Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information (ESI)

Synthesis and Oxidation of Cp*Ir^{III} Compounds: Functionalization of a Cp* Methyl Group

Lisa S. Park-Gehrke,[a] John Freudenthal,[b] Werner Kaminsky,[b] Antonio G. DiPasquale[c] and James M. Mayer[a]*

Table S1. Selected bond distances and angles for Cp*Ir(ppy)Cl (**4Cl**),

	2Cl
Ir(1)–C(1)	2.156(11)
Ir(1)–C(2)	2.179(11)
Ir(1)–C(3)	2.228(10)
Ir(1)–C(4)	2.216(14)
Ir(1)–C(5)	2.188(13)
Ir(1)–Cl(1)	2.401(3)
Ir(1)–N(1)	2.076(11)
Ir(1)–C(11)	2.067(12)
N(1)–Ir(1)–C(11)	79.3(4)
N(1)–Ir(1)–Cl(1)	87.9(3)
Cl(1)–Ir(1)–C(11)	104.6(4)

Table S2. Crystal data and structure refinement for Cp*Ir(ppy)Cl (**4Cl**),

	2Cl
Empirical formula	$C_{21}H_{23}ClIrN$
Formula weight	517.07
Temperature (K)	130(2)
Wavelength (Å)	0.71073
Crystal description/color	cut block/orange
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	
a (Å)	15.3684(10)
b (Å)	7.4007(5)
c (Å)	21.0300(11)
α (°)	90

β (°)	132.246(3)
γ (°)	90
Volume, Å^3	1770.63(19)
Z	4
Calculated density (g/cm^3)	1.940
Abs coeff, mm^{-1}	7.693
F(000)	1000
Crystal size (mm)	0.26×0.25×0.24
Reflections for indexing	382
θ range for data coll.(deg)	1.79 to 25.03
Index ranges	$-18 \leq h \leq 18$
	$-8 \leq k \leq 8$
	$-24 \leq l \leq 24$
Reflns collected	5440
Unique reflns	3109 $R_{int} = 0.104$
Completeness to $\theta = 25.00$	99.1%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3109 / 0 / 224
Goodness-of-fit on F^2	$S = 0.845$
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.049$
R indices (all data)	$wR_2 = 0.099$