1.1545 (15)	C34—H34	0.9500
O2—C2	1.1428 (16)	C34—C35	1.3889 (19)
O3—C3	1.2071 (15)	C35—H35	0.9500
O4—C3	1.3621 (16)	C35—C36	1.383 (3)
O4—C45	1.4382 (15)	C36—H36	0.9500
C3—C4	1.4719 (17)	C36—C37	1.381 (3)
C4—H4	0.966 (16)	C37—H37	0.9500
C4—C5	1.4312 (17)	C37—C38	1.399 (2)
C5—H5	0.969 (17)	C38—H38	0.9500
C5—C6	1.4052 (16)	C39—C40	1.3996 (17)
C6—H6	0.982 (16)	C39—C44	1.3974 (18)
C6—C7	1.4260 (17)	C40—H40	0.9500
C7—H7	0.987 (16)	C40—C41	1.3871 (19)
C7—C8	1.5097 (16)	C41—H41	0.9500
C8—H8A	0.9900	C41—C42	1.384 (2)
C8—H8B	0.9900	C42—H42	0.9500
C9—C10	1.3928 (17)	C42—C43	1.384 (2)
C9—C14	1.4005 (17)	C43—H43	0.9500
C10—H10	0.9500	C43—C44	1.3917 (19)
C10—C11	1.3979 (17)	C44—H44	0.9500
C11—H11	0.9500	C45—H45A	0.9800
C11—C12	1.381 (2)	C45—H45B	0.9800
C12—H12	0.9500	C45—H45C	0.9800
C12—C13	1.388 (2)	F1—P3	1.6054 (10)
C13—H13	0.9500	F1—P3A	1.6054 (10)
C13—C14	1.3932 (17)	F1—P3B	1.6054 (10)
C14—H14	0.9500	F1—P3C	1.6054 (10)
C15—C16	1.3987 (17)	F2—P3	1.6099 (10)
C15—C20	1.3987 (18)	F2—P3A	1.6099 (10)
C16—H16	0.9500	F2—P3B	1.6099 (10)
C16—C17	1.3929 (18)	F2—P3C	1.6099 (10)
C17—H17	0.9500	P3—F3	1.583 (3)
C17—C18	1.387 (2)	P3—F4	1.644 (3)
C18—H18	0.9500	P3—F5	1.587 (3)
C18—C19	1.384 (2)	P3—F6	1.593 (3)
C19—H19	0.9500	P3A—F3A	1.609 (2)
C19—C20	1.3937 (18)	P3A—F4A	1.614 (3)
C20—H20	0.9500	P3A—F5A	1.577 (3)
C21—C22	1.4023 (16)	P3A—F6A	1.625 (2)

C21—C26	1.4003 (17)	P3B—F3B	1.560 (6)
C22—H22	0.9500	P3B—F4B	1.562 (6)
C22—C23	1.3929 (18)	P3B—F5B	1.647 (7)
C23—H23	0.9500	P3B—F6B	1.664 (6)
C23—C24	1.393 (2)	P3C—F3C	1.546 (9)
C24—H24	0.9500	P3C—F4C	1.576 (10)
C24—C25	1.3871 (19)	P3C—F5C	1.643 (10)
C25—H25	0.9500	P3C—F6C	1.663 (10)
C25—C26	1.3964 (17)		

C1—Fe1—P1	102.27 (4)	C25—C26—H26	119.8
C1—Fe1—C4	97.93 (5)	C28—C27—P2	119.38 (9)
C1—Fe1—C5	94.19 (5)	C32—C27—P2	120.49 (9)
C1—Fe1—C6	120.19 (5)	C32—C27—C28	120.12 (11)
C1—Fe1—C7	159.30 (5)	C27—C28—H28	120.4
C2—Fe1—P1	95.53 (4)	C29—C28—C27	119.30 (12)
C2—Fe1—C1	88.28 (6)	C29—C28—H28	120.4
C2—Fe1—C4	167.12 (5)	C28—C29—H29	119.8
C2—Fe1—C5	128.65 (5)	C30—C29—C28	120.38 (12)
C2—Fe1—C6	96.57 (5)	C30—C29—H29	119.8
C2—Fe1—C7	90.50 (5)	C29—C30—H30	119.8
C4—Fe1—P1	94.16 (3)	C31—C30—C29	120.47 (12)
C4—Fe1—C7	79.70 (4)	C31—C30—H30	119.8
C5—Fe1—P1	133.35 (4)	C30—C31—H31	120.0
C5—Fe1—C4	39.98 (5)	C30—C31—C32	120.00 (12)
C5—Fe1—C6	39.87 (5)	C32—C31—H31	120.0
C5—Fe1—C7	70.66 (5)	C27—C32—H32	120.2
C6—Fe1—P1	136.02 (4)	C31—C32—C27	119.69 (11)
C6—Fe1—C4	70.55 (5)	C31—C32—H32	120.2
C6—Fe1—C7	39.51 (5)	C34—C33—P2	119.26 (9)
C7—Fe1—P1	98.42 (3)	C38—C33—P2	120.41 (11)
C9—P1—Fe1	119.63 (4)	C38—C33—C34	120.30 (12)
C9—P1—C15	98.79 (5)	C33—C34—H34	120.1
C15—P1—Fe1	115.04 (4)	C35—C34—C33	119.82 (14)
C21—P1—Fe1	111.13 (4)	C35—C34—H34	120.1
C21—P1—C9	103.52 (5)	C34—C35—H35	120.2
C21—P1—C15	107.24 (6)	C36—C35—C34	119.60 (15)
C27—P2—C8	110.34 (5)	C36—C35—H35	120.2
C27—P2—C33	110.54 (6)	C35—C36—H36	119.4
C27—P2—C39	109.64 (6)	C37—C36—C35	121.12 (13)
C33—P2—C8	106.77 (6)	C37—C36—H36	119.4
C39—P2—C8	110.13 (6)	C36—C37—H37	119.9
C39—P2—C33	109.37 (6)	C36—C37—C38	120.14 (14)
C3—O4—C45	116.27 (11)	C38—C37—H37	119.9
O1—C1—Fe1	175.30 (11)	C33—C38—C37	119.01 (15)
O2—C2—Fe1	177.73 (12)	C33—C38—H38	120.5
O3—C3—O4	122.80 (12)	C37—C38—H38	120.5
O3—C3—C4	125.21 (13)	C40—C39—P2	119.17 (10)

O4—C3—C4	111.99 (10)	C44—C39—P2	120.74 (9)
Fe1—C4—H4	109.7 (10)	C44—C39—C40	120.06 (12)
C3—C4—Fe1	120.97 (8)	C39—C40—H40	120.2
C3—C4—H4	111.5 (10)	C41—C40—C39	119.55 (12)
C5—C4—Fe1	66.94 (7)	C41—C40—H40	120.2
C5—C4—C3	119.94 (11)	C40—C41—H41	119.9
C5—C4—H4	120.6 (10)	C42—C41—C40	120.16 (12)
Fe1—C5—H5	124.0 (9)	C42—C41—H41	119.9
C4—C5—Fe1	73.08 (7)	C41—C42—H42	119.7
C4—C5—H5	120.2 (10)	C41—C42—C43	120.68 (13)
C6—C5—Fe1	70.91 (7)	C43—C42—H42	119.7
C6—C5—C4	117.72 (11)	C42—C43—H43	120.1
C6—C5—H5	122.0 (10)	C42—C43—C44	119.88 (13)
Fe1—C6—H6	121.7 (9)	C44—C43—H43	120.1
C5—C6—Fe1	69.22 (7)	C39—C44—H44	120.2
C5—C6—H6	120.3 (10)	C43—C44—C39	119.65 (12)
C5—C6—C7	117.91 (11)	C43—C44—H44	120.2
C7—C6—Fe1	72.95 (7)	O4—C45—H45A	109.5
C7—C6—H6	121.2 (10)	O4—C45—H45B	109.5
Fe1—C7—H7	104.3 (9)	O4—C45—H45C	109.5
C6—C7—Fe1	67.55 (6)	H45A—C45—H45B	109.5
C6—C7—H7	120.7 (10)	H45A—C45—H45C	109.5
C6—C7—C8	118.60 (10)	H45B—C45—H45C	109.5
C8—C7—Fe1	125.88 (8)	F1—P3—F2	179.14 (6)
C8—C7—H7	112.7 (10)	F1—P3—F4	89.00 (11)
P2—C8—H8A	108.9	F2—P3—F4	90.69 (11)
P2—C8—H8B	108.9	F3—P3—F1	90.72 (11)
C7—C8—P2	113.49 (8)	F3—P3—F2	88.47 (12)
C7—C8—H8A	108.9	F3—P3—F4	88.98 (19)
C7—C8—H8B	108.9	F3—P3—F5	175.89 (19)
H8A—C8—H8B	107.7	F3—P3—F6	91.6 (2)
C10—C9—P1	120.27 (9)	F5—P3—F1	92.47 (14)
C10—C9—C14	118.61 (11)	F5—P3—F2	88.32 (14)
C14—C9—P1	121.02 (9)	F5—P3—F4	88.5 (2)
C9—C10—H10	119.6	F5—P3—F6	90.9 (2)
C9—C10—C11	120.73 (12)	F6—P3—F1	91.86 (13)
C11—C10—H10	119.6	F6—P3—F2	88.46 (13)
C10—C11—H11	120.0	F6—P3—F4	178.96 (19)
C12—C11—C10	120.10 (12)	F1—P3A—F2	179.14 (6)
C12—C11—H11	120.0	F1—P3A—F3A	88.75 (10)
C11—C12—H12	120.1	F1—P3A—F4A	88.19 (11)
C11—C12—C13	119.87 (12)	F1—P3A—F6A	88.20 (10)
C13—C12—H12	120.1	F2—P3A—F4A	92.49 (11)
C12—C13—H13	119.9	F2—P3A—F6A	91.11 (10)
C12—C13—C14	120.25 (12)	F3A—P3A—F2	90.73 (10)
C14—C13—H13	119.9	F3A—P3A—F4A	89.47 (19)
C9—C14—H14	119.8	F3A—P3A—F6A	89.29 (18)
C13—C14—C9	120.43 (12)	F4A—P3A—F6A	176.20 (14)

C13—C14—H14	119.8	F5A—P3A—F1	90.32 (11)
C16—C15—P1	117.00 (9)	F5A—P3A—F2	90.20 (11)
C16—C15—C20	118.59 (11)	F5A—P3A—F3A	179.02 (16)
C20—C15—P1	124.37 (9)	F5A—P3A—F4A	90.2 (2)
C15—C16—H16	119.5	F5A—P3A—F6A	91.00 (19)
C17—C16—C15	121.04 (13)	F1—P3B—F2	179.14 (6)
C17—C16—H16	119.5	F1—P3B—F5B	87.6 (3)
C16—C17—H17	120.1	F1—P3B—F6B	88.9 (3)
C18—C17—C16	119.71 (13)	F2—P3B—F5B	93.1 (3)
C18—C17—H17	120.1	F2—P3B—F6B	90.6 (3)
C17—C18—H18	120.1	F3B—P3B—F1	92.1 (3)
C19—C18—C17	119.85 (12)	F3B—P3B—F2	87.2 (3)
C19—C18—H18	120.1	F3B—P3B—F4B	93.0 (5)
C18—C19—H19	119.6	F3B—P3B—F5B	179.5 (5)
C18—C19—C20	120.72 (13)	F3B—P3B—F6B	89.3 (5)
C20—C19—H19	119.6	F4B—P3B—F1	94.3 (3)
C15—C20—H20	120.0	F4B—P3B—F2	86.2 (3)
C19—C20—C15	120.05 (12)	F4B—P3B—F5B	87.5 (5)
C19—C20—H20	120.0	F4B—P3B—F6B	176.0 (4)
C22—C21—P1	119.24 (9)	F5B—P3B—F6B	90.3 (5)
C26—C21—P1	121.00 (9)	F1—P3C—F2	179.14 (6)
C26—C21—C22	119.09 (11)	F1—P3C—F5C	90.3 (5)
C21—C22—H22	119.9	F1—P3C—F6C	90.0 (5)
C23—C22—C21	120.17 (12)	F2—P3C—F5C	90.6 (5)
C23—C22—H22	119.9	F2—P3C—F6C	89.9 (5)
C22—C23—H23	119.9	F3C—P3C—F1	96.1 (5)
C24—C23—C22	120.28 (12)	F3C—P3C—F2	83.0 (5)
C24—C23—H23	119.9	F3C—P3C—F4C	91.3 (8)
C23—C24—H24	120.0	F3C—P3C—F5C	173.6 (7)
C25—C24—C23	119.96 (12)	F3C—P3C—F6C	90.3 (8)
C25—C24—H24	120.0	F4C—P3C—F1	92.1 (6)
C24—C25—H25	119.9	F4C—P3C—F2	88.0 (6)
C24—C25—C26	120.13 (12)	F4C—P3C—F5C	88.7 (9)
C26—C25—H25	119.9	F4C—P3C—F6C	177.2 (9)
C21—C26—H26	119.8	F5C—P3C—F6C	89.6 (8)
C25—C26—C21	120.34 (11)		

Fe1—P1—C9—C10	25.81 (11)	C15—P1—C21—C26	41.49 (11)
Fe1—P1—C9—C14	−158.01 (8)	C15—C16—C17—C18	−0.7 (2)
Fe1—P1—C15—C16	−43.04 (10)	C16—C15—C20—C19	2.36 (18)
Fe1—P1—C15—C20	139.46 (9)	C16—C17—C18—C19	1.4 (2)
Fe1—P1—C21—C22	85.53 (10)	C17—C18—C19—C20	−0.2 (2)
Fe1—P1—C21—C26	−85.02 (10)	C18—C19—C20—C15	−1.7 (2)
Fe1—C4—C5—C6	−56.90 (9)	C20—C15—C16—C17	−1.17 (18)
Fe1—C5—C6—C7	−56.23 (10)	C21—P1—C9—C10	150.09 (9)
Fe1—C6—C7—C8	119.80 (10)	C21—P1—C9—C14	−33.73 (11)
Fe1—C7—C8—P2	167.38 (6)	C21—P1—C15—C16	−167.19 (9)
P1—C9—C10—C11	177.44 (9)	C21—P1—C15—C20	15.30 (12)

P1—C9—C14—C13	−177.68 (10)	C21—C22—C23—C24	0.21 (19)
P1—C15—C16—C17	−178.82 (10)	C22—C21—C26—C25	2.07 (18)
P1—C15—C20—C19	179.83 (10)	C22—C23—C24—C25	0.73 (19)
P1—C21—C22—C23	−172.32 (9)	C23—C24—C25—C26	−0.25 (19)
P1—C21—C26—C25	172.62 (9)	C24—C25—C26—C21	−1.16 (19)
P2—C27—C28—C29	177.59 (9)	C26—C21—C22—C23	−1.59 (18)
P2—C27—C32—C31	−178.52 (9)	C27—P2—C8—C7	55.85 (10)
P2—C33—C34—C35	177.10 (10)	C27—P2—C33—C34	71.33 (11)
P2—C33—C38—C37	−176.86 (10)	C27—P2—C33—C38	−110.66 (11)
P2—C39—C40—C41	−179.33 (9)	C27—P2—C39—C40	−166.48 (9)
P2—C39—C44—C43	179.03 (11)	C27—P2—C39—C44	15.56 (12)
O3—C3—C4—Fe1	121.25 (12)	C27—C28—C29—C30	0.92 (19)
O3—C3—C4—C5	−159.20 (12)	C28—C27—C32—C31	0.91 (17)
O4—C3—C4—Fe1	−57.61 (13)	C28—C29—C30—C31	0.95 (19)
O4—C3—C4—C5	21.94 (15)	C29—C30—C31—C32	−1.91 (19)
C3—C4—C5—Fe1	−113.59 (10)	C30—C31—C32—C27	0.97 (18)
C3—C4—C5—C6	−170.50 (11)	C32—C27—C28—C29	−1.85 (18)
C4—C5—C6—Fe1	58.01 (9)	C33—P2—C8—C7	176.03 (9)
C4—C5—C6—C7	1.78 (16)	C33—P2—C27—C28	174.08 (9)
C5—C6—C7—Fe1	54.38 (9)	C33—P2—C27—C32	−6.48 (11)
C5—C6—C7—C8	174.18 (10)	C33—P2—C39—C40	72.15 (11)
C6—C7—C8—P2	85.57 (12)	C33—P2—C39—C44	−105.80 (11)
C8—P2—C27—C28	−68.04 (11)	C33—C34—C35—C36	0.1 (2)
C8—P2—C27—C32	111.40 (10)	C34—C33—C38—C37	1.13 (19)
C8—P2—C33—C34	−48.72 (11)	C34—C35—C36—C37	0.5 (2)
C8—P2—C33—C38	129.30 (10)	C35—C36—C37—C38	−0.3 (2)
C8—P2—C39—C40	−44.89 (11)	C36—C37—C38—C33	−0.5 (2)
C8—P2—C39—C44	137.16 (10)	C38—C33—C34—C35	−0.92 (19)
C9—P1—C15—C16	85.61 (10)	C39—P2—C8—C7	−65.33 (10)
C9—P1—C15—C20	−91.89 (11)	C39—P2—C27—C28	53.43 (11)
C9—P1—C21—C22	−44.12 (11)	C39—P2—C27—C32	−127.14 (10)
C9—P1—C21—C26	145.34 (10)	C39—P2—C33—C34	−167.85 (10)
C9—C10—C11—C12	0.00 (18)	C39—P2—C33—C38	10.16 (12)
C10—C9—C14—C13	−1.45 (18)	C39—C40—C41—C42	0.33 (19)
C10—C11—C12—C13	−0.93 (19)	C40—C39—C44—C43	1.10 (19)
C11—C12—C13—C14	0.7 (2)	C40—C41—C42—C43	1.0 (2)
C12—C13—C14—C9	0.5 (2)	C41—C42—C43—C44	−1.2 (2)
C14—C9—C10—C11	1.18 (18)	C42—C43—C44—C39	0.2 (2)
C15—P1—C9—C10	−99.69 (10)	C44—C39—C40—C41	−1.36 (18)
C15—P1—C9—C14	76.49 (11)	C45—O4—C3—O3	−3.63 (17)
C15—P1—C21—C22	−147.96 (9)	C45—O4—C3—C4	175.26 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C26—H26···F1	0.95	2.43	3.1353 (15)	131
C28—H28···F5*B*^{i}	0.95	2.49	3.322 (8)	146
C28—H28···F5*C*^{i}	0.95	2.55	3.320 (15)	139

C32—H32···O4^{ii}	0.95	2.56	3.3659 (16)	143
C34—H34···F1	0.95	2.41	3.1349 (16)	133
C40—H40···F2^{iii}	0.95	2.40	3.2586 (16)	150

Symmetry codes: (i) $-x+3/2, y-1/2, -z+1/2$; (ii) $-x+3/2, y+1/2, -z+1/2$; (iii) $-x+1/2, y-1/2, -z+1/2$.