TABLE 1. Cartesian coordinates (in Angstrom) of eclipsed ferrocene.

	$^1A_1$			$^3B_2$			$^5A_1$		
atom	x	y	z	x	y	z	x	y	z
C	1.209358	0.000000	1.658315	-1.198571	0.000000	1.742034	-1.346852	0.000000	1.959365
C	1.209358	0.000000	-1.658315	-1.198571	0.000000	-1.742034	-1.346852	0.000000	-1.959365
C	0.373712	-1.150168	1.658315	-0.372681	1.163937	1.809968	-0.517477	1.144729	1.963818
C	0.373712	1.150168	1.658315	-0.372681	-1.163937	1.809968	-0.517477	-1.144729	1.963818
C	0.373712	1.150168	-1.658315	-0.372681	-1.163937	-1.809968	-0.517477	-1.144729	-1.963818
C	0.373712	-1.150168	-1.658315	-0.372681	1.163937	-1.809968	-0.517477	1.144729	-1.963818
C	-0.978391	-0.710843	1.658315	0.960440	0.721076	1.783433	0.833051	0.711200	1.972742
C	-0.978391	0.710843	1.658315	0.960440	-0.721076	1.783433	0.833051	-0.711200	1.972742
C	-0.978391	0.710843	-1.658315	0.960440	-0.721076	-1.783433	0.833051	-0.711200	-1.972742
C	-0.978391	-0.710843	-1.658315	0.960440	0.721076	-1.783433	0.833051	0.711200	-1.972742
H	2.287829	0.000000	1.641304	-2.277672	0.000000	1.707696	-2.426015	0.000000	1.936450
H	2.287829	0.000000	-1.641304	-2.277672	0.000000	-1.707696	-2.426015	0.000000	-1.936450
H	0.706978	-2.175855	1.641304	-0.711177	2.187068	1.809691	-0.853225	2.170583	1.959565
H	0.706978	2.175855	1.641304	-0.711177	-2.187068	1.809691	-0.853225	-2.170583	1.959565
H	0.706978	2.175855	-1.641304	-0.711177	-2.187068	-1.809691	-0.853225	-2.170583	-1.959565
H	0.706978	-2.175855	-1.641304	-0.711177	2.187068	-1.809691	-0.853225	2.170583	-1.959565
H	-1.850892	-1.344752	1.641304	1.839490	1.346662	1.776587	1.704837	1.346394	2.008769
H	-1.850892	1.344752	1.641304	1.839490	-1.346662	1.776587	1.704837	-1.346394	2.008769
H	-1.850892	1.344752	-1.641304	1.839490	-1.346662	-1.776587	1.704837	-1.346394	-2.008769
H	-1.850892	-1.344752	-1.641304	1.839490	1.346662	-1.776587	1.704837	1.346394	-2.008769
Fe	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

TABLE 2. Cartesian coordinates (in Angstrom) of staggered ferrocene.

	^1A_g			^3B_g			^5A_g		
atom	x	y	z	x	y	z	x	y	z
C	1.208914	0.000000	1.662016	0.822816	0.000000	1.957409	0.799115	0.000000	2.253385
C	-1.208914	0.000000	-1.662016	-0.822816	0.000000	-1.957409	-0.799115	0.000000	-2.253385
C	0.373575	1.149745	1.662016	0.000000	1.162856	1.852504	0.000000	1.144923	2.035491
C	0.373575	-1.149745	1.662016	0.000000	-1.162856	1.852504	0.000000	-1.144923	2.035491
C	-0.373575	1.149745	-1.662016	0.000000	1.162856	-1.852504	0.000000	1.144923	-2.035491
C	-0.373575	-1.149745	-1.662016	0.000000	-1.162856	-1.852504	0.000000	-1.144923	-2.035491
C	-0.978032	0.710582	1.662016	-1.299359	0.721232	1.554295	-1.304902	0.711530	1.684435
C	-0.978032	-0.710582	1.662016	-1.299359	-0.721232	1.554295	-1.304902	-0.711530	1.684435
C	0.978032	0.710582	-1.662016	1.299359	0.721232	-1.554295	1.304902	0.711530	-1.684435
C	0.978032	-0.710582	-1.662016	1.299359	-0.721232	-1.554295	1.304902	-0.711530	-1.684435
H	2.287264	0.000000	1.640907	1.885698	0.000000	2.147056	1.845736	0.000000	2.518006
H	-2.287264	0.000000	-1.640907	-1.885698	0.000000	-2.147056	-1.845736	0.000000	-2.518006
H	0.706803	2.175317	1.640907	0.331797	2.186151	1.919606	0.324066	2.170793	2.122847
H	0.706803	-2.175317	1.640907	0.331797	-2.186151	1.919606	0.324066	-2.170793	2.122847
H	-0.706803	2.175317	-1.640907	-0.331797	2.186151	-1.919606	-0.324066	2.170793	-2.122847
H	-0.706803	-2.175317	-1.640907	-0.331797	-2.186151	-1.919606	-0.324066	-2.170793	-2.122847
H	-1.850435	1.344420	1.640907	-2.157801	1.347370	1.367033	-2.155414	1.346817	1.490249
H	-1.850435	-1.344420	1.640907	-2.157801	-1.347370	1.367033	-2.155414	-1.346817	1.490249
H	1.850435	1.344420	-1.640907	2.157801	1.347370	-1.367033	2.155414	1.346817	-1.490249
H	1.850435	-1.344420	-1.640907	2.157801	-1.347370	-1.367033	2.155414	-1.346817	-1.490249
Fe	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000