Supplementary Materials for:

[(η^5-pentamethylcyclopentadienyl)(3-fluoro-*N*-methylbenzylamine-κ^1,*N*)dichlorido]iridium(III)

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Supporting Information

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EXPERIMENTAL SECTION

X-ray Crystallography. X-ray Diffraction data were collected at 298(2) K on a Bruker Smart CCD area detector (Bruker, Karlsruhe, Germany) with graphite-monochromated MoKα radiation (λ = 0.71073 Å). Absorption corrections were applied using SADABS program. The structures were solved by direct methods using SHELXS (TREF) with additional light atoms found by Fourier methods. Complexes were refined against F^2 using SHELXL, and hydrogen atoms were added at calculated positions and refined riding on their parent atoms.

X-ray crystallographic data for complexes [(η^5-Cp*)Ir($C_6H_4FCH_2NHCH_3$)Cl_2] is available as **Figure 1**, **Table S1** and have been deposited in the Cambridge Crystallographic Data Centre under the accession numbers CCDC 1842677. X-ray crystallographic data in CIF format are available from the Cambridge Crystallographic Data Centre (http://www.ccdc.cam.ac.uk/).

NMR Spectroscopy. NMR-spectra were measured in the given solvent at RT on *Bruker DPX 500* (500.13 MHz, ^{1}H; 125.8 MHz, ^{13}C) instrument operating at the denoted spectrometer frequency given in mega Hertz (MHz) for the specified nucleus. Chemical shifts are given in parts per million (ppm) relative to tetramethylsilane (TMS) as an external standard for ^{1}H- and ^{13}C-NMR spectra and calibrated against the solvent residual peak. Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, or as combination of them. Coupling constants *J* are given in Hertz (Hz).

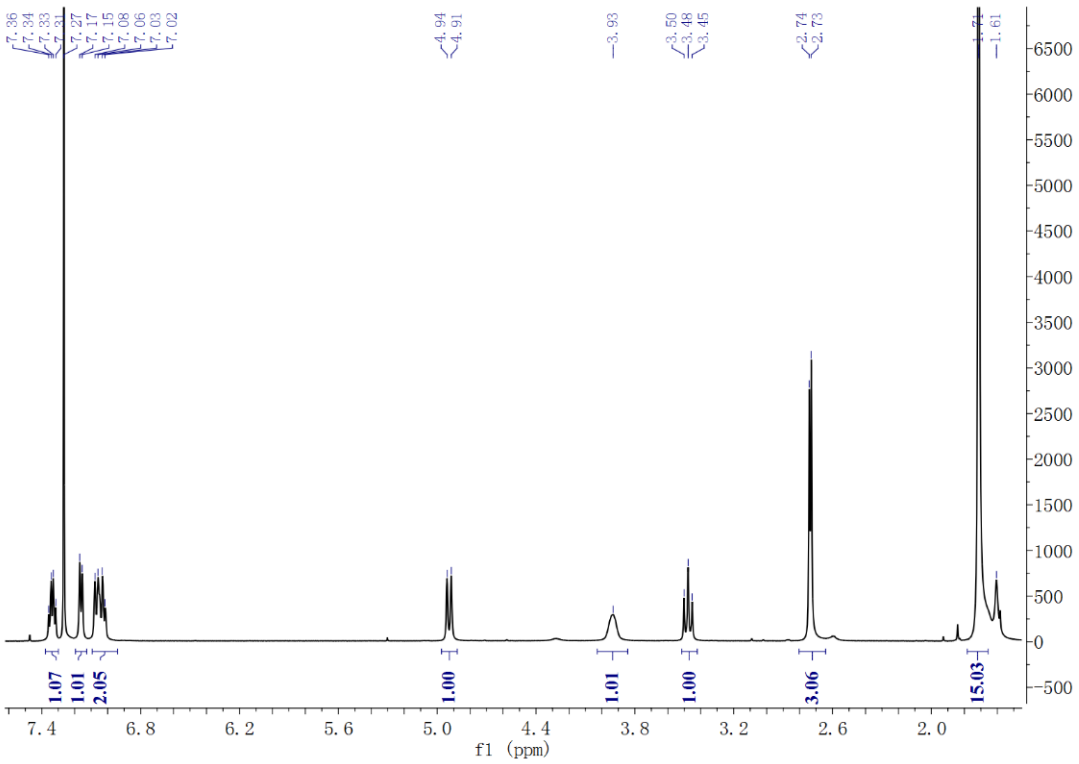

Figure S1: ^{1}H-NMR spectrum of [(η^5-Cp*)Ir($C_6H_4FCH_2NHCH_3$)Cl_2] in $CDCl_3$.

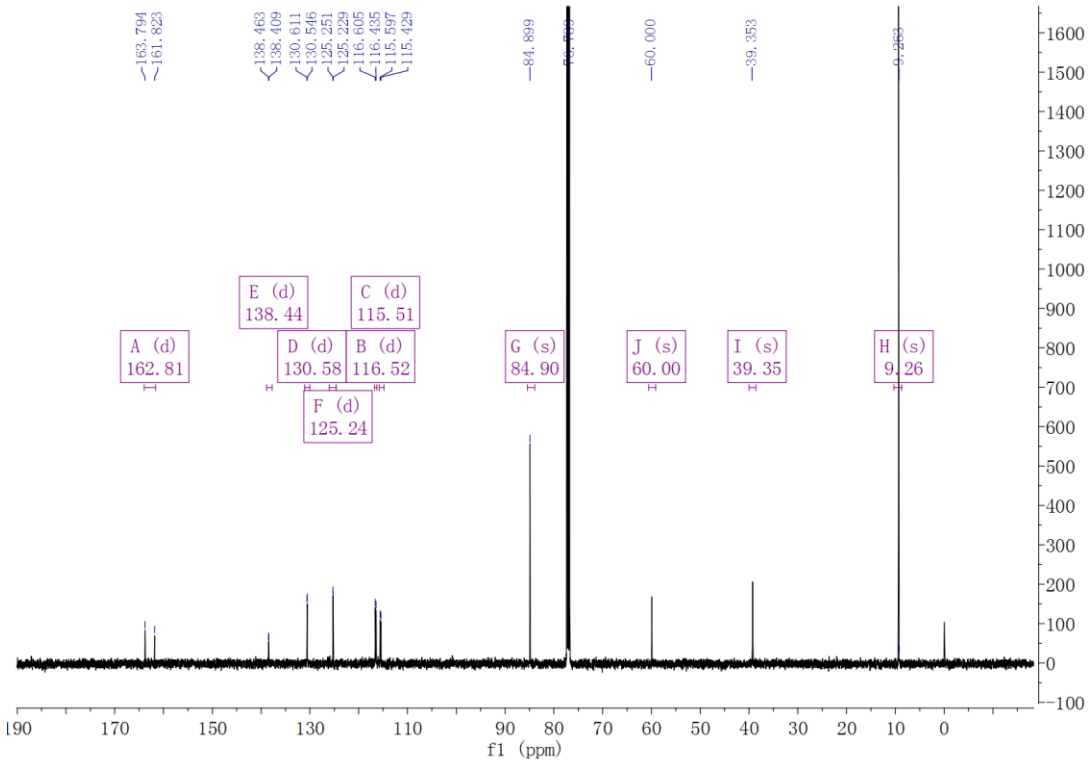

Figure S2: ^{13}C-NMR spectrum of [(η^5-Cp*)Ir($C_6H_4FCH_2NHCH_3$)Cl_2] in $CDCl_3$.

	Complex
Empirical formula	$C_{18}H_{25}Cl_2FIrN$
MW	537.49
Cryst	yellow plate
Cryst size(mm)	0.88 x 0.38 x 0.08
λ (Å)	0.71073
Temp(K)	293(2)
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
a (Å)	9.0825(18)
b (Å)	12.552(3)
c (Å)	17.516(4)
α (°)	90
β (°)	90
γ (°)	90
vol($Å^3$)	1996.9(7)
Z	4
F(000)	1040
Density(mg/m^{-3})	1.788
M/mm^{-1}	6.961
*Θ*range(°)	2.00 - 28.3
R_{int}	0.0602
Data	4932
restraints	0
parameters	320
$R_1/\omega R_2$ [I > 2σ(I)]	0.0419/0.1028
$R_1/\omega R_2$(all date)	0.0453/0.1050
Goodness of fit	1.013
Largest diff. peak and hole ($e.A^{-3}$)	1.503 / -1.085

Table S1: Crystal data an d structure refinement for [(η^5-Cp*)Ir($C_6H_4FCH_2NHCH_3$)Cl_2].