

Coordination Chemistry and Catalytic Activity of N-Heterocyclic Carbene Iridium(I) Complexes

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Supporting infromations

Table S1 Kinetic data for CO exchanging on **3b-3d** and [(PCy₃)Ir(CO)₂Cl].

[CO] (mM)	[complex] (mM)	Half-height Width (Hz) ^b	$\Delta\nu$ (Hz)	k_{obs} (s ⁻¹)	k (M ⁻¹ .s ⁻¹) ^c	$\Delta G^\ddagger$ (kcal/mol)	$\Delta G^\ddagger$ (kcal/mol) (average)
0	[3b], 9.7	1.47	0	-	-	-	
3.3	[3b], 9.7	9.86	8.39	26.36	2707	12.8	12.9
1.5	[3b], 19.8	9.97	8.51	26.72	1372	13.2	
0.9	[3b], 9.7	9.43	7.96	25.02	2569	12.8	
0	[3c], 9.8	0.94	0	-	-	-	
4.3	[3c], 9.8	13.37	12.43	39.1	4.0 x10 ³	12.6	12.8
3.1	[3c], 19.6	11.59	10.65	33.4	1.7 x10 ³	13.1	
1.9	[3c], 9.8	9.93	8.99	28.2	2.9 x10 ³	12.7	
0	[3d], 9.8	0.88	0	-			
4.3	[3d], 9.8	10.22	9.33	29.33	3.0 x10 ³	12.7	12.9
3.9	[3d], 19.5	9.74	8.85	27.82	1.4 x10 ³	13.2	
2.1	[3d], 9.8	8.44	7.56	23.74	2.4 x10 ³	12.9	