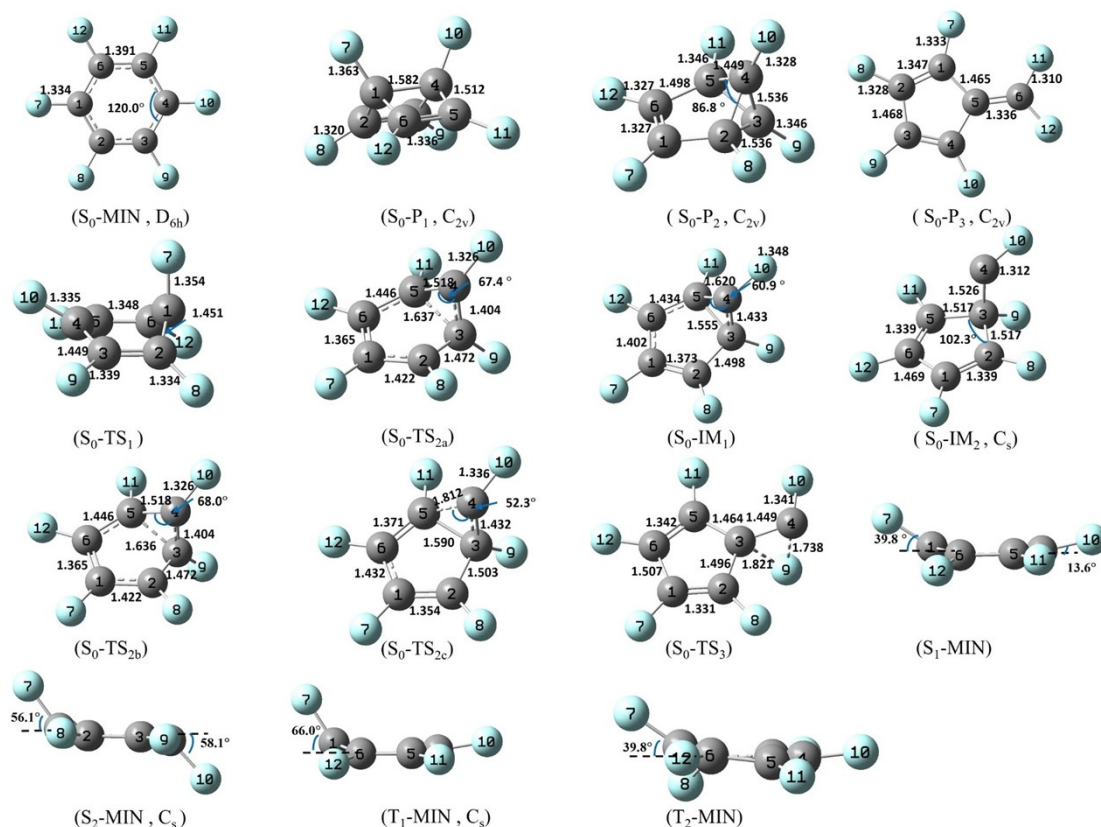


# Photochemical mechanistic study of hexafluorobenzene involving the low-lying states

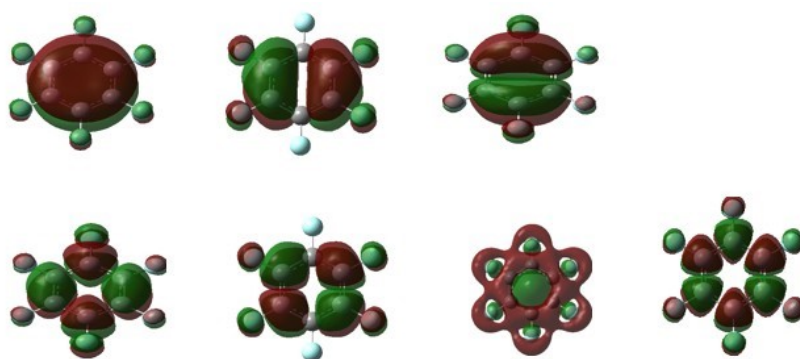
Duoduo Li,<sup>a,b</sup> Xinli Song,<sup>\*,a,b</sup> Jinming Liu,<sup>a,b</sup> Song Zhang,<sup>\*,a,b</sup>

<sup>a</sup>State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Innovation, Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan 430071, P R China

<sup>b</sup>University of Chinese Academy of Sciences, Beijing 100049, P R China



**Fig. S1** Optimized geometries of all the possible stationary points at the B3LYP/6-311G\*\* level (Unit: Å, °).



**Fig. S2** Orbitals included in the CASSCF active space at the CAS(6,7)/6-31G\* level.

**Table S1.** The HOMO and LUMO orbitals of HFBCl<sub>3</sub> at different theoretical levels.

	CAS(6,7)/ 6-31G*	CAS(6,7)/ /6-31+G*	B3LYP/ 6-31G*	B3LYP/ 6-31+G*	BP86/ 6-31G*	EOM-CCSD/ 6-31G*
HOMO						
LUMO						

**Table S2.** The structural parameters of the critical points in Cartesian coordinates (Å) at the CAS(6, 7)/6-31G\* level.

$S_0$			
C	-1.0755965698	-0.8763097126	0.0000065298
C	0.2209864456	-1.3696452742	0.0000037780
C	1.2966189679	-0.4935640532	0.0000072298
C	1.0757390629	0.8761961339	0.0000221356
C	-0.2209928667	1.3696897843	0.0000451497
C	-1.2967188219	0.4934112245	0.0000226168
F	-2.0962179699	-1.7070846788	-0.0000057095
F	0.4306460345	-2.6691005189	-0.0000037460
F	2.5267330019	-0.9611941726	-0.0000060436
F	2.0957379839	1.7074168010	-0.0000085581
F	-0.4305751448	2.6686540317	-0.0000111167
F	-2.5263811234	0.9616584340	-0.0000082659

**HFB-P<sub>1</sub>**

---

C	-0.0275987499	-0.9475035501	-0.0001042243
C	-0.5668512407	-0.4191113559	1.2987797338
C	0.1906899298	0.6786644778	1.2990225006
C	0.8758554654	0.3624460510	-0.0001044085
C	0.1913545999	0.6791994603	-1.2993548345
C	-0.5671202553	-0.4199171744	-1.2991076238
F	0.5317654716	-2.1611900403	0.0001477600
F	-1.5926432616	-0.8082543751	2.0068892951
F	0.1890672424	1.7763049458	2.0063795820
F	2.2091022090	0.2705848018	0.0001490271
F	0.1895627420	1.7773180095	-2.0060948303
F	-1.5934141527	-0.8090752505	-2.0066019773

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**HFB-P<sub>2</sub>**

---

C	1.2702878042	-0.6721045822	0.0150795339
C	-0.1832392012	-1.0500717161	0.0204095579
C	-0.9937413355	-0.0075732446	0.7283812521
C	-1.0178214665	0.0131180400	-0.7363382099
C	-0.1892053334	1.0344947436	-0.0031163542
C	1.2673303832	0.6610316103	-0.0004485515
F	2.2571782216	-1.5335865859	-0.0353991254
F	-0.5583855041	-2.3215756356	0.0234404594
F	-1.7045377282	0.0068771832	1.8278440631
F	-1.7701759490	0.0355497194	-1.8072518978
F	-0.5607272413	2.3089424201	0.0260577487
F	2.2508983500	1.5252150477	-0.0593514762

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**HFB-P<sub>3</sub>**

---

C	-0.2415366696	1.1695225238	0.0000319846
C	-1.5070196922	0.7361231736	-0.0000174146
C	-1.5077236987	-0.7360929225	-0.0000251285
C	-0.2407304848	-1.1699211320	0.0000336134
C	0.6490271689	-0.0000385615	0.0000659133
C	1.9795291874	-0.0000067674	-0.0000095527
F	0.1925504663	2.4107557872	0.0000392469
F	-2.6132375799	1.4392543153	-0.0000588375
F	-2.6145052583	-1.4389033877	-0.0000426983
F	0.1938049630	-2.4106091376	0.0000501611
F	2.7100976929	1.0712276646	-0.0000170539
F	2.7100679051	-1.0713125558	-0.0000172336

---

**S<sub>0</sub>-TS<sub>1</sub>**

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C	-0.3190845272	0.0000473129	1.1613286994
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C	0.2008010774	-1.2888761821	0.6633984449
C	0.2008010832	-1.2888759856	-0.6633983327
C	-0.3190849333	0.0000474133	-1.1613283869
C	0.2019333320	1.2885135724	-0.6633984303
C	0.2019332401	1.2885135637	0.6633983508
F	-1.4912485669	0.0005623641	1.7760744949
F	0.7155741874	-2.1854594097	1.4758602457
F	0.7155740324	-2.1854592455	-1.4758602103
F	-1.4912485573	0.0005621830	-1.7760748782
F	0.7174938544	2.1846442558	-1.4758602267
F	0.7174937779	2.1846441575	1.4758602296

### **S<sub>0</sub>-TS<sub>2a</sub> (B3LYP)**

C	1.48067700	-0.25867800	-0.01208300
C	0.39059500	-1.16046100	0.10956800
C	-0.86894900	-0.53185400	0.55669100
C	-1.21086000	-0.23117700	-0.77428800
C	-0.47174500	0.91627100	-0.09579000
C	0.97046500	1.01260800	-0.07530200
F	2.73911700	-0.63458400	-0.23317200
F	0.48329400	-2.45880700	-0.17013300
F	-1.48941600	-0.67584200	1.74359900
F	-2.35573300	-0.19702900	-1.44930400
F	-1.20781100	1.97475000	0.31394900
F	1.63709200	2.16037400	-0.01080200

### **S<sub>0</sub>-TS<sub>2b</sub>**

C	1.4957605138	-0.2200998552	-0.0101959727
C	0.4571756428	-1.1592752561	0.0703316064
C	-0.8308634399	-0.5318065532	0.4558321992
C	-1.2195643109	-0.2222207295	-0.8706415678
C	-0.4885453894	0.8909575818	0.0103848966
C	0.9466258766	1.0361208036	0.0125245783
F	2.7480575114	-0.5200282861	-0.2553931993
F	0.5901864805	-2.4411045110	-0.1589365086
F	-1.4848367010	-0.8217445776	1.5707034845
F	-2.4258697067	-0.1417249506	-1.3702518430
F	-1.2630098959	1.8833785961	0.4381016752
F	1.5844254187	2.1780747379	0.0107856513

### **S<sub>0</sub>-TS<sub>2c</sub>**

C	1.5576728462	-0.2014349316	-0.0587635389
C	0.6048132771	-1.1146092819	0.1004332642
C	-0.7681756413	-0.4494540337	0.1735333040

C	-1.392581138	-0.5117990532	-1.1883980368
C	-0.3673124032	1.0204362978	0.3055312172
C	0.9259114856	1.1494785927	0.0777244339
F	2.8191364391	-0.3657364507	-0.3432248775
F	0.7053915604	-2.4348125356	-0.0495737460
F	-1.5324176379	-0.8818855919	1.1649339708
F	-2.7367386804	-0.4726588099	-0.9692445994
F	-1.2838728708	1.9374358903	0.5459227600
F	1.6141697640	2.2470689178	0.0345168485

### **S<sub>0</sub>-TS<sub>3</sub>**

C	1.53064300	-0.17573200	-0.04170300
C	0.60404400	-1.16604700	0.10967400
C	-0.77179600	-0.60476000	0.31754600
C	-1.31382700	-0.26046600	-0.96460300
C	-0.50424600	0.88926600	-0.00863600
C	0.89317000	1.08382600	-0.03210600
F	2.83798500	-0.36080900	-0.29813100
F	0.80749000	-2.47822900	-0.11264400
F	-1.46458300	-0.98626200	1.43061100
F	-2.65192600	-0.14408600	-1.10210700
F	-1.33859600	1.85525700	0.45839100
F	1.51763900	2.27007100	0.03709900

### **S<sub>0</sub>-IM<sub>1</sub>**

C	-1.54639500	0.01198200	-0.10664900
C	-0.78169200	1.10010000	0.10595800
C	0.68205000	0.73997900	0.30446100
C	1.30457500	0.33760200	-0.90321100
C	0.64101200	0.79660900	-0.14321500
C	-0.74266300	1.17537300	-0.18347400
F	-2.82829700	0.02362100	-0.37805000
F	-1.13911600	2.34797900	-0.09009200
F	1.28900100	1.17728600	1.39261600
F	2.61497300	0.30084100	-0.99959700
F	1.49634500	1.66785500	0.37871300
F	-1.13749700	2.32699300	0.31383000

### **S<sub>0</sub>-IM<sub>2</sub>**

C	-1.3580487156	0.7395702722	-0.0479319369
C	-0.1111549297	1.1734077112	0.1236329785
C	0.8460572839	0.0030430530	0.1861177397
C	1.6908636768	0.0036753976	-1.0851688816
C	-0.1086198021	-1.1692837904	0.1178795725

C	-1.3557850981	-0.7388049309	-0.0480823385
F	-2.4582791131	1.4297287109	-0.1949804693
F	0.3352363809	2.4081674008	0.1437282401
F	1.5735173438	0.0013170342	1.3280444363
F	2.9268760061	-0.0156238235	-0.7196784381
F	0.3402166474	-2.4034288900	0.1412105069
F	-2.4537816801	-1.4317531451	-0.1955414096

### S<sub>1</sub>-MIN

C	0.0936554723	0.0000001830	-1.4577258324
C	0.0014961967	1.2122355540	-0.7128344645
C	0.0014962067	1.2122355565	0.7128344668
C	0.0936554766	0.0000001839	1.4577258320
C	0.0014976552	1.2122353340	0.7128345090
C	0.0014976679	1.2122353362	-0.7128345124
F	0.3177706583	0.0000000437	-2.7187229740
F	0.1275920863	2.3585956000	-1.3393481644
F	0.1275921182	2.3585956023	1.3393481641
F	0.3177706528	0.0000000458	2.7187229748
F	0.1275961923	2.3585951592	1.3393480526
F	0.1275962387	2.3585951608	-1.3393480516

### S<sub>1</sub>-TS<sub>1</sub>

C	1.4949167040	-0.0109047616	-0.1083535142
C	0.7465675811	-1.1747297233	-0.0400212051
C	-0.7020883887	-0.9898221374	0.0026686529
C	-1.3741052388	-0.0001863611	-0.8392608167
C	-0.6921840318	0.9936397286	0.0131752196
C	0.7330252776	1.1406433330	0.0332228147
F	2.8069859236	0.0343927025	-0.2100340592
F	1.2643038087	-2.3785535681	0.0446596077
F	-1.4118798414	-1.8258791579	0.7290985871
F	-2.6940600602	-0.0365484078	-0.7011822155
F	-1.3327746874	1.8838024027	0.7464244485
F	1.2265179531	2.3641459504	0.0184094802

### S<sub>0</sub>/S<sub>1</sub>-MSX

C	0.1021828172	0.0000915466	-1.5034747327
C	0.0280088704	1.1536950447	-0.7402895141
C	-0.0699422495	0.9512357410	0.7008831887
C	0.7877526636	-0.0001281637	1.3986155533
C	-0.0700363857	-0.9513184631	0.7007617715
C	0.0278936385	-1.1536021422	-0.7404371818
F	0.3140827042	0.0001638916	-2.8000536406

F	-0.0394250737	2.3614752856	-1.2462049023
F	-0.8164542507	1.7986915156	1.3794855268
F	0.6603682814	-0.0002059865	2.7179650592
F	-0.8166356953	-1.7987844300	1.3792552127
F	-0.0396613206	-2.3613108395	-1.2465073407

### S<sub>2</sub>-MIN

C	0.0000000448	1.4641632088	0.2784356243
C	1.2371032540	0.6711155042	0.1950783447
C	1.2392034532	-0.6674046716	-0.1867214822
C	-0.0000000463	-1.4587688575	-0.2905550370
C	-1.2392035082	-0.6674046470	-0.1867212245
C	-1.2371031982	0.6711155254	0.1950786116
F	-0.0000000434	2.5456526303	-0.5057470636
F	2.3727653153	1.3296964558	0.2511396157
F	2.3722916293	-1.3297738198	-0.2321703855
F	0.0000000400	-2.5583141317	0.4632120620
F	-2.3722917142	-1.3297737393	-0.2321700320
F	-2.3727652263	1.3296965425	0.2511399664

### S<sub>2</sub>/S<sub>1</sub>-MSX

C	-0.0004738878	1.4115923903	0.0040201345
C	1.2488523094	0.6758119098	-0.1396258929
C	1.2748718673	-0.6943164652	-0.0291049830
C	0.0000021073	-1.2795280793	0.3321137306
C	-1.2743319102	-0.6951631541	-0.0323515980
C	-1.2489410936	0.6749822807	-0.1428070584
F	-0.0019430182	2.3977981458	0.9003619779
F	2.3331022254	1.3667199948	-0.3909476131
F	2.2105221866	-1.4418104421	-0.6028518150
F	-0.0006326760	-2.3379787087	1.1065624953
F	-2.2080210499	1.4432780491	-0.6084790818
F	-2.3330060604	1.3651701775	-0.3968902963

### T<sub>1</sub>-MIN

C	-0.0000000560	-1.4880611797	-0.0597809075
C	-1.2474500666	-0.7108796623	-0.2159687521
C	-1.2440624895	0.6285891325	-0.0460434015
C	-0.0000000072	1.3290992020	0.0451034887
C	1.2440624124	0.6285891028	-0.0460442065
C	1.2474499668	-0.7108797368	-0.2159691101
F	0.0000001283	-2.2918187406	1.0063023916
F	-2.3575052125	-1.3824351616	-0.4437373184
F	-2.3468191545	1.3459055054	-0.0925559729

F	0.0000001611	2.5871555463	0.4212408790
F	2.3468191557	1.3459053727	-0.0925560659
F	2.3575051619	-1.3824353805	-0.4437370244

### T<sub>2</sub>-MIN

C	-0.0000000290	-1.5142137883	-0.0805533168
C	-1.2248796657	-0.7234788874	-0.1346044549
C	-1.2155148330	0.6668876788	-0.0333825662
C	0.0000000227	1.3723373021	0.0419546646
C	1.2155148526	0.6668876404	-0.0333826846
C	1.2248796267	-0.7234789329	-0.1346045297
F	-0.0000000205	-2.5026446616	0.8248129455
F	-2.3596981799	-1.3445634027	-0.3738966253
F	-2.3416466005	1.3378554946	-0.0762052009
F	0.0000000504	2.6698536488	0.2662178451
F	2.3416466570	1.3378553970	-0.0762053583
F	2.3596981192	-1.3445634886	-0.3738967187

### T<sub>2</sub>/S<sub>1</sub>-MSX

C	0.0246476714	-0.0114353357	1.3631247375
C	-0.1046150883	-1.2515066697	0.6410303523
C	0.0321486855	-1.2111626201	-0.7883596783
C	0.0629646056	0.0090879948	-1.5096830170
C	0.0209227401	1.2261604331	-0.8074843524
C	-0.0295294223	1.2102691867	0.6094658283
F	-0.4277219502	0.0258515397	2.6079728077
F	0.2763712393	-2.3629478346	1.2534601320
F	-0.0055882702	-2.3391077799	-1.4532841459
F	-0.0761945876	-0.0078975787	-2.8187870247
F	0.2329482796	2.3634800572	-1.4358524254
F	0.0098140471	2.3481279272	1.2572066257

### T<sub>2</sub>/T<sub>1</sub>-MSX

C	0.0000000906	-1.5633147493	0.2120648283
C	-1.0875581768	-0.7719039102	-0.1850347352
C	-1.1580694185	0.6880336253	-0.0299821995
C	-0.0000006943	1.4268077381	0.0665102106
C	1.1580691205	0.6880319443	-0.0299817877
C	1.0875592218	-0.7719044766	-0.1850341169
F	-0.0000004175	-2.5011507483	1.1736561047
F	-2.1284570413	-1.2831711368	-0.8155964349
F	-2.3380378629	1.2437592728	0.0059318431
F	0.0000006733	2.7119391981	0.3715760971
F	2.3380365576	1.2437596041	0.0059309571



F	2.1284579474	-1.2831715116	-0.8155970168
<b>T<sub>1</sub>/S<sub>1</sub>-MSX</b>			
C	-0.0002400583	-1.3977090843	0.0948175991
C	-1.2501431736	-0.6822668307	0.0420260657
C	-1.2518528225	0.6696623515	-0.0002930623
C	0.0002380219	1.4015747826	-0.0616541168
C	1.2519101814	0.6700007602	-0.0005453463
C	1.2500968931	-0.6818781633	0.0422647026
F	-0.0000717113	-2.7072545137	0.2590887016
F	-2.3574649347	-1.3732496507	-0.1573504917
F	-2.3660683519	1.3405583110	-0.2299967764
F	0.0000583319	2.6918589482	0.2152691871
F	2.3661003518	1.3405594637	-0.2309247709
F	2.3574372720	-1.3731223744	-0.1564476917
<b>T<sub>1</sub>/S<sub>0</sub>-MSX</b>			
C	-0.1147291641	-0.0009524639	1.3778510210
C	0.2829732453	-1.2378481393	0.6589154472
C	0.0362875295	-1.2492930732	-0.6709128074
C	-0.1574498555	-0.0001181984	-1.3381935202
C	0.0363627145	1.2501880638	-0.6702750730
C	0.2823654426	1.2375681958	0.6603622425
F	-1.4296263407	0.0002674913	1.6498634534
F	0.7048965379	-2.2906473553	1.3263135101
F	0.1202927101	-2.3349110135	-1.4113222525
F	-0.5740835367	0.0003794184	-2.5818957668
F	0.1242842694	2.3353605436	-1.4109691997
F	0.7045943976	2.2889258507	1.3290727852

**S1.** The details for the optimization of S<sub>1</sub>/S<sub>0</sub>-MSX, S<sub>2</sub>/S<sub>1</sub>-MSX, S<sub>0</sub>/T<sub>1</sub>-MSX and T<sub>2</sub>/T<sub>1</sub>-MSX.

① Optimization of S<sub>1</sub>/S<sub>0</sub>-MSX

\*\*\*, C6F6 CAS67-S1/S0 conical intersection optimization  
memory, 500, m  
symmetry, nosym  
geomtyp=xyz  
geom={  
12  
C6F6

C	0.1021828172	0.0000915466	-1.5034747327
C	0.0280088704	1.1536950447	-0.7402895141
C	-0.0699422495	0.9512357410	0.7008831887
C	0.7877526636	-0.0001281637	1.3986155533
C	-0.0700363857	-0.9513184631	0.7007617715
C	0.0278936385	-1.1536021422	-0.7404371818
F	0.3140827042	0.0001638916	-2.8000536406
F	-0.0394250737	2.3614752856	-1.2462049023
F	-0.8164542507	1.7986915156	1.3794855268
F	0.6603682814	-0.0002059865	2.7179650592
F	-0.8166356953	-1.7987844300	1.3792552127
F	-0.0396613206	-2.3613108395	-1.2465073407

}

basis=6-31g\*

{hf  
wf, 90, 1, 0  
}

{multi,  
occ, 49  
closed, 42  
wf, 90, 1, 0  
state, 2

CPMCSCF, NACM, 1.1, 2.1, accu=1.0d-6, record=5100.1

CPMCSCF, GRAD, 1.1, spin=0, accu=1.0d-6, record=5101.1

CPMCSCF, GRAD, 2.1, spin=0, accu=1.0d-6, record=5102.1

}

{Force  
SAMC, 5100.1  
CONICAL,6100.1}

{Force  
SAMC, 5101.1  
CONICAL,6100.1}

{Force  
SAMC, 5102.1  
CONICAL,6100.1}

optg, startcmd=multi

② Optimization of the S<sub>2</sub>/S<sub>1</sub>-MSX

\*\*\*,C6F6 cas67-S2/S1 conical optimization

memory, 500, m

symmetry, nosym

geomtyp=xyz

geom={

12

C6F6

C	-0.0004738878	1.4115923903	0.0040201345
C	1.2488523094	0.6758119098	-0.1396258929
C	1.2748718673	-0.6943164652	-0.0291049830
C	0.0000021073	-1.2795280793	0.3321137306
C	-1.2743319102	-0.6951631541	-0.0323515980
C	-1.2489410936	0.6749822807	-0.1428070584
F	-0.0019430182	2.3977981458	0.9003619779
F	2.3331022254	1.3667199948	-0.3909476131
F	2.2105221866	-1.4418104421	-0.6028518150
F	-0.0006326760	-2.3379787087	1.1065624953
F	-2.2080210499	-1.4432780491	-0.6084790818
F	-2.3330060604	1.3651701775	-0.3968902963

}

basis=6-311G\*\*

{hf

wf, 90, 1, 0

}

{multi,

occ, 49

closed, 42

wf, 90, 1, 0

state, 3

CPMCSCF, NACM, 2.1, 3.1, accu=1.0d-7, record=5100.1

CPMCSCF, GRAD, 2.1, spin=0, accu=1.0d-7, record=5101.1

CPMCSCF, GRAD, 3.1, spin=0, accu=1.0d-7, record=5102.1

}

{Force

SAMC, 5100.1

CONICAL,6100.1}

```
{Force
SAMC, 5101.1
CONICAL,6100.1}
```

```
{Force
SAMC, 5102.1
CONICAL,6100.1}
```

```
optg, startcmd=multi
```

### ③ Optimization of the $S_0/T_1$ -MSX

```
***, C6F6 CAS67-S0/T1 conical optimization
```

```
memory, 500, m
```

```
symmetry, nosym
```

```
geomtyp=xyz
```

```
geom={
```

```
12
```

```
C6F6
```

C	-0.1147255239	-0.0009522995	1.3778513963
C	0.2829713823	-1.2378493956	0.6589137745
C	0.0362877583	-1.2492929342	-0.6709145517
C	-0.1574491183	-0.0001181109	-1.3381949407
C	0.0363623470	1.2501880327	-0.6702766587
C	0.2823629971	1.2375696119	0.6603606086
F	-1.4296196870	0.0002670901	1.6498796584
F	0.7048892762	-2.2906492447	1.3263132175
F	0.1202941524	-2.3349108213	-1.4113248062
F	-0.5740793241	0.0003795761	-2.5818983829
F	0.1242867263	2.3353599732	-1.4109719167
F	0.7045869635	2.2889278422	1.3290724416

```
}
```

```
basis=6-31G*
```

```
{hf
```

```
wf, 90, 1, 0
```

```
}
```

```
{multi,
```

```
occ, 49
```

```
closed, 42
```

```
wf, 90, 1, 0
```

```
wf, 90, 1, 2
CPMCSCF, GRAD, 1.1, spin=0, accu=1.0d-6, record=5101.1
CPMCSCF, GRAD, 1.1, spin=1, accu=1.0d-6, record=5100.1
}
```

```
{Force
SAMC, 5101.1
CONICAL,6100.1, NODC}
```

```
{Force
SAMC, 5100.1
CONICAL, 6100.1, NODC}
```

```
optg, startcmd=multi
```

#### ④ Optimization of the $T_2/T_1$ -MSX

```
***,C6F6 cas67-T2/T1 conical optimization
```

```
memory, 500, m
```

```
symmetry, nosym
```

```
geomtyp=xyz
```

```
geom={
```

```
12
```

```
C6F6
```

C	0.0000000906	-1.5633147493	0.2120648283
C	-1.0875581768	-0.7719039102	-0.1850347352
C	-1.1580694185	0.6880336253	-0.0299821995
C	-0.0000006943	1.4268077381	0.0665102106
C	1.1580691205	0.6880319443	-0.0299817877
C	1.0875592218	-0.7719044766	-0.1850341169
F	-0.0000004175	-2.5011507483	1.1736561047
F	-2.1284570413	-1.2831711368	-0.8155964349
F	-2.3380378629	1.2437592728	0.0059318431
F	0.0000006733	2.7119391981	0.3715760971
F	2.3380365576	1.2437596041	0.0059309571
F	2.1284579474	-1.2831715116	-0.8155970168

```
}
```

```
basis=6-31G*
```

```
{hf
```

wf, 90, 1, 2  
}

{multi,  
occ, 49  
closed, 42  
wf, 90, 1, 2  
state, 2  
CPMCSCF, NACM, 1.1, 2.1, accu=1.0d-7, record=5100.1  
CPMCSCF, GRAD, 1.1, spin=1, accu=1.0d-7, record=5101.1  
CPMCSCF, GRAD, 2.1, spin=1, accu=1.0d-7, record=5102.1  
}

{Force  
SAMC, 5100.1  
CONICAL,6100.1}

{Force  
SAMC, 5101.1  
CONICAL,6100.1}

{Force  
SAMC, 5102.1  
CONICAL,6100.1}

optg, startcmd=multi