

	ML Shifts (GBR)	Experimental Shifts	ML Shifts (GBR)	Hexafluorobenzene	
doublemontecarlogen3D333	-130.2654428	-112.02	293.2654428	-163	130.2654428
doublemontecarlogen3D135	-93.8998733	-68.08	<u>256.8998733</u>	-163	93.8998733
doublemontecarlogen3D330	-132.6925431	-117.35	295.6925431	-163	132.6925431
doublemontecarlogen3D606	-91.80987483	-62.91	254.8098748	-163	91.80987483
doublemontecarlogen3D214	-116.8554966	-80.67	279.8554966	-163	116.8554966
doublemontecarlogen3D358	-98.94496903	-69.02	261.944969	-163	98.94496903

