Aromatic Stabilization Energy Calculations for the Antiaromatic Fluorenyl Cation. Issues in the
Choice of Reference Systems for Positively Charged Species

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Table S1 Total energies and Cartesian coordinates for structures optimized at B3LYP/6-31G(d)
ASE calculations for C_6H_6^+ , B3LYP/6-31G(d) pp. S2-S11.

Table S1 Total energies and Cartesian coordinates for structures optimized at B3LYP/6-31G(d)

1

Total energy, -500.5447563 hartrees

H	-0.34151	-3.61148	0.00000
H	2.12509	-4.02384	0.00000
C	2.62465	-1.93048	0.00000
C	2.17314	-0.58104	0.00000
H	1.34621	2.57572	0.00000
C	0.35962	-2.78192	0.00000
C	-2.08512	2.7823	0.00000
H	-3.45586	1.10304	0.00000
C	1.74085	-3.00964	0.00000
C	0.82024	-0.34984	0.00000
H	-2.86718	3.53371	0.00000
C	0.00000	0.89162	0.00000
C	-1.41558	-0.93507	0.00000
H	2.89751	0.22749	0.00000
C	-0.09429	-1.45367	0.00000
C	-1.37417	0.4837	0.00000
C	-2.41775	1.42252	0.00000
H	-2.32228	-1.53426	0.00000
H	3.69393	-2.12083	0.00000
C	-0.74569	3.1716	0.00000
C	0.3183	2.2267	0.00000
H	-0.50121	4.22981	0.00000

2

Total energy, -540.7350859 hartrees

C	3.78532	0.00000	0.00000
C	2.72254	0.89592	0.00000
C	1.39086	0.45078	-0.00088
C	1.13223	-0.92506	-0.00177
C	2.21138	-1.82338	-0.00168
C	3.52695	-1.37452	-0.00086
C	0.27757	1.47664	-0.00103
C	-0.27757	-1.47664	-0.00292
C	-1.39086	-0.45078	-0.00055
C	-1.13223	0.92506	0.00038
C	-2.21138	1.82337	0.00251
H	-2.00585	2.89239	0.00330
C	-3.52695	1.37452	0.00360
C	-3.78532	0.00000	0.00265
C	-2.72254	-0.89593	0.00065
H	0.40236	2.13816	0.86991
H	4.80833	0.36703	0.00069
H	2.91921	1.96660	0.00068

H	2.00585	-2.89239	-0.00237
H	4.34685	-2.08797	-0.00080
H	-0.40175	-2.1394	0.86716
H	-4.34685	2.08797	0.00524
H	-4.80833	-0.36703	0.00355
H	-2.91921	-1.9666	-0.00009
H	-0.40181	-2.13543	-0.87604
H	0.40120	2.13668	-0.87330

3

Total energy, -539.8894796 hartrees

C	3.67068	-0.7883	-0.00033
C	2.45582	-1.44163	0.00000
C	1.24476	-0.69397	0.00035
C	1.28026	0.7346	0.00017
C	2.51879	1.36958	-0.00034
C	3.69699	0.61892	-0.00052
C	0.00000	-1.35146	0.0005
C	0.00000	1.52216	0.00083
C	-1.28026	0.7346	0.00019
C	-1.24476	-0.69397	0.00026
C	-2.45582	-1.44163	-0.00007
H	-2.40743	-2.52691	0.00000
C	-3.67068	-0.7883	-0.0004
C	-3.69699	0.61892	-0.00051
C	-2.51879	1.36958	-0.0002
H	0.00000	-2.44064	0.0005
H	4.59929	-1.34913	-0.00051
H	2.40743	-2.52691	0.00012
H	2.57262	2.45472	-0.00053
H	4.65328	1.13399	-0.00096
H	0.00000	2.20139	-0.86626
H	-4.59929	-1.34913	-0.00061
H	-4.65328	1.13399	-0.0008
H	-2.57262	2.45472	-0.00025
H	0.00000	2.19926	0.86963

4

Total energy, -501.4231871 hartrees

H	0.00033	2.49241	-1.17913
C	3.01703	-1.21186	-0.3000
C	3.46242	0.11445	-0.3000
C	2.54557	1.17211	-0.3000
C	1.18513	0.88664	-0.3000
C	0.73516	-0.45022	-0.3000

C	1.65137	-1.50426	-0.3000
H	3.74043	-2.02294	-0.3000
H	4.52835	0.32588	-0.3000
H	2.89846	2.20094	-0.3000
H	1.31246	-2.53719	-0.29999
C	0.00033	1.83285	-0.3000
H	0.00033	2.49241	0.57914
C	-1.18447	0.88664	-0.3000
C	-2.5449	1.17211	-0.3000
C	-3.46176	0.11445	-0.3000
C	-3.01636	-1.21186	-0.3000
C	-1.65071	-1.50426	-0.3000
C	-0.7345	-0.45022	-0.3000
H	-2.89779	2.20094	-0.3000
H	-4.52769	0.32588	-0.29999
H	-3.73977	-2.02294	-0.30001
H	-1.3118	-2.53719	-0.3000

5

Total energy, -539.8696856 hartrees

H	2.05142	2.83873	0.0000
H	4.00957	1.30788	-0.00001
C	2.83119	-0.49368	-0.00001
C	1.51052	-1.0539	-0.00001
H	-1.36041	-2.59151	-0.00001
C	1.9087	1.76189	0.0000
C	-3.83971	-0.2154	0.0000
H	-3.53755	1.9322	0.00001
C	3.00399	0.90038	-0.00001
C	0.42747	-0.21826	0.0000
H	-4.92241	-0.14979	0.0000
C	-1.04063	-0.45896	0.0000
C	-0.6518	1.82288	0.0000
H	1.39856	-2.13478	-0.00001
C	0.61672	1.20629	0.0000
C	-1.67158	0.8256	0.0000
C	-3.0663	0.95359	0.0000
H	-0.82766	2.8952	0.0000
C	-3.21918	-1.46347	0.0000
C	-1.80426	-1.60069	0.0000
H	-3.8305	-2.36107	0.0000
C	4.01022	-1.41787	0.00001
H	3.98407	-2.07494	0.87965
H	3.98393	-2.07516	-0.87947

6

Total energy, -540.7408599 hartrees

H	-0.81898	2.60467	0.87954
C	-3.13401	-1.57378	-0.00001
C	-3.80609	-0.3466	0.00001
C	-3.09011	0.85608	0.00001
C	-1.70054	0.81524	0.00001
C	-1.02215	-0.42177	0.00000
C	-1.7384	-1.62074	-0.00001
H	-3.70359	-2.49948	-0.00001
H	-4.89269	-0.32677	0.00001
H	-3.61871	1.80674	0.00002
H	-1.22239	-2.57767	-0.00002
C	-0.70124	1.95602	0.00001
H	-0.81898	2.60468	-0.87950
C	0.63102	1.23262	0.00000
C	1.92252	1.74138	-0.00001
C	3.00534	0.85393	-0.00002
C	2.81666	-0.53585	-0.00002
C	1.508	-1.04051	-0.00002
C	0.42469	-0.16319	0.00000
H	2.10045	2.81447	-0.00001
H	4.01844	1.24939	-0.00004
H	1.34635	-2.11684	-0.00004
C	3.99814	-1.47957	0.00004
H	3.99055	-2.13197	0.88229
H	3.98972	-2.13313	-0.88135
H	4.94683	-0.93364	-0.00075

7

Total energy, -539.865526 hartrees

C	-3.02204	0.53399	-0.00053
C	-3.29224	-0.83167	-0.0006
C	-2.23586	-1.74881	0.00001
C	-0.92959	-1.2397	0.00046
C	-0.66119	0.16888	0.00048
C	-1.69925	1.08139	0.00012
H	-3.85643	1.23049	-0.00103
H	-4.31982	-1.17881	-0.0011
H	-2.42035	-2.81903	0.00014
C	0.30719	-1.93446	0.00033
H	0.41642	-3.01566	0.00009
C	1.3767	-1.00487	0.00032
C	2.76268	-1.22608	-0.00012
C	3.61194	-0.11458	-0.00049
C	3.06948	1.17027	-0.00036
C	1.66647	1.40405	0.00011

C	0.821	0.31885	0.0004
H	3.16432	-2.23533	-0.00012
H	4.68808	-0.24928	-0.00091
H	3.73727	2.02695	-0.00071
H	1.29965	2.42371	0.00025
C	-1.50229	2.57483	0.0003
H	-0.9431	2.90166	0.88509
H	-0.94414	2.902	-0.88506
H	-2.45997	3.10075	0.00093

8

Total energy, -540.7397501 hartrees

H	-0.36964	-2.71641	0.87894
C	3.00863	0.62733	0.00018
C	3.30796	-0.73682	0.00013
C	2.28025	-1.68326	0.00004
C	0.96489	-1.23729	0.00000
C	0.65837	0.14178	0.00004
C	1.6894	1.10047	0.00014
H	3.82103	1.35057	0.00025
H	4.34529	-1.06065	0.00016
H	2.50839	-2.74648	0.00001
C	-0.30539	-2.05968	-0.00010
H	-0.36955	-2.71634	-0.87920
C	-1.38864	-1.00459	-0.00011
C	-2.76729	-1.17172	-0.00019
C	-3.5919	-0.04102	-0.00019
C	-3.02961	1.23791	-0.00011
C	-1.6429	1.41203	-0.00003
C	-0.81108	0.28589	-0.00003
H	-3.20416	-2.16785	-0.00026
H	-4.67207	-0.15945	-0.00025
H	-3.67633	2.11143	-0.00011
H	-1.23275	2.41511	0.00003
C	1.42448	2.58657	0.00020
H	0.85146	2.89805	-0.88262
H	0.85135	2.89795	0.88299
H	2.36400	3.14853	0.00028

9

Total energy, -542.2308924 hartrees

C	-3.75312	-0.86555	0.00068
C	-2.39225	-1.44591	-0.00061
C	-1.23575	-0.69658	-0.00090
C	-1.29643	0.77796	-0.00045
C	-2.49554	1.38113	0.00074

C	-3.82667	0.68116	0.00172
C	0.00001	-1.37544	-0.00131
C	0.00001	1.57565	-0.00200
C	1.29644	0.77796	-0.00058
C	1.23576	-0.69658	-0.00075
C	2.39224	-1.44591	0.00005
H	2.31499	-2.53253	-0.00014
C	3.75311	-0.86556	0.00161
C	3.82666	0.68116	0.00077
C	2.49553	1.38112	0.00017
H	0.00001	-2.46303	-0.00164
H	-4.28796	-1.29564	0.86333
H	-2.31501	-2.53254	-0.00123
H	-2.53927	2.46926	0.00099
H	-4.40012	1.02522	0.87212
H	0.00003	2.24153	0.87029
H	4.28728	-1.29461	0.86520
H	4.40114	1.02532	-0.86891
H	2.53927	2.46925	0.00013
H	-0.00003	2.23800	-0.87703
H	4.40096	1.02625	0.87019
H	4.29007	-1.29574	-0.85964
H	-4.40199	1.02635	-0.86698
H	-4.28943	-1.29470	-0.86151

10

Total energy, -502.9093676 hartrees

C	-3.14387	-1.20213	-0.00131
C	-3.55815	0.29944	0.00256
C	-2.46147	1.30133	-0.00049
C	-1.14675	0.91432	-0.00087
C	-0.73853	-0.51253	0.00036
C	-1.66033	-1.48553	0.00027
H	-3.58820	-1.70022	-0.87272
H	-4.20942	0.53276	-0.85563
H	-2.72977	2.35659	-0.00123
H	-1.36856	-2.53321	0.00037
C	0.00004	1.73904	-0.00186
H	0.00003	2.82473	-0.00296
C	1.14678	0.91431	-0.00087
C	2.46146	1.30131	-0.00042
C	3.55812	0.29945	0.00277
C	3.14385	-1.20213	-0.00157
C	1.66032	-1.48553	0.00015
C	0.73855	-0.51253	0.00034
H	2.72974	2.35654	-0.00111

H	4.20040	0.53040	0.86853
H	3.59154	-1.70558	0.86494
H	1.36854	-2.53321	0.00018
H	4.20972	0.53292	-0.85509
H	3.58803	-1.69992	-0.87323
H	-3.59140	-1.70527	0.86547
H	-4.20078	0.53059	0.86802

11

Total energy, -502.5569887 hartrees

H	0.00703	2.54967	0.88017
C	-3.12299	-1.13362	-0.00001
C	-3.49031	0.161	-0.00002
C	-2.51638	1.24706	-0.00001
C	-1.19276	0.95739	0.00001
C	-0.71102	-0.4111	0.00002
C	-1.67586	-1.5726	0.00006
H	-3.87489	-1.91921	-0.00002
H	-4.54637	0.42178	-0.00006
H	-2.87001	2.27499	-0.00003
H	-1.49182	-2.22466	-0.87066
C	0.00412	1.89352	-0.00001
H	0.00701	2.54964	-0.88022
C	1.18776	0.93913	-0.00001
C	2.50463	1.19640	-0.00001
C	3.52479	0.08474	0.00006
C	2.92288	-1.29659	-0.00006
C	1.59571	-1.52964	-0.00005
C	0.66035	-0.42553	0.00000
H	2.87869	2.21873	-0.00003
H	4.19985	0.18781	0.86892
H	3.61881	-2.13333	-0.00013
H	1.21796	-2.54979	-0.00012
H	-1.49188	-2.22454	0.87089
H	4.20010	0.18788	-0.86860

12

Total energy, -501.7080058 hartrees

C	3.12725	-1.05558	-0.00005
C	3.48016	0.26726	-0.00064
C	2.48305	1.28009	-0.00022
C	1.13269	0.94019	0.00014
C	0.69671	-0.46147	0.00031
C	1.72066	-1.55610	0.00132
H	3.91157	-1.80940	-0.00028

H	4.52692	0.55266	-0.00137
H	2.78371	2.32545	-0.00005
H	1.60895	-2.22974	0.86924
C	0.01344	1.79054	-0.00010
H	0.01598	2.87361	-0.00007
C	-1.12880	0.93553	-0.00020
C	-2.45634	1.25307	-0.00023
C	-3.48759	0.18510	0.00096
C	-2.97113	-1.22469	-0.00095
C	-1.65648	-1.52845	-0.00107
C	-0.66996	-0.47493	-0.00029
H	-2.78605	2.29036	-0.00045
H	-4.16227	0.35357	-0.85832
H	-3.71741	-2.01342	-0.00192
H	-1.33491	-2.56607	-0.00206
H	1.60790	-2.23262	-0.86415
H	-4.15633	0.35223	0.86544

13

Total energy, -540.105521 hartrees

C	-3.69145800	0.75111243	-0.00048249
C	-2.47704300	1.41859043	-0.00000249
C	-1.24960500	0.70868443	0.00033851
C	-1.28461000	-0.71378757	0.00024251
C	-2.51747200	-1.36477257	-0.00029549
C	-3.71769600	-0.65023357	-0.00066049
C	-0.00000000	1.39229743	0.00061951
C	-0.00000000	-1.51730457	0.00102151
C	1.28461000	-0.71378757	0.00025051
C	1.24960500	0.70868443	0.00034551
C	2.47704300	1.41859043	0.00001151
H	2.44945200	2.50585543	0.00009351
C	3.69145800	0.75111243	-0.00046249
C	3.71769600	-0.65023357	-0.00063749
C	2.51747200	-1.36477257	-0.00027949
H	-0.00000000	2.47956043	0.00071451
H	-4.62117500	1.31394343	-0.00074749
H	-2.44945200	2.50585543	0.00008051
H	-2.54147000	-2.45313457	-0.00040649
H	-4.66592600	-1.18047457	-0.00107849
H	0.00000300	-2.19276357	-0.86910049
H	4.62117500	1.31394343	-0.00072249
H	4.66592600	-1.18047457	-0.00104849
H	2.54147000	-2.45313457	-0.00038849
H	-0.00000300	-2.19080657	0.87269351

14

Total energy, -500.78239 hartrees

H	-0.38859200	-3.62187800	0.00000000
H	2.06051000	-4.04487300	0.00000000
C	2.59514500	-1.95615900	0.00000000
C	2.14425100	-0.62623900	0.00000000
H	1.41977000	2.49275100	0.00000000
C	0.31173600	-2.79023100	0.00000000
C	-1.98504100	2.83818100	0.00000000
H	-3.42858700	1.23005400	0.00000000
C	1.68800500	-3.02414200	0.00000000
C	0.77931700	-0.37786300	0.00000000
H	-2.74102100	3.61864200	0.00000000
C	0.00000000	0.86596900	0.00000000
C	-1.47929200	-0.92672200	0.00000000
H	2.86235200	0.19027600	0.00000000
C	-0.15350000	-1.46687000	0.00000000
C	-1.38686900	0.50184700	0.00000000
C	-2.37480400	1.49773600	0.00000000
H	-2.39814600	-1.50260500	0.00000000
H	3.66281300	-2.15814300	0.00000000
C	-0.62825400	3.18841400	0.00000000
C	0.37182900	2.20250200	0.00000000
H	-0.34424000	4.23725500	0.00000000

ASE calculations for $C_6H_6^+$, B3LYP/6-31G(d)
 For methodology using radical species, see Scheme 6

$\Delta E = +0.005787$ (a.u.); ASE, hexadienyl cation = +3.6 kcal/mole

Scheme I

$\Delta E (C_2) = +0.00735$ (a.u.); ASE, hexadienyl cation = +4.6 kcal/mole

$\Delta E (C_{2v}) = +0.006200$ (a.u.); ASE, hexadienyl cation = +3.9 kcal/mole

Scheme II