

Supporting Information for
Rationalization and Design of Enhanced
Photoinduced Cycloreversion in Photochromic
Dimethyldihdropyrenes by Theoretical Calculations

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Table S1. B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-GS in DHP_{parent}.

C	-0.071385728398	2.829459449281	1.223997938634
C	-0.085863458712	3.506379174713	0.000000000000
C	-0.071385728398	2.829459449281	-1.223997938634
C	0.027653880586	1.442232294133	-1.283064739466
C	0.027653880586	1.442232294133	1.283064739466
C	-0.027356717528	0.697768117369	-2.467070269930
C	0.027356717528	-0.697768117369	-2.467070269930
C	-0.027653880586	-1.442232294133	-1.283064739466
C	0.071385728398	-2.829459449281	-1.223997938634
C	0.085863458712	-3.506379174713	0.000000000000
C	0.071385728398	-2.829459449281	1.223997938634
C	-0.027653880586	-1.442232294133	1.283064739466
C	0.027356717528	-0.697768117369	2.467070269930
C	-0.027356717528	0.697768117369	2.467070269930
C	0.357539732851	0.683721261968	0.000000000000
C	-0.357539732851	-0.683721261968	0.000000000000
C	1.920064774871	0.531404022874	0.000000000000
C	-1.920064774871	-0.531404022874	0.000000000000
H	-0.186185584216	3.391756124396	2.145834454220
H	-0.186185584216	3.391756124396	-2.145834454220
H	0.186185584216	-3.391756124396	-2.145834454220
H	0.186185584216	-3.391756124396	2.145834454220
H	-0.176037417410	4.587205393298	0.000000000000
H	0.176037417410	-4.587205393298	0.000000000000
H	-0.086306996554	1.228354617362	-3.412687024624
H	0.086306996554	-1.228354617362	-3.412687024624
H	0.086306996554	-1.228354617362	3.412687024624
H	-0.086306996554	1.228354617362	3.412687024624
H	2.262140676654	-0.001839455716	-0.887782955981
H	2.262140676654	-0.001839455716	0.887782955981
H	-2.262140676654	0.001839455716	-0.887782955981
H	-2.262140676654	0.001839455716	0.887782955981
H	2.370224269262	1.525519761854	0.000000000000
H	-2.370224269262	-1.525519761854	0.000000000000

B3LYP energy:

$$E(S_0) = -695.670276 \text{ a.u.}$$

CAM-B3LYP energy:

$$E(S_0) = -695.247632 \text{ a.u.}$$

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-LE in DHP_{parent}.

C	-0.091231518098	2.832800256841	1.219042857158	E(S ₁) = -695.168659 a.u.
C	-0.120648949894	3.511986676695	0.000000000000	
C	-0.091231518098	2.832800256841	-1.219042857158	
C	0.036165560711	1.441942437710	-1.269447853570	
C	0.036165560711	1.441942437710	1.269447853570	
C	-0.024371874377	0.697705320488	-2.453883769218	
C	0.024371874377	-0.697705320487	-2.453883769218	
C	-0.036165560711	-1.441942437710	-1.269447853570	
C	0.091231518098	-2.832800256841	-1.219042857158	
C	0.120648949894	-3.511986676695	0.000000000000	
C	0.091231518098	-2.832800256841	1.219042857158	
C	-0.036165560711	-1.441942437710	1.269447853570	
C	0.024371874377	-0.697705320488	2.453883769218	
C	-0.024371874377	0.697705320487	2.453883769218	
C	0.361967702588	0.686547715265	0.000000000000	
C	-0.361967702588	-0.686547715265	0.000000000000	
C	1.907605582514	0.482781293691	0.000000000000	
C	-1.907605582514	-0.482781293691	0.000000000000	
H	-0.206969011911	3.384786311449	2.145065873328	
H	-0.206969011911	3.384786311449	-2.145065873328	
H	0.206969011911	-3.384786311449	-2.145065873328	
H	0.206969011911	-3.384786311449	2.145065873328	
H	-0.223704166419	4.590510597022	0.000000000000	
H	0.223704166419	-4.590510597022	0.000000000000	
H	-0.101290901387	1.227204744077	-3.397565490686	
H	0.101290901387	-1.227204744077	-3.397565490686	
H	0.101290901387	-1.227204744077	3.397565490686	
H	-0.101290901387	1.227204744077	3.397565490686	
H	2.220497212261	-0.068519877430	-0.886753499245	
H	2.220497212261	-0.068519877430	0.886753499245	
H	-2.220497212261	0.068519877430	-0.886753499245	
H	-2.220497212261	0.068519877430	0.886753499245	
H	2.401411629018	1.454848398053	0.000000000000	
H	-2.401411629018	-1.454848398053	0.000000000000	

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of CPD* in DHP_{parent}.

C	-0.136692316908	2.808954949874	1.212589274729	E(S ₁) = -695.160828 a.u.
C	-0.192380206195	3.501659461494	0.000000000000	
C	-0.136692316908	2.808954949874	-1.212589274729	
C	0.068572904630	1.444677560795	-1.255850568977	
C	0.068572904630	1.444677560795	1.255850568977	
C	0.019581571352	0.681312841696	-2.470069813591	
C	-0.019581571352	-0.681312841696	-2.470069813591	
C	-0.068572904630	-1.444677560795	-1.255850568977	
C	0.136692316908	-2.808954949874	-1.212589274729	
C	0.192380206195	-3.501659461494	0.000000000000	
C	0.136692316908	-2.808954949874	1.212589274729	
C	-0.068572904630	-1.444677560795	1.255850568977	
C	-0.019581571352	-0.681312841696	2.470069813591	
C	0.019581571352	0.681312841696	2.470069813591	
C	0.397104579856	0.699081767393	0.000000000000	
C	-0.397104579856	-0.699081767393	0.000000000000	
C	1.921879736655	0.382232561863	0.000000000000	
C	-1.921879736655	-0.382232561863	0.000000000000	
H	-0.286584331542	3.347163979022	2.142964785846	
H	-0.286584331542	3.347163979022	-2.142964785846	
H	0.286584331542	-3.347163979022	-2.142964785846	
H	0.286584331542	-3.347163979022	2.142964785846	
H	-0.342739370263	4.574031978177	0.000000000000	
H	0.342739370263	-4.574031978177	0.000000000000	
H	-0.000374498745	1.220524366869	-3.411277076889	
H	0.000374498745	-1.220524366869	-3.411277076889	
H	0.000374498745	-1.220524366869	3.411277076889	
H	-0.000374498745	1.220524366869	3.411277076889	
H	2.189485319027	-0.191934488665	-0.886957774143	
H	2.189485319027	-0.191934488665	0.886957774143	
H	-2.189485319027	0.191934488665	-0.886957774143	
H	-2.189485319027	0.191934488665	0.886957774143	
H	2.485092287114	1.316240000464	0.000000000000	
H	-2.485092287114	-1.316240000464	0.000000000000	

Table S1 (continued). B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-GS in

DHP-1_{model}.

C	-2.844191941140	0.067622683045	-2.030832337687
C	-3.509831714158	0.143339458282	-0.834813046906
C	-2.816728005240	0.159636008084	0.410762772838
C	-1.461369088530	-0.001241214442	0.497819463218
C	-1.433536839792	-0.034137927494	-2.069973436587
C	-0.715454448941	0.018253598377	1.744243120288
C	0.715454447683	-0.018253598377	1.744243120804
C	1.461369088171	0.001241214442	0.497819464272
C	2.816728004944	-0.159636008084	0.410762774869
C	3.509831714760	-0.143339458282	-0.834813044374
C	2.844191942605	-0.067622683045	-2.030832335635
C	1.433536841285	0.034137927494	-2.069973435553
C	0.707861818239	-0.029641133678	-3.238050370227
C	-0.707861815903	0.029641133678	-3.238050370738
C	-0.686791036340	-0.354903480379	-0.770817513050
C	0.686791036896	0.354903480379	-0.770817512555
C	-0.535640443325	-1.917043021767	-0.751120162990
C	0.535640443867	1.917043021767	-0.751120162604
H	-3.389426283632	0.145083835828	-2.966528038232
H	-3.405443360117	0.345001640146	1.300718181703
H	3.405443359179	-0.345001640146	1.300718184160
H	3.389426285771	-0.145083835828	-2.966528035787
H	-4.588279175238	0.256767912645	-0.826468521885
H	4.588279175834	-0.256767912645	-0.826468518576
H	1.236821404689	-0.107732265102	-4.183093084727
H	-1.236821401671	0.107732265102	-4.183093085619
H	-0.020637179840	-2.255996013066	0.149097693371
H	0.017783777520	-2.264523523656	-1.624633937250
H	0.020637179733	2.255996013066	0.149097693386
H	-0.017783776348	2.264523523656	-1.624633937262
H	-1.529447984818	-2.367575012030	-0.768575551154
H	1.529447985372	2.367575012030	-0.768575550050
C	1.384329094710	-0.031583593992	2.995020957056
H	2.466011966304	-0.032705363755	3.016627613994
C	-1.384329096870	0.031583593992	2.995020956058
H	-2.466011968480	0.032705363755	3.016627612216
C	0.703037728245	-0.015772625624	4.189398338418
H	1.249074984383	-0.022375608116	5.125919159726
C	-0.703037731267	0.015772625624	4.189398337911
H	-1.249074988080	0.022375608116	5.125919158825

B3LYP energy:

$E(S_0) = -849.339402$ a.u.

CAM-B3LYP energy:

$E(S_0) = -848.833659$ a.u.

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-LE in DHP-**1**_{model}.

C	-2.819005185686	0.097651779542	-2.017876232087	E(S ₁) = -848.749996 a.u.
C	-3.511586406650	0.132200810795	-0.802480231902	
C	-2.851256777169	0.108562661672	0.416369951852	
C	-1.452809311074	-0.013755266239	0.502231346927	
C	-1.437650250052	-0.031352173249	-2.043596190703	
C	-0.727055448913	0.040102897113	1.711892196833	
C	0.727055447678	-0.040102897113	1.711892197358	
C	1.452809310711	0.013755266239	0.502231347975	
C	2.851256776869	-0.108562661672	0.416369953909	
C	3.511586407229	-0.132200810795	-0.802480229369	
C	2.819005187142	-0.097651779542	-2.017876230054	
C	1.437650251526	0.031352173249	-2.043596189666	
C	0.692203896620	-0.020767860361	-3.233330989175	
C	-0.692203894288	0.020767860361	-3.233330989674	
C	-0.690106381126	-0.352665488683	-0.762490892973	
C	0.690106381676	0.352665488683	-0.762490892475	
C	-0.505422311541	-1.901280898411	-0.752391585320	
C	0.505422312084	1.901280898411	-0.752391584955	
H	-3.358115454732	0.213778194052	-2.951196890219	
H	-3.441474137489	0.224351468626	1.314197199410	
H	3.441474136541	-0.224351468626	1.314197201893	
H	3.358115456861	-0.213778194052	-2.951196887797	
H	-4.590197194401	0.235100712630	-0.812148599053	
H	4.590197194987	-0.235100712630	-0.812148595742	
H	1.227433474395	-0.085832310321	-4.174533362297	
H	-1.227433471383	0.085832310321	-4.174533363182	
H	0.031875524904	-2.217379447186	0.142140282182	
H	0.053063990965	-2.225871040224	-1.630786738663	
H	-0.031875525006	2.217379447186	0.142140282159	
H	-0.053063989788	2.225871040224	-1.630786738701	
H	-1.483378521449	-2.383062931302	-0.761064332632	
H	1.483378521998	2.383062931302	-0.761064331562	
C	1.383717447826	-0.132356587206	2.974074027664	
H	2.459978194455	-0.225747332630	3.002401226379	
C	-1.383717449971	0.132356587206	2.974074026666	
H	-2.459978196621	0.225747332630	3.002401224605	
C	0.704685973903	-0.075834107626	4.152089949353	
H	1.241172937316	-0.134840985620	5.091201164431	
C	-0.704685976898	0.075834107626	4.152089948845	
H	-1.241172940989	0.134840985620	5.091201163536	

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of CPD* in DHP-1_{model}.

C	-2.809178379937	0.069893164332	-2.007544728103	E(S ₁) = -848.758408 a.u.
C	-3.493893262232	0.164456689867	-0.806031938908	
C	-2.798032010778	0.129472875655	0.412327529499	
C	-1.448993546329	-0.118222440844	0.478366673346	
C	-1.434784795703	-0.116148150835	-2.038671685061	
C	-0.705335786740	-0.094400500212	1.741840845133	
C	0.705335786740	0.094400500212	1.741840845133	
C	1.448993546329	0.118222440844	0.478366673346	
C	2.798032010778	-0.129472875655	0.412327529499	
C	3.493893262232	-0.164456689867	-0.806031938908	
C	2.809178379937	-0.069893164332	-2.007544728103	
C	1.434784795703	0.116148150835	-2.038671685061	
C	0.685218606750	0.036670480589	-3.240624363552	
C	-0.685218606750	-0.036670480589	-3.240624363552	
C	-0.686719090882	-0.425339318102	-0.770464879272	
C	0.686719090882	0.425339318102	-0.770464879272	
C	-0.315017245801	-1.934175456765	-0.771583121809	
C	0.315017245801	1.934175456765	-0.771583121809	
H	-3.340832720684	0.197536112333	-2.944842943889	
H	-3.349704412817	0.334838261528	1.321186436682	
H	3.349704412817	-0.334838261528	1.321186436682	
H	3.340832720684	-0.197536112333	-2.944842943889	
H	-4.563361110496	0.334545471148	-0.803762407556	
H	4.563361110496	-0.334545471148	-0.803762407556	
H	1.225646426195	0.015535502931	-4.181083884118	
H	-1.225646426195	-0.015535502931	-4.181083884118	
H	0.257684935728	-2.184086631315	0.122402018234	
H	0.280082814411	-2.181511585548	-1.650926621690	
H	-0.257684935728	2.184086631315	0.122402018234	
H	-0.280082814411	2.181511585548	-1.650926621690	
H	-1.226765347737	-2.532890618043	-0.781484235322	
H	1.226765347737	2.532890618043	-0.781484235322	
C	1.357723208499	0.230263542771	2.969798677098	
H	2.418366392044	0.443715945830	2.984279343284	
C	-1.357723208499	-0.230263542771	2.969798677098	
H	-2.418366392044	-0.443715945830	2.984279343284	
C	0.681662973060	0.124152288048	4.175124340604	
H	1.221296096003	0.233126782280	5.107979525757	
C	-0.681662973060	-0.124152288048	4.175124340604	
H	-1.221296096003	-0.233126782280	5.107979525757	

Table S1 (continued). B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-GS in

DHP-2.

C	-1.954274305530	2.887883147340	-0.342042734247
C	-1.281360376531	2.667019603019	0.861626114146
C	-0.548652795331	1.503442508070	1.077722645436
C	0.255132818664	1.283157692901	2.201672875673
C	1.035051191290	0.134477775792	2.342421259755
C	1.211709313606	-0.771004060382	1.291168482702
C	1.883389802954	-1.983163520477	1.406906156405
C	1.954274305530	-2.887883147340	0.342042734247
C	1.281360376531	-2.667019603019	-0.861626114146
C	0.548652795331	-1.503442508070	-1.077722645436
C	-0.255132818664	-1.283157692901	-2.201672875673
C	-1.035051191290	-0.134477775792	-2.342421259755
C	-1.211709313606	0.771004060382	-1.291168482702
C	-1.883389802954	1.983163520477	-1.406906156405
C	-0.698253051101	0.344043713896	0.082283117353
C	0.698253051101	-0.344043713896	-0.082283117353
C	-1.675203942348	-0.631414173063	0.786157506758
C	1.675203942348	0.631414173063	-0.786157506758
H	-2.487379722987	3.821868806641	-0.482435877966
H	-1.273378974309	3.443786860637	1.620293926097
H	0.239992847662	2.018683851745	3.000399336413
H	1.536914774763	-0.057392036582	3.286284854640
H	2.329073490090	-2.249014019136	2.361268792820
H	2.487379722987	-3.821868806641	0.482435877966
H	1.273378974309	-3.443786860637	-1.620293926097
H	-0.239992847662	-2.018683851745	-3.000399336413
H	-1.536914774763	0.057392036582	-3.286284854640
H	-2.329073490090	2.249014019136	-2.361268792820
C	-2.940781404578	-1.028059931636	0.591366055469
H	-1.213751822771	-1.045524675702	1.675616779603
C	2.940781404578	1.028059931636	-0.591366055469
H	1.213751822771	1.045524675702	-1.675616779603
C	-3.918673338260	-0.657930351026	-0.495496310262
C	-3.541213788705	-2.003543954135	1.584463045062
C	3.918673338260	0.657930351026	0.495496310262
C	3.541213788705	2.003543954135	-1.584463045062
H	-4.175950001910	-1.546387693719	-1.084833106508
H	-4.853190293703	-0.308692466859	-0.040877179157
H	4.853190293703	0.308692466859	0.040877179157
H	-3.564927066643	0.110388945273	-1.171514096519
H	3.564927066643	-0.110388945273	1.171514096519
H	4.175950001910	1.546387693719	1.084833106508
H	-3.881516382411	-2.913787472378	1.076244141803
H	-2.830808621260	-2.293281436348	2.360370661186
H	-4.423081144258	-1.569661373242	2.071217307541
H	3.881516382411	2.913787472378	-1.076244141803
H	4.423081144258	1.569661373242	-2.071217307541
H	2.830808621260	2.293281436348	-2.360370661186

B3LYP energy:

 $E(S_0) = -929.129673$ a.u.

CAM-B3LYP energy:

 $E(S_0) = -928.562881$ a.u.

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-LE in DHP-2.

C	-2.030973814329	2.734854021380	-0.798918603390	E(S ₁) = -928.489776 a.u.
C	-1.562249466128	2.588255787052	0.507167143985	
C	-0.861159256872	1.448937525561	0.912300000659	
C	-0.209040084332	1.362682166203	2.146274852489	
C	0.669864908138	0.319487038243	2.440538006508	
C	1.099356362707	-0.579304121838	1.459170933563	
C	1.789831058154	-1.755857686903	1.763546618289	
C	2.030973814329	-2.734854021380	0.798918603390	
C	1.562249466128	-2.588255787052	-0.507167143985	
C	0.861159256872	-1.448937525561	-0.912300000659	
C	0.209040084332	-1.362682166203	-2.146274852489	
C	-0.669864908138	-0.319487038243	-2.440538006508	
C	-1.099356362707	0.579304121838	-1.459170933563	
C	-1.789831058154	1.755857686903	-1.763546618289	
C	-0.747416361495	0.249195413804	-0.016330672839	
C	0.747416361495	-0.249195413804	0.016330672839	
C	-1.614293264054	-0.917437193092	0.498938426327	
C	1.614293264054	0.917437193092	-0.498938426327	
H	-2.550691649877	3.642676912160	-1.079612414325	
H	-1.692264576072	3.397292704524	1.217702193082	
H	-0.391917441678	2.133792129082	2.887020573571	
H	1.029153708795	0.192471292011	3.456188158368	
H	2.093819399072	-1.928091671642	2.790303078617	
H	2.550691649877	-3.642676912160	1.079612414325	
H	1.692264576072	-3.397292704524	-1.217702193082	
H	0.391917441678	-2.133792129082	-2.887020573571	
H	-1.029153708795	-0.192471292011	-3.456188158368	
H	-2.093819399072	1.928091671642	-2.790303078617	
C	-2.929881911811	-1.023585640805	0.669603492147	
H	-1.035868601627	-1.795770708604	0.764139534745	
C	2.929881911811	1.023585640805	-0.669603492147	
H	1.035868601627	1.795770708604	-0.764139534745	
C	-3.968966821237	0.021365087143	0.389780645446	
C	-3.502490963569	-2.312360741427	1.201077435147	
C	3.968966821237	-0.021365087143	-0.389780645446	
C	3.502490963569	2.312360741427	-1.201077435147	
H	-4.697574242119	-0.362713979913	-0.331827486104	
H	-4.526426827892	0.245857131905	1.305211425464	
H	4.526426827892	-0.245857131905	-1.305211425464	
H	-3.564604360666	0.948686810338	0.002813296178	
H	3.564604360666	-0.948686810338	-0.002813296178	
H	4.697574242119	0.362713979913	0.331827486104	
H	-4.216133503773	-2.740737686941	0.489772757582	
H	-2.728089686330	-3.054084213807	1.397069594509	
H	-4.052695337649	-2.136410861079	2.131175162173	
H	4.216133503773	2.740737686941	-0.489772757582	
H	4.052695337649	2.136410861079	-2.131175162173	
H	2.728089686330	3.054084213807	-1.397069594509	

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of CPD* in DHP-2.

C	-1.951060757692	2.765313341125	-0.831584225465	E(S ₁) = -928.490884 a.u.
C	-1.488080289300	2.608994363612	0.476186522969	
C	-0.877208021806	1.443376342468	0.895255981956	
C	-0.220153749843	1.341362699435	2.169876161901	
C	0.714252643345	0.389806999278	2.427749872737	
C	1.127816629040	-0.565447727186	1.436181674297	
C	1.730290898096	-1.760912801120	1.775769903321	
C	1.951060757692	-2.765313341125	0.831584225465	
C	1.488080289300	-2.608994363612	-0.476186522969	
C	0.877208021806	-1.443376342468	-0.895255981956	
C	0.220153749843	-1.341362699435	-2.169876161901	
C	-0.714252643345	-0.389806999278	-2.427749872737	
C	-1.127816629040	0.565447727186	-1.436181674297	
C	-1.730290898096	1.760912801120	-1.775769903321	
C	-0.800012134133	0.257690644809	-0.011052639012	
C	0.800012134133	-0.257690644809	0.011052639012	
C	-1.592527456402	-0.943932877428	0.526486130786	
C	1.592527456402	0.943932877428	-0.526486130786	
H	-2.430306040141	3.689934739130	-1.128257593346	
H	-1.575107208501	3.432368565789	1.177660924954	
H	-0.465495222487	2.075840668077	2.929617607867	
H	1.147758572549	0.314742146893	3.419359805402	
H	2.004265501441	-1.929822879274	2.812107827538	
H	2.430306040141	-3.689934739130	1.128257593346	
H	1.575107208501	-3.432368565789	-1.177660924954	
H	0.465495222487	-2.075840668077	-2.929617607867	
H	-1.147758572549	-0.314742146893	-3.419359805402	
H	-2.004265501441	1.929822879274	-2.812107827538	
C	-2.904959427784	-1.056429962028	0.710708498011	
H	-0.981309474561	-1.803689190789	0.783622086521	
C	2.904959427784	1.056429962028	-0.710708498011	
H	0.981309474561	1.803689190789	-0.783622086521	
C	-3.935495183693	-0.004144596033	0.426231983590	
C	-3.471656369846	-2.340953497869	1.255365895684	
C	3.935495183693	0.004144596033	-0.426231983590	
C	3.471656369846	2.340953497869	-1.255365895684	
H	-4.668020674379	-0.384098942701	-0.293500380477	
H	-4.489934327194	0.232116159284	1.340433960539	
H	4.489934327194	-0.232116159284	-1.340433960539	
H	-3.519037871225	0.917213565049	0.033366663539	
H	3.519037871225	-0.917213565049	-0.033366663539	
H	4.668020674379	0.384098942701	0.293500380477	
H	-4.190681895052	-2.774464689671	0.552791133375	
H	-2.694324926140	-3.080180668011	1.449411343566	
H	-4.013553827268	-2.158743479137	2.189013142953	
H	4.190681895052	2.774464689671	-0.552791133375	
H	4.013553827268	2.158743479137	-2.189013142953	
H	2.694324926140	3.080180668011	-1.449411343566	

Table S1 (continued). B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-GS in**DHP-3.**

C	-0.146594811838	5.770938163644	0.753308244493
C	-0.160987032118	4.842983690016	1.792379395738
C	-0.173587437044	3.472047586687	1.534741315677
C	-0.049102357661	2.490158543825	2.522136856430
C	-0.000269656500	1.128952098607	2.210590905038
C	0.118360152189	0.678687267504	0.892067163028
C	0.014189237400	-0.656478885687	0.520283554037
C	0.060187950720	-1.061571961882	-0.825064625975
C	0.131843471943	-0.104686230880	-1.859072260125
C	0.175802909269	1.251646818811	-1.597645371122
C	0.070526558676	2.238627797121	-2.593494111299
C	0.006779632916	3.592759624011	-2.287764266218
C	-0.137215509161	4.048449169093	-0.967317014463
C	-0.091455364083	5.383371013194	-0.594117036421
C	-0.440234091317	2.999772530927	0.098638361899
C	0.435614267103	1.730915985936	-0.166086773937
C	-1.940980992740	2.613116016876	0.114289130765
C	1.930172537244	2.139316844234	-0.144547446829
H	-0.103189955660	6.827607221422	0.994033802327
H	-0.094024381080	5.187206127004	2.819715073806
H	-0.030075767398	2.800511198842	3.562280495634
H	-0.051772041135	0.396576078133	3.010819135087
H	-0.118871113714	-1.402085543354	1.296005359789
H	0.082312691509	-0.462162762359	-2.881516237044
H	0.065541011460	1.923160167077	-3.632258055008
H	0.045834584505	4.324610318690	-3.088958756026
H	0.034504639492	6.143044778184	-1.359978518287
C	-3.061818954294	3.084505117026	-0.450444165418
H	-2.101373968274	1.781666486956	0.791527005261
C	3.058170165974	1.584742919211	0.320707484541
H	2.082226466392	3.070281349091	-0.678816441501
C	-3.261383041862	4.231744147697	-1.408484902420
C	-4.369839845289	2.396224967414	-0.113296217363
C	3.262363680876	0.290150649324	1.065835690940
C	4.363238063952	2.319371077391	0.088640703871
H	-3.659017586116	3.857460791602	-2.359307949254
H	-4.018310126935	4.914720844403	-1.005527179562
H	4.005367835810	-0.319366928954	0.538700625739
H	-2.366073870949	4.804737158726	-1.614298607642
H	2.364786821470	-0.304096630446	1.184965128969
H	3.678642334165	0.491816247435	2.060213750896
H	-4.857684996701	2.025167519574	-1.022393393676
H	-4.230918252749	1.553916889104	0.566289695694
H	-5.070265781688	3.100050452475	0.352023725239
H	4.864030384880	2.529762290812	1.041194467720
H	5.055474916354	1.704740562413	-0.499051790402
H	4.217647509988	3.265490485225	-0.435093197591
C	0.035508706522	-2.499404274575	-1.231184701004
O	0.454387667652	-2.831160098481	-2.330805543218
C	-0.520966233885	-3.531442223301	-0.286450833028
C	0.138111685067	-4.790312565677	-0.084380124455
C	-1.740741734721	-3.292569133382	0.317784628190
C	1.393048733423	-5.119220846522	-0.665048675491
C	-0.485147507889	-5.757146255258	0.770906180505
C	-2.363223019914	-4.262949408955	1.130548580427
H	-2.241964722359	-2.347108803160	0.146728246584
C	1.994742541474	-6.327645630783	-0.407720875238
H	1.863028631523	-4.413390425602	-1.334401480757
C	0.165125736781	-6.995854890012	1.011324649001
C	-1.743464870669	-5.465238436810	1.357701546110
H	-3.329742900720	-4.050100446217	1.572733604425
C	1.379012929235	-7.277540409313	0.437275013532
H	2.951481475347	-6.557429864740	-0.863217109161
H	-0.318280820838	-7.717908703040	1.661159602408
H	-2.209560725884	-6.214418722220	1.989301268103
H	1.866609621871	-8.227073984108	0.627315788030

B3LYP energy:

 $E(S_0) = -1427.269888$ a.u.

CAM-B3LYP energy:

 $E(S_0) = -1426.437917$ a.u.

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-LE in DHP-3.

C	-0.100657998104	5.778740338465	0.502396752040	E(S ₁) = -1426.368637 a.u.
C	-0.280725093888	4.878324270410	1.554182857646	
C	-0.390191896850	3.503328133840	1.336063392185	
C	-0.370757472566	2.569712409096	2.377659829628	
C	-0.252916413977	1.201468587764	2.133013733775	
C	0.057909148226	0.708291675211	0.859554163416	
C	-0.038300305588	-0.643991957795	0.542890923373	
C	0.088432372747	-1.116536338902	-0.775198971803	
C	0.289654637483	-0.196334326594	-1.819006334319	
C	0.380640659651	1.173811888255	-1.599834839439	
C	0.359262246666	2.103302837060	-2.645593679420	
C	0.238546247683	3.473138197609	-2.403819210635	
C	-0.076162334815	3.969386114475	-1.135620633566	
C	0.012919442733	5.326223013778	-0.812477655578	
C	-0.492670098143	2.957448025982	-0.079466838631	
C	0.477447752206	1.725215262890	-0.187966264899	
C	-1.915884334353	2.439349773813	-0.363895056558	
C	1.899834948411	2.242675472124	0.098204813116	
H	-0.003446973646	6.835994512947	0.714361693255	
H	-0.287560080420	5.243169088880	2.575734725189	
H	-0.44822959639	2.925905834238	3.399266995924	
H	-0.407153310411	0.496523070290	2.942814790469	
H	-0.241055550033	-1.344920587560	1.343169234570	
H	0.329568193851	-0.584938983499	-2.829846135169	
H	0.439134557637	1.742224498732	-3.665055819023	
H	0.394324309934	4.175336710371	-3.215673936573	
H	0.229352105977	6.034121630491	-1.605404339401	
C	-3.091844734160	3.063011149591	-0.372335618199	
H	-1.947669968241	1.381735985950	-0.602439665534	
C	3.070424318602	1.609481283809	0.131509000046	
H	1.938139470412	3.305639463331	0.310836502078	
C	-3.354227967890	4.512890353868	-0.090865072264	
C	-4.338918511721	2.281387121142	-0.696238569224	
C	3.324162080808	0.151484179433	-0.114896096321	
C	4.320160480178	2.387566397961	0.453642968365	
H	-3.842620643138	4.975891946545	-0.954584270229	
H	-4.050968989344	4.609022901859	0.748368576081	
H	4.085853194722	0.033000017706	-0.891907582257	
H	-2.463433421956	5.083809517609	0.140654960963	
H	2.445818093438	-0.404461544647	-0.418669999644	
H	3.727682903595	-0.314575000880	0.790170929195	
H	-4.844279540385	2.704760023073	-1.570183158432	
H	-4.123473944394	1.232791030690	-0.901857242370	
H	-5.051852626413	2.329709449274	0.133230235943	
H	4.817918653648	1.970658504169	1.335120288439	
H	5.037306039117	2.325221719583	-0.371095493797	
H	4.109628727083	3.439790369393	0.645486559719	
C	0.051210898543	-2.552208623653	-1.135653722159	
O	0.478857695431	-2.923676225211	-2.214975439250	
C	-0.528056595724	-3.545329483108	-0.170111037967	
C	0.134523990659	-4.783861051999	0.100372502424	
C	-1.754974802761	-3.291635858708	0.390171141602	
C	1.400486720131	-5.123636879946	-0.442295174241	
C	-0.492871735813	-5.710250638735	0.976681193630	
C	-2.384974506351	-4.228332326727	1.232541876893	
H	-2.259438327510	-2.359310251459	0.167033270159	
C	2.003931202036	-6.306950833084	-0.123019891094	
H	1.873724220124	-4.443072142323	-1.134430832523	
C	0.160297056143	-6.929041528892	1.283719457761	
C	-1.762817916717	-5.406028513483	1.524198904980	
H	-3.361220305480	-4.004671411117	1.645011576133	
C	1.380767004806	-7.222528169288	0.749635000456	
H	2.970137073223	-6.548350638120	-0.549704002281	
H	-0.330839330180	-7.625528215221	1.954067586774	
H	-2.233656422572	-6.131154131042	2.178624217768	
H	1.872324747283	-8.157572169715	0.990154448802	

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of CPD* in DHP-3.

C	-0.038899321438	5.752500538721	0.505855249527	E(S ₁) = -1426.371742 a.u.
C	-0.234145600051	4.850511645063	1.554034473250	
C	-0.407240956035	3.501130854173	1.322589322427	
C	-0.409599967532	2.538287627622	2.388885587680	
C	-0.175964054481	1.218773843138	2.168826738684	
C	0.111133921082	0.704434318082	0.857125790120	
C	-0.054283832728	-0.627474466672	0.546331812465	
C	0.054140583989	-1.104131388481	-0.770340563332	
C	0.264863443308	-0.178367779338	-1.814000802029	
C	0.424739942028	1.162004417323	-1.581622798083	
C	0.430292545652	2.128077921757	-2.651654235585	
C	0.189344893697	3.444409811895	-2.434082861638	
C	-0.101970484196	3.960651940955	-1.123980405809	
C	0.058959822559	5.295111128713	-0.809357049757	
C	-0.514316977621	2.976794305490	-0.075702452645	
C	0.529644637129	1.691841618160	-0.185047923015	
C	-1.902225387347	2.377819830324	-0.366549768405	
C	1.917204682340	2.289135499936	0.103059259239	
H	0.092888278134	6.805867177641	0.720233334345	
H	-0.211707858924	5.206502245518	2.578593927068	
H	-0.571413038622	2.897616908523	3.399373738891	
H	-0.235638287130	0.514848499830	2.991902694421	
H	-0.281071858161	-1.319002075913	1.348424911384	
H	0.268059041139	-0.559013137487	-2.828686511379	
H	0.604249324552	1.767894409963	-3.659636549493	
H	0.249894944675	4.148428342908	-3.256944409036	
H	0.303976892174	5.993089520728	-1.602914101904	
C	-3.086755948974	2.982244880395	-0.390673225735	
H	-1.885458170246	1.314133864966	-0.583064937901	
C	3.096697359753	1.675503949113	0.145747807460	
H	1.910544809424	3.358122664609	0.292763736000	
C	-3.352228484018	4.435313856936	-0.130967608888	
C	-4.321540592580	2.179821888844	-0.705510274601	
C	3.351740948207	0.215286647858	-0.082757099658	
C	4.336604990676	2.474219840620	0.450024485710	
H	-3.841334484409	4.885482137417	-1.000811155455	
H	-4.046989652131	4.543516478286	0.708224128979	
H	4.067758298981	0.085600341409	-0.900414032548	
H	-2.458844467326	5.008535119425	0.091080638205	
H	2.459321774672	-0.351933982440	-0.322599141153	
H	3.810515920141	-0.226964065739	0.807457239477	
H	-4.828564079578	2.583030493046	-1.587768585366	
H	-4.091088296401	1.131194126687	-0.893711737297	
H	-5.036901857818	2.232403117723	0.121389278038	
H	4.836325582721	2.084648254701	1.342579626489	
H	5.055072138946	2.398288551128	-0.372216964821	
H	4.114082261440	3.528616820498	0.614571533742	
C	-0.023779197652	-2.534190418378	-1.136311227035	
O	0.355569435370	-2.910903159693	-2.232889115394	
C	-0.579920012747	-3.524952160606	-0.153958445660	
C	0.085098092993	-4.767122584450	0.093864969736	
C	-1.788243117520	-3.268183206368	0.444374730108	
C	1.331687079991	-5.111047095299	-0.489443501677	
C	-0.517842593446	-5.692532984702	0.988141664483	
C	-2.395312381644	-4.204066004523	1.304314939341	
H	-2.296193753390	-2.334008439423	0.237814427141	
C	1.940602102676	-6.297079039467	-0.191200032506	
H	1.784420404020	-4.431147437754	-1.195909288081	
C	0.140224506899	-6.914208122899	1.272685178825	
C	-1.768955287429	-5.384516088974	1.575434094198	
H	-3.357695872465	-3.977539364455	1.746894572268	
C	1.342048248854	-7.211494104412	0.699755978282	
H	2.891654352933	-6.541679635935	-0.649038839253	
H	-0.332052731170	-7.609901434473	1.957312209164	
H	-2.222043829502	-6.108801536161	2.243228308776	
H	1.837397253562	-8.148790796080	0.923291779216	

Table S1 (continued). B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-GS in

DHP-4.

C	2.049473480003	5.202735337932	0.359229681587
C	2.855490095367	4.172173633464	0.753341537889
C	2.399432245965	2.830174667836	0.669768323528
C	3.244712361307	1.751641333493	0.781399563668
C	2.780510513403	0.422433853493	0.611719062631
C	1.514200578067	0.156666868067	0.144094276121
C	0.954596910099	-1.139301768282	0.213866287887
C	-0.397282020989	-1.347785471805	0.042926961747
C	-1.263692715702	-0.239900692549	-0.267420392424
C	-0.810487978422	1.023754501777	-0.469920387114
C	-1.683404644364	2.153556471038	-0.764501190540
C	-1.205438215171	3.490611181575	-0.635273506554
C	0.135676750027	3.753624517834	-0.130614584370
C	0.729413457210	4.980673709615	-0.146030871514
C	0.885548824181	2.580705895602	0.502677238383
C	0.686858455640	1.327259516161	-0.414699167399
C	0.405905748827	2.260241136228	1.936726932499
C	1.234896883397	1.688398944336	-1.819406206767
H	2.434138616460	6.216776801129	0.363357577003
H	3.883662274553	4.358895090726	1.046700065101
H	4.285580553135	1.924267350785	1.036559468288
H	3.424408523099	-0.405592911627	0.892735237866
H	1.606389222197	-1.965375137014	0.473677228126
H	-2.319278737339	-0.470650376684	-0.319335496779
H	0.214262481980	5.832497735833	-0.572985295602
C	-0.329617641683	2.894895884160	2.859780757513
H	0.815908843905	1.308758578380	2.260214126926
C	1.171378350324	1.036145560297	-2.987054764037
H	1.780158602159	2.624933579965	-1.844522077773
C	-1.022361396368	4.231200924538	2.781929343997
C	-0.535763992593	2.218438287100	4.199473123656
C	0.515728375980	-0.290248388547	-3.261898377905
C	1.827764150711	1.644588642480	-4.205980097728
H	-2.104519405407	4.097771359471	2.894609398263
H	-0.698747044462	4.859730022438	3.619840556801
H	-0.211798167433	-0.188561943379	-4.075577386370
H	-0.839045305643	4.773738379672	1.862599307520
H	0.006534500565	-0.716581282453	-2.405290786730
H	1.267068659440	-1.010605752990	-3.607275516712
H	-1.603934559128	2.071286392950	4.397517816181
H	-0.043352883663	1.246109481656	4.251633266753
H	-0.149640831510	2.843091404943	5.013795003133
H	2.584491153451	0.967116487510	-4.619217254976
H	1.090680660778	1.811594928310	-5.000244998220
H	2.308851922465	2.598040618673	-3.981358113863
C	-1.023680095212	-2.696611407134	0.105058511354
O	-2.127244206361	-2.881839044785	-0.392411534554
C	-0.298390284926	-3.827847782580	0.784654862202
C	-0.226628430538	-5.130884215513	0.187193374205
C	0.221265959559	-3.625795142223	2.049139495294
C	-0.734490716046	-5.427115919178	-1.106789189802
C	0.416624744368	-6.182826121475	0.917997771284
C	0.822712004292	-4.675211930364	2.775324521734
H	0.145333144506	-2.645064954395	2.503500085350
C	-0.605663688940	-6.685058272038	-1.644852552062
H	-1.248128290119	-4.653406761457	-1.658871146416
C	0.528731241514	-7.470437808607	0.331049969535
C	0.924798655032	-5.923735971543	2.217135010334
H	1.202240047499	-4.486155461247	3.772975360656
C	0.031026869189	-7.719054305791	-0.923144165752
H	-1.002412042075	-6.888319161638	-2.633247574036
H	1.018463632793	-8.257003833204	0.895701089500
H	1.394083755200	-6.735012200594	2.763975141223
H	0.121815267560	-8.706472355077	-1.361629447440
C	-2.084101589796	4.550976427247	-0.961071469207
C	-3.003803628590	1.950231340517	-1.224847499934
C	-3.369121510877	4.322264184861	-1.403102460718
C	-3.834317828747	3.004900063376	-1.538307739115
H	-4.840043478417	2.814945336312	-1.895556407951
H	-3.363831228633	0.939159691103	-1.363575073563
H	-1.752206190410	5.574198080155	-0.841728149051
H	-4.017169796644	5.157798271138	-1.642021222760

B3LYP energy:

$E(S_0) = -1580.944287$ a.u.

CAM-B3LYP energy:

$E(S_0) = -1580.030723$ a.u.

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of CPD* in DHP-4.

C	1.817694066010	5.202503556071	0.019927871533
C	2.635523683001	4.188696762350	0.490209597776
C	2.151417270630	2.899556096761	0.666467930682
C	3.029430831019	1.804325707083	0.897442919405
C	2.644183961395	0.512729659920	0.672344512145
C	1.362999480110	0.187606680334	0.142661343006
C	0.831232860132	-1.079894048592	0.292718872553
C	-0.505025443127	-1.357408802416	-0.001801215727
C	-1.340873123600	-0.292176893257	-0.418175976422
C	-0.880467917704	0.971760937066	-0.642762565852
C	-1.801222991747	2.081887770830	-0.935447160863
C	-1.450644448238	3.408600720402	-0.585554969218
C	-0.095016445969	3.709785736702	-0.110537863348
C	0.482485578655	4.937603499395	-0.322968631102
C	0.685274338625	2.607103364216	0.519150788308
C	0.571269715241	1.291976192453	-0.500725404110
C	0.054246288938	2.139126037626	1.839367535425
C	1.197668144541	1.761794552562	-1.820930422674
H	2.223200616111	6.193353820400	-0.143843531975
H	3.688997083822	4.378676266432	0.665055350427
H	4.040975295961	2.018840838395	1.224401549651
H	3.312840203192	-0.301718694500	0.930187525851
H	1.473153510339	-1.862482014150	0.678382321002
H	-2.390440015264	-0.525507328553	-0.538535454130
H	-0.094502639705	5.721213976153	-0.797571343233
C	-0.115658297510	2.824691680874	2.966681784970
H	-0.302757753715	1.114516844983	1.820792321192
C	1.331339390747	1.085163040493	-2.958898600906
H	1.568760134628	2.781769927081	-1.807380932623
C	0.292764347258	4.247168751250	3.210123124669
C	-0.776197071465	2.162781464838	4.146432651872
C	0.895822423418	-0.328451546947	-3.207377403595
C	1.977242531171	1.747691801906	-4.146605300807
H	-0.584448214716	4.847796391380	3.471531696847
H	0.972746199457	4.298767374367	4.066481563186
H	0.191552046958	-0.360353089999	-4.044777574036
H	0.782149453561	4.710563340217	2.360102579846
H	0.424474336774	-0.797054398350	-2.350331050876
H	1.757181513298	-0.937430409777	-3.500063581433
H	-1.671665248882	2.715898034469	4.446646423062
H	-1.066967759222	1.135192141386	3.928426893421
H	-0.104597173849	2.155262173085	5.010789644925
H	2.861078121040	1.187238626590	-4.467347252529
H	1.289574892097	1.766768293443	-4.997920448835
H	2.281113754613	2.771678421380	-3.928609761354
C	-1.111263471290	-2.698853419519	0.087769953390
O	-2.202719008199	-2.921889508076	-0.411021807826
C	-0.379865252314	-3.800131024301	0.802971370639
C	-0.235043643610	-5.091733360629	0.206273297072
C	0.075337577548	-3.584845050147	2.079440487499
C	-0.685243036969	-5.395720766734	-1.104242018346
C	0.413336979091	-6.114372700331	0.949982496692
C	0.688249336200	-4.612542543084	2.822988442929
H	-0.054407019980	-2.609679687989	2.532957512406
C	-0.491162306306	-6.636956328271	-1.640722312130
H	-1.208886430348	-4.636870579123	-1.666891444831
C	0.595571303430	-7.390910607148	0.363570119907
C	0.860271820122	-5.845378401941	2.266430449473
H	1.021299236721	-4.414514179433	3.834582538527
C	0.156833824513	-7.648518977998	-0.902212747656
H	-0.844367982202	-6.849728452220	-2.642685207402
H	1.092472838068	-8.161128851268	0.942913192816
H	1.339131416341	-6.641401922891	2.825778911021
H	0.300535598158	-8.628328270807	-1.341777790432
C	-2.398005373217	4.420861901035	-0.750910741556
C	-3.048807258234	1.853093025407	-1.515417059205
C	-3.644603657542	4.165717141148	-1.297344504749
C	-3.963933814258	2.877393970081	-1.698417685315
H	-4.925906618970	2.665692705338	-2.149100870120
H	-3.303682214382	0.853621017719	-1.842823362140
H	-2.161469200808	5.425512975586	-0.424481988834
H	-4.360361199587	4.970544739249	-1.411654357933

$$E(S_1) = -1579.970710 \text{ a.u.}$$

Table S1 (continued). TD-CAM-B3LYP/6-311G(d,p) Cartesian coordinates and energies of DHP-LE in DHP-4.

C	2.037207772238	5.208892566866	0.338512391578
C	2.861857107791	4.134049945300	0.691915836920
C	2.392122201909	2.830263146766	0.652549444646
C	3.249192387653	1.721881046814	0.774426983609
C	2.806130761898	0.426276860418	0.581840685804
C	1.499080053831	0.149464094675	0.136914153044
C	0.958116539789	-1.118419890519	0.228984242064
C	-0.415172700181	-1.354812009435	0.010791791550
C	-1.253550448931	-0.284997806983	-0.307872797329
C	-0.797401538996	1.025373009016	-0.467563532111
C	-1.660510728209	2.120226211116	-0.694845503520
C	-1.144915611914	3.478405482639	-0.636003148443
C	0.143850248075	3.729414200296	-0.122514607779
C	0.741682227177	5.002200585361	-0.107835224794
C	0.895676306142	2.569371627407	0.504986509793
C	0.692409595797	1.315942457442	-0.414316413378
C	0.395283168491	2.212205740143	1.913771542444
C	1.255404474341	1.689684960964	-1.800695713618
H	2.441488349112	6.213561584661	0.342461238124
H	3.905960930981	4.310506710960	0.925643703598
H	4.286790290146	1.901783288958	1.033755480177
H	3.463114805444	-0.406421280070	0.809178561332
H	1.603311070584	-1.936605841713	0.523512787427
H	-2.303116660823	-0.521409999862	-0.409564400106
H	0.192332939505	5.857244619249	-0.476862098596
C	-0.344557543954	2.846206938394	2.822690034205
H	0.752211115743	1.231295650672	2.211005879273
C	1.168132448130	1.069443190014	-2.975595923568
H	1.837724131605	2.604919113151	-1.795464322067
C	-0.972206598148	4.210579592062	2.743716150425
C	-0.648365705327	2.142863886071	4.122517580293
C	0.462256030975	-0.220240644549	-3.274585442052
C	1.840206431387	1.676066199709	-4.180249821215
H	-2.048758197825	4.120833867106	2.565193816333
H	-0.853526917066	4.721837512131	3.703211763703
H	-0.296037648145	-0.061508167471	-4.048020387018
H	-0.551563663109	4.843096408123	1.971011656393
H	-0.020516547345	-0.669677007713	-2.415287482270
H	1.175450822591	-0.944334888242	-3.681630984277
H	-1.730054709451	2.073023983676	4.275917150459
H	-0.234683542151	1.134862405766	4.151880580094
H	-0.245827298287	2.706256637318	4.970413580819
H	2.573705233391	0.982501097848	-4.603803552199
H	1.107794774790	1.879360268546	-4.968002384012
H	2.349884421996	2.608860832667	-3.938668143124
C	-1.034352307145	-2.699260377720	0.080406361170
O	-2.129754673233	-2.898704779605	-0.415360268806
C	-0.309893102887	-3.813428163708	0.778991839624
C	-0.218539294354	-5.115784188430	0.195007659718
C	0.192259726541	-3.592713303867	2.036926020722
C	-0.715570199578	-5.425598091649	-1.097088295389
C	0.425178463905	-6.145276036661	0.933568738240
C	0.800142948791	-4.626257793431	2.775901264737
H	0.103718335071	-2.607909157853	2.479581677097
C	-0.570698383547	-6.679113778591	-1.620471699405
H	-1.234274756328	-4.661125267187	-1.656334572643
C	0.555361291391	-7.434385053998	0.361162835096
C	0.920122554104	-5.870650379430	2.231525170987
H	1.170636733251	-4.423905144352	3.773404398122
C	0.071646183316	-7.697691230567	-0.886877329679
H	-0.958832743801	-6.895832768819	-2.608535358692
H	1.049161674121	-8.209402881897	0.936650331541
H	1.394527360604	-6.672048733505	2.786931389436
H	0.175773938050	-8.686961549091	-1.316160519742
C	-2.014158005253	4.533508134966	-1.043524799444
C	-3.031504798782	1.940284718836	-1.035642264061
C	-3.307672338332	4.305081852217	-1.396638938604
C	-3.830752901388	2.986733359863	-1.377969951390
H	-4.863379786163	2.812920128691	-1.654405819549
H	-3.440267021560	0.940339069681	-1.066540544550
H	-1.650185212227	5.551031207513	-1.043684554807
H	-3.945084296217	5.132368122845	-1.684129202364

$E(S_2) = -1579.949501$ a.u.

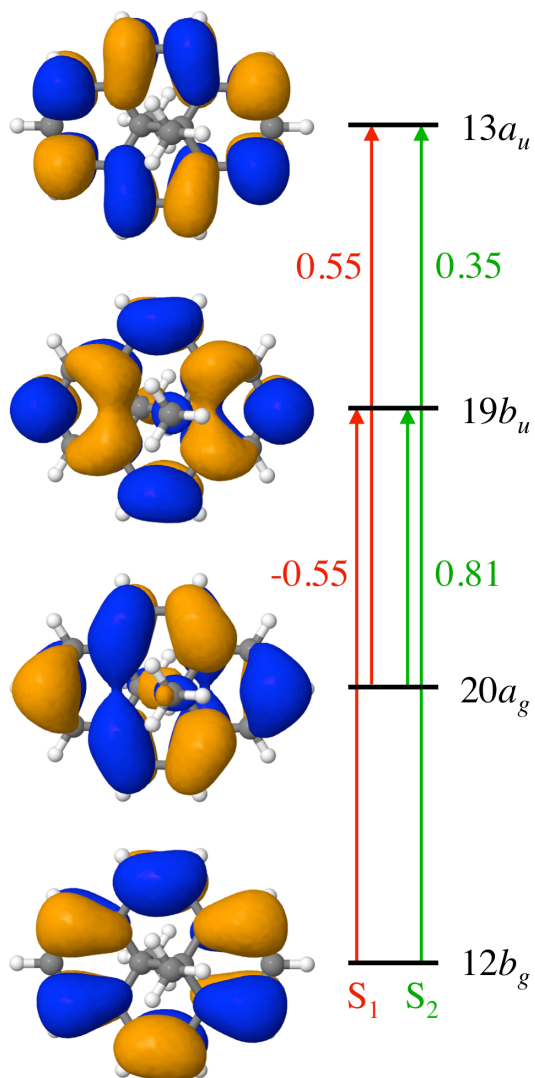


Figure S1. Representation of the CASSCF molecular orbitals involved in the electronic configurations of the S_1 and S_2 excited states of $\text{DHP}_{\text{parent}}$. The main transitions are indicated by vertical arrows along with the corresponding configuration interaction coefficients for each state.