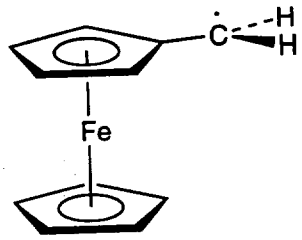
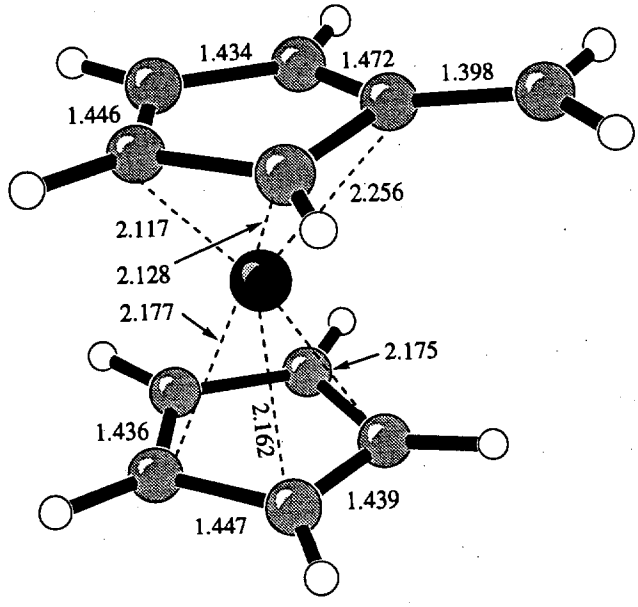


5

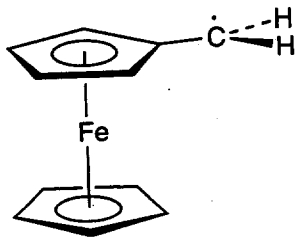


B3LYP/LANL2DZ Optimized Geometry of **5**.

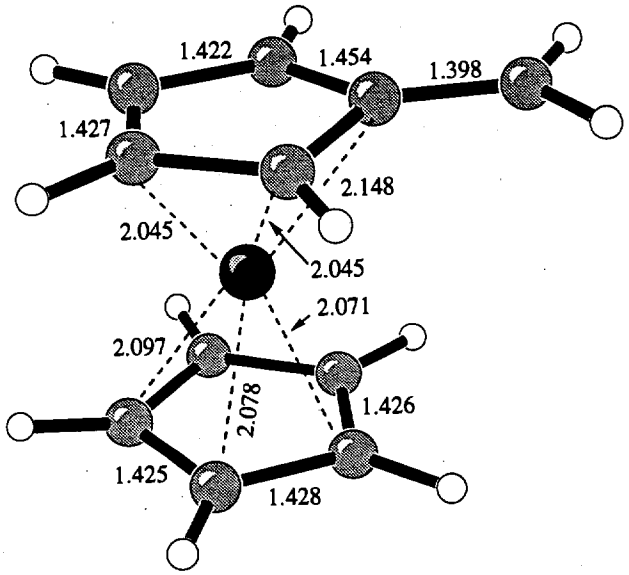
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.159200	-0.128386	0.063852
2	6	0	-0.628252	-1.956134	0.904765
3	6	0	0.351418	-1.868021	-1.204919
4	6	0	-0.904704	-1.937613	-0.506737
5	6	0	0.807696	-1.939402	1.080134
6	6	0	1.412316	-1.886159	-0.221187
7	1	0	-1.362957	-2.004193	1.696856
8	1	0	0.482213	-1.838368	-2.278041
9	1	0	-1.885665	-1.933755	-0.962284
10	1	0	1.331680	-1.958797	2.026147
11	1	0	2.472828	-1.857920	-0.431702
12	6	0	1.364072	1.603256	-0.116468
13	6	0	-0.648943	1.570495	1.058673
14	6	0	0.777665	1.545189	1.203661
15	6	0	0.298641	1.664441	-1.074843
16	6	0	-0.984117	1.768982	-0.360645
17	1	0	2.421522	1.588216	-0.341523
18	1	0	-1.370750	1.556703	1.864267
19	1	0	1.320659	1.478436	2.136274
20	1	0	0.411971	1.733990	-2.148380
21	6	0	-2.259085	1.884493	-0.921882
22	1	0	-3.149276	1.896002	-0.298674
23	1	0	-2.395195	1.970360	-1.996604

E(UB+HF-LYP) = -549.105090966 au

Zero-point correction = 0.182900 (Hartree/Particle)



5

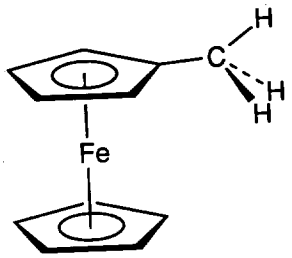


B3LYP/6-31G* Optimized Geometry of **5**.

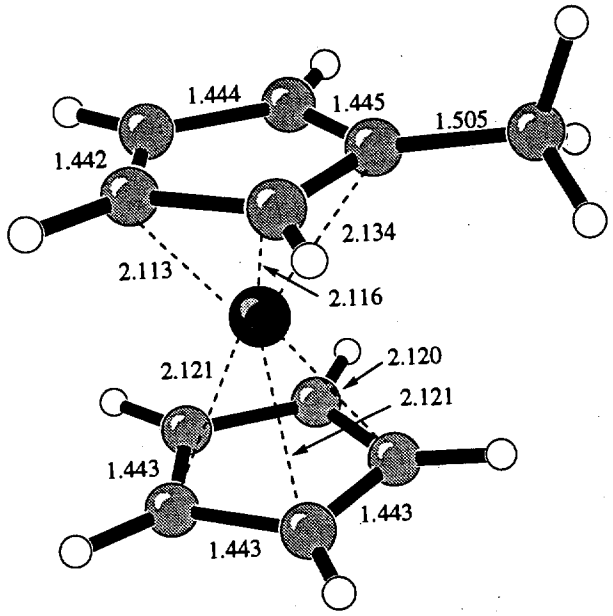
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.171839	-0.121304	0.031374
2	6	0	-0.910546	-1.811109	0.544325
3	6	0	0.760351	-1.798017	-1.046316
4	6	0	-0.654729	-1.799020	-0.858689
5	6	0	0.347338	-1.817670	1.219234
6	6	0	1.379509	-1.823618	0.236840
7	1	0	-1.884931	-1.802472	1.015178
8	1	0	1.274180	-1.774778	-1.998932
9	1	0	-1.400316	-1.779196	-1.642857
10	1	0	0.491921	-1.812308	2.292130
11	1	0	2.444150	-1.813349	0.431043
12	6	0	1.304721	1.505283	-0.472575
13	6	0	-0.364069	1.525540	1.119465
14	6	0	1.045355	1.494620	0.931030
15	6	0	0.055619	1.542823	-1.151746
16	6	0	-1.014861	1.657268	-0.174271
17	1	0	2.280498	1.458665	-0.939010
18	1	0	-0.878839	1.527916	2.072118
19	1	0	1.790128	1.438625	1.714647
20	1	0	-0.084734	1.560374	-2.225309
21	6	0	-2.386640	1.752610	-0.427005
22	1	0	-3.104864	1.782020	0.385293
23	1	0	-2.767286	1.796156	-1.441772

E(UB+HF-LYP) = -1689.36809033 au

Zero-point correction = 0.184259 (Hartree/Particle)



6

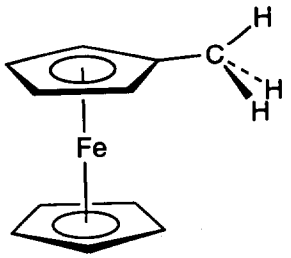


B3LYP/LANL2DZ Optimized Geometry of **6**.

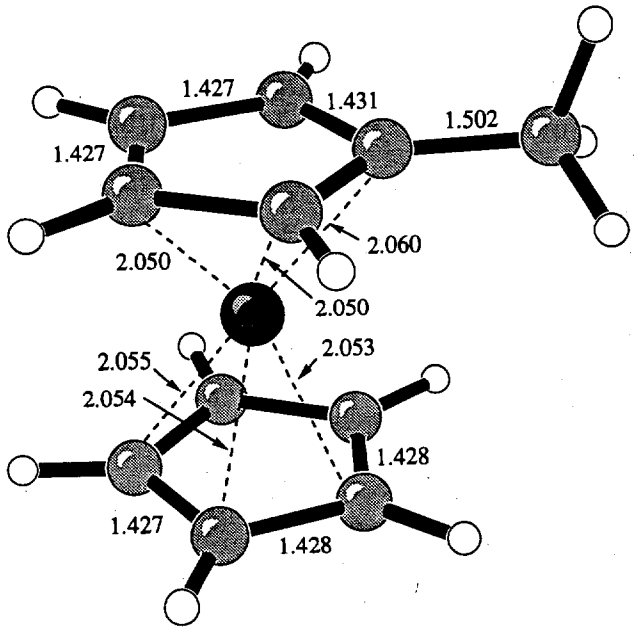
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.203586	-0.148772	0.083248
2	6	0	-0.662897	-1.893497	0.921489
3	6	0	0.264886	-1.820517	-1.220123
4	6	0	-0.977190	-1.815066	-0.484993
5	6	0	0.773049	-1.946100	1.055678
6	6	0	1.346568	-1.900951	-0.268114
7	1	0	-1.377455	-1.904506	1.732834
8	1	0	0.367554	-1.767251	-2.295125
9	1	0	-1.968728	-1.758946	-0.912613
10	1	0	1.322765	-2.002865	1.984927
11	1	0	2.401374	-1.917955	-0.504765
12	6	0	1.457353	1.541458	-0.102120
13	6	0	-0.551881	1.556498	1.081700
14	6	0	0.883851	1.496443	1.220572
15	6	0	0.372905	1.629095	-1.050956
16	6	0	-0.875712	1.646185	-0.323765
17	1	0	2.511105	1.508271	-0.341416
18	1	0	-1.270298	1.539233	1.890394
19	1	0	1.430672	1.423489	2.150316
20	1	0	0.471856	1.676022	-2.127256
21	6	0	-2.253178	1.776606	-0.916651
22	1	0	-2.540762	2.834578	-1.004650
23	1	0	-3.006740	1.280299	-0.293199
24	1	0	-2.301099	1.336790	-1.920212

E(RB+HF-LYP) = -549.751964685 au

Zero-point correction = 0.196614 (Hartree/Particle)



6

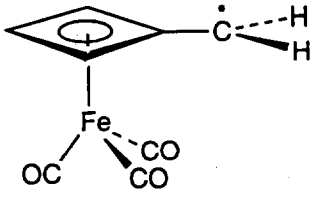


B3LYP/6-31G* Optimized Geometry of **6**.

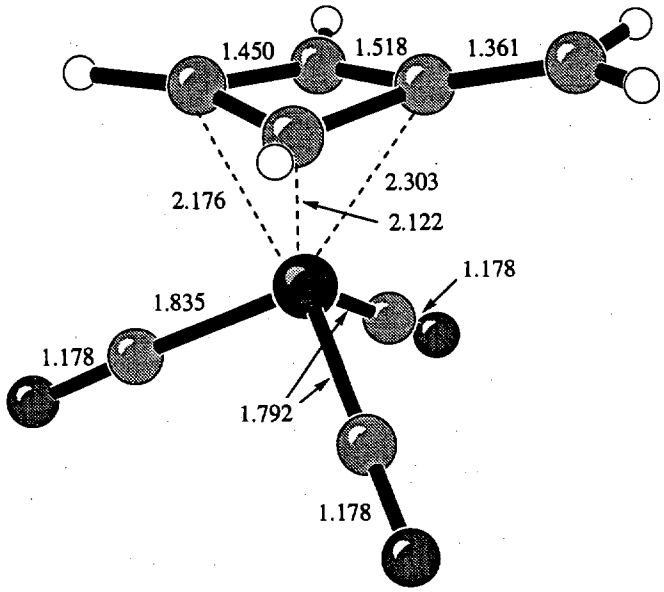
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.216055	-0.143475	0.038529
2	6	0	-0.954567	-1.754602	0.536615
3	6	0	0.716476	-1.807109	-1.057294
4	6	0	-0.697176	-1.743307	-0.867444
5	6	0	0.300011	-1.825431	1.214492
6	6	0	1.332199	-1.857932	0.229311
7	1	0	-1.928678	-1.702858	1.005652
8	1	0	1.231466	-1.801335	-2.009336
9	1	0	-1.441700	-1.681489	-1.650659
10	1	0	0.443932	-1.835899	2.287251
11	1	0	2.396269	-1.896548	0.424098
12	6	0	1.387577	1.463456	-0.457952
13	6	0	-0.284751	1.518618	1.129445
14	6	0	1.129182	1.451900	0.945273
15	6	0	0.131775	1.537216	-1.132554
16	6	0	-0.912844	1.568929	-0.155182
17	1	0	2.360725	1.404899	-0.928204
18	1	0	-0.802864	1.512116	2.080739
19	1	0	1.871203	1.382944	1.730279
20	1	0	-0.013398	1.547392	-2.205989
21	6	0	-2.383798	1.707187	-0.425485
22	1	0	-2.675022	2.765198	-0.471659
23	1	0	-2.982574	1.235019	0.360889
24	1	0	-2.661302	1.247343	-1.380190

E(RB+HF-LYP) = -1690.02154679 au

Zero-point correction = 0.198316 (Hartree/Particle)



7

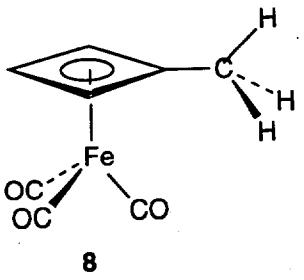


B3LYP/LANL2DZ Optimized Geometry of **7**.

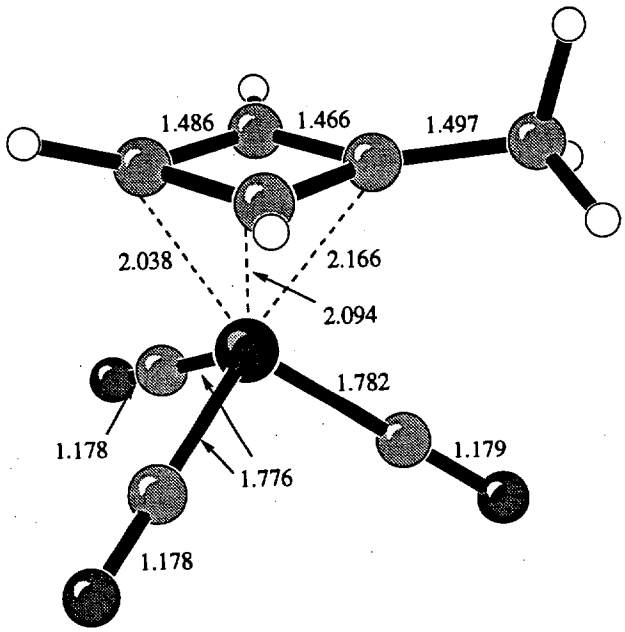
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.128870	1.781292	0.269654
2	6	0	0.056188	1.785709	1.074981
3	6	0	1.021606	1.676854	-0.001588
4	1	0	0.139088	1.912112	2.145035
5	1	0	2.085803	1.850225	-0.064926
6	6	0	-0.109301	1.801277	-1.006135
7	6	0	-1.062951	1.642671	0.163880
8	6	0	-0.219046	2.001207	-2.348211
9	1	0	0.661649	2.103631	-2.976457
10	1	0	-1.190623	2.073681	-2.829449
11	26	0	0.015279	-0.184728	0.153634
12	6	0	0.159056	-0.934635	1.822052
13	8	0	0.250771	-1.444016	2.880653
14	6	0	1.340382	-1.100478	-0.632104
15	8	0	2.215705	-1.696332	-1.148299
16	6	0	-1.386194	-1.144945	-0.417206
17	8	0	-2.311819	-1.770149	-0.791399

E(UB+HF-LYP) = -656.819464809 au

Zero-point correction = 0.105162 (Hartree/Particle)



8



B3LYP/LANL2DZ Optimized Geometry of **8**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.149801	1.713878	0.070585
2	6	0	0.050596	1.679615	0.886240
3	6	0	0.989723	1.648956	-0.239217
4	6	0	0.185699	1.912740	2.358563
5	1	0	2.055220	1.797676	-0.328727
6	6	0	-0.145433	1.592246	-1.196284
7	6	0	-1.081421	1.608080	-0.042544
8	1	0	-0.249514	1.780925	-2.252357
9	1	0	0.183979	2.992985	2.563092
10	1	0	1.123513	1.502374	2.749412
11	1	0	-0.645352	1.467777	2.917158
12	26	0	-0.016223	-0.186853	-0.209863
13	6	0	0.149369	-1.103173	1.309893
14	8	0	0.259492	-1.699572	2.321179
15	6	0	1.263152	-0.986169	-1.146883
16	8	0	2.112225	-1.497157	-1.784425
17	6	0	-1.418847	-1.040106	-0.886971
18	8	0	-2.353375	-1.587091	-1.351692

E(RB+HF-LYP) = -657.456537116 au

Zero-point correction = 0.118409 (Hartree/Particle)