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I. Spectroscopic and Analytical Data

NMR, infrared and analytical data are provided below.

[Cp'(PMe$_3$)Ir≡CPh]BArf (1). Dark green solid: ^{1}H NMR (CD_2Cl_2): δ 7.89 (t, J = 1.4 Hz, 1H), 7.83 (d, J = 7.7, 2H), 7.71 (s, 8H), 7.55 (s, 4H), 7.45 (t, J = 7.7, 2H), 2.49 (q, J = 7.9 Hz, 2H), 2.25 (s, 6H), 2.22 (s, 6H), 1.65 (d, J = 10.9 Hz, 9H), 1.15 (t, J = 7.9 Hz, 3H); ^{13}C{^{1}H} (CD_2Cl_2): δ 296.9 (d, J = 11.5 Hz), 162.6 (d, J = 15 Hz), 161.9 (d, J = 15 Hz), 137.0 (s), 135.4 (s), 133.4 (s), 130.1 (s), 129.1 (s), 129.5 (d, J = 40.5 Hz), 128.4 (s), 124.1 (s), 121.9 (s), 118.0 (s), 107.7 (s), 101.3 (s), 100.4 (s), 20.4 (d, J = 55 Hz), 18.9 (s), 17.3 (s), 10.6 (s), 10.5 (s); ^{31}P{^{1}H} (CD_2Cl_2): δ -49.7 (s); ^{19}F{^{1}H} (CD_2Cl_2): δ -63.3 (s). IR (CD_2Cl_2, cm^{-1}) 3089 (s), 3050 (s), 2977 (m), 2629 (w), 1985 (w), 1874 (vw), 1784 (m) 1617 (s). Anal. Calcd for $C_{53}H_{43}BF_{24}IrP$: C, 46.47; H, 3.16. Found: C, 46.28; H, 2.93.

Cp'(PMe3)IrCO(Ph)(H) (2). Yellow-orange solid: ^{1}H NMR (C_6D_6): δ 8.26 (d, J = 7 Hz, 2H), 7.27 (t, J = 15 Hz, 2H), 7.23 (t, J = 15 Hz, 1H), 2.21 (q, J = 7.7 Hz, 2H), 1.78 (s, 6H), 1.75 (s, 6H), 1.24 (d, J = 9 Hz, 9H), 0.89 (t, J = 7.7 Hz, 3H), -16.28 (d, J = 36.1 Hz, 1H); ^{13}C{^{1}H} (C_6D_6): δ 129.1 (s), 128.4 (s), 128.3 (s), 128.0 (s), 127.1 (s), 94.5 (s), 93.2 (s), 92.9 (s), 92.5 (s), 92.1 (s), 18.62 (d, J = 42.1 Hz), 12.7 (s), 11.4 (s), 10.5 (s), 10.2 (s), 9.8 (s), 9.5 (s); ^{31}P{^{1}H} (C_6D_6): δ -38.2 (s). IR (C_6D_6, cm^{-1}) 3090 (s), 2162 (w), 1556 (s), 1505 (s) . HRMS (EI) *m/z* Calcd for $C_{21}H_{32}OPIr$: calcd 523.1824, obsvd 523.1830.

[Cp'(PMe3)(H)Ir=C(OMe)Ph]OTf (3). Yellow solid: ^{1}H NMR (CD_2Cl_2): δ 7.50 (s, 3H), 7.48 (s, 2H), 4.35 (s, 3H), 2.21 (m, 2H), 1.90 (s, 3H), 1.87 (s, 3H), 1.82 (s, 3H), 1.79 (s, 3H), 1.60 (d, J = 10.7 Hz, 9H), 1.02 (t, J = 7.6 Hz, 9H), -16.21(d, J = 35.3 Hz, 1H); ^{13}C{^{1}H} (CD_2Cl_2): δ 261.2 (s), 152.1 (s), 134.4 (s), 130.4 (s), 129.0 (s), 125.5 (s), 103.2 (s), 100.7 (s), 100.1 (s), 99.0 (s), 98.6 (s), 69.4 (s), 19.4 (d, J = 34.0 Hz), 18.6 (s), 14.8 (s), 10.0 (s), 9.9 (s), 9.8 (s), 9.7 (s); ^{31}P{^{1}H} (CD_2Cl_2): δ -44 (s); ^{19}F{^{1}H} (CD_2Cl_2): δ -77.1 (s). IR (CD_2Cl_2, cm^{-1}) 2974 (s), 2145 (s), 1973

(w), 1714 (s), 1445 (s), 1253 (s) . Anal. Calcd for $C_{23}H_{35}O_4SF_3PIr$: C, 40.17; H, 5.13. Found: C, 40.05; H, 5.22.

Cp'(PMe$_3$)Ir=C(OMe)Ph (4). Orange solid: ^{1}H NMR (C_6D_6): δ 7.22 (d, J = 12.1 Hz, 2H), 7.09 (t, J = 9.7 Hz, 2H), 7.00 (t, J = 10.9 Hz, 1H), 3.07 (s, 3H), 2.21 (q, J = 12.4 Hz, 2H), 1.84 (s, 6H), 1.76 (s, 6H) 1.57 (d, J = 11.2 Hz, 9H); $^{13}C\{^1H\}$ (C_6D_6): δ 216.6 (d, J = 17.4 Hz), 156.1 (s), 126.9 (s), 125.5 (s), 122.8 (s), 100.0 (s), 93.6 (s), 92.4 (s), 54.8 (s), 22.5 (d, J = 35.8 Hz), 19.0 (s), 17.2 (s), 10.9 (s), 10.3 (s); $^{31}P\{^1H\}$ (C_6D_6): δ -31.3 (s). IR (nujol, cm^{-1}) 2960 (s), 1969 (w), 1723 (s), 1452 (s), 1278 (s). HRMS (EI) *m/z* Calcd for $C_{22}H_{34}OPIr$: calcd 536.1953, obsvd 536.1949.

[Cp'(PMe$_3$)Ir(CO)(Ph)]BArf (6). colorless solid: ^{1}H NMR (CD_2Cl_2): δ 7.71 (s, 8H), 7.55 (s, 4H), 7.19 (d, J = 7.2 Hz, 2H), 7.11(m, 3H), 2.15 (m, 2H), 1.87 (s, 3H), 1.85 (s), 1.82 (s), 1.76 (s), 1.69 (d, J = 11.4 Hz, 9H), (t, J = 7.6 Hz, 3H); $^{13}C\{^1H\}$ (CD_2Cl_2): δ 167.5 (d, J = 12.5 Hz), 162.3 (q, J = 50.1 Hz), 140.0 (s), 135.4 (s), 130.8 (s), 129.3 (m), 126.5 (s), 125.9 (s), 123.8 (s), 122.0 (s), 121.1 (s), 118.0 (s), 107.7 (s), 104.5 (s), 104.4 (s), 104.3 (s), 104.2 (s), 103.8 (s), 18.1 (s), 16.3 (s), 15.8 (s), 13.9 (s), 9.2 (d, J = 10.3 Hz); 31P{1H} (CD_2Cl_2): δ -35.2 (s); $^{19}F\{^1H\}$ (CD_2Cl_2): δ -62.9 (s), -77.4 (s). IR (CD_2Cl_2, cm^{-1}) 2925 (w), 2033 (vs), 1275 (s), 1037 (s), 637 (w) . Anal. Calcd for $C_{53}H_{43}BF_{24}IrOP$: C, 45.93; H, 3.13. Found: C, 46.22; H, 2.86.

[Cp'Ir(CH(Ph)(PMe$_3$))(OTf)]BArf (12). Dark green solid: ^{1}H NMR (CD_2Cl_2): δ 7.75 (s, 8H), 7.58 (s, 4H), 7.54 (m, 1H), 6.72 (m, 4H), 4.33 (d, J = 16.5 Hz, 1H), 1.87 (dq, J = 1.4 Hz, 2H), 1.63 (d, J = 12.6 Hz, 9H), 1.47 (s, 3H), 1.42 (s, 3H), 1.38 (s, 3H), 1.35 (s, 3H), 1.01 (t, J = 1.4 Hz, 3H); $^{31}P\{^1H\}$ (CD_2Cl_2): δ -25.6 (s); $^{19}F\{^1H\}$ (CD_2Cl_2): δ - 63.1 (s), -77.1 (s). While **12** appears to be quite thermally stable in the solid state, gradual decomposition to unknown products occurs in both CH_2Cl_2 and THF.

[Cp'(PMe$_3$)Ir=CH(Ph)(OTf)]BArf (13). Dark green solid: ^{1}H NMR (CD_2Cl_2): δ 18.74 (s, 1H), 8.23 (t, J = 1.7 Hz, 1H), 7.9 (s, 4H), 7.68 (s, 12H), 7.51 (s,

8H), 2.10 (m, 2H), 1.78 (s, 6H), 1.76(s, 6H), 1.61 (d, J = 9.4 Hz, 9H), 1.09 (vt, J = 1.7 Hz, 3H); $^{31}P\{^{1}H\}$ (CD_2Cl_2): δ -45 (s); $^{19}F\{^{1}H\}$ (CD_2Cl_2): δ -62.9 (s), -77.3 (s). Due to thermal instability of **15** elemental analysis could not be obtained.

Cp'Ir(CH(Ph)(PMe$_3$))(Cl)$_2$ (14). Orange solid: ^{1}H NMR (CD_2Cl_2): δ 7.43 (s, 2H), 7.20 (t, J = 7.32 Hz, 2H), 7.06 (m, 1H), 3.92 (d, J = 16.2 Hz, 2H), 1.65 (q,J = 7.8 Hz, 2H), 1.63 (d, J = 12.8 Hz, 9H), 1.25 (s, 6H), 1.22 (s, 3H), 1.19 (s, 3H), 0.93 (t, J = 7.44 Hz, 3H); $^{13}C\{^{1}H\}$ (CD_2Cl_2): δ 145.8 (d, J = 10 Hz), 130.5 (d, J = 11.3 Hz), 127.6 (s), 125.1 (s), 88.0 (s), 86.7 (s), 86.5 (s), 85.8 (s), 85.3 (s), 16.6 (s), 15.1 (s), 14.6 (s), 11.8 (s), 9.0 (d, J = 48 Hz), 8.1 (s), 8.0 (s), 7.9 (s), 7.8 (s); $^{31}P\{^{1}H\}$ (CD_2Cl_2): δ -35.4 (s); IR (CD_2Cl_2, cm^{-1}) 2954 (s), 2947 (m), 1632 (m), 1265 (w), 1047 (w). Anal. Calcd for $C_{21}H_{32}Cl_2IrP$: C, 43.58; H, 5.57. Found: C, 43.18; H, 5.63.

Figure S-1. ORTEP Diagram of **1** (cation).

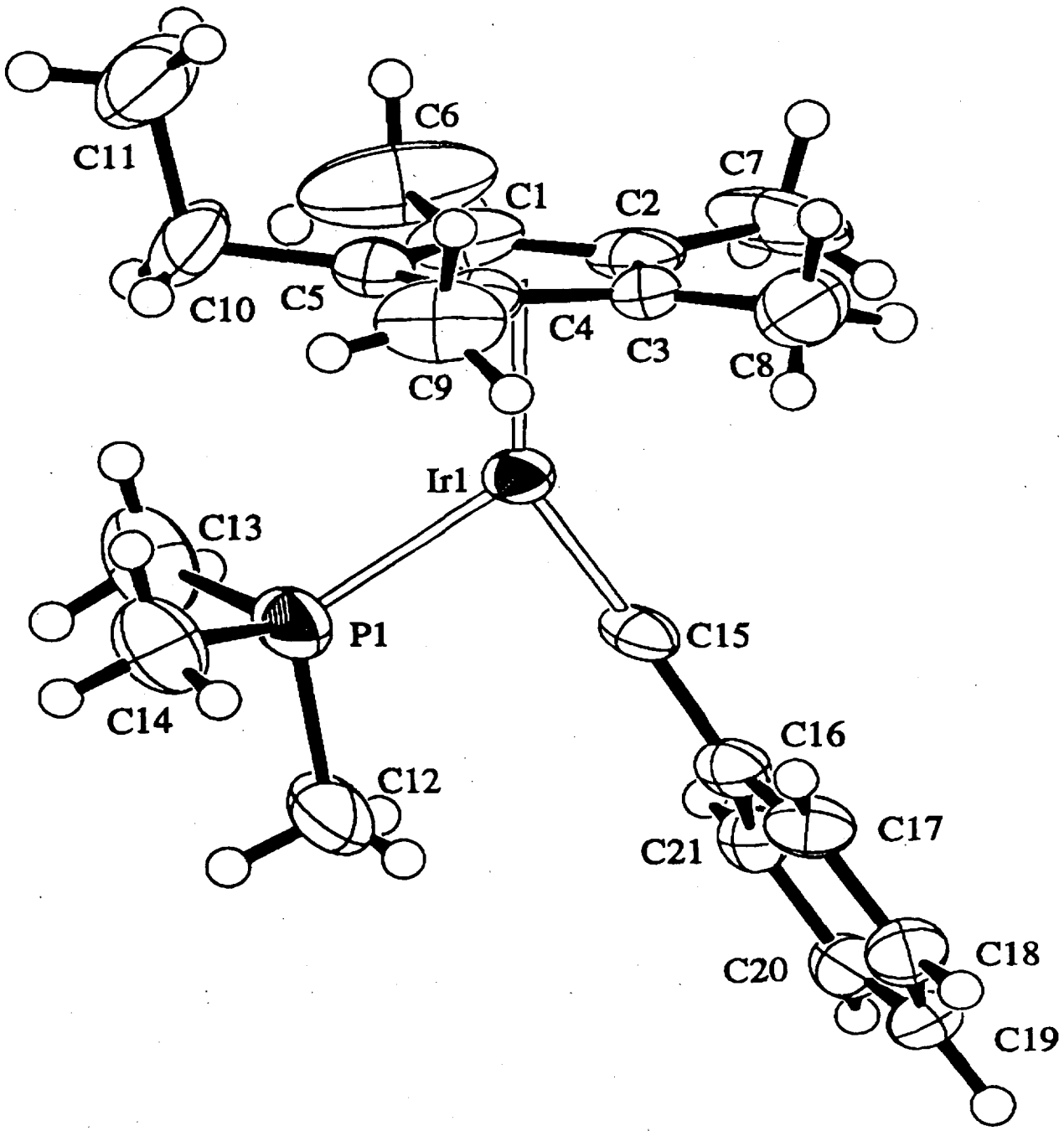

Figure S-2. ORTEP Diagram of **1** (cation and anion).

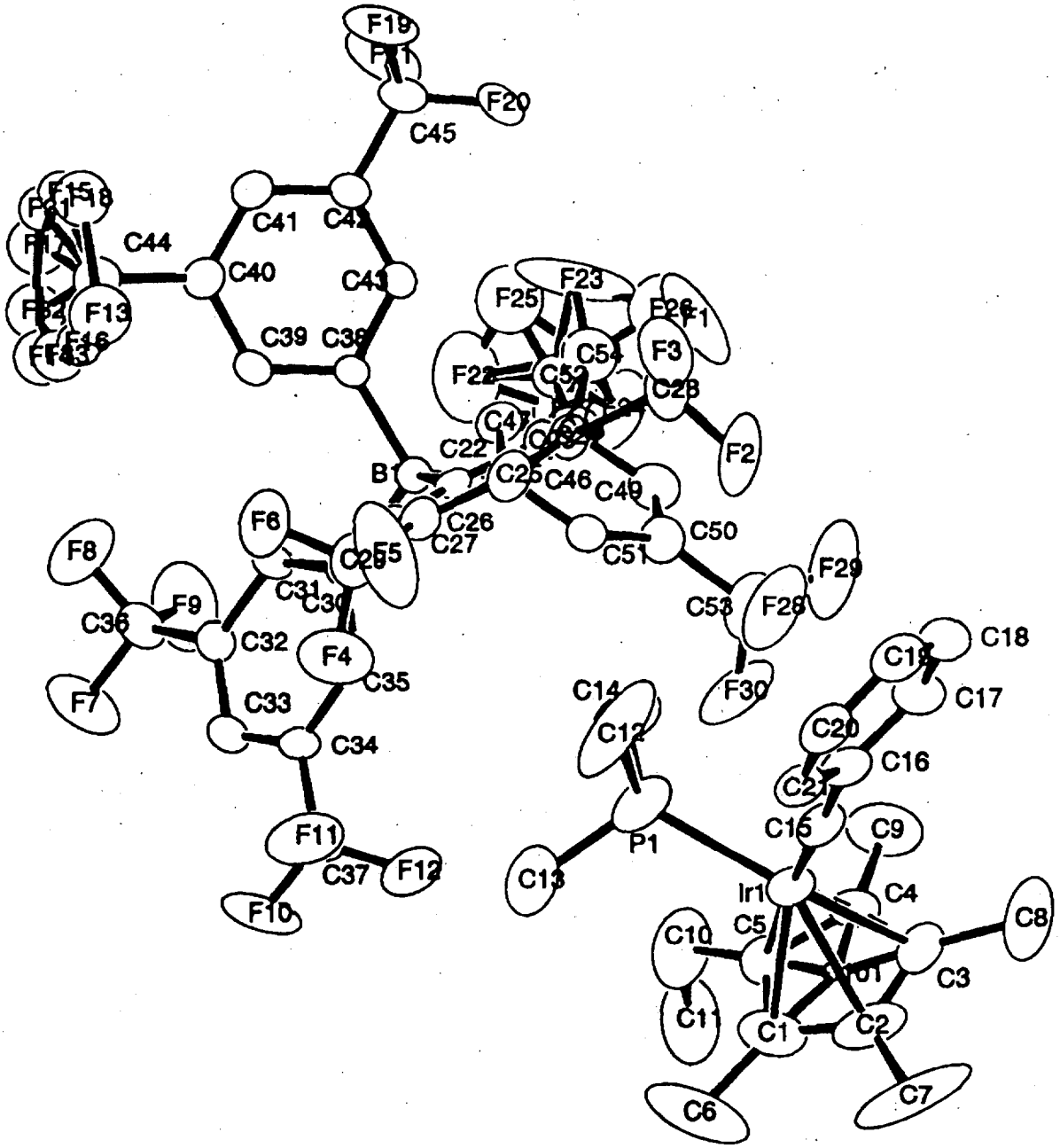

Table S-1. Crystal and Data Collection Parameters for **1**.
Empirical formula: $IrPF_{24}C_{53}H_{43}B$

(A) Crystal Parameters at T= -120° C

a = 12.7002(5) Å	Space Group: P1 (#2)
b = 14.5937(6) Å	Formula Weight = 1369.89
c = 16.2986(6) Å	Z = 2
α = 105.152(1) Å	D_{calc} = 1.637 g/cm^3
β = 106.924(1) °	μ(MoKα) = 25.54 cm $^{-1}$
γ = 90.423(1) °	
V = 2778.11(18) Å^3	

Size: 0.20 x 0.22 x 0.30 mm

(B) Data Measurement Parameters

Diffractometer: SMART CCD

Radiation: MoKα (λ = 0.71069 Å)

Monochromator: graphite ($2\theta_{max}$ = 52.2°)

Scan type: ω (0.3° per frame)

Scan rate: 10.0 s per frame

Crystal to detector distance: 60 mm

No. of reflections measured: Total: 15206 (Unique: 9385 (R_{int} = 0.022))

Corrections: Lorentz-polarization absorption (Tmax = 0.93, Tmin = 0.72);

(C) Data Reduction and Refinement

Structure Solution	Direct Methods (SIR92)	
Refinement	Full-matrix least-squares	
p-factor	0.0300	
Reflection/Parameter	10.79	
Final Residuals:	R= 4.0 %	Rw = 4.6 %

G.O.F = 1.54

Table S-2. Positional Parameters and B_{iso}/B_{eq}.

Atom	x	y	z	B
Ir(1)	0.26897(2)	0.222962(16)	0.249977(15)	2.662(5)
P(1)	0.31485(18)	0.30749(13)	0.39714(11)	4.28(4)
F(1)	-0.0986(3)	0.3017(3)	0.5682(4)	7.56(14)
F(2)	-0.0374(4)	0.3108(4)	0.4646(3)	8.62(14)
F(3)	-0.0816(3)	0.4344(3)	0.5436(3)	4.88(10)
F(4)	0.4132(4)	0.5438(3)	0.6738(3)	6.86(13)
F(5)	0.2720(4)	0.6198(3)	0.6537(4)	8.75(15)
F(6)	0.3576(4)	0.6072(3)	0.7817(3)	5.83(11)
F(7)	0.7631(3)	0.1818(4)	0.9805(3)	7.09(13)
F(8)	0.6369(4)	0.2293(3)	1.0377(3)	6.64(12)
F(9)	0.6247(4)	0.0888(3)	0.9594(3)	7.19(13)
F(10)	0.7473(3)	0.2565(5)	0.7068(3)	8.36(16)
F(11)	0.6272(4)	0.3529(3)	0.6737(3)	6.30(13)
F(12)	0.5954(4)	0.2079(3)	0.6034(3)	6.31(12)
F(13)	0.3526(13)	0.5696(10)	1.0325(9)	5.6(4)
F(14)	0.4603(10)	0.4739(10)	1.0921(9)	4.5(3)
F(15)	0.3032(9)	0.5375(8)	1.1313(7)	2.85(18)
F(16)	0.3966(11)	0.5503(9)	1.0436(7)	2.9(2)
F(17)	0.3842(12)	0.4540(10)	1.1512(9)	5.3(3)
F(18)	0.2837(9)	0.5590(8)	1.1045(8)	4.6(3)
F(19)	-0.0573(3)	0.3577(3)	0.9690(3)	5.60(11)
F(20)	-0.0737(3)	0.2399(4)	0.8577(3)	6.35(11)
F(21)	-0.0022(3)	0.2279(3)	0.9892(3)	5.92(12)
F(22)	0.2444(8)	-0.0748(6)	0.8538(5)	7.6(3)
F(23)	0.0753(10)	-0.0778(9)	0.8002(11)	9.5(4)
F(24)	0.1651(9)	-0.1838(4)	0.7344(6)	5.8(2)
F(25)	0.1428(16)	-0.0584(11)	0.8443(10)	6.9(4)
F(26)	0.0350(13)	-0.1367(10)	0.7225(10)	7.4(4)
F(27)	0.2043(12)	-0.1608(12)	0.7732(10)	6.1(4)
F(28)	0.1208(5)	0.0323(3)	0.4420(3)	7.73(15)
F(29)	0.0758(6)	-0.1016(4)	0.4439(3)	9.22(16)
F(30)	0.2423(5)	-0.0617(6)	0.4644(3)	14.1(2)
F(31)	0.3405(16)	0.5052(14)	1.1507(11)	2.8(3)
F(32)	0.4356(14)	0.4576(10)	1.1236(10)	4.5(3)
F(33)	0.4340(13)	0.5154(12)	1.0671(10)	3.8(3)
C(1)	0.4175(6)	0.1493(4)	0.2211(5)	4.39(18)
C(2)	0.3296(7)	0.1388(5)	0.1403(5)	4.42(18)
C(3)	0.2384(6)	0.0858(4)	0.1446(4)	3.70(14)
C(4)	0.2711(5)	0.0627(4)	0.2272(4)	2.94(13)
C(5)	0.3791(5)	0.1024(4)	0.2735(4)	3.35(14)
C(6)	0.5334(8)	0.1919(6)	0.2413(9)	10.2(4)
C(7)	0.3370(11)	0.1710(7)	0.0614(6)	9.8(4)
C(8)	0.1320(8)	0.0514(6)	0.0713(5)	7.8(2)
C(9)	0.2010(7)	-0.0010(5)	0.2536(6)	5.7(2)
C(10)	0.4483(7)	0.0836(6)	0.3590(5)	6.4(2)
C(11)	0.5175(8)	0.0016(6)	0.3417(6)	7.4(3)
C(12)	0.2520(10)	0.4183(6)	0.4231(5)	9.2(3)
C(13)	0.4597(8)	0.3457(6)	0.4516(5)	6.2(2)
C(14)	0.2784(7)	0.2439(6)	0.4677(5)	5.9(2)

Table S-2. Positional Parameters and B_{iso}/B_{eq} (cont'd)

Atom	x	y	z	B
C(15)	0.1744(5)	0.3050(4)	0.2272(4)	2.83(13)
C(16)	0.0921(5)	0.3711(4)	0.2127(4)	2.85(13)
C(17)	-0.0192(5)	0.3396(4)	0.1896(4)	3.34(14)
C(18)	-0.0989(5)	0.4021(5)	0.1728(4)	3.77(15)
C(19)	-0.0686(6)	0.4956(5)	0.1800(4)	3.63(15)
C(20)	0.0407(6)	0.5274(4)	0.2042(4)	3.43(14)
C(21)	0.1221(5)	0.4658(4)	0.2190(4)	2.90(13)
C(22)	0.2346(4)	0.3167(3)	0.7092(3)	1.85(10)
C(23)	0.1273(4)	0.3037(3)	0.6510(3)	2.19(11)
C(24)	0.0828(5)	0.3725(4)	0.6095(3)	2.46(11)
C(25)	0.1438(5)	0.4560(4)	0.6224(4)	2.90(13)
C(26)	0.2515(5)	0.4705(4)	0.6797(3)	2.57(12)
C(27)	0.2955(4)	0.4024(4)	0.7222(3)	2.20(11)
C(28)	-0.0327(5)	0.3553(4)	0.5472(4)	3.60(14)
C(29)	0.3203(6)	0.5603(4)	0.6964(4)	3.57(15)
C(30)	0.4171(4)	0.2397(3)	0.7910(3)	1.98(10)
C(31)	0.4808(4)	0.2141(4)	0.8660(3)	2.15(11)
C(32)	0.5941(4)	0.2059(4)	0.8834(3)	2.39(11)
C(33)	0.6487(4)	0.2235(4)	0.8264(4)	2.84(12)
C(34)	0.5868(4)	0.2483(4)	0.7506(4)	2.55(12)
C(35)	0.4744(4)	0.2547(4)	0.7338(3)	2.23(11)
C(36)	0.6547(5)	0.1776(5)	0.9647(4)	3.25(14)
C(37)	0.6405(5)	0.2661(5)	0.6851(4)	3.90(16)
C(38)	0.2476(4)	0.2881(3)	0.8594(3)	1.68(10)
C(39)	0.3131(4)	0.3616(4)	0.9304(3)	2.17(11)
C(40)	0.2760(5)	0.4097(4)	1.0006(4)	2.64(12)
C(41)	0.1726(5)	0.3860(4)	1.0034(3)	2.53(12)
C(42)	0.1060(4)	0.3133(4)	0.9348(3)	2.20(11)
C(43)	0.1429(4)	0.2655(3)	0.8641(3)	1.90(10)
C(44)	0.3491(6)	0.4912(5)	1.0731(5)	4.47(17)
C(45)	-0.0059(5)	0.2850(4)	0.9378(4)	2.98(13)
C(46)	0.2317(4)	0.1323(3)	0.7183(3)	1.92(10)
C(47)	0.2129(5)	0.0682(4)	0.7640(4)	2.58(12)
C(48)	0.1774(5)	-0.0269(4)	0.7212(4)	3.32(14)
C(49)	0.1578(5)	-0.0618(4)	0.6306(4)	3.49(14)
C(50)	0.1762(5)	0.0002(4)	0.5832(4)	3.15(13)
C(51)	0.2128(4)	0.0947(4)	0.6276(4)	2.47(12)
C(52)	0.1694(11)	-0.0887(8)	0.7793(9)	2.7(2)
C(53)	0.1581(8)	-0.0359(5)	0.4839(5)	5.1(2)
C(54)	0.125(2)	-0.0981(15)	0.7585(15)	4.5(5)
C(101)	0.3271	0.1078	0.2014	0.3
B(1)	0.2822(5)	0.2428(4)	0.7690(4)	1.89(10)
H(1)	0.5648	0.2174	0.304	12.262
H(2)	0.5321	0.2413	0.2131	12.262
H(3)	0.5765	0.1439	0.2198	12.262
H(4)	0.3851	0.2279	0.0817	11.7281
H(5)	0.2656	0.1827	0.0289	11.7281
H(6)	0.3651	0.1227	0.0239	11.7281
H(7)	0.1233	0.0875	0.0293	9.3276
H(8)	0.0721	0.0589	0.0956	9.3276

Table S-2. Positional Parameters and B_{iso}/B_{eq} (cont'd)

Atom	x	y	z	B
H(9)	0.133	-0.014	0.0424	9.3276
H(10)	0.2261	0.0094	0.3164	6.8119
H(11)	0.1262	0.013	0.2358	6.8119
H(12)	0.2065	-0.0657	0.2252	6.8119
H(13)	0.4007	0.0691	0.3902	7.7076
H(14)	0.4958	0.1392	0.3946	7.7076
H(15)	0.5588	-0.0087	0.3968	8.9135
H(16)	0.4707	-0.0542	0.3056	8.9135
H(17)	0.5666	0.0161	0.3117	8.9135
H(18)	0.174	0.4069	0.3977	11.0188
H(19)	0.2791	0.463	0.3993	11.0188
H(20)	0.2698	0.4431	0.486	11.0188
H(21)	0.5018	0.2925	0.4424	7.4452
H(22)	0.4817	0.3924	0.4273	7.4452
H(23)	0.4718	0.3722	0.5137	7.4452
H(24)	0.2003	0.2343	0.4523	7.0446
H(25)	0.3084	0.184	0.4597	7.0446
H(26)	0.3075	0.2801	0.5283	7.0446
H(27)	-0.0402	0.2755	0.1854	4.007
H(28)	-0.1749	0.3805	0.1563	4.5299
H(29)	-0.1238	0.5381	0.1681	4.3596
H(30)	0.061	0.5924	0.2109	4.1141
H(31)	0.1976	0.4876	0.2334	3.4822
H(32)	0.0834	0.2461	0.6395	2.6296
H(33)	0.1134	0.5024	0.5931	3.4793
H(34)	0.3691	0.4143	0.7612	2.643
H(35)	0.4456	0.2017	0.9066	2.5832
H(36)	0.726	0.2189	0.8384	3.412
H(37)	0.4343	0.2699	0.6808	2.6784
H(38)	0.3852	0.3792	0.9304	2.6026
H(39)	0.1473	0.419	1.0515	3.0361
H(40)	0.0953	0.216	0.8176	2.2802
H(41)	0.2248	0.0905	0.8265	3.0926
H(42)	0.1321	-0.1268	0.601	4.1872
H(43)	0.2254	0.1357	0.5941	2.9683

Table S-3. Anisotropic Parameters.

Atom	U11	U22	U33	U12	U13	U23
Ir(1)	0.04253(14)	0.03154(13)	0.03475(13)	0.01209(9)	0.01866(10)	0.01409(9)
P(1)	0.0866(14)	0.0481(10)	0.0368(9)	0.0233(10)	0.0259(10)	0.0178(8)
F(1)	0.037(2)	0.098(3)	0.146(5)	-0.015(2)	-0.028(3)	0.085(3)
F(2)	0.077(3)	0.139(5)	0.050(3)	0.038(3)	-0.027(2)	-0.027(3)
F(3)	0.050(2)	0.049(2)	0.074(3)	0.015(2)	-0.006(2)	0.025(2)
F(4)	0.094(4)	0.062(3)	0.120(4)	-0.024(3)	0.065(3)	0.015(3)
F(5)	0.097(4)	0.063(3)	0.146(5)	-0.032(3)	-0.043(3)	0.076(3)
F(6)	0.098(3)	0.053(2)	0.057(3)	-0.039(2)	0.019(2)	-0.003(2)
F(7)	0.028(2)	0.172(5)	0.088(3)	0.025(3)	0.006(2)	0.081(3)
F(8)	0.095(4)	0.120(4)	0.036(2)	0.059(3)	0.014(2)	0.025(2)
F(9)	0.102(4)	0.069(3)	0.095(4)	-0.002(3)	-0.009(3)	0.053(3)
F(10)	0.033(2)	0.234(6)	0.088(3)	0.027(3)	0.034(2)	0.091(4)
F(11)	0.106(4)	0.080(3)	0.084(3)	0.004(3)	0.065(3)	0.035(3)
F(12)	0.084(3)	0.108(4)	0.049(3)	-0.010(3)	0.039(2)	0.004(2)
F(19)	0.048(2)	0.071(3)	0.112(4)	0.022(2)	0.054(3)	0.023(3)
F(20)	0.026(2)	0.143(4)	0.055(3)	-0.020(2)	0.014(2)	-0.004(3)
F(21)	0.042(2)	0.103(3)	0.111(4)	0.008(2)	0.029(2)	0.075(3)
F(22)	0.127(8)	0.087(6)	0.082(6)	-0.027(5)	0.000(5)	0.071(5)
F(23)	0.089(8)	0.163(10)	0.225(14)	0.074(8)	0.122(10)	0.166(11)
F(24)	0.138(8)	0.019(3)	0.058(5)	-0.007(4)	0.022(5)	0.014(3)
F(28)	0.159(5)	0.077(3)	0.046(3)	-0.001(3)	0.021(3)	0.009(2)
F(29)	0.171(6)	0.080(3)	0.056(3)	-0.044(4)	-0.011(3)	-0.001(3)
F(30)	0.101(5)	0.346(11)	0.048(3)	0.106(6)	0.026(3)	-0.023(4)
C(1)	0.053(4)	0.034(3)	0.094(6)	0.015(3)	0.042(4)	0.020(4)
C(2)	0.091(6)	0.045(4)	0.062(5)	0.044(4)	0.052(4)	0.032(3)
C(3)	0.052(4)	0.047(4)	0.034(3)	0.028(3)	0.007(3)	0.003(3)
C(4)	0.038(3)	0.037(3)	0.044(3)	0.009(3)	0.022(3)	0.012(3)
C(5)	0.049(4)	0.031(3)	0.045(4)	0.011(3)	0.015(3)	0.004(3)
C(6)	0.074(7)	0.070(6)	0.269(15)	0.007(5)	0.104(9)	0.030(8)
C(7)	0.253(14)	0.101(7)	0.106(7)	0.114(8)	0.145(9)	0.074(6)
C(8)	0.090(7)	0.085(6)	0.064(5)	0.044(5)	-0.021(5)	-0.025(5)
C(9)	0.080(6)	0.047(4)	0.111(7)	0.004(4)	0.058(5)	0.026(4)
C(10)	0.092(6)	0.067(5)	0.063(5)	0.045(5)	-0.009(5)	0.018(4)
C(11)	0.087(7)	0.067(5)	0.092(7)	0.031(5)	-0.015(5)	0.007(5)
C(12)	0.210(12)	0.086(6)	0.039(4)	0.092(7)	0.022(6)	0.009(4)
C(13)	0.099(7)	0.074(5)	0.051(5)	-0.015(5)	0.014(5)	0.006(4)
C(14)	0.095(6)	0.097(6)	0.049(4)	0.014(5)	0.039(4)	0.031(4)
C(15)	0.054(4)	0.022(3)	0.034(3)	0.006(3)	0.021(3)	0.003(2)
C(16)	0.048(4)	0.036(3)	0.035(3)	0.012(3)	0.024(3)	0.015(3)
C(17)	0.043(4)	0.039(3)	0.050(4)	0.005(3)	0.024(3)	0.010(3)
C(18)	0.035(4)	0.066(4)	0.045(4)	0.013(3)	0.016(3)	0.015(3)
C(19)	0.054(4)	0.050(4)	0.039(3)	0.028(3)	0.017(3)	0.018(3)
C(20)	0.064(5)	0.035(3)	0.035(3)	0.015(3)	0.018(3)	0.014(3)
C(21)	0.047(4)	0.039(3)	0.033(3)	0.007(3)	0.019(3)	0.017(3)
C(22)	0.026(3)	0.027(3)	0.020(3)	0.002(2)	0.013(2)	0.004(2)
C(23)	0.029(3)	0.024(3)	0.028(3)	0.002(2)	0.007(2)	0.005(2)
C(24)	0.034(3)	0.028(3)	0.029(3)	0.007(2)	0.005(2)	0.008(2)
C(25)	0.051(4)	0.029(3)	0.030(3)	0.006(3)	0.009(3)	0.013(2)
C(26)	0.042(3)	0.028(3)	0.028(3)	-0.001(3)	0.010(3)	0.008(2)

Table S-3. Anisotropic Parameters (cont'd)

Atom	U11	U22	U33	U12	U13	U23
C(27)	0.026(3)	0.036(3)	0.024(3)	0.005(2)	0.010(2)	0.009(2)
C(28)	0.043(4)	0.039(3)	0.046(4)	0.006(3)	-0.005(3)	0.017(3)
C(29)	0.056(4)	0.034(3)	0.044(4)	-0.005(3)	0.010(3)	0.013(3)
C(30)	0.024(3)	0.025(3)	0.024(3)	0.005(2)	0.006(2)	0.005(2)
C(31)	0.021(3)	0.031(3)	0.033(3)	0.004(2)	0.011(2)	0.012(2)
C(32)	0.025(3)	0.033(3)	0.031(3)	0.008(2)	0.005(2)	0.008(2)
C(33)	0.023(3)	0.039(3)	0.041(3)	0.003(2)	0.011(3)	0.002(3)
C(34)	0.025(3)	0.040(3)	0.033(3)	0.004(2)	0.015(3)	0.006(3)
C(35)	0.025(3)	0.034(3)	0.028(3)	0.007(2)	0.010(2)	0.009(2)
C(36)	0.026(3)	0.054(4)	0.045(4)	0.008(3)	0.006(3)	0.021(3)
C(37)	0.031(4)	0.076(5)	0.049(4)	0.007(3)	0.018(3)	0.023(4)
C(38)	0.018(3)	0.025(3)	0.023(3)	0.006(2)	0.006(2)	0.010(2)
C(39)	0.021(3)	0.033(3)	0.029(3)	0.001(2)	0.008(2)	0.010(2)
C(40)	0.035(3)	0.035(3)	0.030(3)	0.002(3)	0.012(3)	0.006(2)
C(41)	0.034(3)	0.036(3)	0.028(3)	0.007(3)	0.012(3)	0.007(2)
C(42)	0.024(3)	0.034(3)	0.029(3)	0.008(2)	0.009(2)	0.012(2)
C(43)	0.019(3)	0.030(3)	0.024(3)	0.005(2)	0.005(2)	0.011(2)
C(44)	0.043(4)	0.065(5)	0.051(4)	-0.004(4)	0.021(4)	-0.010(4)
C(45)	0.028(3)	0.051(4)	0.042(3)	0.010(3)	0.018(3)	0.019(3)
C(46)	0.018(3)	0.023(3)	0.033(3)	0.004(2)	0.009(2)	0.009(2)
C(47)	0.038(3)	0.031(3)	0.034(3)	0.011(3)	0.015(3)	0.012(2)
C(48)	0.054(4)	0.028(3)	0.056(4)	0.010(3)	0.028(3)	0.019(3)
C(49)	0.047(4)	0.025(3)	0.060(4)	-0.004(3)	0.023(3)	0.003(3)
C(50)	0.045(4)	0.030(3)	0.043(3)	-0.006(3)	0.014(3)	0.005(3)
C(51)	0.031(3)	0.031(3)	0.032(3)	-0.002(2)	0.013(3)	0.006(2)
C(53)	0.093(6)	0.037(4)	0.052(4)	-0.013(4)	0.017(4)	-0.001(3)

Table S-4. Bond Lengths (Å).

Atom	Atom	Distance	Atom	Atom	Distance	Atom	Atom	Distance
IR1	P1	2.290(2)	F20	C45	1.329(7)	C38	B1	1.636(7)
IR1	C1	2.284(6)	F21	C45	1.318(7)	C39	C40	1.387(7)
IR1	C2	2.227(6)	F22	F25	1.29(2)	C40	C41	1.372(8)
IR1	C3	2.216(6)	F22	F27	1.52(2)	C40	C44	1.510(8)
IR1	C4	2.272(6)	F22	C52	1.27(2)	C41	C42	1.380(7)
IR1	C5	2.297(6)	F22	C54	1.78(3)	C42	C43	1.390(7)
IR1	C15	1.734(6)	F23	F25	0.93(2)	C42	C45	1.496(7)
IR1	C101	1.9130(2)	F23	F26	1.29(2)	C46	C47	1.397(7)
P1	C12	1.814(8)	F23	C52	1.34(1)	C46	C51	1.382(7)
P1	C13	1.805(9)	F23	C54	1.04(2)	C46	B1	1.636(7)
P1	C14	1.805(7)	F24	F27	0.68(1)	C47	C48	1.384(8)
F1	C28	1.315(7)	F24	C52	1.38(1)	C48	C49	1.375(8)
F2	C28	1.316(7)	F24	C54	1.36(2)	C48	C52	1.49(1)
F3	C28	1.321(7)	F25	C52	1.18(2)	C48	C54	1.57(2)
F4	C29	1.340(8)	F25	C54	1.32(3)	C49	C50	1.391(8)
F5	C29	1.301(7)	F26	C52	1.73(2)	C50	C51	1.384(7)
F6	C29	1.319(7)	F26	C54	1.18(3)	C3	C4	1.419(8)
F7	C36	1.322(7)	F27	C52	1.14(2)	C3	C8	1.50(1)
F8	C36	1.315(7)	F27	C54	1.38(3)	C3	C101	1.209(6)
F9	C36	1.322(7)	F28	C53	1.363(9)	C4	C5	1.394(8)
F10	C37	1.316(7)	F29	C53	1.303(8)	C4	C9	1.504(9)
F11	C37	1.333(8)	F30	C53	1.24(1)	C4	C101	1.195(6)
F12	C37	1.334(7)	F31	F32	1.52(2)	C5	C10	1.51(1)
F13	F16	0.63(2)	F31	C44	1.27(2)	C5	C101	1.192(6)
F13	F18	1.69(2)	F32	F33	1.40(2)	C10	C11	1.51(1)
F13	F33	1.39(2)	F32	C44	1.35(2)	C15	C16	1.439(8)
F13	C44	1.47(2)	F33	C44	1.17(1)	C16	C17	1.393(8)
F14	F16	1.62(2)	C1	C2	1.43(1)	C16	C21	1.400(8)
F14	F17	1.62(2)	C1	C5	1.407(9)	C17	C18	1.384(9)
F14	F32	0.76(2)	C1	C6	1.50(1)	C18	C19	1.381(9)
F14	F33	0.84(2)	C1	C101	1.209(7)	C19	C20	1.369(9)
F14	C44	1.40(1)	C2	C3	1.42(1)	C20	C21	1.384(8)
F15	F17	1.64(2)	C2	C7	1.506(9)	C22	C23	1.394(7)
F15	F18	0.60(1)	C2	C101	1.204(6)	C22	C27	1.400(7)
F15	F31	0.74(2)	C30	C35	1.395(7)	C22	B1	1.642(7)
F15	C44	1.30(1)	C30	B1	1.648(7)	C23	C24	1.388(7)
F16	F33	0.79(1)	C31	C32	1.396(7)	C24	C25	1.374(7)
F16	C44	1.31(1)	C32	C33	1.380(7)	C24	C28	1.496(8)
F17	F31	0.93(2)	C32	C36	1.489(8)	C25	C26	1.391(8)
F17	F32	0.90(2)	C33	C34	1.395(8)	C26	C27	1.386(7)
F17	C44	1.47(1)	C34	C35	1.382(7)	C26	C29	1.488(8)
F18	F31	1.31(2)	C34	C37	1.496(8)	C30	C31	1.399(7)
F18	C44	1.39(1)	C38	C39	1.400(7)	C50	C53	1.512(9)
F19	C45	1.316(6)	C38	C43	1.396(7)	C52	C54	0.57(2)

Table S-5. Bond Angles (°)

Atom	Atom	Atom	Angle
P1	IR1	C15	87.7(2)
P1	IR1	C101	126.63(5)
C15	IR1	C101	145.6(2)
IR1	P1	C12	116.9(3)
IR1	P1	C13	115.8(3)
IR1	P1	C14	114.2(3)
C12	P1	C13	101.8(5)
C12	P1	C14	102.4(4)
C13	P1	C14	103.9(4)
C2	C1	C5	107.1(6)
C2	C1	C6	126.2(8)
C5	C1	C6	126.3(8)
C1	C2	C3	108.1(5)
C1	C2	C7	125.5(8)
C3	C2	C7	126.3(8)
C2	C3	C4	107.3(6)
C2	C3	C8	126.1(7)
C4	C3	C8	126.3(7)
C3	C4	C5	108.5(5)
C3	C4	C9	123.8(6)
C5	C4	C9	127.6(6)
C1	C5	C4	109.0(6)
C1	C5	C10	125.8(7)
C4	C5	C10	124.5(6)
C5	C10	C11	111.9(6)
IR1	C15	C16	175.7(4)
C15	C16	C17	119.4(5)
C15	C16	C21	120.9(5)
C17	C16	C21	119.7(5)
C16	C17	C18	119.6(6)
C17	C18	C19	120.4(6)
C18	C19	C20	120.2(5)
C19	C20	C21	120.6(6)
C16	C21	C20	119.4(6)
C23	C22	C27	116.2(5)
C23	C22	B1	122.1(4)
C27	C22	B1	121.2(4)
C22	C23	C24	121.8(5)
C23	C24	C25	121.3(5)
C23	C24	C28	120.1(5)
C25	C24	C28	118.6(5)
C24	C25	C26	118.0(5)
C25	C26	C27	120.8(5)
C25	C26	C29	119.9(5)
C27	C26	C29	119.3(5)
C22	C27	C26	121.9(5)
F1	C28	F2	104.9(6)
F1	C28	F3	105.6(6)

Atom	Atom	Atom	Angle
F1	C28	C24	113.3(5)
F2	C28	F3	106.1(5)
F2	C28	C24	112.7(5)
F3	C28	C24	113.5(5)
F4	C29	F5	105.7(6)
F4	C29	F6	103.0(6)
F4	C29	C26	112.1(5)
F5	C29	F6	107.3(5)
F5	C29	C26	114.9(5)
F6	C29	C26	112.9(5)
C31	C30	C35	115.2(5)
C31	C30	B1	121.4(4)
C35	C30	B1	123.2(4)
C30	C31	C32	122.4(5)
C31	C32	C33	120.7(5)
C31	C32	C36	118.4(5)
C33	C32	C36	120.8(5)
C32	C33	C34	118.0(5)
C33	C34	C35	120.4(5)
C33	C34	C37	120.6(5)
C35	C34	C37	118.9(5)
C30	C35	C34	123.1(5)
F7	C36	F8	106.6(5)
F7	C36	F9	105.3(5)
F7	C36	C32	113.9(5)
F8	C36	F9	104.9(5)
F8	C36	C32	113.3(5)
F9	C36	C32	112.1(5)
F10	C37	F11	107.1(6)
F10	C37	F12	106.8(6)
F10	C37	C34	113.9(5)
F11	C37	F12	103.8(5)
F11	C37	C34	112.3(5)
F12	C37	C34	112.3(5)
C39	C38	C43	115.8(4)
C39	C38	B1	122.4(4)
C43	C38	B1	121.1(4)
C38	C39	C40	122.2(5)
C39	C40	C41	120.7(5)
C39	C40	C44	119.4(5)
C41	C40	C44	119.8(5)
C40	C41	C42	118.7(5)
C41	C42	C43	120.6(5)
C41	C42	C45	119.4(5)
C43	C42	C45	119.9(5)
C38	C43	C42	122.0(4)
F13	C44	F14	99(1)
F13	C44	F15	95(1)

Table S-5. Bond Angles (°) (cont'd)

Atom	Atom	Atom	Angle
F13	C44	F16	25.3(7)
F13	C44	F17	149.2(9)
F13	C44	F18	72.4(9)
F13	C44	F31	122(1)
F13	C44	F32	127(1)
F13	C44	F33	62(1)
F13	C44	C40	106.4(8)
F14	C44	F15	124.9(9)