

Electronic Supplementary Information for:

QALE Analysis of CO Dissociative Kinetics of Ru(CO)₄L (L = P-donor ligands): Accelerating Effects of Hydrogen in PH_nR_{3-n} Ligands (n = 1-2)[†]

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Table S1. Rate data for the reaction of Ru(CO)₄L With L or L' ^a in heptane

L	T, °C	10 ² [L']/M	10 ⁴ k _{obs} /s ⁻¹			
			v ₁	v ₂	v ₃	v ₄
PMe ₃	50.0	2.50	0.375	0.382		
		5.00	0.380	0.356		
		7.50	0.389	0.398		
	60.0	2.50	1.68	1.72		
		4.50	1.67	1.73		
		5.00	1.67	1.73		
	70.0	3.00	6.68	6.95		
		5.00	6.93	7.09		
		7.50	6.96	7.09		
P(NMe ₂) ₃	50.0	3.30	1.15	1.17		
		5.50	1.15	1.20		
		8.25	1.15	1.15		
	60.0	2.72	4.72	4.68	4.93	4.99
		9.79	4.78	4.85	4.83	4.17
		15.0	5.10	5.15	4.97	4.81
	70.0	3.30	18.67	18.53		
		5.50	18.78	18.98		
		8.25	18.75	18.97		
PH ₂ Ph ^b	50.2	1.16	2.30	2.73	2.50	
		2.03	2.39	2.63	2.49	
		2.90	2.26	2.92	2.54	
	60.0	1.00	11.4	12.2	11.4	
		4.34	10.4	12.4	11	
		4.96	9.79	11.1	10.4	
	70.0	4.67	15.31	16.11	15.98	15.13
		5.2	14.66	14.14	14.04	
		5.2	14.66	14.14	14.04	
PHPh ₂ ^b	60.0	1.24	9.01	10.5	10.8	
		3.91	8.88	8.76	11.1	
		4.56	7.45	6.88	9.02	

		5.14	9.38	8.32	8.38	
		8.65	8.9	9.33	6.81	
		5.83	5.99	6.4	5.97	
PH ₂ Cy	60.0	1.68	12.9	13.7		
		4.19	9.69	10.2		
		6.71	11.6	9.97		
PHCy ₂	60.0	1.45	15	15.2		
		6.53	15.4	16.5		
		9.07	17.7	17.8		
PD ₂ Ph ^b	60.0	8.76	8.37	8.07	8.56	8.2
		29.19	8.62	8.58	9.14	8.59
PDPPh ₂	60.0	4	4.89	4.8	5.27	5.08
		8.01	4.76	4.51	5.23	5.05

^a L = L' unless otherwise indicated. ^b L = P(OEt)₃.
