						ML Shifts (GBR)	Experimental Shifts	ML Shifts (GBR)	Hexafluorobenzene	
doublemontecarlogen3D333						-130.2654428	-112.02	293.2654428	-163	130.265442
doublemontecarlogen3D135						-93.8998733	-68.08	256.8998733	-163	93.899873
doublemontecarlogen3D330						-132.6925431	-117.35	295.6925431	-163	132.692543
doublemontecarlogen3D606						-91.80987483	-62.91	254.8098748	-163	91.8098748
doublemontecarlogen3D214						-116.8554966	-80.67	279.8554966	-163	116.855496
doublemontecarlogen3D358						-98.94496903	-69.02	261.944969	-163	98.94496903
	Exp	erimental	Shifts	vs. ML S	hifts					
		0								
		-25								
	Experimental Shifts	-50								
	riment	-75					• •			
		-100								
		•								
		-125 -130)	-120	-1	10 -1	00			
				ML Shifts - R	Recalibrated wit	h C6F6 = -163ppm				