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Table 1. Crystal data and structure refinement for [Cp*IrCl(dab)](PF$_6$).

Empirical formula	$C_{28}H_{35}ClF_6IrN_2P$
Formula weight	772.20
Temperature	173 K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	Pnma
Unit cell dimensions	a = 16.187(2) Å
	b = 15.823(2) Å
	c = 11.6770(10) Å
Volume	2990.8(6) Å^3
Z	4
Density (calculated)	1.715 Mg/m^3
Absorption coefficient	4.665 mm^{-1}
F(000)	1520
Crystal size	0.4 x 0.3 x 0.3 mm
θ range for data collection	2.15 to 29.00°
Index ranges	$-14 \le h \le 22$, $-21 \le k \le 21$, $-4 \le l \le 15$
Reflections collected	5052
Independent reflections	4083 (R_{int} = 0.0389)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4081 / 0 / 185
Goodness-of-fit on F^2	1.041
Final R indices [I>2σ(I)]	R1 = 0.0588, wR2 = 0.1454
R indices (all data)	R1 = 0.0843, wR2 = 0.1644
Largest diff. peak and hole	4.152 and -5.061 e Å^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [Å^2 x 10^3] for [Cp*IrCl(dab)](PF$_6$). U(eq) is defined as one third of the trace of the orthogonalized U$_{ij}$ tensor.

	x	y	z	U(eq)
Ir	361(1)	2500	2022(1)	19(1)
Cl	-1059(2)	2500	2460(3)	35(1)
N	486(3)	1686(4)	3422(6)	23(1)
C(1)	1384(14)	2500	762(17)	29(4)
C(2)	880(10)	1770(10)	591(11)	23(3)
C(3)	64(10)	2052(10)	290(13)	32(3)
C(4)	2279(16)	2500	899(23)	54(7)
C(5)	1168(13)	860(13)	577(18)	59(6)
C(6)	-632(14)	1496(16)	-79(21)	71(7)

C(6)	-632(14)	1496(16)	-79(21)	71(7)
C(1A)	59(18)	2500	197(23)	32(6)
C(2A)	565(11)	1787(12)	480(13)	21(3)
C(3A)	1331(11)	2050(12)	845(14)	27(4)
C(4A)	-744(21)	2500	-318(32)	63(10)
C(5A)	359(16)	876(21)	272(27)	71(8)
C(6A)	2074(15)	1487(18)	1029(21)	60(7)
C(7)	-841(7)	422(7)	3160(10)	55(3)
C(8)	49(6)	196(5)	3207(7)	32(2)
C(9)	295(7)	-645(6)	3098(8)	45(2)
C(10)	1107(8)	-880(6)	3201(9)	53(3)
C(11)	1694(7)	-288(6)	3422(9)	50(2)
C(12)	1496(5)	569(5)	3529(8)	35(2)
C(13)	677(5)	792(5)	3380(7)	29(2)
C(14)	2158(5)	1205(7)	3794(9)	51(3)
C(15)	398(4)	2032(5)	4405(7)	28(2)
P	1740(2)	2500	-2628(3)	35(1)
F(1)	1673(8)	1787(5)	-1730(7)	111(3)
F(2)	1694(8)	1781(6)	-3548(9)	136(4)
F(3)	2656(8)	2500	-2679(21)	179(10)
F(4)	752(8)	2500	-2637(21)	144(7)

Table 3. Selected bond lengths [Å] and angles [°] for [Cp*IrCl(dab)](PF$_6$).

Cp-Ir	1.834(9)	Cp-Cl	2.908(25)
CpA-Ir	1.820(11)	CpA-Cl	3.083(30)
Cp-Ir-Cl	117.1	CpA-Ir-Cl	122.4
Cp-IrNC15C15#1N#1	74.66(63)	CpA-IrNC15C15#1N#1	69.38(76)
Aryl-IrNC15C15#1N#1	81.69(28)		

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Carbon atoms and Cp indicated by A belong to the eclipsed form

Table 4. Bond lengths [Å] and angles [°] for [Cp*IrCl(dab)](PF$_6$).

Ir-Cl	2.354(3)	Ir-N	2.091(7)
Ir-N#1	2.091(7)	Ir-C(1)	2.215(21)
Ir-C(2)	2.198(14)	Ir-C(3)	2.196(15)
Ir-C(2)#1	2.198(14)	Ir-C(3)#1	2.296(15)
Ir-C(1A)	2.187(27)	Ir-C(2A)	2.150(16)

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Ir-C(3A)	2.205(17)	Ir-C(2A)#1	2.150(16)
Ir-C(3A)#1	2.205(17)	N-C(13)	1.450(10)
N-C(15)	1.280(10)	C(1)-C(2)	1.43(2)
C(1)-C(2)#1	1.43(2)	C(2)-C(3)	1.44(2)
C(3)-C(3)#1	1.42(3)	C(1)-C(4)	1.46(3)
C(2)-C(5)	1.51(2)	C(3)-C(6)	1.49(3)
C(1A)-C(2A)	1.43(3)	C(1A)-C(2A)#1	1.43(3)
C(2A)-C(3A)	1.38(2)	C(3A)-C(3A)#1	1.42(4)
C(1A)-C(4A)	1.43(4)	C(2A)-C(5A)	1.50(4)
C(3A)-C(6A)	1.51(3)	C(7)-C(8)	1.485(15)
C(8)-C(9)	1.395(13)	C(8)-C(13)	1.401(12)
C(9)-C(10)	1.371(15)	C(10)-C(11)	1.359(15)
C(11)-C(12)	1.398(13)	C(12)-C(13)	1.383(11)
C(12)-C(14)	1.502(13)	C(15)-C(15)#1	1.482(15)
P-F(1)	1.544(8)	P-F(1)#1	1.544(8)
P-F(2)	1.567(9)	P-F(2)#1	1.567(9)
P-F(3)	1.483(14)	P-F(4)	1.599(14)

N-Ir-N#1	76.0(4)	N#1-Ir-C(2A)	164.3(5)
N-Ir-C(2A)	108.5(5)	N#1-Ir-C(2A)#1	108.5(5)
N-Ir-C(2A)#1	164.3(5)	C(2A)-Ir-C(2A)#1	63.3(10)
N#1-Ir-C(1A)	141.6(2)	N-Ir-C(1A)	141.6(2)
C(2A)-Ir-C(1A)	38.6(7)	C(2A)#1-Ir-C(1A)	38.6(7)
N#1-Ir-C(3)	160.1(5)	N-Ir-C(3)	122.8(5)
N#1-Ir-C(3)#1	122.8(5)	N-Ir-C(3)#1	160.1(5)
C(3)-Ir-C(3)#1	37.7(9)	N#1-Ir-C(2)	151.7(4)
N-Ir-C(2)	103.5(4)	C(3)-Ir-C(2)	38.2(6)
C(3)#1-Ir-C(2)	63.5(6)	N#1-Ir-C(2)#1	103.5(4)
N-Ir-C(2)#1	151.7(4)	C(3)-Ir-C(2)#1	63.5(6)
C(3)#1-Ir-C(2)#1	38.2(6)	C(2)-Ir-C(2)#1	63.4(8)
N#1-Ir-C(3A)#1	102.7(5)	N-Ir-C(3A)#1	128.1(5)
C(2A)-Ir-C(3A)#1	62.5(6)	C(2A)#1-Ir-C(3A)#1	36.8(6)
C(1A)-Ir-C(3A)#1	63.4(9)	N#1-Ir-C(3A)	128.1(5)
N-Ir-C(3A)	102.7(5)	C(2A)-Ir-C(3A)	36.8(6)
C(2A)#1-Ir-C(3A)	62.5(6)	C(1A)-Ir-C(3A)	63.4(9)
C(3A)#1-Ir-C(3A)	37.7(10)	N#1-Ir-C(1)	116.5(4)
N-Ir-C(1)	116.5(4)	C(3)-Ir-C(1)	63.4(7)
C(3)#1-Ir-C(1)	63.4(7)	C(2)-Ir-C(1)	37.8(5)
C(2)#1-Ir-C(1)	37.8(5)	C(15)-N-C(13)	118.1(7)
C(15)-N-Ir	115.3(5)	C(13)-N-Ir	126.6(5)
C(2)-C(1)-C(2)#1	108(2)	C(2)-C(1)-C(4)	125.7(10)
C(2)#1-C(1)-C(4)	125.7(10)	C(2)-C(1)-Ir	70.5(10)
C(2)#1-C(1)-Ir	70.5(10)	C(4)-C(1)-Ir	132(2)
C(1)-C(2)-C(3)	108.0(14)	C(1)-C(2)-C(5)	127(2)
C(3)-C(2)-C(5)	125(2)	C(1)-C(2)-Ir	71.8(10)
C(3)-C(2)-Ir	70.8(8)	C(5)-C(2)-Ir	128.8(11)

C(3)#1-C(3)-C(2)	108.1(9)	C(3)#1-C(3)-C(6)	126.1(12)
C(2)-C(3)-C(6)	126(2)	C(3)#1-C(3)-Ir	71.1(4)
C(2)-C(3)-Ir	71.0(8)	C(6)-C(3)-Ir	128.4(13)
C(4A)-C(1A)-C(2A)#1	128.0(12)	C(4A)-C(1A)-C(2A)	128.0(12)
C(2A)#1-C(1A)-C(2A)	104(2)	C(4A)-C(1A)-Ir	128(2)
C(2A)#1-C(1A)-Ir	69.3(12)	C(2A)-C(1A)-Ir	69.3(12)
C(3A)-C(2A)-C(1A)	111(2)	C(3A)-C(2A)-C(5A)	123(2)
C(1A)-C(2A)-C(5A)	126(2)	C(3A)-C(2A)-Ir	73.8(10)
C(1A)-C(2A)-Ir	72.1(12)	C(5A)-C(2A)-Ir	127(2)
C(2A)-C(3A)-C(3A)#1	107.6(11)	C(2A)-C(3A)-C(6A)	126(2)
C(3A)#1-C(3A)-C(6A)	126.1(12)	C(2A)-C(3A)-Ir	69.4(9)
C(3A)#1-C(3A)-Ir	71.2(5)	C(6A)-C(3A)-Ir	131.9(13)
C(9)-C(8)-C(13)	116.5(9)	C(9)-C(8)-C(7)	120.3(8)
C(13)-C(8)-C(7)	123.2(8)	C(10)-C(9)-C(8)	121.7(9)
C(11)-C(10)-C(9)	119.9(9)	C(10)-C(11)-C(12)	121.7(10)
C(13)-C(12)-C(11)	117.1(9)	C(13)-C(12)-C(14)	122.6(8)
C(11)-C(12)-C(14)	120.3(8)	C(12)-C(13)-C(8)	122.9(8)
C(12)-C(13)-N	116.6(7)	C(8)-C(13)-N	120.5(7)
N-C(15)-C(15)#1	115.3(4)	F(3)-P-F(1)#1	95.6(8)
F(3)-P-F(1)	95.6(8)	F(1)#1-P-F(1)	94.0(7)
F(3)-P-F(2)	91.1(8)	F(1)#1-P-F(2)	173.2(7)
F(1)-P-F(2)	86.0(6)	F(3)-P-F(2)#1	91.1(8)
F(1)#1-P-F(2)#1	86.0(6)	F(1)-P-F(2)#1	173.2(7)
F(2)-P-F(2)#1	93.1(9)	F(3)-P-F(4)	177.3(13)
F(1)#1-P-F(4)	86.3(8)	F(1)-P-F(4)	86.3(8)
F(2)-P-F(4)	87.0(8)	F(2)#1-P-F(4)	87.0(8)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

Table 5. Anisotropic displacement parameters [Å^2 x 10^3] for [Cp*IrCl(dab)](PF$_6$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Ir	19(1)	8(1)	30(1)	0	2(1)	0
Cl	21(1)	30(2)	54(2)	0	1(1)	0
N	19(3)	16(3)	36(3)	2(3)	1(2)	-3(2)
C(7)	46(5)	32(5)	88(8)	13(5)	-5(5)	-13(5)
C(8)	37(4)	15(4)	44(4)	4(3)	2(4)	-4(4)
C(9)	68(7)	12(4)	54(5)	3(4)	2(5)	-14(4)
C(10)	79(7)	18(4)	61(6)	3(4)	10(6)	10(5)
C(11)	50(5)	35(5)	65(6)	8(5)	5(5)	18(5)

C(12)	35(4)	22(4)	47(5)	6(4)	4(4)	10(4)
C(13)	34(4)	14(4)	38(4)	2(3)	0(3)	7(3)
C(14)	34(4)	41(6)	78(7)	0(5)	-9(5)	5(4)
C(15)	33(4)	14(4)	37(4)	0(3)	4(3)	-2(3)
P	40(2)	23(2)	42(2)	0	4(1)	0
F(1)	184(10)	62(5)	88(5)	38(5)	13(7)	-2(7)
F(2)	187(10)	100(7)	120(7)	-58(6)	21(8)	-41(8)
F(3)	33(5)	80(11)	423(31)	0	-12(11)	0
F(4)	49(6)	52(8)	331(23)	0	-5(11)	0

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Cp*IrCl(dab)](PF$_6$).

	x	y	z	U(eq)
H(4A)	2446(16)	3002	1298(23)	81
H(4B)	2537(16)	2486	159(23)	81
H(4C)	2444(16)	2012	1330(23)	81
H(5A)	1446(13)	746(13)	-132(18)	89
H(5B)	700(13)	492(13)	650(18)	89
H(5C)	1540(13)	766(13)	1204(18)	89
H(6A)	-500(14)	918(16)	91(21)	107
H(6B)	-718(14)	1558(16)	-888(21)	107
H(6C)	-1126(14)	1655(16)	322(21)	107
H(4AA)	-1042(21)	2007	-77(32)	95
H(4BB)	-688(21)	2495	-1137(32)	95
H(4CC)	-1039(21)	2998	-87(32)	95
H(5AA)	540(16)	716(21)	-480(27)	107
H(5BB)	-227(16)	797(21)	332(27)	107
H(5CC)	633(16)	532(21)	832(27)	107
H(6AA)	2533(15)	1823(18)	1281(21)	90
H(6BB)	2213(15)	1211(18)	323(21)	90
H(6CC)	1947(15)	1070(18)	1600(21)	90
H(7A)	-923(7)	862(7)	2606(10)	83
H(7B)	-1019(7)	615(7)	3899(10)	83
H(7C)	-1157(7)	-66(7)	2945(10)	83
H(9)	-101(7)	-1056(6)	2950(8)	54
H(10)	1256(8)	-1445(6)	3120(9)	63
H(11)	2241(7)	-456(6)	3505(9)	60
H(14A)	2690(5)	962(7)	3641(9)	76
H(14B)	2125(5)	1363(7)	4587(9)	76
H(14C)	2081(5)	1697(7)	3324(9)	76
H(15)	337(4)	1717(5)	5073(7)	34

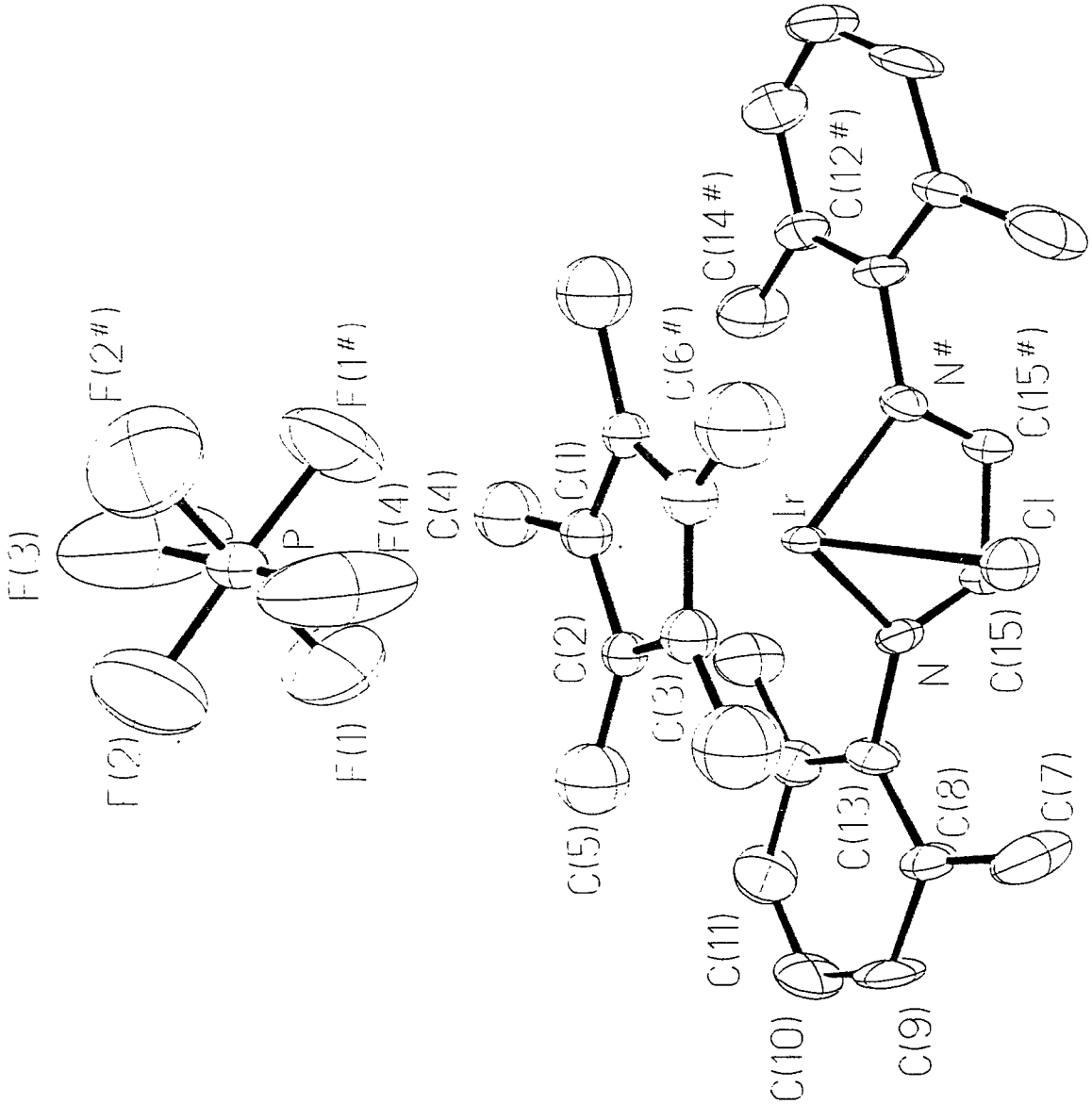

Figure 2: ORTEP plot of $[Cp^*IrCl(dab)]PF_6$, staggered form

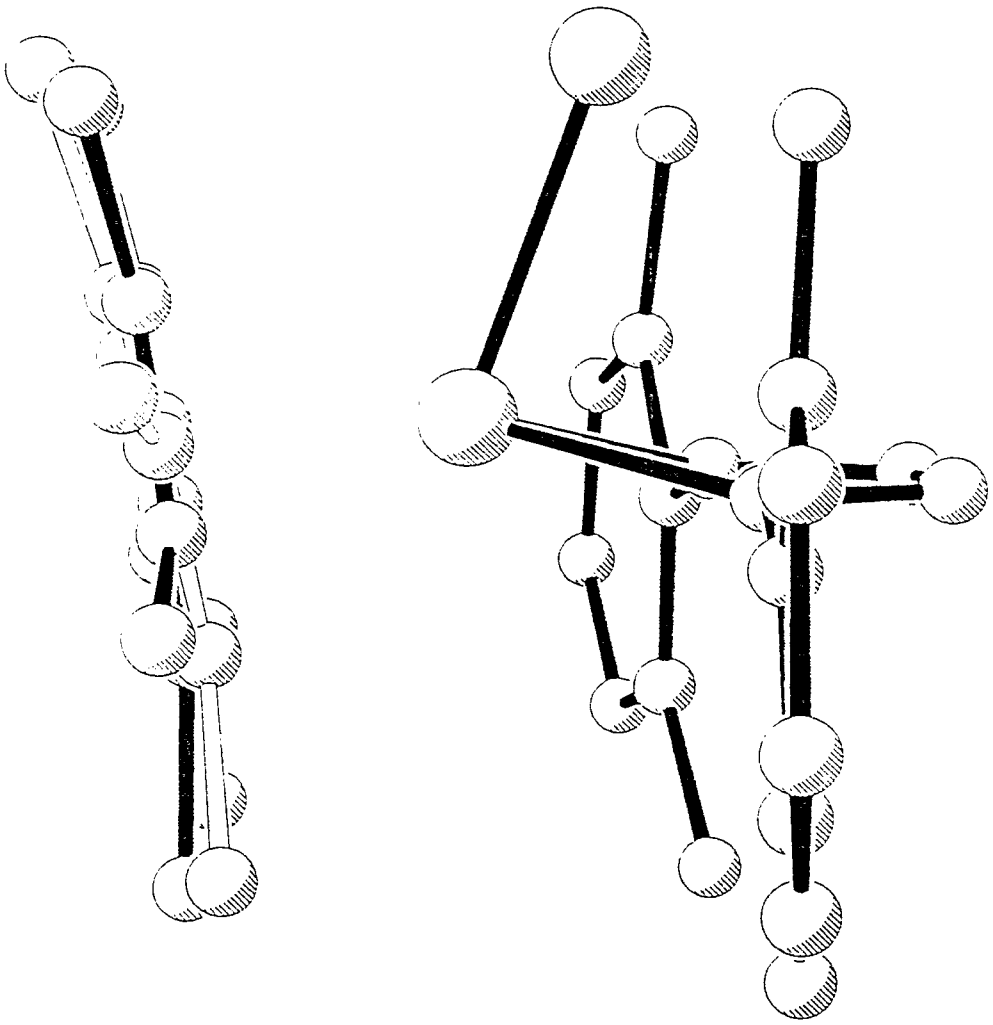

Figure 3: Molecular structure of [Cp*IrCl(dab)]PF_6 in the crystal, staggered and eclipsed form

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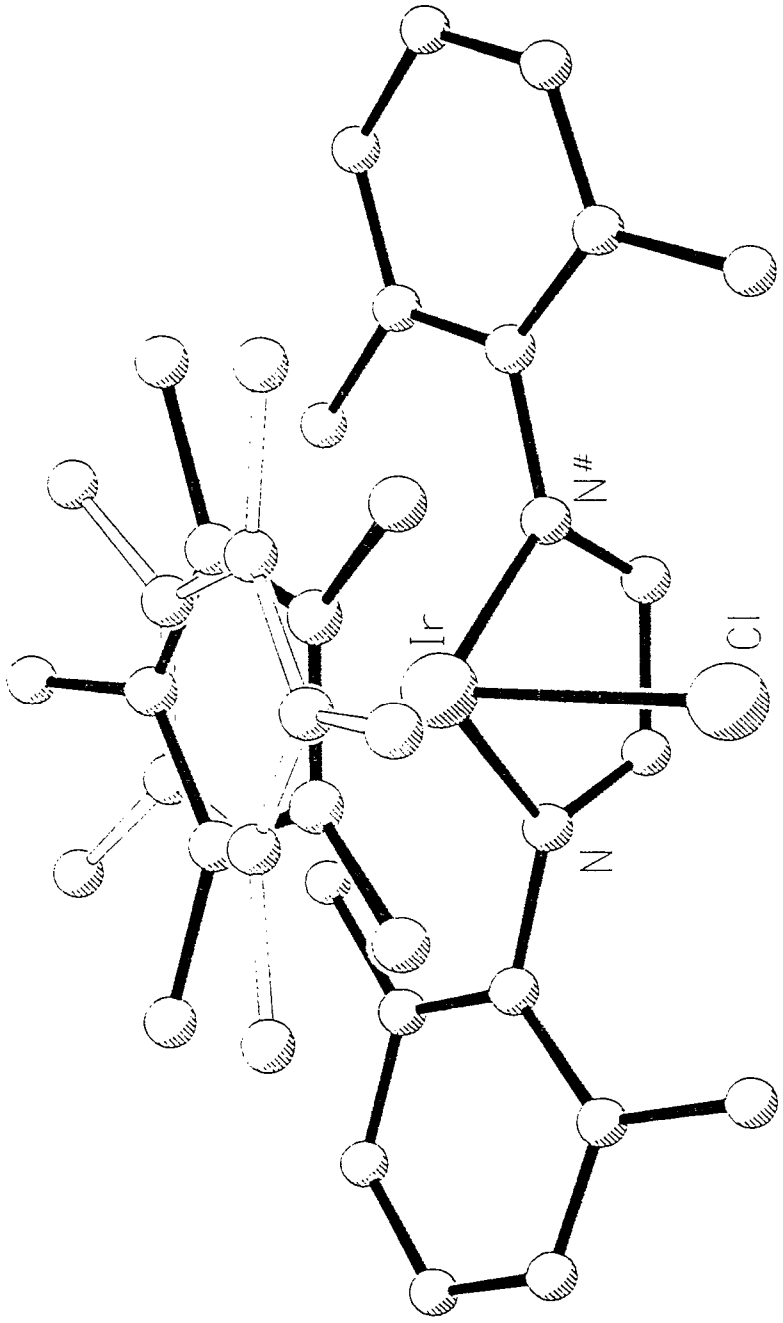

Figure 4: Molecular structure of [Cp*IrCl(dab)]PF_6 in the crystal, staggered and eclipsed form

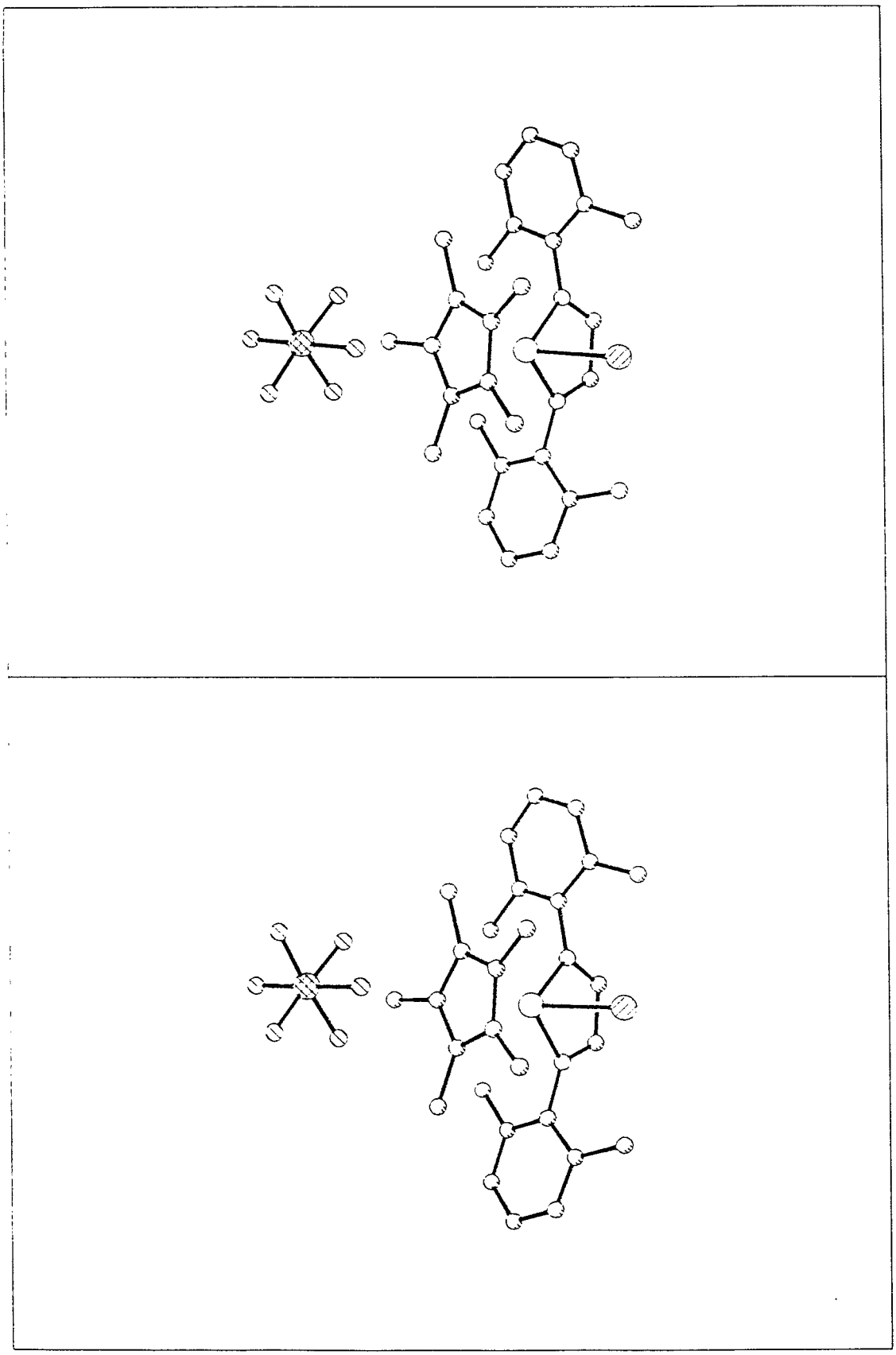

Figure 5: Stereo view of [Cp*IrCl(dab)]PF_6 (staggered form)

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Table 1. Crystal data and structure refinement for Cp*Ir(dab).

Empirical formula	$C_{28}H_{35}IrN_2$
Formula weight	591.78
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 8.484(2) Å
	b = 14.535(3) Å
	c = 20.956(4) Å
	β = 98.88(3)°
Volume	2553.2(9) $Å^3$
Z	4
Density (calculated)	1.540 Mg/m^3
Absorption coefficient	5.246 mm^{-1}
F(000)	1176
Crystal size	0.4 x 0.3 x 0.1 mm
q range for data collection	1.71 to 28.00°
Index ranges	$0 \le h \le 11$, $0 \le k \le 19$, $-27 \le l \le 27$
Reflections collected	6466
Independent reflections	6075 (R_{int} = 0.0199)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6060 / 0 / 280
Goodness-of-fit on F^2	1.329
Final R indices [I>2s(I)]	R1 = 0.0586, wR2 = 0.1479
R indices (all data)	R1 = 0.0687, wR2 = 0.1590
Largest diff. peak and hole	2.321 and -2.117 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Cp*Ir(dab). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ir	4568(1)	2295(1)	1578(1)	28(1)
N(1)	4801(11)	1344(6)	924(4)	34(2)
N(2)	4409(12)	1131(6)	2053(4)	35(2)
C(1)	5818(15)	3512(8)	1998(6)	43(3)
C(2)	5486(14)	3640(8)	1321(6)	40(3)
C(3)	3792(17)	3626(8)	1142(6)	46(3)
C(4)	3102(14)	3455(10)	1729(7)	49(3)
C(5)	4394(19)	3448(8)	2250(6)	50(3)
C(6)	7512(20)	3515(10)	2384(9)	72(5)
C(7)	6668(21)	3822(11)	866(8)	70(5)

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C(8)	2902(24)	3801(11)	468(7)	84(6)
C(9)	1317(19)	3491(13)	1754(10)	81(6)
C(10)	4237(25)	3372(10)	2965(7)	75(6)
C(11)	2034(17)	1505(12)	-58(7)	62(4)
C(12)	3712(16)	1662(8)	-201(6)	42(3)
C(13)	3984(21)	1907(10)	-818(6)	59(4)
C(14)	5466(24)	2037(10)	-966(7)	70(5)
C(15)	6752(19)	1888(10)	-493(8)	61(4)
C(16)	6631(15)	1638(9)	145(6)	46(3)
C(17)	5015(15)	1550(8)	282(5)	39(3)
C(18)	8014(16)	1461(14)	662(8)	72(5)
C(19)	4728(14)	439(8)	1094(5)	38(2)
C(20)	4542(13)	333(8)	1710(5)	35(2)
C(21)	7224(16)	1079(9)	3006(6)	51(3)
C(22)	5584(16)	1061(8)	3186(6)	43(3)
C(23)	5374(21)	1038(9)	3847(6)	58(4)
C(24)	3891(23)	999(10)	4015(7)	65(4)
C(25)	2549(21)	988(10)	3541(8)	62(4)
C(26)	2674(17)	1032(9)	2883(7)	50(3)
C(27)	4228(14)	1069(7)	2720(5)	35(2)
C(28)	1242(16)	1022(11)	2368(9)	66(4)

Table 3. Selected bond lengths [Å] and angles [°] for Cp*Ir(dab).

Cp-IrN1C19C20N2	88.87(44)	C12-C17)-IrN1C19C20N2	89.04(37)
C22-C27)-IrN1C19C20N2	89.00(36)		

Table 4. Bond lengths [Å] and angles[°] for Cp*Ir(dab).

Ir-N(1)	1.977(9)	Ir-N(2)	1.978(9)
Ir-C(4)	2.151(14)	Ir-C(1)	2.175(12)
Ir-C(3)	2.199(12)	Ir-C(2)	2.199(12)
Ir-C(5)	2.209(12)	N(1)-C(19)	1.366(14)
N(1)-C(17)	1.419(14)	N(2)-C(20)	1.379(13)
N(2)-C(27)	1.432(14)	C(1)-C(5)	1.394(19)
C(1)-C(2)	1.416(17)	C(1)-C(6)	1.536(19)
C(2)-C(3)	1.428(18)	C(2)-C(7)	1.509(18)
C(3)-C(4)	1.463(18)	C(3)-C(8)	1.518(17)
C(4)-C(5)	1.423(19)	C(4)-C(9)	1.525(18)
C(5)-C(10)	1.528(17)	C(11)-C(12)	1.515(18)
C(12)-C(17)	1.389(17)	C(12)-C(13)	1.395(17)
C(13)-C(14)	1.353(23)	C(14)-C(15)	1.374(23)
C(15)-C(16)	1.405(19)	C(16)-C(17)	1.448(17)
C(16)-C(18)	1.493(20)	C(19)-C(20)	1.334(15)

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C(21)-C(22)	1.498(19)	C(22)-C(27)	1.389(16)
C(22)-C(23)	1.423(17)	C(23)-C(24)	1.359(23)
C(24)-C(25)	1.391(23)	C(25)-C(26)	1.402(20)
C(26)-C(27)	1.413(17)	C(26)-C(28)	1.495(21)
N(1)-Ir-N(2)	76.9(4)	N(1)-Ir-C(4)	140.7(5)
N(2)-Ir-C(4)	120.8(4)	N(1)-Ir-C(1)	138.9(4)
N(2)-Ir-C(1)	123.8(4)	C(4)-Ir-C(1)	63.8(5)
N(1)-Ir-C(3)	112.6(4)	N(2)-Ir-C(3)	157.4(5)
C(4)-Ir-C(3)	39.3(5)	C(1)-Ir-C(3)	63.2(5)
N(1)-Ir-C(2)	112.0(4)	N(2)-Ir-C(2)	159.4(4)
C(4)-Ir-C(2)	64.7(5)	C(1)-Ir-C(2)	37.8(4)
C(3)-Ir-C(2)	37.9(5)	N(1)-Ir-C(5)	174.8(4)
N(2)-Ir-C(5)	108.1(4)	C(4)-Ir-C(5)	38.1(5)
C(1)-Ir-C(5)	37.1(5)	C(3)-Ir-C(5)	63.3(5)
C(2)-Ir-C(5)	62.8(4)	C(19)-N(1)-C(17)	117.9(9)
C(19)-N(1)-Ir	118.7(7)	C(17)-N(1)-Ir	123.4(7)
C(20)-N(2)-C(27)	119.1(9)	C(20)-N(2)-Ir	116.0(7)
C(27)-N(2)-Ir	124.9(7)	C(5)-C(1)-C(2)	109.8(11)
C(5)-C(1)-C(6)	126.6(13)	C(2)-C(1)-C(6)	123.5(13)
C(5)-C(1)-Ir	72.8(7)	C(2)-C(1)-Ir	72.1(7)
C(6)-C(1)-Ir	124.8(9)	C(1)-C(2)-C(3)	107.4(11)
C(1)-C(2)-C(7)	127.4(12)	C(3)-C(2)-C(7)	125.2(12)
C(1)-C(2)-Ir	70.2(7)	C(3)-C(2)-Ir	71.0(7)
C(7)-C(2)-Ir	127.1(9)	C(2)-C(3)-C(4)	107.3(10)
C(2)-C(3)-C(8)	125.4(14)	C(4)-C(3)-C(8)	127.3(14)
C(2)-C(3)-Ir	71.1(7)	C(4)-C(3)-Ir	68.6(7)
C(8)-C(3)-Ir	127.6(9)	C(5)-C(4)-C(3)	106.6(11)
C(5)-C(4)-C(9)	128.7(13)	C(3)-C(4)-C(9)	123.5(13)
C(5)-C(4)-Ir	73.2(8)	C(3)-C(4)-Ir	72.1(7)
C(9)-C(4)-Ir	129.4(11)	C(1)-C(5)-C(4)	108.6(11)
C(1)-C(5)-C(10)	126(2)	C(4)-C(5)-C(10)	125.4(14)
C(1)-C(5)-Ir	70.1(7)	C(4)-C(5)-Ir	68.7(7)
C(10)-C(5)-Ir	126.5(9)	C(17)-C(12)-C(13)	118.6(13)
C(17)-C(12)-C(11)	120.4(11)	C(13)-C(12)-C(11)	121.1(13)
C(14)-C(13)-C(12)	122.7(14)	C(13)-C(14)-C(15)	118.3(13)
C(14)-C(15)-C(16)	124.2(13)	C(15)-C(16)-C(17)	114.9(13)
C(15)-C(16)-C(18)	124.9(12)	C(17)-C(16)-C(18)	120.2(11)
C(12)-C(17)-N(1)	120.8(11)	C(12)-C(17)-C(16)	121.2(11)
N(1)-C(17)-C(16)	118.1(11)	C(20)-C(19)-N(1)	112.2(10)
C(19)-C(20)-N(2)	116.1(10)	C(27)-C(22)-C(23)	118.0(13)
C(27)-C(22)-C(21)	121.6(11)	C(23)-C(22)-C(21)	120.4(12)
C(24)-C(23)-C(22)	120.9(14)	C(23)-C(24)-C(25)	120.2(13)
C(24)-C(25)-C(26)	121.7(14)	C(25)-C(26)-C(27)	117.0(14)
C(25)-C(26)-C(28)	122.3(13)	C(27)-C(26)-C(28)	120.7(12)
C(22)-C(27)-C(26)	122.2(11)	C(22)-C(27)-N(2)	119.0(11)

C(26)-C(27)-N(2) 118.8(11)

Table 5'. Anisotropic displacement parameters [$Å^2$ x 10^3] for Cp*Ir(dab).The anisotropic displacement factor exponent takes the form: $-2p^2$ [$(ha^*)^2U_{11}$ + ... + 2hka*b*U_{12}

	U11	U22	U33	U23	U13	U12
Ir	29(1)	28(1)	27(1)	-1(1)	4(1)	0(1)
N(1)	38(5)	33(5)	34(5)	-6(4)	11(4)	-4(4)
N(2)	43(5)	26(4)	35(5)	3(4)	8(4)	1(4)
C(1)	46(7)	32(6)	50(7)	6(5)	1(5)	-6(5)
C(2)	42(6)	42(6)	36(6)	-2(5)	11(5)	3(5)
C(3)	62(8)	31(6)	41(6)	-3(5)	-7(6)	6(6)
C(4)	32(6)	62(8)	55(8)	0(6)	11(5)	-5(6)
C(5)	85(10)	30(6)	39(6)	-8(5)	19(7)	-3(6)
C(6)	70(10)	42(8)	92(12)	7(8)	-25(9)	-14(7)
C(7)	81(11)	58(9)	78(11)	1(8)	34(9)	-16(8)
C(8)	129(16)	49(9)	55(9)	1(7)	-43(10)	15(10)
C(9)	64(10)	82(12)	107(14)	17(11)	49(10)	26(9)
C(10)	154(18)	39(7)	40(7)	-3(6)	41(9)	0(9)
C(11)	48(8)	81(11)	55(8)	-4(8)	-1(6)	-9(8)
C(12)	50(7)	41(6)	33(6)	-6(5)	3(5)	0(5)
C(13)	94(12)	50(8)	32(6)	1(6)	5(7)	4(8)
C(14)	127(15)	49(8)	43(7)	-1(6)	38(9)	-23(9)
C(15)	67(9)	55(8)	71(10)	-20(8)	45(8)	-16(7)
C(16)	47(7)	44(7)	52(7)	-7(6)	26(6)	-5(5)
C(17)	56(7)	31(5)	33(5)	-8(4)	17(5)	-13(5)
C(18)	32(7)	113(15)	72(10)	-9(10)	15(7)	-6(8)
C(19)	49(7)	30(5)	34(5)	-7(4)	7(5)	2(5)
C(20)	39(6)	33(5)	35(6)	-4(4)	5(5)	2(5)
C(21)	60(8)	42(7)	45(7)	2(6)	-14(6)	-1(6)
C(22)	59(8)	38(6)	32(6)	3(5)	5(5)	5(6)
C(23)	96(12)	46(7)	28(6)	-3(5)	-1(7)	6(8)
C(24)	106(13)	53(9)	39(7)	4(6)	26(8)	6(9)
C(25)	80(11)	43(7)	72(10)	4(7)	46(9)	8(7)
C(26)	54(8)	34(6)	68(9)	-2(6)	31(7)	0(6)
C(27)	45(6)	27(5)	32(5)	1(4)	5(5)	5(5)
C(28)	37(7)	61(9)	108(13)	12(9)	29(8)	6(6)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Cp*Ir(dab).

	x	y	z	U(eq)
H(6A)	7725(20)	4101(10)	2591(9)	108
H(6B)	8270(20)	3406(10)	2096(9)	108
H(6C)	7598(20)	3039(10)	2705(9)	108
H(7A)	6695(21)	4468(11)	775(8)	105
H(7B)	6354(21)	3488(11)	472(8)	105
H(7C)	7709(21)	3625(11)	1063(8)	105
H(8A)	3036(24)	4433(11)	353(7)	126
H(8B)	1788(24)	3671(11)	458(7)	126
H(8C)	3319(24)	3409(11)	165(7)	126
H(9A)	795(19)	2985(13)	1513(10)	121
H(9B)	891(19)	4059(13)	1570(10)	121
H(9C)	1142(19)	3450(13)	2195(10)	121
H(10A)	3240(25)	3083(10)	3007(7)	113
H(10B)	4273(25)	3976(10)	3152(7)	113
H(10C)	5099(25)	3010(10)	3184(7)	113
H(11A)	1280(17)	1631(12)	-439(7)	93
H(11B)	1839(17)	1906(12)	285(7)	93
H(11C)	1921(17)	877(12)	70(7)	93
H(13)	3112(21)	1983(10)	-1141(6)	71
H(14)	5610(24)	2224(10)	-1378(7)	84
H(15)	7767(19)	1958(10)	-602(8)	73
H(18A)	8544(16)	908(14)	564(8)	108
H(18B)	7640(16)	1392(14)	1069(8)	108
H(18C)	8747(16)	1969(14)	686(8)	108
H(19)	4800(14)	-48(8)	812(5)	45
H(20)	4505(13)	-245(8)	1898(5)	42
H(21A)	7564(16)	461(9)	2942(6)	77
H(21B)	7950(16)	1363(9)	3346(6)	77
H(21C)	7210(16)	1423(9)	2614(6)	77
H(23)	6263(21)	1051(9)	4167(6)	69
H(24)	3774(23)	980(10)	4449(7)	77
H(25)	1544(21)	951(10)	3665(8)	74
H(28A)	753(16)	424(11)	2349(9)	100
H(28B)	1561(16)	1162(11)	1959(9)	100
H(28C)	492(16)	1475(11)	2465(9)	100

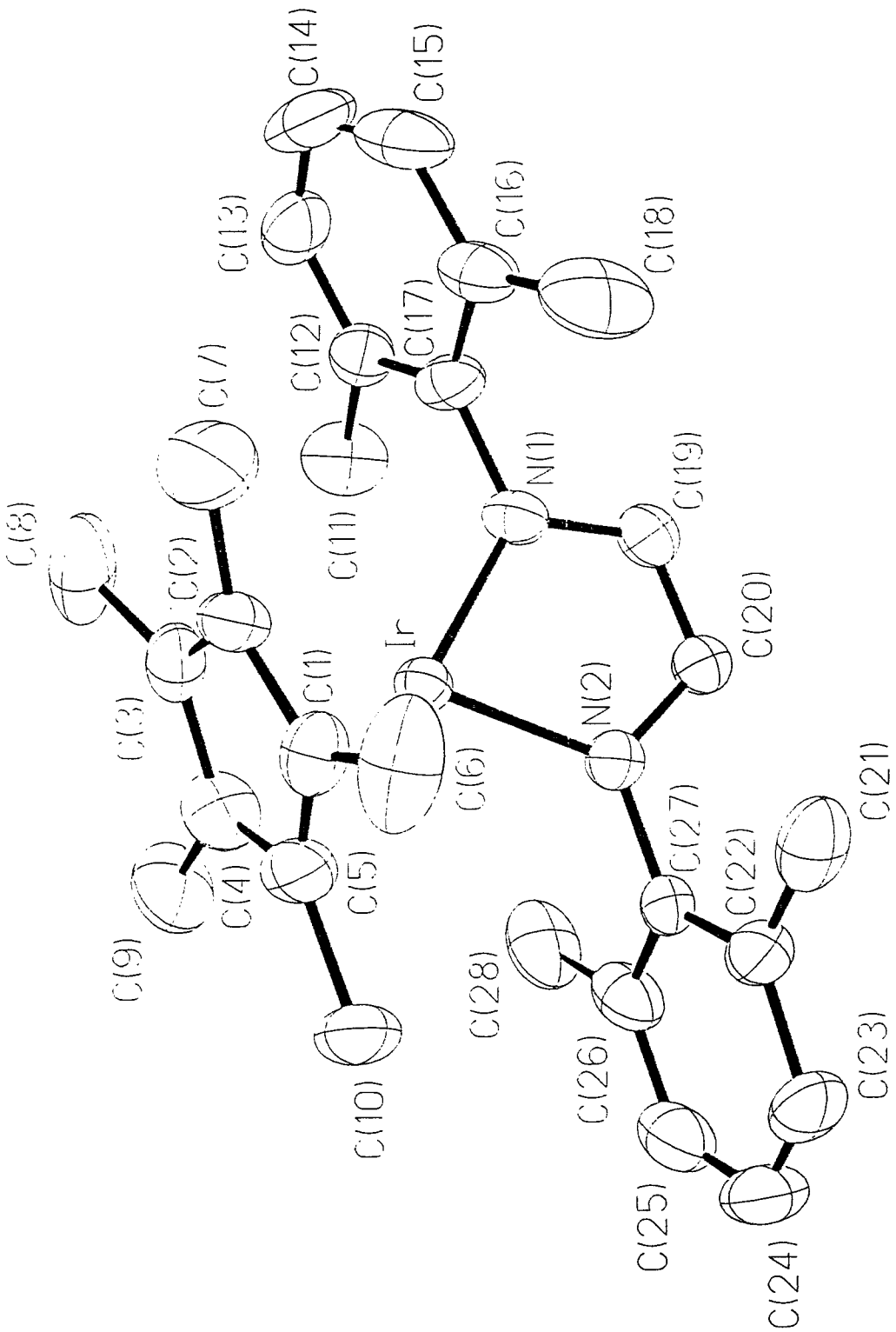

Figure 6: ORTEP plot of [Cp*IrCl(dab)]

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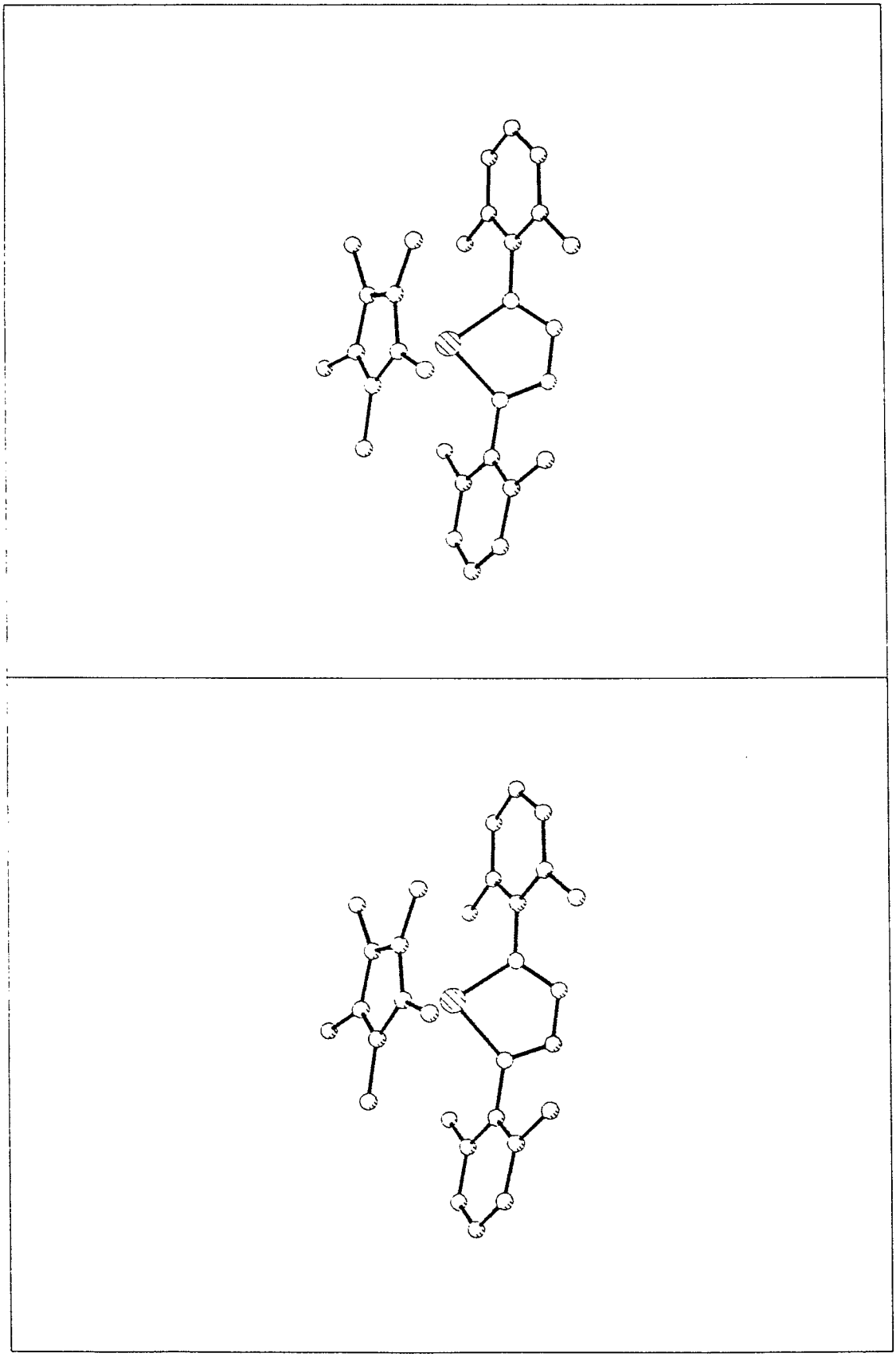

Figure 7: stereo view of [Cp*IrCl(dab)]