

## Supplementary Information

# **N-Alkyl Functionalised Expanded Ring N-Heterocyclic Carbene Complexes of Rhodium & Iridium(I): Structural Investigations & Catalytic Application**

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**Structure Refinement Data for Compounds 4, 5, 6, 10 and 14**

**S2**

	<b>4</b>	<b>5</b>	<b>6</b>
Empirical formula	C14 H28 Br N2	C12 H25 Cl2 I N2	C15 H30 I N2
Fw/g mol <sup>-1</sup>	304.29	395.14	365.31
Cryst syst, space group	Orthorhombic, P212121	Orthorhombic, Pna21	Monoclinic, P21/n
a/Å	7.0089(5)	25.0834(6)	13.2298(2)
b/Å	13.0334(12)	10.1732(3)	8.9506(2)
c/Å	18.072(2)	13.7406(3)	15.5722(3)
α/deg	90	90	90
β/deg	90	90	103.0750(10)
γ/deg	90	90	90
Vol/Å <sup>3</sup>	1650.9(3)	3506.31(15)	1796.17(6)
Z, calc density (Mg m <sup>-3</sup> )	4, 1.224	8, 1.497	4, 1.351
Abs coeff (mm <sup>-1</sup> )	2.476	2.117	1.773
F(000)	644	1584	748
Cryst	Needle, colourless	Block, colourless	Needle, colourless
Cryst dimens/mm <sup>3</sup>	0.35 x 0.08 x 0.08	0.25 x 0.25 x 0.13	0.35 x 0.12 x 0.10
θ range (deg)	2.74 - 25.24	1.62 - 30.48	2.64 - 28.27
No. of reflns collected/unique	2897/2897	19185/8832	8565/4426
R <sub>int</sub>	0.0100	0.0377	0.0689
No. of data/restraints/parameters	2897/0/161	8832/1/317	4426/0/170
Final R indices [F <sup>2</sup> < 2θ(F <sup>2</sup> )]:	0.0559, 0.1079	0.0731, 0.1873	0.0689, 0.1380
R indices (all data): R1, wR2	0.1654, 0.1178	0.1184, 0.2361	0.1126, 0.1554
Largest diff peak and hole/e Å <sup>-3</sup>	0.869, -0.432	1.019, -1.178	1.170, -1.032

	<b>10</b>	<b>14</b>
Empirical formula	C22 H40 Cl Ir N2	C23 H42 Cl Ir N2
Fw/g mol <sup>-1</sup>	560.21	574.24
Cryst syst, space group	Orthorhombic, Pbca	Monoclinic, P21/a
a/Å	18.6021(3)	11.5140(3)
b/Å	12.6261(2)	15.0802(5)
c/Å	19.3427(3)	14.4033(5)
α/deg	90	90
β/deg	90	107.804(2)
γ/deg	90	90
Vol/Å <sup>3</sup>	4543.06(12)	2381.12(13)
Z, calc density (Mg m <sup>-3</sup> )	8, 1.638	4, 1.602
Abs coeff (mm <sup>-1</sup> )	6.004	5.730
F(000)	2240	1152
Cryst	Needle, yellow	Plate, yellow
Cryst dimens/mm <sup>3</sup>	0.30 x 0.25 x 0.20	0.15 x 0.15 x 0.06
θ range (deg)	2.72 - 28.31	2.70 - 28.27
No. of reflns collected/unique	18940/5622	11361/5876
R <sub>int</sub>	0.0630	0.0526
No. of data/restraints/parameters	5622/0/241	5876/0/251
Final R indices [F <sup>2</sup> < 2θ(F <sup>2</sup> )]:	0.0646, 0.1163	0.0628, 0.1515
R indices (all data): R1, wR2	0.0891, 0.1249	0.0928, 0.1759
Largest diff peak and hole/e Å <sup>-3</sup>	2.658, -2.313	1.993, -1.504