

	DFT Isotropic Shielding Constants	Experimental Shifts	Hexafluorobenzene		
doublemontecarlogen3D333	-130.241	-112.02	-163	293.241	130.241
doublemontecarlogen3D135	-93.285	-68.08	-163	256.285	93.285
doublemontecarlogen3D330	-132.692	-117.35	-163	295.692	132.692
doublemontecarlogen3D606	-91.792	-62.91	-163	254.792	91.792
doublemontecarlogen3D214	-116.852	-80.67	-163	279.852	116.852
doublemontecarlogen3D358	-99.012	-69.02	-163	262.012	99.012

