Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2020

Chemoselective and efficient catalytic hydrogenation of furfural by iridium and ruthenium half-sandwich complexes

Novisi K. Oklu^a and Banothile C. E. Makhubela^{a*}

^a University of Johannesburg, Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, Auckland Park 2006, Johannesburg,South Africa. *E-mail: bmakhubela@uj.ac.za

SUPPORTING INFORMATION

1. ¹H NMR spectra of complexes **1** to **4**



Figure S1: ¹H NMR spectra of complex 1



Figure S2: ¹H NMR spectra of complex 2



Figure S3: ¹H and ³¹P{¹H} NMR spectra of complex 3



Figure S4: ¹H and ³¹P{¹H} NMR spectra of complex 4

2. High Resolution - Mass Spectra of complexes 1 to 4



Figure S5: HR-MS (ESI^+) of complex 1



Figure S6: HR-MS (ESI⁺) of complex 2



Figure S7: HR-MS (ESI⁺) of complex 3



Figure S8: HR-MS (ESI^+) of complex **4**

3. ¹H NMR Spectrum of catalysis product showing DFE when ruthenium complex was used



Figure S9: ¹H NMR Spectrum of catalysis products using complex 2

4. Time- dependent ¹H NMR spectra collected during the hydrogenation FFR to FFA in J Young NMR tube.



Figure S10: ¹H NMR Spectrum (10 ppm to -11 ppm) of *in situ* reaction using complex **3**.

5. Crystallographic data obtained for complex **3**.

Empirical formula	$C_{23}H_{25}ClF_6IrN_2O_2P$
Formula weight	734.07
Temperature/K	100.01
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.9192(12)
b/Å	19.809(2)
c/Å	11.7104(12)
$\alpha /^{\circ}$	90
β/°	93.931(3)
$\gamma/^{\circ}$	90
Volume/Å ³	2526.9(5)
Z	4
$\rho_{calc}g/cm^3$	1.930
μ/mm^{-1}	5.522
F(000)	1424.0
Crystal size/mm ³	$0.3\times0.27\times0.2$
Radiation	MoKa ($\lambda = 0.71073$)
2Θ range for data collection/°	3.738 to 55.24
Index ranges	$-14 \le h \le 14, -24 \le k \le 25, -15 \le l \le 15$
Reflections collected	91002
Independent reflections	5846 [$R_{int} = 0.0804$, $R_{sigma} = 0.0270$]
Data/restraints/parameters	5846/0/334
Goodness-of-fit on F ²	1.202
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0334, wR_2 = 0.0840$
Final R indexes [all data]	$R_1 = 0.0427, wR_2 = 0.0984$

 Table S1: Crystallographic data for complex 3.