

Supporting information

**Excited-state E→Z photoisomerization mechanism unveiled by *ab initio*  
nonadiabatic molecular dynamics simulation for hemithioindigo-  
hemistilbene**

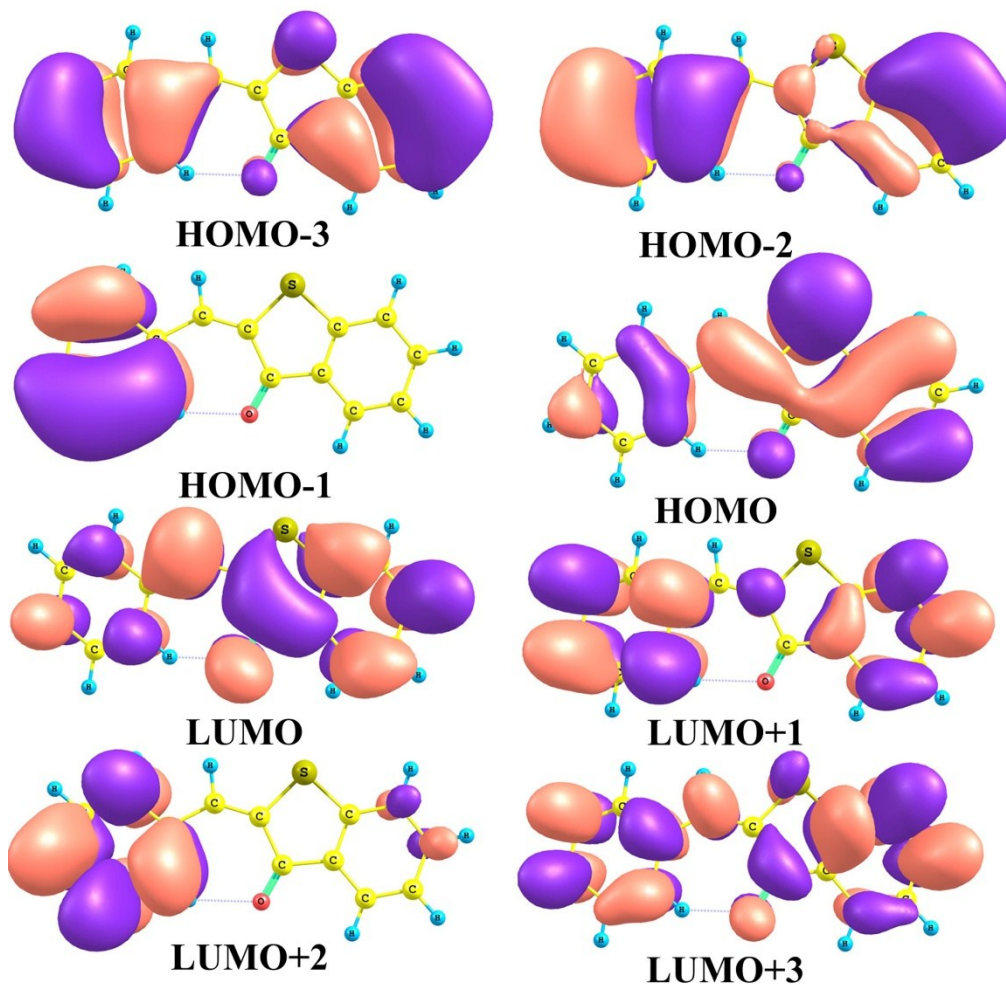
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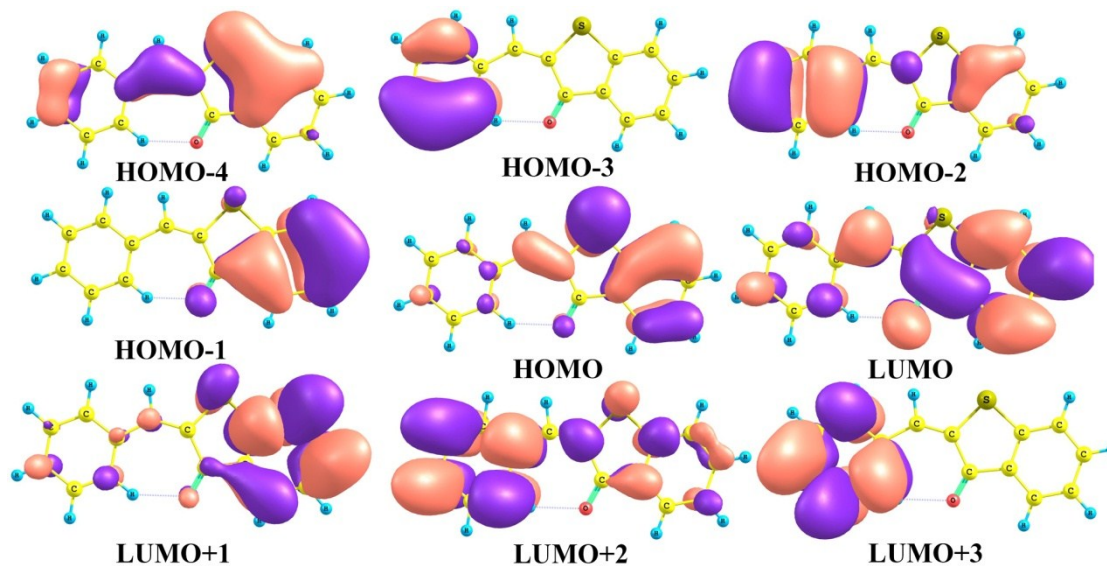
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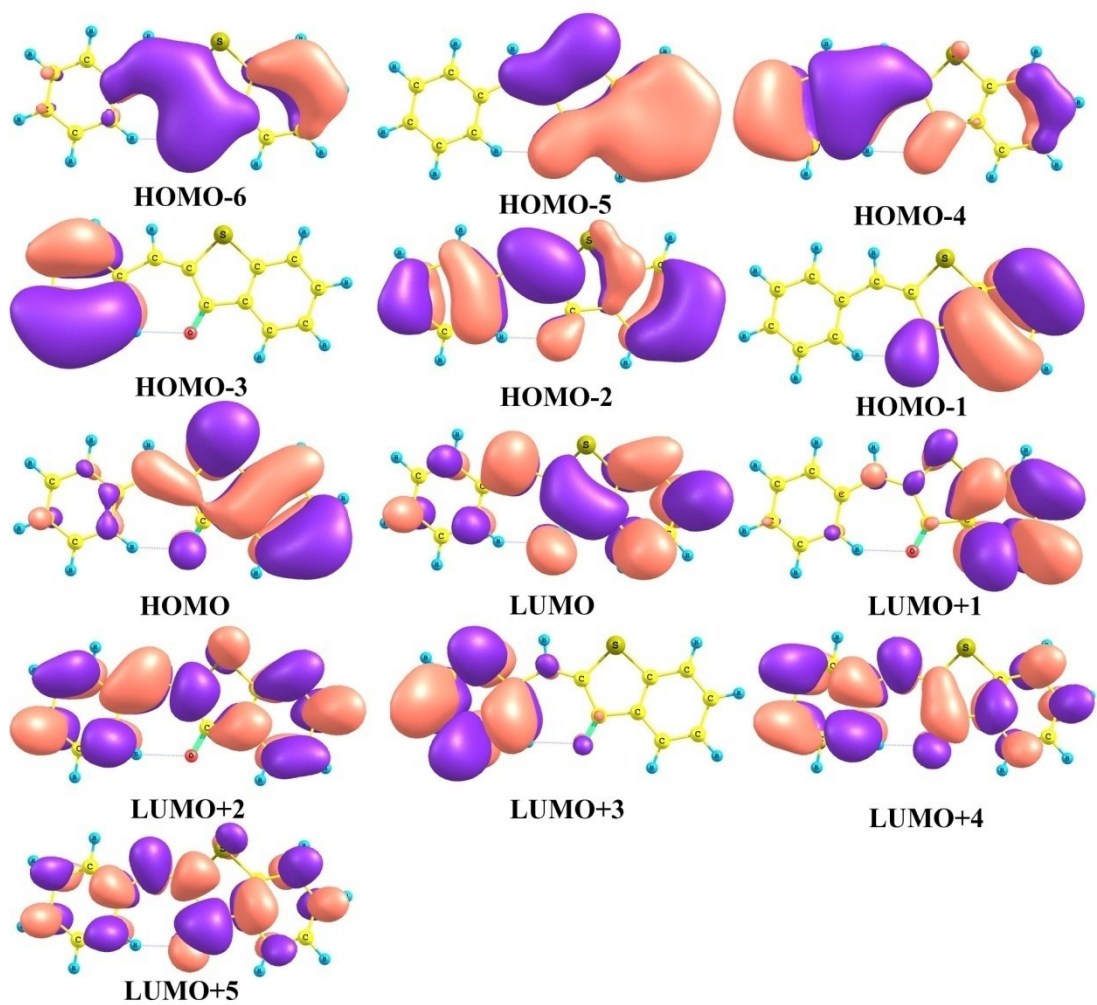
**S1. Molecular orbitals calculated at SA-2-CAS(8,8), SA-2-CAS(14,13), SA-2-CAS(10,9) and SA-3-CAS(14,13) with 6-31G\*.**



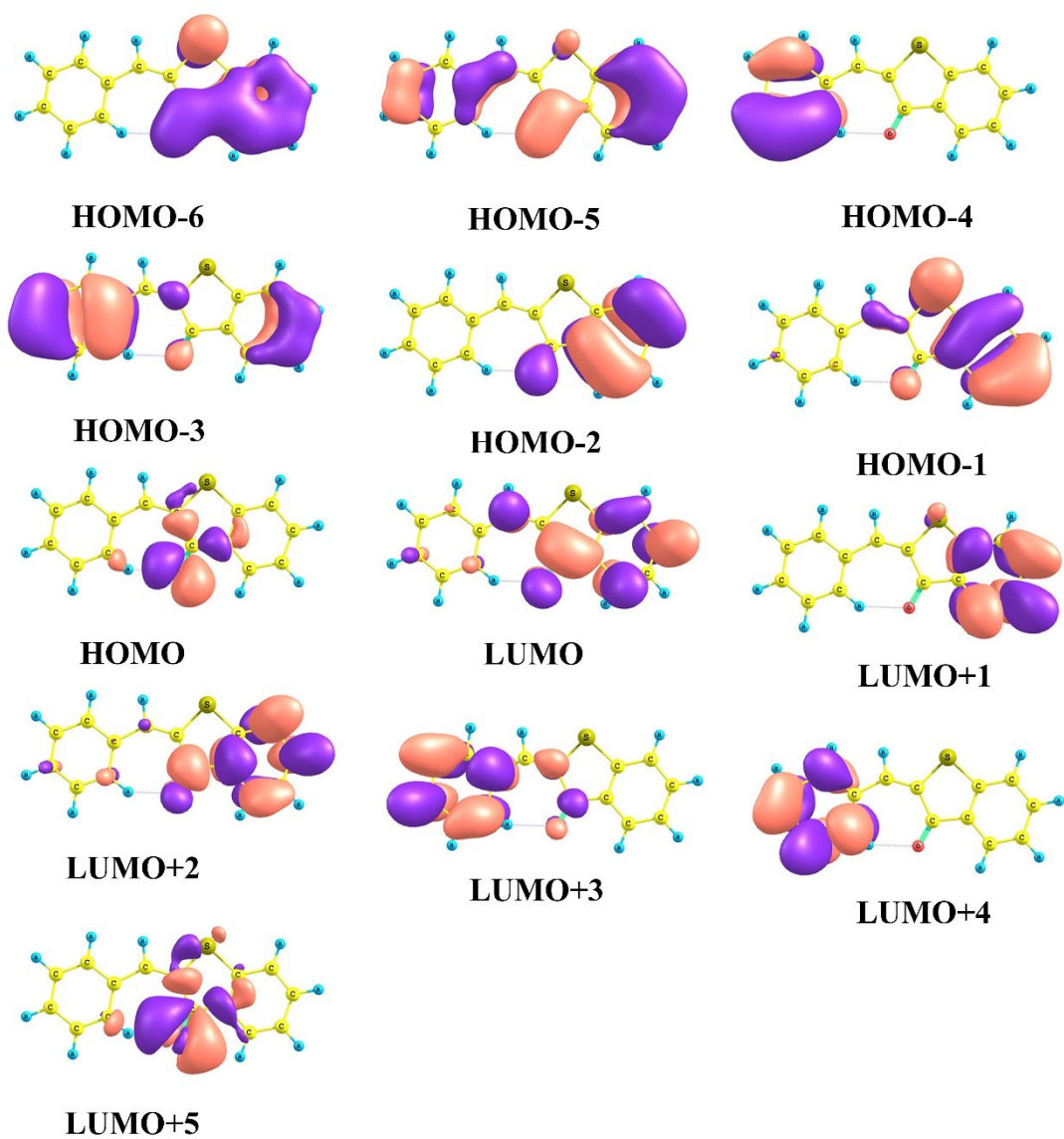
**Figure S1a.** SA-2-CASSCF(8,8)/6-31G\* computed HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2 and LUMO+3 of E-HTI.



**Figure S1b.** SA-2-CASSCF(10,9)/6-31G\* computed HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2 and LUMO+3 of E-HTI.

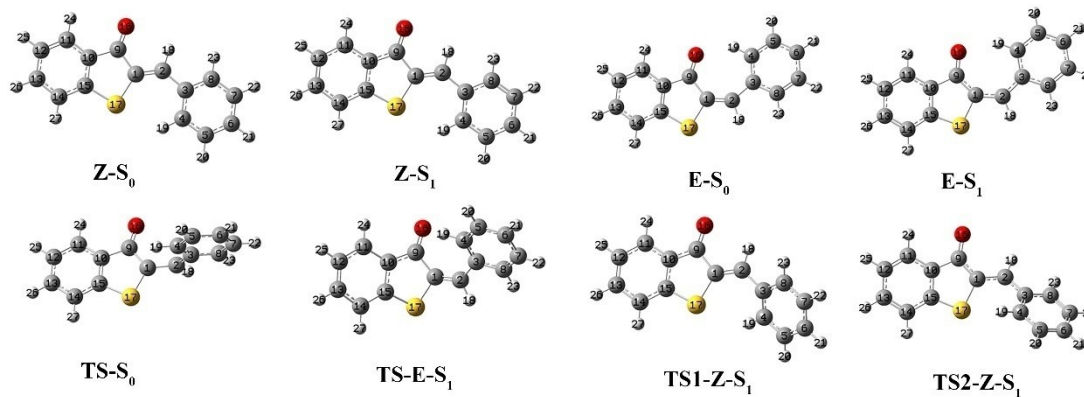


**Figure S1c.** SA-2-CASSCF(14,13)/6-31G\* computed HOMO-6, HOMO-5, HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2, LUMO+3, LUMO+4 and LUMO+5 of E-HTI.



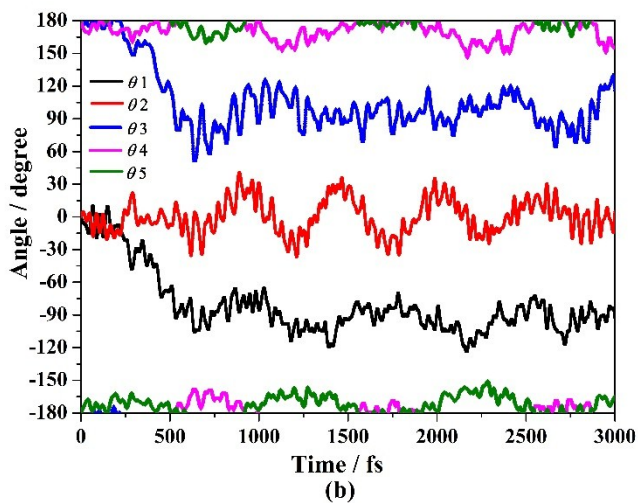
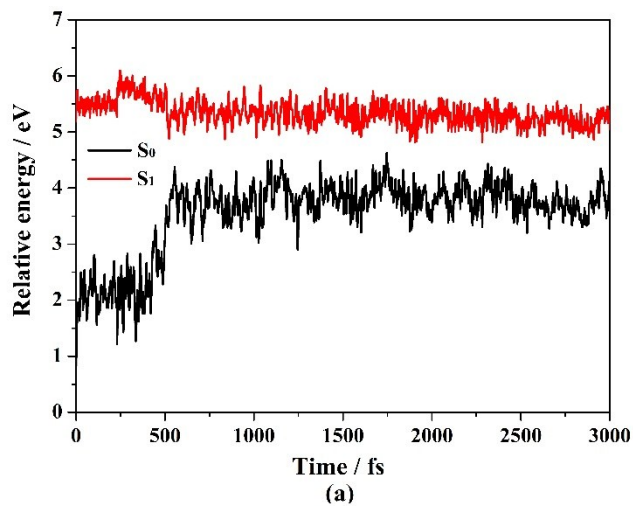
**Figure S1d.** SA-3-CASSCF(14,13)/6-31G\* computed HOMO-6, HOMO-5, HOMO-4, HOMO-3, HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1, LUMO+2, LUMO+3, LUMO+4 and LUMO+5 of E-HTI.

**S2. Structures for optimized stationary geometries at CASSCF(8,8)/6-31G\*.**



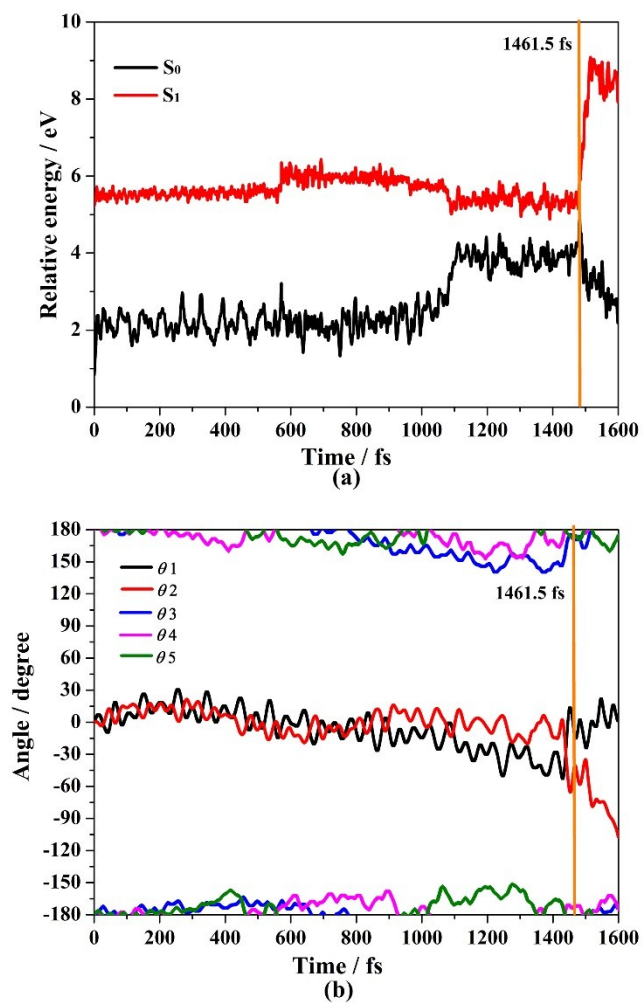
**Figure S2.** Geometries of stationary points optimized at SA-2-CASSCF(8,8)/6-31G\* level.

### S3. A sample resonance trajectory.



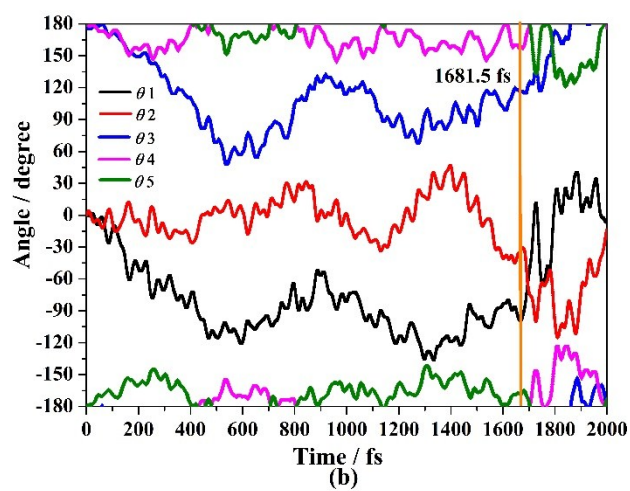
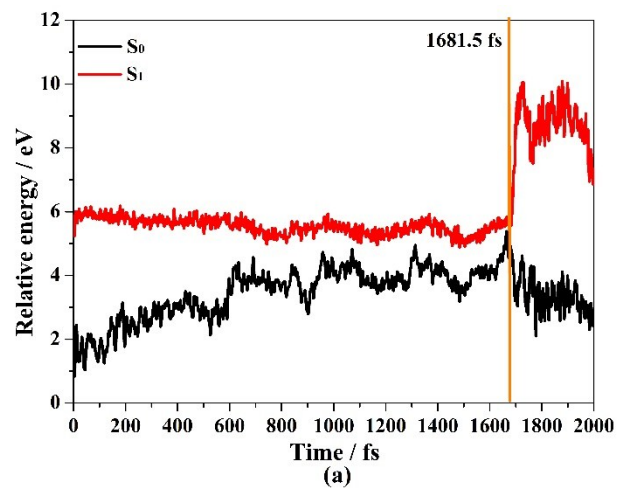
**Figure S3.** Time evolution of potential energies and key dihedral angles along a typical resonance trajectory.

#### S4. The supplemented typical trajectories for mechanism E-1.



**Figure S4.** Time evolution of dihedral angles ( $\theta_1$ ~ $\theta_5$ ) and potential energies along a nonreactive trajectory of E-1 case 4.





**Figure S5.** Time evolution of dihedral angles ( $\theta_1\sim\theta_5$ ) and potential energies along trajectory in E-1 case 3. An example for symmetrically oscillation towards  $\theta_1$ ,  $\theta_2$  and  $\theta_3$ .

**S5. Key dihedral angles and relative energies for Z-S<sub>0</sub> and E-S<sub>0</sub> calculate at CASSCF(8,8) with 6-31G\* and 6-31G\*(S,O), respectively**

**Table S1.** Key dihedral angles (°) and relative energies (eV) for Z-S<sub>0</sub> and E-S<sub>0</sub> optimized at CASSCF(8,8) with 6-31G\* and 6-31G\*(S,O), respectively.

geometry	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$	$\theta_5$	CASSCF(S <sub>0</sub> /S <sub>1</sub> )
Z-S <sub>0</sub> -6-31G*	-179.9	0.0	0.0	-179.9	179.9	0.00/5.67
Z-S <sub>0</sub> -6-31G*(S,O)	-179.9	0.0	0.0	-179.9	179.9	0.00/4.70
E-S <sub>0</sub> -6-31G*	0.0	0.0	-180.0	-179.9	179.9	0.84/5.24
E-S <sub>0</sub> -6-31G*(S,O)	0.0	0.0	-180.0	-179.9	179.9	0.90/4.32

**S6. Key internal coordinates that involve in photoisomerization processes for optimized geometries at SA-2-CASSCF(8,8)/6-31G\*.**

**Table S2a.** Key parameter for the structures optimized at CASSCF(8,8)/6-31G\*.<sup>a</sup>

Species	Z-S <sub>0</sub>	Z-S <sub>1</sub>	E-S <sub>0</sub>	E-S <sub>1</sub>	TS1-Z-S <sub>1</sub>	TS2-Z-S <sub>1</sub>	TS-S <sub>0</sub>
$\theta_1$	-179.9	-179.9	0.0	0.0	178.7	161.5	92.6
$\theta_2$	-0.0	-0.0	0.0	0.0	33.7	-16.9	-0.9
$\theta_3$	-0.0	-0.0	-180.0	-179.9	1.8	-48.6	-90.2
$\theta_4$	-179.9	-179.9	-179.9	-179.9	176.8	-160.8	-177.8
$\theta_5$	179.9	179.9	179.9	179.9	-176.9	160.1	177.8
$\theta_6$	179.9	179.9	-179.9	-179.9	-147.5	162.9	179.0
$\theta_7$	179.9	179.9	179.9	179.9	-179.9	178.3	179.9
$\theta_8$	-179.9	-179.9	180.0	-180.0	179.5	-178.4	179.9
$\alpha_1$	132.5	133.2	136.5	132.1	130.2	125.5	124.8
$\alpha_2$	118.8	121.3	131.3	137.4	122.4	125.7	125.4
$\alpha_3$	124.6	125.2	126.7	125.3	123.4	122.6	122.4

**Table S2b.** Key parameter for the structures optimized at CASSCF(8,8)/6-31G\*.

Species	CI1	CI2	CI3	CI4	CI5	CI6	CI7
$\theta_1$	42.5	34.8	92.5	87.7	-110.5	152.3	37.3
$\theta_2$	-7.6	-14.6	-77.0	76.0	-2.6	-55.6	0.8
$\theta_3$	-74.0	-78.0	-94.6	-98.6	122.6	-32.4	-124.7
$\theta_4$	131.2	123.7	-174.7	-177.9	133.4	-172.9	165.7
$\theta_5$	-123.1	-106.8	174.4	177.9	-151.8	172.7	-166.0
$\theta_6$	-177.4	172.8	121.3	-120.6	177.7	127.4	-165.7
$\theta_7$	-170.4	-174.0	-127.3	132.8	-178.7	-177.5	-162.3
$\theta_8$	171.3	174.8	125.0	-127.6	178.7	177.7	161.9
$\alpha_1$	132.2	132.6	91.9	92.3	126.0	134.8	118.9
$\alpha_2$	119.4	123.8	127.1	122.5	98.9	123.2	118.5
$\alpha_3$	123.3	123.0	125.2	125.7	120.0	119.7	121.1

<sup>a</sup> In table,  $\alpha_1$ =C1C2C3,  $\alpha_2$ =C9C1C2 and  $\alpha_3$ =C2C3C4.

### S7. Cartesian coordinates for interested geometries optimized by SA-2-CASSCF(8,8) with 6-31G\*.

#### Z-S<sub>0</sub>

C	0.4244002780	-0.0002814662	-0.0187641646
C	0.9426588959	-0.0004023274	-1.2434783519
C	0.3332559456	-0.0002327432	-2.5820080602
C	-1.0493433281	-0.0010532131	-2.8311562660
C	-1.5288276877	-0.0007891718	-4.1346850959
C	-0.6435887316	0.0002800490	-5.2131329214
C	0.7259658105	0.0010820231	-4.9736783916
C	1.1993425373	0.0007811955	-3.6685139289
C	1.3553010415	-0.0004680767	1.1618956153
C	0.5772180026	-0.0001561211	2.4297092057
C	1.1221319883	-0.0002129616	3.7079760231
C	0.2819602584	0.0001084870	4.7897199094
C	-1.1202989831	0.0004871310	4.5974041668
C	-1.6744243311	0.0005456392	3.3168120005
C	-0.7983922348	0.0002152287	2.2244182592
O	2.5443481123	-0.0008140156	1.0873949714
S	-1.2754638301	0.0002106680	0.5019190540
H	2.0190646505	-0.0005878304	-1.2464204493
H	-1.7540983779	-0.0020139372	-2.0247518445
H	-2.5897036907	-0.0014168783	-4.3087765746
H	-1.0181255839	0.0004278819	-6.2208450040
H	1.4206901626	0.0019361817	-5.7939184387
H	2.2608878403	0.0013393182	-3.4948852493
H	2.1904816344	-0.0005045517	3.8229606710
H	0.6778941751	0.0000720708	5.7885577776
H	-1.7705900365	0.0007369262	5.4531708592
H	-2.7396676364	0.0008339937	3.1790283128

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

C	0.5003703813	-0.0004175496	-0.0168474358
C	0.9777564584	-0.0005830720	-1.2572170499
C	0.3405517496	-0.0003238287	-2.5812101350
C	-1.0441540135	-0.0013567365	-2.8132891574
C	-1.5458640658	-0.0009875167	-4.1109857480
C	-0.6808795522	0.0004246047	-5.2024330160
C	0.6942162691	0.0013662589	-4.9808256749
C	1.1881116162	0.0009849711	-3.6915945482
C	1.4195739139	-0.0006739772	1.1751752511

C	0.6589758416	-0.0002545366	2.3721976813
C	1.1294938014	-0.0002970673	3.7220049736
C	0.1876445029	0.0001753282	4.8077318610
C	-1.1521741125	0.0006722197	4.6149943183
C	-1.6860983353	0.0007565707	3.2880338967
C	-0.7637079465	0.0002915972	2.1833714576
O	2.6324266391	-0.0011514514	1.0845594295
S	-1.1957227593	0.0003118594	0.5315613306
H	2.0540070709	-0.0008622221	-1.2754377014
H	-1.7415401913	-0.0025951550	-1.9997120847
H	-2.6098700728	-0.0018281907	-4.2666253708
H	-1.0702762784	0.0007426384	-6.2044328035
H	1.3752408197	0.0023839937	-5.8128534923
H	2.2522957592	0.0017288587	-3.5355231572
H	2.1846250816	-0.0006730579	3.9097380928
H	0.5794704054	0.0001182131	5.8086536815
H	-1.8282194489	0.0010162713	5.4488957865
H	-2.7431766523	0.0011544760	3.1080216996

### E-S<sub>0</sub>

C	-0.6060501813	-0.0000661216	0.0172182266
C	-0.9892443603	-0.0000657343	-1.2608829273
C	-0.3250612919	-0.0000336633	-2.5763739094
C	1.0584603646	-0.0002231481	-2.8189366034
C	1.5361248045	-0.0001794378	-4.1260257969
C	0.6580897394	0.0000236409	-5.2067598646
C	-0.7147874684	0.0002361950	-4.9723224448
C	-1.189990331	0.0001773522	-3.6782839972
C	0.7718687969	0.0000043224	0.6512544049
C	0.6440727905	0.0000277840	2.1060999264
C	1.7212897022	0.0000979438	3.0111747355
C	1.4722069987	0.0001064435	4.3532787875
C	0.1391751270	0.0000437676	4.8237414400
C	-0.9309276324	-0.0000261796	3.9424242257
C	-0.6591043222	-0.0000328819	2.5638809689
O	1.8093422503	0.0000401267	0.0549911879
S	-1.8547827070	-0.0001165434	1.2879999586
H	-2.0605880067	-0.0000840586	-1.3796542230
H	1.7436363927	-0.0003931713	-2.0011970944
H	2.5976249219	-0.0003039055	-4.2964857963
H	1.0354324589	0.0000149614	-6.2134441588

H	-1.4056122560	0.0004408575	-5.7960100100
H	-2.2532290712	0.0003000944	-3.5146863382
H	2.7241759528	0.0001435755	2.6259797465
H	2.2832225378	0.0001598381	5.0581038283
H	-0.0489595055	0.0000502818	5.8820718556
H	-1.9429150155	-0.0000739287	4.3029071395

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

C	-0.4514429319	0.0000268535	0.0144955750
C	-0.9876572788	0.0000588100	-1.2895541310
C	-0.3726095127	0.0000246972	-2.5814247938
C	1.0215778515	-0.0001359916	-2.8243122713
C	1.5082215703	-0.0001687290	-4.1280463856
C	0.6425277413	-0.0000515463	-5.2201210949
C	-0.7395454349	0.0001124223	-4.9900421989
C	-1.2286259563	0.0001428213	-3.7123347542
C	0.8306084978	0.0000746747	0.6136536307
C	0.6777803331	0.0000384409	2.1060066904
C	1.7251082955	0.0000700551	3.0218520476
C	1.4331531203	0.0000374160	4.3642749459
C	0.0922833977	-0.0000258828	4.8424461645
C	-0.9549065119	-0.0000556427	3.9541265680
C	-0.6406119834	-0.0000201504	2.5691394547
O	1.9496325486	0.0001430925	0.1202500107
S	-1.7102691253	-0.0000437973	1.2760737685
H	-2.0636311486	0.0001286042	-1.3315523088
H	1.7000769849	-0.0002184966	-1.9962763930
H	2.5721128086	-0.0002857408	-4.2887602746
H	1.0266931519	-0.0000874043	-6.2242787865
H	-1.4217185391	0.0002146471	-5.8223292540
H	-2.2943602130	0.0002637216	-3.5576128542
H	2.7342492290	0.0001185371	2.6574728325
H	2.2338460559	0.0000591839	5.0813378864
H	-0.0925654810	-0.0000499237	5.9000107536
H	-1.9764654828	-0.0001022612	4.2855684398

### TS1-Z-S<sub>1</sub>

C	0.1194000684	0.2878749740	0.0659420759
C	1.2609740470	0.4000576466	-0.6003715788
C	1.5375828775	0.2813828442	-2.0432880924
C	0.6431802042	0.6796320934	-3.0309841481

C	0.9569271020	0.5433970614	-4.3741168344
C	2.1817443250	0.0072074069	-4.7601758691
C	3.0978485709	-0.3798551963	-3.7830399597
C	2.7814232555	-0.2351605400	-2.4378065560
C	0.0415454475	0.4174598130	1.5629555770
C	-1.2870997971	0.1834363806	1.9965336068
C	-1.7988557361	0.1952626201	3.3301653502
C	-3.1927110168	-0.0668224140	3.5647872735
C	-4.0654023164	-0.3345461717	2.5657398296
C	-3.6133786446	-0.3660459283	1.2085309929
C	-2.2230949468	-0.1068721900	0.9476417328
O	1.0039562572	0.6764849651	2.2611192203
S	-1.4926028138	-0.0981372647	-0.5946191399
H	2.1129052630	0.5736925853	0.0348340379
H	-0.2935533747	1.1298875672	-2.7599904296
H	0.2508380839	0.8642438309	-5.1189193690
H	2.4229841941	-0.0976618952	-5.8025748247
H	4.0517307029	-0.7867354180	-4.0671608166
H	3.4916447211	-0.5305446463	-1.6860793970
H	-1.1339040849	0.4003012023	4.1452815714
H	-3.5404574568	-0.0460374324	4.5816720862
H	-5.1007201921	-0.5259799828	2.7752345845
H	-4.2833395700	-0.5779021714	0.3984939265

### TS2-Z-S<sub>1</sub>

C	-0.0336061253	0.6537525942	0.0635019270
C	1.2639919411	1.1450056575	-0.3109721705
C	2.5159911261	0.4635632387	-0.0865096683
C	2.6475868061	-0.5814901451	0.8143398790
C	3.8736569347	-1.2420747295	0.9805124205
C	4.9735695040	-0.8598405912	0.2632581637
C	4.8723169107	0.2164593138	-0.6426116265
C	3.6733031922	0.8662275222	-0.8114342949
C	-1.2020643179	1.4284162393	0.1898719675
C	-2.3919262701	0.5329736810	0.1130874367
C	-3.7289613131	0.9243672569	0.2956209315
C	-4.7123443199	-0.0072083456	0.1549889507
C	-4.4182349972	-1.3716088895	-0.1774182918
C	-3.1276277022	-1.7716690137	-0.3674639769
C	-2.1011351354	-0.7883687232	-0.2141053513
O	-1.3141384769	2.6435399851	0.3392196436

S	-0.4449673781	-1.0204171204	-0.3774915147
H	1.2915365088	2.1372526253	-0.7242678679
H	1.8148842087	-0.8596015704	1.4335477500
H	3.9443632912	-2.0462697355	1.6913613817
H	5.9139777432	-1.3640216734	0.3949553760
H	5.7366213021	0.5285525064	-1.2011056860
H	3.5948006951	1.6848863319	-1.5046133468
H	-3.9366921222	1.9499108391	0.5331076411
H	-5.7408774393	0.2759234843	0.2879261294
H	-5.2253120285	-2.0725802650	-0.2806440025
H	-2.8799795376	-2.7856494727	-0.6206228000

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

C	-0.0083177217	-0.0691963343	-0.7698178203
C	1.3605238887	0.0005306703	-1.2479577528
C	2.5312389427	-0.0084618314	-0.4024385836
C	2.4499091955	-0.0683166870	0.9934661995
C	3.5957301942	-0.0754017936	1.7663656875
C	4.8458804666	-0.0226932047	1.1697322200
C	4.9436490912	0.0378270241	-0.2129516930
C	3.8024917319	0.0445759364	-0.9892580303
C	-0.8607844634	1.0764375748	-0.4796176953
C	-2.2087489215	0.6241555262	-0.0620971229
C	-3.2818252324	1.4404809239	0.2978343500
C	-4.4819238181	0.8464026245	0.6640679702
C	-4.6040769125	-0.5495115679	0.6689292458
C	-3.5333827946	-1.3604410685	0.3096341967
C	-2.3380951015	-0.7478647301	-0.0548866936
O	-0.5035829037	2.2392604797	-0.5738219153
S	-0.8523696361	-1.5844818344	-0.5465630271
H	1.5122104931	0.0486958178	-2.3117556155
H	1.4892844426	-0.1086921313	1.4716313469
H	3.5130262068	-0.1211011040	2.8374960075
H	5.7344428198	-0.0278807178	1.7748412495
H	5.9095971305	0.0800501138	-0.6835490163
H	3.8859673006	0.0928970651	-2.0606660370
H	-3.1644315404	2.5081271261	0.2862632613
H	-5.3213358126	1.4559089032	0.9450314873
H	-5.5368908263	-1.0018005174	0.9536029900
H	-3.6287482190	-2.4307762637	0.3136657905



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

C	-0.4909090438	0.9859406489	2.4562795780
C	-1.3574613055	0.7279146714	3.4333519454
C	-2.8402932517	0.7214357075	3.4421673266
C	-3.6053547424	0.6737216931	2.2682847304
C	-4.9550657167	0.4062621418	2.3128232782
C	-5.6011131750	0.1852156078	3.5322245070
C	-4.8671257238	0.2493808899	4.7130623512
C	-3.4963677946	0.5094784826	4.6666956316
C	-0.7108729925	1.5331482482	1.0666114385
C	0.1704776632	0.8678354098	0.1837400321
C	0.0780439428	0.7498140179	-1.2914205084
C	0.8562356075	-0.2275423973	-1.9782754765
C	1.6889819688	-1.0867707143	-1.3412941819
C	1.8766339931	-1.0078885231	0.0771554622
C	1.1431652943	0.0118227075	0.8207896037
O	-1.5422281927	2.3469723597	0.7580834140
S	1.1719758375	0.2897377963	2.5212523432
H	-0.9384507705	0.2989728777	4.3286094298
H	-3.1398734694	0.8321007845	1.3164058795
H	-5.5076155479	0.3509086867	1.3904904858
H	-6.6515296838	-0.0495415630	3.5543164788
H	-5.3496658571	0.0721260927	5.6607351530
H	-2.9335698118	0.5187070769	5.5850696648
H	-0.5406050294	1.4528449208	-1.8028043350
H	0.7935868292	-0.2317286192	-3.0206926721
H	2.2472395335	-1.8065816849	-1.8871122828
H	2.5162546386	-1.6919971097	0.5997409725

**CI1**

C	-1.6328408974	0.2162208619	-0.1195885374
C	-1.4604670221	0.3386408154	1.2939160335
C	-0.3382358239	0.1356738075	2.1408393437
C	0.8989646153	-0.4202118100	1.6865080719
C	1.8553111308	-0.7625066270	2.6013707128
C	1.6059052145	-0.5693771121	3.9833094526
C	0.4223025538	-0.0477132674	4.4392611327
C	-0.5552246210	0.2994803427	3.5075490937
C	-1.0648797451	-0.8853024131	-0.7955833271
C	-0.1458627122	-0.4177205226	-1.8875072722
C	0.4165866799	-1.2245770799	-2.8840447530

C	1.3300352230	-0.6670816560	-3.7646528951
C	1.6921681550	0.6876720227	-3.6488187575
C	1.1464293292	1.4847213161	-2.6547346228
C	0.2350404970	0.8943499508	-1.7658861364
O	-1.1658388421	-2.0748933393	-0.5196439623
S	-0.7233246757	1.7388287903	-0.5445629190
H	-2.3240626256	0.6260999845	1.8935424302
H	1.0606730163	-0.5699789982	0.6402800885
H	2.7882914263	-1.1888053443	2.2863980080
H	2.3655411915	-0.8486439499	4.6911903331
H	0.2469266759	0.0855221557	5.4895140909
H	-1.4927960593	0.6985506296	3.8494363246
H	0.1267519000	-2.2569185239	-2.9430102743
H	1.7695036270	-1.2679745316	-4.5407849601
H	2.4056916563	1.1088925571	-4.3348222369
H	1.4173441328	2.5210239403	-2.5648334628

## CI2

C	-1.8475750822	0.0569525373	-0.1339127083
C	-1.5711295011	0.2471711814	1.2627416723
C	-0.3733903997	0.0520820815	2.0673220777
C	0.7386647602	-0.6760399359	1.6183769494
C	1.7895711822	-0.9271753839	2.4732958246
C	1.7489526732	-0.4665009164	3.7845967928
C	0.6496603796	0.2382018877	4.2507155699
C	-0.4077150702	0.4847491520	3.3982219538
C	-1.2622493151	-1.0028360162	-0.9369604764
C	-0.2178221217	-0.4609665918	-1.8769367612
C	0.4539470324	-1.1933676872	-2.8548249113
C	1.4676359270	-0.5770786914	-3.5793990298
C	1.8078574435	0.7594106956	-3.3287677756
C	1.1375834932	1.4901086562	-2.3538146907
C	0.1335486484	0.8474430657	-1.6312250256
O	-1.4538645355	-2.1959827116	-0.8211111573
S	-1.0103097323	1.5985574833	-0.4943402812
H	-2.3945614076	0.5732969500	1.8920239244
H	0.7667411105	-1.0562776225	0.6185060636
H	2.6364892144	-1.4906736231	2.1281122155
H	2.5715978365	-0.6705217746	4.4460760313
H	0.6176358342	0.5839430322	5.2673454474
H	-1.2672941502	1.0226653850	3.7568250774

H	0.1814334481	-2.2178573588	-3.0272726623
H	1.9990140073	-1.1269452520	-4.3351893646
H	2.5972074566	1.2239090269	-3.8921592718
H	1.3883048683	2.5177044306	-2.1636044841

### CI3

C	1.6306666906	-0.0890565393	1.1646005173
C	0.1691286039	-0.0303488123	1.0041557711
C	0.2771656055	0.0284184413	-0.3962738831
C	0.6617304248	1.2501818980	-1.1887445671
C	-0.1580036323	1.5967297135	-2.1680146885
C	-1.2745030799	0.7334742221	-2.5560221148
C	-1.2493579946	-0.6609323026	-2.1553919014
C	-0.3957006326	-1.0462447834	-1.2158954828
C	2.5491236696	1.0443107990	1.3662501287
C	3.9183859102	0.5407757736	1.6147105990
C	5.0437587462	1.3413024996	1.8444677990
C	6.2643141456	0.7285366472	2.0736346144
C	6.3564714679	-0.6734894795	2.0750260173
C	5.2391583114	-1.4648085163	1.8493916107
C	4.0153400026	-0.8308459336	1.6161305993
O	2.2298305380	2.2007976455	1.3184808533
S	2.4768346864	-1.6489981754	1.3205366064
H	-0.4211006731	-0.8191127070	1.4408361439
H	1.5018608910	1.8509000955	-0.9101295738
H	0.0004254400	2.5054023344	-2.7208090299
H	-2.0154417912	1.0877288316	-3.2456207421
H	-1.8760708519	-1.3658600023	-2.6739529661
H	-0.2440546122	-2.0746513178	-0.9474164127
H	4.9386477585	2.4100450470	1.8403919906
H	7.1431707955	1.3206339291	2.2524519537
H	7.3071451995	-1.1430111469	2.2536153531
H	5.3138813813	-2.5366921611	1.8524168049

### CI4

C	0.9496703289	0.0646702514	-0.1552225538
C	1.5446960683	-0.0617282533	-1.4833614037
C	0.2820305373	-0.0408690595	-2.1155290213
C	-0.5667519714	1.1694966225	-2.3305631941
C	-1.0815373235	1.3411395566	-3.5376086961
C	-0.9441119492	0.3168181426	-4.5925533360

C	-0.5255460989	-0.9814406848	-4.2438599321
C	-0.1039722985	-1.2254094974	-2.9512282867
C	0.5157902219	-1.1101208425	0.6385923814
C	0.0031303908	-0.6565826284	1.9535859675
C	-0.5268452010	-1.4817841175	2.9589284708
C	-0.9692151979	-0.9089852027	4.1181677773
C	-0.8907830151	0.4874936339	4.2956492806
C	-0.3754778397	1.3019529495	3.3234883595
C	0.0741147230	0.7090508254	2.1340201011
O	0.5746074365	-2.2482105665	0.2675567209
S	0.8062931734	1.5644934444	0.7605394174
H	2.1812112773	-0.9133581242	-1.6527195805
H	-0.6933245641	1.8999126149	-1.5560638089
H	-1.6438566091	2.2288678944	-3.7669247783
H	-1.2967016476	0.5333290685	-5.5826633061
H	-0.6197814590	-1.7835201005	-4.9544316254
H	0.0913955182	-2.2072672198	-2.5683567008
H	-0.5726306251	-2.5427753503	2.7972587924
H	-1.3792069053	-1.5181243880	4.9029743416
H	-1.2439337900	0.9198245472	5.2147842563
H	-0.3176281800	2.3654574841	3.4660493565

## CI5

C	-0.0005906782	-0.2931904375	0.4553063775
C	-1.1674031847	-0.6721122874	-0.3150599705
C	-2.4987766042	-0.2607997079	-0.0664393040
C	-2.7895245388	0.5486996861	1.0462296606
C	-4.0924896403	0.9238217756	1.2968701301
C	-5.0982667679	0.5019289412	0.4379250880
C	-4.8312921025	-0.2943608619	-0.6766143633
C	-3.5372596910	-0.6715208486	-0.9303385772
C	0.6183552850	0.5102117309	-0.4743967097
C	2.0782654292	0.5235175794	-0.2938029791
C	3.0196844557	1.3390571635	-0.9429282242
C	4.3615394264	1.1753454604	-0.6535238425
C	4.7704540916	0.1975709925	0.2760361006
C	3.8460833272	-0.6155466589	0.9082844821
C	2.4867832932	-0.4517993790	0.5917409668
O	-0.0598668080	0.9792220749	-1.4277839559
S	1.1482194958	-1.3752662781	1.2741315571
H	-1.0605145600	-1.3331243419	-1.1688364885

H	-1.9741418166	0.8559856288	1.6703816940
H	-4.3295075791	1.5404551517	2.1429452730
H	-6.1131900803	0.7982789831	0.6343990909
H	-5.6308019928	-0.5999681183	-1.3244969960
H	-3.3021122784	-1.2774095611	-1.7863174441
H	2.6797993137	2.0751020197	-1.6479168330
H	5.0996522078	1.7925661608	-1.1337159762
H	5.8170469541	0.0780146514	0.4940925141
H	4.1609720433	-1.3624365196	1.6143157297

## CI6

C	-0.0118983786	-0.4553854458	-0.0442829777
C	-0.0379105914	-0.9556915326	-1.3020738541
C	-0.0533650022	-0.3749528251	-2.6421046471
C	-1.0563985219	0.5437684082	-2.9911055028
C	-1.1163987457	1.0675349106	-4.2800634479
C	-0.1842508274	0.6897071414	-5.2414412481
C	0.8075710596	-0.2281698677	-4.8961372108
C	0.8692018269	-0.7538642954	-3.6254881625
C	-0.6030967289	-1.2024351074	1.1823405642
C	-0.2776132619	-0.4964031033	2.4360968912
C	-0.6414533975	-0.9223167979	3.7236423828
C	-0.2866983170	-0.1541953327	4.7974708159
C	0.4269922739	1.0446754590	4.6056885725
C	0.7833832865	1.4714387051	3.3532179654
C	0.4255716750	0.6755762556	2.2569253101
O	-1.2207989137	-2.2054360297	1.0741953407
S	0.7734118093	1.0643602278	0.5566533341
H	1.0770771284	-0.9681048838	-0.9046375858
H	-1.7868455786	0.8381287219	-2.2590163004
H	-1.8920004654	1.7708502605	-4.5272865414
H	-0.2297169151	1.0946023031	-6.2360966641
H	1.5329383076	-0.5343195156	-5.6292938865
H	1.6319873303	-1.4733467957	-3.3837501361
H	-1.1904930930	-1.8382483133	3.8395396696
H	-0.5518746431	-0.4580805847	5.7933348466
H	0.6969647527	1.6370008538	5.4613752974
H	1.3256959311	2.3883511846	3.2147861754

## CI7

C	1.0937631958	1.5327138331	-1.7086613378
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C	0.8043576943	1.8431215021	-0.2855675266
C	-0.2479907419	1.2103828206	0.3320388878
C	-1.0693508674	0.2284715815	-0.3854240287
C	-2.3568231114	-0.1164427608	0.1453419175
C	-2.7977511501	0.4314347715	1.2873206277
C	-1.9666493908	1.3514752561	2.0521908157
C	-0.7594955724	1.7025828887	1.6133530784
C	0.0386276641	1.3201753433	-2.5615353311
C	0.4722557687	0.7120263088	-3.8220856573
C	-0.3154522344	0.3750473856	-4.9348277074
C	0.3000709017	-0.1505397419	-6.0574369953
C	1.6954289358	-0.3337613567	-6.0879326618
C	2.4772781375	0.0012910956	-4.9942369626
C	1.8388120116	0.5149754867	-3.8592491359
O	-1.1598515597	1.4314503288	-2.1506773977
S	2.6076100680	0.9827299390	-2.3453614297
H	1.2382994577	2.7151645176	0.1697335158
H	-0.5950272015	-0.4746294329	-1.0346611097
H	-2.9549261858	-0.8278755585	-0.3933730642
H	-3.7694157949	0.1773291522	1.6709585510
H	-2.3484512063	1.7436451436	2.9773015611
H	-0.1478672622	2.3926743216	2.1666957601
H	-1.3777322784	0.5310167468	-4.8994028617
H	-0.2878237350	-0.4181238510	-6.9169495405
H	2.1600883073	-0.7384403241	-6.9690252241
H	3.5429049254	-0.1370034999	-5.0142057164