Supporting Information

Influence of Excited State Aromaticity in the Lowest Excited Singlet States of Fulvene Derivatives

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Contents:

6,6-Dimethylfulvene (1)
Cartesian coordinates (Å)

C	0.000000	1.260973	2.095176
C	0.000000	-1.260973	2.095176
C	0.000000	0.000000	1.276542
C	0.000000	0.000000	-0.080732
C	0.000000	1.172357	-0.972103
C	0.000000	-1.172357	-0.972103
C	0.000000	0.732135	-2.254631
C	0.000000	-0.732135	-2.254631
H	0.000000	2.205512	-0.655055
H	0.000000	-2.205512	-0.655055
H	0.000000	1.351719	-3.143138
H	0.000000	-1.351719	-3.143138
H	0.000000	2.167502	1.493422
H	0.000000	-2.167502	1.493422
H	0.876477	1.288999	2.753345
H	-0.876477	1.288999	2.753345
H	0.876477	-1.288999	2.753345
H	-0.876477	-1.288999	2.753345

Point group: C_{2v}
***E*(B3LYP/6-311+G(d)) = - 310.898279000 a. u.**

6,6-Dimethylfulvene (1)
Cartesian coordinates (Å)

C	0.000000	1.260621	2.101095
C	0.000000	-1.260621	2.101095
C	0.000000	0.000000	1.281392
C	0.000000	0.000000	-0.085198
C	0.000000	1.171845	-0.974358
C	0.000000	-1.171845	-0.974358
C	0.000000	0.730703	-2.260961
C	0.000000	-0.730703	-2.260961
H	0.000000	2.206694	-0.657892
H	0.000000	-2.206694	-0.657892
H	0.000000	1.351559	-3.151450
H	0.000000	-1.351559	-3.151450
H	0.000000	2.170106	1.502018
H	0.000000	-2.170106	1.502018
H	0.877307	1.284720	2.762043
H	-0.877307	1.284720	2.762043
H	0.877307	-1.284720	2.762043
H	-0.877307	-1.284720	2.762043

Point group: C_{2v}
***E*(UOLYP/cc-pVTZ) = -310.801406048 a. u**.

6,6-Dimethylfulvene (1)
Cartesian coordinates (Å)

C	0.000000	1.260486	2.096324
C	0.000000	-1.260486	2.096324
C	0.000000	0.000000	1.279125
C	0.000000	0.000000	-0.081099
C	0.000000	1.173105	-0.971667
C	0.000000	-1.173105	-0.971667
C	0.000000	0.732259	-2.257578
C	0.000000	-0.732259	-2.257578
H	0.000000	2.209002	-0.654690
H	0.000000	-2.209002	-0.654690
H	0.000000	1.352977	-3.148816
H	0.000000	-1.352977	-3.148816
H	0.000000	2.168672	1.496305
H	0.000000	-2.168672	1.496305
H	0.875973	1.283771	2.755326
H	-0.875973	1.283771	2.755326
H	0.875973	-1.283771	2.755326
H	-0.875973	-1.283771	2.755326

Point group: C_{2v}
***E*(IEF-PCM/B3LYP/6-311+G(d)) = -310.904954789 a. u.**

T_1 state 6,6-Dimethylfulvene (1)
Cartesian coordinates (Å)

C	-0.064333	1.267818	2.135613
C	0.064333	-1.267818	2.135613
C	0.000000	0.000000	1.334908
C	0.000000	0.000000	-0.075286
C	0.000000	1.131135	-0.958680
C	0.000000	-1.131135	-0.958680
C	-0.000124	0.681975	-2.347365
C	0.000124	-0.681975	-2.347365
H	0.012008	2.173044	-0.660041
H	-0.012008	-2.173044	-0.660041
H	0.001262	1.336944	-3.211199
H	-0.001262	-1.336944	-3.211199
H	-0.345829	2.141607	1.543886
H	0.345829	-2.141607	1.543886
H	0.900995	1.495850	2.617558
H	-0.900995	-1.495850	2.617558
H	-0.794030	1.179455	2.953524
H	0.794030	-1.179455	2.953524

Point group: C_2
***E*(UOLYP/cc-pVTZ) = -310.738308602 a. u**.

1,2,3,4-Tetrachloro-6,6-dimethylfulvene (2)
Cartesian coordinates (Å)

C	-0.256069	1.226895	3.245676
C	0.256069	-1.226895	3.245676
C	0.000000	0.000000	2.411114
C	0.000000	0.000000	1.048433
C	0.000000	1.164839	0.134307
C	0.000000	-1.164839	0.134307
C	0.016550	0.727855	-1.150555
C	-0.016550	-0.727855	-1.150555
Cl	0.222994	2.831176	0.561136
Cl	-0.222994	-2.831176	0.561136
Cl	0.135189	1.685886	-2.573807
Cl	-0.135189	-1.685886	-2.573807
H	-0.881303	1.968957	2.758603
H	0.881303	-1.968957	2.758603
H	0.687700	1.713716	3.519618
H	-0.687700	-1.713716	3.519618
H	-0.736056	0.928708	4.181961
H	0.736056	-0.928708	4.181961

Point group: C_2
***E*(B3LYP/6-311+G(d)) = -2149.37705067 a. u.**

1,2,3,4-Tetrachloro-6,6-dimethylfulvene (2)
Cartesian coordinates (Å)

C	-0.262848	1.224095	3.246851
C	0.262848	-1.224095	3.246851
C	0.000000	0.000000	2.414610
C	0.000000	0.000000	1.048836
C	0.000000	1.163052	0.136165
C	0.000000	-1.163052	0.136165
C	0.016025	0.725742	-1.150141
C	-0.016025	-0.725742	-1.150141
Cl	0.225649	2.830554	0.561009
Cl	-0.225649	-2.830554	0.561009
Cl	0.136814	1.688042	-2.575909
Cl	-0.136814	-1.688042	-2.575909
H	-0.889745	1.964923	2.759525
H	0.889745	-1.964923	2.759525
H	0.681888	1.708856	3.523270
H	-0.681888	-1.708856	3.523270
H	-0.741052	0.922931	4.182933
H	0.741052	-0.922931	4.182933

Point group: C_2
***E*(IEF-PCM/B3LYP/6-311+G(d)) = -2149.38153596 a. u.**

1,2,3,4-Tetrachloro-6,6-dimethylfulvene (2)
Cartesian coordinates (Å)

C	-0.292050	1.216300	3.256120
C	0.292050	-1.216300	3.256120
C	0.000000	0.000000	2.419520
C	0.000000	0.000000	1.047130
C	0.000000	1.166570	0.135530
C	0.000000	-1.166570	0.135530
C	0.019140	0.727610	-1.158770
C	-0.019140	-0.727610	-1.158770
Cl	0.234880	2.822850	0.554440
Cl	-0.234880	-2.822850	0.554440
Cl	0.145460	1.681280	-2.572070
Cl	-0.145460	-1.681280	-2.572070
H	-0.895600	1.966340	2.751800
H	0.895600	-1.966340	2.751800
H	0.640920	1.696780	3.581910
H	-0.640920	-1.696780	3.581910
H	-0.810660	0.901480	4.168780
H	0.810660	-0.901480	4.168780

Point group: C_2
***E*(UOLYP/cc-pVTZ) = -2149.35217261 a. u.**

1,2,3,4-Tetrachloro-6,6-(*N*,*N*'-dipyrrolidino)fulvene (3)
Cartesian coordinates (Å)

C	0.000000	0.000000	1.157486
C	0.000000	0.000000	-0.257545
C	-0.103307	1.139352	-1.132308
C	0.103307	-1.139352	-1.132308
C	0.048428	-0.714644	-2.441558
Cl	0.000000	-2.808179	-0.630327
C	-0.048428	0.714644	-2.441558
Cl	0.000000	2.808179	-0.630327
Cl	-0.004791	1.712855	-3.853291
Cl	0.004791	-1.712855	-3.853291
N	-0.856728	0.788174	1.862159
N	0.856728	-0.788174	1.862159
C	-0.482031	1.554655	3.071817
C	-1.793134	2.207336	3.518655
C	-2.551670	2.420125	2.201859
C	-2.211003	1.169921	1.388140
H	2.228822	-1.342735	0.316330
H	0.265718	2.305965	2.793838
H	-0.047005	0.929058	3.850606
H	-2.347929	1.526786	4.172926
H	-1.620304	3.131551	4.073562
H	-2.178851	3.310069	1.688249
H	-3.627869	2.539111	2.340780
H	-2.228822	1.342735	0.316330
H	-2.902816	0.348719	1.610655
C	0.482031	-1.554655	3.071817
C	1.793134	-2.207336	3.518655
C	2.551670	-2.420125	2.201859
C	2.211003	-1.169921	1.388140
H	2.902816	-0.348719	1.610655
H	-0.265718	-2.305965	2.793838
H	0.047005	-0.929058	3.850606
H	2.347929	-1.526786	4.172926
H	1.620304	-3.131551	4.073562
H	2.178851	-3.310069	1.688249
H	3.627869	-2.539111	2.340780

Point group: C_2
***E*(B3LYP/6-311+G(d)) = - 2493.61882918 a. u.**

1,2,3,4-Tetrachloro-6,6-(*N*,*N*'-dipyrrolidino)fulvene (3)
Cartesian coordinates (Å)

C	0.000000	0.000000	1.227249
C	0.000000	0.000000	-0.229077
C	-0.070081	1.132003	-1.085978
C	0.070081	-1.132003	-1.085978
C	0.034706	-0.707364	-2.411120
Cl	0.004318	-2.800963	-0.566874
C	-0.034706	0.707364	-2.411120
Cl	-0.004318	2.800963	-0.566874
Cl	0.000000	1.724724	-3.824234
Cl	0.000000	-1.724724	-3.824234
N	-1.037251	0.535498	1.890407
N	1.037251	-0.535498	1.890407
C	-0.980934	1.138587	3.248840
C	-2.276330	1.966926	3.373904
C	-2.816665	2.090059	1.941399
C	-2.370967	0.785782	1.287790
H	2.306709	-0.824827	0.205079
H	-0.076822	1.749362	3.315615
H	-0.939536	0.376815	4.026500
H	-2.993768	1.434272	4.004114
H	-2.085124	2.935410	3.840120
H	-2.362557	2.939058	1.424647
H	-3.901265	2.213288	1.909098
H	-2.306709	0.824827	0.205079
H	-3.033699	-0.042206	1.567301
C	0.980934	-1.138587	3.248840
C	2.276330	-1.966926	3.373904
C	2.816665	-2.090059	1.941399
C	2.370967	-0.785782	1.287790
H	3.033699	0.042206	1.567301
H	0.076822	-1.749362	3.315615
H	0.939536	-0.376815	4.026500
H	2.993768	-1.434272	4.004114
H	2.085124	-2.935410	3.840120
H	2.362557	-2.939058	1.424647
H	3.901265	-2.213288	1.909098

Point group: C_2
***E*(IEF-PCM/B3LYP/6-311+G(d)) = -2493.63573835 a. u.**

1,2,3,4-Tetrachloro-6,6-(*N*,*N*'-dipyrrolidino)fulvene (3)
Cartesian coordinates (Å)

C	0.000000	0.000000	1.149540
C	0.000000	0.000000	-0.270640
C	-0.106670	1.142650	-1.146050
C	0.106670	-1.142650	-1.146050
C	0.048650	-0.716210	-2.462170
Cl	0.000000	-2.803010	-0.653350
C	-0.048650	0.716210	-2.462170
Cl	0.000000	2.803010	-0.653350
Cl	-0.002670	1.708460	-3.865140
Cl	0.002670	-1.708460	-3.865140
N	-0.901120	0.746190	1.855200
N	0.901120	-0.746190	1.855200
C	-0.591990	1.531620	3.066310
C	-1.957500	2.012190	3.560090
C	-2.762460	2.170720	2.264900
C	-2.287790	1.000150	1.401700
H	2.331630	-1.218550	0.336360
H	0.050730	2.378120	2.787400
H	0.060050	0.953340	3.824020
H	-2.414640	1.252500	4.205350
H	-1.880350	2.937340	4.138270
H	-2.515960	3.119570	1.777960
H	-3.843760	2.147100	2.425850
H	-2.331630	1.218550	0.336360
H	-2.889820	0.098930	1.587340
C	0.591990	-1.531620	3.066310
C	1.957500	-2.012190	3.560090
C	2.762460	-2.170720	2.264900
C	2.287790	-1.000150	1.401700
H	2.889820	-0.098930	1.587340
H	-0.050730	-2.378120	2.787400
H	0.060050	-0.953340	3.824020
H	2.414640	-1.252500	4.205350
H	1.880350	-2.937340	4.138270
H	2.515960	-3.119570	1.777960
H	3.843760	-2.147100	2.425850

Point group: C_2
***E*(UOLYP/cc-pVTZ) = -2493.47891334 a. u.**

1,2,3,4-Tetrachloro-6,6-dicyanofulvene (4)
Cartesian coordinates (Å)

C	0.000000	0.000000	2.117024
C	0.000000	0.000000	0.752524
C	0.000000	1.179208	-0.141413
C	0.000000	-1.179208	-0.141413
C	0.000000	0.740255	-1.419941
C	0.000000	-0.740255	-1.419941
C	0.000000	-1.184107	2.922765
C	0.000000	1.184107	2.922765
N	0.000000	-2.065588	3.668975
N	0.000000	2.065588	3.668975
Cl	0.000000	2.827084	0.342008
Cl	0.000000	-2.827084	0.342008
Cl	0.000000	1.686497	-2.839651
Cl	0.000000	-1.686497	-2.839651

Point group: C_{2v}
***E*(B3LYP/6-311+G(d)) = -2255.24060355 a. u.**

1,2,3,4-Tetrachloro-6,6-dicyanofulvene (4)
Cartesian coordinates (Å)

C	0.000000	0.000000	2.113796
C	0.000000	0.000000	0.750526
C	0.000000	1.178998	-0.142471
C	0.000000	-1.178998	-0.142471
C	0.000000	0.741640	-1.419353
C	0.000000	-0.741640	-1.419353
C	0.000000	-1.182001	2.922013
C	0.000000	1.182001	2.922013
N	0.000000	-2.060257	3.671372
N	0.000000	2.060257	3.671372
Cl	0.000000	2.828052	0.340869
Cl	0.000000	-2.828052	0.340869
Cl	0.000000	1.686178	-2.838146
Cl	0.000000	-1.686178	-2.838146

Point group: C_{2v}
***E*(IEF-PCM/B3LYP/6-311+G(d)) = -2255.25248020 a. u.**