

Supporting Information

Carbon-Hydrogen Bond Activation in Bis(2,6-dimethylbenzenethiolato)- tris(trimethylphosphine)Ruthenium(II): Ligand Dances and Solvent Transformations

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Table S1. Single Point ω B97XD//B97D Relative Electronic Energies for the Axial and Equatorial Mechanisms

Axial Mechanism		Equatorial Mechanism	
Structure	ΔE	Structure	ΔE
1	0	1	0
2^{A-TS}	8.41	2^{E-TS}	0.68
3^A	5.28	3^E	-0.16
		4^{E-TS}	0.85
		5^E	0.6
4^{A-TS}	6.61	6^{E-TS}	1.20
5^A	6.54	7^E	-0.6
6^{A-TS}	28.84	8^{E-TS}	21.34
7^A	12.51	9^E	14.74
Separated Products	28.12	Separated Products	28.12
10b	0.76	10b	0.76

Raw electronic energies, enthalpies, entropies, and free energies from the optimization and frequency calculations for the axial and equatorial reaction pathways

	Axial Mechanism			
	E	H	S(cal)	G
1	-2894.614046	-2893.939746	0.000391051	-2894.056338
2^{A-TS}	-2894.602292	-2893.928301	0.000381419	-2894.042021
3^A	-2894.605935	-2893.930685	0.000381046	-2894.044294
4^{A-TS}	-2894.603364	-2893.929159	0.000373845	-2894.040621
5^A	-2894.603387	-2893.928117	0.000381482	-2894.041856
6^{A-TS}	-2894.571036	-2893.902264	0.000374147	-2894.013816
7^A	-2894.595918	-2893.924427	0.000389334	-2894.040507
Separated Products	-2185.717698	-2185.212456	0.000313822	-2185.306022
10b	-2646.773654	-2646.14391	0.000344783	-2646.246707
10m	-3355.645184	-3354.844947	0.000415868	-3354.968938

	Equatorial Mechanism			
	E	H	S(cal)	G
1	-2894.614148	-2893.939868	0.000391746	-2894.056667
2^{E-TS}	-2894.614074	-2893.93999	0.000372007	-2894.050904
3^E	-2894.614365	-2893.939627	0.000378135	-2894.052368
4^{E-TS}	-2894.612646	-2893.938899	0.000374842	-2894.050658
5^E	-2894.611951	-2893.937459	0.00038263	-2894.05154
6^{E-TS}	-2894.611039	-2893.936952	0.000380895	-2894.050516
7^E	-2894.613251	-2893.938736	0.000378414	-2894.05156
8^{E-TS}	-2894.582499	-2893.913463	0.000369582	-2894.023654
9^E	-2894.595168	-2893.924731	0.000392051	-2894.041621
Separated Products	-2185.717698	-2185.212456	0.000313822	-2185.306022
10b	-2646.773654	-2646.14391	0.000344783	-2646.246707
10m	-3355.645184	-3354.844947	0.000415868	-3354.968938