Electronic Supplementary Material (ESI) for RSC Advances.

The d-electrons of Fe in ferrocene: exceed orbital energy spectrum (EOES)

Supplementary Materials

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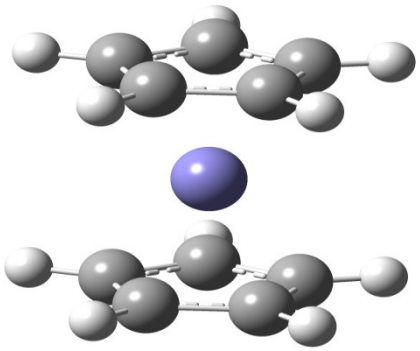
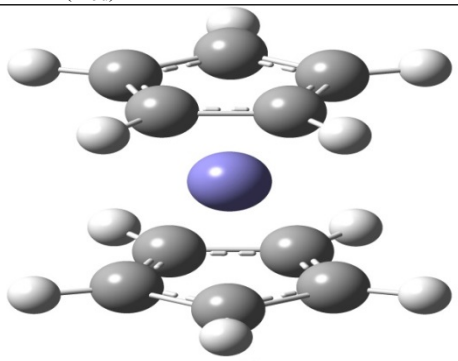
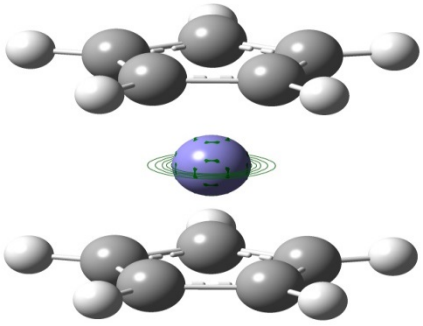
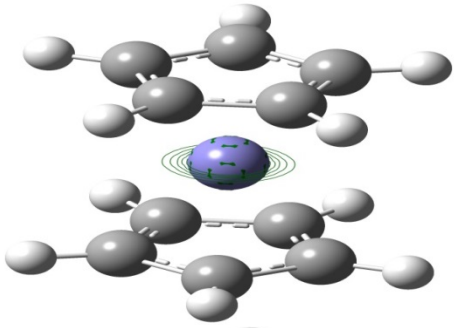
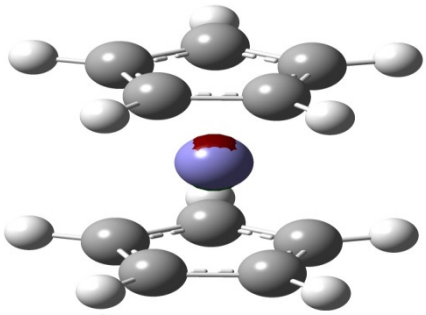
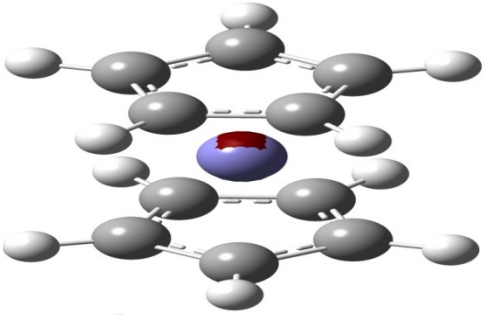
Table S1 Comparison of the calculated orbital energies of Fc using HF the B3LYP models.

MO	B3LYP/m6-31G*					HF/m6-31G*				
		D_{5h}		D_{5d}	Δε (Kcal•mol^{-1})		D_{5h}		D_{5d}	Δε (Kcal•mol^{-1})
		E (a.u.)		E (a.u.)			E (a.u.)		E(a.u.)	
1	a_1'	-256.07902	a_{1g}	-256.07788	-0.72	a_1'	-261.35039	a_{1g}	-261.34976	-0.40
2	a_1'	-30.03923	a_{1g}	-30.03787	-0.85	a_1'	-31.93078	a_{1g}	-31.92999	-0. 50
3	a_2''	-25.91638	a_{2u}	-25.91536	-0.64	a_2''	-27.42944	a_{2u}	-27.42878	-0.41
4	e_1'	-25.89751	e_{1u}	-25.89601	-0.94	e_1'	-27.40418	e_{1u}	-27.40335	-0.52
5	e_1'	-25.89751	e_{1u}	-25.89601	-0.94	e_1'	-27.40418	e_{1u}	-27.40335	-0.52
6	a_1'	-10.18289	a_{1g}	-10.18299	0.06	a_1'	-11.22748	a_{1g}	-11.22765	0.11
7	a_2''	-10.18287	a_{2u}	-10.18298	0.06	a_2''	-11.22747	a_{2u}	-11.22765	0.11
8	e_1'	-10.18264	e_{1u}	-10.18274	0.06	e_1'	-11.22682	e_{1u}	-11.22699	0.11
9	e_1'	-10.18264	e_{1u}	-10.18274	0.06	e_1'	-11.22682	e_{1u}	-11.22699	0.11
10	e_1''	-10.18261	e_{1g}	-10.18271	0.06	e_1''	-11.22681	e_{1g}	-11.22699	0.11
11	e_1''	-10.18261	e_{1g}	-10.18271	0.06	e_1''	-11.22681	e_{1g}	-11.22699	0.11
12	e_2''	-10.18219	e_{2u}	-10.18229	0.06	e_2''	-11.22566	e_{2u}	-11.22583	0.11
13	e_2''	-10.18219	e_{2u}	-10.18229	0.06	e_2''	-11.22566	e_{2u}	-11.22583	0.11
14	e_2'	-10.18216	e_{2g}	-10.18227	0.07	e_2'	-11.22565	e_{2g}	-11.22583	0.11
15	e_2'	-10.18216	e_{2g}	-10.18227	0.07	e_2'	-11.22565	e_{2g}	-11.22583	0.11
16	a_1'	-3.41056	a_{1g}	-3.40949	-0.67	a_1'	-4.11094	a_{1g}	-4.11048	-0.29
17	a_2''	-2.21232	a_{2u}	-2.21169	-0.40	a_2''	-2.71397	a_{2u}	-2.71348	-0.31
18	e_1'	-2.16587	e_{1u}	-2.16459	-0.80	e_1'	-2.67898	e_{1u}	-2.67853	-0.28
19	e_1'	-2.16587	e_{1u}	-2.16459	-0.80	e_1'	-2.67898	e_{1u}	-2.67853	-0.28
20	a_1'	-0.88364	a_{1g}	-0.88343	-0.13	a_1'	-1.18319	a_{1g}	-1.18304	-0.09
21	a_2''	-0.86796	a_{2u}	-0.86798	0.01	a_2''	-1.1629	a_{2u}	-1.16303	0.08
22	e_1''	-0.70583	e_{1g}	-0.70575	-0.05	e_1''	-0.9602	e_{1g}	-0.96021	0.01
23	e_1''	-0.70583	e_{1g}	-0.70575	-0.05	e_1''	-0.9602	e_{1g}	-0.96021	0.01
24	e_1'	-0.70498	e_{1u}	-0.70488	-0.06	e_1'	-0.9598	e_{1u}	-0.95977	-0.02
25	e_1'	-0.70498	e_{1u}	-0.70488	-0.06	e_1'	-0.9598	e_{1u}	-0.95977	-0.02
26	e_2'	-0.54204	e_{2g}	-0.54168	-0.23	e_2'	-0.74315	e_{2g}	-0.74272	-0.27
27	e_2'	-0.54204	e_{2g}	-0.54168	-0.23	e_2'	-0.74315	e_{2g}	-0.74272	-0.27
28	e_2''	-0.53415	e_{2u}	-0.53453	0.24	e_2''	-0.73117	e_{2u}	-0.73169	0.33
29	e_2''	-0.53415	e_{2u}	-0.53453	0.24	e_2''	-0.73117	e_{2u}	-0.73169	0.33
30	a_1'	-0.5315	a_{1g}	-0.53125	-0.16	a_1'	-0.7242	a_{1g}	-0.72384	-0.23
31	a_2''	-0.51875	a_{2u}	-0.51888	0.08	a_2''	-0.69948	a_{2u}	-0.69967	0.12
32	e_1''	-0.40515	e_{1g}	-0.40513	-0.01	e_1''	-0.55802	e_{1g}	-0.55828	0.16
33	e_1''	-0.40515	e_{1g}	-0.40513	-0.01	e_1''	-0.55802	e_{1g}	-0.55828	0.16
34	a_1'	-0.40351	a_{1g}	-0.40341	-0.06	a_1'	-0.56217	a_{1g}	-0.56232	0.09
35	e_1'	-0.39664	e_{1u}	-0.3961	-0.34	e_1'	-0.55251	e_{1u}	-0.55186	-0.41
36	e_1'	-0.39664	e_{1u}	-0.3961	-0.34	e_1'	-0.55251	e_{1u}	-0.55186	-0.41
37	e_2'	-0.37516	e_{2u}	-0.37316	-1.26	e_2'	-0.52637	e_{2g}	-0.52334	-1.90
38	e_2'	-0.37516	e_{2u}	-0.37316	-1.26	e_2'	-0.52637	e_{2g}	-0.52334	-1.90
39	e_2''	-0.3705	e_{2g}	-0.37251	1.26	e_2''	-0.51755	e_{2u}	-0.52087	2.08
40	e_2''	-0.3705	e_{2g}	-0.37251	1.26	e_2''	-0.51755	e_{2u}	-0.52087	2.08
41	a_2''	-0.35211	a_{2u}	-0.35249	0.24	a_2''	-0.49016	a_{2u}	-0.49072	0.35
42	e_1''	-0.26125	e_{1g}	-0.26139	0.09	e_1''	-0.33588	e_{1g}	-0.3361	0.14
43	e_1''	-0.26125	e_{1g}	-0.26139	0.09	e_1''	-0.33588	e_{1g}	-0.3361	0.14
44	e_1'	-0.24297	e_{1u}	-0.24265	-0.20	e_1'	-0.33681	e_{1u}	-0.33649	-0.20
45	e_1'	-0.24297	e_{1u}	-0.24265	-0.20	e_1'	-0.33681	e_{1u}	-0.33649	-0.20
46	a_1'	-0.22052	a_{1g}	-0.22	-0.33	a_1'	-0.50021	a_{1g}	-0.50003	-0.11
47	e_2'	-0.18877	e_{2g}	-0.18744	-0.83	e_2'	-0.41485	e_{2g}	-0.41484	-0.01
48	e_2'	-0.18877	e_{2g}	-0.18744	-0.83	e_2'	-0.41485	e_{2g}	-0.41484	-0.01

Figure S1 Core EOES of the E-Fc and S-Fc ferrocene conformers using B3LYP/m6-31G (d) model

MO	Δε (Kcal•mol^{-1})	E-Fc (D_{5h})	S-Fc (D_{5d})
1 a_1' (a_{1g})	-0.72		
2 a_1' (a_{1g})	-0.85		
3 a_2'' (a_{2u})	-0.64		
4 , 5 e_1' (e_{1u})	-0.94