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(*OC*-6-13)-Bis(acetone)dihydrido-bis(tricyclohexylphosphine)iridium(III) tetrafluoridoborate acetone solvate

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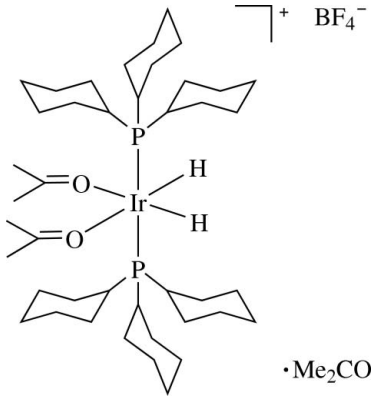
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.024; wR factor = 0.043; data-to-parameter ratio = 23.4.

The title solvated salt, $[Ir(H)_2\{P(C_6H_{11})_3\}_2\{OC(CH_3)_2\}_2]BF_4\cdot(CH_3)_2CO$, was obtained by the protonation of $[Ir(H)_5\{P(C_6H_{11})_3\}_2]$ with HBF_4 in acetone. The cation features *OC*-6-13 stereochemistry, with Ir—P = 2.3159 (6) and 2.3267 (6) Å, and Ir—O = 2.238 (1) and 2.276 (1) Å. The BF_4^- anion shows threefold rotational disorder about a B—F bond, with site occupancies of 0.65, 0.25 and 0.10. While there are several intramolecular C—H···O and intermolecular C—H···F hydrogen-bonding interactions [C···O = 3.207 (3)–3.358 (3) Å, and C···F = 3.434 (3) and 3.441 (3) Å], the O atom of the acetone solvent molecule does not act as a C—H acceptor.

Related literature

For the corresponding solvent-free bis(triphenylphosphine) complex, $[Ir(H)_2\{P(C_6H_5)_3\}_2\{OC(CH_3)_2\}_2][BF_4]$, see Crabtree *et al.* (1984). For data analysis techniques, see Orpen (1980).



Experimental

Crystal data

$[IrH_2(C_{18}H_{33}P)_2(C_3H_6O)_2]BF_4\cdot C_3H_6O$
M_r = 1016.09
Monoclinic, $P2_1/c$
a = 10.218 (1) Å
b = 25.199 (4) Å
c = 19.621 (1) Å
β = 102.060 (5)°
V = 4940.6 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.82 mm^{-1}
T = 100 (2) K
0.20 × 0.18 × 0.17 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: integration (Gaussian; Coppens *et al.*, 1965)
T_{min} = 0.562, T_{max} = 0.687
111705 measured reflections
12737 independent reflections
10353 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.043
S = 1.04
12737 reflections
544 parameters
39 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ir1—O2	2.2379 (13)	Ir1—P2	2.3159 (6)
Ir1—O1	2.2762 (14)	Ir1—P1	2.3267 (6)
O2—Ir1—O1	83.00 (5)	O2—Ir1—P1	94.84 (4)
O2—Ir1—P2	97.03 (4)	O1—Ir1—P1	92.05 (4)
O1—Ir1—P2	96.06 (4)	P2—Ir1—P1	166.350 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8*A*···O1	0.99	2.49	3.358 (3)	146
C18—H18*A*···O2	0.99	2.45	3.207 (3)	133
C36—H36*B*···O1	0.99	2.50	3.347 (3)	144
C39—H39*A*···O2	0.98	2.45	3.304 (3)	146
C39—H39*B*···F4^{i}	0.98	2.54	3.441 (3)	153
C40—H40*B*···F1^{ii}	0.98	2.51	3.434 (3)	156

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

Data collection: *COLLECT* (Bruker–Nonius, 2002); cell refinement: *COLLECT*; data reduction: *COLLECT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2038).

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supplementary materials

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(*OC*-6-13)-Bis(acetone)dihydridobis(tricyclohexylphosphine)iridium(III) tetrafluoridoborate acetone solvate

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Comment

The cation of the title complex (Fig. 1), adopts a slightly distorted *OC*-6–13 coordination geometry, where the two monodentate phosphines lie *trans* to each other [Ir—P = 2.3159 (6) and 2.3267 (6) Å] and the hydrides are opposite to the O-bound acetone groups [Ir—O = 2.238 (1) and 2.276 (1) Å] (Table 1). The tetrafluoridoborate anion exhibts threefold rotational disorder about the B1—F1 axis. The acetone molecule of solvation, by contrast, is located in fully ordered atomic positions.

The ionic components are linked by C—H···F hydrogen-bonding contacts, in which atoms C39 and C40 of the acetone ligands act as donors, *via* H39B and H40B, to fluorine atoms F4 and F1 with C39···F4($-x+1, y-1/2, -z+1/2$) = 3.441 (3) Å and C40···F1($x-1, -y+3/2, z-1/2+z$) = 3.434 (3) Å, respectively. Even though the cation displays several intramolecular C—H···O interactions with C···O distances in the range 3.207 (3)–3.358 (3) Å (Table 2), the oxygen atom of the solvate molecule does not function as a carbon—hydrogen bond acceptor.

In the corresponding solvate-free bis(triphenylphosphine) complex $[Ir(H)_2\{P(C_6H_5)_3\}_2\{OC(CH_3)_2\}_2][BF_4]$, the cation also has pseudooctahedral geometry with the two phosphines in mutual *trans* coordination and the hydrido ligands opposite to the acetone molecules (Crabtree *et al.*, 1984).

Experimental

Single crystals of the title compound were obtained by protonation of $[Ir(H)_5\{P(C_6H_{11})_3\}_2]$ with tetrafluoridoboric acid (54% in diethyl ether) in acetone, followed by slow evaporation of the solvent at ambient temperature.

Refinement

The rotational disorder of the BF_4^- anion about the B1—F1 axis was modelled using one major and two minor orientations of the remaining BF_3 fragment with fluorine site occupancies fixed at 0.65, 1/4, and 0.10, respectively. Standard SADI restraints with subsequent rigid-group refinement were applied for the tetrahedral dimensions of the disordered ion. The two hydride ligands were placed, with Ir—H restrained to 1.55 Å, at the positions calculated by the HYDEX energy-minimizing procedure (Orpen, 1980). Carbon-bound H atoms were positioned geometrically (C—H = 0.96–0.99 Å) and refined using appropriate riding models. All hydrogen U_{iso} values were fixed at 1.2 times U_{eq} of the preceding carrier atom.

Figures

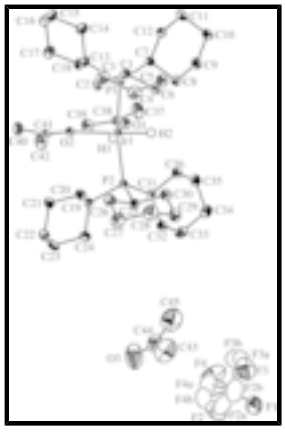


Fig. 1. Molecular structures of the ionic and solvate components of (I), including the major (octant-shaded) and minor (boundary) atomic positions of the disordered BF_4^- ion. Displacement ellipsoids are drawn at the 50% probability level. Carbon-bonded H atoms are omitted for clarity.

(*OC*-6–13)-Bis(acetone)dihydridobis(tricyclohexylphosphine)iridium(III) tetrafluoridoborate acetone solvate

Crystal data

$[IrH_2(C_{18}H_{33}P)_2(C_3H_6O)_2]BF_4{\cdot}C_3H_6O$	F_{000} = 2112
M_r = 1016.09	D_x = 1.366 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 244 reflections
a = 10.218 (1) Å	θ = 6–20º
b = 25.199 (4) Å	μ = 2.82 mm^{-1}
c = 19.621 (1) Å	T = 100 (2) K
β = 102.060 (5)º	Irregular, yellow
V = 4940.6 (10) Å^3	0.20 × 0.18 × 0.17 mm
Z = 4	

Data collection

Nonius KappaCCD area-detector diffractometer	12737 independent reflections
Monochromator: graphite	10353 reflections with $I > 2\sigma(I)$
Detector resolution: 9 pixels mm^{-1}	R_{int} = 0.049
T = 100(2) K	θ_{max} = 28.7º
φ– and ω–rotations with 1.10 ° and 55 sec per frame scans	θ_{min} = 3.0º
Absorption correction: integration (Gaussian; Coppens *et al.*, 1965)	h = −13→13
T_{min} = 0.562, T_{max} = 0.687	k = −34→34
111705 measured reflections	l = −26→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.024$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0135P)^2 + 3.6535P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.004$
12737 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}
544 parameters	$\Delta\rho_{min} = -0.52$ e Å^{-3}
39 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ir1	0.284245 (8)	0.460836 (3)	0.267476 (4)	0.00798 (2)	
H1	0.2025 (16)	0.4558 (8)	0.3224 (9)	0.010*	
H2	0.4088 (14)	0.4555 (8)	0.3262 (9)	0.010*	
P1	0.28670 (6)	0.368517 (19)	0.26606 (3)	0.00904 (10)	
P2	0.29923 (5)	0.549912 (19)	0.29715 (3)	0.00913 (10)	
O1	0.41473 (14)	0.46566 (6)	0.18679 (7)	0.0136 (3)	
O2	0.11784 (13)	0.46847 (5)	0.17367 (7)	0.0108 (3)	
C1	0.2342 (2)	0.33866 (8)	0.34236 (10)	0.0113 (4)	
H1A	0.2436	0.2993	0.3390	0.014*	
C2	0.0868 (2)	0.35053 (8)	0.34315 (10)	0.0141 (4)	
H2A	0.0731	0.3894	0.3430	0.017*	
H2B	0.0290	0.3359	0.3005	0.017*	
C3	0.0458 (2)	0.32642 (9)	0.40740 (10)	0.0159 (4)	
H3A	−0.0470	0.3372	0.4082	0.019*	
H3B	0.0480	0.2872	0.4043	0.019*	
C4	0.1392 (2)	0.34446 (9)	0.47470 (11)	0.0160 (5)	
H4A	0.1309	0.3833	0.4800	0.019*	
H4B	0.1128	0.3271	0.5150	0.019*	
C5	0.2838 (2)	0.33051 (9)	0.47383 (10)	0.0150 (4)	
H5A	0.2933	0.2915	0.4710	0.018*	
H5B	0.3430	0.3429	0.5175	0.018*	
C6	0.3258 (2)	0.35675 (8)	0.41109 (10)	0.0137 (4)	
H6A	0.4196	0.3472	0.4107	0.016*	
H6B	0.3207	0.3958	0.4153	0.016*	
C7	0.4517 (2)	0.33716 (8)	0.26411 (10)	0.0111 (4)	
H7	0.4538	0.3330	0.2137	0.013*	
C8	0.5737 (2)	0.37216 (8)	0.29526 (11)	0.0131 (4)	
H8A	0.5615	0.4080	0.2741	0.016*	
H8B	0.5804	0.3760	0.3461	0.016*	

C9	0.7031 (2)	0.34750 (8)	0.28166 (11)	0.0161 (5)
H9A	0.7802	0.3696	0.3041	0.019*
H9B	0.6998	0.3472	0.2309	0.019*
C10	0.7234 (2)	0.29056 (8)	0.30994 (12)	0.0184 (5)
H10A	0.8034	0.2750	0.2966	0.022*
H10B	0.7392	0.2913	0.3615	0.022*
C11	0.6014 (2)	0.25610 (9)	0.28129 (12)	0.0178 (5)
H11A	0.6143	0.2205	0.3031	0.021*
H11B	0.5927	0.2516	0.2304	0.021*
C12	0.4729 (2)	0.28085 (8)	0.29554 (11)	0.0149 (4)
H12A	0.4784	0.2827	0.3465	0.018*
H12B	0.3955	0.2582	0.2750	0.018*
C13	0.1699 (2)	0.33971 (8)	0.18943 (10)	0.0124 (4)
H13	0.0807	0.3562	0.1889	0.015*
C14	0.1472 (2)	0.27940 (8)	0.18914 (11)	0.0180 (5)
H14A	0.2318	0.2609	0.1872	0.022*
H14B	0.1200	0.2688	0.2327	0.022*
C15	0.0383 (2)	0.26304 (9)	0.12626 (12)	0.0232 (5)
H15A	0.0275	0.2240	0.1260	0.028*
H15B	−0.0480	0.2793	0.1303	0.028*
C16	0.0744 (2)	0.28069 (9)	0.05804 (12)	0.0242 (5)
H16A	0.1555	0.2615	0.0516	0.029*
H16B	0.0004	0.2715	0.0186	0.029*
C17	0.1001 (2)	0.34030 (9)	0.05797 (11)	0.0202 (5)
H17A	0.0161	0.3596	0.0592	0.024*
H17B	0.1287	0.3503	0.0145	0.024*
C18	0.2081 (2)	0.35652 (9)	0.12081 (10)	0.0147 (5)
H18A	0.2204	0.3955	0.1206	0.018*
H18B	0.2941	0.3397	0.1174	0.018*
C19	0.1703 (2)	0.59093 (8)	0.23935 (10)	0.0115 (4)
H19	0.0854	0.5701	0.2341	0.014*
C20	0.1990 (2)	0.59394 (8)	0.16537 (10)	0.0144 (4)
H20A	0.2749	0.6183	0.1653	0.017*
H20B	0.2242	0.5584	0.1510	0.017*
C21	0.0750 (2)	0.61381 (9)	0.11372 (11)	0.0165 (5)
H21A	0.0008	0.5882	0.1119	0.020*
H21B	0.0950	0.6161	0.0666	0.020*
C22	0.0319 (2)	0.66848 (9)	0.13532 (11)	0.0188 (5)
H22A	0.1011	0.6950	0.1310	0.023*
H22B	−0.0527	0.6791	0.1036	0.023*
C23	0.0118 (2)	0.66789 (9)	0.21033 (11)	0.0199 (5)
H23A	−0.0665	0.6455	0.2129	0.024*
H23B	−0.0075	0.7044	0.2241	0.024*
C24	0.1351 (2)	0.64662 (8)	0.26185 (11)	0.0160 (5)
H24A	0.2119	0.6708	0.2630	0.019*
H24B	0.1161	0.6451	0.3093	0.019*
C25	0.2682 (2)	0.56519 (8)	0.38504 (10)	0.0115 (4)
H25	0.2741	0.6046	0.3905	0.014*
C26	0.1266 (2)	0.54915 (8)	0.39223 (11)	0.0157 (5)

H26A	0.0602	0.5654	0.3539	0.019*
H26B	0.1172	0.5101	0.3880	0.019*
C27	0.0977 (2)	0.56690 (10)	0.46231 (11)	0.0209 (5)
H27A	0.0081	0.5540	0.4664	0.025*
H27B	0.0966	0.6062	0.4642	0.025*
C28	0.2031 (2)	0.54562 (10)	0.52352 (11)	0.0234 (5)
H28A	0.1864	0.5604	0.5677	0.028*
H28B	0.1955	0.5065	0.5256	0.028*
C29	0.3438 (2)	0.56049 (9)	0.51579 (11)	0.0173 (5)
H29A	0.4100	0.5444	0.5544	0.021*
H29B	0.3544	0.5995	0.5190	0.021*
C30	0.3711 (2)	0.54132 (9)	0.44602 (10)	0.0134 (4)
H30A	0.3660	0.5021	0.4439	0.016*
H30B	0.4625	0.5520	0.4421	0.016*
C31	0.4636 (2)	0.57988 (8)	0.29324 (10)	0.0102 (4)
H31	0.4598	0.5878	0.2429	0.012*
C32	0.4943 (2)	0.63318 (8)	0.33186 (11)	0.0146 (4)
H32A	0.4197	0.6582	0.3154	0.018*
H32B	0.5011	0.6275	0.3824	0.018*
C33	0.6248 (2)	0.65754 (9)	0.31986 (12)	0.0194 (5)
H33A	0.6437	0.6906	0.3475	0.023*
H33B	0.6144	0.6669	0.2700	0.023*
C34	0.7431 (2)	0.61922 (9)	0.34073 (12)	0.0183 (5)
H34A	0.7610	0.6133	0.3917	0.022*
H34B	0.8242	0.6352	0.3290	0.022*
C35	0.7132 (2)	0.56596 (9)	0.30276 (11)	0.0162 (5)
H35A	0.7054	0.5714	0.2521	0.019*
H35B	0.7882	0.5411	0.3192	0.019*
C36	0.58314 (19)	0.54158 (8)	0.31571 (10)	0.0133 (4)
H36A	0.5937	0.5332	0.3659	0.016*
H36B	0.5648	0.5080	0.2892	0.016*
C37	0.5669 (2)	0.46118 (11)	0.11183 (12)	0.0256 (5)
H37A	0.6069	0.4950	0.1022	0.031*
H37B	0.5582	0.4379	0.0711	0.031*
H37C	0.6242	0.4442	0.1522	0.031*
C38	0.4313 (2)	0.47117 (8)	0.12710 (11)	0.0144 (4)
C39	0.3235 (2)	0.48740 (9)	0.06649 (11)	0.0192 (5)
H39A	0.2376	0.4890	0.0812	0.023*
H39B	0.3178	0.4614	0.0288	0.023*
H39C	0.3445	0.5224	0.0499	0.023*
C40	−0.0856 (2)	0.46968 (9)	0.08943 (11)	0.0190 (5)
H40A	−0.0248	0.4696	0.0568	0.023*
H40B	−0.1409	0.5018	0.0823	0.023*
H40C	−0.1433	0.4383	0.0813	0.023*
C41	−0.0053 (2)	0.46875 (8)	0.16295 (11)	0.0131 (4)
C42	−0.0809 (2)	0.46771 (10)	0.22023 (11)	0.0232 (5)
H42A	−0.0183	0.4717	0.2652	0.028*
H42B	−0.1283	0.4338	0.2193	0.028*
H42C	−0.1456	0.4969	0.2139	0.028*

O3	0.2746 (2)	0.84436 (9)	0.41579 (13)	0.0681 (7)	
C43	0.3208 (3)	0.80391 (15)	0.52688 (16)	0.0534 (9)	
H43A	0.2404	0.8229	0.5331	0.064*	
H43B	0.3983	0.8165	0.5614	0.064*	
H43C	0.3089	0.7658	0.5332	0.064*	
C44	0.3432 (3)	0.81387 (11)	0.45587 (14)	0.0342 (6)	
C45	0.4556 (3)	0.78411 (16)	0.43585 (17)	0.0606 (10)	
H45A	0.4384	0.7459	0.4374	0.073*	
H45B	0.5394	0.7926	0.4685	0.073*	
H45C	0.4629	0.7942	0.3886	0.073*	
B1	0.63333 (11)	0.88431 (5)	0.59616 (6)	0.0282 (6)	
F1	0.74063 (11)	0.91865 (5)	0.61781 (7)	0.0412 (4)	
F2	0.52168 (13)	0.90752 (10)	0.61630 (14)	0.0564 (10)	0.65
F3	0.6589 (2)	0.83624 (6)	0.62953 (14)	0.0490 (9)	0.65
F4	0.6068 (2)	0.87863 (10)	0.52580 (6)	0.0632 (12)	0.65
F2A	0.53400 (16)	0.89281 (10)	0.63199 (12)	0.040 (3)	0.25
F3A	0.6728 (2)	0.83142 (4)	0.60168 (16)	0.047 (3)	0.25
F4A	0.5812 (2)	0.89353 (10)	0.52508 (7)	0.042 (3)	0.25
F2B	0.5769 (2)	0.86477 (11)	0.64814 (9)	0.045 (5)	0.10
F3B	0.6844 (2)	0.84045 (7)	0.56388 (15)	0.061 (6)	0.10
F4B	0.53435 (17)	0.90809 (8)	0.54592 (12)	0.051 (6)	0.10

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.00797 (4)	0.00727 (3)	0.00852 (4)	0.00048 (4)	0.00131 (2)	−0.00013 (3)
P1	0.0090 (2)	0.0085 (2)	0.0092 (2)	0.0000 (2)	0.00099 (18)	−0.0004 (2)
P2	0.0093 (2)	0.0083 (3)	0.0095 (2)	0.00102 (19)	0.00132 (19)	0.00001 (18)
O1	0.0153 (7)	0.0139 (7)	0.0122 (7)	−0.0019 (6)	0.0046 (6)	−0.0008 (6)
O2	0.0083 (7)	0.0106 (7)	0.0129 (7)	0.0007 (6)	0.0008 (5)	−0.0003 (5)
C1	0.0118 (10)	0.0098 (10)	0.0122 (10)	−0.0011 (8)	0.0027 (8)	0.0001 (8)
C2	0.0124 (11)	0.0166 (11)	0.0127 (10)	−0.0005 (8)	0.0009 (8)	0.0002 (8)
C3	0.0152 (11)	0.0178 (11)	0.0156 (11)	−0.0030 (9)	0.0055 (9)	0.0013 (8)
C4	0.0177 (12)	0.0177 (11)	0.0137 (11)	−0.0019 (9)	0.0061 (9)	0.0012 (8)
C5	0.0178 (11)	0.0170 (11)	0.0098 (10)	−0.0002 (9)	0.0021 (8)	0.0024 (8)
C6	0.0138 (11)	0.0153 (11)	0.0122 (10)	−0.0004 (9)	0.0032 (8)	−0.0010 (8)
C7	0.0104 (10)	0.0113 (10)	0.0117 (10)	0.0023 (8)	0.0026 (8)	−0.0016 (8)
C8	0.0117 (11)	0.0129 (10)	0.0140 (11)	0.0003 (8)	0.0014 (8)	−0.0007 (8)
C9	0.0112 (11)	0.0172 (11)	0.0193 (11)	0.0006 (9)	0.0021 (9)	0.0014 (9)
C10	0.0124 (11)	0.0151 (11)	0.0266 (13)	0.0041 (9)	0.0017 (9)	−0.0002 (9)
C11	0.0167 (12)	0.0136 (11)	0.0218 (12)	0.0051 (9)	0.0009 (9)	−0.0005 (9)
C12	0.0129 (11)	0.0106 (10)	0.0197 (11)	0.0006 (8)	−0.0004 (9)	−0.0013 (8)
C13	0.0100 (10)	0.0142 (10)	0.0118 (10)	−0.0016 (8)	−0.0001 (8)	−0.0025 (8)
C14	0.0209 (12)	0.0141 (11)	0.0168 (11)	−0.0025 (9)	−0.0011 (9)	−0.0010 (8)
C15	0.0248 (13)	0.0176 (12)	0.0239 (13)	−0.0068 (10)	−0.0025 (10)	−0.0051 (9)
C16	0.0279 (14)	0.0217 (12)	0.0180 (12)	0.0010 (10)	−0.0063 (10)	−0.0101 (9)
C17	0.0246 (13)	0.0206 (12)	0.0129 (11)	0.0007 (10)	−0.0019 (9)	−0.0033 (9)
C18	0.0152 (11)	0.0169 (11)	0.0113 (10)	0.0002 (9)	0.0013 (8)	−0.0018 (8)

C19	0.0096 (10)	0.0114 (10)	0.0121 (10)	0.0012 (8)	−0.0009 (8)	0.0007 (8)
C20	0.0161 (11)	0.0147 (11)	0.0122 (10)	0.0028 (9)	0.0024 (8)	0.0019 (8)
C21	0.0190 (12)	0.0163 (11)	0.0126 (11)	0.0037 (9)	−0.0002 (9)	0.0003 (8)
C22	0.0200 (12)	0.0153 (11)	0.0177 (11)	0.0045 (9)	−0.0039 (9)	0.0029 (9)
C23	0.0202 (12)	0.0167 (11)	0.0209 (12)	0.0108 (9)	−0.0001 (9)	−0.0014 (9)
C24	0.0190 (12)	0.0133 (10)	0.0141 (11)	0.0049 (9)	0.0000 (9)	−0.0015 (8)
C25	0.0137 (11)	0.0111 (10)	0.0101 (10)	0.0014 (8)	0.0033 (8)	−0.0006 (8)
C26	0.0139 (11)	0.0176 (12)	0.0164 (11)	0.0010 (8)	0.0050 (8)	−0.0018 (8)
C27	0.0172 (12)	0.0259 (13)	0.0224 (12)	−0.0008 (10)	0.0106 (10)	−0.0046 (10)
C28	0.0282 (13)	0.0285 (14)	0.0159 (11)	0.0005 (11)	0.0101 (10)	−0.0011 (10)
C29	0.0203 (12)	0.0194 (11)	0.0118 (11)	0.0031 (9)	0.0023 (9)	−0.0001 (8)
C30	0.0148 (10)	0.0140 (10)	0.0117 (10)	0.0003 (9)	0.0033 (8)	0.0017 (8)
C31	0.0100 (10)	0.0105 (10)	0.0103 (10)	−0.0006 (8)	0.0028 (8)	0.0009 (7)
C32	0.0136 (11)	0.0107 (10)	0.0192 (11)	−0.0008 (8)	0.0028 (9)	−0.0003 (8)
C33	0.0200 (12)	0.0131 (11)	0.0250 (12)	−0.0061 (9)	0.0044 (10)	−0.0011 (9)
C34	0.0138 (11)	0.0207 (12)	0.0207 (12)	−0.0052 (9)	0.0045 (9)	−0.0018 (9)
C35	0.0106 (11)	0.0206 (12)	0.0177 (11)	0.0006 (9)	0.0036 (9)	−0.0019 (9)
C36	0.0104 (10)	0.0116 (9)	0.0176 (10)	0.0008 (9)	0.0022 (8)	−0.0006 (9)
C37	0.0163 (11)	0.0397 (14)	0.0225 (12)	0.0032 (12)	0.0082 (9)	0.0049 (11)
C38	0.0135 (11)	0.0119 (11)	0.0181 (11)	−0.0014 (8)	0.0043 (8)	0.0000 (8)
C39	0.0200 (12)	0.0241 (12)	0.0141 (11)	0.0031 (10)	0.0053 (9)	0.0017 (9)
C40	0.0141 (11)	0.0242 (13)	0.0167 (11)	0.0025 (9)	−0.0015 (9)	−0.0010 (9)
C41	0.0132 (10)	0.0074 (10)	0.0176 (11)	0.0016 (8)	0.0010 (8)	−0.0001 (8)
C42	0.0154 (11)	0.0352 (15)	0.0190 (12)	0.0022 (10)	0.0034 (9)	0.0022 (10)
O3	0.0511 (15)	0.0535 (15)	0.0860 (18)	−0.0109 (12)	−0.0170 (13)	0.0303 (13)
C43	0.045 (2)	0.076 (3)	0.0460 (19)	−0.0144 (18)	0.0257 (16)	−0.0103 (17)
C44	0.0280 (15)	0.0336 (15)	0.0383 (16)	−0.0072 (12)	0.0011 (12)	0.0046 (12)
C45	0.054 (2)	0.089 (3)	0.044 (2)	−0.001 (2)	0.0210 (17)	−0.0189 (19)
B1	0.0293 (16)	0.0300 (16)	0.0256 (16)	−0.0019 (13)	0.0059 (13)	0.0038 (12)
F1	0.0244 (8)	0.0388 (10)	0.0593 (11)	−0.0064 (7)	0.0062 (8)	−0.0015 (8)
F2	0.0292 (19)	0.0468 (18)	0.097 (3)	0.0002 (14)	0.0225 (18)	−0.0071 (19)
F3	0.048 (2)	0.0413 (19)	0.056 (2)	−0.0039 (15)	0.0060 (15)	0.0273 (14)
F4	0.111 (3)	0.055 (2)	0.025 (2)	−0.029 (2)	0.0166 (19)	0.0024 (13)
F2A	0.033 (5)	0.073 (6)	0.019 (3)	−0.008 (4)	0.018 (3)	−0.019 (4)
F3A	0.047 (5)	0.033 (4)	0.057 (6)	0.000 (3)	0.000 (4)	0.023 (3)
F4A	0.053 (5)	0.046 (5)	0.024 (5)	−0.010 (4)	0.000 (4)	0.010 (3)
F2B	0.045 (8)	0.054 (9)	0.035 (8)	−0.016 (7)	0.003 (7)	0.016 (7)
F3B	0.052 (9)	0.067 (9)	0.063 (9)	0.013 (7)	0.009 (7)	−0.026 (8)
F4B	0.048 (9)	0.040 (8)	0.055 (9)	0.000 (7)	−0.010 (7)	0.012 (7)

Geometric parameters (Å, °)

Ir1—O2	2.2379 (13)	C22—H22B	0.9900
Ir1—O1	2.2762 (14)	C23—C24	1.537 (3)
Ir1—P2	2.3159 (6)	C23—H23A	0.9900
Ir1—P1	2.3267 (6)	C23—H23B	0.9900
Ir1—H1	1.501 (14)	C24—H24A	0.9900
Ir1—H2	1.534 (14)	C24—H24B	0.9900
P1—C1	1.852 (2)	C25—C26	1.537 (3)

P1—C13	1.861 (2)	C25—C30	1.541 (3)
P1—C7	1.870 (2)	C25—H25	1.0000
P2—C25	1.858 (2)	C26—C27	1.532 (3)
P2—C31	1.858 (2)	C26—H26A	0.9900
P2—C19	1.862 (2)	C26—H26B	0.9900
O1—C38	1.226 (2)	C27—C28	1.533 (3)
O2—C41	1.232 (2)	C27—H27A	0.9900
C1—C2	1.539 (3)	C27—H27B	0.9900
C1—C6	1.541 (3)	C28—C29	1.524 (3)
C1—H1A	1.0000	C28—H28A	0.9900
C2—C3	1.534 (3)	C28—H28B	0.9900
C2—H2A	0.9900	C29—C30	1.531 (3)
C2—H2B	0.9900	C29—H29A	0.9900
C3—C4	1.528 (3)	C29—H29B	0.9900
C3—H3A	0.9900	C30—H30A	0.9900
C3—H3B	0.9900	C30—H30B	0.9900
C4—C5	1.523 (3)	C31—C32	1.542 (3)
C4—H4A	0.9900	C31—C36	1.547 (3)
C4—H4B	0.9900	C31—H31	1.0000
C5—C6	1.535 (3)	C32—C33	1.531 (3)
C5—H5A	0.9900	C32—H32A	0.9900
C5—H5B	0.9900	C32—H32B	0.9900
C6—H6A	0.9900	C33—C34	1.534 (3)
C6—H6B	0.9900	C33—H33A	0.9900
C7—C12	1.544 (3)	C33—H33B	0.9900
C7—C8	1.545 (3)	C34—C35	1.534 (3)
C7—H7	1.0000	C34—H34A	0.9900
C8—C9	1.533 (3)	C34—H34B	0.9900
C8—H8A	0.9900	C35—C36	1.532 (3)
C8—H8B	0.9900	C35—H35A	0.9900
C9—C10	1.537 (3)	C35—H35B	0.9900
C9—H9A	0.9900	C36—H36A	0.9900
C9—H9B	0.9900	C36—H36B	0.9900
C10—C11	1.527 (3)	C37—C38	1.498 (3)
C10—H10A	0.9900	C37—H37A	0.9800
C10—H10B	0.9900	C37—H37B	0.9800
C11—C12	1.531 (3)	C37—H37C	0.9800
C11—H11A	0.9900	C38—C39	1.500 (3)
C11—H11B	0.9900	C39—H39A	0.9800
C12—H12A	0.9900	C39—H39B	0.9800
C12—H12B	0.9900	C39—H39C	0.9800
C13—C14	1.537 (3)	C40—C41	1.503 (3)
C13—C18	1.538 (3)	C40—H40A	0.9800
C13—H13	1.0000	C40—H40B	0.9800
C14—C15	1.535 (3)	C40—H40C	0.9800
C14—H14A	0.9900	C41—C42	1.491 (3)
C14—H14B	0.9900	C42—H42A	0.9800
C15—C16	1.527 (3)	C42—H42B	0.9800
C15—H15A	0.9900	C42—H42C	0.9800

C15—H15B	0.9900	O3—C44	1.212 (3)
C16—C17	1.525 (3)	C43—C44	1.480 (4)
C16—H16A	0.9900	C43—H43A	0.9800
C16—H16B	0.9900	C43—H43B	0.9800
C17—C18	1.529 (3)	C43—H43C	0.9800
C17—H17A	0.9900	C44—C45	1.491 (4)
C17—H17B	0.9900	C45—H45A	0.9800
C18—H18A	0.9900	C45—H45B	0.9800
C18—H18B	0.9900	C45—H45C	0.9800
C19—C24	1.536 (3)	B1—F4	1.3577
C19—C20	1.542 (3)	B1—F2B	1.3643
C19—H19	1.0000	B1—F2A	1.3669
C20—C21	1.532 (3)	B1—F3	1.3759
C20—H20A	0.9900	B1—F3A	1.3901
C20—H20B	0.9900	B1—F1	1.3917
C21—C22	1.533 (3)	B1—F4B	1.3918
C21—H21A	0.9900	B1—F4A	1.4045
C21—H21B	0.9900	B1—F2	1.4100
C22—C23	1.528 (3)	B1—F3B	1.4257
C22—H22A	0.9900		
O2—Ir1—O1	83.00 (5)	H21A—C21—H21B	108.0
O2—Ir1—P2	97.03 (4)	C23—C22—C21	111.20 (17)
O1—Ir1—P2	96.06 (4)	C23—C22—H22A	109.4
O2—Ir1—P1	94.84 (4)	C21—C22—H22A	109.4
O1—Ir1—P1	92.05 (4)	C23—C22—H22B	109.4
P2—Ir1—P1	166.350 (19)	C21—C22—H22B	109.4
O2—Ir1—H1	99.0 (7)	H22A—C22—H22B	108.0
O1—Ir1—H1	177.4 (7)	C22—C23—C24	112.36 (18)
P2—Ir1—H1	85.3 (8)	C22—C23—H23A	109.1
P1—Ir1—H1	86.2 (8)	C24—C23—H23A	109.1
O2—Ir1—H2	173.7 (7)	C22—C23—H23B	109.1
O1—Ir1—H2	90.7 (7)	C24—C23—H23B	109.1
P2—Ir1—H2	84.0 (8)	H23A—C23—H23B	107.9
P1—Ir1—H2	84.9 (8)	C19—C24—C23	109.76 (17)
H1—Ir1—H2	87.2 (8)	C19—C24—H24A	109.7
C1—P1—C13	104.43 (9)	C23—C24—H24A	109.7
C1—P1—C7	105.05 (9)	C19—C24—H24B	109.7
C13—P1—C7	104.34 (9)	C23—C24—H24B	109.7
C1—P1—Ir1	113.01 (7)	H24A—C24—H24B	108.2
C13—P1—Ir1	113.14 (7)	C26—C25—C30	109.23 (16)
C7—P1—Ir1	115.77 (7)	C26—C25—P2	112.17 (14)
C25—P2—C31	106.58 (9)	C30—C25—P2	114.74 (14)
C25—P2—C19	102.35 (9)	C26—C25—H25	106.7
C31—P2—C19	106.27 (9)	C30—C25—H25	106.7
C25—P2—Ir1	114.78 (7)	P2—C25—H25	106.7
C31—P2—Ir1	113.35 (6)	C27—C26—C25	111.55 (17)
C19—P2—Ir1	112.56 (7)	C27—C26—H26A	109.3
C38—O1—Ir1	152.71 (14)	C25—C26—H26A	109.3
C41—O2—Ir1	135.60 (13)	C27—C26—H26B	109.3

C2—C1—C6	110.51 (17)	C25—C26—H26B	109.3
C2—C1—P1	112.25 (14)	H26A—C26—H26B	108.0
C6—C1—P1	111.20 (14)	C26—C27—C28	111.42 (18)
C2—C1—H1A	107.6	C26—C27—H27A	109.3
C6—C1—H1A	107.6	C28—C27—H27A	109.3
P1—C1—H1A	107.6	C26—C27—H27B	109.3
C3—C2—C1	111.52 (17)	C28—C27—H27B	109.3
C3—C2—H2A	109.3	H27A—C27—H27B	108.0
C1—C2—H2A	109.3	C29—C28—C27	111.06 (18)
C3—C2—H2B	109.3	C29—C28—H28A	109.4
C1—C2—H2B	109.3	C27—C28—H28A	109.4
H2A—C2—H2B	108.0	C29—C28—H28B	109.4
C4—C3—C2	111.36 (17)	C27—C28—H28B	109.4
C4—C3—H3A	109.4	H28A—C28—H28B	108.0
C2—C3—H3A	109.4	C28—C29—C30	111.33 (18)
C4—C3—H3B	109.4	C28—C29—H29A	109.4
C2—C3—H3B	109.4	C30—C29—H29A	109.4
H3A—C3—H3B	108.0	C28—C29—H29B	109.4
C5—C4—C3	110.73 (17)	C30—C29—H29B	109.4
C5—C4—H4A	109.5	H29A—C29—H29B	108.0
C3—C4—H4A	109.5	C29—C30—C25	110.38 (17)
C5—C4—H4B	109.5	C29—C30—H30A	109.6
C3—C4—H4B	109.5	C25—C30—H30A	109.6
H4A—C4—H4B	108.1	C29—C30—H30B	109.6
C4—C5—C6	110.10 (17)	C25—C30—H30B	109.6
C4—C5—H5A	109.6	H30A—C30—H30B	108.1
C6—C5—H5A	109.6	C32—C31—C36	109.65 (16)
C4—C5—H5B	109.6	C32—C31—P2	115.24 (14)
C6—C5—H5B	109.6	C36—C31—P2	113.67 (14)
H5A—C5—H5B	108.2	C32—C31—H31	105.8
C5—C6—C1	110.74 (17)	C36—C31—H31	105.8
C5—C6—H6A	109.5	P2—C31—H31	105.8
C1—C6—H6A	109.5	C33—C32—C31	111.58 (17)
C5—C6—H6B	109.5	C33—C32—H32A	109.3
C1—C6—H6B	109.5	C31—C32—H32A	109.3
H6A—C6—H6B	108.1	C33—C32—H32B	109.3
C12—C7—C8	109.43 (16)	C31—C32—H32B	109.3
C12—C7—P1	115.57 (14)	H32A—C32—H32B	108.0
C8—C7—P1	114.02 (14)	C32—C33—C34	111.71 (18)
C12—C7—H7	105.6	C32—C33—H33A	109.3
C8—C7—H7	105.6	C34—C33—H33A	109.3
P1—C7—H7	105.6	C32—C33—H33B	109.3
C9—C8—C7	110.68 (17)	C34—C33—H33B	109.3
C9—C8—H8A	109.5	H33A—C33—H33B	107.9
C7—C8—H8A	109.5	C33—C34—C35	110.77 (18)
C9—C8—H8B	109.5	C33—C34—H34A	109.5
C7—C8—H8B	109.5	C35—C34—H34A	109.5
H8A—C8—H8B	108.1	C33—C34—H34B	109.5
C8—C9—C10	111.84 (18)	C35—C34—H34B	109.5

C8—C9—H9A	109.2	H34A—C34—H34B	108.1
C10—C9—H9A	109.2	C36—C35—C34	111.23 (17)
C8—C9—H9B	109.2	C36—C35—H35A	109.4
C10—C9—H9B	109.2	C34—C35—H35A	109.4
H9A—C9—H9B	107.9	C36—C35—H35B	109.4
C11—C10—C9	111.07 (17)	C34—C35—H35B	109.4
C11—C10—H10A	109.4	H35A—C35—H35B	108.0
C9—C10—H10A	109.4	C35—C36—C31	111.27 (17)
C11—C10—H10B	109.4	C35—C36—H36A	109.4
C9—C10—H10B	109.4	C31—C36—H36A	109.4
H10A—C10—H10B	108.0	C35—C36—H36B	109.4
C10—C11—C12	111.50 (18)	C31—C36—H36B	109.4
C10—C11—H11A	109.3	H36A—C36—H36B	108.0
C12—C11—H11A	109.3	C38—C37—H37A	109.5
C10—C11—H11B	109.3	C38—C37—H37B	109.5
C12—C11—H11B	109.3	H37A—C37—H37B	109.5
H11A—C11—H11B	108.0	C38—C37—H37C	109.5
C11—C12—C7	110.79 (17)	H37A—C37—H37C	109.5
C11—C12—H12A	109.5	H37B—C37—H37C	109.5
C7—C12—H12A	109.5	O1—C38—C37	119.36 (19)
C11—C12—H12B	109.5	O1—C38—C39	124.26 (19)
C7—C12—H12B	109.5	C37—C38—C39	116.38 (18)
H12A—C12—H12B	108.1	C38—C39—H39A	109.5
C14—C13—C18	109.56 (17)	C38—C39—H39B	109.5
C14—C13—P1	117.35 (14)	H39A—C39—H39B	109.5
C18—C13—P1	111.25 (14)	C38—C39—H39C	109.5
C14—C13—H13	106.0	H39A—C39—H39C	109.5
C18—C13—H13	106.0	H39B—C39—H39C	109.5
P1—C13—H13	106.0	C41—C40—H40A	109.5
C15—C14—C13	110.60 (18)	C41—C40—H40B	109.5
C15—C14—H14A	109.5	H40A—C40—H40B	109.5
C13—C14—H14A	109.5	C41—C40—H40C	109.5
C15—C14—H14B	109.5	H40A—C40—H40C	109.5
C13—C14—H14B	109.5	H40B—C40—H40C	109.5
H14A—C14—H14B	108.1	O2—C41—C42	122.86 (19)
C16—C15—C14	111.05 (19)	O2—C41—C40	119.81 (19)
C16—C15—H15A	109.4	C42—C41—C40	117.32 (19)
C14—C15—H15A	109.4	C41—C42—H42A	109.5
C16—C15—H15B	109.4	C41—C42—H42B	109.5
C14—C15—H15B	109.4	H42A—C42—H42B	109.5
H15A—C15—H15B	108.0	C41—C42—H42C	109.5
C17—C16—C15	111.14 (18)	H42A—C42—H42C	109.5
C17—C16—H16A	109.4	H42B—C42—H42C	109.5
C15—C16—H16A	109.4	C44—C43—H43A	109.5
C17—C16—H16B	109.4	C44—C43—H43B	109.5
C15—C16—H16B	109.4	H43A—C43—H43B	109.5
H16A—C16—H16B	108.0	C44—C43—H43C	109.5
C16—C17—C18	110.96 (19)	H43A—C43—H43C	109.5
C16—C17—H17A	109.4	H43B—C43—H43C	109.5

C18—C17—H17A	109.4	O3—C44—C43	122.4 (3)
C16—C17—H17B	109.4	O3—C44—C45	121.4 (3)
C18—C17—H17B	109.4	C43—C44—C45	116.2 (3)
H17A—C17—H17B	108.0	C44—C45—H45A	109.5
C17—C18—C13	111.08 (18)	C44—C45—H45B	109.5
C17—C18—H18A	109.4	H45A—C45—H45B	109.5
C13—C18—H18A	109.4	C44—C45—H45C	109.5
C17—C18—H18B	109.4	H45A—C45—H45C	109.5
C13—C18—H18B	109.4	H45B—C45—H45C	109.5
H18A—C18—H18B	108.0	F4—B1—F3	111.6
C24—C19—C20	109.13 (16)	F2A—B1—F3A	110.2
C24—C19—P2	120.69 (14)	F4—B1—F1	110.7
C20—C19—P2	110.55 (14)	F2B—B1—F1	115.2
C24—C19—H19	105.0	F2A—B1—F1	111.6
C20—C19—H19	105.0	F3—B1—F1	110.0
P2—C19—H19	105.0	F3A—B1—F1	112.0
C21—C20—C19	110.18 (17)	F2B—B1—F4B	109.1
C21—C20—H20A	109.6	F1—B1—F4B	111.0
C19—C20—H20A	109.6	F2A—B1—F4A	108.5
C21—C20—H20B	109.6	F3A—B1—F4A	106.2
C19—C20—H20B	109.6	F1—B1—F4A	108.1
H20A—C20—H20B	108.1	F4—B1—F2	109.1
C20—C21—C22	110.89 (17)	F3—B1—F2	108.4
C20—C21—H21A	109.5	F1—B1—F2	106.8
C22—C21—H21A	109.5	F2B—B1—F3B	107.7
C20—C21—H21B	109.5	F1—B1—F3B	106.2
C22—C21—H21B	109.5	F4B—B1—F3B	107.4
O2—Ir1—P1—C1	−113.65 (8)	C7—P1—C13—C18	−64.65 (16)
O1—Ir1—P1—C1	163.20 (8)	Ir1—P1—C13—C18	62.02 (16)
P2—Ir1—P1—C1	36.70 (12)	C18—C13—C14—C15	−57.5 (2)
O2—Ir1—P1—C13	4.77 (8)	P1—C13—C14—C15	174.38 (15)
O1—Ir1—P1—C13	−78.38 (8)	C13—C14—C15—C16	57.1 (3)
P2—Ir1—P1—C13	155.12 (10)	C14—C15—C16—C17	−55.8 (3)
O2—Ir1—P1—C7	125.13 (8)	C15—C16—C17—C18	55.6 (3)
O1—Ir1—P1—C7	41.98 (8)	C16—C17—C18—C13	−56.9 (3)
P2—Ir1—P1—C7	−84.52 (11)	C14—C13—C18—C17	57.7 (2)
O2—Ir1—P2—C25	119.70 (8)	P1—C13—C18—C17	−170.95 (15)
O1—Ir1—P2—C25	−156.63 (8)	C25—P2—C19—C24	38.12 (19)
P1—Ir1—P2—C25	−30.52 (12)	C31—P2—C19—C24	−73.49 (18)
O2—Ir1—P2—C31	−117.50 (8)	Ir1—P2—C19—C24	161.87 (15)
O1—Ir1—P2—C31	−33.83 (8)	C25—P2—C19—C20	167.12 (14)
P1—Ir1—P2—C31	92.28 (11)	C31—P2—C19—C20	55.51 (16)
O2—Ir1—P2—C19	3.16 (8)	Ir1—P2—C19—C20	−69.13 (15)
O1—Ir1—P2—C19	86.82 (8)	C24—C19—C20—C21	−60.8 (2)
P1—Ir1—P2—C19	−147.07 (10)	P2—C19—C20—C21	164.19 (14)
O2—Ir1—O1—C38	3.7 (3)	C19—C20—C21—C22	58.3 (2)
P2—Ir1—O1—C38	−92.7 (3)	C20—C21—C22—C23	−54.1 (2)
P1—Ir1—O1—C38	98.3 (3)	C21—C22—C23—C24	53.6 (3)
O1—Ir1—O2—C41	177.91 (18)	C20—C19—C24—C23	59.1 (2)

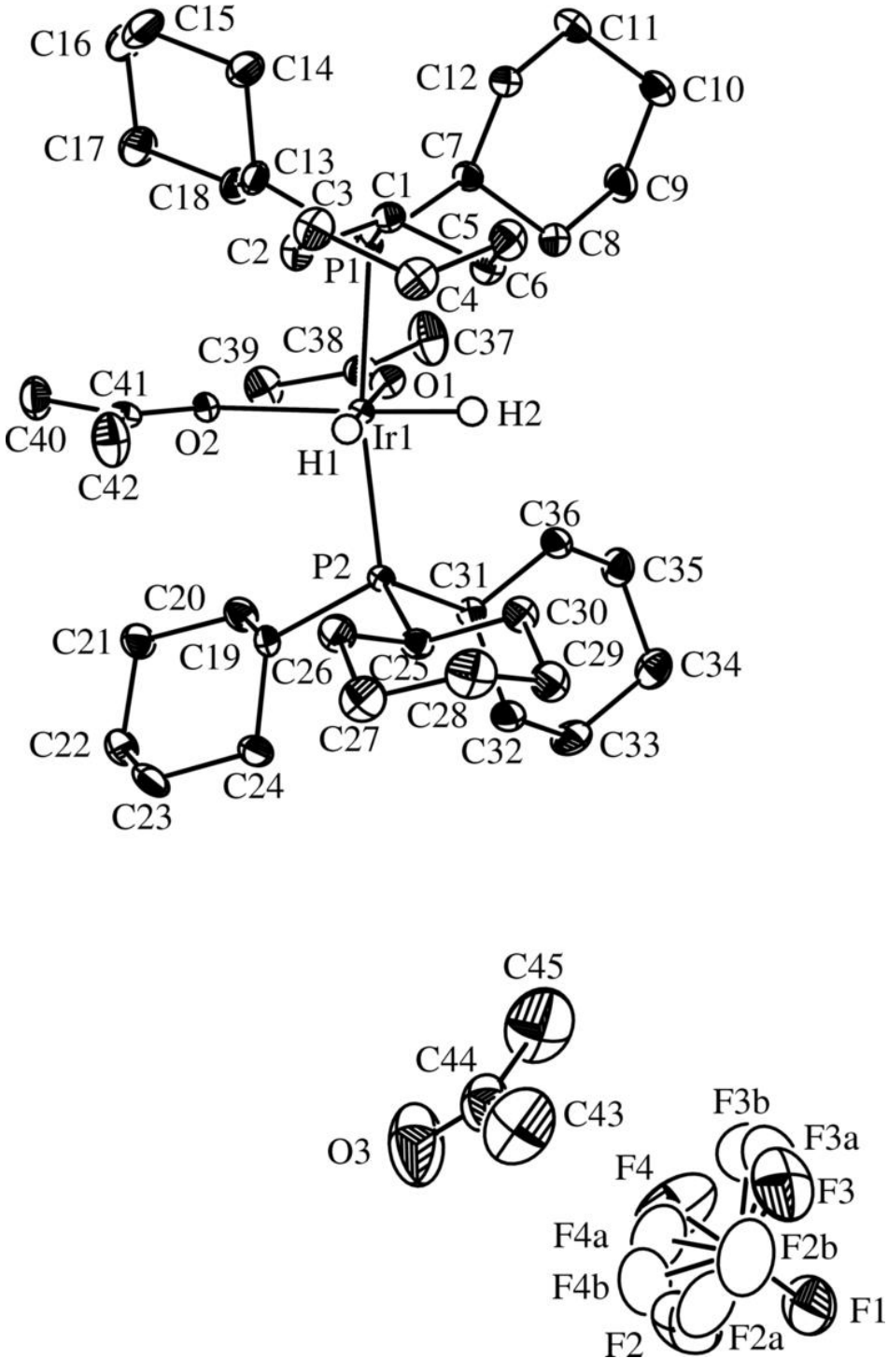
P2—Ir1—O2—C41	−86.80 (18)	P2—C19—C24—C23	−171.23 (16)
P1—Ir1—O2—C41	86.44 (18)	C22—C23—C24—C19	−56.3 (2)
C13—P1—C1—C2	−58.05 (16)	C31—P2—C25—C26	172.35 (14)
C7—P1—C1—C2	−167.56 (14)	C19—P2—C25—C26	60.98 (16)
Ir1—P1—C1—C2	65.33 (15)	Ir1—P2—C25—C26	−61.28 (15)
C13—P1—C1—C6	177.58 (15)	C31—P2—C25—C30	−62.25 (17)
C7—P1—C1—C6	68.06 (16)	C19—P2—C25—C30	−173.62 (15)
Ir1—P1—C1—C6	−59.04 (16)	Ir1—P2—C25—C30	64.12 (16)
C6—C1—C2—C3	−54.1 (2)	C30—C25—C26—C27	57.2 (2)
P1—C1—C2—C3	−178.89 (14)	P2—C25—C26—C27	−174.40 (15)
C1—C2—C3—C4	54.5 (2)	C25—C26—C27—C28	−55.4 (2)
C2—C3—C4—C5	−56.7 (2)	C26—C27—C28—C29	53.9 (3)
C3—C4—C5—C6	58.6 (2)	C27—C28—C29—C30	−55.6 (2)
C4—C5—C6—C1	−58.6 (2)	C28—C29—C30—C25	58.3 (2)
C2—C1—C6—C5	56.3 (2)	C26—C25—C30—C29	−58.3 (2)
P1—C1—C6—C5	−178.36 (14)	P2—C25—C30—C29	174.77 (14)
C1—P1—C7—C12	28.15 (17)	C25—P2—C31—C32	−35.95 (17)
C13—P1—C7—C12	−81.44 (16)	C19—P2—C31—C32	72.68 (16)
Ir1—P1—C7—C12	153.54 (12)	Ir1—P2—C31—C32	−163.16 (12)
C1—P1—C7—C8	−99.95 (15)	C25—P2—C31—C36	91.82 (15)
C13—P1—C7—C8	150.47 (14)	C19—P2—C31—C36	−159.55 (14)
Ir1—P1—C7—C8	25.45 (16)	Ir1—P2—C31—C36	−35.39 (16)
C12—C7—C8—C9	57.5 (2)	C36—C31—C32—C33	55.9 (2)
P1—C7—C8—C9	−171.33 (14)	P2—C31—C32—C33	−174.35 (14)
C7—C8—C9—C10	−56.1 (2)	C31—C32—C33—C34	−55.8 (2)
C8—C9—C10—C11	54.2 (2)	C32—C33—C34—C35	54.9 (2)
C9—C10—C11—C12	−54.6 (2)	C33—C34—C35—C36	−55.5 (2)
C10—C11—C12—C7	57.3 (2)	C34—C35—C36—C31	57.0 (2)
C8—C7—C12—C11	−58.2 (2)	C32—C31—C36—C35	−56.5 (2)
P1—C7—C12—C11	171.50 (14)	P2—C31—C36—C35	172.86 (14)
C1—P1—C13—C14	−47.42 (18)	Ir1—O1—C38—C37	−171.0 (2)
C7—P1—C13—C14	62.62 (18)	Ir1—O1—C38—C39	8.8 (4)
Ir1—P1—C13—C14	−170.71 (14)	Ir1—O2—C41—C42	5.3 (3)
C1—P1—C13—C18	−174.69 (15)	Ir1—O2—C41—C40	−174.12 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8A···O1	0.99	2.49	3.358 (3)	146
C18—H18A···O2	0.99	2.45	3.207 (3)	133
C36—H36B···O1	0.99	2.50	3.347 (3)	144
C39—H39A···O2	0.98	2.45	3.304 (3)	146
C39—H39B···F4^{i}	0.98	2.54	3.441 (3)	153
C40—H40B···F1^{ii}	0.98	2.51	3.434 (3)	156

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

Fig. 1


C15
C16
C14
C11
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C13
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C18
C3
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C9
C5
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P1
C8
C4
C6
C39
C38
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O1
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O2
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Ir1
C42
C36
P2
C31
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C28
C27
C22
C32
C33
C24
C23
C45
C44
C43
O3
F3b
F3a
F4
F3
F4a
F2b
F4b
F1
F2
F2a