				DFT Isotropic	Shielding Consta	nts	Experimental Shifts	Hexafluorobenzene		
doublemontecarlogen3D333					-130.241			-163	293.241	130.241
doublemontecarlogen3D135					-93.285			-163	256.285	93.285
doublemontecarlogen3D330					-132.692			-163	295.692	132.692
doublemontecarlogen3D606					-91.792			-163	254.792	91.792
doublemontecarlogen3D214					-116.852			-163	279.852	116.852
doublemontecarlogen3D358					-99.012			-163	262.012	99.012
	Experime	ntal Shifts vs	. DFT Shifts							
	0 —					_				
	0									
	-25									
	£									
	Experimental Shiffs — 25-					_				
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	.⊑ -75 —				•					
	ф		•							
	ய் -100 —									
	-100									
	•									
	-125	-130	-120	110	-100					
	DFT Shifts- Recalibrated with C6F6 = -163ppm									