

Agostic Complexes							
Agostic	Pt-Me	Pt-H	Pt-O	Pt-P1	Pt-P2	Energy (au)	Energy (kJ mol-1)
Silicon	2.05126	2.76285		2.34383	2.35725	-2379.275	-6246785.458
Sulfur	2.05185	2.82847		2.35022	2.36334	-2486.734	-6528919.118
Carbon	2.05139	2.86822		2.35747	2.37283	-2127.839	-5586640.324

Pincer Complexes							
Pincer	Pt-Me	Pt-H	Pt-O	Pt-P1	Pt-P2	Energy	Energy (kJ mol-1)
Silicon	2.05183	-	2.32339	2.32916	-	-2379.318	-6246898.416
Sulfur	2.05275	-	2.27702	2.34069	2.34067	-2486.777	-6529031.843
Carbon	2.05317	-	2.25641	2.34262	-	-2127.886	-5586765.573

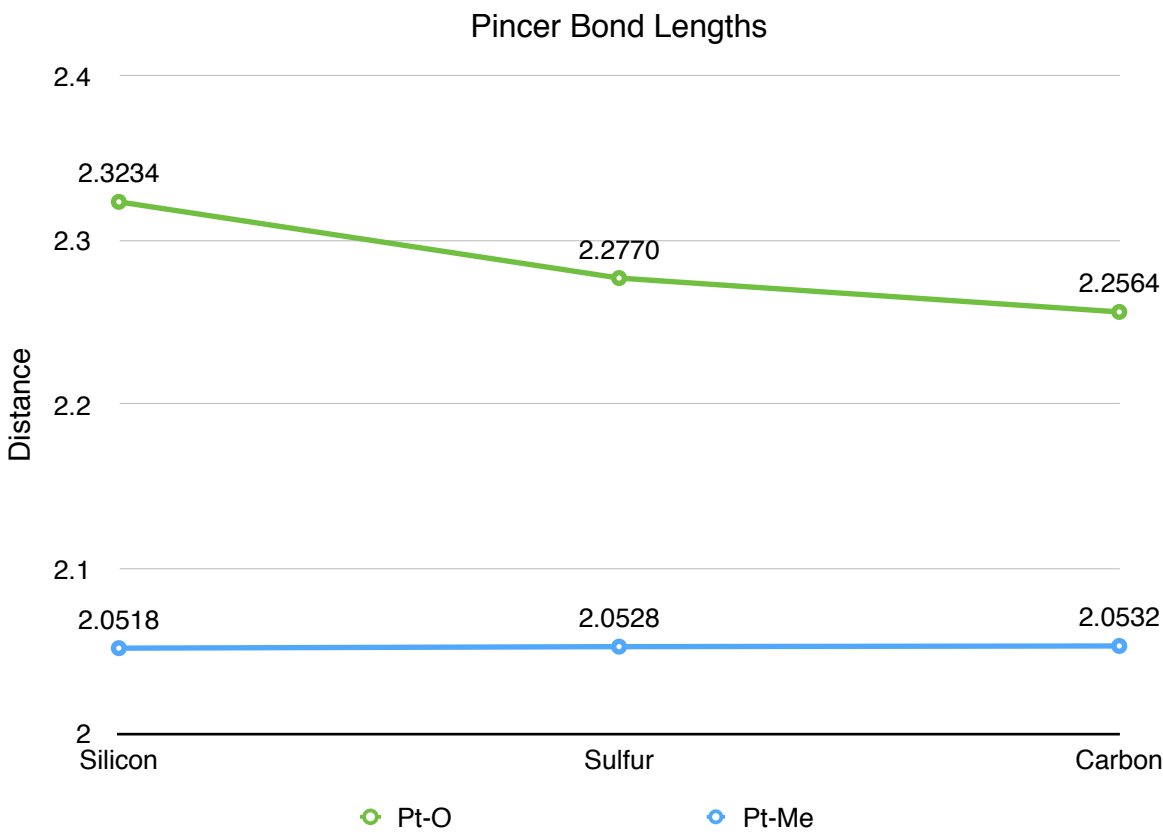
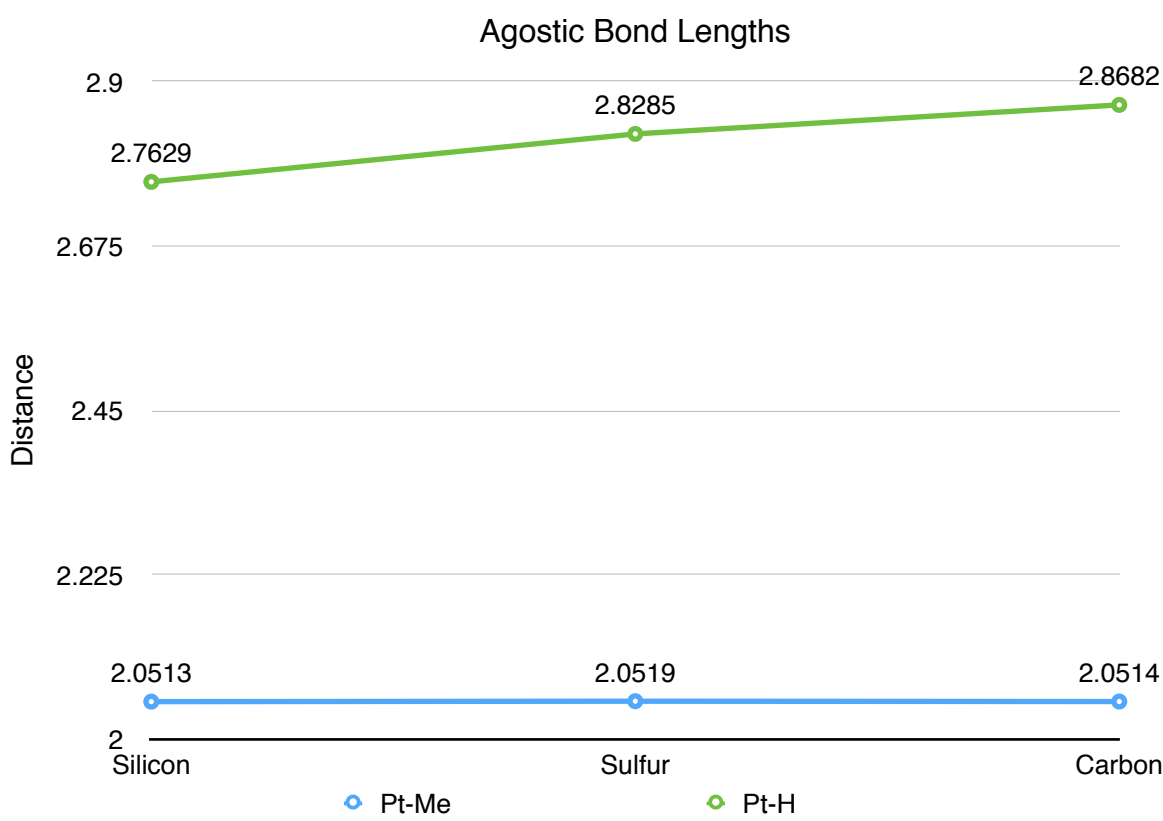


Table 2				
Experimental	13C CH3	1J Pt-CH3	1H CH3	2H Pt-CH3
Silicon	-22.7	780.5	2.01	98.6
Sulfur	-23.8	777.2	1.94	97.4
Carbon	-23.9	774.6	1.92	97.4

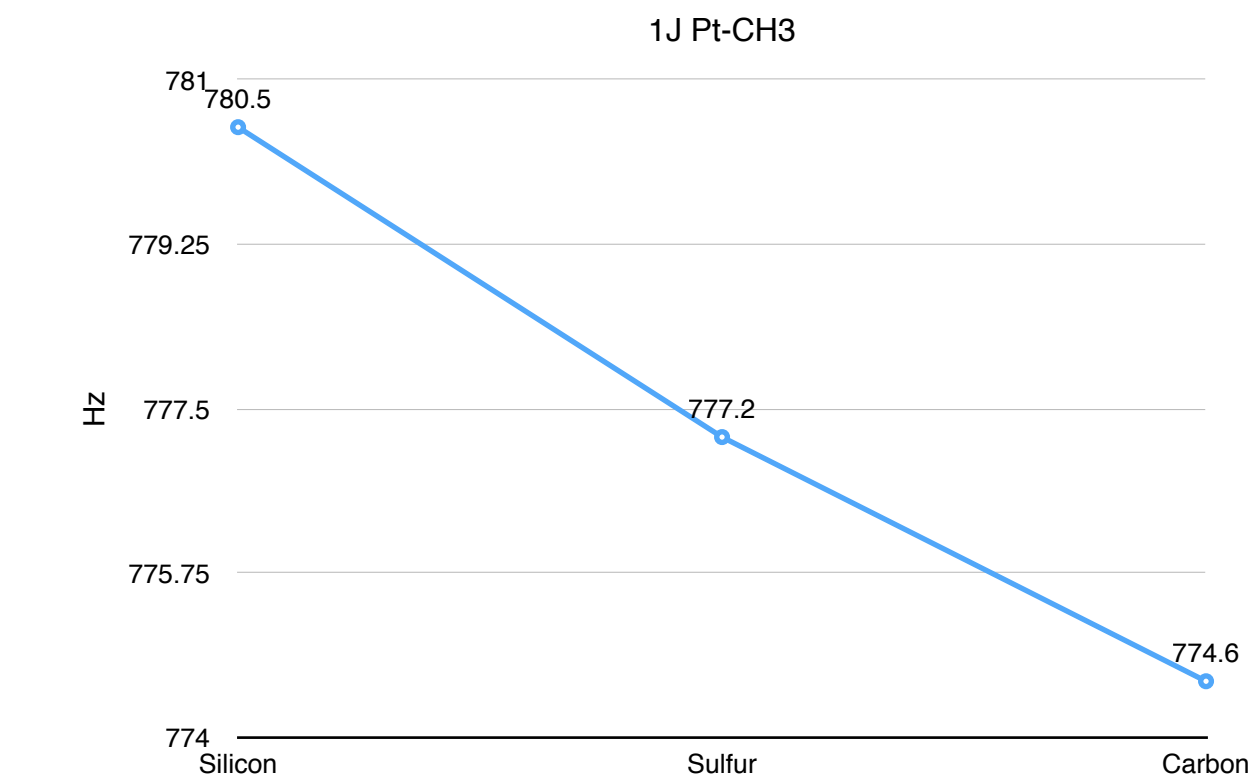


Table 3				
	Agostic	Pincer	Difference	
Silicon	-6246785.45783665	-6246898.41564208	-112.957805424929	
Sulfur	-6528919.11831231	-6529031.84297333	-112.724661025219	
Carbon	-5586640.3238789	-5586765.57259501	-125.248716104776	