Symmetrical Hydrogen Bonds in Iridium(III) Alkoxides with Relevance to Outer Sphere Hydrogen Transfer

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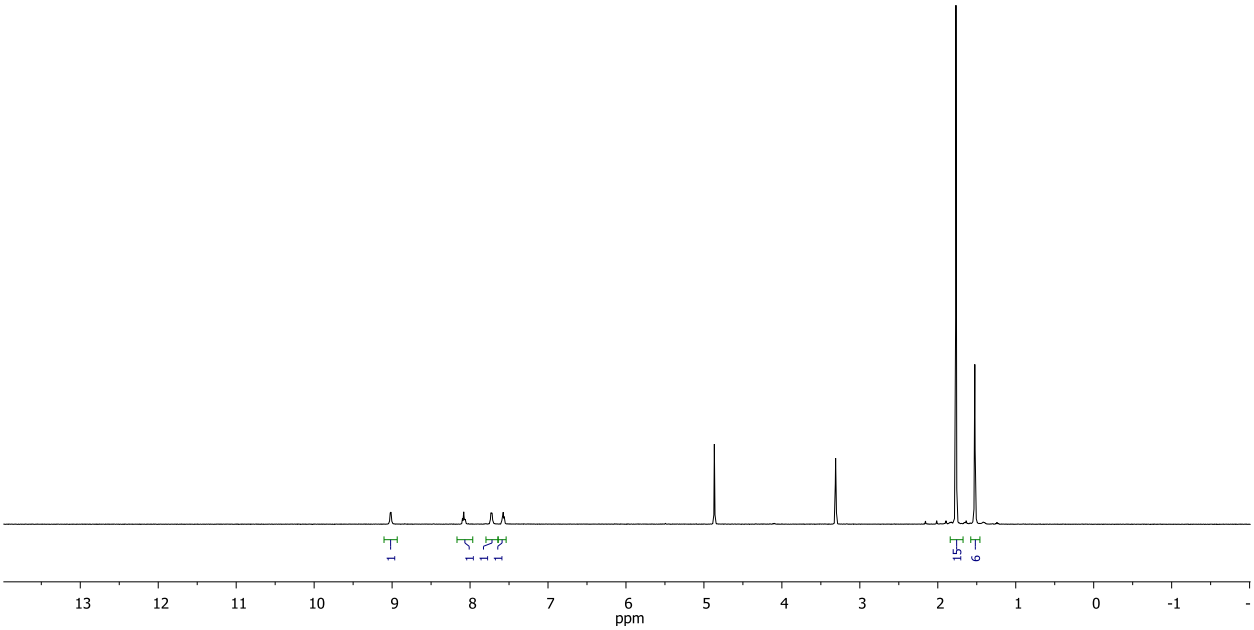

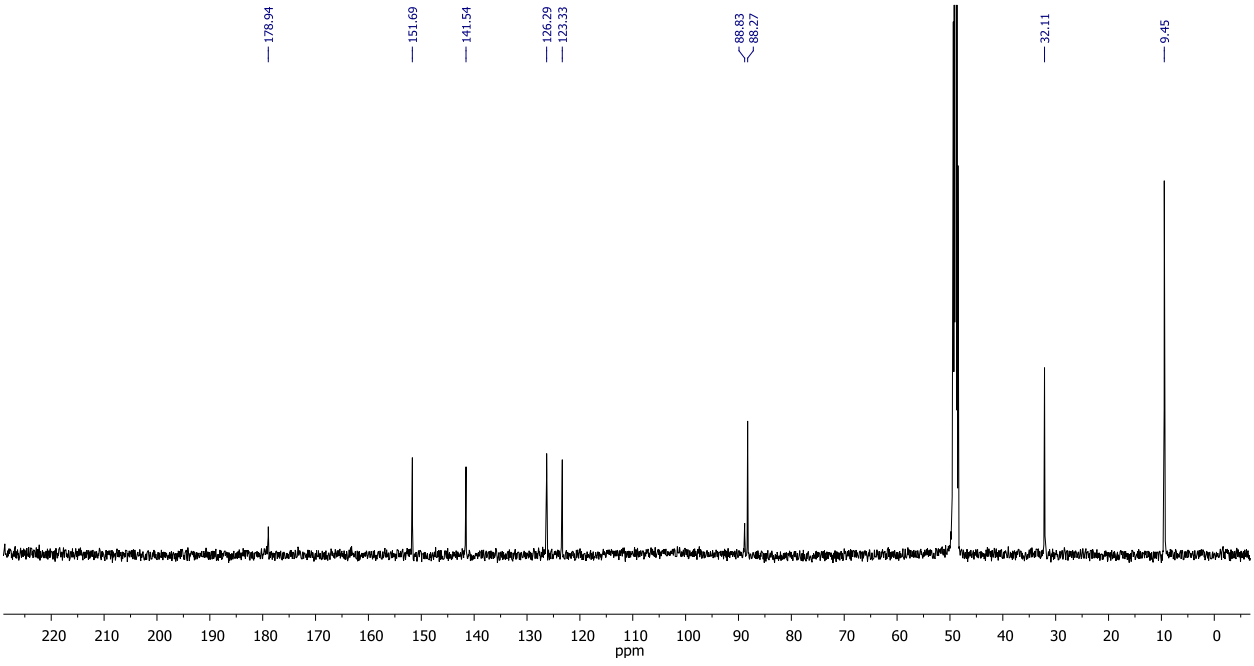

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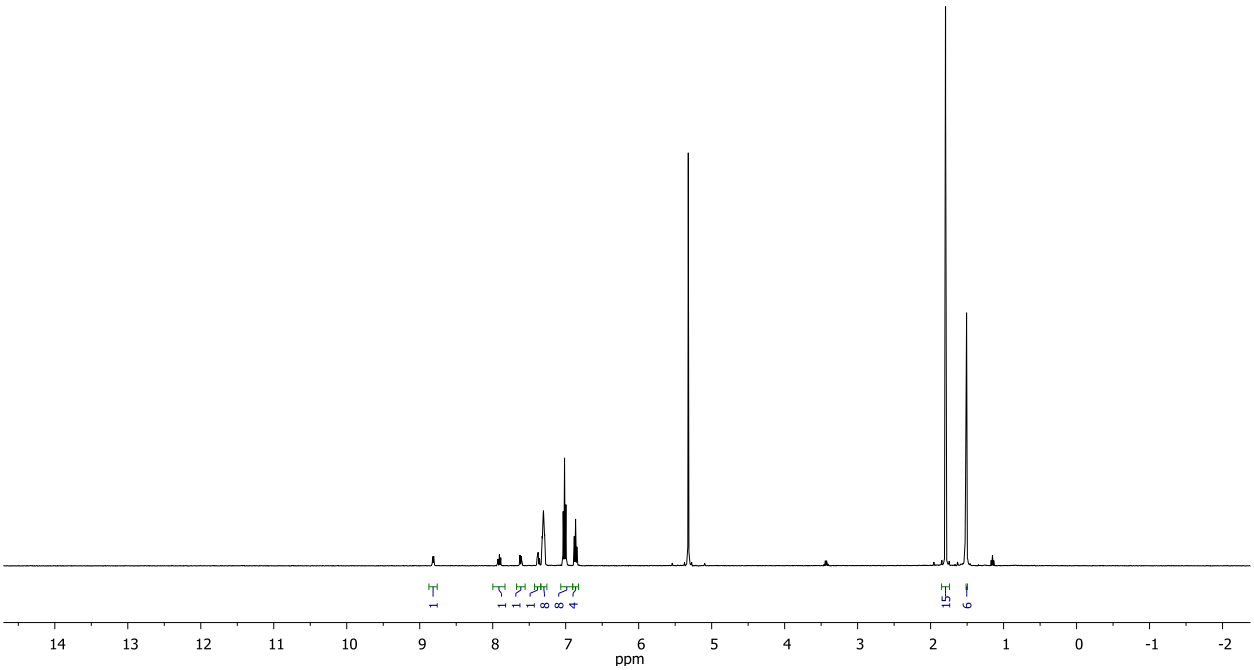

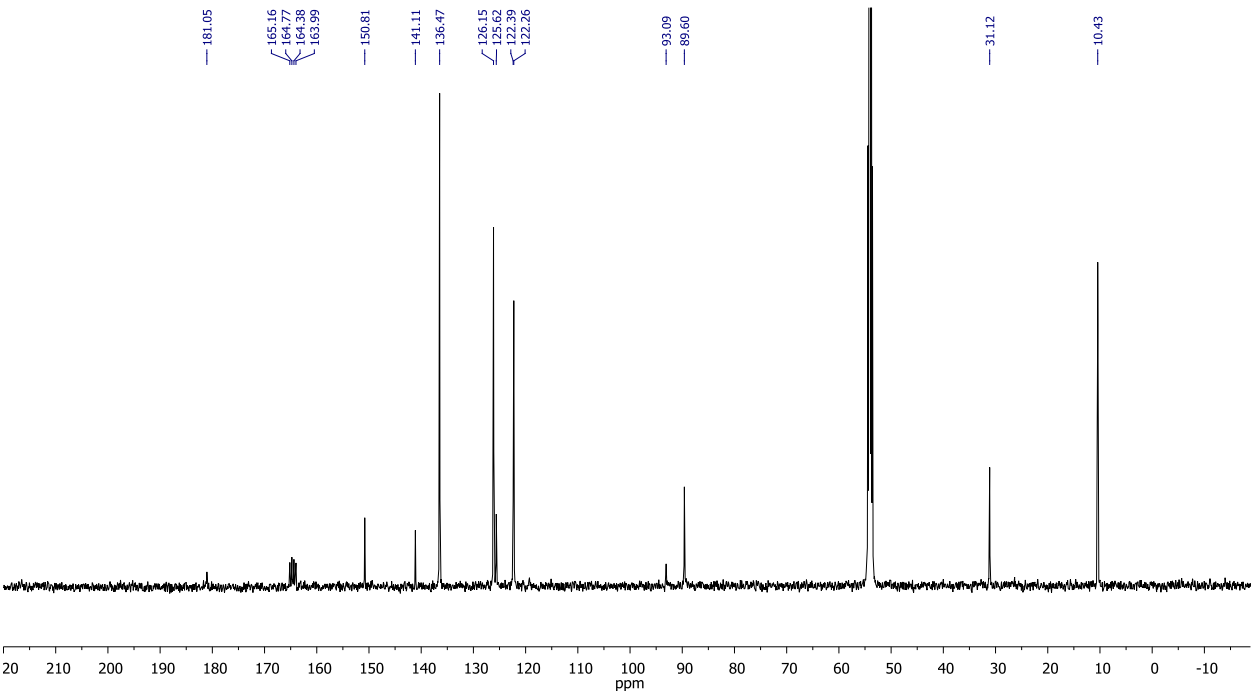

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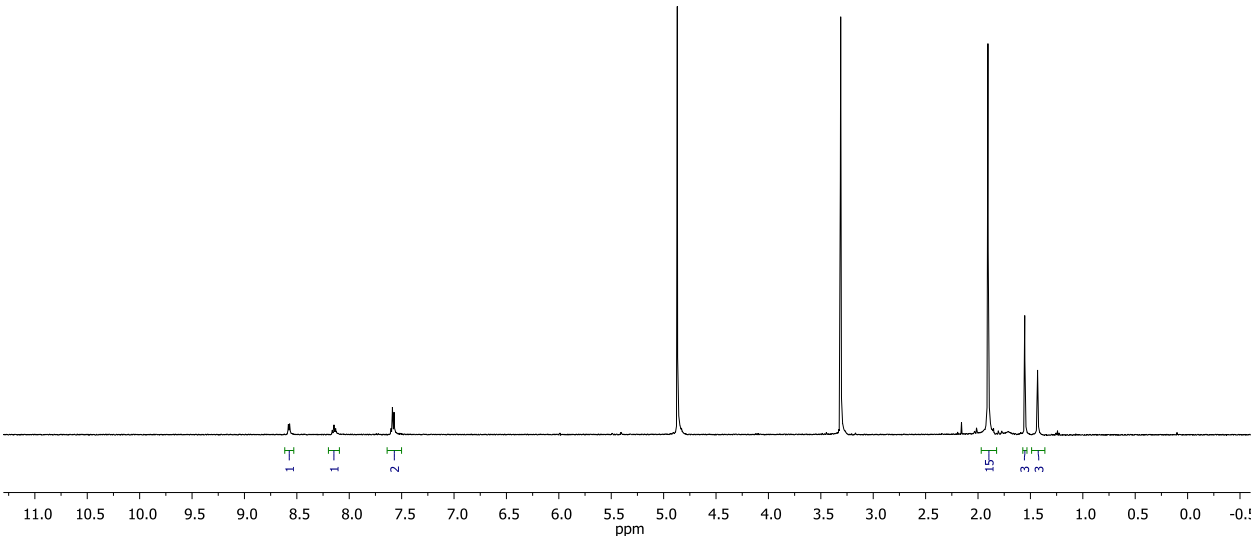

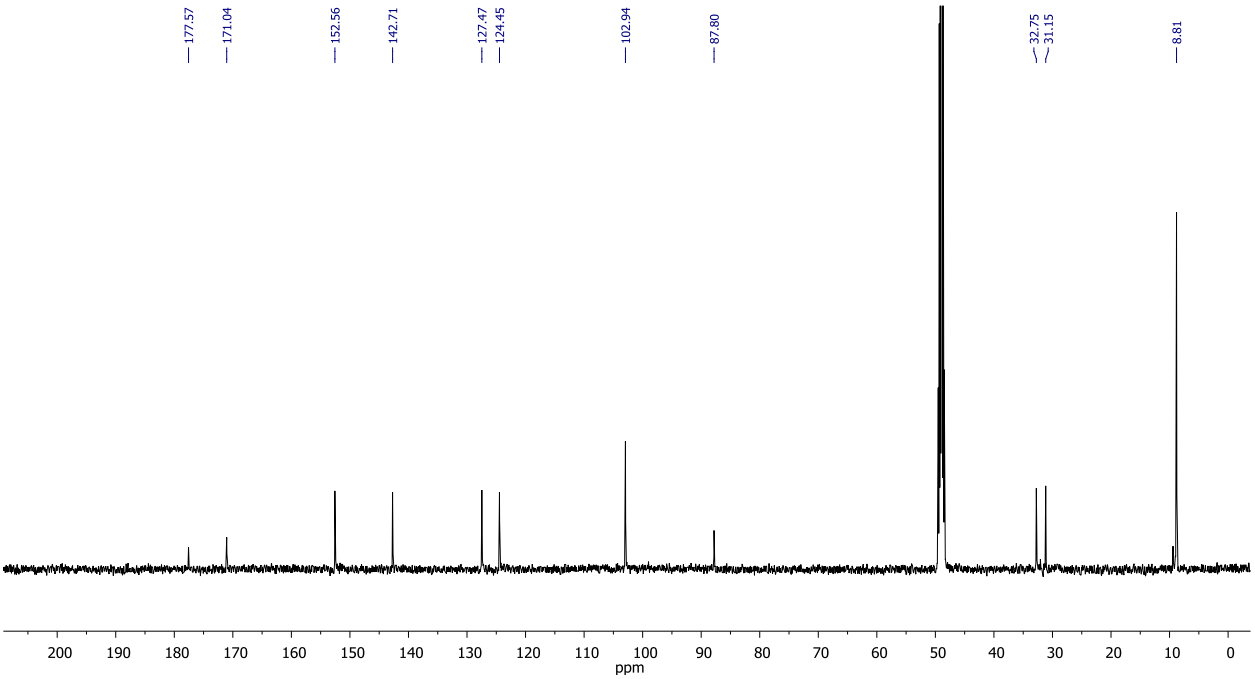

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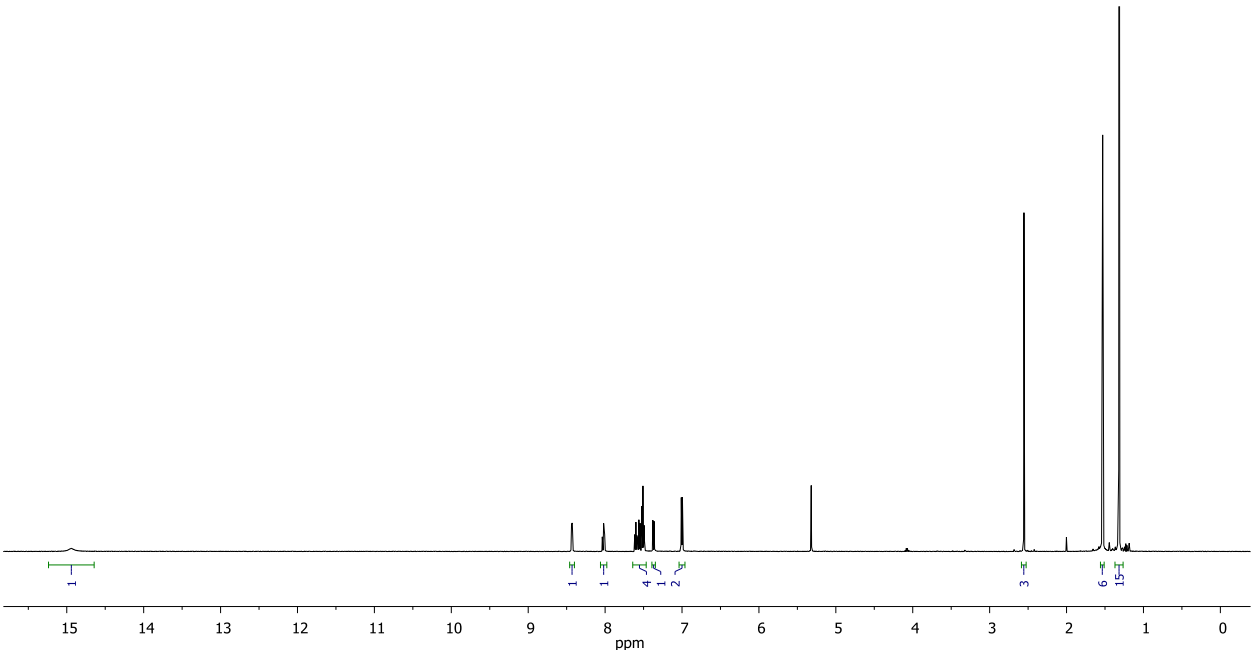

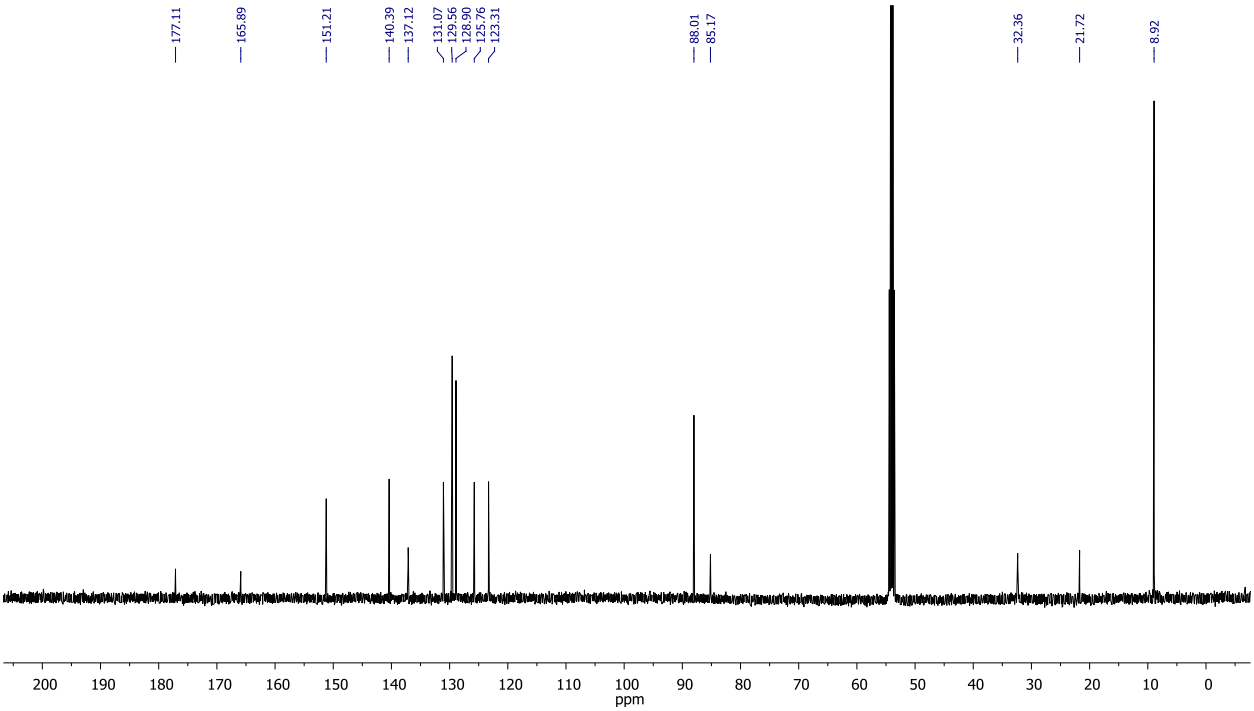

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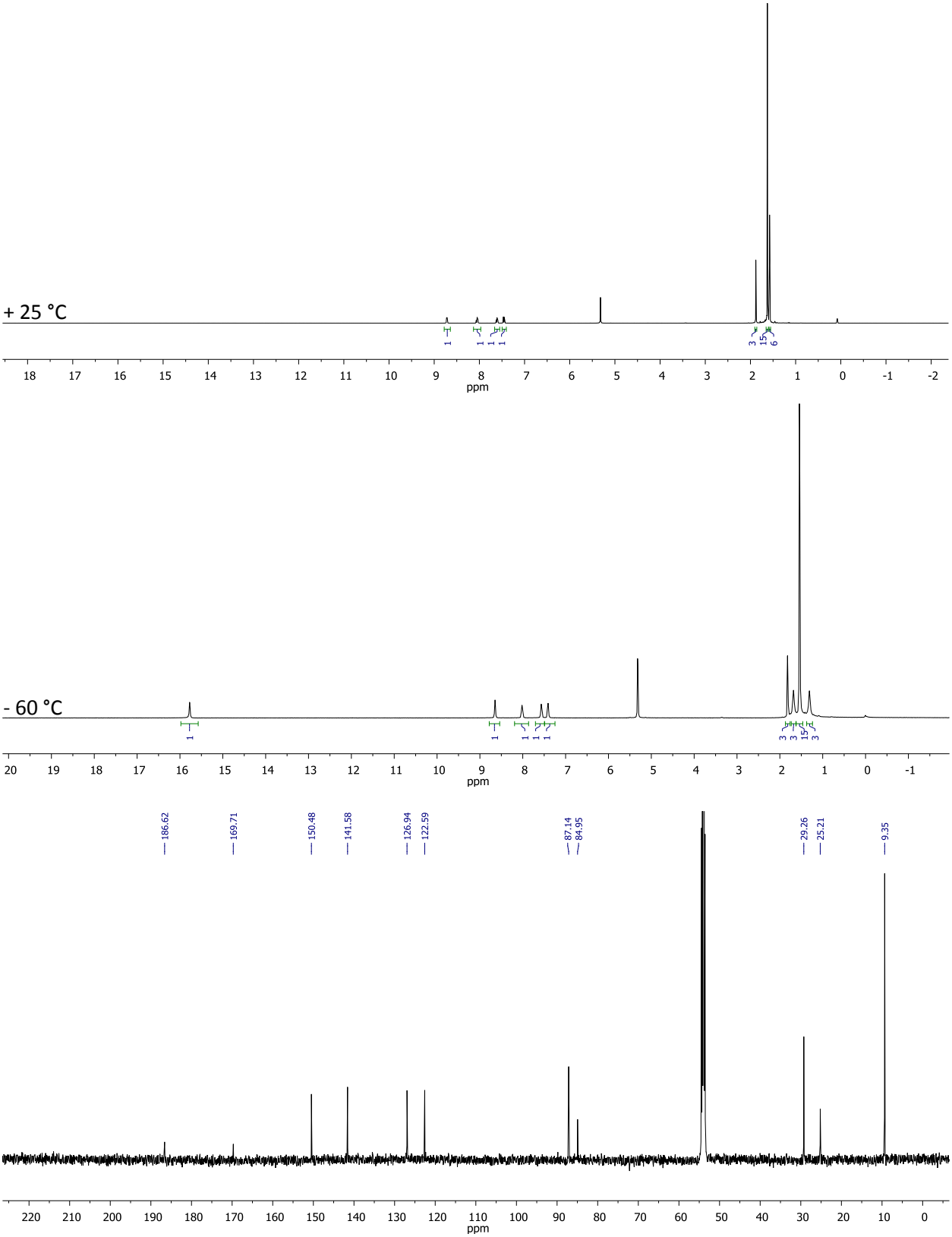

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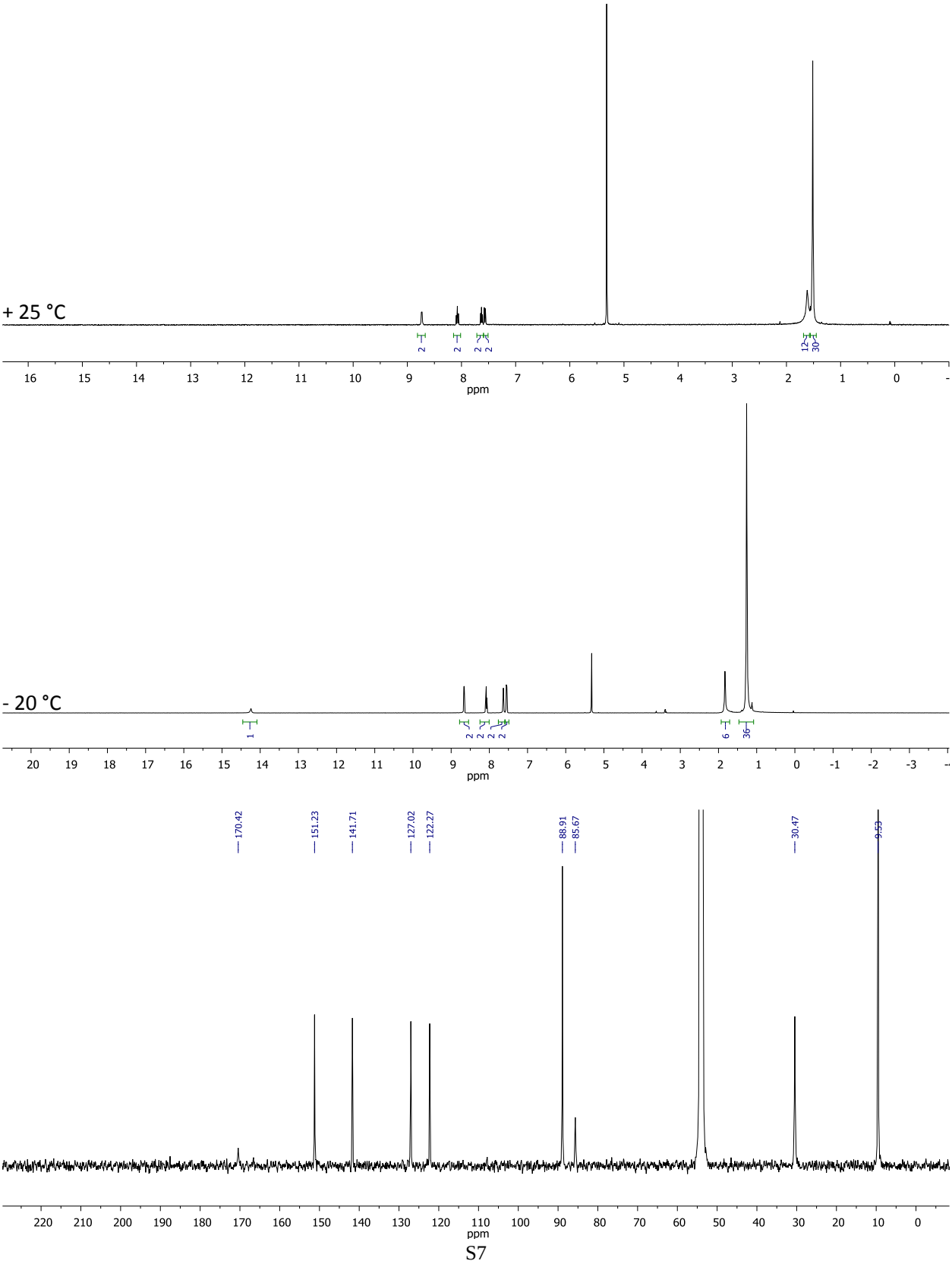
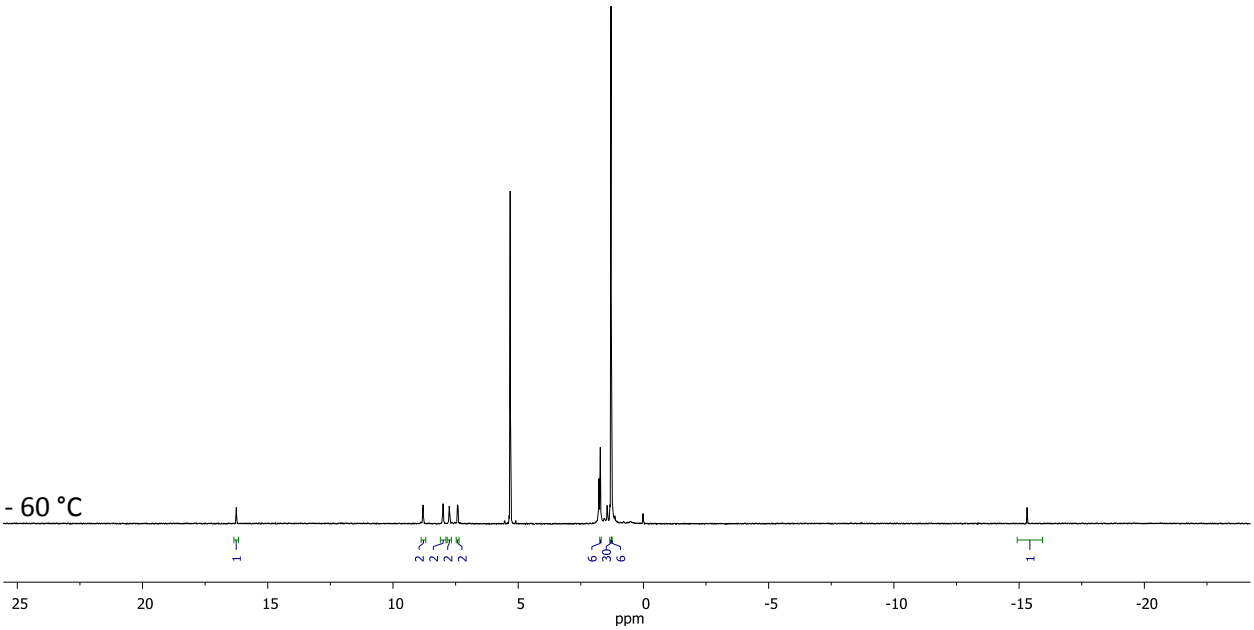


^{1}H NMR Spectrum of 6



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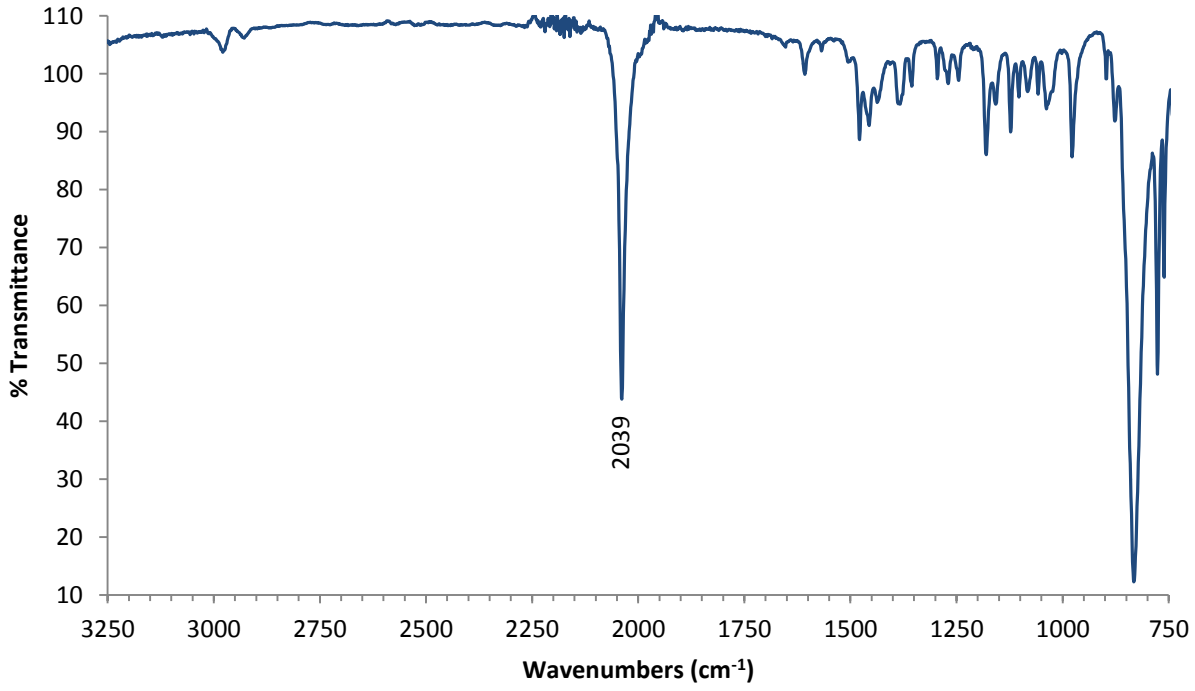
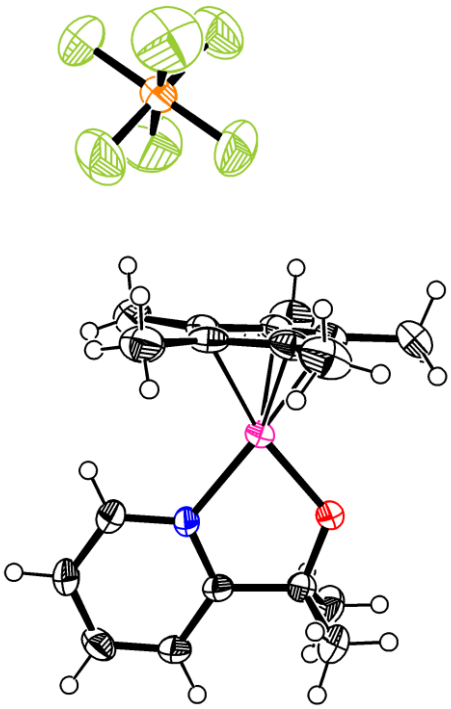


X-ray crystal structure of Cp*Ir(2-(2'-pyridyl)-2-propanolate)PF_6 (1[PF_6])



A. Crystal Data

Empirical Formula	$C_{18}H_{25}IrNPF_6O$	
Formula Weight	608.59	
Crystal Color, Habit	red, prism	
Crystal Dimensions	0.20 X 0.15 X 0.06 mm	
Crystal System	triclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 8.0923(11) Å	α = 100.005(4) °
	b = 11.3570(13) Å	β = 90.790(3) °
	c = 12.7166(17) Å	γ = 110.572(8) °
	V = 1074.0(2) Å^3	
Space Group	P-1 (#2)	
Z value	2	
D_{calc}	1.882 g/cm^3	
F_{000}	588.00	
μ(MoKα)	63.662 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku SCX-MINI
Radiation	MoKα (λ = 0.71075 Å)
Detector Aperture	75 mm (diameter)
Data Images	540 images
Exposure Rate	10.0 sec./°
Detector Swing Angle	-28.40°

Detector Position	49.90 mm
$2\theta_{max}$	54.9°
No. of Reflections Measured	Total: 11238 Unique: 4872 (R_{int} = 0.0491)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.346 - 0.683)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.0192 \cdot P)^2 + 0.0000 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4872
No. Variables	260
Reflection/Parameter Ratio	18.74
Residuals: R1 (I>2.00σ(I))	0.0432
Residuals: R (All reflections)	0.0577
Residuals: wR2 (All reflections)	0.0659
Goodness of Fit Indicator	1.101
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.82 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.00 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a MiTeGen polyimide loop with immersion oil. All measurements were made on a Rigaku Mercury2 CCD diffractometer with filtered Mo-Kα radiation at a temperature of -50°C. The structure was solved by Patterson methods[a] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 4872 observed reflections and 260 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0432$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 - Fc^2)^2\ )/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.0659$$

The standard deviation of an observation of unit weight[d] was 1.10. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.82 and -1.00 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]
Ir(1)	0.04197(3)	0.196218(19)	0.275441(15)	2.230(6)
P(1)	0.6455(2)	0.33482(14)	0.73595(11)	3.10(3)
F(1)	0.5361(5)	0.2223(4)	0.7946(3)	6.51(10)
F(2)	0.4827(6)	0.3818(4)	0.7382(4)	7.14(11)
F(3)	0.5668(6)	0.2430(5)	0.6250(3)	7.91(12)
F(4)	0.7506(6)	0.4452(4)	0.6780(4)	8.24(13)
F(5)	0.8092(5)	0.2869(4)	0.7337(3)	5.95(9)
F(6)	0.7238(6)	0.4221(4)	0.8492(3)	7.82(12)
O(1)	-0.1681(5)	0.2173(4)	0.2192(3)	3.41(8)
N(1)	0.1281(5)	0.2544(4)	0.1350(3)	2.34(8)
C(1)	0.2925(7)	0.2732(6)	0.1024(4)	3.50(12)
C(2)	0.3388(8)	0.3100(6)	0.0060(4)	3.64(12)
C(3)	0.2170(7)	0.3309(5)	-0.0578(4)	3.15(11)
C(4)	0.0517(7)	0.3146(5)	-0.0238(4)	2.83(10)
C(5)	0.0095(7)	0.2770(5)	0.0735(4)	2.36(9)
C(6)	-0.1666(7)	0.2555(5)	0.1185(4)	2.64(10)
C(7)	-0.3126(7)	0.1502(6)	0.0430(5)	3.92(12)
C(8)	-0.2010(7)	0.3824(5)	0.1370(5)	3.48(11)
C(9)	0.0234(7)	0.0371(5)	0.3485(4)	2.64(10)
C(10)	-0.0381(7)	0.1231(5)	0.4191(4)	2.85(10)
C(11)	0.1083(8)	0.2440(5)	0.4453(4)	3.07(11)
C(12)	0.2607(8)	0.2309(5)	0.3926(4)	2.77(10)
C(13)	0.2075(7)	0.1020(5)	0.3346(4)	2.69(10)
C(14)	-0.0819(8)	-0.0989(5)	0.3000(5)	4.23(13)
C(15)	-0.2208(8)	0.0945(6)	0.4550(5)	4.53(14)
C(16)	0.1072(10)	0.3649(6)	0.5157(5)	4.76(15)
C(17)	0.4410(8)	0.3335(6)	0.4013(5)	4.22(13)
C(18)	0.3245(8)	0.0433(6)	0.2708(5)	4.11(13)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1)	0.3769	0.2608	0.1465	4.20
H(2)	0.4527	0.3207	-0.016	4.37
H(3)	0.2469	0.3561	-0.124	3.78
H(4)	-0.033	0.3288	-0.066	3.40
H(7A)	-0.288	0.0716	0.0329	4.70
H(7B)	-0.318	0.1758	-0.026	4.70
H(7C)	-0.426	0.1364	0.0737	4.70
H(8A)	-0.312	0.3704	0.1698	4.17
H(8B)	-0.208	0.4086	0.0689	4.17
H(8C)	-0.105	0.4480	0.1840	4.17
H(14A)	-0.039	-0.122	0.2316	5.07
H(14B)	-0.206	-0.109	0.2892	5.07
H(14C)	-0.07	-0.154	0.3475	5.07
H(15A)	-0.224	0.0721	0.5253	5.44
H(15B)	-0.304	0.0235	0.4045	5.44
H(15C)	-0.253	0.1695	0.4585	5.44
H(16A)	0.1697	0.3769	0.5847	5.71
H(16B)	-0.014	0.3583	0.5259	5.71
H(16C)	0.1653	0.4375	0.4820	5.71
H(17A)	0.4987	0.3468	0.4721	5.07
H(17B)	0.4293	0.4126	0.3901	5.07
H(17C)	0.5115	0.3073	0.3476	5.07
H(18A)	0.4318	0.1106	0.2586	4.93
H(18B)	0.2620	-0.006	0.2026	4.93
H(18C)	0.3551	-0.013	0.3103	4.93

Table 3. Anisotropic displacement parameters[j]

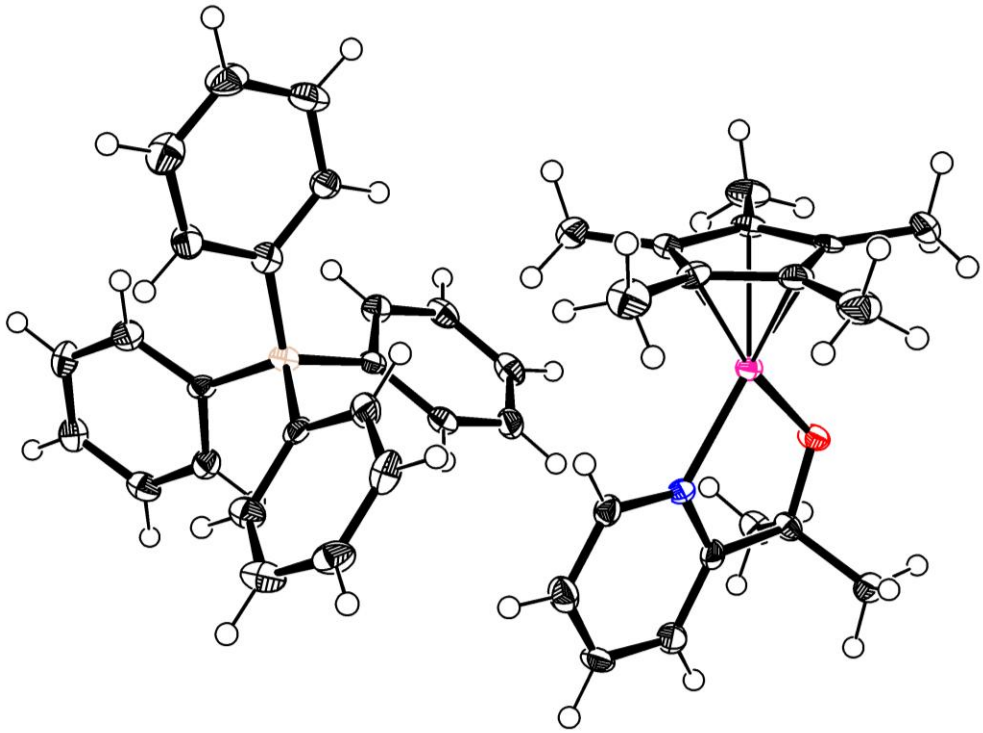
atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.02877(12)	0.03390(12)	0.02473(11)	0.01245(9)	0.00347(8)	0.00993(8)
P(1)	0.0415(9)	0.0446(9)	0.0357(8)	0.0176(8)	0.0079(7)	0.0127(7)
F(1)	0.086(3)	0.076(3)	0.088(3)	0.018(3)	0.027(3)	0.044(2)
F(2)	0.073(3)	0.115(4)	0.121(4)	0.067(3)	0.037(3)	0.048(3)
F(3)	0.111(4)	0.130(4)	0.049(2)	0.045(3)	-0.012(2)	-0.016(2)
F(4)	0.095(4)	0.105(4)	0.150(4)	0.045(3)	0.062(3)	0.096(3)
F(5)	0.063(3)	0.094(3)	0.091(3)	0.051(2)	0.011(2)	0.026(2)
F(6)	0.120(4)	0.085(3)	0.069(3)	0.029(3)	-0.018(3)	-0.029(2)
O(1)	0.031(2)	0.070(3)	0.043(2)	0.025(2)	0.0129(18)	0.033(2)
N(1)	0.024(2)	0.042(3)	0.026(2)	0.014(2)	0.0056(18)	0.0102(19)
C(1)	0.031(3)	0.068(4)	0.044(3)	0.025(3)	0.008(3)	0.022(3)
C(2)	0.035(3)	0.070(4)	0.045(4)	0.028(3)	0.019(3)	0.022(3)
C(3)	0.045(4)	0.047(3)	0.029(3)	0.014(3)	0.010(3)	0.014(3)
C(4)	0.038(3)	0.047(3)	0.029(3)	0.020(3)	0.002(2)	0.014(2)
C(5)	0.031(3)	0.035(3)	0.027(3)	0.015(3)	0.001(2)	0.009(2)
C(6)	0.025(3)	0.040(3)	0.037(3)	0.010(3)	0.003(2)	0.016(2)
C(7)	0.032(3)	0.059(4)	0.054(4)	0.013(3)	-0.004(3)	0.006(3)
C(8)	0.029(3)	0.055(4)	0.053(4)	0.019(3)	0.005(3)	0.013(3)
C(9)	0.038(3)	0.035(3)	0.029(3)	0.012(3)	0.001(2)	0.014(2)
C(10)	0.038(3)	0.046(3)	0.030(3)	0.016(3)	0.007(3)	0.020(2)
C(11)	0.061(4)	0.037(3)	0.022(3)	0.021(3)	0.001(3)	0.005(2)
C(12)	0.048(4)	0.033(3)	0.024(3)	0.014(3)	-0.008(2)	0.007(2)
C(13)	0.042(3)	0.037(3)	0.031(3)	0.020(3)	0.005(2)	0.015(2)
C(14)	0.059(4)	0.041(4)	0.052(4)	0.008(3)	-0.008(3)	0.010(3)
C(15)	0.057(4)	0.077(5)	0.051(4)	0.028(4)	0.023(3)	0.035(3)
C(16)	0.097(6)	0.047(4)	0.041(4)	0.033(4)	0.010(4)	0.005(3)
C(17)	0.045(4)	0.052(4)	0.056(4)	0.002(3)	-0.010(3)	0.022(3)
C(18)	0.058(4)	0.059(4)	0.056(4)	0.035(4)	0.014(3)	0.020(3)

Table 4. Bond lengths (Å)

atom	atom	distance
Ir(1)	O(1)	1.942(4)
Ir(1)	C(9)	2.133(6)
Ir(1)	C(11)	2.145(5)
Ir(1)	C(13)	2.183(7)
P(1)	F(2)	1.585(6)
P(1)	F(4)	1.558(5)
P(1)	F(6)	1.580(4)
N(1)	C(1)	1.355(7)
C(1)	C(2)	1.378(8)
C(3)	C(4)	1.372(8)
C(5)	C(6)	1.498(8)
C(6)	C(8)	1.542(9)
C(9)	C(13)	1.441(7)
C(10)	C(11)	1.445(7)
C(11)	C(12)	1.452(9)
C(12)	C(13)	1.430(7)
C(13)	C(18)	1.509(9)

atom	atom	distance
Ir(1)	N(1)	2.057(4)
Ir(1)	C(10)	2.151(5)
Ir(1)	C(12)	2.177(6)
P(1)	F(1)	1.590(4)
P(1)	F(3)	1.575(4)
P(1)	F(5)	1.598(5)
O(1)	C(6)	1.421(7)
N(1)	C(5)	1.350(7)
C(2)	C(3)	1.377(9)
C(4)	C(5)	1.386(7)
C(6)	C(7)	1.524(6)
C(9)	C(10)	1.434(8)
C(9)	C(14)	1.491(7)
C(10)	C(15)	1.494(9)
C(11)	C(16)	1.507(8)
C(12)	C(17)	1.502(7)

X-ray crystal structure of Cp*Ir(2-(2'-pyridyl)-2-propanolate)BPh_4 (1[BPh_4])



A. Crystal Data

Empirical Formula	$C_{42}H_{45}IrNOB$	
Formula Weight	782.85	
Crystal Color, Habit	orange, block	
Crystal Dimensions	0.10 X 0.08 X 0.06 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 16.3596(12) Å	α = 90 °
	b = 15.4413(3) Å	β = 112.699(8) °
	c = 14.6362(3) Å	γ = 90 °
	V = 3410.9(3) $Å^3$	
Space Group	$P2_1/c$ (#14)	
Z value	4	
D_{calc}	1.524 g/cm^3	
F_{000}	1576.00	
μ(CuKα)	76.563 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku Saturn944+ CCD
Radiation	CuKα (λ = 1.54187 Å)
Detector Aperture	94 mm x 94 mm
Data Images	792 exposures (1°)
Exposure Rate	3.0 sec./ °
Detector Swing Angles	42°, 90°
Detector Position	50.00 mm
$2\theta_{max}$	127.3°

No. of Reflections Measured	Total: 15751 Unique: 5432 (R_{int} = 0. 0685)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.472 - 0.632)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.0164 \cdot P)^2\ + 12.8067 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	127.3°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	5432
No. Variables	422
Reflection/Parameter Ratio	12.87
Residuals: R1 (I>2.00σ(I))	0.0356
Residuals: R (All reflections)	0.0397
Residuals: wR2 (All reflections)	0.0889
Goodness of Fit Indicator	0.993
Max Shift/Error in Final Cycle	0.003
Maximum peak in Final Diff. Map	0.94 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.90 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a Hampton Research loop with immersion oil. All measurements were made on a Rigaku Saturn944+ CCD diffractometer with filtered Cu-Kα radiation at a temperature of -180°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 5432 observed reflections and 422 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0356$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 – Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.0889$$

The standard deviation of an observation of unit weight[d] was 0.99. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.94 and -0.90 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]
Ir(1)	0.756177(12)	0.424811(12)	0.081264(13)	1.201(8)
O(1)	0.6569(2)	0.3601(2)	-0.0103(2)	1.61(5)
N(1)	0.7384(2)	0.3349(2)	0.1769(3)	1.23(6)
C(1)	0.7868(3)	0.3305(3)	0.2756(3)	1.52(8)
C(2)	0.7686(3)	0.2710(3)	0.3346(3)	1.93(9)
C(3)	0.7000(3)	0.2124(3)	0.2921(4)	1.87(8)
C(4)	0.6514(3)	0.2167(3)	0.1919(3)	1.71(8)
C(5)	0.6712(3)	0.2787(3)	0.1346(3)	1.40(8)
C(6)	0.6194(3)	0.2903(3)	0.0257(3)	1.39(8)
C(7)	0.6226(3)	0.2077(3)	-0.0310(3)	2.00(9)
C(8)	0.5239(3)	0.3146(4)	0.0085(4)	2.08(9)
C(9)	0.8789(3)	0.4659(3)	0.0744(4)	1.73(8)
C(10)	0.8052(3)	0.5047(3)	-0.0078(3)	1.72(8)
C(11)	0.7585(3)	0.5573(3)	0.0350(4)	1.41(8)
C(12)	0.8020(3)	0.5514(3)	0.1424(3)	1.53(8)
C(13)	0.8775(3)	0.4979(3)	0.1661(3)	1.48(8)
C(14)	0.9465(4)	0.4058(4)	0.0652(5)	2.57(10)
C(15)	0.7871(4)	0.4947(4)	-0.1148(4)	2.61(10)
C(16)	0.6781(3)	0.6100(3)	-0.0188(4)	2.30(9)
C(17)	0.7758(4)	0.6003(3)	0.2151(4)	2.21(9)
C(18)	0.9457(3)	0.4784(4)	0.2668(4)	2.48(10)
C(19)	0.6767(3)	0.5650(3)	0.4078(3)	1.22(8)
C(20)	0.6156(3)	0.6325(3)	0.3619(3)	1.55(8)
C(21)	0.5502(3)	0.6242(3)	0.2677(3)	1.77(8)
C(22)	0.5414(3)	0.5477(3)	0.2140(4)	1.89(9)
C(23)	0.5986(3)	0.4808(3)	0.2569(3)	1.83(8)
C(24)	0.6651(3)	0.4894(3)	0.3517(3)	1.59(8)
C(25)	0.8131(3)	0.4895(3)	0.5541(3)	1.38(8)
C(26)	0.8724(3)	0.4733(3)	0.5069(3)	1.78(8)
C(27)	0.9266(3)	0.4002(3)	0.5275(4)	1.98(9)
C(28)	0.9240(3)	0.3415(3)	0.5973(4)	2.14(9)
C(29)	0.8685(3)	0.3559(3)	0.6469(4)	2.30(9)
C(30)	0.8138(3)	0.4290(3)	0.6250(4)	1.81(9)
C(31)	0.6914(3)	0.5909(3)	0.5903(3)	1.30(8)
C(32)	0.6253(3)	0.5317(3)	0.5866(3)	1.77(8)
C(33)	0.5715(3)	0.5422(3)	0.6400(3)	1.83(8)
C(34)	0.5819(3)	0.6145(3)	0.6998(3)	1.79(8)
C(35)	0.6449(3)	0.6751(3)	0.7047(4)	1.88(9)
C(36)	0.6985(3)	0.6629(3)	0.6511(4)	1.90(9)
C(37)	0.8173(3)	0.6582(3)	0.5336(3)	1.45(8)
C(38)	0.8804(3)	0.6784(3)	0.6270(4)	1.83(8)
C(39)	0.9407(3)	0.7459(4)	0.6436(4)	2.49(10)
C(40)	0.9408(4)	0.7960(4)	0.5654(4)	2.51(10)
C(41)	0.8808(3)	0.7764(3)	0.4708(4)	2.31(9)
C(42)	0.8205(3)	0.7095(3)	0.4563(4)	1.66(8)
B(1)	0.7498(4)	0.5767(3)	0.5211(4)	1.41(9)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1)	0.8346	0.3697	0.3047	1.83
H(2)	0.8026	0.2698	0.4039	2.32
H(3)	0.6868	0.1701	0.3315	2.24
H(4)	0.6041	0.1773	0.1617	2.05
H(7A)	0.5925	0.2180	-0.102	2.40
H(7B)	0.5929	0.1606	-0.011	2.40
H(7C)	0.6845	0.1918	-0.016	2.40
H(8A)	0.4893	0.3210	-0.063	2.50
H(8B)	0.5235	0.3695	0.0420	2.50
H(8C)	0.4977	0.2690	0.0351	2.50
H(14A)	0.9939	0.4394	0.0567	3.08
H(14B)	0.9187	0.3680	0.0077	3.08
H(14C)	0.9715	0.3704	0.1253	3.08
H(15A)	0.8142	0.5428	-0.137	3.14
H(15B)	0.7229	0.4949	-0.153	3.14
H(15C)	0.8121	0.4398	-0.126	3.14
H(16A)	0.6954	0.6701	-0.023	2.76
H(16B)	0.6382	0.6077	0.0167	2.76
H(16C)	0.6477	0.5867	-0.086	2.76
H(17A)	0.8067	0.6561	0.2298	2.65
H(17B)	0.7917	0.5666	0.2763	2.65
H(17C)	0.7116	0.6103	0.1869	2.65
H(18A)	0.9218	0.4921	0.3171	2.98
H(18B)	0.9987	0.5135	0.2785	2.98
H(18C)	0.9614	0.4169	0.2710	2.98
H(20)	0.6196	0.6851	0.3970	1.86
H(21)	0.5110	0.6711	0.2394	2.13
H(22)	0.4968	0.5420	0.1494	2.26
H(23)	0.5931	0.4279	0.2218	2.19
H(24)	0.7038	0.4419	0.3790	1.91
H(26)	0.8754	0.5138	0.4594	2.13
H(27)	0.9651	0.3909	0.4937	2.38
H(28)	0.9603	0.2913	0.6113	2.57
H(29)	0.8675	0.3161	0.6959	2.76
H(30)	0.7759	0.4378	0.6597	2.17
H(32)	0.6167	0.4819	0.5458	2.12
H(33)	0.5279	0.5000	0.6355	2.20
H(34)	0.5458	0.6220	0.7369	2.15
H(35)	0.6520	0.7253	0.7445	2.26
H(36)	0.7418	0.7056	0.6561	2.28
H(38)	0.8822	0.6445	0.6820	2.19
H(39)	0.9820	0.7576	0.7088	2.99
H(40)	0.9810	0.8429	0.5762	3.01
H(41)	0.8811	0.8088	0.4157	2.77
H(42)	0.7795	0.6979	0.3908	1.99

Table 3. Anisotropic displacement parameters[j]

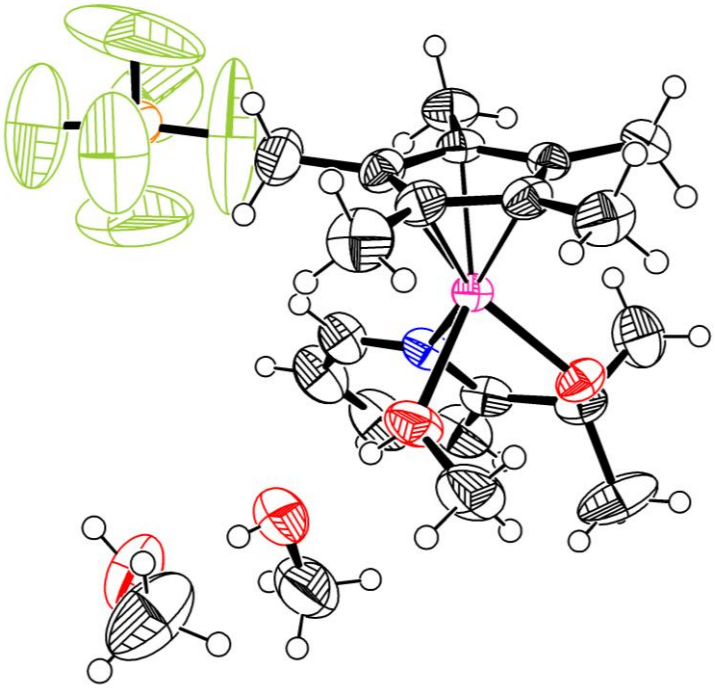
atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.01558(13)	0.01483(14)	0.01530(13)	-0.00093(7)	0.00606(9)	0.00030(7)
O(1)	0.0218(17)	0.0192(17)	0.0182(16)	-0.0025(14)	0.0057(14)	0.0044(13)
N(1)	0.0156(19)	0.014(2)	0.0165(19)	-0.0033(15)	0.0057(16)	-0.0015(15)
C(1)	0.023(3)	0.018(3)	0.014(2)	0.0023(19)	0.0035(19)	-0.0013(18)
C(2)	0.027(3)	0.028(3)	0.017(2)	0.004(2)	0.007(2)	0.003(2)
C(3)	0.033(3)	0.016(3)	0.026(3)	0.003(2)	0.016(2)	0.008(2)
C(4)	0.022(2)	0.022(3)	0.022(2)	-0.003(2)	0.010(2)	-0.002(2)
C(5)	0.020(2)	0.018(2)	0.018(2)	0.0009(20)	0.0104(19)	-0.0032(19)
C(6)	0.016(2)	0.021(3)	0.014(2)	0.0004(19)	0.0042(18)	0.0033(19)
C(7)	0.034(3)	0.021(3)	0.020(2)	-0.006(2)	0.009(2)	-0.0027(20)
C(8)	0.025(3)	0.031(3)	0.023(2)	-0.000(2)	0.009(2)	0.004(2)
C(9)	0.024(3)	0.015(3)	0.031(3)	-0.0035(20)	0.015(2)	0.001(2)
C(10)	0.031(3)	0.015(3)	0.025(2)	-0.012(2)	0.017(2)	0.0003(19)
C(11)	0.012(2)	0.015(2)	0.025(3)	-0.0003(18)	0.0067(20)	0.0065(19)
C(12)	0.024(3)	0.017(2)	0.022(2)	-0.005(2)	0.013(2)	0.0005(19)
C(13)	0.012(2)	0.018(3)	0.024(2)	-0.0074(19)	0.0046(19)	-0.0032(20)
C(14)	0.032(3)	0.026(3)	0.049(3)	0.000(2)	0.026(3)	0.003(2)
C(15)	0.056(4)	0.028(3)	0.020(3)	-0.012(3)	0.020(3)	-0.001(2)
C(16)	0.026(3)	0.019(3)	0.042(3)	0.007(2)	0.012(2)	0.013(2)
C(17)	0.038(3)	0.019(3)	0.032(3)	-0.001(2)	0.020(2)	-0.003(2)
C(18)	0.020(3)	0.037(3)	0.030(3)	-0.006(2)	0.002(2)	0.001(2)
C(19)	0.018(2)	0.013(2)	0.018(2)	0.0005(18)	0.0095(20)	0.0028(17)
C(20)	0.019(2)	0.019(3)	0.022(2)	0.0014(19)	0.0083(20)	0.0010(19)
C(21)	0.019(2)	0.028(3)	0.020(2)	0.001(2)	0.0064(20)	0.008(2)
C(22)	0.019(2)	0.033(3)	0.019(2)	-0.003(2)	0.007(2)	0.004(2)
C(23)	0.026(3)	0.027(3)	0.019(2)	-0.006(2)	0.012(2)	-0.003(2)
C(24)	0.020(2)	0.021(3)	0.021(2)	-0.0016(20)	0.011(2)	0.0033(19)
C(25)	0.019(2)	0.013(2)	0.016(2)	-0.0027(19)	0.0021(19)	-0.0040(18)
C(26)	0.023(3)	0.025(3)	0.015(2)	0.001(2)	0.0026(20)	0.0008(20)
C(27)	0.018(2)	0.031(3)	0.022(2)	0.005(2)	0.003(2)	-0.008(2)
C(28)	0.025(3)	0.018(3)	0.031(3)	0.004(2)	0.002(2)	0.004(2)
C(29)	0.023(3)	0.026(3)	0.033(3)	-0.003(2)	0.005(2)	0.010(2)
C(30)	0.019(2)	0.024(3)	0.023(3)	-0.0005(20)	0.005(2)	0.005(2)
C(31)	0.018(2)	0.011(2)	0.017(2)	0.0024(18)	0.0037(19)	0.0026(17)
C(32)	0.023(3)	0.023(3)	0.020(2)	-0.004(2)	0.0072(20)	-0.003(2)
C(33)	0.017(2)	0.027(3)	0.022(2)	-0.002(2)	0.0032(20)	0.007(2)
C(34)	0.019(2)	0.028(3)	0.022(2)	0.004(2)	0.009(2)	-0.001(2)
C(35)	0.023(3)	0.028(3)	0.021(2)	0.001(2)	0.009(2)	-0.007(2)
C(36)	0.024(3)	0.024(3)	0.024(3)	-0.004(2)	0.009(2)	-0.001(2)
C(37)	0.015(2)	0.019(3)	0.023(2)	0.0048(19)	0.0093(20)	0.0011(19)
C(38)	0.019(2)	0.030(3)	0.021(2)	-0.005(2)	0.0080(20)	-0.002(2)
C(39)	0.023(3)	0.038(3)	0.036(3)	-0.007(2)	0.014(2)	-0.010(2)
C(40)	0.028(3)	0.028(3)	0.045(3)	-0.011(2)	0.021(3)	-0.006(2)
C(41)	0.033(3)	0.021(3)	0.042(3)	-0.000(2)	0.024(3)	0.006(2)
C(42)	0.026(3)	0.017(3)	0.024(2)	0.0021(20)	0.014(2)	-0.0000(19)
B(1)	0.017(3)	0.016(3)	0.021(3)	-0.000(2)	0.008(2)	0.003(2)

Table 4. Bond lengths (Å)

atom	atom	distance
Ir(1)	O(1)	1.937(3)
Ir(1)	C(9)	2.144(5)
Ir(1)	C(11)	2.159(5)
Ir(1)	C(13)	2.203(4)
N(1)	C(1)	1.355(5)
C(1)	C(2)	1.370(7)
C(3)	C(4)	1.373(6)
C(5)	C(6)	1.500(6)
C(6)	C(8)	1.531(7)
C(9)	C(13)	1.439(8)
C(10)	C(11)	1.417(8)
C(11)	C(12)	1.456(6)
C(12)	C(13)	1.414(7)
C(13)	C(18)	1.497(6)
C(19)	C(24)	1.398(7)
C(20)	C(21)	1.388(5)
C(22)	C(23)	1.373(7)
C(25)	C(26)	1.412(8)
C(25)	B(1)	1.653(7)
C(27)	C(28)	1.378(8)
C(29)	C(30)	1.398(7)
C(31)	C(36)	1.401(7)
C(32)	C(33)	1.394(8)
C(34)	C(35)	1.373(7)
C(37)	C(38)	1.394(6)
C(37)	B(1)	1.637(7)
C(39)	C(40)	1.382(9)
C(41)	C(42)	1.388(7)

atom	atom	distance
Ir(1)	N(1)	2.070(4)
Ir(1)	C(10)	2.162(6)
Ir(1)	C(12)	2.160(5)
O(1)	C(6)	1.438(6)
N(1)	C(5)	1.350(6)
C(2)	C(3)	1.389(7)
C(4)	C(5)	1.390(7)
C(6)	C(7)	1.532(7)
C(9)	C(10)	1.462(6)
C(9)	C(14)	1.490(8)
C(10)	C(15)	1.485(7)
C(11)	C(16)	1.488(6)
C(12)	C(17)	1.497(8)
C(19)	C(20)	1.421(6)
C(19)	B(1)	1.638(6)
C(21)	C(22)	1.394(7)
C(23)	C(24)	1.400(6)
C(25)	C(30)	1.393(7)
C(26)	C(27)	1.396(7)
C(28)	C(29)	1.383(9)
C(31)	C(32)	1.401(7)
C(31)	B(1)	1.654(9)
C(33)	C(34)	1.387(7)
C(35)	C(36)	1.396(9)
C(37)	C(42)	1.399(7)
C(38)	C(39)	1.391(7)
C(40)	C(41)	1.387(7)

X-ray crystal structure of Cp*Ir(2-(2'-pyridyl)-2-propanolate)(MeOH)PF_6 ([1·MeOH]PF_6)



A. Crystal Data

Empirical Formula	$C_{19}H_{29}IrPF_6NO_2 \cdot 2(CH_3OH)$	
Formula Weight	704.71	
Crystal Color, Habit	yellow, prism	
Crystal Dimensions	0.26 X 0.26 X 0.26 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Detector Position	49.90 mm	
Lattice Parameters	a = 12.6701(12) Å	α = 90 º
	b = 12.9965(12) Å	β = 99.222(3) º
	c = 16.9027(16) Å	γ = 90 º
	V = 2747.3(4) $Å^3$	
Space Group	$P2_1/c$ (#14)	
Z value	4	
D_{calc}	1.704 g/cm^3	
F_{000}	1392.00	
μ(MoKα)	49.976 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku SCXmini
Radiation	MoKα (λ = 0.71075 Å)
Detector Aperture	75 mm round
Data Images	540 exposures
Exposure Rate	10.0 sec./ °
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm

$2\theta_{max}$	57.4°
No. of Reflections Measured	Total: 30479 Unique: 7060 (R_{int} = 0.0499)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.225 - 0.273)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.0370 \cdot P)^2\ + 5.6098 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	57.4°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	7060
No. Variables	320
Reflection/Parameter Ratio	22.06
Residuals: R1 (I>2.00σ(I))	0.0449
Residuals: R (All reflections)	0.0670
Residuals: wR2 (All reflections)	0.0940
Goodness of Fit Indicator	1.088
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.08 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.92 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a MiTeGen polyimide loop with immersion oil. All measurements were made on a Rigaku Mercury2 CCD area detector with filtered Mo-Kα radiation at a temperature of -50°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. Protic hydrogen atoms on methanol molecules were modeled as idealized hydroxyls using a rotating group refinement. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 7060 observed reflections and 320 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0449$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 - Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.0940$$

The standard deviation of an observation of unit weight[d] was 1.09. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.08 and -0.92 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	Z	B_{eq}[j]
Ir(1)	0.237620(15)	0.301537(15)	0.028119(12)	2.526(6)
P(1)	-0.17593(15)	0.24000(14)	0.21587(12)	4.43(3)
F(1)	-0.0759(6)	0.3004(6)	0.2559(4)	13.7(3)
F(2)	-0.1233(9)	0.1384(7)	0.2381(7)	18.9(4)
F(3)	-0.2042(8)	0.2399(8)	0.3007(5)	15.8(3)
F(4)	-0.2739(5)	0.1774(6)	0.1801(6)	14.5(3)
F(5)	-0.1358(10)	0.2315(10)	0.1387(5)	21.1(6)
F(6)	-0.2284(12)	0.3358(7)	0.1983(8)	26.3(8)
O(1)	0.3166(3)	0.2092(3)	-0.0415(3)	3.48(7)
O(2)	0.3747(3)	0.2645(4)	0.1196(3)	4.45(9)
O(3)	0.3665(5)	0.1347(4)	0.2335(3)	5.99(12)
O(4)	0.4572(5)	0.2098(4)	0.3755(4)	6.72(14)
N(1)	0.1842(4)	0.1535(4)	0.0536(3)	3.20(8)
C(1)	0.1268(5)	0.1327(5)	0.1126(4)	4.18(12)
C(2)	0.0946(6)	0.0345(6)	0.1266(5)	5.28(16)
C(3)	0.1204(7)	-0.0432(6)	0.0800(5)	6.16(19)
C(4)	0.1781(6)	-0.0231(5)	0.0190(5)	5.43(16)
C(5)	0.2107(5)	0.0773(4)	0.0067(4)	3.41(11)
C(6)	0.2720(5)	0.1094(5)	-0.0592(4)	3.93(11)
C(7)	0.3644(6)	0.0363(6)	-0.0641(6)	7.3(2)
C(8)	0.1946(6)	0.1125(6)	-0.1377(4)	5.73(17)
C(9)	0.2353(5)	0.4592(4)	0.0701(4)	3.43(10)
C(10)	0.1343(4)	0.4120(4)	0.0736(3)	3.24(10)
C(11)	0.0890(4)	0.3800(4)	-0.0070(3)	2.93(9)
C(12)	0.1632(4)	0.4088(4)	-0.0596(3)	2.87(9)
C(13)	0.2543(4)	0.4572(4)	-0.0117(4)	3.24(10)
C(14)	0.3097(6)	0.5029(5)	0.1402(4)	5.34(16)
C(15)	0.0805(6)	0.4072(6)	0.1461(4)	4.95(14)
C(16)	-0.0178(5)	0.3296(5)	-0.0304(4)	4.02(12)
C(17)	0.1489(5)	0.3956(5)	-0.1484(4)	4.37(13)
C(18)	0.3464(5)	0.5067(5)	-0.0436(4)	4.71(14)
C(19)	0.4826(5)	0.2679(7)	0.1049(5)	6.23(19)
C(20)	0.3961(8)	0.0322(7)	0.2235(5)	7.7(2)
C(21)	0.5528(8)	0.2634(8)	0.3826(8)	9.3(3)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1)	0.1086	0.1868	0.1447	5.02
H(2)	0.0550	0.0214	0.1680	6.33
H(3)	0.0990	-0.111	0.0892	7.39
H(4)	0.1953	-0.077	-0.014	6.52
H(7A)	0.4125	0.0361	-0.013	8.76
H(7B)	0.4027	0.0587	-0.106	8.76
H(7C)	0.3369	-0.033	-0.076	8.76
H(8A)	0.1355	0.1580	-0.132	6.87
H(8B)	0.1676	0.0438	-0.151	6.87
H(8C)	0.2313	0.1378	-0.18	6.87
H(14A)	0.3125	0.4571	0.1858	6.41
H(14B)	0.2839	0.5699	0.1538	6.41
H(14C)	0.3807	0.5099	0.1263	6.41
H(15A)	0.0602	0.4760	0.1599	5.94
H(15B)	0.1294	0.3781	0.1905	5.94
H(15C)	0.0172	0.3644	0.1348	5.94
H(16A)	-0.021	0.2966	-0.082	4.83
H(16B)	-0.074	0.3812	-0.034	4.83
H(16C)	-0.028	0.2784	0.0095	4.83
H(17A)	0.1378	0.4623	-0.174	5.24
H(17B)	0.0872	0.3522	-0.166	5.24
H(17C)	0.2122	0.3637	-0.163	5.24
H(18A)	0.3212	0.5670	-0.075	5.65
H(18B)	0.3766	0.4581	-0.077	5.65
H(18C)	0.4008	0.5268	0.0008	5.65
H(19A)	0.4924	0.3279	0.0728	7.47
H(19B)	0.4979	0.2062	0.0765	7.47
H(19C)	0.5308	0.2717	0.1556	7.47
H(20A)	0.4680	0.0209	0.2518	9.28
H(20B)	0.3939	0.0180	0.1669	9.28
H(20C)	0.3468	-0.013	0.2449	9.28
H(21A)	0.5383	0.3367	0.3795	11.16
H(21B)	0.5909	0.2435	0.3396	11.16
H(21C)	0.5962	0.2475	0.4338	11.16
H(2A)	0.3696	0.2215	0.1551	5.34
H(3A)	0.3979	0.1566	0.2771	7.19
H(4A)	0.4126	0.2445	0.3949	8.06

Table 3. Anisotropic displacement parameters[j]

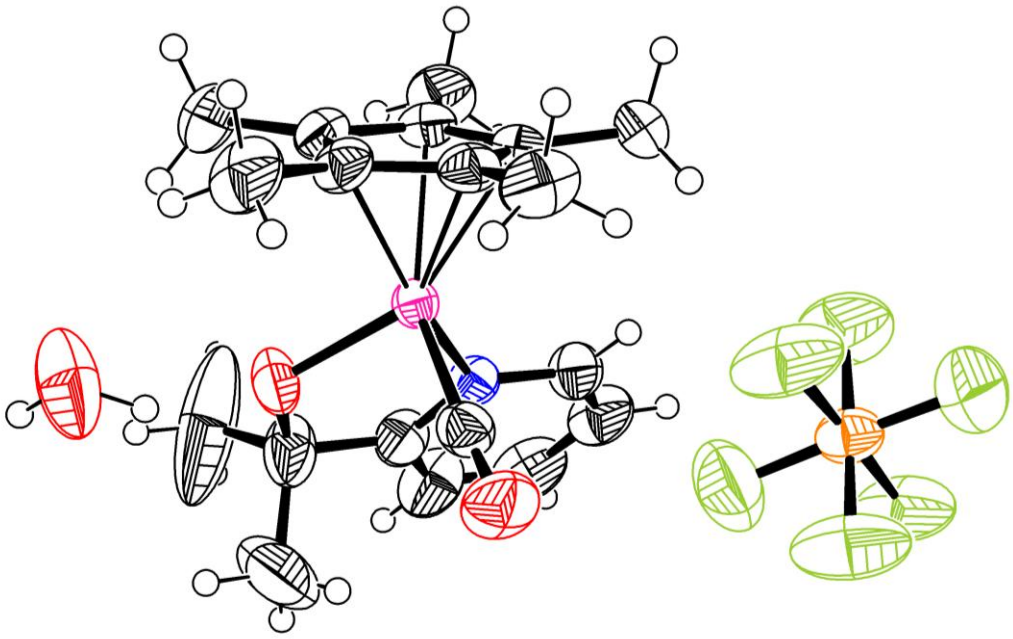
atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03014(11)	0.03046(11)	0.03519(11)	0.00043(9)	0.00462(7)	0.00151(9)
P(1)	0.0549(10)	0.0490(10)	0.0656(12)	-0.0010(8)	0.0132(9)	-0.0009(8)
F(1)	0.158(7)	0.246(9)	0.124(5)	-0.135(6)	0.042(5)	-0.050(5)
F(2)	0.235(10)	0.147(8)	0.305(13)	0.099(7)	-0.054(9)	-0.045(8)
F(3)	0.241(10)	0.243(9)	0.147(7)	-0.125(8)	0.117(7)	-0.052(7)
F(4)	0.082(4)	0.201(8)	0.253(10)	-0.043(5)	-0.017(5)	-0.099(7)
F(5)	0.351(15)	0.365(15)	0.123(7)	-0.217(12)	0.150(8)	-0.103(8)
F(6)	0.49(2)	0.113(6)	0.303(14)	0.159(10)	-0.213(15)	-0.047(8)
O(1)	0.043(2)	0.035(2)	0.056(2)	0.0046(17)	0.0146(18)	-0.0052(17)
O(2)	0.039(2)	0.066(3)	0.059(3)	0.001(2)	-0.0046(20)	0.017(2)
O(3)	0.082(4)	0.084(4)	0.062(3)	0.009(3)	0.014(3)	0.021(3)
O(4)	0.093(4)	0.082(4)	0.092(4)	-0.014(3)	0.050(4)	-0.019(3)
N(1)	0.037(2)	0.037(3)	0.046(3)	-0.007(2)	-0.001(2)	0.008(2)
C(1)	0.057(4)	0.049(4)	0.052(4)	-0.012(3)	0.006(3)	0.006(3)
C(2)	0.075(5)	0.057(5)	0.066(5)	-0.024(4)	0.003(4)	0.015(4)
C(3)	0.105(6)	0.042(4)	0.081(6)	-0.028(4)	-0.004(5)	0.017(4)
C(4)	0.086(5)	0.043(4)	0.071(5)	-0.006(4)	-0.007(4)	-0.005(3)
C(5)	0.042(3)	0.029(3)	0.054(4)	-0.003(2)	-0.007(3)	-0.004(2)
C(6)	0.046(3)	0.041(3)	0.061(4)	0.003(3)	0.005(3)	-0.007(3)
C(7)	0.070(5)	0.047(4)	0.165(9)	0.017(4)	0.031(5)	-0.025(5)
C(8)	0.081(5)	0.077(5)	0.057(4)	-0.014(4)	0.004(4)	-0.006(4)
C(9)	0.047(3)	0.033(3)	0.051(4)	0.002(2)	0.008(3)	-0.005(2)
C(10)	0.043(3)	0.033(3)	0.049(3)	0.002(2)	0.014(3)	-0.001(2)
C(11)	0.033(3)	0.029(3)	0.049(3)	0.007(2)	0.005(2)	0.003(2)
C(12)	0.037(3)	0.033(3)	0.040(3)	0.006(2)	0.007(2)	0.007(2)
C(13)	0.039(3)	0.029(3)	0.057(4)	0.001(2)	0.015(3)	0.004(2)
C(14)	0.073(5)	0.054(4)	0.071(5)	-0.008(4)	-0.003(4)	-0.022(4)
C(15)	0.071(5)	0.064(4)	0.057(4)	0.004(4)	0.025(3)	-0.005(3)
C(16)	0.033(3)	0.048(4)	0.070(4)	-0.002(2)	-0.000(3)	0.001(3)
C(17)	0.060(4)	0.059(4)	0.046(4)	0.016(3)	0.005(3)	0.011(3)
C(18)	0.050(4)	0.048(4)	0.085(5)	-0.005(3)	0.023(3)	0.010(3)
C(19)	0.038(4)	0.112(7)	0.082(6)	-0.005(4)	-0.006(4)	0.025(5)
C(20)	0.127(8)	0.088(7)	0.074(6)	0.024(6)	-0.001(5)	0.011(5)
C(21)	0.111(8)	0.079(7)	0.184(12)	-0.012(6)	0.087(8)	-0.003(7)

Table 4. Bond lengths (Å)

atom	atom	distance
Ir(1)	O(1)	2.051(4)
Ir(1)	N(1)	2.107(5)
Ir(1)	C(10)	2.166(6)
Ir(1)	C(12)	2.141(5)
P(1)	F(1)	1.551(8)
P(1)	F(3)	1.532(9)
P(1)	F(5)	1.478(10)
O(1)	C(6)	1.427(7)
O(3)	C(20)	1.401(11)
N(1)	C(1)	1.351(8)
C(1)	C(2)	1.372(10)
C(3)	C(4)	1.383(12)
C(5)	C(6)	1.514(9)
C(6)	C(8)	1.519(9)
C(9)	C(13)	1.440(9)
C(10)	C(11)	1.452(8)
C(11)	C(12)	1.443(8)
C(12)	C(13)	1.444(7)
C(13)	C(18)	1.507(9)

atom	atom	Distance
Ir(1)	O(2)	2.186(4)
Ir(1)	C(9)	2.170(6)
Ir(1)	C(11)	2.140(5)
Ir(1)	C(13)	2.152(6)
P(1)	F(2)	1.499(10)
P(1)	F(4)	1.526(7)
P(1)	F(6)	1.420(10)
O(2)	C(19)	1.429(8)
O(4)	C(21)	1.385(12)
N(1)	C(5)	1.344(8)
C(2)	C(3)	1.351(11)
C(4)	C(5)	1.394(9)
C(6)	C(7)	1.520(10)
C(9)	C(10)	1.430(8)
C(9)	C(14)	1.502(9)
C(10)	C(15)	1.495(9)
C(11)	C(16)	1.499(8)
C(12)	C(17)	1.492(8)

X-ray crystal structure of Cp*Ir(2-(2'-pyridyl)-2-propanolate)CO(PF_6) (2)



A. Crystal Data

Empirical Formula	$C_{19}H_{25}IrNO_2PF_6 \cdot H_2O$	
Formula Weight	654.61	
Crystal Color, Habit	yellow, prism	
Crystal Dimensions	0.20 X 0.10 X 0.08 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 8.5250(9) Å	α = 90 °
	b = 20.792(2) Å	β = 98.695(3) °
	c = 13.5964(14) Å	γ = 90 °
	V = 2382.3(4) $Å^3$	
Space Group	$P2_1/c$ (#14)	
Z value	4	
D_{calc}	1.825 g/cm^3	
F_{000}	1272.00	
μ(MoKα)	57.529 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku SCXmini
Radiation	MoKα (λ = 0.71075 Å)
Detector Aperture	75 mm round
Data Images	540 exposures
Exposure Rate	30.0 sec./ °
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm
$2\theta_{max}$	57.3°

No. of Reflections Measured	Total: 26376 Unique: 6094 (R_{int} = 0.0522)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.368 - 0.631)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.0199 \cdot P)^2\ + 1.7105 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	57.3°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	6094
No. Variables	329
Reflection/Parameter Ratio	18.52
Residuals: R1 (I>2.00σ(I))	0.0399
Residuals: R (All reflections)	0.0636
Residuals: wR2 (All reflections)	0.0641
Goodness of Fit Indicator	1.100
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	0.89 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.71 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a MiTeGen polyimide loop with immersion oil. All measurements were made on a Rigaku Mercury2 CCD area detector with filtered Mo-Kα radiation at a temperature of -50°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. Four of the fluorine atoms in the PF_6 anion are disordered and modeled over two sites with occupancy of 0.55 and 0.45. Hydrogen atoms H3A and H3B bound to oxygen in the water molecule were located in the difference map and refined in x, y, and z with a distance restraint placed on the O-H distances and with thermal parameters riding on the parent oxygen atom. The remainder of the hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 6094 observed reflections and 329 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0399$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 – Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.0641$$

The standard deviation of an observation of unit weight[d] was 1.10. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.89 and -0.71 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]	occ
Ir(1)	1.055297(19)	0.128692(7)	0.762720(12)	2.589(5)	
P(1)	0.60454(16)	-0.04637(7)	0.76291(10)	4.06(3)	
F(1)	0.6864(5)	-0.0636(2)	0.6685(3)	7.96(10)	
F(2)	0.5257(5)	-0.0273(2)	0.8564(3)	9.10(12)	
F(3)	0.617(2)	0.0294(4)	0.7528(9)	8.5(3)	0.55
F(3')	0.505(3)	-0.0002(12)	0.6871(13)	11.4(6)	0.45
F(4)	0.7711(11)	-0.0461(10)	0.8298(8)	8.2(3)	0.55
F(4')	0.741(3)	0.0040(11)	0.7772(17)	11.3(5)	0.45
F(5)	0.4391(11)	-0.0439(9)	0.6980(9)	7.6(3)	0.55
F(5')	0.468(3)	-0.0957(14)	0.7366(13)	13.3(6)	0.45
F(6)	0.589(2)	-0.1195(4)	0.7766(14)	9.8(4)	0.55
F(6')	0.705(3)	-0.0946(12)	0.8299(12)	10.8(6)	0.45
O(1)	0.8287(5)	0.11806(19)	0.9126(3)	5.70(9)	
O(2)	1.0539(4)	0.22682(14)	0.7531(3)	4.35(7)	
N(1)	0.8687(4)	0.14583(17)	0.6442(3)	3.01(7)	
C(1)	0.9114(6)	0.1238(2)	0.8551(4)	3.55(9)	
C(2)	0.7840(6)	0.0987(3)	0.5917(4)	4.00(10)	
C(3)	0.6691(6)	0.1132(3)	0.5127(4)	5.18(12)	
C(4)	0.6364(7)	0.1760(4)	0.4879(4)	5.93(14)	
C(5)	0.7195(6)	0.2238(3)	0.5432(4)	5.60(14)	
C(6)	0.8371(6)	0.2077(2)	0.6221(4)	3.94(10)	
C(7)	0.9319(7)	0.2566(3)	0.6901(5)	5.44(13)	
C(8)	0.8182(9)	0.2867(4)	0.7583(7)	11.8(3)	
C(9)	1.0006(12)	0.3069(4)	0.6328(7)	15.6(5)	
C(10)	1.2294(5)	0.0844(2)	0.6727(3)	3.24(9)	
C(11)	1.1585(5)	0.0353(2)	0.7283(3)	3.12(8)	
C(12)	1.2030(5)	0.0492(2)	0.8318(3)	3.33(9)	
C(13)	1.2934(5)	0.1075(2)	0.8411(3)	3.49(9)	
C(14)	1.3146(5)	0.1275(2)	0.7417(3)	3.37(8)	
C(15)	1.2201(7)	0.0864(3)	0.5622(4)	5.13(12)	
C(16)	1.0776(6)	-0.0240(2)	0.6851(4)	4.72(11)	
C(17)	1.1692(6)	0.0069(3)	0.9158(4)	5.04(12)	
C(18)	1.3757(6)	0.1371(3)	0.9365(4)	5.44(13)	
C(19)	1.4079(6)	0.1851(3)	0.7191(5)	5.38(13)	
O(3)	1.2460(7)	0.2979(2)	0.8920(4)	8.60(14)	

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(2)	0.8041	0.0555	0.6096	4.80
H(3)	0.6130	0.0800	0.4758	6.21
H(4)	0.5582	0.1864	0.4338	7.12
H(5)	0.6970	0.2672	0.5277	6.72
H(8A)	0.8782	0.3152	0.8066	14.22
H(8B)	0.7709	0.2527	0.7928	14.22
H(8C)	0.7351	0.3109	0.7177	14.22
H(9A)	1.0690	0.2871	0.5906	18.68
H(9B)	1.0620	0.3366	0.6783	18.68
H(9C)	0.9159	0.3300	0.5918	18.68
H(15A)	1.2410	0.1298	0.5415	6.15
H(15B)	1.1150	0.0733	0.5313	6.15
H(15C)	1.2985	0.0573	0.5421	6.15
H(16A)	0.9999	-0.0377	0.7260	5.67
H(16B)	1.1555	-0.0578	0.6831	5.67
H(16C)	1.0248	-0.0151	0.6182	5.67
H(17A)	1.2530	-0.0248	0.9305	6.05
H(17B)	1.0685	-0.0149	0.8968	6.05
H(17C)	1.1642	0.0330	0.9744	6.05
H(18A)	1.3909	0.1827	0.9264	6.53
H(18B)	1.4779	0.1166	0.9557	6.53
H(18C)	1.3110	0.1310	0.9886	6.53
H(19A)	1.3857	0.1944	0.6485	6.46
H(19B)	1.5203	0.1765	0.7378	6.46
H(19C)	1.3783	0.2217	0.7564	6.46
H(3A)	1.1544	0.2753	0.8629	10.32
H(3B)	1.2344	0.3401	0.8655	10.32

Table 3. Anisotropic displacement parameters[j]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03413(9)	0.03278(9)	0.03085(9)	-0.00129(9)	0.00294(6)	-0.00169(8)
P(1)	0.0411(7)	0.0655(9)	0.0465(8)	0.0074(7)	0.0024(6)	-0.0016(7)
F(1)	0.097(3)	0.147(4)	0.064(2)	0.007(3)	0.030(2)	-0.025(2)
F(2)	0.095(3)	0.178(4)	0.081(3)	0.041(3)	0.038(2)	-0.009(3)
F(3)	0.147(10)	0.070(5)	0.111(8)	-0.019(7)	0.036(8)	-0.024(5)
F(3')	0.153(16)	0.161(15)	0.127(12)	0.098(12)	0.046(12)	0.081(13)
F(4)	0.048(5)	0.186(14)	0.070(6)	0.022(8)	-0.016(4)	-0.019(8)
F(4')	0.117(13)	0.151(15)	0.172(17)	-0.081(11)	0.061(13)	-0.078(12)
F(5)	0.050(5)	0.151(11)	0.079(7)	0.026(7)	-0.022(5)	-0.038(7)
F(5')	0.135(15)	0.197(19)	0.170(15)	-0.123(14)	0.015(13)	-0.004(14)
F(6)	0.110(9)	0.064(5)	0.205(16)	-0.001(7)	0.044(9)	0.015(7)
F(6')	0.164(19)	0.156(16)	0.099(11)	0.107(12)	0.044(11)	0.073(12)
O(1)	0.072(3)	0.091(3)	0.061(2)	-0.006(2)	0.033(2)	-0.008(2)
O(2)	0.057(2)	0.0334(17)	0.069(2)	-0.0036(16)	-0.0122(18)	-0.0042(16)
N(1)	0.0337(20)	0.042(2)	0.037(2)	0.0026(16)	-0.0012(17)	0.0001(16)
C(1)	0.046(3)	0.046(3)	0.043(3)	0.002(2)	0.006(2)	-0.007(2)
C(2)	0.047(3)	0.057(3)	0.046(3)	-0.004(2)	0.000(2)	-0.010(2)
C(3)	0.045(3)	0.096(5)	0.052(3)	-0.005(3)	-0.006(3)	-0.017(3)
C(4)	0.050(3)	0.117(6)	0.053(4)	0.007(4)	-0.007(3)	0.018(4)
C(5)	0.051(3)	0.077(4)	0.078(4)	0.004(3)	-0.012(3)	0.031(3)
C(6)	0.043(3)	0.047(3)	0.058(3)	-0.000(2)	0.003(2)	0.013(2)
C(7)	0.058(4)	0.042(3)	0.099(5)	-0.005(3)	-0.015(3)	0.013(3)
C(8)	0.091(6)	0.110(6)	0.235(11)	0.034(5)	-0.021(7)	-0.103(7)
C(9)	0.201(10)	0.159(9)	0.190(10)	-0.129(8)	-0.105(8)	0.118(8)
C(10)	0.034(2)	0.051(3)	0.038(2)	0.008(2)	0.008(2)	-0.001(2)
C(11)	0.033(2)	0.036(2)	0.050(3)	0.0084(19)	0.010(2)	-0.002(2)
C(12)	0.037(3)	0.045(3)	0.045(3)	0.011(2)	0.007(2)	0.010(2)
C(13)	0.032(2)	0.057(3)	0.042(3)	0.001(2)	-0.002(2)	-0.002(2)
C(14)	0.034(2)	0.048(3)	0.047(3)	-0.001(2)	0.0096(20)	0.004(2)
C(15)	0.071(4)	0.077(4)	0.050(3)	0.002(3)	0.019(3)	-0.005(3)
C(16)	0.056(3)	0.041(3)	0.084(4)	-0.002(2)	0.016(3)	-0.015(3)
C(17)	0.059(3)	0.071(4)	0.063(4)	0.010(3)	0.017(3)	0.028(3)
C(18)	0.052(3)	0.094(5)	0.054(3)	-0.005(3)	-0.013(3)	-0.011(3)
C(19)	0.057(3)	0.065(4)	0.088(4)	-0.019(3)	0.026(3)	0.006(3)
O(3)	0.140(5)	0.073(3)	0.098(4)	-0.025(3)	-0.031(3)	-0.014(3)

Table 4. Bond lengths (Å)

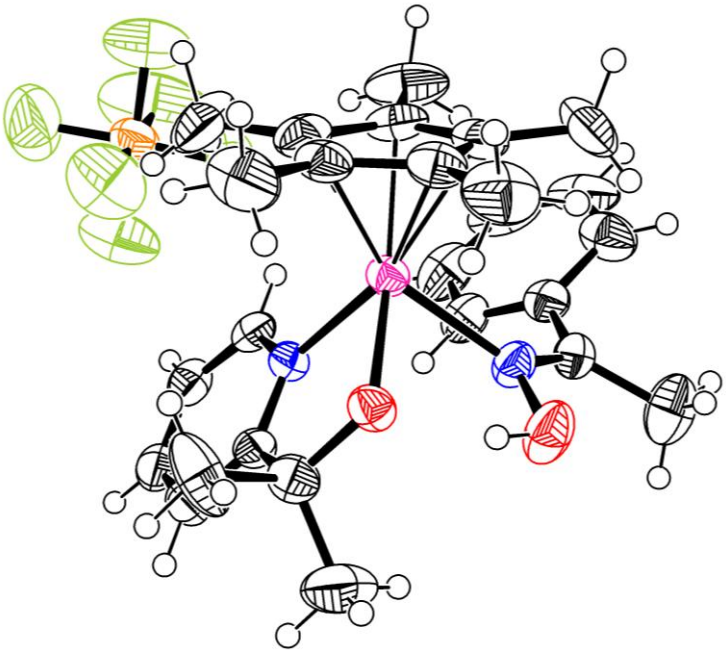
atom	atom	distance
Ir(1)	O(2)	2.044(3)
Ir(1)	C(1)	1.886(5)
Ir(1)	C(11)	2.211(4)
Ir(1)	C(13)	2.190(4)
P(1)	F(1)	1.592(4)
P(1)	F(3)	1.586(9)
P(1)	F(4)	1.566(9)
P(1)	F(5)	1.548(9)
P(1)	F(6)	1.541(9)
F(3)	F(3')	1.35(2)
F(3')	F(5)	1.09(3)
F(4)	F(6')	1.16(3)

atom	atom	distance
Ir(1)	N(1)	2.116(3)
Ir(1)	C(10)	2.258(5)
Ir(1)	C(12)	2.200(4)
Ir(1)	C(14)	2.272(4)
P(1)	F(2)	1.575(4)
P(1)	F(3')	1.56(2)
P(1)	F(4')	1.56(2)
P(1)	F(5')	1.55(3)
P(1)	F(6')	1.53(2)
F(3)	F(4')	1.19(3)
F(4)	F(4')	1.27(3)
F(5)	F(5')	1.21(3)

atom	atom	distance
F(5')	F(6)	1.20(3)
O(1)	C(1)	1.136(7)
N(1)	C(2)	1.355(6)
C(2)	C(3)	1.373(7)
C(4)	C(5)	1.376(9)
C(6)	C(7)	1.522(7)
C(7)	C(9)	1.476(12)
C(10)	C(14)	1.416(6)
C(11)	C(12)	1.430(6)
C(12)	C(13)	1.431(7)
C(13)	C(14)	1.451(7)
C(14)	C(19)	1.495(7)

atom	atom	distance
F(6)	F(6')	1.25(3)
O(2)	C(7)	1.389(6)
N(1)	C(6)	1.339(6)
C(3)	C(4)	1.366(10)
C(5)	C(6)	1.394(7)
C(7)	C(8)	1.570(11)
C(10)	C(11)	1.455(7)
C(10)	C(15)	1.493(7)
C(11)	C(16)	1.490(6)
C(12)	C(17)	1.505(7)
C(13)	C(18)	1.509(7)

X-ray crystal structure of Cp*Ir(2-(2'-pyridyl)-2-propanolate)(acetophenone oxime)PF_6 (3)



A. Crystal Data

Empirical Formula	$C_{26}H_{34}IrN_2O_2PF_6$	
Formula Weight	743.75	
Crystal Color, Habit	yellow, prism	
Crystal Dimensions	0.26 X 0.06 X 0.05 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 10.5483(10) Å	α = 90 °
	b = 12.4161(11) Å	β = 91.432(6) °
	c = 21.8014(19) Å	γ = 90 °
	V = 2854.4(4) $Å^3$	
Space Group	$P2_1/c$ (#14)	
Z value	4	
D_{calc}	1.731 g/cm^3	
F_{000}	1464.00	
μ(MoKα)	48.116 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku SCXmini
Radiation	MoKα (λ = 0.71075 Å)
Detector Aperture	75 mm round
Data Images	540 exposures
Exposure Rate	30.0 sec./ °
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm
$2\theta_{max}$	54.2°

No. of Reflections Measured	Total: 28630 Unique: 6294 (R_{int} = 0.0763)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.516 - 0.786)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\, w\,(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/[\,\sigma^2(Fo^2) + (0.0266 \cdot P)^2 + 4.7031 \cdot P\,]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.2°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	6294
No. Variables	355
Reflection/Parameter Ratio	17.73
Residuals: R1 (I>2.00σ(I))	0.0489
Residuals: R (All reflections)	0.0745
Residuals: wR2 (All reflections)	0.0870
Goodness of Fit Indicator	1.074
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.07 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.07 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a MiTeGen polyimide loop with immersion oil. All measurements were made on a Rigaku Mercury2 CCD area detector with filtered Mo-Kα radiation at a temperature of -50°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. H1A was located in the difference density map and refined without restraint. The remaining hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 6294 observed reflections and 355 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\, ||Fo| - |Fc|| \,/\, \Sigma\, |Fo| = 0.0489$$

$$wR2 = [\,\Sigma\,(\,w\,(Fo^2 - Fc^2)^2)/\,\Sigma\, w(Fo^2)^2]^{1/2} = 0.0870$$

The standard deviation of an observation of unit weight[d] was 1.07. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.07 and -1.07 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]
Ir(1)	0.66449(2)	0.196525(18)	0.402447(11)	2.556(6)
P(1)	0.8690(2)	0.66385(17)	0.31389(9)	4.75(5)
F(1)	1.0080(6)	0.7030(7)	0.3084(3)	13.7(3)
F(2)	0.8116(9)	0.7619(6)	0.2824(3)	14.7(3)
F(3)	0.8644(6)	0.7165(4)	0.3792(2)	8.72(15)
F(4)	0.7420(6)	0.6106(8)	0.3229(3)	13.5(3)
F(5)	0.8757(7)	0.6141(7)	0.2495(3)	12.6(2)
F(6)	0.9332(6)	0.5619(4)	0.3491(3)	9.16(16)
O(1)	0.7059(4)	0.1147(3)	0.48350(18)	3.00(8)
O(2)	0.4721(5)	0.1157(4)	0.4869(3)	4.66(11)
N(1)	0.7400(4)	0.3190(4)	0.4585(2)	2.63(9)
N(2)	0.4829(5)	0.2026(4)	0.4470(2)	3.11(10)
C(1)	0.7542(6)	0.4224(5)	0.4406(3)	3.04(12)
C(2)	0.8118(6)	0.4986(6)	0.4767(3)	3.54(13)
C(3)	0.8574(6)	0.4690(6)	0.5338(3)	3.61(13)
C(4)	0.8452(6)	0.3641(6)	0.5528(3)	3.46(13)
C(5)	0.7873(5)	0.2896(5)	0.5143(3)	2.78(11)
C(6)	0.7772(6)	0.1708(5)	0.5295(3)	3.39(13)
C(7)	0.7138(9)	0.1544(7)	0.5910(3)	6.0(2)
C(8)	0.9113(7)	0.1236(6)	0.5316(4)	6.0(2)
C(9)	0.7919(6)	0.1117(5)	0.3437(3)	3.46(13)
C(10)	0.7818(7)	0.2189(6)	0.3235(3)	4.04(15)
C(11)	0.6511(7)	0.2390(6)	0.3061(3)	3.81(14)
C(12)	0.5811(7)	0.1395(6)	0.3162(3)	3.67(14)
C(13)	0.6688(7)	0.0621(5)	0.3401(3)	3.49(13)
C(14)	0.9106(7)	0.0534(7)	0.3634(4)	5.9(2)
C(15)	0.8864(8)	0.2989(7)	0.3182(4)	6.4(2)
C(16)	0.6000(9)	0.3375(6)	0.2745(3)	6.2(2)
C(17)	0.4454(7)	0.1215(7)	0.3009(4)	5.9(2)
C(18)	0.6382(9)	-0.0522(6)	0.3581(4)	5.68(19)
C(19)	0.2572(7)	0.2077(6)	0.4641(4)	5.58(19)
C(20)	0.3761(6)	0.2508(5)	0.4365(3)	3.10(12)
C(21)	0.3707(6)	0.3515(5)	0.4004(3)	3.19(12)
C(22)	0.2807(7)	0.3637(7)	0.3527(3)	4.80(17)
C(23)	0.2730(9)	0.4587(9)	0.3211(4)	6.0(2)
C(24)	0.3504(10)	0.5435(8)	0.3349(4)	6.2(2)
C(25)	0.4391(8)	0.5324(6)	0.3824(4)	5.28(18)
C(26)	0.4477(6)	0.4370(5)	0.4153(3)	3.65(13)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1A)	0.550(8)	0.096(7)	0.493(4)	8.1(28)
H(1)	0.7231	0.4427	0.4015	3.65
H(2)	0.8200	0.5699	0.4629	4.25
H(3)	0.8967	0.5201	0.5597	4.34
H(4)	0.8762	0.3431	0.5918	4.16
H(7A)	0.6269	0.1796	0.5880	7.25
H(7B)	0.7596	0.1946	0.6226	7.25
H(7C)	0.7147	0.0784	0.6014	7.25
H(8A)	0.9514	0.1362	0.4927	7.16
H(8B)	0.9069	0.0467	0.5393	7.16
H(8C)	0.9607	0.1579	0.5643	7.16
H(14A)	0.8943	0.0107	0.3996	7.03
H(14B)	0.9770	0.1053	0.3727	7.03
H(14C)	0.9373	0.0065	0.3305	7.03
H(15A)	0.9218	0.2942	0.2777	7.69
H(15B)	0.9520	0.2837	0.3490	7.69
H(15C)	0.8533	0.3708	0.3246	7.69
H(16A)	0.5980	0.3260	0.2305	7.39
H(16B)	0.6541	0.3986	0.2844	7.39
H(16C)	0.5148	0.3518	0.2882	7.39
H(17A)	0.4078	0.0782	0.3327	7.11
H(17B)	0.4373	0.0842	0.2619	7.11
H(17C)	0.4021	0.1903	0.2980	7.11
H(18A)	0.6738	-0.102	0.3286	6.82
H(18B)	0.5469	-0.061	0.3586	6.82
H(18C)	0.6742	-0.067	0.3986	6.82
H(19A)	0.2569	0.2253	0.5075	6.69
H(19B)	0.2541	0.1302	0.4590	6.69
H(19C)	0.1838	0.2400	0.4436	6.69
H(22)	0.2255	0.3067	0.3424	5.76
H(23)	0.2126	0.4656	0.2889	7.24
H(24)	0.3438	0.6082	0.3126	7.49
H(25)	0.4937	0.5899	0.3925	6.33
H(26)	0.5069	0.4308	0.4480	4.38

Table 3. Anisotropic displacement parameters[j]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03278(14)	0.03386(13)	0.03036(13)	0.00275(12)	-0.00123(9)	-0.00054(13)
P(1)	0.0678(15)	0.0668(14)	0.0455(12)	-0.0145(11)	-0.0069(10)	0.0075(10)
F(1)	0.105(5)	0.302(10)	0.112(5)	-0.088(6)	-0.029(4)	0.097(6)
F(2)	0.316(11)	0.127(6)	0.112(5)	0.104(7)	-0.046(6)	0.036(5)
F(3)	0.159(6)	0.105(4)	0.066(3)	0.017(4)	-0.018(3)	-0.021(3)
F(4)	0.098(5)	0.306(10)	0.106(5)	-0.093(6)	-0.027(4)	0.047(6)
F(5)	0.183(7)	0.229(8)	0.068(4)	-0.012(6)	0.015(4)	-0.053(5)
F(6)	0.141(5)	0.089(4)	0.118(5)	0.010(4)	-0.022(4)	0.015(4)
O(1)	0.043(3)	0.035(2)	0.036(2)	-0.0024(19)	-0.0063(19)	0.0074(20)
O(2)	0.045(3)	0.058(3)	0.074(4)	-0.004(3)	0.006(3)	0.027(3)
N(1)	0.032(3)	0.037(3)	0.030(3)	-0.001(2)	0.000(2)	-0.003(2)
N(2)	0.038(3)	0.039(3)	0.041(3)	-0.004(3)	0.005(2)	0.007(3)
C(1)	0.038(4)	0.043(4)	0.035(4)	0.000(3)	0.010(3)	0.005(3)
C(2)	0.042(4)	0.044(4)	0.050(4)	-0.003(3)	0.012(3)	-0.004(3)
C(3)	0.039(4)	0.052(4)	0.046(4)	-0.009(3)	0.009(3)	-0.018(4)
C(4)	0.038(4)	0.055(4)	0.038(4)	0.001(3)	-0.004(3)	-0.007(3)
C(5)	0.032(3)	0.044(4)	0.030(3)	0.004(3)	0.005(3)	-0.006(3)
C(6)	0.047(4)	0.041(4)	0.041(4)	0.005(3)	-0.003(3)	0.002(3)
C(7)	0.118(8)	0.070(5)	0.042(5)	-0.017(5)	0.009(5)	0.005(4)
C(8)	0.059(5)	0.059(5)	0.106(7)	0.017(4)	-0.043(5)	-0.014(5)
C(9)	0.051(4)	0.049(4)	0.032(3)	0.013(3)	0.002(3)	-0.012(3)
C(10)	0.062(5)	0.052(5)	0.040(4)	-0.000(4)	0.017(3)	-0.012(3)
C(11)	0.064(5)	0.054(4)	0.028(4)	0.021(4)	0.011(3)	0.004(3)
C(12)	0.051(4)	0.060(5)	0.029(4)	0.012(4)	-0.002(3)	-0.009(3)
C(13)	0.057(5)	0.039(4)	0.037(4)	0.011(3)	0.001(3)	-0.008(3)
C(14)	0.067(6)	0.089(6)	0.066(5)	0.038(5)	-0.010(4)	-0.017(5)
C(15)	0.080(6)	0.079(6)	0.087(6)	-0.019(5)	0.051(5)	-0.023(5)
C(16)	0.122(8)	0.072(6)	0.041(4)	0.043(5)	0.014(5)	0.016(4)
C(17)	0.052(5)	0.106(7)	0.066(5)	0.006(5)	-0.019(4)	-0.044(5)
C(18)	0.107(7)	0.044(4)	0.065(6)	-0.002(4)	0.004(5)	-0.013(4)
C(19)	0.046(5)	0.064(5)	0.102(7)	0.003(4)	0.013(4)	0.009(5)
C(20)	0.033(4)	0.042(4)	0.042(4)	-0.000(3)	0.002(3)	0.000(3)
C(21)	0.033(4)	0.050(4)	0.039(4)	0.014(3)	0.005(3)	-0.005(3)
C(22)	0.053(5)	0.078(6)	0.051(5)	0.022(4)	-0.008(4)	-0.008(4)
C(23)	0.084(7)	0.110(8)	0.035(4)	0.044(6)	0.001(4)	0.001(5)
C(24)	0.106(8)	0.067(6)	0.066(6)	0.042(6)	0.033(6)	0.025(5)
C(25)	0.067(6)	0.048(5)	0.086(6)	0.010(4)	0.028(5)	-0.002(5)
C(26)	0.042(4)	0.041(4)	0.057(4)	0.010(3)	0.014(3)	-0.001(3)

Table 4. Bond lengths (Å)

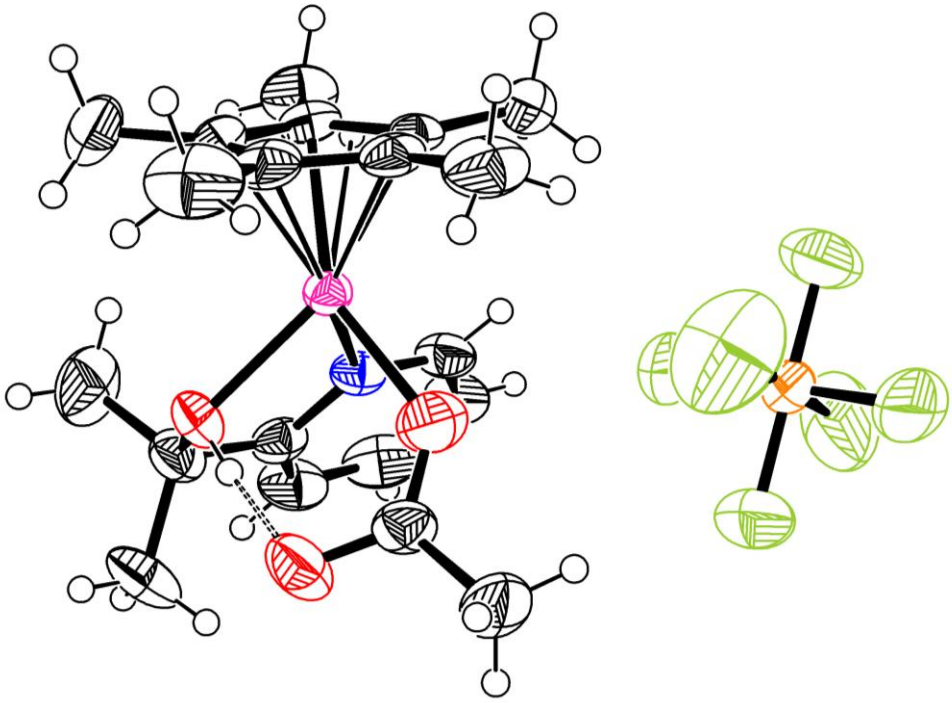
atom	atom	distance
Ir(1)	O(1)	2.075(4)
Ir(1)	N(2)	2.171(5)
Ir(1)	C(10)	2.163(7)
Ir(1)	C(12)	2.175(6)
P(1)	F(1)	1.552(7)
P(1)	F(3)	1.569(5)
P(1)	F(5)	1.537(7)
O(1)	C(6)	1.421(7)
N(1)	C(1)	1.351(8)
N(2)	C(20)	1.291(8)
C(2)	C(3)	1.373(9)
C(4)	C(5)	1.381(9)
C(6)	C(7)	1.526(10)
C(9)	C(10)	1.405(10)

atom	atom	Distance
Ir(1)	N(1)	2.095(5)
Ir(1)	C(9)	2.155(7)
Ir(1)	C(11)	2.166(6)
Ir(1)	C(13)	2.153(6)
P(1)	F(2)	1.517(8)
P(1)	F(4)	1.512(7)
P(1)	F(6)	1.619(6)
O(2)	N(2)	1.392(7)
N(1)	C(5)	1.354(7)
C(1)	C(2)	1.364(9)
C(3)	C(4)	1.373(10)
C(5)	C(6)	1.515(9)
C(6)	C(8)	1.532(10)
C(9)	C(13)	1.437(10)

atom	atom	distance
C(9)	C(14)	1.500(10)
C(10)	C(15)	1.491(11)
C(11)	C(16)	1.498(11)
C(12)	C(17)	1.479(10)
C(19)	C(20)	1.503(10)
C(21)	C(22)	1.399(9)
C(22)	C(23)	1.368(13)
C(24)	C(25)	1.386(13)
O(2)	H(1A)	0.86(9)

atom	atom	Distance
C(10)	C(11)	1.443(11)
C(11)	C(12)	1.459(10)
C(12)	C(13)	1.424(10)
C(13)	C(18)	1.509(9)
C(20)	C(21)	1.478(9)
C(21)	C(26)	1.370(9)
C(23)	C(24)	1.362(14)
C(25)	C(26)	1.386(10)

X-ray crystal structure of Cp*Ir(2-(2'-pyridyl)-2-propanol)(acetate)PF_6 (4)



A. Crystal Data

Empirical Formula	$IrC_{20}H_{29}NO_3PF_6$	
Formula Weight	668.64	
Crystal Color, Habit	yellow, prism	
Crystal Dimensions	0.11 X 0.08 X 0.04 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 7.9352(15) Å	α = 90 °
	b = 18.617(4) Å	β = 98.978(4) °
	c = 16.983(3) Å	γ = 90 °
	V = 2478.2(8) $Å^3$	
Space Group	$P2_1/c$ (#14)	
Z value	4	
D_{calc}	1.792 g/cm^3	
F_{000}	1304.00	
μ(MoKα)	55.324 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku SCXmini
Radiation	MoKα (λ = 0.71075 Å)
Detector Aperture	75 mm round
Data Images	535 exposures
Exposure Rate	50.0 sec./ °
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm
$2\theta_{max}$	51.4°

No. of Reflections Measured	Total: 19807 Unique: 4676 (R_{int} = 0.0657)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.537 - 0.801)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.\ 0238 \cdot P)^2\ + 2.7848 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	51.4°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4676
No. Variables	298
Reflection/Parameter Ratio	15.69
Residuals: R1 (I>2.00σ(I))	0.0467
Residuals: R (All reflections)	0.0708
Residuals: wR2 (All reflections)	0.0791
Goodness of Fit Indicator	1.125
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.65 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.61 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a MiTeGen polyimide loop with immersion oil. All measurements were made on a Rigaku Mercury2 CCD area detector with filtered Mo-Kα radiation at a temperature of -50°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. H1A was placed on O1 on the basis of the observed O1-Ir bond distance, which is somewhat elongated relative to other Iridium 2-pyridyl-2-propanolate complexes. H1A was modeled as an idealized hydroxyl using a rotating group refinement. The remaining hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 4676 observed reflections and 298 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0467$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 – Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.0791$$

The standard deviation of an observation of unit weight[d] was 1.13. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.65 and -0.61 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]
Ir(1)	0.20587(3)	0.081958(13)	0.753729(14)	2.586(7)
P(1)	-0.0398(3)	0.28783(11)	0.53393(12)	4.34(5)
F(1)	-0.0342(10)	0.3653(3)	0.4991(4)	10.1(2)
F(2)	0.0978(7)	0.2604(3)	0.4823(3)	7.89(15)
F(3)	0.1023(10)	0.3071(4)	0.6046(4)	12.1(2)
F(4)	-0.0442(7)	0.2082(3)	0.5701(3)	7.13(13)
F(5)	-0.1846(8)	0.3116(3)	0.5822(4)	8.64(17)
F(6)	-0.1835(8)	0.2635(3)	0.4630(4)	9.74(18)
O(1)	0.3928(6)	0.0033(2)	0.7359(3)	3.50(9)
O(2)	0.2951(7)	0.1409(3)	0.6618(3)	5.01(12)
O(3)	0.5286(7)	0.0768(3)	0.6451(3)	5.12(12)
N(1)	0.0769(7)	0.0154(3)	0.6630(3)	2.87(10)
C(1)	-0.0777(9)	0.0311(4)	0.6214(4)	3.75(15)
C(2)	-0.1646(10)	-0.0145(4)	0.5669(4)	4.27(16)
C(3)	-0.0901(11)	-0.0786(5)	0.5530(5)	5.24(19)
C(4)	0.0700(11)	-0.0961(4)	0.5935(5)	4.64(18)
C(5)	0.1544(10)	-0.0481(4)	0.6492(4)	3.31(14)
C(6)	0.3247(10)	-0.0630(4)	0.6999(5)	3.80(15)
C(7)	0.4523(11)	-0.0918(4)	0.6487(5)	6.0(2)
C(8)	0.3014(13)	-0.1153(4)	0.7660(5)	6.4(2)
C(9)	0.1991(10)	0.0632(4)	0.8806(4)	3.52(14)
C(10)	0.0309(9)	0.0721(4)	0.8407(4)	3.24(13)
C(11)	0.0167(9)	0.1425(4)	0.8033(4)	3.11(13)
C(12)	0.1797(10)	0.1775(4)	0.8237(4)	3.57(15)
C(13)	0.2951(10)	0.1290(4)	0.8687(4)	3.79(15)
C(14)	0.2734(12)	0.0028(4)	0.9322(5)	5.9(2)
C(15)	-0.1115(11)	0.0202(4)	0.8387(5)	5.25(19)
C(16)	-0.1446(10)	0.1762(5)	0.7638(4)	5.10(19)
C(17)	0.2189(12)	0.2529(4)	0.8011(5)	5.8(2)
C(18)	0.4752(10)	0.1441(5)	0.9069(5)	6.7(2)
C(19)	0.4316(9)	0.1320(4)	0.6284(4)	3.78(15)
C(20)	0.4797(10)	0.1860(5)	0.5707(5)	5.21(19)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1)	-0.1277	0.0755	0.6304	4.50
H(2)	-0.2730	-0.0022	0.5395	5.12
H(3)	-0.1479	-0.1110	0.5157	6.28
H(4)	0.1213	-0.1400	0.5836	5.57
H(7A)	0.5645	-0.0949	0.6808	7.21
H(7B)	0.4568	-0.0595	0.6042	7.21
H(7C)	0.4167	-0.1391	0.6287	7.21
H(8A)	0.2265	-0.0943	0.7997	7.66
H(8B)	0.4113	-0.1256	0.7977	7.66
H(8C)	0.2515	-0.1596	0.7428	7.66
H(14A)	0.2843	0.0169	0.9877	7.09
H(14B)	0.3851	-0.0092	0.9194	7.09
H(14C)	0.1993	-0.0388	0.9229	7.09
H(15A)	-0.1860	0.0355	0.8757	6.30
H(15B)	-0.0660	-0.0270	0.8539	6.30
H(15C)	-0.1757	0.0182	0.7852	6.30
H(16A)	-0.2199	0.1394	0.7377	6.12
H(16B)	-0.1192	0.2108	0.7245	6.12
H(16C)	-0.1998	0.2005	0.8034	6.12
H(17A)	0.3349	0.2552	0.7897	7.01
H(17B)	0.2070	0.2851	0.8448	7.01
H(17C)	0.1402	0.2671	0.7541	7.01
H(18A)	0.4769	0.1566	0.9625	8.05
H(18B)	0.5202	0.1838	0.8795	8.05
H(18C)	0.5448	0.1018	0.9034	8.05
H(20A)	0.5001	0.1618	0.5225	6.25
H(20B)	0.5825	0.2110	0.5945	6.25
H(20C)	0.3877	0.2204	0.5577	6.25
H(1A)	0.4408	0.0259	0.7035	4.21

Table 3. Anisotropic displacement parameters[j]

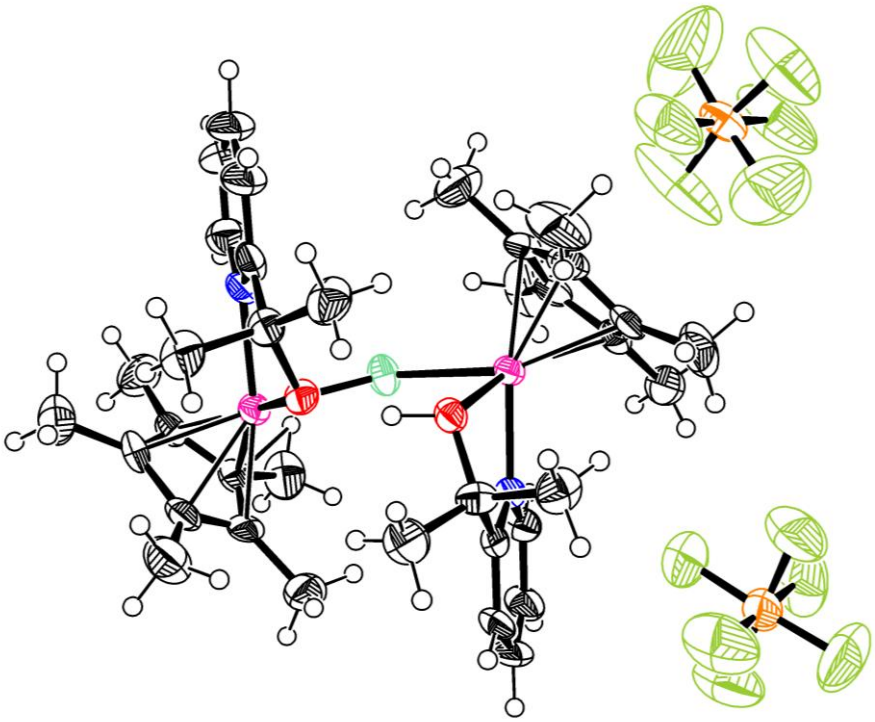
atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03722(16)	0.03061(14)	0.03109(14)	0.00022(14)	0.00739(10)	-0.00193(13)
P(1)	0.0778(16)	0.0492(13)	0.0410(12)	0.0166(11)	0.0194(11)	0.0081(9)
F(1)	0.224(7)	0.055(3)	0.129(5)	0.031(4)	0.109(5)	0.038(3)
F(2)	0.118(4)	0.096(4)	0.103(4)	0.029(4)	0.069(4)	0.018(3)
F(3)	0.178(7)	0.155(6)	0.106(5)	-0.057(5)	-0.039(5)	-0.021(5)
F(4)	0.135(5)	0.056(3)	0.087(4)	0.026(3)	0.042(3)	0.026(3)
F(5)	0.154(6)	0.071(4)	0.125(5)	0.030(4)	0.093(4)	0.007(3)
F(6)	0.130(5)	0.129(5)	0.094(4)	0.041(4)	-0.037(4)	-0.014(4)
O(1)	0.041(3)	0.035(3)	0.057(3)	0.009(2)	0.009(2)	-0.002(2)
O(2)	0.077(4)	0.061(4)	0.056(3)	-0.002(3)	0.021(3)	-0.001(3)
O(3)	0.048(3)	0.055(4)	0.097(4)	0.010(3)	0.029(3)	0.009(3)
N(1)	0.039(3)	0.034(3)	0.040(3)	-0.007(3)	0.015(3)	-0.005(2)
C(1)	0.037(4)	0.062(5)	0.046(4)	-0.001(4)	0.015(4)	-0.007(4)
C(2)	0.041(5)	0.067(6)	0.054(5)	-0.012(4)	0.008(4)	-0.016(4)
C(3)	0.066(6)	0.080(7)	0.056(5)	-0.027(5)	0.017(5)	-0.025(5)
C(4)	0.076(6)	0.042(5)	0.063(5)	-0.010(4)	0.025(5)	-0.022(4)
C(5)	0.057(5)	0.033(4)	0.040(4)	-0.008(4)	0.020(4)	-0.000(3)
C(6)	0.051(5)	0.037(4)	0.058(5)	0.005(3)	0.017(4)	-0.002(3)
C(7)	0.064(6)	0.064(6)	0.106(7)	0.021(5)	0.033(5)	-0.019(5)
C(8)	0.117(8)	0.042(5)	0.082(7)	-0.003(5)	0.012(6)	0.016(4)
C(9)	0.052(5)	0.054(5)	0.027(4)	0.004(4)	0.004(3)	-0.003(3)
C(10)	0.046(4)	0.049(5)	0.033(4)	-0.011(4)	0.018(3)	-0.005(3)
C(11)	0.046(4)	0.047(4)	0.027(4)	0.009(4)	0.011(3)	-0.010(3)
C(12)	0.071(6)	0.037(4)	0.032(4)	-0.005(4)	0.020(4)	-0.012(3)
C(13)	0.054(5)	0.060(5)	0.030(4)	-0.005(4)	0.005(4)	-0.017(3)
C(14)	0.103(8)	0.073(6)	0.046(5)	0.019(5)	0.005(5)	0.017(4)
C(15)	0.072(6)	0.064(6)	0.068(6)	-0.023(5)	0.026(5)	-0.010(4)
C(16)	0.067(6)	0.083(6)	0.043(5)	0.029(5)	0.007(4)	0.003(4)
C(17)	0.119(8)	0.044(5)	0.068(6)	-0.015(5)	0.042(5)	-0.017(4)
C(18)	0.059(6)	0.124(9)	0.069(6)	-0.024(6)	0.001(5)	-0.038(6)
C(19)	0.039(4)	0.057(5)	0.051(5)	-0.006(4)	0.017(4)	0.003(4)
C(20)	0.052(5)	0.082(6)	0.069(6)	-0.006(5)	0.024(4)	0.020(5)

Table 4. Bond lengths (Å)

atom	atom	distance
Ir(1)	O(1)	2.140(5)
Ir(1)	N(1)	2.113(5)
Ir(1)	C(10)	2.186(7)
Ir(1)	C(12)	2.168(7)
P(1)	F(1)	1.562(6)
P(1)	F(3)	1.554(7)
P(1)	F(5)	1.576(7)
O(1)	C(6)	1.445(8)
O(3)	C(19)	1.289(9)
N(1)	C(5)	1.370(9)
C(2)	C(3)	1.369(12)
C(4)	C(5)	1.394(10)
C(6)	C(7)	1.530(12)
C(9)	C(10)	1.409(10)
C(9)	C(14)	1.490(10)
C(10)	C(15)	1.484(11)
C(11)	C(16)	1.488(10)
C(12)	C(17)	1.501(10)
C(19)	C(20)	1.495(11)

atom	atom	distance
Ir(1)	O(2)	2.119(6)
Ir(1)	C(9)	2.192(7)
Ir(1)	C(11)	2.151(7)
Ir(1)	C(13)	2.156(7)
P(1)	F(2)	1.588(6)
P(1)	F(4)	1.606(5)
P(1)	F(6)	1.591(6)
O(2)	C(19)	1.309(10)
N(1)	C(1)	1.348(8)
C(1)	C(2)	1.361(10)
C(3)	C(4)	1.386(12)
C(5)	C(6)	1.510(10)
C(6)	C(8)	1.519(11)
C(9)	C(13)	1.472(11)
C(10)	C(11)	1.454(9)
C(11)	C(12)	1.442(10)
C(12)	C(13)	1.421(10)
C(13)	C(18)	1.501(11)

X-ray crystal structure of $[Cp^*Ir(2\text{-}(2'\text{-pyridyl})\text{-}2\text{-propanolate})]_2HCl(PF_6)_2$ (5)



A. Crystal Data

Empirical Formula	$Ir_2ClP_2F_{12}O_2N_2C_{36}H_{51}$	
Formula Weight	1253.63	
Crystal Color, Habit	yellow, prism	
Crystal Dimensions	0.07 X 0.07 X 0.04 mm	
Crystal System	monoclinic	
Lattice Type	C-centered	
Lattice Parameters	a = 18.578(6) Å	α = 90 °
	b = 20.340(6) Å	β = 112.035(8) °
	c = 24.619(7) Å	γ = 90 °
	V = 8623.4(45) $Å^3$	
Space Group	C2/c (#15)	
Z value	8	
D_{calc}	1.931 g/cm^3	
F_{000}	4848.00	
μ(MoKα)	64.058 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku SCXmini
Radiation	MoKα (λ = 0.71075 Å)
Detector Aperture	75 mm round
Data Images	540 exposures
Exposure Rate	30.0 sec./ °
Detector Swing Angle	-28.40°
Detector Position	49.90 mm
Pixel Size	0.146 mm

$2\theta_{max}$	52.7°
No. of Reflections Measured	Total: 29537 Unique: 8791 (R_{int} = 0.0943)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.501 - 0.774)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.0244 \cdot P)^2\ + 47.2422 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	52.7°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	8791
No. Variables	532
Reflection/Parameter Ratio	16.52
Residuals: R1 (I>2.00σ(I))	0.0683
Residuals: R (All reflections)	0.1111
Residuals: wR2 (All reflections)	0.1030
Goodness of Fit Indicator	1.139
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.17 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.79 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a MiTeGen polyimide loop with immersion oil. All measurements were made on a Rigaku Mercury2 CCD area detector with filtered Mo-Kα radiation at a temperature of -50°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. H1A was located in the difference density map and refined without restraint. The remaining hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 8791 observed reflections and 532 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0683$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 - Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.1030$$

The standard deviation of an observation of unit weight[d] was 1.14. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.17 and -0.79 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]
Ir(1)	0.74604(2)	0.166984(17)	0.210779(17)	2.437(9)
Ir(2)	0.74887(2)	0.066418(17)	0.368639(17)	2.339(9)
Cl(1)	0.68752(14)	0.13092(12)	0.27899(11)	3.10(5)
P(1)	0.9215(2)	0.13868(19)	0.61178(15)	5.10(8)
P(2)	0.56738(19)	-0.13748(15)	0.42512(17)	4.50(7)
F(1)	0.9950(5)	0.1400(4)	0.5963(4)	9.2(3)
F(2)	0.9216(5)	0.2150(4)	0.6123(4)	9.1(3)
F(3)	0.8672(5)	0.1393(4)	0.5454(3)	8.6(2)
F(4)	0.8464(5)	0.1392(6)	0.6273(4)	10.9(3)
F(5)	0.9217(6)	0.0614(4)	0.6102(4)	11.2(3)
F(6)	0.9723(6)	0.1361(5)	0.6786(4)	10.7(3)
F(7)	0.6272(6)	-0.1421(4)	0.3946(5)	9.4(3)
F(8)	0.5553(6)	-0.0655(4)	0.4117(7)	13.9(5)
F(9)	0.5057(7)	-0.1664(9)	0.3743(5)	19.6(7)
F(10)	0.5086(6)	-0.1332(4)	0.4565(6)	12.0(4)
F(11)	0.5893(6)	-0.2077(4)	0.4507(5)	11.6(4)
F(12)	0.6369(7)	-0.1138(6)	0.4811(5)	14.2(4)
O(1)	0.8352(4)	0.0997(3)	0.2535(3)	2.53(12)
O(2)	0.8536(4)	0.0715(3)	0.3546(3)	2.58(12)
N(1)	0.7055(5)	0.0776(4)	0.1676(4)	2.91(16)
N(2)	0.7985(5)	0.1555(4)	0.4072(3)	2.59(15)
C(1)	0.7762(6)	0.2672(4)	0.2383(4)	3.3(2)
C(2)	0.8150(6)	0.2477(5)	0.2008(5)	3.2(2)
C(3)	0.7576(7)	0.2309(5)	0.1445(5)	3.6(2)
C(4)	0.6824(6)	0.2399(4)	0.1480(5)	3.1(2)
C(5)	0.6934(6)	0.2633(5)	0.2051(5)	3.3(2)
C(6)	0.8149(7)	0.2931(5)	0.2995(5)	4.7(3)
C(7)	0.8999(7)	0.2471(6)	0.2167(6)	5.3(3)
C(8)	0.7700(7)	0.2135(6)	0.0891(5)	4.8(3)
C(9)	0.6053(7)	0.2345(6)	0.0982(5)	4.7(3)
C(10)	0.6332(7)	0.2817(5)	0.2282(5)	5.0(3)
C(11)	0.6308(7)	0.0683(5)	0.1319(5)	3.9(2)
C(12)	0.6071(7)	0.0080(6)	0.1057(5)	4.6(3)
C(13)	0.6578(8)	-0.0424(5)	0.1161(5)	4.7(3)
C(14)	0.7331(7)	-0.0314(5)	0.1508(5)	4.2(2)
C(15)	0.7567(6)	0.0287(5)	0.1778(4)	3.3(2)
C(16)	0.8385(6)	0.0449(4)	0.2166(4)	2.90(20)
C(17)	0.8845(6)	0.0665(5)	0.1798(5)	3.9(2)
C(18)	0.8802(7)	-0.0116(5)	0.2567(5)	4.4(3)
C(19)	0.6701(7)	-0.0150(5)	0.3358(5)	3.3(2)
C(20)	0.6380(6)	0.0314(5)	0.3646(5)	3.5(2)
C(21)	0.6883(6)	0.0361(5)	0.4234(5)	3.2(2)
C(22)	0.7525(7)	-0.0080(5)	0.4331(5)	3.7(2)
C(23)	0.7386(7)	-0.0394(5)	0.3775(5)	3.7(2)
C(24)	0.6328(8)	-0.0368(7)	0.2732(5)	6.2(3)
C(25)	0.5627(7)	0.0678(7)	0.3372(6)	6.1(3)
C(26)	0.6742(8)	0.0746(6)	0.4702(5)	5.4(3)
C(27)	0.8124(7)	-0.0272(6)	0.4908(5)	6.2(3)
C(28)	0.7915(8)	-0.0903(5)	0.3677(7)	6.6(4)
C(29)	0.7575(6)	0.2037(5)	0.4204(4)	3.2(2)
C(30)	0.7940(7)	0.2607(5)	0.4473(5)	3.8(2)
C(31)	0.8697(7)	0.2698(5)	0.4596(5)	4.0(2)
C(32)	0.9124(6)	0.2211(5)	0.4445(4)	3.3(2)
C(33)	0.8742(6)	0.1648(4)	0.4175(4)	2.75(19)
C(34)	0.9141(6)	0.1092(5)	0.3988(5)	3.2(2)
C(35)	0.9716(6)	0.1338(6)	0.3722(5)	4.4(3)
C(36)	0.9538(6)	0.0630(5)	0.4511(5)	4.1(2)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1A)	0.843(7)	0.091(6)	0.316(5)	6.8(34)
H(6A)	0.8164	0.3408	0.2986	5.63
H(6B)	0.8675	0.2762	0.3165	5.63
H(6C)	0.7859	0.2792	0.3231	5.63
H(7A)	0.9255	0.2382	0.2582	6.37
H(7B)	0.9166	0.2896	0.2078	6.37
H(7C)	0.9134	0.2132	0.1944	6.37
H(8A)	0.8239	0.2011	0.0987	5.73
H(8B)	0.7576	0.2511	0.0630	5.73
H(8C)	0.7367	0.1769	0.0699	5.73
H(9A)	0.5922	0.2764	0.0781	5.61
H(9B)	0.5658	0.2226	0.1132	5.61
H(9C)	0.6082	0.2010	0.0710	5.61
H(10A)	0.5896	0.2517	0.2129	6.01
H(10B)	0.6157	0.3262	0.2162	6.01
H(10C)	0.6548	0.2791	0.2706	6.01
H(11)	0.5948	0.1029	0.1249	4.64
H(12)	0.5551	0.0020	0.0804	5.51
H(13)	0.6413	-0.084	0.0997	5.63
H(14)	0.7698	-0.065	0.1566	5.01
H(17A)	0.9363	0.0797	0.2055	4.65
H(17B)	0.8584	0.1034	0.1553	4.65
H(17C)	0.8880	0.0303	0.1553	4.65
H(18A)	0.8505	-0.025	0.2798	5.25
H(18B)	0.9314	0.0028	0.2826	5.25
H(18C)	0.8853	-0.048	0.2332	5.25
H(24A)	0.5872	-0.063	0.2684	7.46
H(24B)	0.6694	-0.063	0.2628	7.46
H(24C)	0.6177	0.0014	0.2478	7.46
H(25A)	0.5642	0.1076	0.3593	7.34
H(25B)	0.5203	0.0401	0.3374	7.34
H(25C)	0.5549	0.0792	0.2971	7.34
H(26A)	0.6450	0.0479	0.4874	6.48
H(26B)	0.6448	0.1139	0.4532	6.48
H(26C)	0.7235	0.0868	0.5002	6.48
H(27A)	0.7926	-0.063	0.5077	7.48
H(27B)	0.8248	0.0103	0.5170	7.48
H(27C)	0.8589	-0.042	0.4853	7.48
H(28A)	0.7801	-0.095	0.3261	7.98
H(28B)	0.7835	-0.132	0.3834	7.98
H(28C)	0.8451	-0.077	0.3875	7.98
H(29)	0.7040	0.1983	0.4111	3.84
H(30)	0.7653	0.2934	0.4571	4.61
H(31)	0.8943	0.3086	0.4782	4.80
H(32)	0.9656	0.2267	0.4526	3.95
H(35A)	0.9441	0.1594	0.3373	5.32
H(35B)	0.9966	0.0966	0.3620	5.32
H(35C)	1.0106	0.1612	0.4005	5.32
H(36A)	0.9775	0.0266	0.4387	4.95
H(36B)	0.9154	0.0464	0.4656	4.95
H(36C)	0.9934	0.0871	0.4821	4.95

Table 3. Anisotropic displacement parameters[j]

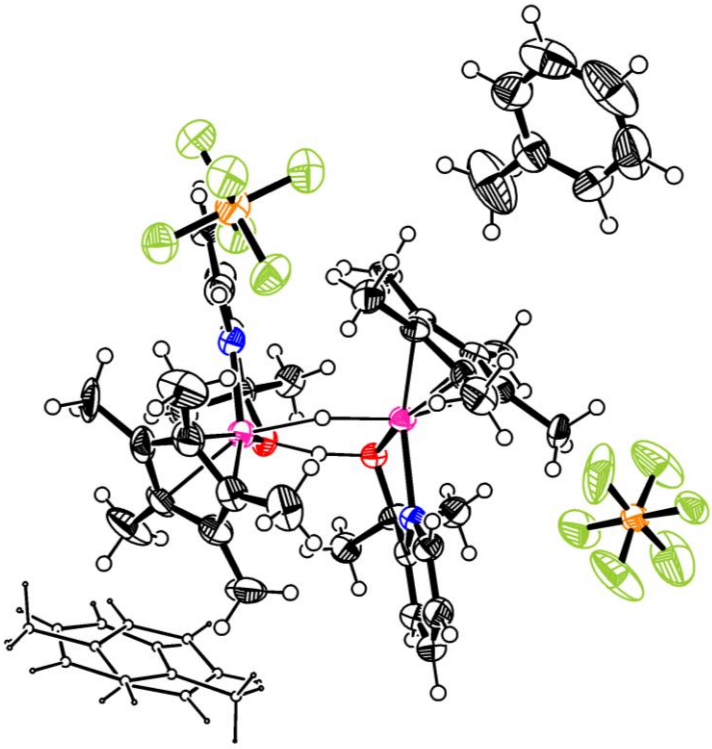
atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.0350(3)	0.0269(2)	0.0319(2)	0.00001(17)	0.01407(18)	0.00045(17)
Ir(2)	0.0346(2)	0.02567(19)	0.0318(2)	-0.00355(17)	0.01612(18)	-0.00229(18)
Cl(1)	0.0368(16)	0.0449(14)	0.0423(15)	0.0058(12)	0.0219(13)	0.0092(12)
P(1)	0.057(2)	0.082(3)	0.047(2)	-0.0290(19)	0.0109(18)	0.0085(18)
P(2)	0.049(2)	0.0442(18)	0.083(3)	-0.0080(15)	0.0302(20)	0.0088(17)
F(1)	0.093(7)	0.116(7)	0.175(10)	-0.023(5)	0.090(7)	-0.020(6)
F(2)	0.133(8)	0.068(6)	0.163(9)	-0.030(5)	0.077(7)	-0.021(5)
F(3)	0.122(8)	0.123(7)	0.057(5)	-0.032(6)	0.004(5)	0.016(5)
F(4)	0.081(7)	0.236(12)	0.107(7)	-0.031(7)	0.049(6)	0.045(8)
F(5)	0.179(10)	0.083(7)	0.126(8)	-0.046(6)	0.015(7)	0.036(6)
F(6)	0.127(8)	0.196(10)	0.049(5)	-0.025(7)	-0.007(5)	0.006(6)
F(7)	0.152(9)	0.082(6)	0.188(10)	-0.017(5)	0.138(8)	-0.004(6)
F(8)	0.152(10)	0.075(6)	0.379(18)	0.041(6)	0.187(12)	0.097(9)
F(9)	0.146(11)	0.47(3)	0.100(9)	-0.152(14)	0.008(8)	-0.057(13)
F(10)	0.174(10)	0.077(6)	0.301(15)	0.008(6)	0.197(11)	0.027(8)
F(11)	0.156(10)	0.090(7)	0.248(13)	0.033(6)	0.135(10)	0.062(8)
F(12)	0.137(10)	0.202(13)	0.155(11)	-0.034(9)	0.002(9)	-0.022(9)
O(1)	0.040(4)	0.028(3)	0.033(4)	0.005(3)	0.019(3)	-0.003(3)
O(2)	0.042(4)	0.028(4)	0.035(4)	0.000(3)	0.022(3)	-0.001(3)
N(1)	0.053(6)	0.027(5)	0.042(5)	-0.010(4)	0.030(5)	-0.001(4)
N(2)	0.040(6)	0.029(4)	0.029(5)	-0.003(4)	0.013(4)	-0.000(4)
C(1)	0.059(8)	0.016(5)	0.036(6)	-0.008(5)	0.002(6)	0.007(4)
C(2)	0.045(7)	0.029(6)	0.047(7)	-0.010(5)	0.019(6)	0.007(5)
C(3)	0.060(8)	0.044(6)	0.040(7)	-0.005(6)	0.026(6)	0.016(5)
C(4)	0.054(8)	0.024(5)	0.038(6)	0.000(5)	0.017(6)	0.011(5)
C(5)	0.054(8)	0.025(5)	0.043(7)	0.000(5)	0.013(6)	0.010(5)
C(6)	0.081(10)	0.038(6)	0.047(7)	-0.008(6)	0.009(7)	0.002(6)
C(7)	0.059(9)	0.068(9)	0.074(10)	-0.012(7)	0.024(7)	0.013(7)
C(8)	0.078(10)	0.060(8)	0.052(8)	0.007(6)	0.035(7)	0.010(6)
C(9)	0.063(9)	0.057(7)	0.045(7)	0.008(6)	0.005(7)	0.000(6)
C(10)	0.086(10)	0.048(7)	0.068(9)	0.021(6)	0.043(8)	0.005(6)
C(11)	0.048(8)	0.046(7)	0.048(7)	-0.005(6)	0.012(6)	-0.002(6)
C(12)	0.067(9)	0.056(8)	0.043(7)	-0.027(7)	0.011(6)	-0.015(6)
C(13)	0.085(11)	0.033(6)	0.068(9)	-0.017(7)	0.037(8)	-0.021(6)
C(14)	0.072(9)	0.031(6)	0.062(8)	-0.010(6)	0.032(7)	-0.011(6)
C(15)	0.056(8)	0.038(6)	0.040(6)	-0.007(5)	0.029(6)	0.007(5)
C(16)	0.049(7)	0.029(5)	0.042(6)	0.007(5)	0.028(6)	-0.003(5)
C(17)	0.049(7)	0.054(7)	0.058(7)	0.014(6)	0.036(6)	-0.007(6)
C(18)	0.074(9)	0.047(7)	0.049(7)	0.013(6)	0.028(7)	-0.006(6)
C(19)	0.057(8)	0.028(5)	0.045(7)	-0.019(5)	0.023(6)	-0.008(5)
C(20)	0.040(7)	0.043(6)	0.052(7)	-0.023(5)	0.021(6)	-0.001(5)
C(21)	0.047(7)	0.038(6)	0.045(7)	-0.011(5)	0.027(6)	0.002(5)
C(22)	0.058(8)	0.031(6)	0.048(7)	-0.016(5)	0.016(6)	0.014(5)
C(23)	0.055(8)	0.030(6)	0.058(8)	-0.011(5)	0.024(7)	-0.002(5)
C(24)	0.087(11)	0.095(10)	0.051(8)	-0.038(8)	0.021(8)	-0.026(7)
C(25)	0.038(8)	0.112(11)	0.087(10)	-0.000(7)	0.030(7)	0.029(9)
C(26)	0.108(11)	0.063(8)	0.056(8)	-0.029(7)	0.055(8)	-0.019(7)
C(27)	0.080(10)	0.078(9)	0.062(9)	-0.009(8)	0.007(8)	0.041(8)
C(28)	0.110(12)	0.023(6)	0.135(14)	0.014(7)	0.064(11)	0.001(7)
C(29)	0.042(7)	0.035(6)	0.048(7)	-0.002(5)	0.021(6)	-0.002(5)
C(30)	0.075(9)	0.028(6)	0.061(8)	-0.009(6)	0.045(7)	-0.011(5)
C(31)	0.076(9)	0.031(6)	0.052(7)	-0.026(6)	0.031(7)	-0.018(5)
C(32)	0.040(7)	0.039(6)	0.045(7)	-0.018(5)	0.015(5)	0.005(5)
C(33)	0.050(7)	0.027(5)	0.026(5)	-0.005(5)	0.012(5)	0.005(4)
C(34)	0.034(6)	0.038(6)	0.044(7)	-0.007(5)	0.010(5)	-0.006(5)
C(35)	0.045(8)	0.073(8)	0.062(8)	-0.011(6)	0.032(7)	-0.008(7)
C(36)	0.044(7)	0.054(7)	0.049(7)	0.009(6)	0.007(6)	0.004(6)

Table 4. Bond lengths (Å)

atom	atom	distance
Ir(1)	Cl(1)	2.431(3)
Ir(1)	N(1)	2.097(7)
Ir(1)	C(2)	2.153(11)
Ir(1)	C(4)	2.148(9)
Ir(2)	Cl(1)	2.450(2)
Ir(2)	N(2)	2.092(7)
Ir(2)	C(20)	2.145(12)
Ir(2)	C(22)	2.177(11)
P(1)	F(1)	1.551(12)
P(1)	F(3)	1.565(7)
P(1)	F(5)	1.572(10)
P(2)	F(7)	1.560(13)
P(2)	F(9)	1.466(12)
P(2)	F(11)	1.552(10)
O(1)	C(16)	1.455(12)
N(1)	C(11)	1.349(13)
N(2)	C(29)	1.353(14)
C(1)	C(2)	1.425(19)
C(1)	C(6)	1.501(14)
C(2)	C(7)	1.476(17)
C(3)	C(8)	1.509(18)
C(4)	C(9)	1.500(13)
C(11)	C(12)	1.378(16)
C(13)	C(14)	1.358(17)
C(15)	C(16)	1.497(14)
C(16)	C(18)	1.523(13)
C(19)	C(23)	1.392(14)
C(20)	C(21)	1.401(14)
C(21)	C(22)	1.439(16)
C(22)	C(23)	1.445(17)
C(23)	C(28)	1.507(19)
C(30)	C(31)	1.336(18)
C(32)	C(33)	1.379(13)
C(34)	C(35)	1.532(18)
O(1)	H(1A)	1.51(14)

atom	atom	distance
Ir(1)	O(1)	2.101(6)
Ir(1)	C(1)	2.156(9)
Ir(1)	C(3)	2.160(12)
Ir(1)	C(5)	2.171(10)
Ir(2)	O(2)	2.103(8)
Ir(2)	C(19)	2.156(10)
Ir(2)	C(21)	2.145(13)
Ir(2)	C(23)	2.180(10)
P(1)	F(2)	1.552(9)
P(1)	F(4)	1.578(12)
P(1)	F(6)	1.560(8)
P(2)	F(8)	1.499(9)
P(2)	F(10)	1.558(15)
P(2)	F(12)	1.569(11)
O(2)	C(34)	1.455(11)
N(1)	C(15)	1.335(13)
N(2)	C(33)	1.346(14)
C(1)	C(5)	1.449(15)
C(2)	C(3)	1.438(13)
C(3)	C(4)	1.444(18)
C(4)	C(5)	1.425(16)
C(5)	C(10)	1.48(2)
C(12)	C(13)	1.351(18)
C(14)	C(15)	1.381(14)
C(16)	C(17)	1.524(18)
C(19)	C(20)	1.438(17)
C(19)	C(24)	1.501(15)
C(20)	C(25)	1.501(15)
C(21)	C(26)	1.495(18)
C(22)	C(27)	1.491(14)
C(29)	C(30)	1.381(14)
C(31)	C(32)	1.403(17)
C(33)	C(34)	1.515(15)
C(34)	C(36)	1.539(14)
O(2)	H(1A)	0.97(13)

X-ray crystal structure of $[Cp^*Ir(2\text{-}(2'\text{-pyridyl})\text{-}2\text{-propanolate})]_2H_2(PF_6)_2$ (6)



A. Crystal Data

Empirical Formula	$Ir_2C_{36}H_{52}N_2O_2P_2F_{12} \cdot 2(CH_3C_6H_5)$	
Formula Weight	1403.47	
Crystal Color, Habit	orange, prism	
Crystal Dimensions	0.04 X 0.02 X 0.02 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 18.5780(3) Å	α = 90 °
	b = 13.3039(2) Å	β = 110.182(8) °
	c = 22.7037(16) Å	γ = 90 °
	V = 5266.9(5) Å^3	
Space Group	$P2_1/c$ (#14)	
Z value	4	
D_{calc}	1.770 g/cm^3	
F_{000}	2760.00	
μ(CuKα)	107.210 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku Saturn944+ CCD
Radiation	CuKα (λ = 1.54187 Å)
Detector Aperture	94 mm x 94 mm
Data Images	893 exposures (2°)
Exposure Rate	2.0 sec./ °
Detector Swing Angles	42°, 90°
Detector Position	50.00 mm
$2\theta_{max}$	130.2°

No. of Reflections Measured	Total: 58608 Unique: 8823 (R_{int} = 0.0878)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.613 - 0.807)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.\ 0543 \cdot P)^2\ + 37.0008 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	130.2°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	8823
No. Variables	717
Reflection/Parameter Ratio	12.31
Residuals: R1 (I>2.00σ(I))	0.0523
Residuals: R (All reflections)	0.0625
Residuals: wR2 (All reflections)	0.1320
Goodness of Fit Indicator	1.086
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.95 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.72 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a Hampton Research loop with immersion oil. All measurements were made on a Rigaku Saturn944+ CCD diffractometer with filtered Cu-Kα radiation at a temperature of -180°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. Disorder in the cocrystalized toluene molecule was modeled with appropriate similarity restraints placed on the C-C bond distances and thermal parameters. H2A was located in the difference density map and refined in x, y, and z without restraint but with a thermal parameter fixed to ride on its parent oxygen atom. H1A was placed at an idealized location and allowed to refine in x, y and z with Ir-H distance restraints and a riding thermal parameter. The remaining hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 8823 observed reflections and 717 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0524$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 – Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.1320$$

The standard deviation of an observation of unit weight[d] was 1.09. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.95 and -1.72 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}^{j}	occ
Ir(1)	0.69219(2)	0.14329(2)	0.418194(15)	2.435(10)	
Ir(2)	0.78021(2)	0.23120(3)	0.319418(15)	2.692(10)	
P(1)	0.39719(15)	0.25980(17)	0.52176(11)	3.45(4)	
P(2)	0.98153(14)	-0.16557(19)	0.36788(11)	3.57(4)	
F(1)	0.4456(8)	0.1942(7)	0.4962(5)	12.8(4)	
F(2)	0.4583(5)	0.3416(6)	0.5510(4)	9.8(3)	
F(3)	0.4253(4)	0.1976(4)	0.5850(2)	4.88(12)	
F(4)	0.3409(6)	0.3219(7)	0.5452(6)	10.9(3)	
F(5)	0.3283(5)	0.1819(6)	0.4953(4)	9.4(3)	
F(6)	0.3698(5)	0.3236(5)	0.4596(3)	7.5(2)	
F(7)	0.9976(3)	-0.0948(4)	0.4279(2)	4.84(12)	
F(8)	0.9040(3)	-0.1069(4)	0.3322(2)	4.31(11)	
F(9)	0.9360(3)	-0.2415(4)	0.3971(3)	4.84(12)	
F(10)	1.0589(3)	-0.2253(4)	0.4014(3)	4.32(11)	
F(11)	1.0272(3)	-0.0888(4)	0.3394(2)	4.31(11)	
F(12)	0.9646(3)	-0.2366(4)	0.3075(3)	4.45(11)	
O(1)	0.6135(3)	0.2463(4)	0.3602(3)	2.65(10)	
O(2)	0.6642(3)	0.2728(4)	0.2778(3)	2.85(10)	
N(1)	0.7176(4)	0.2795(5)	0.4697(3)	2.53(12)	
N(2)	0.7320(4)	0.1127(5)	0.2567(3)	2.86(12)	
C(1)	0.7787(5)	0.2892(6)	0.5229(4)	2.89(15)	
C(2)	0.7923(5)	0.3766(7)	0.5574(4)	3.42(17)	
C(3)	0.7414(6)	0.4561(7)	0.5359(4)	3.62(18)	
C(4)	0.6800(5)	0.4457(6)	0.4818(4)	3.43(17)	
C(5)	0.6695(5)	0.3559(6)	0.4486(4)	2.91(15)	
C(6)	0.5987(5)	0.3358(6)	0.3903(4)	2.96(15)	
C(7)	0.5834(5)	0.4235(6)	0.3440(4)	3.49(17)	
C(8)	0.5314(5)	0.3168(8)	0.4117(5)	3.85(18)	
C(9)	0.6096(5)	0.0287(6)	0.4247(4)	2.93(15)	
C(10)	0.6638(5)	0.0500(6)	0.4857(4)	2.80(15)	
C(11)	0.7399(5)	0.0255(6)	0.4868(4)	2.76(15)	
C(12)	0.7329(5)	-0.0134(5)	0.4261(4)	2.73(15)	
C(13)	0.6523(5)	-0.0077(5)	0.3866(4)	2.70(14)	
C(14)	0.5262(5)	0.0403(6)	0.4044(5)	3.56(17)	
C(15)	0.6445(7)	0.0856(7)	0.5413(4)	4.4(2)	
C(16)	0.8118(5)	0.0236(7)	0.5429(4)	3.87(18)	
C(17)	0.7963(5)	-0.0549(7)	0.4083(4)	3.69(18)	
C(18)	0.6181(6)	-0.0458(6)	0.3214(4)	3.66(19)	
C(19)	0.7714(5)	0.0289(6)	0.2539(4)	3.29(16)	
C(20)	0.7421(6)	-0.0433(7)	0.2092(4)	3.80(18)	
C(21)	0.6704(6)	-0.0299(7)	0.1657(4)	3.78(18)	
C(22)	0.6288(6)	0.0557(7)	0.1677(4)	3.70(18)	
C(23)	0.6614(5)	0.1259(6)	0.2147(4)	2.86(15)	
C(24)	0.6220(5)	0.2241(6)	0.2192(4)	2.82(15)	
C(25)	0.6250(6)	0.2931(7)	0.1655(4)	4.19(20)	
C(26)	0.5409(5)	0.2075(7)	0.2162(4)	3.53(17)	
C(27)	0.8701(5)	0.2723(8)	0.2811(4)	3.79(19)	
C(28)	0.8337(6)	0.3628(7)	0.2924(5)	3.77(18)	
C(29)	0.8437(5)	0.3679(7)	0.3577(4)	3.44(17)	
C(30)	0.8878(5)	0.2841(7)	0.3882(4)	3.28(17)	
C(31)	0.9037(6)	0.2217(7)	0.3419(5)	3.99(19)	
C(32)	0.8718(7)	0.2369(10)	0.2199(5)	6.2(3)	
C(33)	0.7941(7)	0.4402(8)	0.2453(5)	6.2(3)	
C(34)	0.8172(6)	0.4526(7)	0.3878(5)	4.7(2)	
C(35)	0.9181(6)	0.2606(9)	0.4567(4)	4.9(2)	
C(36)	0.9551(6)	0.1326(8)	0.3541(7)	6.0(3)	
C(37)	0.9091(6)	-0.3750(8)	0.5720(5)	4.24(20)	
C(38)	0.9144(9)	-0.3626(9)	0.6345(6)	6.3(3)	
C(39)	0.9583(11)	-0.4327(14)	0.6798(6)	8.3(5)	

atom	x	y	z	B_{eq}[j]	occ
C(40)	0.9899(8)	-0.5121(12)	0.6613(8)	7.5(4)	
C(41)	0.9850(7)	-0.5231(9)	0.6012(8)	6.1(3)	
C(42)	0.9446(6)	-0.4550(8)	0.5588(5)	4.8(2)	
C(43)	0.8626(8)	-0.3033(12)	0.5226(8)	8.6(5)	
C(44)	0.7330(9)	0.6838(13)	0.2089(9)	4.7(2)	0.645(11)
C(44a)	0.7081(17)	0.688(3)	0.2784(13)	4.9(3)	0.355(11)
C(45)	0.778(4)	0.701(5)	0.275(2)	4.8(3)	0.645(11)
C(45a)	0.778(8)	0.695(10)	0.275(4)	4.8(3)	0.355(11)
C(46)	0.7376(9)	0.6976(12)	0.3151(9)	4.7(2)	0.645(11)
C(46a)	0.7981(17)	0.696(2)	0.2223(13)	4.8(3)	0.355(11)
C(47)	0.6608(9)	0.6786(13)	0.2969(9)	4.9(2)	0.645(11)
C(47a)	0.7373(19)	0.680(3)	0.1683(16)	4.9(3)	0.355(11)
C(48)	0.6228(11)	0.6623(16)	0.2356(9)	5.5(3)	0.645(11)
C(48a)	0.664(2)	0.678(3)	0.1676(16)	5.0(3)	0.355(11)
C(49)	0.6564(9)	0.6644(17)	0.1906(10)	5.1(3)	0.645(11)
C(49a)	0.6487(19)	0.684(3)	0.2224(13)	5.2(3)	0.355(11)
C(50a)	0.6940(17)	0.686(2)	0.3404(13)	4.3(4)	0.355(11)
C(50)	0.7717(12)	0.6821(17)	0.1600(9)	5.6(3)	0.645(11)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}	occ
H(1)	0.8132	0.2343	0.5369	3.47	
H(1a)	0.755(2)	0.167(4)	0.377(3)	3.410	
H(2)	0.8353	0.3824	0.5950	4.10	
H(2a)	0.640(5)	0.268(6)	0.321(4)	3.420	
H(3)	0.7493	0.5173	0.5588	4.34	
H(4)	0.6448	0.4995	0.4668	4.11	
H(7A)	0.5384	0.4083	0.3070	4.18	
H(7B)	0.6281	0.4337	0.3312	4.18	
H(7C)	0.5737	0.4847	0.3642	4.18	
H(8A)	0.5423	0.2584	0.4397	4.62	
H(8B)	0.4854	0.3039	0.3751	4.62	
H(8C)	0.5230	0.3760	0.4342	4.62	
H(14A)	0.5132	0.0865	0.4329	4.27	
H(14B)	0.5025	-0.025	0.4051	4.27	
H(14C)	0.5070	0.0676	0.3617	4.27	
H(15A)	0.6423	0.0278	0.5675	5.22	
H(15B)	0.5946	0.1195	0.5268	5.22	
H(15C)	0.6840	0.1326	0.5660	5.22	
H(16A)	0.8554	0.0427	0.5304	4.65	
H(16B)	0.8199	-0.044	0.5608	4.65	
H(16C)	0.8072	0.0712	0.5744	4.65	
H(17A)	0.8100	-0.122	0.4270	4.43	
H(17B)	0.8409	-0.01	0.4236	4.43	
H(17C)	0.7800	-0.06	0.3625	4.43	
H(18A)	0.5736	-0.005	0.2984	4.40	
H(18B)	0.6020	-0.116	0.3222	4.40	
H(18C)	0.6563	-0.042	0.3005	4.40	
H(19)	0.8212	0.0197	0.2841	3.94	
H(20)	0.7710	-0.102	0.2084	4.56	
H(21)	0.6492	-0.079	0.1341	4.53	
H(22)	0.5791	0.0661	0.1377	4.44	
H(25A)	0.6784	0.3009	0.1678	5.03	
H(25B)	0.6038	0.3591	0.1695	5.03	
H(25C)	0.5949	0.2631	0.1250	5.03	
H(26A)	0.5182	0.2719	0.2217	4.24	
H(26B)	0.5405	0.1612	0.2497	4.24	
H(26C)	0.5109	0.1787	0.1754	4.24	
H(32A)	0.8606	0.1648	0.2156	7.49	
H(32B)	0.9227	0.2493	0.2175	7.49	
H(32C)	0.8331	0.2733	0.1860	7.49	
H(33A)	0.8273	0.4993	0.2506	7.43	
H(33B)	0.7462	0.4597	0.2511	7.43	
H(33C)	0.7828	0.4128	0.2030	7.43	
H(34A)	0.8543	0.5077	0.3961	5.59	
H(34B)	0.8127	0.4297	0.4274	5.59	
H(34C)	0.7671	0.4760	0.3597	5.59	
H(35A)	0.8937	0.3047	0.4788	5.85	
H(35B)	0.9737	0.2713	0.4730	5.85	
H(35C)	0.9069	0.1903	0.4632	5.85	
H(36A)	0.9489	0.0930	0.3884	7.21	
H(36B)	1.0084	0.1550	0.3658	7.21	
H(36C)	0.9418	0.0912	0.3161	7.21	
H(38)	0.8892	-0.308	0.6465	7.53	
H(39)	0.9654	-0.424	0.7229	10.00	
H(40)	1.0163	-0.561	0.6913	9.03	
H(41)	1.0095	-0.578	0.5889	7.35	
H(42)	0.9411	-0.464	0.5164	5.73	
H(43A)	0.8082	-0.321	0.5100	10.36	
H(43B)	0.8791	-0.307	0.4860	10.36	
H(43C)	0.8700	-0.235	0.5394	10.36	
H(45A)	0.8192	0.7008	0.3137	5.71	0.355
H(46)	0.7647	0.7091	0.3584	5.62	0.645
H(46A)	0.8491	0.7057	0.2232	5.81	0.355
H(47)	0.6351	0.6771	0.3265	5.86	0.645
H(47A)	0.7466	0.6716	0.1300	5.86	0.355
H(48)	0.5695	0.6483	0.2228	6.57	0.645
H(48A)	0.6226	0.6713	0.1288	6.05	0.355
H(49)	0.6271	0.6526	0.1478	6.07	0.645
H(49A)	0.5972	0.6849	0.2215	6.26	0.355
H(50A)	0.8264	0.6973	0.1801	6.76	0.645
H(50B)	0.7480	0.7325	0.1277	6.76	0.645
H(50C)	0.7659	0.6153	0.1407	6.76	0.645
H(50D)	0.6388	0.6834	0.3324	5.14	0.355
H(50E)	0.7153	0.7476	0.3640	5.14	0.355
H(50F)	0.7190	0.6274	0.3648	5.14	0.355
H(45)	0.8313	0.7143	0.2891	5.80	0.645

Table 3. Anisotropic displacement parameters[j]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.0334(2)	0.02980(19)	0.02729(19)	0.00087(14)	0.00780(15)	-0.00084(13)
Ir(2)	0.0387(2)	0.0333(2)	0.0282(2)	-0.00033(14)	0.00899(16)	0.00189(14)
P(1)	0.0593(16)	0.0350(11)	0.0350(12)	0.0019(11)	0.0143(11)	0.0039(9)
P(2)	0.0422(14)	0.0514(14)	0.0390(12)	0.0077(11)	0.0101(11)	0.0044(10)
F(1)	0.289(14)	0.118(7)	0.173(9)	0.116(8)	0.198(10)	0.072(7)
F(2)	0.118(7)	0.099(6)	0.093(5)	-0.062(5)	-0.043(5)	0.054(5)
F(3)	0.086(4)	0.048(3)	0.043(3)	-0.016(3)	0.010(3)	0.009(2)
F(4)	0.162(9)	0.089(6)	0.219(11)	0.056(6)	0.136(9)	0.058(7)
F(5)	0.119(7)	0.091(5)	0.092(5)	-0.045(5)	-0.034(5)	0.042(4)
F(6)	0.149(7)	0.065(4)	0.045(4)	-0.011(4)	-0.000(4)	0.023(3)
F(7)	0.069(4)	0.071(4)	0.041(3)	0.014(3)	0.016(3)	-0.003(3)
F(8)	0.043(3)	0.062(3)	0.053(3)	0.016(3)	0.011(3)	0.010(3)
F(9)	0.055(4)	0.070(4)	0.061(4)	0.006(3)	0.023(3)	0.012(3)
F(10)	0.042(3)	0.064(4)	0.051(3)	0.018(3)	0.008(3)	0.010(3)
F(11)	0.051(3)	0.062(3)	0.049(3)	-0.001(3)	0.016(3)	0.004(3)
F(12)	0.050(3)	0.067(4)	0.052(3)	0.002(3)	0.017(3)	-0.011(3)
O(1)	0.038(3)	0.029(3)	0.037(3)	-0.001(2)	0.017(3)	-0.002(2)
O(2)	0.038(3)	0.042(3)	0.029(3)	0.003(2)	0.012(3)	0.005(2)
N(1)	0.039(4)	0.027(3)	0.031(4)	-0.001(3)	0.013(3)	-0.000(3)
N(2)	0.045(4)	0.037(4)	0.030(4)	-0.001(3)	0.016(3)	-0.001(3)
C(1)	0.036(5)	0.040(5)	0.031(4)	-0.002(4)	0.008(4)	-0.005(4)
C(2)	0.042(5)	0.049(5)	0.040(5)	-0.008(4)	0.016(4)	-0.005(4)
C(3)	0.059(6)	0.039(5)	0.046(5)	-0.013(4)	0.027(5)	-0.011(4)
C(4)	0.049(6)	0.033(4)	0.048(5)	-0.003(4)	0.017(4)	-0.002(4)
C(5)	0.050(6)	0.031(4)	0.038(5)	-0.004(4)	0.024(4)	0.002(3)
C(6)	0.036(5)	0.036(4)	0.036(5)	0.006(4)	0.008(4)	-0.006(4)
C(7)	0.052(6)	0.036(5)	0.044(5)	0.012(4)	0.015(4)	0.009(4)
C(8)	0.037(5)	0.058(6)	0.051(6)	-0.013(4)	0.015(4)	-0.015(5)
C(9)	0.041(5)	0.024(4)	0.044(5)	-0.005(3)	0.013(4)	-0.001(3)
C(10)	0.046(5)	0.028(4)	0.033(4)	0.000(4)	0.014(4)	0.004(3)
C(11)	0.043(5)	0.035(4)	0.026(4)	0.004(4)	0.011(4)	0.010(3)
C(12)	0.045(5)	0.020(4)	0.042(5)	0.011(3)	0.019(4)	0.006(3)
C(13)	0.050(5)	0.020(4)	0.032(4)	-0.007(3)	0.014(4)	-0.005(3)
C(14)	0.032(5)	0.034(5)	0.061(6)	-0.008(4)	0.005(4)	-0.003(4)
C(15)	0.094(8)	0.049(6)	0.040(5)	0.004(5)	0.045(5)	0.006(4)
C(16)	0.046(6)	0.051(5)	0.037(5)	0.004(4)	-0.003(4)	0.014(4)
C(17)	0.050(6)	0.041(5)	0.056(6)	0.020(4)	0.026(5)	0.008(4)
C(18)	0.071(7)	0.031(4)	0.028(4)	-0.019(4)	0.005(4)	-0.006(3)
C(19)	0.045(5)	0.044(5)	0.038(5)	0.004(4)	0.015(4)	0.003(4)
C(20)	0.068(7)	0.041(5)	0.039(5)	-0.004(5)	0.022(5)	-0.012(4)
C(21)	0.061(6)	0.054(6)	0.028(4)	-0.016(5)	0.014(4)	-0.016(4)
C(22)	0.047(6)	0.057(6)	0.031(5)	-0.010(5)	0.006(4)	-0.005(4)
C(23)	0.030(5)	0.046(5)	0.034(4)	0.001(4)	0.012(4)	0.008(4)
C(24)	0.040(5)	0.042(5)	0.024(4)	0.001(4)	0.009(4)	0.009(3)
C(25)	0.064(7)	0.051(6)	0.042(5)	-0.000(5)	0.016(5)	0.013(4)
C(26)	0.038(5)	0.056(6)	0.035(5)	0.004(4)	0.006(4)	0.000(4)
C(27)	0.040(5)	0.070(7)	0.041(5)	-0.024(5)	0.022(4)	-0.008(4)
C(28)	0.057(6)	0.036(5)	0.052(6)	-0.017(4)	0.022(5)	0.007(4)
C(29)	0.035(5)	0.042(5)	0.049(5)	-0.009(4)	0.008(4)	-0.003(4)
C(30)	0.031(5)	0.053(5)	0.033(5)	-0.010(4)	0.001(4)	0.003(4)
C(31)	0.039(6)	0.053(6)	0.067(7)	-0.004(4)	0.027(5)	-0.001(5)
C(32)	0.086(9)	0.114(10)	0.068(7)	-0.051(8)	0.066(7)	-0.028(7)
C(33)	0.096(9)	0.047(6)	0.068(7)	-0.029(6)	-0.002(7)	0.024(5)
C(34)	0.059(7)	0.038(5)	0.081(7)	-0.012(5)	0.025(6)	-0.022(5)
C(35)	0.039(6)	0.093(8)	0.039(5)	-0.025(5)	-0.005(4)	0.007(5)
C(36)	0.037(6)	0.052(6)	0.140(12)	0.009(5)	0.031(7)	-0.004(7)
C(37)	0.046(6)	0.054(6)	0.063(7)	0.004(5)	0.021(5)	0.012(5)
C(38)	0.122(12)	0.057(7)	0.086(9)	-0.014(7)	0.069(9)	-0.024(7)
C(39)	0.155(16)	0.119(13)	0.044(7)	-0.089(12)	0.035(9)	-0.023(8)
C(40)	0.075(9)	0.083(10)	0.090(11)	-0.047(8)	-0.020(8)	0.029(9)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(41)	0.054(7)	0.049(7)	0.120(12)	-0.004(5)	0.018(7)	-0.001(7)
C(42)	0.058(7)	0.062(7)	0.062(7)	-0.021(6)	0.022(6)	-0.018(6)
C(43)	0.068(9)	0.109(11)	0.152(15)	0.022(8)	0.039(9)	0.076(11)
C(44)	0.051(5)	0.055(6)	0.065(6)	-0.003(5)	0.009(5)	0.000(6)
C(44a)	0.051(6)	0.059(7)	0.067(6)	-0.006(6)	0.008(5)	-0.007(7)
C(45)	0.050(5)	0.055(7)	0.068(6)	-0.005(6)	0.006(4)	0.001(6)
C(45a)	0.051(6)	0.055(8)	0.066(6)	-0.004(7)	0.008(5)	-0.000(7)
C(46)	0.055(6)	0.051(6)	0.062(6)	-0.001(6)	0.007(5)	-0.008(6)
C(46a)	0.052(7)	0.055(8)	0.068(7)	-0.003(7)	0.010(6)	0.004(7)
C(47)	0.055(6)	0.060(6)	0.064(6)	-0.009(6)	0.012(5)	-0.013(6)
C(47a)	0.053(8)	0.057(8)	0.067(7)	-0.001(9)	0.009(7)	0.003(9)
C(48)	0.054(6)	0.080(7)	0.067(7)	-0.012(6)	0.012(5)	-0.014(7)
C(48a)	0.052(7)	0.063(8)	0.067(7)	-0.006(7)	0.008(7)	0.001(8)
C(49)	0.049(6)	0.072(7)	0.064(7)	-0.001(6)	0.010(5)	-0.008(7)
C(49a)	0.054(7)	0.067(7)	0.068(7)	-0.010(7)	0.009(6)	-0.007(8)
C(50a)	0.042(12)	0.045(11)	0.067(9)	-0.005(10)	0.007(8)	0.000(11)
C(50)	0.060(10)	0.073(10)	0.079(8)	-0.007(10)	0.020(8)	0.005(8)
C(46a)	0.052(7)	0.055(8)	0.068(7)	-0.003(7)	0.010(6)	0.004(7)
C(47)	0.055(6)	0.060(6)	0.064(6)	-0.009(6)	0.012(5)	-0.013(6)
C(47a)	0.053(8)	0.057(8)	0.067(7)	-0.001(9)	0.009(7)	0.003(9)
C(48)	0.054(6)	0.080(7)	0.067(7)	-0.012(6)	0.012(5)	-0.014(7)
C(48a)	0.052(7)	0.063(8)	0.067(7)	-0.006(7)	0.008(7)	0.001(8)
C(49)	0.049(6)	0.072(7)	0.064(7)	-0.001(6)	0.010(5)	-0.008(7)
C(49a)	0.054(7)	0.067(7)	0.068(7)	-0.010(7)	0.009(6)	-0.007(8)
C(50a)	0.042(12)	0.045(11)	0.067(9)	-0.005(10)	0.007(8)	0.000(11)
C(50)	0.060(10)	0.073(10)	0.079(8)	-0.007(10)	0.020(8)	0.005(8)

Table 4. Bond lengths (Å)

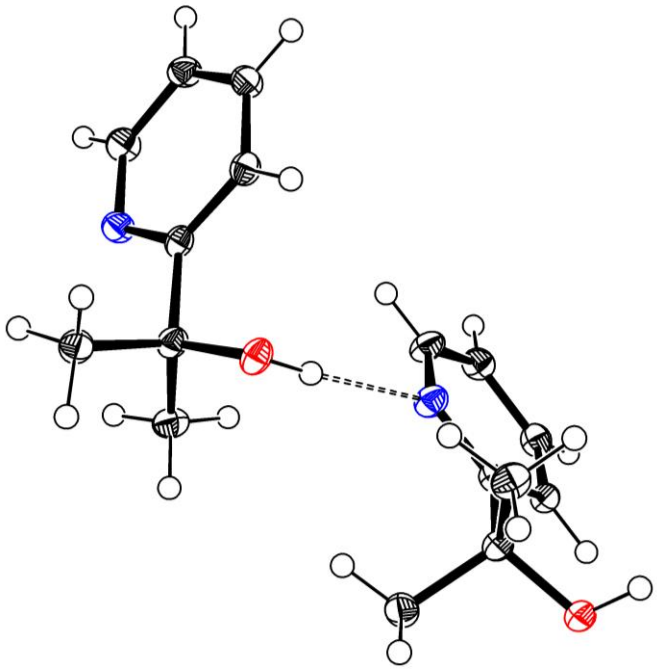
atom	atom	distance
Ir(1)	O(1)	2.103(5)
Ir(1)	C(9)	2.204(9)
Ir(1)	C(11)	2.171(7)
Ir(1)	C(13)	2.175(7)
Ir(2)	N(2)	2.105(6)
Ir(2)	C(28)	2.203(10)
Ir(2)	C(30)	2.185(8)
P(1)	F(1)	1.506(14)
P(1)	F(3)	1.581(6)
P(1)	F(5)	1.594(9)
P(2)	F(7)	1.597(6)
P(2)	F(9)	1.600(7)
P(2)	F(11)	1.599(7)
O(1)	C(6)	1.446(10)
N(1)	C(1)	1.349(9)
N(2)	C(19)	1.347(12)
C(1)	C(2)	1.376(12)
C(3)	C(4)	1.366(11)
C(5)	C(6)	1.534(10)
C(6)	C(8)	1.510(15)
C(9)	C(13)	1.446(14)
C(10)	C(11)	1.443(13)
C(11)	C(12)	1.435(12)
C(12)	C(13)	1.458(11)

atom	atom	distance
Ir(1)	N(1)	2.120(6)
Ir(1)	C(10)	2.173(9)
Ir(1)	C(12)	2.203(7)
Ir(2)	O(2)	2.107(6)
Ir(2)	C(27)	2.202(11)
Ir(2)	C(29)	2.178(8)
Ir(2)	C(31)	2.175(10)
P(1)	F(2)	1.547(8)
P(1)	F(4)	1.562(13)
P(1)	F(6)	1.574(7)
P(2)	F(8)	1.593(5)
P(2)	F(10)	1.588(6)
P(2)	F(12)	1.605(6)
O(2)	C(24)	1.444(9)
N(1)	C(5)	1.328(10)
N(2)	C(23)	1.341(10)
C(2)	C(3)	1.390(13)
C(4)	C(5)	1.389(12)
C(6)	C(7)	1.530(12)
C(9)	C(10)	1.431(10)
C(9)	C(14)	1.465(12)
C(10)	C(15)	1.504(15)
C(11)	C(16)	1.494(10)
C(12)	C(17)	1.478(15)

atom	atom	distance
C(13)	C(18)	1.485(11)
C(20)	C(21)	1.370(12)
C(22)	C(23)	1.390(12)
C(24)	C(25)	1.543(13)
C(27)	C(28)	1.446(14)
C(27)	C(32)	1.477(17)
C(28)	C(33)	1.483(14)
C(29)	C(34)	1.487(15)
C(30)	C(35)	1.492(13)
C(37)	C(38)	1.399(19)
C(37)	C(43)	1.499(18)
C(39)	C(40)	1.34(3)
C(41)	C(42)	1.347(16)
C(44)	C(49)	1.36(2)
C(44a)	C(45a)	1.33(15)
C(44a)	C(50a)	1.52(5)
C(45a)	C(46a)	1.37(13)
C(46a)	C(47a)	1.37(4)
C(47a)	C(48a)	1.36(6)
C(48a)	C(49a)	1.37(5)
O(2)	H(2a)	1.21(11)

atom	atom	distance
C(19)	C(20)	1.367(12)
C(21)	C(22)	1.385(14)
C(23)	C(24)	1.519(12)
C(24)	C(26)	1.501(14)
C(27)	C(31)	1.467(13)
C(28)	C(29)	1.431(14)
C(29)	C(30)	1.415(12)
C(30)	C(31)	1.448(15)
C(31)	C(36)	1.487(14)
C(37)	C(42)	1.340(16)
C(38)	C(39)	1.418(20)
C(40)	C(41)	1.34(3)
C(44)	C(45)	1.46(5)
C(44)	C(50)	1.52(3)
C(44a)	C(49a)	1.37(4)
C(45)	C(46)	1.36(8)
C(46)	C(47)	1.36(2)
C(47)	C(48)	1.34(3)
C(48)	C(49)	1.37(3)
O(1)	H(2a)	1.19(11)

X-ray crystal structure of 2-(2'-pyridyl)-2-propanol



One molecule in the asymmetric unit, two shown

A. Crystal Data

Empirical Formula	$C_8H_{11}ON$	
Formula Weight	137.18	
Crystal Color, Habit	colorless, prism	
Crystal Dimensions	0.17 X 0.14 X 0.12 mm	
Crystal System	monoclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 8.14463(15) Å	α = 90 °
	b = 10.9211(2) Å	β = 107.018(8) °
	c = 8.7179(6) Å	γ = 90 °
	V = 741.48(6) Å^3	
Space Group	$P2_1/n$ (#14)	
Z value	4	
D_{calc}	1.229 g/cm^3	
F_{000}	296.00	
μ(CuKα)	6.502 cm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku Saturn944+ CCD
Radiation	CuKα (λ = 1.54187 Å)
Detector Aperture	94 mm x 94 mm
Data Images	1447 exposures (1°)
Exposure Rate (42°)	2.0 sec./ °
Exposure Rate (90°)	4.0 sec./ °
Detector Swing Angles	42°, 90°
Detector Position	50.00 mm

$2\theta_{max}$	130.1°
No. of Reflections Measured	Total: 6512 Unique: 1244 (R_{int} = 0.0222)
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.848 - 0.925)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2\ (Fo^2) + (0.0379 \cdot P)^2\ + 0.2245 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	130.1°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	1244
No. Variables	97
Reflection/Parameter Ratio	12.82
Residuals: R1 (I>2.00σ(I))	0.0314
Residuals: R (All reflections)	0.0336
Residuals: wR2 (All reflections)	0.0799
Goodness of Fit Indicator	1.069
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.21 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.15 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a Hampton Research loop with immersion oil. All measurements were made on a Rigaku Saturn944+ CCD diffractometer with filtered Cu-Kα radiation at a temperature of -180°C. The structure was solved by direct methods[k] and expanded using Fourier techniques.[b] The non-hydrogen atoms were refined anisotropically. H1A was located in the difference map and refined freely without restraint. The remaining hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[c] on F^2 was based on 1244 observed reflections and 97 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ ||Fo| - |Fc||\ /\ \Sigma\ |Fo| = 0.0314$$

$$wR2 = [\ \Sigma\ (\ w\ (Fo^2 - Fc^2)^2)/\ \Sigma\ w(Fo^2)^2]^{1/2} = 0.0799$$

The standard deviation of an observation of unit weight[d] was 1.07. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.21 and -0.15 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[e] Anomalous dispersion effects were included in Fcalc[f]; the values for Δf' and Δf'' were those of Creagh and McAuley.[g] The values for the mass attenuation coefficients are those of Creagh and Hubbell.[h] All calculations were performed using the CrystalStructure[i] crystallographic software package except for refinement, which was performed using SHELXL-97.[k]

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}[j]
O(1)	0.75148(9)	0.14997(7)	0.29498(9)	1.582(18)
N(1)	0.30191(11)	0.21940(9)	0.09167(11)	1.628(20)
C(1)	0.14808(14)	0.18819(11)	0.10645(14)	1.80(2)
C(2)	0.12318(14)	0.10122(11)	0.21195(13)	1.71(2)
C(3)	0.26660(14)	0.04139(11)	0.30727(13)	1.66(2)
C(4)	0.42721(13)	0.07337(10)	0.29556(13)	1.48(2)
C(5)	0.44132(13)	0.16344(10)	0.18782(12)	1.33(2)
C(6)	0.61551(13)	0.20162(10)	0.16855(12)	1.43(2)
C(7)	0.63492(14)	0.14680(11)	0.01369(13)	1.71(2)
C(8)	0.63164(14)	0.34087(10)	0.16753(14)	1.80(2)

Table 2. Atomic coordinates and B_{iso} of hydrogen atoms

atom	x	y	z	B_{iso}
H(1A)	0.7696(18)	0.1924(14)	0.3847(20)	2.8(3)
H(1)	0.0498	0.2287	0.0398	2.16
H(2)	0.0116	0.0830	0.2190	2.05
H(3)	0.2552	-0.0207	0.3797	1.99
H(4)	0.5272	0.0338	0.3610	1.78
H(7A)	0.5359	0.1700	-0.0764	2.05
H(7B)	0.6410	0.0574	0.0230	2.05
H(7C)	0.7403	0.1779	-0.0049	2.05
H(8A)	0.6164	0.3744	0.2667	2.15
H(8B)	0.5433	0.3744	0.0752	2.15
H(8C)	0.7456	0.3632	0.1600	2.15

Table 3. Anisotropic displacement parameters[j]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.0156(4)	0.0232(5)	0.0193(4)	0.0022(3)	0.0019(3)	-0.0029(3)
N(1)	0.0168(5)	0.0231(5)	0.0217(5)	0.0006(4)	0.0052(4)	0.0032(4)
C(1)	0.0153(5)	0.0265(7)	0.0254(6)	0.0033(5)	0.0042(5)	0.0042(5)
C(2)	0.0180(5)	0.0244(6)	0.0240(6)	-0.0025(4)	0.0083(5)	-0.0016(5)
C(3)	0.0242(6)	0.0204(6)	0.0197(5)	-0.0017(5)	0.0083(5)	0.0010(5)
C(4)	0.0182(5)	0.0189(6)	0.0178(5)	0.0019(4)	0.0031(4)	-0.0004(4)
C(5)	0.0174(5)	0.0170(6)	0.0156(5)	0.0006(4)	0.0041(4)	-0.0036(4)
C(6)	0.0143(5)	0.0205(6)	0.0183(5)	0.0003(4)	0.0029(4)	-0.0006(4)
C(7)	0.0171(5)	0.0276(7)	0.0210(6)	-0.0014(4)	0.0068(4)	-0.0021(5)
C(8)	0.0183(6)	0.0221(6)	0.0271(6)	-0.0023(4)	0.0055(5)	0.0007(5)

Table 4. Bond lengths (Å)

atom	atom	distance
O(1)	C(6)	1.4300(11)
N(1)	C(5)	1.3447(13)
C(2)	C(3)	1.3834(15)
C(4)	C(5)	1.3879(16)
C(6)	C(7)	1.5268(16)
O(1)	H(1A)	0.883(17)

atom	atom	distance
N(1)	C(1)	1.3405(16)
C(1)	C(2)	1.3778(18)
C(3)	C(4)	1.3863(17)
C(5)	C(6)	1.5344(16)
C(6)	C(8)	1.5267(15)

Coordinates, E and G in a.u. of All Calculated Extrema

1-T - DFT

(E = -934.998845968, G = -934.657047)

Ir	6.237466	6.772121	4.353548
O	6.082767	6.742601	6.268833
N	6.113275	8.803299	4.758895
C	7.126133	4.902986	3.747756
C	5.709102	4.805904	3.636181
C	5.267534	5.823076	2.678604
C	6.426205	6.493436	2.163583
C	7.570831	5.981045	2.859940
C	8.019176	4.051861	4.588751
H	8.875871	4.616601	4.962899
H	8.403181	3.215621	3.992587
H	7.488135	3.638575	5.447798
C	4.821130	3.828075	4.332659
H	5.253168	3.495393	5.278029
H	4.672221	2.945920	3.698791
H	3.839061	4.256294	4.544670
C	3.858135	6.022508	2.229558
H	3.148525	5.853583	3.042388
H	3.622682	5.310781	1.428603
H	3.694085	7.028882	1.838986
C	6.442485	7.499899	1.058198
H	5.518574	8.082331	1.018747
H	6.540809	6.986403	0.094691
H	7.286732	8.188955	1.141059
C	8.992748	6.375578	2.634555
H	9.076244	7.402819	2.273839
H	9.443811	5.718730	1.880593
H	9.584410	6.287887	3.548289
C	6.142462	9.791354	3.835354
H	6.239550	9.475297	2.804851
C	6.054533	11.125074	4.180564
H	6.081991	11.884114	3.406736
C	5.930835	11.462839	5.530927
H	5.859047	12.502517	5.835280
C	5.901203	10.450345	6.477668
H	5.806615	10.679989	7.533368
C	5.994368	9.118690	6.071138
C	5.977466	7.941455	7.014807
C	4.655671	7.890823	7.796438
H	3.804227	7.837365	7.112507
H	4.534411	8.765323	8.441960
H	4.654758	6.996023	8.423489
C	7.180293	8.001414	7.969411
H	7.174633	7.105758	8.595209
H	7.136771	8.879122	8.620454
H	8.116971	8.026734	7.405711

1-T[PF_6] – DFT – A[1]

(E = -1540.72311842, G = -1540.374583)

Ir	-0.277263	1.635510	3.535952
P	2.617277	0.122747	8.061492
F	1.798035	-0.619558	9.264422
F	1.325894	1.161831	7.838938
F	1.925483	-0.917713	6.951452
F	3.399038	0.874776	6.789726
F	3.879946	-0.900117	8.224948
F	3.284064	1.192082	9.101390
O	-1.907416	1.197372	2.566214
N	-0.058763	2.830786	1.848242
C	0.991086	3.644520	1.601419
C	1.073717	4.415060	0.457570
C	0.034686	4.346936	-0.473487
C	-1.041337	3.510039	-0.219714
C	-1.070656	2.754145	0.953683
C	-2.190404	1.809292	1.331615
C	-2.326386	0.702084	0.273017
C	-3.508254	2.588452	1.479822
C	0.171426	0.047315	4.938817
C	-0.547392	1.071094	5.607488
C	0.242425	2.294394	5.520645
C	1.466417	1.996666	4.845164
C	1.415985	0.627744	4.443361
C	-0.222418	-1.383800	4.811518
C	-1.830460	0.926065	6.350681
C	-0.101378	3.580095	6.187342
C	2.628335	2.920036	4.692344
C	2.516181	-0.138644	3.799787
H	1.765468	3.654292	2.358009
H	1.935683	5.054217	0.301206
H	0.068342	4.939427	-1.382909
H	-1.863123	3.434206	-0.923671
H	-1.387225	0.150254	0.176770
H	-2.604377	1.102197	-0.707052
H	-3.103514	0.005880	0.598167
H	-4.288316	1.892628	1.798833
H	-3.819603	3.054593	0.539753
H	-3.405026	3.365045	2.242865
H	0.112660	-1.810670	3.863033
H	-1.304172	-1.512924	4.880496
H	0.256010	-1.933609	5.628471
H	-1.595408	0.727973	7.402796
H	-2.429401	0.097911	5.967347
H	-2.433635	1.835690	6.299178
H	0.265478	3.523102	7.219191
H	-1.180072	3.750946	6.212940
H	0.373557	4.434832	5.700762
H	3.263087	2.791980	5.575013
H	2.320423	3.967783	4.633010
H	3.234223	2.677479	3.814662
H	3.149312	0.495909	3.175745
H	2.139434	-0.963842	3.191503
H	3.127820	-0.548594	4.611543

1-T[PF_6] – DFT – B

(E = -1540.70852111, G = -1540.362222)

C	-0.294621	1.326811	3.418916
C	-1.660411	1.557652	2.997088
C	-1.648111	2.272173	1.733904
C	-0.276586	2.405488	1.344962
C	0.564510	1.815338	2.387311
Ir	-0.740867	0.315524	1.518148
N	0.024070	-1.582663	1.585039
C	0.937812	-2.014188	2.490965
C	1.420380	-3.302467	2.496769
C	0.941037	-4.197368	1.532269
C	0.012546	-3.754888	0.600278
C	-0.437011	-2.436601	0.640888
C	-1.443787	-1.839634	-0.311783
C	-0.932798	-1.904483	-1.757571
C	-2.876560	1.202865	3.786016
C	-2.844103	2.777791	0.993164
C	0.232872	3.081633	0.115390
C	2.059017	1.823833	2.394004
C	0.109798	0.727861	4.728504
O	-1.644964	-0.470040	0.009884
C	-2.799268	-2.549603	-0.177173
F	1.277179	-5.766798	4.061420
P	2.874032	-6.193619	4.256539
F	3.221172	-4.586189	4.582299
F	3.113787	-5.869628	2.634418
F	2.505478	-7.744869	3.890636
F	4.459979	-6.558412	4.411435
F	2.611420	-6.454465	5.849142
H	1.259388	-1.280330	3.218626
H	2.136968	-3.634239	3.243202

[1] A, B, and C refer to different PF_6 anion locations tested: near the Cp*, pyridyl ring, and iridium atom respectively.

H	1.316923	-5.214656	1.550993
H	-0.374485	-4.425679	-0.159939
H	-3.163431	-2.484864	0.851929
H	-2.725783	-3.605267	-0.453675
H	-3.523607	-2.064803	-0.837057
H	-1.656243	-1.412836	-2.413329
H	-0.807470	-2.938937	-2.090023
H	0.027903	-1.390332	-1.848402
H	-2.704536	0.325841	4.413396
H	-3.731160	0.997468	3.138233
H	-3.145198	2.039320	4.443442
H	-3.095638	3.793917	1.318731
H	-3.716127	2.143261	1.165810
H	-2.665049	2.801029	-0.083805
H	0.492211	4.121727	0.348585
H	-0.515098	3.090666	-0.679427
H	1.131019	2.592699	-0.268760
H	2.430392	2.774699	2.794646
H	2.464835	1.703184	1.386976
H	2.467115	1.021704	3.012498
H	1.165694	0.450522	4.742599
H	-0.475106	-0.163113	4.971667
H	-0.043187	1.456458	5.533057

1-T[PF_6] – DFT – C

(E = -1540.708521, G = -1540.362222)

C	-0.294621	1.326811	3.418916
C	-1.660411	1.557652	2.997088
C	-1.648111	2.272173	1.733904
C	-0.276586	2.405488	1.344962
C	0.564510	1.815338	2.387311
Ir	-0.740867	0.315524	1.518148
N	0.024070	-1.582663	1.585039
C	0.937812	-2.014188	2.490965
C	1.420380	-3.302467	2.496769
C	0.941037	-4.197368	1.532269
C	0.012546	-3.754888	0.600278
C	-0.437011	-2.436601	0.640888
C	-1.443787	-1.839634	-0.311783
C	-0.932798	-1.904483	-1.757571
C	-2.876560	1.202865	3.786016
C	-2.844103	2.777791	0.993164
C	0.232872	3.081633	0.115390
C	2.059017	1.823833	2.394004
C	0.109798	0.727861	4.728504
O	-1.644964	-0.470040	0.009884
C	-2.799268	-2.549603	-0.177173
F	1.277179	-5.766798	4.061420
P	2.874032	-6.193619	4.256539
F	3.221172	-4.586189	4.582299
F	3.113787	-5.869628	2.634418
F	2.505478	-7.744869	3.890636
F	4.459979	-6.558412	4.411435
F	2.611420	-6.454465	5.849142
H	1.259388	-1.280330	3.218626
H	2.136968	-3.634239	3.243202
H	1.316923	-5.214656	1.550993
H	-0.374485	-4.425679	-0.159939
H	-3.163431	-2.484864	0.851929
H	-2.725783	-3.605267	-0.453675
H	-3.523607	-2.064803	-0.837057
H	-1.656243	-1.412836	-2.413329
H	-0.807470	-2.938937	-2.090023
H	0.027903	-1.390332	-1.848402
H	-2.704536	0.325841	4.413396
H	-3.731160	0.997468	3.138233
H	-3.145198	2.039320	4.443442
H	-3.095638	3.793917	1.318731
H	-3.716127	2.143261	1.165810
H	-2.665049	2.801029	-0.083805
H	0.492211	4.121727	0.348585
H	-0.515098	3.090666	-0.679427
H	1.131019	2.592699	-0.268760
H	2.430392	2.774699	2.794646
H	2.464835	1.703184	1.386976
H	2.467115	1.021704	3.012498
H	1.165694	0.450522	4.742599
H	-0.475106	-0.163113	4.971667
H	-0.043187	1.456458	5.533057

1-T – DFTD

(E = -935.061768471098, G = -934.719545)

Ir	6.232331	6.764577	4.350867
O	6.050097	6.724228	6.260057
N	6.131191	8.789648	4.750060
C	7.132980	4.909867	3.743874
C	5.717490	4.799429	3.638681
C	5.264319	5.813535	2.685571
C	6.413809	6.494295	2.165667
C	7.564522	5.992037	2.855626
C	8.035753	4.078780	4.592256
H	8.877899	4.664203	4.967108
H	8.436748	3.247677	4.001311
H	7.505544	3.664628	5.450981
C	4.839468	3.825548	4.350748
H	5.280929	3.510744	5.297574
H	4.689677	2.936490	3.728103
H	3.859759	4.257199	4.565341
C	3.851108	6.012463	2.253447
H	3.154787	5.840252	3.076618
H	3.609174	5.302909	1.453327
H	3.684652	7.021448	1.871535
C	6.411378	7.508180	1.068885
H	5.493688	8.101383	1.064477
H	6.476590	7.000679	0.100229
H	7.266029	8.185377	1.137406
C	8.979764	6.408510	2.635384
H	9.044492	7.439662	2.282792
H	9.442218	5.762170	1.880268
H	9.565786	6.326501	3.552967
C	6.186776	9.777586	3.827690
H	6.294773	9.461202	2.799096
C	6.110588	11.111157	4.175306
H	6.158721	11.871524	3.403936
C	5.971402	11.448225	5.525036
H	5.908035	12.488241	5.829717
C	5.915885	10.434836	6.469680
H	5.809663	10.660544	7.524903
C	5.998145	9.104221	6.060487
C	5.956233	7.926726	7.001130
C	4.626824	7.895348	7.765709
H	3.788331	7.853172	7.065378
H	4.509232	8.772111	8.408512
H	4.605993	6.999483	8.390391
C	7.156090	7.971107	7.956812
H	7.135803	7.076176	8.582869
H	7.126122	8.852164	8.603794
H	8.089503	7.979160	7.387295

1-T[PF_6] - DFTD – A

(E = -1540.806957, G = -1540.456026)

Ir	-0.369294	1.632130	3.596657
P	2.770956	0.402158	7.898421
F	1.995621	-0.122559	9.238111
F	1.651041	1.638198	7.747144
F	1.780879	-0.566122	6.959934
F	3.499860	0.949318	6.498179
F	3.859737	-0.813230	7.985712
F	3.727372	1.394462	8.776653

O	-2.118246	1.535635	2.742600
N	0.043850	2.588627	1.816920
C	1.250875	3.090014	1.473407
C	1.465702	3.708568	0.257456
C	0.398726	3.816570	-0.639479
C	-0.838460	3.301980	-0.281739
C	-0.996860	2.686237	0.960413
C	-2.292821	2.084965	1.459249
C	-2.733065	0.952095	0.520396
C	-3.366399	3.178535	1.558858
C	0.246986	-0.018631	4.838550
C	-0.634135	0.823129	5.581437
C	-0.007145	2.119560	5.657514
C	1.265699	2.061575	4.987212
C	1.416754	0.752560	4.459512
C	0.061538	-1.466521	4.563065
C	-1.904499	0.415653	6.245960
C	-0.524937	3.296394	6.401637
C	2.269578	3.161084	4.992163
C	2.611112	0.193878	3.771112
H	2.033969	2.976677	2.212870
H	2.449144	4.097665	0.018455
H	0.536396	4.296971	-1.603456
H	-1.686704	3.369291	-0.954215
H	-1.953492	0.186946	0.470619
H	-2.944835	1.313221	-0.490681
H	-3.638697	0.497639	0.929189
H	-4.278025	2.732094	1.963051
H	-3.593059	3.623936	0.585243
H	-3.032065	3.964028	2.242240
H	0.470333	-1.747088	3.589975
H	-0.989114	-1.758231	4.600963
H	0.611641	-2.007743	5.341013
H	-1.680823	0.046184	7.252525
H	-2.408235	-0.375928	5.687544
H	-2.596615	1.256030	6.330053
H	-0.104955	3.239804	7.412043
H	-1.614525	3.292835	6.466180
H	-0.200887	4.234539	5.946083
H	2.703045	3.184793	5.995736
H	1.817555	4.130523	4.764331
H	3.085129	2.973150	4.291210
H	3.216938	0.978022	3.312473
H	2.331631	-0.525873	2.998139
H	3.221315	-0.299830	4.532872

1-T[PF_6] – DFTD - C

(E = -1540.827028, G = -1540.472213)

C	0.286199	0.758842	3.770842
C	-1.160595	0.862932	3.611056
C	-1.445826	1.498209	2.363105
C	-0.173069	1.718991	1.684547
C	0.888601	1.302602	2.598531
Ir	-0.385489	-0.315542	1.983583
N	0.851573	-1.705041	1.071755
C	2.136567	-1.924035	1.408194
C	2.883117	-2.930664	0.828961
C	2.273863	-3.751520	-0.120929
C	0.945665	-3.532035	-0.450055
C	0.243679	-2.496403	0.164967
C	-1.213021	-2.186157	-0.102857
C	-1.408013	-1.844920	-1.587870
C	-2.143488	0.337343	4.603064
C	-2.785588	1.794848	1.772795
C	0.005910	2.417849	0.377860
C	2.348532	1.458310	2.325465
C	0.970151	0.246973	4.994080
O	-1.616729	-1.062508	0.641436
C	-2.071878	-3.395563	0.305422
F	-1.093733	-2.302281	3.100695
P	-0.238522	-3.466816	4.037221
F	1.104806	-2.496807	3.942062
F	0.210122	-4.190922	2.628400
F	-1.612765	-4.341796	4.072133
F	0.571708	-4.554438	4.927912
F	-0.710363	-2.629254	5.382621
H	2.537905	-1.283378	2.180579
H	3.911508	-3.082545	1.136334
H	2.829025	-4.559662	-0.587686
H	0.436882	-4.163420	-1.169684
H	-1.888428	-3.652840	1.347628
H	-1.860939	-4.268294	-0.321506
H	-3.122900	-3.121664	0.181445
H	-2.456561	-1.577613	-1.743689
H	-1.161173	-2.684749	-2.245312
H	-0.786722	-0.986211	-1.859548
H	-1.820063	-0.636380	4.976413
H	-3.131077	0.213190	4.156172
H	-2.225420	1.029377	5.449152
H	-2.945471	2.876733	1.710851
H	-3.586344	1.363612	2.375397
H	-2.862233	1.367509	0.768845
H	0.046101	3.503637	0.526947
H	-0.824405	2.192056	-0.294486
H	0.931672	2.104958	-0.110294
H	2.644387	2.505422	2.455253
H	2.593292	1.163119	1.301359
H	2.950173	0.855936	3.009314
H	1.996881	-0.054070	4.781291
H	0.457785	-0.628266	5.393242
H	0.991046	1.031843	5.759820

2-T – DFT

(E = -1048.291205, G = -1047.943251)

C	7.404060	2.708019	10.204902
C	6.370978	1.732452	10.226657
C	6.588011	0.809394	9.110858
C	7.765546	1.240219	8.415474
C	8.331010	2.367456	9.139436
Ir	8.345245	0.629138	10.460262
C	9.758827	-0.440089	9.870137
O	10.589156	-1.076917	9.389981
C	5.203654	1.691298	11.160368
C	5.614802	-0.224616	8.641490
C	8.272654	0.691353	7.120701
C	9.503337	3.198767	8.722430
C	7.621586	3.803901	11.188088
O	9.220811	1.360608	12.133665
C	9.421481	0.477918	13.210962
C	9.278996	1.308062	14.493617
N	7.799509	-0.790129	11.931142
C	6.925648	-1.794402	11.722638
C	6.567832	-2.674074	12.728973
C	7.142522	-2.512515	13.989859
C	8.058061	-1.487667	14.189315
C	8.382211	-0.628354	13.138721
C	10.821539	-0.164112	13.148567
H	6.528158	-1.880793	10.718473
H	5.860892	-3.469939	12.522642
H	6.884368	-3.183654	14.803356
H	8.529181	-1.347263	15.155744
H	11.570183	0.632417	13.141783
H	10.950629	-0.763981	12.243433
H	11.009011	-0.812241	14.010272
H	8.270704	1.721298	14.580303
H	9.990670	2.136086	14.449056
H	9.502303	0.723149	15.390592
H	5.403150	2.248329	12.077149
H	4.943981	0.666950	11.440166
H	4.323210	2.134080	10.680429

H	6.111496	-1.060802	8.143823
H	4.919091	0.221914	7.920871
H	5.012272	-0.618203	9.463281
H	7.818201	1.250609	6.294448
H	8.013977	-0.361546	6.991701
H	9.355787	0.791876	7.027288
H	10.025387	3.607718	9.589980
H	9.170515	4.036779	8.098689
H	10.223312	2.617888	8.142688
H	6.700232	4.065223	11.711174
H	8.001620	4.699561	10.690356
H	8.363908	3.475867	11.929457

2-T – DFTD

(E = -1048.366538, G = -1048.017381)

C	7.390811	2.686770	10.225085
C	6.384502	1.684870	10.245317
C	6.606405	0.786146	9.112178
C	7.767896	1.252823	8.413617
C	8.313893	2.381718	9.146723
Ir	8.367477	0.628865	10.437522
C	9.781376	-0.430474	9.831240
O	10.610966	-1.060013	9.340277
C	5.259315	1.573985	11.221728
C	5.660765	-0.269472	8.638741
C	8.289508	0.718109	7.120394
C	9.477749	3.230611	8.748291
C	7.598777	3.764412	11.228601
O	9.256799	1.367831	12.095018
C	9.431772	0.489212	13.178630
C	9.324366	1.339898	14.447571
N	7.799044	-0.763679	11.908066
C	6.902625	-1.748108	11.704289
C	6.497426	-2.587438	12.726816
C	7.049127	-2.406469	13.995932
C	7.990843	-1.403730	14.188449
C	8.359703	-0.584066	13.122741
C	10.802485	-0.208019	13.104604
H	6.529072	-1.850651	10.693014
H	5.772849	-3.368829	12.527009
H	6.753416	-3.046910	14.821175
H	8.447917	-1.250106	15.159304
H	11.580258	0.558918	13.073186
H	10.885925	-0.821095	12.202983
H	10.975377	-0.854206	13.970534
H	8.328274	1.782833	14.527150
H	10.059552	2.145252	14.381821
H	9.535099	0.763570	15.352825
H	5.498617	2.077012	12.159994
H	5.035750	0.528908	11.450535
H	4.351779	2.027142	10.808495
H	6.188624	-1.116923	8.195277
H	4.994462	0.146450	7.874624
H	5.029750	-0.637588	9.450232
H	7.835433	1.275543	6.293756
H	8.045397	-0.337900	6.990990
H	9.372534	0.830941	7.043363
H	9.990374	3.621516	9.629562
H	9.140013	4.077397	8.140425
H	10.202921	2.661923	8.163514
H	6.673892	4.008187	11.753410
H	7.976546	4.669496	10.747523
H	8.342251	3.422368	11.962863

2-T[PF_6] – DFT

(E = -1654.028295, G = -1653.670680)

C	7.512204	2.660033	10.113006
C	6.448544	1.720812	10.263441
C	6.558518	0.737282	9.187092
C	7.714360	1.060546	8.411091
C	8.352727	2.221764	9.023017
Ir	8.380931	0.600640	10.491204
C	9.910049	-0.354310	9.967224
O	10.854029	-0.862260	9.553407
C	5.331552	1.796269	11.256382
C	5.532397	-0.290722	8.850002
C	8.126594	0.396478	7.137912
C	9.527730	2.973166	8.477517
C	7.805858	3.803669	11.023508
O	9.144621	1.353260	12.223881
C	9.288963	0.475405	13.310298
C	8.974922	1.280092	14.579215
N	7.858129	-0.881162	11.893217
C	7.102878	-1.954893	11.595867
C	6.753188	-2.883015	12.565147
C	7.204580	-2.697637	13.867553
C	8.009105	-1.599249	14.154166
C	8.336598	-0.698226	13.144270
C	10.728049	-0.075601	13.375573
P	7.526308	-3.673043	8.192145
H	6.820010	-2.092388	10.560563
H	6.160529	-3.741363	12.270717
H	6.950150	-3.408059	14.648826
H	8.397030	-1.441774	15.154672
H	11.422970	0.766360	13.441240
H	10.970467	-0.652000	12.479031
H	10.877582	-0.724637	14.244659
H	7.940081	1.632989	14.564447
H	9.637144	2.149444	14.612505
H	9.136810	0.697284	15.491329
H	5.633454	2.335439	12.156823
H	4.997647	0.800003	11.556437
H	4.467863	2.315070	10.823397
H	5.961266	-1.161074	8.354043
H	4.792454	0.159102	8.175351
H	4.995424	-0.632124	9.737761
H	7.623727	0.894370	6.299481
H	7.857324	-0.660499	7.128548
H	9.203119	0.477353	6.970940
H	10.101388	3.448392	9.276388
H	9.192900	3.754724	7.784693
H	10.203125	2.313164	7.929030
H	6.884107	4.232912	11.423408
H	8.356045	4.590825	10.503236
H	8.415955	3.442032	11.863401
F	8.127944	-2.234743	8.843181
F	8.893209	-3.822371	7.314610
F	6.835996	-2.761492	6.985732
F	6.897782	-5.035653	7.568755
F	6.142954	-3.437710	9.103971
F	8.192886	-4.482273	9.452382

2-T[PF_6] – DFTD

(E = -1654.125732, G =-1653.765513)

C	7.486130	2.653326	10.124470
C	6.443054	1.692347	10.262548
C	6.562132	0.731805	9.167124
C	7.713266	1.082380	8.399466
C	8.334354	2.242603	9.029296
Ir	8.374989	0.604749	10.464656
C	9.891509	-0.361000	9.925267
O	10.823503	-0.875815	9.493306
C	5.358764	1.691876	11.291759
C	5.545231	-0.295800	8.810915
C	8.154620	0.424439	7.133830
C	9.512651	3.004856	8.511333
C	7.767633	3.778569	11.060066
O	9.155351	1.346866	12.187713
C	9.299816	0.452608	13.259568

C	9.044786	1.257365	14.537970
N	7.817537	-0.854590	11.860698
C	7.026519	-1.900047	11.564747
C	6.664512	-2.827361	12.528805
C	7.134946	-2.663180	13.827623
C	7.967680	-1.585168	14.115422
C	8.309246	-0.688881	13.107802
C	10.716119	-0.153025	13.270767
P	7.576807	-3.602043	8.319150
H	6.726880	-2.014011	10.534710
H	6.051045	-3.669399	12.230877
H	6.873270	-3.374410	14.605586
H	8.370164	-1.443169	15.112215
H	11.444060	0.661996	13.303714
H	10.894155	-0.739749	12.365899
H	10.870948	-0.807543	14.134523
H	8.020436	1.639533	14.544176
H	9.733144	2.106309	14.554503
H	9.210999	0.665722	15.443343
H	5.663499	2.243435	12.183486
H	5.114978	0.670613	11.596114
H	4.445789	2.149514	10.894762
H	5.979240	-1.139549	8.279105
H	4.787736	0.172232	8.170176
H	5.033579	-0.679543	9.695540
H	7.685996	0.934439	6.284108
H	7.877018	-0.629649	7.113979
H	9.237622	0.491499	7.008876
H	10.075504	3.457437	9.330624
H	9.186890	3.800647	7.831551
H	10.191610	2.350198	7.961237
H	6.839990	4.192754	11.461420
H	8.318563	4.577183	10.559210
H	8.373916	3.399410	11.895100
F	8.089937	-2.095404	8.879118
F	9.021968	-3.792571	7.585792
F	6.974898	-2.821715	6.983464
F	7.040530	-5.038050	7.780104
F	6.111137	-3.331192	9.084822
F	8.145521	-4.263242	9.713254

3-T – DFT

(E = -1375.057662, G = -1374.570503)

C	6.853899	2.399376	8.824534
C	7.278397	3.657726	8.380338
C	8.654567	3.935425	8.349361
C	9.581585	2.957107	8.699739
C	9.147982	1.697980	9.117434
C	7.782780	1.426373	9.189451
C	6.298807	4.726093	8.087994
C	6.392970	6.025512	8.833422
N	5.328194	4.548554	7.245500
O	4.463440	5.602984	7.195738
Ir	4.936307	3.223782	5.565443
C	5.549051	4.164898	3.721700
C	4.837090	2.926765	3.428160
C	5.583683	1.846044	4.003956
C	6.753501	2.390467	4.668809
C	6.734548	3.820005	4.450611
C	3.617010	2.829726	2.573731
C	5.267792	0.392941	3.861124
C	7.885546	1.596550	5.237338
C	7.797648	4.780938	4.867926
C	5.145533	5.522078	3.242842
O	3.092716	4.152909	5.792605
C	2.044980	3.427164	6.411580
C	1.035777	2.997467	5.333263
N	3.899536	1.888320	6.813488
C	4.436906	0.747504	7.293203
C	3.714284	-0.150224	8.058985
C	2.383038	0.144935	8.352117
C	1.831823	1.316662	7.853358
C	2.604871	2.177529	7.070906
C	1.362262	4.337782	7.443532
H	5.481861	0.585649	7.057965
H	4.189644	-1.055190	8.421143
H	1.785155	-0.531024	8.955752
H	0.796289	1.567712	8.055016
H	2.056645	4.630914	8.235304
H	0.493498	3.857527	7.902432
H	1.013799	5.241287	6.935491
H	1.514250	2.344416	4.598921
H	0.669071	3.889750	4.818900
H	0.179520	2.467402	5.761282
H	2.925281	3.648482	2.781049
H	3.087350	1.886810	2.722599
H	3.903082	2.887607	1.516715
H	5.800374	-0.007067	2.990162
H	4.201555	0.216674	3.706951
H	5.588366	-0.185939	4.729854
H	8.613171	1.359786	4.451256
H	7.543360	0.647793	5.657426
H	8.407571	2.139131	6.027183
H	7.379921	5.745845	5.163675
H	8.473613	4.955211	4.022262
H	8.390086	4.389142	5.694886
H	5.401679	5.641380	2.183616
H	5.651314	6.312261	3.800667
H	4.068611	5.673124	3.350215
H	5.503128	6.157423	9.458762
H	6.404609	6.873301	8.141041
H	7.277274	6.046911	9.469890
H	9.000877	4.921795	8.051988
H	10.643090	3.183349	8.662940
H	9.871223	0.942279	9.408985
H	7.439698	0.463004	9.556479
H	5.791728	2.210228	8.931310
H	3.716295	5.202662	6.608437

3-T – DFTD

(E = -1375.171893, G = -1374.680200)

C	6.763338	2.391421	8.685261
C	7.246975	3.654183	8.325130
C	8.632138	3.876379	8.322690
C	9.511986	2.835815	8.611427
C	9.020061	1.569644	8.932825
C	7.643089	1.353995	8.981184
C	6.307910	4.756067	8.051847
C	6.458552	6.069718	8.755559
N	5.317660	4.579518	7.234231
O	4.467108	5.643661	7.167902
Ir	4.951667	3.236572	5.586491
C	5.553414	4.157076	3.743064
C	4.879735	2.892564	3.472935
C	5.653468	1.848317	4.079112
C	6.797313	2.440360	4.745351
C	6.735198	3.866352	4.498450
C	3.649219	2.746372	2.642936
C	5.341091	0.390408	3.999507
C	7.927205	1.698103	5.378780
C	7.736999	4.875114	4.950199
C	5.081971	5.491730	3.267825
O	3.112267	4.164346	5.768980
C	2.072228	3.440730	6.402862
C	1.070089	3.000766	5.325265
N	3.917544	1.893275	6.796859
C	4.448192	0.737479	7.246901
C	3.722738	-0.163964	8.003562
C	2.397599	0.143049	8.315695
C	1.852281	1.326848	7.838280

C	2.627537	2.190047	7.062195
C	1.405047	4.356776	7.435813
H	5.489015	0.573301	6.998098
H	4.190602	-1.080537	8.345180
H	1.798773	-0.535547	8.915167
H	0.820204	1.584313	8.048178
H	2.115429	4.642962	8.215893
H	0.537647	3.885413	7.905778
H	1.062704	5.261907	6.927201
H	1.561549	2.339467	4.607020
H	0.714981	3.888606	4.795992
H	0.209563	2.476585	5.751487
H	2.929278	3.531510	2.883223
H	3.169297	1.778841	2.801819
H	3.904941	2.827408	1.580555
H	5.677461	-0.002422	3.033915
H	4.267817	0.205944	4.085131
H	5.850183	-0.176975	4.780191
H	8.654436	1.391218	4.618374
H	7.581305	0.797891	5.891212
H	8.442846	2.310149	6.119496
H	7.254899	5.807244	5.251830
H	8.424134	5.097756	4.126630
H	8.321455	4.501178	5.790021
H	5.284837	5.608390	2.197716
H	5.580127	6.303530	3.800210
H	4.005599	5.595535	3.428134
H	5.572867	6.261089	9.370665
H	6.509733	6.889635	8.031620
H	7.341793	6.075285	9.393843
H	9.022094	4.862787	8.086449
H	10.582550	3.015687	8.593949
H	9.707813	0.763208	9.168309
H	7.253284	0.383226	9.274694
H	5.693234	2.250112	8.774257
H	3.725445	5.243589	6.577392

3-T[PF_6] – DFT

(E = -1980.790501, G = -1980.292182)

Ir	6.852821	2.463709	8.787623
P	8.336520	8.077245	7.268595
F	8.987444	9.501983	7.708806
F	7.065149	8.819300	6.540821
F	7.461464	8.020102	8.688728
F	7.651964	6.581407	6.867574
F	9.167183	8.050194	5.865004
F	9.556823	7.250502	8.021869
O	7.063293	1.383326	10.558197
O	4.723440	1.988825	10.771860
N	7.753578	3.859705	10.080737
N	4.927382	2.887094	9.760156
C	8.009804	5.140055	9.743773
C	8.599484	6.034993	10.625743
C	8.933856	5.593191	11.899724
C	8.684692	4.267895	12.239056
C	8.100917	3.410682	11.310669
C	7.894800	1.928490	11.567962
C	7.226000	1.674074	12.926600
C	9.263914	1.231298	11.517885
C	8.245781	1.425540	7.526012
C	8.049945	2.741140	6.968433
C	6.660650	2.897200	6.625749
C	5.995033	1.645243	6.955051
C	6.958718	0.740604	7.496850
C	9.557287	0.783073	7.843861
C	9.131793	3.738812	6.716623
C	6.076222	4.011425	5.822451
C	4.556464	1.342739	6.686102
C	6.727337	-0.665466	7.946705
C	2.626427	3.332777	10.317364
C	3.870918	3.600402	9.516237
C	3.831937	4.675947	8.504155
C	2.760654	4.699192	7.592713
C	2.640295	5.735194	6.671920
C	3.571785	6.774795	6.665283
C	4.623875	6.776425	7.578548
C	4.750675	5.731375	8.493247
H	7.734364	5.462013	8.746980
H	8.772212	7.044755	10.277809
H	9.390324	6.267683	12.618324
H	8.950983	3.887504	13.219316
H	6.270527	2.200010	13.000019
H	7.861463	1.987691	13.759748
H	7.042769	0.600628	13.030793
H	9.745817	1.412888	10.554808
H	9.121538	0.153629	11.642145
H	9.929421	1.590353	12.309222
H	9.454777	0.020940	8.619015
H	10.297343	1.514728	8.175019
H	9.957191	0.295129	6.945997
H	9.560378	3.545953	5.724817
H	9.941706	3.651750	7.444536
H	8.769594	4.768141	6.723358
H	6.198791	3.780679	4.755806
H	6.569670	4.962514	6.020185
H	5.009796	4.136902	6.015761
H	4.152498	0.616637	7.395044
H	4.452109	0.925080	5.677361
H	3.947824	2.247140	6.735658
H	7.137282	-1.368852	7.212355
H	5.662660	-0.879114	8.059990
H	7.209619	-0.851518	8.909796
H	2.836055	3.483869	11.381458
H	2.312850	2.288463	10.216138
H	1.819818	3.999469	10.014087
H	2.022870	3.900495	7.604820
H	1.814953	5.734196	5.965120
H	3.477994	7.587620	5.950987
H	5.360244	7.571002	7.570660
H	5.552275	5.756370	9.221272
H	5.667400	1.570921	10.851160

3-T[PF_6] – DFTD

(E= -1980.925986, G = -1980.423422)

Ir	6.828450	2.493294	8.780845
P	8.379523	7.965647	7.170284
F	9.214559	9.314508	7.528968
F	7.154009	8.822216	6.497972
F	7.591633	8.042099	8.643039
F	7.510569	6.548930	6.856074
F	9.118290	7.803945	5.723936
F	9.541244	7.018130	7.880967
O	7.084445	1.395204	10.524035
O	4.693149	1.815142	10.680647
N	7.717361	3.895876	10.049616
N	4.900969	2.790114	9.742322
C	7.998870	5.164329	9.688070
C	8.619274	6.055979	10.551078
C	8.947267	5.627170	11.831612
C	8.670419	4.313457	12.194419
C	8.067448	3.455342	11.280695
C	7.867825	1.975387	11.550016
C	7.156362	1.736066	12.886590
C	9.247468	1.301989	11.535303
C	8.224891	1.489469	7.518947
C	8.004528	2.802729	6.969129
C	6.609417	2.936889	6.636283
C	5.967153	1.674319	6.970455
C	6.949794	0.782509	7.498983
C	9.541718	0.881383	7.870524

C	9.073376	3.821745	6.755506
C	5.988321	4.045964	5.858378
C	4.519740	1.368320	6.765848
C	6.744464	-0.611043	7.994444
C	2.542004	3.079487	10.141234
C	3.827875	3.464699	9.469771
C	3.848944	4.608045	8.543460
C	2.839579	4.731905	7.573963
C	2.825615	5.826196	6.713568
C	3.799348	6.819311	6.830135
C	4.784836	6.722967	7.810533
C	4.809597	5.618940	8.658619
H	7.715319	5.471646	8.690397
H	8.818825	7.054369	10.187809
H	9.424240	6.302443	12.535810
H	8.937861	3.939515	13.176665
H	6.189290	2.245423	12.903743
H	7.751040	2.081442	13.736809
H	6.988340	0.661728	13.004307
H	9.739262	1.497388	10.580036
H	9.115714	0.222197	11.648665
H	9.890957	1.669723	12.340438
H	9.434030	0.141442	8.666163
H	10.255393	1.640810	8.196634
H	9.966301	0.378803	6.993249
H	9.622233	3.569985	5.840366
H	9.788831	3.824420	7.581286
H	8.679887	4.831051	6.648959
H	6.104101	3.835911	4.787711
H	6.455493	5.004527	6.070728
H	4.923216	4.137658	6.070339
H	4.144715	0.687736	7.533182
H	4.372399	0.901254	5.785731
H	3.924007	2.281627	6.798848
H	7.191402	-1.331339	7.300505
H	5.682802	-0.843819	8.095024
H	7.209543	-0.733448	8.976720
H	2.662848	3.141955	11.227488
H	2.291065	2.036426	9.921002
H	1.728398	3.735691	9.833439
H	2.076525	3.962661	7.484314
H	2.053073	5.903252	5.953651
H	3.793891	7.673699	6.160121
H	5.545663	7.486582	7.898817
H	5.558913	5.548856	9.437228
H	5.655532	1.455881	10.785795

4-T – DFT

(E = -1164.027930, G = -1163.630012)

C	-0.435678	1.517160	12.548545
C	-0.773229	2.622706	11.655533
C	-0.020085	3.770243	12.072250
C	0.810776	3.387817	13.202635
C	0.504692	2.002616	13.510142
Ir	1.346590	2.182188	11.513647
N	2.636004	3.146023	10.158651
C	3.416525	4.179848	10.527170
C	4.323685	4.768577	9.661813
C	4.435614	4.261457	8.369369
C	3.641888	3.182491	7.998364
C	2.746153	2.631996	8.913426
C	1.810200	1.478238	8.581910
C	0.565339	2.032506	7.885437
C	-1.844197	2.576921	10.615826
C	-0.101338	5.137783	11.477651
C	1.656678	4.293706	14.039976
C	1.113607	1.228267	14.630345
C	-1.046233	0.154197	12.492799
O	1.390730	0.872925	9.818981
O	3.151652	1.261365	12.126861
C	3.600923	0.130211	11.719873
C	4.801058	-0.414614	12.444522
C	2.478872	0.400459	7.726708
O	3.092159	-0.543241	10.786075
H	3.305826	4.517542	11.550756
H	4.932150	5.598872	10.002594
H	5.137138	4.694486	7.662985
H	3.717034	2.761713	7.002248
H	1.783271	-0.434251	7.607759
H	3.393381	0.025213	8.192069
H	2.717280	0.776259	6.728569
H	0.075389	2.780359	8.513394
H	-0.136815	1.217315	7.692136
H	0.828929	2.500293	6.932724
H	-2.823888	2.661340	11.101381
H	-1.829634	1.635934	10.062120
H	-1.760986	3.398189	9.901664
H	-0.849426	5.729838	12.017724
H	-0.394224	5.105850	10.426506
H	0.850353	5.669339	11.548105
H	1.979185	5.178179	13.485040
H	2.547243	3.780178	14.409935
H	1.089290	4.647674	14.908829
H	1.020815	0.152056	14.476667
H	0.602064	1.480774	15.566476
H	2.172814	1.466649	14.747409
H	-2.026062	0.160525	12.984475
H	-0.424224	-0.588623	12.995558
H	-1.188868	-0.173422	11.460885
H	5.439631	-0.961438	11.748987
H	4.457178	-1.124058	13.204901
H	5.358668	0.380798	12.939481
H	2.134112	0.151670	10.186276

4-T – DFTD

(E = -1164.114390321929, G = -1163.714139)

C	-0.439677	1.501965	12.563940
C	-0.790088	2.581960	11.645843
C	-0.047204	3.746643	12.028936
C	0.784574	3.400007	13.171807
C	0.493805	2.021536	13.513865
Ir	1.323850	2.166902	11.520813
N	2.632202	3.127247	10.203142
C	3.432217	4.133656	10.600676
C	4.372440	4.703293	9.757935
C	4.497693	4.202063	8.463950
C	3.680990	3.149528	8.065054
C	2.751252	2.621288	8.956391
C	1.769791	1.516436	8.598954
C	0.535022	2.157439	7.967548
C	-1.831467	2.469780	10.583064
C	-0.099538	5.086981	11.374774
C	1.640599	4.322982	13.976526
C	1.150664	1.280482	14.628736
C	-1.019176	0.126549	12.516367
O	1.348100	0.875566	9.819064
O	3.109065	1.246448	12.150817
C	3.600729	0.149808	11.695971
C	4.798838	-0.386048	12.428761
C	2.377032	0.447281	7.694556
O	3.132899	-0.493322	10.722992
H	3.308930	4.461138	11.626006
H	4.996894	5.513570	10.117078
H	5.226684	4.620300	7.776914
H	3.763145	2.735262	7.067110
H	1.651007	-0.360484	7.574702
H	3.289753	0.033026	8.129544
H	2.600746	0.844930	6.701767
H	0.112943	2.902861	8.645812
H	-0.215276	1.387311	7.772969

H	0.793469	2.648774	7.025869
H	-2.821402	2.418150	11.049607
H	-1.690519	1.563461	9.990131
H	-1.824272	3.327410	9.908879
H	-0.805825	5.735199	11.904588
H	-0.418496	5.011217	10.333538
H	0.878572	5.573791	11.390742
H	1.937813	5.203382	13.401743
H	2.544379	3.815649	14.322514
H	1.093746	4.678195	14.857075
H	0.948993	0.210068	14.575354
H	0.776189	1.654080	15.587643
H	2.233768	1.424940	14.599371
H	-2.009042	0.116257	12.985700
H	-0.386363	-0.593386	13.037881
H	-1.127343	-0.211365	11.483494
H	5.409404	-0.991548	11.758196
H	4.446075	-1.029377	13.241955
H	5.383468	0.424712	12.865309
H	2.107955	0.177104	10.154184

4-T[PF_6] – DFT

(E = -1769.757851, G = -1769.350475)

Ir	-0.336688	1.536646	12.771955
P	-1.785677	4.514007	8.803316
F	-1.640530	4.773738	7.202230
F	-0.781453	3.192592	8.689616
F	-0.476038	5.454363	9.129570
F	-1.937555	4.208373	10.461588
F	-2.786253	5.791090	8.977407
F	-3.082485	3.509094	8.560280
O	1.063969	0.009954	12.382753
O	0.761653	2.711266	11.391835
O	2.411621	1.308143	10.820733
N	-1.085264	0.570853	11.057090
C	-1.985921	1.135081	10.234684
C	-2.442017	0.487031	9.094373
C	-1.950500	-0.778658	8.804864
C	-0.992858	-1.343991	9.645458
C	-0.558527	-0.641329	10.763189
C	0.503620	-1.131326	11.737719
C	1.639301	-1.874730	11.025728
C	-0.147058	-2.046749	12.782074
C	-0.516677	1.286547	14.906483
C	-1.825818	1.247256	14.302950
C	-2.050488	2.536858	13.656373
C	-0.883616	3.340752	13.858748
C	0.087040	2.564968	14.613490
C	0.127981	0.210740	15.717715
C	-2.866990	0.186453	14.471608
C	-3.324341	2.981101	13.013646
C	-0.694114	4.733181	13.356765
C	1.412675	3.044975	15.114257
C	1.780153	2.426875	10.712865
C	2.300462	3.450721	9.756455
H	-2.296896	2.144522	10.468517
H	-3.129696	1.015769	8.445999
H	-2.283222	-1.313439	7.919907
H	-0.569068	-2.317405	9.424653
H	2.424425	-2.090728	11.755497
H	2.067881	-1.271869	10.221293
H	1.298697	-2.826073	10.607002
H	-0.944374	-1.515214	13.306364
H	0.606657	-2.362883	13.509010
H	-0.578203	-2.936630	12.312693
H	0.103933	0.486302	16.778597
H	1.171367	0.069542	15.425656
H	-0.384304	-0.746017	15.605886
H	-3.588797	0.491907	15.238894
H	-2.435152	-0.765206	14.787944
H	-3.422227	0.015197	13.545956
H	-3.880273	2.136863	12.597894
H	-3.141143	3.695534	12.209325
H	-3.965720	3.459551	13.764344
H	0.362926	5.001346	13.318005
H	-1.196966	5.434936	14.033392
H	-1.107782	4.852302	12.353058
H	1.307304	3.516088	16.099296
H	1.849254	3.783127	14.437956
H	2.122325	2.219620	15.209581
H	2.944652	2.984091	9.010701
H	2.886976	4.187263	10.316371
H	1.456867	3.966161	9.293940
H	1.877022	0.676331	11.535444

4-T[PF_6] – DFTD

(E = -1769.867533, G = -1769.456358)

Ir	-0.358097	1.566899	12.761888
P	-1.610073	4.435663	8.964666
F	-1.491300	4.685687	7.359113
F	-0.711428	3.037211	8.815441
F	-0.224858	5.275072	9.250924
F	-1.730970	4.135776	10.620094
F	-2.508329	5.783670	9.168625
F	-2.987584	3.531491	8.756497
O	1.042382	0.045331	12.372697
O	0.743556	2.763418	11.418474
O	2.347099	1.333708	10.775328
N	-1.130542	0.613588	11.068209
C	-2.074222	1.164249	10.289630
C	-2.529166	0.536988	9.138302
C	-1.991825	-0.695893	8.794160
C	-1.004546	-1.257358	9.603676
C	-0.578307	-0.576550	10.736077
C	0.476408	-1.080782	11.708108
C	1.611079	-1.824365	11.000272
C	-0.201371	-1.990122	12.738805
C	-0.574161	1.208688	14.863764
C	-1.872993	1.264821	14.246429
C	-2.029909	2.593974	13.664302
C	-0.829664	3.331376	13.925217
C	0.092491	2.474857	14.645448
C	0.042404	0.056461	15.586872
C	-2.953068	0.232642	14.280326
C	-3.279079	3.118952	13.037704
C	-0.560424	4.724571	13.465958
C	1.448501	2.840555	15.156095
C	1.741827	2.470886	10.713144
C	2.251271	3.490048	9.752483
H	-2.419427	2.148201	10.569081
H	-3.246499	1.060946	8.519465
H	-2.316845	-1.210269	7.894577
H	-0.555906	-2.211218	9.350693
H	2.393426	-2.036304	11.733640
H	2.038025	-1.216869	10.198606
H	1.271989	-2.775686	10.580735
H	-0.995715	-1.442702	13.250045
H	0.536786	-2.313706	13.477614
H	-0.639286	-2.871060	12.259922
H	0.238094	0.333924	16.627862
H	0.989480	-0.221459	15.115680
H	-0.606315	-0.820203	15.580955
H	-3.761719	0.558399	14.944061
H	-2.587847	-0.729469	14.643977
H	-3.377109	0.080367	13.284097
H	-3.847180	2.316044	12.561057
H	-3.059758	3.871770	12.281044
H	-3.917071	3.564293	13.810315
H	0.504958	4.954615	13.509601
H	-1.093771	5.431641	14.111261

H	-0.893104	4.859966	12.435263
H	1.388414	3.250957	16.170925
H	1.920054	3.588160	14.515074
H	2.100402	1.963941	15.178007
H	3.199526	3.175692	9.317704
H	2.347122	4.451258	10.260548
H	1.485166	3.627220	8.985717
H	1.833079	0.706898	11.504732

5-T – DFT

(E = -1885.608499, G = -1884.891008)

Ir	11.941612	3.427604	4.759574
Ir	10.459246	1.380731	8.465275
Cl	10.196352	2.847712	6.476644
O	13.164439	2.059275	5.780737
O	12.559131	1.537178	8.105621
N	11.504730	1.574254	3.865348
N	11.044508	3.127836	9.476955
C	12.236331	5.522103	5.273767
C	13.345574	5.074502	4.481104
C	12.841457	4.616368	3.202594
C	11.403325	4.848740	3.192860
C	11.035581	5.398241	4.457020
C	12.301673	6.173882	6.616939
H	11.412533	5.953197	7.211064
H	12.367252	7.262520	6.502487
H	13.177383	5.848574	7.181719
C	14.783196	5.118251	4.875509
H	14.909445	5.091309	5.958635
H	15.224074	6.054599	4.512414
H	15.350914	4.292497	4.444618
C	13.650508	4.244063	2.002043
H	14.674690	3.971141	2.261177
H	13.705639	5.104295	1.323871
H	13.203086	3.416591	1.445968
C	10.512188	4.677396	2.006305
H	10.832008	3.851582	1.367055
H	10.543865	5.589167	1.397759
H	9.469859	4.517411	2.291855
C	9.671602	5.853937	4.855352
H	8.887188	5.312864	4.322759
H	9.565130	6.918816	4.615120
H	9.500159	5.732201	5.926000
C	10.434864	1.360952	3.075540
H	9.750129	2.193432	2.968592
C	10.216447	0.152060	2.435042
H	9.345988	0.027342	1.800196
C	11.137983	-0.876761	2.623909
H	11.008889	-1.833621	2.127080
C	12.226469	-0.660388	3.462087
H	12.955464	-1.446045	3.626482
C	12.390990	0.577541	4.083844
C	13.562139	0.941618	4.986017
C	14.762709	1.317427	4.105278
H	14.505808	2.135736	3.430872
H	15.088905	0.467992	3.497823
H	15.596815	1.627202	4.740794
C	13.955881	-0.217907	5.904050
H	14.769882	0.102334	6.559042
H	14.323745	-1.071904	5.329593
H	13.120266	-0.542415	6.525580
C	9.274004	-0.269880	7.667104
C	8.417674	0.666705	8.393081
C	8.849454	0.687813	9.758775
C	10.000702	-0.184065	9.889855
C	10.224268	-0.798095	8.592344
C	9.092196	-0.669936	6.240965
H	8.742685	0.168707	5.636594
H	8.346081	-1.470597	6.173053
H	10.022190	-1.037378	5.803382
C	7.223181	1.360500	7.826305
H	6.954965	2.248538	8.402338
H	6.362481	0.681329	7.843225
H	7.390502	1.667693	6.792332
C	8.183486	1.394311	10.892087
H	8.900368	1.754774	11.632992
H	7.516485	0.687548	11.400628
H	7.567909	2.231861	10.558783
C	10.622152	-0.608502	11.180996
H	11.608828	-1.051748	11.035059
H	9.990195	-1.370989	11.653175
H	10.714045	0.220477	11.886418
C	11.243732	-1.851851	8.319722
H	11.414320	-1.986882	7.251112
H	10.882444	-2.806925	8.719799
H	12.198900	-1.632245	8.801610
C	10.156566	4.033534	9.932315
H	9.117055	3.836971	9.700969
C	10.540768	5.154848	10.648995
H	9.789112	5.851967	11.002845
C	11.897279	5.351151	10.900122
H	12.237241	6.209876	11.470911
C	12.813061	4.432590	10.399171
H	13.874519	4.569484	10.572588
C	12.366259	3.327485	9.675870
C	13.296699	2.263845	9.110610
C	14.546151	2.874045	8.477241
H	15.151171	2.082370	8.030362
H	15.162098	3.366844	9.232980
H	14.290086	3.593553	7.698010
C	13.690111	1.282201	10.217388
H	12.805166	0.813140	10.649868
H	14.232962	1.793374	11.017387
H	14.336873	0.504058	9.803168
H	12.820429	1.795459	7.076733

5-T – DFTD

(E = -1885.801580, G = -1885.076943)

Ir	11.881761	3.453970	4.853911
Ir	10.544213	1.353524	8.385935
Cl	10.139052	2.817516	6.458116
O	13.119672	2.005719	5.723700
O	12.591915	1.515519	8.003397
N	11.328447	1.679889	3.887841
N	11.091276	3.127675	9.353205
C	12.241126	5.479031	5.513888
C	13.352471	5.050411	4.713052
C	12.864001	4.691430	3.399716
C	11.436081	4.969834	3.375795
C	11.054939	5.448765	4.666459
C	12.263318	5.961253	6.927086
H	11.426050	5.542235	7.490743
H	12.188692	7.053482	6.960329
H	13.182687	5.668403	7.434973
C	14.782859	4.954327	5.127499
H	14.927525	5.266920	6.161702
H	15.389064	5.608150	4.492201
H	15.154601	3.932510	5.019535
C	13.690543	4.336615	2.207896
H	14.696135	4.022187	2.492350
H	13.788777	5.213013	1.557093
H	13.229774	3.537477	1.621718
C	10.568741	4.862623	2.166926
H	10.850539	4.010358	1.544340
H	10.684689	5.767222	1.559504
H	9.511648	4.775687	2.426460
C	9.695884	5.898356	5.083545
H	8.911001	5.413725	4.500285
H	9.611863	6.980633	4.933359
H	9.514848	5.683729	6.138060

C	10.198803	1.562774	3.164188
H	9.575991	2.447064	3.110869
C	9.847947	0.381266	2.531965
H	8.932414	0.330750	1.953065
C	10.696488	-0.718106	2.656149
H	10.461951	-1.656402	2.163101
C	11.845764	-0.598575	3.430023
H	12.516954	-1.441143	3.550953
C	12.137725	0.612068	4.054225
C	13.370136	0.850982	4.910621
C	14.563837	1.150412	4.002218
H	14.352196	2.022733	3.382026
H	14.783150	0.304552	3.345016
H	15.444481	1.355134	4.616591
C	13.666387	-0.330133	5.830712
H	14.505825	-0.075040	6.481282
H	13.945712	-1.219560	5.261652
H	12.805521	-0.555442	6.460582
C	9.610059	-0.448684	7.648048
C	8.584430	0.450532	8.163898
C	8.844892	0.681993	9.548432
C	10.037230	-0.066126	9.916621
C	10.472530	-0.790648	8.742821
C	9.661116	-0.969349	6.249060
H	9.472224	-0.167098	5.531430
H	8.905292	-1.748324	6.101611
H	10.637480	-1.396295	6.017368
C	7.435007	0.986273	7.379542
H	7.118331	1.964677	7.745964
H	6.586194	0.298508	7.464942
H	7.688029	1.088195	6.323416
C	7.997346	1.457613	10.499920
H	8.599638	1.955984	11.262753
H	7.316095	0.770934	11.014929
H	7.384377	2.203275	9.989322
C	10.548437	-0.235184	11.309002
H	11.535291	-0.700450	11.324296
H	9.867293	-0.883993	11.871541
H	10.605848	0.720851	11.835062
C	11.640709	-1.718511	8.721515
H	11.802070	-2.146947	7.732365
H	11.460305	-2.543743	9.418105
H	12.553503	-1.204146	9.031193
C	10.195479	4.038113	9.779431
H	9.155323	3.806959	9.586141
C	10.578916	5.204751	10.420437
H	9.825124	5.909302	10.754052
C	11.938595	5.436892	10.624832
H	12.275938	6.333396	11.135697
C	12.859216	4.505565	10.156729
H	13.922337	4.666533	10.294560
C	12.413212	3.356680	9.507473
C	13.330038	2.270816	8.969649
C	14.564221	2.852557	8.284598
H	15.135929	2.040922	7.829258
H	15.217446	3.359234	8.998406
H	14.277478	3.549959	7.497451
C	13.733151	1.339076	10.114889
H	12.845170	0.904174	10.576189
H	14.293619	1.876343	10.884868
H	14.360312	0.534898	9.721089
H	12.844199	1.770360	6.842474

5-T[PF_6]$_2$ – DFT – A

(E = -3097.132488, G = -3096.394181)

C	11.792626	3.379652	5.000558
N	11.412687	2.702280	6.106697
C	10.126846	2.745875	6.507070
C	9.170159	3.489658	5.836985
C	9.554548	4.207474	4.706675
C	10.879419	4.156107	4.292078
Ir	12.862128	1.597530	7.146154
C	14.478205	1.042338	8.528357
C	13.284800	0.366584	8.932560
C	12.261133	1.360865	9.190292
C	12.864761	2.670610	9.012693
C	14.224754	2.473339	8.589401
C	13.120656	-1.101342	9.073395
C	10.912070	1.077392	9.771177
C	12.205178	3.981117	9.292943
C	15.275879	3.517938	8.409854
C	15.809559	0.419148	8.273105
C	13.263758	3.281964	4.627124
C	13.994931	4.500416	5.194618
Cl	11.924491	-0.343530	5.967736
Ir	12.569892	-1.278219	3.707450
C	10.606770	-2.183814	3.451981
C	10.609739	-0.884379	2.779241
C	11.606451	-0.919084	1.759801
C	12.259847	-2.219306	1.808027
C	11.595353	-3.005650	2.835019
C	9.630319	0.207156	3.057196
C	11.933087	0.147941	0.770187
C	13.179380	-2.771475	0.766987
C	11.857751	-4.451191	3.107336
C	9.640867	-2.592496	4.515837
O	14.088483	0.156462	3.697302
C	15.397198	-0.405334	3.720729
C	16.385341	0.644291	4.238229
N	14.131079	-2.193280	4.740444
C	13.955913	-3.260090	5.546288
C	14.996347	-3.834366	6.250389
C	16.270690	-3.287846	6.110936
C	16.447600	-2.186356	5.281465
C	15.353864	-1.633014	4.617974
O	13.802484	2.098593	5.273699
C	15.814414	-0.824378	2.304171
C	13.495326	3.169973	3.124761
F	14.040206	-4.040913	9.112885
P	15.501849	-3.956847	9.908800
F	15.083198	-5.239179	10.822844
F	14.830080	-2.914505	11.002480
F	15.899735	-2.645899	8.942664
F	16.158806	-4.958104	8.758611
F	16.952144	-3.832587	10.648711
F	9.252799	4.753159	1.640295
P	10.383781	4.104388	0.621765
F	10.101946	5.257495	-0.486331
F	11.559617	3.424568	-0.300505
F	9.257609	3.113047	-0.025998
F	10.693811	2.932541	1.800588
F	11.539574	5.067278	1.355447
H	9.512805	0.367997	4.131938
H	8.651007	-0.081955	2.655158
H	9.914940	1.149719	2.589331
H	11.500729	1.115390	1.023628
H	11.535827	-0.141964	-0.210415
H	13.014374	0.269037	0.665605
H	13.727315	-1.981558	0.250430
H	12.589082	-3.306809	0.012206
H	13.899159	-3.479930	1.184928
H	12.923142	-4.689443	3.063839
H	11.350925	-5.058731	2.347870
H	11.476125	-4.762312	4.081964
H	10.021106	-3.423411	5.114039
H	8.697087	-2.911336	4.056665
H	9.421716	-1.764426	5.192861
H	12.938896	-3.620079	5.638846
H	14.815996	-4.635253	6.955026
H	17.089628	-3.701054	6.688234
H	17.425924	-1.731567	5.171465

H	15.122757	-1.568937	1.910780
H	16.822156	-1.252032	2.297607
H	15.799536	0.051171	1.648412
H	16.330344	1.529349	3.599334
H	17.413157	0.272863	4.200191
H	16.155516	0.940713	5.262592
H	12.073702	-1.401132	9.008482
H	13.518047	-1.427372	10.041472
H	13.689902	-1.655395	8.329691
H	10.228071	1.920431	9.645557
H	11.002643	0.888019	10.847378
H	10.457111	0.192591	9.319757
H	12.667771	4.794927	8.730835
H	12.289253	4.216266	10.360607
H	11.142462	3.962753	9.039886
H	15.882922	3.329687	7.521704
H	15.945554	3.499785	9.278396
H	14.855971	4.522266	8.335771
H	15.725229	-0.638031	8.024880
H	16.413899	0.475052	9.186606
H	16.351887	0.942295	7.482150
H	9.880054	2.146524	7.375196
H	8.144259	3.485878	6.189853
H	8.841364	4.773805	4.117982
H	11.179570	4.672721	3.388680
H	14.571483	3.122350	2.937213
H	13.087062	4.026570	2.587373
H	13.027177	2.274932	2.718356
H	13.836677	4.584725	6.272315
H	13.626109	5.412870	4.718228
H	15.066901	4.412448	4.997857
H	13.878791	1.283731	4.607958

5-T[PF_6]$_2$ – DFT – B

(E = -3097.126768, G = -3096.395347)

C	12.140252	3.397471	4.619232
N	11.594747	2.807319	5.703153
C	10.270413	2.903391	5.919115
C	9.432447	3.627972	5.086090
C	9.987201	4.273456	3.983733
C	11.351793	4.149568	3.749183
Ir	12.886614	1.728590	6.990822
C	14.401322	2.186624	8.501004
C	13.981210	0.821594	8.631837
C	12.568473	0.829091	8.950302
C	12.118493	2.182669	8.964721
C	13.253568	3.037972	8.671172
C	14.866669	-0.375123	8.700434
C	11.752140	-0.370120	9.283810
C	10.777722	2.663021	9.404055
C	13.260732	4.522345	8.814516
C	15.796424	2.655774	8.281183
C	13.646260	3.223599	4.462109
C	14.348870	4.446243	5.063661
Cl	11.970886	-0.270820	5.836457
Ir	12.796585	-1.232369	3.682084
C	10.745214	-1.568754	2.989923
C	11.367300	-0.533538	2.197715
C	12.493004	-1.122341	1.524431
C	12.602956	-2.494272	1.940179
C	11.506856	-2.766868	2.852059
C	10.763771	0.795839	1.895918
C	13.340374	-0.441663	0.507627
C	13.507342	-3.532790	1.368804
C	11.117725	-4.117027	3.352544
C	9.485021	-1.422489	3.768245
O	14.461595	0.076939	3.892522
C	15.692593	-0.594913	4.118960
C	16.677338	0.362133	4.796257
N	14.149643	-2.292428	4.911786
C	13.798091	-3.375301	5.628284
C	14.702558	-4.066771	6.418914
C	16.018620	-3.613692	6.474430
C	16.370941	-2.480515	5.750302
C	15.413518	-1.823829	4.977247
O	14.036729	2.068281	5.208992
C	16.275246	-1.067903	2.777978
C	14.053866	3.040093	3.000117
F	13.570016	0.455981	11.599055
P	14.183915	1.781718	12.414500
F	13.127767	2.756194	11.551797
F	15.295279	1.961116	11.180278
F	15.225512	0.804180	13.204790
F	13.046096	1.592450	13.569588
F	14.789013	3.108593	13.148442
F	10.443730	-3.356638	0.245534
P	9.435916	-2.362080	-0.647761
F	10.014648	-3.027244	-2.022076
F	8.252022	-3.481309	-0.538306
F	8.911185	-1.671166	0.781631
F	8.469070	-1.346256	-1.484745
F	10.657668	-1.221388	-0.689713
H	10.250914	1.216612	2.763229
H	10.033780	0.643822	1.093595
H	11.509650	1.514731	1.550078
H	13.505776	0.608882	0.754814
H	12.799215	-0.496838	-0.442679
H	14.311044	-0.924469	0.387588
H	14.391239	-3.100614	0.896016
H	12.943138	-4.071572	0.598843
H	13.834150	-4.251188	2.124992
H	11.983147	-4.766646	3.506346
H	10.484256	-4.579506	2.587013
H	10.545081	-4.064201	4.282047
H	9.448428	-2.103073	4.621355
H	8.660807	-1.657358	3.086343
H	9.354776	-0.403868	4.137214
H	12.758943	-3.673857	5.556006
H	14.374729	-4.936134	6.978299
H	16.757150	-4.129548	7.080630
H	17.386038	-2.101639	5.785421
H	15.575200	-1.740856	2.279010
H	17.222776	-1.597062	2.920721
H	16.449480	-0.201846	2.133502
H	16.793017	1.252560	4.173321
H	17.666258	-0.091546	4.905670
H	16.319673	0.674978	5.778699
H	14.373751	-1.264905	8.302954
H	15.106278	-0.545381	9.755697
H	15.799288	-0.224131	8.153035
H	10.691578	-0.216074	9.074625
H	11.880814	-0.553289	10.355878
H	12.085245	-1.251380	8.732980
H	10.495700	3.600702	8.918638
H	10.841341	2.844767	10.482941
H	9.993204	1.922444	9.230259
H	14.141888	4.977479	8.358174
H	13.283901	4.746880	9.887150
H	12.367763	4.983019	8.383822
H	16.394791	1.917806	7.744559
H	16.240204	2.804223	9.271237
H	15.833456	3.597891	7.731087
H	9.894195	2.373925	6.785960
H	8.370759	3.678122	5.301310
H	9.365092	4.854285	3.309619
H	11.805447	4.629352	2.889404
H	15.131363	2.867230	2.946096
H	13.834674	3.935655	2.413104
H	13.546415	2.182945	2.554139
H	14.076198	4.559225	6.115143
H	14.068609	5.360818	4.532376

H	15.431929	4.314704	4.991486
H	14.217560	1.141442	4.599231

5-T[PF_6]$_2$ – DFT – C

(E = -3097.121417, G = -3096.384362)

C	11.819203	3.440909	4.881352
N	11.423210	2.781743	5.988525
C	10.141383	2.855203	6.389236
C	9.201561	3.618437	5.722077
C	9.606118	4.340702	4.602869
C	10.920389	4.234344	4.172951
Ir	12.879902	1.780680	7.100098
C	14.616260	1.811625	8.436697
C	13.807662	0.678788	8.736137
C	12.481835	1.164264	9.119188
C	12.512450	2.599929	9.090100
C	13.819945	3.015849	8.625743
C	14.231542	-0.752532	8.738304
C	11.362555	0.302513	9.608390
C	11.434277	3.528462	9.535321
C	14.344559	4.412567	8.642353
C	16.058579	1.807959	8.052808
C	13.288862	3.318460	4.515816
C	14.051482	4.551449	4.995716
Cl	11.902036	-0.270013	6.065459
Ir	12.482153	-1.249256	3.848327
C	10.395346	-1.802487	3.481126
C	10.757709	-0.661570	2.651791
C	11.819803	-1.085356	1.781729
C	12.155640	-2.457365	2.098446
C	11.241578	-2.899883	3.143503
C	10.024756	0.641072	2.604974
C	12.451163	-0.270253	0.703022
C	13.082642	-3.354325	1.341775
C	11.134595	-4.301203	3.653460
C	9.275126	-1.822164	4.468425
O	14.034729	0.120293	3.810189
C	15.341517	-0.479119	3.844246
C	16.351549	0.546649	4.355260
N	14.012690	-2.211418	4.891975
C	13.812738	-3.291688	5.671022
C	14.853633	-3.925980	6.325054
C	16.143346	-3.416472	6.170260
C	16.344953	-2.284635	5.390343
C	15.252391	-1.689162	4.756826
O	13.808261	2.159876	5.216372
C	15.759917	-0.941654	2.444385
C	13.495504	3.113027	3.016382
F	11.781330	5.305402	7.005189
P	11.541178	6.978813	6.981074
F	11.318180	8.587073	6.961417
F	11.735580	6.939117	5.337950
F	9.929511	6.701439	6.792886
F	11.369369	6.919629	8.619276
F	13.172629	7.160434	7.159759
F	19.137895	-1.167921	4.948859
P	19.765198	-1.778144	3.506928
F	19.001733	-0.541198	2.706978
F	20.323709	-2.372843	2.093873
F	21.090038	-0.847562	3.706818
F	20.444447	-3.005234	4.351448
F	18.372474	-2.690225	3.341043
H	9.657067	0.930704	3.591641
H	9.160420	0.566849	1.933185
H	10.660489	1.449285	2.239347
H	12.344325	0.798825	0.891394
H	11.963171	-0.494005	-0.253418
H	13.515263	-0.488385	0.603358
H	13.763950	-2.791359	0.702394
H	12.500733	-4.024189	0.696652
H	13.685476	-3.974417	2.010011
H	12.104541	-4.803751	3.664566
H	10.472546	-4.881915	2.999658
H	10.713839	-4.339371	4.661387
H	9.421735	-2.587515	5.233420
H	8.333685	-2.038877	3.948909
H	9.170669	-0.860391	4.973778
H	12.787262	-3.628712	5.759766
H	14.652822	-4.800414	6.935082
H	16.992422	-3.897065	6.647009
H	17.345306	-1.889761	5.238512
H	15.059867	-1.687861	2.062612
H	16.763786	-1.371210	2.466679
H	15.764741	-0.076773	1.774056
H	16.322357	1.424659	3.704354
H	17.366259	0.145734	4.317927
H	16.113964	0.864324	5.371943
H	13.421661	-1.406423	8.409382
H	14.519489	-1.050261	9.754047
H	15.086823	-0.923156	8.082204
H	10.401691	0.818289	9.546829
H	11.527306	0.033455	10.658798
H	11.289184	-0.621164	9.029428
H	11.389503	4.428747	8.919327
H	11.651994	3.836415	10.565793
H	10.453593	3.047104	9.542999
H	15.232774	4.515470	8.015912
H	14.640235	4.661544	9.670257
H	13.604270	5.145012	8.318176
H	16.394857	0.825153	7.719985
H	16.663118	2.092122	8.922525
H	16.264723	2.527838	7.257990
H	9.889285	2.288448	7.277027
H	8.186949	3.674374	6.099581
H	8.911492	4.992502	4.083724
H	11.266105	4.804733	3.319762
H	14.560129	2.975644	2.813716
H	13.163024	3.993667	2.461774
H	12.963386	2.231112	2.654663
H	13.946911	4.678994	6.070816
H	13.645054	5.457370	4.541194
H	15.107415	4.447935	4.729782
H	13.877016	1.286829	4.607577

5-T[PF_6]$_2$ – DFTD – A

(E = -3097.367922, G = -3096.620525)

C	11.804019	3.419308	5.009240
N	11.428575	2.716124	6.099394
C	10.141794	2.722211	6.495761
C	9.175029	3.457319	5.831669
C	9.555658	4.214148	4.724957
C	10.885158	4.206414	4.324336
Ir	12.875964	1.559709	7.065652
C	14.503770	0.918530	8.372178
C	13.306392	0.247173	8.768295
C	12.308392	1.242258	9.100137
C	12.929279	2.547367	8.962943
C	14.278517	2.348454	8.503683
C	13.117383	-1.221678	8.818346
C	10.953609	0.946001	9.657335
C	12.273890	3.854357	9.262882
C	15.339172	3.379477	8.308707
C	15.800372	0.265842	8.035012
C	13.281860	3.340341	4.665848
C	13.974538	4.522671	5.346945
Cl	11.763792	-0.258856	5.898417
Ir	12.481883	-1.180021	3.729600
C	10.535225	-2.066323	3.432201
C	10.581910	-0.802398	2.699648
C	11.631232	-0.900052	1.735497

C	12.254742	-2.206689	1.868267
C	11.538814	-2.930530	2.903948
C	9.618273	0.319621	2.919908
C	12.058483	0.130078	0.750021
C	13.224076	-2.827975	0.917519
C	11.795285	-4.353791	3.274123
C	9.542299	-2.390733	4.498018
O	14.000984	0.258215	3.704385
C	15.312008	-0.298961	3.776520
C	16.271998	0.755477	4.332646
N	14.020403	-2.063260	4.809472
C	13.828818	-3.117016	5.628311
C	14.866769	-3.712714	6.316152
C	16.151485	-3.193897	6.158651
C	16.339731	-2.096124	5.326886
C	15.249111	-1.524187	4.674455
O	13.799460	2.123464	5.247641
C	15.753675	-0.713981	2.370789
C	13.589494	3.319194	3.173648
F	14.086676	-3.993201	9.150573
P	15.577088	-3.812346	9.879184
F	15.264763	-5.090703	10.839922
F	14.895456	-2.772899	10.970787
F	15.867361	-2.507869	8.868766
F	16.234339	-4.805986	8.720251
F	17.049820	-3.595810	10.552678
F	9.212418	4.228351	1.724189
P	10.477951	3.743087	0.777731
F	9.961290	4.663256	-0.456357
F	11.783774	3.229544	-0.081994
F	9.602290	2.448544	0.250554
F	11.008365	2.797715	2.064040
F	11.387926	5.004077	1.380558
H	9.828471	0.836096	3.860876
H	8.602588	-0.086012	2.976703
H	9.657281	1.052612	2.117947
H	11.667904	1.114739	0.985138
H	11.695266	-0.147680	-0.245727
H	13.149011	0.191684	0.710758
H	13.775605	-2.074349	0.353264
H	12.675687	-3.445457	0.195748
H	13.938354	-3.474667	1.433959
H	12.866167	-4.563573	3.334330
H	11.366376	-5.009984	2.508408
H	11.338912	-4.615720	4.230538
H	9.935690	-3.124402	5.205040
H	8.631549	-2.800402	4.046291
H	9.272624	-1.494357	5.059605
H	12.803022	-3.445239	5.738913
H	14.678920	-4.506959	7.024879
H	16.964079	-3.620658	6.734042
H	17.322880	-1.654257	5.210550
H	15.064059	-1.456376	1.971868
H	16.760513	-1.142287	2.380177
H	15.741505	0.163653	1.718630
H	16.220457	1.645710	3.701820
H	17.303117	0.393091	4.322033
H	16.000366	1.038132	5.349802
H	12.071659	-1.498707	8.678303
H	13.464873	-1.600801	9.784083
H	13.723052	-1.729943	8.071361
H	10.307797	1.827144	9.636719
H	11.037955	0.619346	10.699639
H	10.466094	0.145341	9.095126
H	12.766900	4.677161	8.741620
H	12.313360	4.054858	10.339206
H	11.224614	3.849165	8.956901
H	15.833514	3.252685	7.342883
H	16.095055	3.269209	9.094235
H	14.942894	4.394279	8.360525
H	15.653441	-0.585901	7.372593
H	16.261845	-0.134395	8.941848
H	16.488247	0.970470	7.564090
H	9.906225	2.097272	7.348619
H	8.145469	3.420218	6.170999
H	8.832644	4.774231	4.143330
H	11.187006	4.755314	3.443211
H	14.675474	3.338719	3.047789
H	13.160214	4.176265	2.654984
H	13.190886	2.423632	2.702493
H	13.733601	4.546186	6.412383
H	13.642216	5.460828	4.894528
H	15.057105	4.432964	5.225902
H	13.839680	1.288927	4.534003

5-T[PF_6]$_2$ – DFTD - B

(E = -3097.126768, G = -3096.620978)

C	12.140252	3.397471	4.619232
N	11.594747	2.807319	5.703153
C	10.270413	2.903391	5.919115
C	9.432447	3.627972	5.086090
C	9.987201	4.273456	3.983733
C	11.351793	4.149568	3.749183
Ir	12.886614	1.728590	6.990822
C	14.401322	2.186624	8.501004
C	13.981210	0.821594	8.631837
C	12.568473	0.829091	8.950302
C	12.118493	2.182669	8.964721
C	13.253568	3.037972	8.671172
C	14.866669	-0.375123	8.700434
C	11.752140	-0.370120	9.283810
C	10.777722	2.663021	9.404055
C	13.260732	4.522345	8.814516
C	15.796424	2.655774	8.281183
C	13.646260	3.223599	4.462109
C	14.348870	4.446243	5.063661
Cl	11.970886	-0.270820	5.836457
Ir	12.796585	-1.232369	3.682084
C	10.745214	-1.568754	2.989923
C	11.367300	-0.533538	2.197715
C	12.493004	-1.122341	1.524431
C	12.602956	-2.494272	1.940179
C	11.506856	-2.766868	2.852059
C	10.763771	0.795839	1.895918
C	13.340374	-0.441663	0.507627
C	13.507342	-3.532790	1.368804
C	11.117725	-4.117027	3.352544
C	9.485021	-1.422489	3.768245
O	14.461595	0.076939	3.892522
C	15.692593	-0.594913	4.118960
C	16.677338	0.362133	4.796257
N	14.149643	-2.292428	4.911786
C	13.798091	-3.375301	5.628284
C	14.702558	-4.066771	6.418914
C	16.018620	-3.613692	6.474430
C	16.370941	-2.480515	5.750302
C	15.413518	-1.823829	4.977247
O	14.036729	2.068281	5.208992
C	16.275246	-1.067903	2.777978
C	14.053866	3.040093	3.000117
F	13.570016	0.455981	11.599055
P	14.183915	1.781718	12.414500
F	13.127767	2.756194	11.551797
F	15.295279	1.961116	11.180278
F	15.225512	0.804180	13.204790
F	13.046096	1.592450	13.569588
F	14.789013	3.108593	13.148442
F	10.443730	-3.356638	0.245534
P	9.435916	-2.362080	-0.647761
F	10.014648	-3.027244	-2.022076
F	8.252022	-3.481309	-0.538306

F	8.911185	-1.671166	0.781631
F	8.469070	-1.346256	-1.484745
F	10.657668	-1.221388	-0.689713
H	10.250914	1.216612	2.763229
H	10.033780	0.643822	1.093595
H	11.509650	1.514731	1.550078
H	13.505776	0.608882	0.754814
H	12.799215	-0.496838	-0.442679
H	14.311044	-0.924469	0.387588
H	14.391239	-3.100614	0.896016
H	12.943138	-4.071572	0.598843
H	13.834150	-4.251188	2.124992
H	11.983147	-4.766646	3.506346
H	10.484256	-4.579506	2.587013
H	10.545081	-4.064201	4.282047
H	9.448428	-2.103073	4.621355
H	8.660807	-1.657358	3.086343
H	9.354776	-0.403868	4.137214
H	12.758943	-3.673857	5.556006
H	14.374729	-4.936134	6.978299
H	16.757150	-4.129548	7.080630
H	17.386038	-2.101639	5.785421
H	15.575200	-1.740856	2.279010
H	17.222776	-1.597062	2.920721
H	16.449480	-0.201846	2.133502
H	16.793017	1.252560	4.173321
H	17.666258	-0.091546	4.905670
H	16.319673	0.674978	5.778699
H	14.373751	-1.264905	8.302954
H	15.106278	-0.545381	9.755697
H	15.799288	-0.224131	8.153035
H	10.691578	-0.216074	9.074625
H	11.880814	-0.553289	10.355878
H	12.085245	-1.251380	8.732980
H	10.495700	3.600702	8.918638
H	10.841341	2.844767	10.482941
H	9.993204	1.922444	9.230259
H	14.141888	4.977479	8.358174
H	13.283901	4.746880	9.887150
H	12.367763	4.983019	8.383822
H	16.394791	1.917806	7.744559
H	16.240204	2.804223	9.271237
H	15.833456	3.597891	7.731087
H	9.894195	2.373925	6.785960
H	8.370759	3.678122	5.301310
H	9.365092	4.854285	3.309619
H	11.805447	4.629352	2.889404
H	15.131363	2.867230	2.946096
H	13.834674	3.935655	2.413104
H	13.546415	2.182945	2.554139
H	14.076198	4.559225	6.115143
H	14.068609	5.360818	4.532376
H	15.431929	4.314704	4.991486
H	14.217560	1.141442	4.599231

5-T[PF_6]$_2$ – DFTD – C

(E = -3097.359030, G = -3096.613803)

C	11.804114	3.319323	4.806949
N	11.451634	2.660782	5.926441
C	10.179784	2.693995	6.358379
C	9.206342	3.429828	5.710364
C	9.565725	4.157908	4.578652
C	10.869376	4.081116	4.113713
Ir	12.971863	1.753260	7.014294
C	14.742026	1.922020	8.278274
C	14.045902	0.715176	8.575051
C	12.702862	1.082173	9.030446
C	12.604286	2.512785	9.013776
C	13.856757	3.047364	8.518610
C	14.578770	-0.675710	8.472910
C	11.667568	0.122722	9.516932
C	11.455625	3.342902	9.476041
C	14.285902	4.473614	8.562514
C	16.152742	2.074209	7.818537
C	13.270999	3.249731	4.428902
C	13.981978	4.521269	4.879923
Cl	11.944367	-0.294622	6.106732
Ir	12.449732	-1.164985	3.881210
C	10.362731	-1.630244	3.510331
C	10.751867	-0.452496	2.745072
C	11.789359	-0.856170	1.837159
C	12.090303	-2.250575	2.071178
C	11.173765	-2.728674	3.097012
C	10.091000	0.883075	2.848864
C	12.493363	-0.003373	0.833460
C	13.010016	-3.116536	1.274185
C	11.061453	-4.150044	3.540108
C	9.272035	-1.658037	4.528173
O	14.054554	0.119927	3.822239
C	15.339963	-0.517712	3.933241
C	16.325988	0.490956	4.507325
N	13.915671	-2.212318	4.914582
C	13.644762	-3.270281	5.702262
C	14.632722	-3.911838	6.427288
C	15.938889	-3.427984	6.343320
C	16.208323	-2.313874	5.559232
C	15.170082	-1.715128	4.846815
O	13.852079	2.138825	5.145330
C	15.794691	-0.994718	2.554491
C	13.464891	2.996409	2.936980
F	11.823578	5.039350	6.889751
P	11.475010	6.684821	6.866323
F	11.139347	8.273857	6.857661
F	11.536258	6.641305	5.210845
F	9.873753	6.296192	6.814165
F	11.442994	6.632753	8.519302
F	13.098655	6.977350	6.907267
F	19.003483	-1.229645	5.241175
P	19.646908	-1.863609	3.814233
F	18.909004	-0.624139	2.989426
F	20.219266	-2.477935	2.414844
F	20.978594	-0.944928	4.025992
F	20.295312	-3.090226	4.683106
F	18.245289	-2.761920	3.633285
H	9.930115	1.157375	3.893909
H	9.118888	0.874319	2.342713
H	10.699407	1.668598	2.401069
H	12.072735	1.001951	0.795878
H	12.398176	-0.448487	-0.162035
H	13.555437	0.077409	1.076744
H	13.688980	-2.521843	0.661572
H	12.427790	-3.762549	0.606618
H	13.614883	-3.755951	1.922307
H	12.039780	-4.635734	3.568352
H	10.434003	-4.707709	2.835469
H	10.603870	-4.232437	4.528657
H	9.417338	-2.464349	5.249869
H	8.306658	-1.808231	4.031580
H	9.233070	-0.718142	5.081977
H	12.606530	-3.575283	5.746747
H	14.377936	-4.767965	7.042730
H	16.747149	-3.910113	6.884512
H	17.217931	-1.928252	5.473993
H	15.070557	-1.702645	2.146596
H	16.773916	-1.469825	2.616491
H	15.865484	-0.127942	1.890913
H	16.321182	1.385021	3.878853
H	17.339191	0.089862	4.515779
H	16.022641	0.779451	5.513782
H	13.800445	-1.371658	8.152953
H	14.961956	-1.008792	9.444176

H	15.390121	-0.737733	7.745482
H	10.663773	0.543074	9.423823
H	11.840689	-0.112867	10.573148
H	11.696577	-0.808473	8.947270
H	11.333709	4.233621	8.858308
H	11.653770	3.669355	10.503656
H	10.521713	2.776691	9.485239
H	15.063098	4.679868	7.824750
H	14.711679	4.670390	9.555036
H	13.465257	5.165890	8.394294
H	16.632021	1.114225	7.625332
H	16.726473	2.591472	8.595288
H	16.202320	2.677494	6.908553
H	9.970457	2.128088	7.257619
H	8.201337	3.466896	6.113967
H	8.844003	4.795583	4.080164
H	11.183338	4.659159	3.254041
H	14.529757	2.864941	2.731293
H	13.107137	3.845344	2.349949
H	12.946849	2.088203	2.626365
H	13.905435	4.624287	5.959318
H	13.507719	5.407693	4.455337
H	15.031759	4.471398	4.577834
H	13.924149	1.225253	4.546078

5-T_{TS} - DFT

(E = -1885.608354, G = -1884.891960)

C	12.374907	3.310087	9.682866
N	11.051309	3.124364	9.483465
C	10.169662	4.028140	9.954504
C	10.563072	5.135478	10.687512
C	11.921597	5.317348	10.940146
C	12.830174	4.400250	10.423905
Ir	10.469096	1.387360	8.460798
C	10.240141	-0.790013	8.604714
C	9.300913	-0.275832	7.660448
C	8.424629	0.658519	8.365366
C	8.836887	0.700620	9.733585
C	9.995180	-0.160670	9.890777
C	9.139736	-0.691772	6.236313
C	7.234101	1.338385	7.773616
C	8.147219	1.410340	10.850974
C	10.597845	-0.565108	11.197258
C	11.268044	-1.842580	8.359929
C	13.289164	2.248453	9.088231
C	13.693417	1.249188	10.177641
Cl	10.189812	2.862915	6.464238
Ir	11.925402	3.442283	4.766062
C	11.032332	5.412183	4.463145
C	12.238526	5.535112	5.268642
C	13.339973	5.079344	4.466089
C	12.825575	4.620855	3.193700
C	11.387821	4.852796	3.197094
C	12.320732	6.192550	6.608181
C	14.779810	5.120424	4.851891
C	13.622605	4.236528	1.989018
C	10.484806	4.680606	2.019865
C	9.672067	5.871640	4.868692
O	13.163809	2.064965	5.795823
C	13.558674	0.936945	5.002783
C	13.946930	-0.220972	5.922966
N	11.501732	1.578343	3.876329
C	10.434665	1.363337	3.083158
C	10.219841	0.154670	2.440755
C	11.141513	-0.873207	2.631922
C	12.226082	-0.656344	3.475136
C	12.386468	0.581219	4.098225
O	12.544645	1.555950	8.074245
C	14.759978	1.320370	4.129600
C	14.539905	2.870600	8.464563
H	11.431556	5.988532	7.207979
H	12.402770	7.279401	6.487737
H	13.193825	5.856145	7.170441
H	14.914000	5.068984	5.933158
H	15.212040	6.068099	4.508045
H	15.350104	4.309650	4.396814
H	14.646914	3.957660	2.241312
H	13.678782	5.092551	1.305690
H	13.164877	3.409356	1.441005
H	10.799705	3.856265	1.376368
H	10.508988	5.593286	1.412278
H	9.445719	4.518974	2.316033
H	8.883059	5.320784	4.353234
H	9.562343	6.932240	4.611577
C	12.374907	3.310087	9.682866
N	11.051309	3.124364	9.483465
C	10.169662	4.028140	9.954504
C	10.563072	5.135478	10.687512
C	11.921597	5.317348	10.940146
C	12.830174	4.400250	10.423905
Ir	10.469096	1.387360	8.460798
C	10.240141	-0.790013	8.604714
C	9.300913	-0.275832	7.660448
C	8.424629	0.658519	8.365366
C	8.836887	0.700620	9.733585
C	9.995180	-0.160670	9.890777
C	9.139736	-0.691772	6.236313
C	7.234101	1.338385	7.773616
C	8.147219	1.410340	10.850974
C	10.597845	-0.565108	11.197258
C	11.268044	-1.842580	8.359929
C	13.289164	2.248453	9.088231
C	13.693417	1.249188	10.177641
Cl	10.189812	2.862915	6.464238
Ir	11.925402	3.442283	4.766062
C	11.032332	5.412183	4.463145
C	12.238526	5.535112	5.268642
C	13.339973	5.079344	4.466089
C	12.825575	4.620855	3.193700
C	11.387821	4.852796	3.197094
C	12.320732	6.192550	6.608181
C	14.779810	5.120424	4.851891
C	13.622605	4.236528	1.989018
C	10.484806	4.680606	2.019865
C	9.672067	5.871640	4.868692
O	13.163809	2.064965	5.795823
C	13.558674	0.936945	5.002783
C	13.946930	-0.220972	5.922966
N	11.501732	1.578343	3.876329
C	10.434665	1.363337	3.083158
C	10.219841	0.154670	2.440755
C	11.141513	-0.873207	2.631922
C	12.226082	-0.656344	3.475136
C	12.386468	0.581219	4.098225
O	12.544645	1.555950	8.074245
C	14.759978	1.320370	4.129600
C	14.539905	2.870600	8.464563
H	11.431556	5.988532	7.207979
H	12.402770	7.279401	6.487737
H	13.193825	5.856145	7.170441
H	14.914000	5.068984	5.933158
H	15.212040	6.068099	4.508045
H	15.350104	4.309650	4.396814
H	14.646914	3.957660	2.241312
H	13.678782	5.092551	1.305690
H	13.164877	3.409356	1.441005
H	10.799705	3.856265	1.376368
H	10.508988	5.593286	1.412278
H	9.445719	4.518974	2.316033
H	8.883059	5.320784	4.353234
H	9.562343	6.932240	4.611577

6-T – DFT

(E = -1871.134202, G = -1870.408823)

Ir	11.796909	3.212710	5.202676
Ir	10.717562	1.550197	8.049069
H	10.899668	2.515093	6.565608
O	13.408102	1.997474	5.810231
O	12.810440	1.336149	8.024900
N	11.535159	1.436276	4.102207
N	11.404816	3.169956	9.211465
C	12.187155	5.278547	5.778655
C	12.944197	4.989501	4.579233
C	12.025916	4.624629	3.537024
C	10.677704	4.709574	4.084291
C	10.787211	5.139474	5.447857
C	12.756076	5.864617	7.029989
H	12.128062	5.658196	7.897680
H	12.836073	6.953986	6.929798
H	13.757478	5.479809	7.233126
C	14.425411	5.123420	4.465288
H	14.938263	4.643548	5.301974
H	14.690233	6.187407	4.477296
H	14.810241	4.698099	3.538200
C	12.356152	4.345350	2.107677
H	13.394096	4.035397	1.976836
H	12.206791	5.254388	1.512650
H	11.714423	3.568998	1.683932
C	9.409174	4.615651	3.297098
H	9.519508	3.985234	2.412229
H	9.124351	5.613439	2.942193
H	8.577997	4.234498	3.895796
C	9.637681	5.497992	6.328544
H	8.770792	4.859113	6.148704
H	9.337393	6.532106	6.119952
H	9.905195	5.438370	7.383545
C	10.452554	1.196848	3.332388
H	9.656638	1.928328	3.394842
C	10.354017	0.090709	2.504305
H	9.464721	-0.052685	1.900045
C	11.415459	-0.812970	2.470292
H	11.379355	-1.688877	1.829874
C	12.525377	-0.568996	3.269100
H	13.368831	-1.250501	3.254590
C	12.569015	0.566913	4.079370
C	13.786408	0.947359	4.907293
C	14.878502	1.474820	3.967914
H	14.512052	2.312779	3.370971
H	15.216514	0.692921	3.282246
H	15.734492	1.810970	4.558500
C	14.318726	-0.239811	5.714516
H	15.183195	0.080027	6.301237
H	14.655580	-1.044434	5.056731
H	13.562598	-0.635354	6.395751
C	9.773624	-0.298854	7.382125
C	8.790401	0.761952	7.366692
C	8.653514	1.279938	8.695683
C	9.529126	0.505556	9.566731
C	10.198851	-0.471475	8.753556
C	10.103413	-1.228507	6.259734
H	10.006640	-0.741796	5.288403
H	9.419026	-2.085683	6.271034
H	11.119278	-1.619701	6.346368
C	7.959203	1.168042	6.196224
H	7.680851	2.222812	6.238578
H	7.032625	0.580948	6.197269
H	8.470031	0.976244	5.252481
C	7.621904	2.263204	9.149153
H	7.895298	2.741472	10.092072
H	6.671648	1.743315	9.320469
H	7.436961	3.040694	8.403736
C	9.591028	0.630995	11.053565
H	10.488005	0.168524	11.468719
H	8.724562	0.129465	11.501036
H	9.567750	1.674676	11.376673
C	11.139431	-1.533469	9.214051
H	12.042891	-1.557330	8.600261
H	10.649279	-2.510392	9.128567
H	11.435434	-1.402824	10.255044
C	10.595176	4.141838	9.682018
H	9.570500	4.115080	9.333145
C	11.032984	5.118055	10.561868
H	10.340374	5.873627	10.916793
C	12.365772	5.097088	10.971496
H	12.745809	5.841467	11.664430
C	13.199650	4.100739	10.480041
H	14.237901	4.055182	10.789603
C	12.698482	3.139127	9.600802
C	13.521717	1.962211	9.100729
C	14.900206	2.402159	8.599962
H	15.444488	1.529771	8.230438
H	15.495350	2.833871	9.408020
H	14.822141	3.132469	7.791824
C	13.676651	0.949995	10.243341
H	12.700160	0.628292	10.611865
H	14.230976	1.381802	11.081267
H	14.222667	0.075106	9.881305
H	13.171960	1.648075	6.914140

6-T – DFTD

(E = -1871.329132, G = -1870.597381)

Ir	11.788678	3.204223	5.265542
Ir	10.734915	1.557496	7.981573
H	10.815964	2.532740	6.542623
O	13.417107	2.013398	5.820443
O	12.814235	1.329473	8.006546
N	11.493085	1.455909	4.161204
N	11.381553	3.181249	9.135002
C	12.221185	5.236753	5.870140
C	12.953912	4.949834	4.653313
C	12.012626	4.616111	3.622073
C	10.675612	4.716452	4.194579
C	10.815354	5.126182	5.561192
C	12.828855	5.747633	7.133688
H	12.175582	5.573225	7.988037
H	13.007116	6.826319	7.059136
H	13.786112	5.263414	7.335418
C	14.440479	4.996504	4.550349
H	14.897935	4.360646	5.313042
H	14.784865	6.023757	4.709822
H	14.796468	4.668000	3.574023
C	12.304817	4.291081	2.195305
H	13.352698	4.029608	2.042921
H	12.079877	5.157065	1.563032
H	11.693214	3.454991	1.845071
C	9.385724	4.630048	3.445551
H	9.486827	4.049926	2.526078
H	9.058531	5.635603	3.157565
H	8.593474	4.187703	4.055657
C	9.673478	5.441901	6.468270
H	8.927323	4.643748	6.460076
H	9.188214	6.364988	6.133201
H	10.012057	5.593430	7.491916
C	10.400257	1.242466	3.400161
H	9.627580	1.997342	3.462883
C	10.266012	0.127888	2.589228
H	9.369315	0.000928	1.992665
C	11.300659	-0.807808	2.564254
H	11.233106	-1.692980	1.939668
C	12.425229	-0.582556	3.348550
H	13.251793	-1.283951	3.337190

C	12.505484	0.563377	4.139332
C	13.747067	0.943793	4.925784
C	14.799387	1.459590	3.939653
H	14.396276	2.292117	3.358417
H	15.111163	0.674035	3.246353
H	15.672816	1.807982	4.496012
C	14.288073	-0.226813	5.746824
H	15.160240	0.107892	6.312813
H	14.609305	-1.050568	5.105808
H	13.538102	-0.592525	6.451270
C	9.850341	-0.299965	7.309833
C	8.851359	0.742888	7.265831
C	8.680077	1.270494	8.587147
C	9.549197	0.517067	9.483180
C	10.252284	-0.453165	8.692384
C	10.257242	-1.204596	6.195196
H	10.126511	-0.724879	5.225842
H	9.647614	-2.115265	6.205689
H	11.303498	-1.501485	6.288320
C	8.065129	1.169641	6.072442
H	7.981831	2.257415	6.018181
H	7.053177	0.754794	6.137438
H	8.517382	0.807331	5.150447
C	7.634956	2.253884	9.001835
H	7.873574	2.723312	9.958355
H	6.675920	1.738258	9.126302
H	7.492079	3.035856	8.251463
C	9.610357	0.701527	10.962770
H	10.467619	0.189958	11.402363
H	8.703944	0.296460	11.425867
H	9.676043	1.760221	11.228957
C	11.244546	-1.463032	9.160017
H	12.179618	-1.370545	8.601363
H	10.845614	-2.469337	8.993887
H	11.469162	-1.359720	10.221398
C	10.549820	4.139768	9.590764
H	9.528919	4.085663	9.237119
C	10.969363	5.139078	10.453011
H	10.262304	5.886699	10.795389
C	12.304112	5.153784	10.858704
H	12.669936	5.919718	11.535277
C	13.157730	4.164310	10.386493
H	14.196395	4.141631	10.696239
C	12.673758	3.178799	9.526842
C	13.506548	1.994896	9.068711
C	14.882883	2.419366	8.557118
H	15.421451	1.534191	8.211473
H	15.480039	2.878444	9.347773
H	14.794764	3.118445	7.722746
C	13.630833	1.014409	10.238768
H	12.639314	0.719894	10.590116
H	14.174671	1.460727	11.075444
H	14.166053	0.122484	9.904288
H	13.180297	1.651962	6.924962

7-T – DFT

(E = -936.190594, G = -935.828243)

C	-0.846093	1.182200	3.364211
C	-2.017912	1.491745	2.646518
C	-1.644636	2.371493	1.532717
C	-0.248219	2.666509	1.635558
C	0.287770	1.845394	2.708521
Ir	-0.476115	0.572814	1.190640
N	0.228044	-1.403950	1.316269
C	1.365223	-1.709285	1.972884
C	1.850899	-3.003856	2.066687
C	1.142350	-4.030430	1.450067
C	-0.020871	-3.714282	0.756672
C	-0.457593	-2.392989	0.698405
C	-1.747348	-1.994848	-0.009341
C	-1.937780	-2.701608	-1.348130
C	-3.418805	1.080326	2.966569
C	-2.618464	2.987701	0.579350
C	0.519401	3.664513	0.828362
C	1.674316	1.940342	3.264632
C	-0.733270	0.334255	4.588758
O	-1.686884	-0.560068	-0.269904
C	-2.942553	-2.202599	0.917059
H	1.892298	-0.872964	2.415074
H	2.771717	-3.192539	2.607435
H	1.490752	-5.057153	1.500107
H	-0.590339	-4.492935	0.261802
H	-2.825705	-1.614029	1.830276
H	-3.027622	-3.256565	1.193576
H	-3.862483	-1.896364	0.412339
H	-2.820349	-2.294801	-1.849368
H	-2.105363	-3.772205	-1.211575
H	-1.065407	-2.578600	-1.999180
H	-3.450769	0.212686	3.629292
H	-3.988098	0.841680	2.064424
H	-3.944300	1.898743	3.473570
H	-3.138705	3.825184	1.059293
H	-3.375492	2.266949	0.260112
H	-2.120195	3.371705	-0.312919
H	0.513626	4.634036	1.340551
H	0.082546	3.805555	-0.162031
H	1.559329	3.360199	0.695506
H	1.748083	2.783409	3.962320
H	2.413107	2.095300	2.475161
H	1.953083	1.040572	3.819975
H	0.146263	-0.315037	4.551858
H	-1.612431	-0.296866	4.732602
H	-0.628905	0.969080	5.476622
H	0.549621	0.655906	-0.031979
H	-1.244265	-0.412363	-1.117433

H_2 – DFT

(E = -1.177517, G = -1.178853)

H	0.820511	0.148810	0.000000
H	0.077108	0.148810	0.000000

1·H_2 – DFT

(E = -936.161075, G = -935.802895)

C	-0.436087	1.267391	3.482094
C	-1.830071	1.165282	3.046935
C	-1.990492	2.037051	1.903701
C	-0.704177	2.563528	1.554347
C	0.253660	2.110954	2.559167
Ir	-0.589710	0.370546	1.470997
N	-0.469692	-1.707719	1.809784
C	0.236307	-2.275807	2.806756
C	0.269937	-3.646100	2.997209
C	-0.447703	-4.458073	2.119266
C	-1.160082	-3.866786	1.084208
C	-1.160473	-2.479122	0.940805
C	-1.849546	-1.726152	-0.185822
C	-1.007649	-1.883634	-1.468504
C	-2.940807	0.482830	3.779217
C	-3.263445	2.228342	1.152203
C	-0.422299	3.540043	0.455599
C	1.676587	2.560476	2.660858
C	0.117380	0.702029	4.749226
O	-1.965175	-0.374367	0.180978
C	-3.273354	-2.245357	-0.425259
H	0.784406	-1.597444	3.449145
H	0.851024	-4.062340	3.812574
H	-0.446525	-5.537217	2.238838
H	-1.720835	-4.473265	0.381660
H	-3.862922	-2.196073	0.493811

H	-3.283217	-3.272921	-0.800645
H	-3.749885	-1.609989	-1.175947
H	-1.477615	-1.303642	-2.267261
H	-0.941066	-2.927939	-1.788880
H	0.013086	-1.512877	-1.329943
H	-2.588327	-0.400675	4.316203
H	-3.727971	0.167514	3.091529
H	-3.386029	1.163034	4.514937
H	-3.201300	3.076143	0.468306
H	-4.089993	2.405671	1.846072
H	-3.485683	1.325482	0.569159
H	-0.578015	4.563633	0.815958
H	-1.078267	3.379479	-0.401903
H	0.609486	3.467059	0.105727
H	1.724642	3.502479	3.219899
H	2.118443	2.740265	1.678555
H	2.298451	1.831095	3.183725
H	1.191983	0.515179	4.681847
H	-0.383086	-0.225626	5.035501
H	-0.038494	1.417846	5.565247
H	0.929537	0.064176	0.714806
H	0.392066	0.237613	0.041816

1·H_2-TS – DFT

(E = -936.147723, G = -935.792074)

C	-0.445598	1.303541	3.538260
C	-1.831294	1.118384	3.117518
C	-2.034714	1.896810	1.929886
C	-0.781480	2.526875	1.570829
C	0.182642	2.185369	2.595049
Ir	-0.481929	0.380156	1.565351
N	-0.464755	-1.712392	1.822269
C	0.044930	-2.321666	2.911682
C	0.048026	-3.698075	3.055843
C	-0.487311	-4.476421	2.030789
C	-0.994771	-3.845499	0.902410
C	-0.973269	-2.453754	0.811245
C	-1.530295	-1.676352	-0.372335
C	-1.115439	-2.301195	-1.708549
C	-2.873969	0.365181	3.879289
C	-3.301378	2.038902	1.155320
C	-0.582331	3.489147	0.442818
C	1.582831	2.699997	2.679316
C	0.156006	0.817057	4.817683
O	-1.009724	-0.353255	-0.356622
C	-3.059982	-1.615141	-0.247866
H	0.466701	-1.670318	3.667206
H	0.470255	-4.144483	3.949272
H	-0.501757	-5.559261	2.107628
H	-1.408823	-4.426023	0.085751
H	-3.351273	-1.136306	0.691727
H	-3.506975	-2.613585	-0.276307
H	-3.462724	-1.029833	-1.078731
H	-1.452935	-1.645438	-2.514657
H	-1.567220	-3.285116	-1.864262
H	-0.028289	-2.397797	-1.776381
H	-2.457940	-0.515864	4.373601
H	-3.688001	0.031999	3.232649
H	-3.306062	1.006208	4.656623
H	-3.710083	3.044320	1.310169
H	-4.057977	1.319088	1.470422
H	-3.127256	1.910356	0.083966
H	-0.854456	4.503308	0.758190
H	-1.200916	3.227688	-0.418318
H	0.457703	3.511657	0.110948
H	1.590665	3.630016	3.260217
H	1.994344	2.923014	1.693190
H	2.249004	1.991459	3.175625
H	1.223773	0.608881	4.712455
H	-0.338818	-0.085714	5.183058
H	0.044632	1.581022	5.596307
H	1.020467	0.099809	0.718358
H	0.374768	-0.144745	0.085611

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Endnotes

[a] PATTY: Beurskens, P.T., Admiraal, G., Behm, H., Beurskens, G., Smits, J.M.M. and Smykalla, C. ; *Z. f. Kristallogr. Suppl. 4*, **1991** p.99.

[b] DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

[c] Least Squares function minimized: (SHELXL97) $\Sigma w(Fo^2-Fc^2)^2$ where w = Least Squares weights.

[d] Standard deviation of an observation of unit weight: $[\Sigma w(Fo^2-Fc^2)^2/(No-Nv)]^{1/2}$
where: No = number of observations, Nv = number of variables

[e] Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

[f] Ibers, J. A. & Hamilton, W. C.; *Acta Cryst*. **1964,** 17, 781.

[g] Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

[h] Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

[i] CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku Americas (2000-2007). 9009 New Trails Dr. The Woodlands TX 77381 USA.

[j] $B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

[k] "A short history of SHELX". Sheldrick, G.M. *Acta Cryst.* **2008**, A64, 112-122.