Supporting Information: An Investigation of the Structural and Thermochemical Properties of [2.2.2]-Bicyclooctadienes Photoswitches

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1 Structures

In this section, we have included the CCSD optimized structures and the DFT/6-311++G** structures of the [2.2.2]-bicyclooctadienes, tetracycloctane, and transition states given in Cartesian coordinates with units in Å.

BOD CCSD/cc-pVTZ structure

C	0.00000	1.27254	-0.10847
C	0.00000	0.77014	1.36431
C	-1.22759	0.66413	-0.74226
C	-0.00000	-0.77014	1.36431
H	-0.87774	1.15565	1.87461
H	0.87774	1.15565	1.87461
C	1.22759	0.66413	-0.74226
H	0.00000	2.35545	-0.15105
C	-1.22759	-0.66413	-0.74226
H	-2.03342	1.27305	-1.11304
C	-0.00000	-1.27254	-0.10847
H	-0.87774	-1.15565	1.87461
H	0.87774	-1.15565	1.87461
C	1.22759	-0.66413	-0.74226
H	2.03342	1.27305	-1.11304
H	-2.03342	-1.27305	-1.11304
H	-0.00000	-2.35545	-0.15105
H	2.03342	-1.27305	-1.11304

TCO CCSD/cc-pVTZ structure

C	0.97323	0.77062	-0.75792
C	0.97323	-0.77076	-0.75778
C	-0.18052	-1.34921	0.00013
H	-0.16122	-2.42884	0.00023
C	-0.18052	1.34921	-0.00014
H	-0.16121	2.42884	-0.00023
C	-1.56681	0.76737	-0.00014
H	-2.09857	1.14066	0.87172
H	-2.09846	1.14043	-0.87216
C	-1.56681	-0.76737	0.00006
H	-2.09850	-1.14043	0.87206
H	-2.09853	-1.14066	-0.87182
C	0.97319	0.77076	0.75783
H	1.58181	1.35659	1.42075
C	0.97320	-0.77062	0.75797
H	1.58182	-1.35633	1.42101
H	1.58189	1.35632	-1.42093
H	1.58188	-1.35659	-1.42068

Sub-BOD CCSD/cc-pVTZ structure

C	0.32633	-1.09298	-0.11947
C	1.16008	-1.00449	1.18977
C	1.31388	-0.91054	-1.24493
C	1.89501	0.34824	1.22412
H	1.86684	-1.82785	1.21881
H	0.49660	-1.10612	2.04345
C	-0.58750	0.10032	-0.08911
H	-0.22842	-2.02002	-0.17671
C	1.95063	0.25465	-1.21843
H	1.49962	-1.68961	-1.96329
C	1.54491	1.14538	-0.06765
H	2.97027	0.20524	1.26696
H	1.60165	0.92714	2.09488
C	0.04671	1.27036	-0.06353
H	2.71743	0.54876	-1.91308
H	2.04351	2.10694	-0.08229
H	-0.45272	2.21985	0.00054
C	-2.04036	-0.07558	-0.02684
O	-2.59813	-1.14051	0.01613
O	-2.71755	1.08773	-0.01836
H	-3.64752	0.84576	0.02492

Sub-TCO CCSD/cc-pVTZ structure

C	0.32162	-1.26828	-0.26921
C	-0.50782	-0.00747	0.01030
C	0.33714	1.20153	0.28181
H	-0.28131	2.06242	0.48120
C	1.79702	-1.01598	-0.21790
H	2.36327	-1.91410	-0.41187
C	2.47428	0.24757	-0.67189
H	3.37814	0.37465	-0.08048
H	2.78961	0.13629	-1.70578
C	1.57293	1.47795	-0.52733
H	2.12225	2.29333	-0.06484
H	1.25630	1.82994	-1.50622
C	1.03115	-1.10545	1.06227
H	1.22017	-1.85274	1.80950
C	0.22169	0.17058	1.34352
H	-0.26448	0.37007	2.28052
C	-1.94964	0.11607	-0.15366
O	-2.48496	-0.94898	-0.78091
H	-3.43047	-0.77490	-0.82777
O	-2.61961	1.04070	0.22659
H	-0.10730	-2.15783	-0.68717

Sub-TS CCSD/cc-pVDZ structure

C	0.24160	-1.15174	-0.26929
C	-0.53849	0.13647	-0.38745
C	0.32163	1.13256	0.39149
H	-0.25694	1.99664	0.73852
C	1.71536	-1.06558	-0.34268
H	2.23631	-1.99056	-0.61462
C	2.28111	0.22469	-0.94354
H	3.37854	0.23285	-0.83080
H	2.06125	0.20433	-2.02498
C	1.64997	1.48438	-0.29622
H	2.34148	1.92178	0.44801
H	1.46054	2.25255	-1.06373
C	1.30181	-1.04395	1.13544
H	1.33379	-1.92794	1.77102
C	0.48118	0.07675	1.43040
H	-0.14646	0.08804	2.33183
C	-1.96058	0.15768	-0.20839
O	-2.55205	-1.04619	-0.53595
H	-3.49828	-0.86839	-0.42552
O	-2.64866	1.10912	0.14984
H	-0.26619	-2.12031	-0.29934

BOD B2PLYP/6-311++G structure**

C	0.00000	1.28093	-0.11342
C	0.00000	0.77380	1.37727
C	-1.23488	0.66903	-0.74732
C	-0.00000	-0.77380	1.37727
H	-0.88247	1.16600	1.88738
H	0.88247	1.16600	1.88738
C	1.23488	0.66903	-0.74732
H	0.00000	2.36973	-0.15473
C	-1.23488	-0.66903	-0.74732
H	-2.04648	1.28394	-1.11768
C	-0.00000	-1.28093	-0.11342
H	-0.88247	-1.16600	1.88738
H	0.88247	-1.16600	1.88738
C	1.23488	-0.66903	-0.74732
H	2.04648	1.28394	-1.11768
H	-2.04648	-1.28394	-1.11768
H	-0.00000	-2.36973	-0.15473
H	2.04648	-1.28394	-1.11768

BOD B3LYP/6-311++G structure**

C	0.00000	1.28122	-0.11385
C	0.00000	0.77468	1.38052
C	-1.23632	0.66649	-0.74883
C	-0.00000	-0.77468	1.38052
H	-0.88160	1.16796	1.89201
H	0.88160	1.16796	1.89201
C	1.23632	0.66649	-0.74883
H	0.00000	2.37032	-0.15589
C	-1.23632	-0.66649	-0.74883
H	-2.04628	1.28288	-1.12111
C	-0.00000	-1.28122	-0.11385
H	-0.88160	-1.16796	1.89201
H	0.88160	-1.16796	1.89201
C	1.23632	-0.66649	-0.74883
H	2.04628	1.28288	-1.12111
H	-2.04628	-1.28288	-1.12111
H	-0.00000	-2.37032	-0.15589
H	2.04628	-1.28288	-1.12111

BOD CAM-B3LYP/6-311++G structure**

C	0.00000	1.27542	-0.11153
C	0.00000	0.77152	1.37303
C	-1.23166	0.66338	-0.74545
C	-0.00000	-0.77152	1.37303
H	-0.88035	1.16416	1.88447
H	0.88035	1.16416	1.88447
C	1.23166	0.66338	-0.74545
H	0.00000	2.36353	-0.15342
C	-1.23166	-0.66338	-0.74545
H	-2.04099	1.27803	-1.11956
C	-0.00000	-1.27542	-0.11153
H	-0.88035	-1.16416	1.88447
H	0.88035	-1.16416	1.88447
C	1.23166	-0.66338	-0.74545
H	2.04099	1.27803	-1.11956
H	-2.04099	-1.27803	-1.11956
H	-0.00000	-2.36353	-0.15342
H	2.04099	-1.27803	-1.11956

BOD CAM-B3LYP-D3/6-311++G structure**

C	0.00000	1.27527	-0.11179
C	0.00000	0.77174	1.37308
C	-1.23211	0.66340	-0.74545
C	-0.00000	-0.77174	1.37308
H	-0.88062	1.16453	1.88378
H	0.88062	1.16453	1.88378
C	1.23211	0.66340	-0.74545
H	0.00000	2.36332	-0.15349
C	-1.23211	-0.66340	-0.74545
H	-2.04167	1.27825	-1.11822
C	-0.00000	-1.27527	-0.11179
H	-0.88062	-1.16453	1.88378
H	0.88062	-1.16453	1.88378
C	1.23211	-0.66340	-0.74545
H	2.04167	1.27825	-1.11822
H	-2.04167	-1.27825	-1.11822
H	-0.00000	-2.36332	-0.15349
H	2.04167	-1.27825	-1.11822

BOD CAM-B3LYP-D3BJ/6-311++G structure**

C	0.00000	1.27521	-0.11163
C	0.00000	0.77128	1.37237
C	-1.23154	0.66331	-0.74510
C	-0.00000	-0.77128	1.37237
H	-0.88049	1.16366	1.88339
H	0.88049	1.16366	1.88339
C	1.23154	0.66331	-0.74510
H	0.00000	2.36311	-0.15338
C	-1.23154	-0.66331	-0.74510
H	-2.04095	1.27800	-1.11834
C	-0.00000	-1.27521	-0.11163
H	-0.88049	-1.16366	1.88339
H	0.88049	-1.16366	1.88339
C	1.23154	-0.66331	-0.74510
H	2.04095	1.27800	-1.11834
H	-2.04095	-1.27800	-1.11834
H	-0.00000	-2.36311	-0.15338
H	2.04095	-1.27800	-1.11834

BOD M06-2X/6-311++G structure**

C	0.00000	1.27815	-0.11309
C	0.00000	0.77188	1.37365
C	-1.23378	0.66499	-0.74505
C	-0.00000	-0.77188	1.37365
H	-0.88231	1.16393	1.88217
H	0.88231	1.16393	1.88217
C	1.23378	0.66499	-0.74505
H	0.00000	2.36589	-0.15392
C	-1.23378	-0.66499	-0.74505
H	-2.04434	1.27983	-1.11663
C	-0.00000	-1.27815	-0.11309
H	-0.88231	-1.16393	1.88217
H	0.88231	-1.16393	1.88217
C	1.23378	-0.66499	-0.74505
H	2.04434	1.27983	-1.11663
H	-2.04434	-1.27983	-1.11663
H	-0.00000	-2.36589	-0.15392
H	2.04434	-1.27983	-1.11663

BOD PBE0-DH/6-311++G structure**

C	0.00000	1.27190	-0.11153
C	0.00000	0.76777	1.36509
C	-1.22730	0.66456	-0.74143
C	-0.00000	-0.76777	1.36509
H	-0.88023	1.15927	1.87551
H	0.88023	1.15927	1.87551
C	1.22730	0.66456	-0.74143
H	0.00000	2.35882	-0.15155
C	-1.22730	-0.66456	-0.74143
H	-2.03759	1.27800	-1.11182
C	-0.00000	-1.27190	-0.11153
H	-0.88023	-1.15927	1.87551
H	0.88023	-1.15927	1.87551
C	1.22730	-0.66456	-0.74143
H	2.03759	1.27800	-1.11182
H	-2.03759	-1.27800	-1.11182
H	-0.00000	-2.35882	-0.15155
H	2.03759	-1.27800	-1.11182

BOD PBE0/6-311++G structure**

C	0.00000	1.27521	-0.11280
C	0.00000	0.76955	1.36970
C	-1.23037	0.66558	-0.74356
C	-0.00000	-0.76955	1.36970
H	-0.88234	1.16311	1.88160
H	0.88234	1.16311	1.88160
C	1.23037	0.66558	-0.74356
H	0.00000	2.36528	-0.15247
C	-1.23037	-0.66558	-0.74356
H	-2.04241	1.28171	-1.11471
C	-0.00000	-1.27521	-0.11280
H	-0.88234	-1.16311	1.88160
H	0.88234	-1.16311	1.88160
C	1.23037	-0.66558	-0.74356
H	2.04241	1.28171	-1.11471
H	-2.04241	-1.28171	-1.11471
H	-0.00000	-2.36528	-0.15247
H	2.04241	-1.28171	-1.11471

BOD ωB97X-D/6-311++G structure**

C	0.00000	1.27650	-0.11189
C	0.00000	0.77183	1.37436
C	-1.23258	0.66464	-0.74612
C	-0.00000	-0.77183	1.37436
H	-0.88191	1.16489	1.88500
H	0.88191	1.16489	1.88500
C	1.23258	0.66464	-0.74612
H	0.00000	2.36532	-0.15271
C	-1.23258	-0.66464	-0.74612
H	-2.04247	1.28000	-1.11936
C	-0.00000	-1.27650	-0.11189
H	-0.88191	-1.16489	1.88500
H	0.88191	-1.16489	1.88500
C	1.23258	-0.66464	-0.74612
H	2.04247	1.28000	-1.11936
H	-2.04247	-1.28000	-1.11936
H	-0.00000	-2.36532	-0.15271
H	2.04247	-1.28000	-1.11936

TCO B2PLYP/6-311++G structure**

C	0.98046	0.77567	-0.76366
C	0.98041	-0.77581	-0.76355
C	-0.18212	-1.35917	0.00013
H	-0.16279	-2.44614	0.00025
C	-0.18210	1.35917	-0.00014
H	-0.16276	2.44614	-0.00025
C	-1.57872	0.77246	-0.00015
H	-2.11379	1.15064	0.87610
H	-2.11366	1.15039	-0.87659
C	-1.57873	-0.77244	0.00007
H	-2.11372	-1.15036	0.87649
H	-2.11377	-1.15061	-0.87620
C	0.98038	0.77580	0.76360
H	1.59506	1.36709	1.42930
C	0.98041	-0.77568	0.76371
H	1.59513	-1.36686	1.42948
H	1.59521	1.36683	-1.42942
H	1.59512	-1.36711	-1.42921

TCO B3LYP/6-311++G structure**

C	0.98096	0.77689	-0.76241
C	0.98091	-0.77703	-0.76230
C	-0.18174	-1.36142	0.00014
H	-0.16523	-2.44874	0.00026
C	-0.18172	1.36142	-0.00015
H	-0.16521	2.44874	-0.00026
C	-1.57952	0.77339	-0.00015
H	-2.11678	1.15177	0.87551
H	-2.11665	1.15152	-0.87600
C	-1.57953	-0.77338	0.00008
H	-2.11670	-1.15150	0.87590
H	-2.11674	-1.15175	-0.87561
C	0.98088	0.77702	0.76235
H	1.59752	1.36610	1.42900
C	0.98092	-0.77689	0.76246
H	1.59760	-1.36585	1.42917
H	1.59767	1.36583	-1.42912
H	1.59758	-1.36610	-1.42892

TCO CAM-B3LYP/6-311++G structure**

C	0.97684	0.77356	-0.75836
C	0.97676	-0.77370	-0.75826
C	-0.18080	-1.35510	0.00014
H	-0.16459	-2.44121	0.00026
C	-0.18078	1.35510	-0.00015
H	-0.16455	2.44121	-0.00026
C	-1.57351	0.76955	-0.00016
H	-2.10913	1.14838	0.87441
H	-2.10899	1.14812	-0.87493
C	-1.57352	-0.76953	0.00008
H	-2.10905	-1.14809	0.87482
H	-2.10910	-1.14836	-0.87451
C	0.97674	0.77369	0.75831
H	1.59348	1.36266	1.42302
C	0.97679	-0.77357	0.75841
H	1.59358	-1.36243	1.42316
H	1.59367	1.36240	-1.42310
H	1.59353	-1.36268	-1.42294

TCO CAM-B3LYP-D3/6-311++G structure**

C	0.97673	0.77358	-0.75847
C	0.97666	-0.77372	-0.75838
C	-0.18084	-1.35529	0.00014
H	-0.16477	-2.44141	0.00026
C	-0.18082	1.35529	-0.00015
H	-0.16473	2.44141	-0.00026
C	-1.57363	0.76977	-0.00016
H	-2.10816	1.14894	0.87478
H	-2.10801	1.14868	-0.87530
C	-1.57364	-0.76975	0.00008
H	-2.10807	-1.14865	0.87519
H	-2.10813	-1.14892	-0.87488
C	0.97664	0.77371	0.75843
H	1.59370	1.36213	1.42336
C	0.97668	-0.77359	0.75852
H	1.59380	-1.36190	1.42351
H	1.59389	1.36187	-1.42345
H	1.59376	-1.36214	-1.42328

TCO CAM-B3LYP-D3BJ/6-311++G structure**

C	0.97634	0.77334	-0.75834
C	0.97626	-0.77348	-0.75825
C	-0.18076	-1.35478	0.00014
H	-0.16454	-2.44070	0.00026
C	-0.18074	1.35478	-0.00015
H	-0.16450	2.44070	-0.00026
C	-1.57273	0.76928	-0.00016
H	-2.10794	1.14790	0.87454
H	-2.10779	1.14763	-0.87506
C	-1.57275	-0.76926	0.00008
H	-2.10786	-1.14760	0.87496
H	-2.10791	-1.14787	-0.87464
C	0.97624	0.77346	0.75830
H	1.59283	1.36230	1.42292
C	0.97629	-0.77335	0.75839
H	1.59294	-1.36208	1.42306
H	1.59302	1.36204	-1.42300
H	1.59288	-1.36232	-1.42284

TCO M06-2X/6-311++G structure**

C	0.97624	0.77336	-0.75874
C	0.97619	-0.77351	-0.75862
C	-0.18008	-1.35561	0.00013
H	-0.15836	-2.44135	0.00024
C	-0.18006	1.35561	-0.00014
H	-0.15832	2.44135	-0.00024
C	-1.57523	0.77041	-0.00015
H	-2.10817	1.14871	0.87580
H	-2.10802	1.14846	-0.87630
C	-1.57525	-0.77039	0.00007
H	-2.10809	-1.14843	0.87620
H	-2.10814	-1.14868	-0.87591
C	0.97617	0.77349	0.75867
H	1.59597	1.36329	1.41893
C	0.97618	-0.77337	0.75879
H	1.59601	-1.36306	1.41912
H	1.59610	1.36302	-1.41907
H	1.59603	-1.36331	-1.41885

TCO PBE0-DH/6-311++G structure**

C	0.97431	0.77010	-0.75680
C	0.97426	-0.77026	-0.75668
C	-0.18124	-1.34748	0.00013
H	-0.16058	-2.43241	0.00025
C	-0.18121	1.34748	-0.00014
H	-0.16053	2.43241	-0.00024
C	-1.56872	0.76615	-0.00015
H	-2.10250	1.14561	0.87356
H	-2.10237	1.14537	-0.87404
C	-1.56873	-0.76613	0.00007
H	-2.10244	-1.14533	0.87394
H	-2.10248	-1.14558	-0.87367
C	0.97424	0.77024	0.75673
H	1.58691	1.36093	1.42179
C	0.97426	-0.77012	0.75685
H	1.58696	-1.36070	1.42197
H	1.58705	1.36066	-1.42192
H	1.58696	-1.36095	-1.42171

TCO PBE0/6-311++G structure**

C	0.97663	0.77234	-0.75849
C	0.97657	-0.77249	-0.75837
C	-0.18164	-1.35174	0.00013
H	-0.16210	-2.43981	0.00025
C	-0.18162	1.35174	-0.00014
H	-0.16206	2.43981	-0.00025
C	-1.57237	0.76832	-0.00015
H	-2.10882	1.14891	0.87562
H	-2.10868	1.14867	-0.87611
C	-1.57239	-0.76830	0.00007
H	-2.10875	-1.14863	0.87601
H	-2.10879	-1.14888	-0.87573
C	0.97655	0.77247	0.75842
H	1.59229	1.36359	1.42546
C	0.97657	-0.77235	0.75853
H	1.59235	-1.36336	1.42563
H	1.59244	1.36332	-1.42558
H	1.59234	-1.36360	-1.42538

TCO ωB97X-D/6-311++G structure**

C	0.97808	0.77370	-0.75955
C	0.97801	-0.77384	-0.75945
C	-0.18175	-1.35602	0.00014
H	-0.16354	-2.44275	0.00025
C	-0.18172	1.35602	-0.00014
H	-0.16350	2.44275	-0.00025
C	-1.57544	0.77018	-0.00016
H	-2.10985	1.14932	0.87593
H	-2.10970	1.14905	-0.87645
C	-1.57545	-0.77016	0.00008
H	-2.10976	-1.14902	0.87635
H	-2.10982	-1.14929	-0.87603
C	0.97799	0.77382	0.75950
H	1.59485	1.36325	1.42475
C	0.97803	-0.77371	0.75960
H	1.59493	-1.36303	1.42491
H	1.59502	1.36299	-1.42485
H	1.59490	-1.36327	-1.42467

Sub-BOD B2PLYP/6-311++G structure**

C	0.32821	-1.10001	-0.13142
C	1.17279	-1.02169	1.19307
C	1.31983	-0.90692	-1.26149
C	1.90889	0.33840	1.23830
H	1.88099	-1.85217	1.21021
H	0.50355	-1.13661	2.04823
C	-0.59294	0.10133	-0.08946
H	-0.22896	-2.03198	-0.19519
C	1.96017	0.26706	-1.22652
H	1.50528	-1.68630	-1.99055
C	1.55393	1.15455	-0.06325
H	2.99129	0.20162	1.27757
H	1.61385	0.91820	2.11554
C	0.04974	1.28261	-0.05495
H	2.73107	0.57138	-1.92389
H	2.05740	2.12038	-0.06954
H	-0.45158	2.23960	0.01745
C	-2.05119	-0.07760	-0.02565
O	-2.61655	-1.15153	0.01527
O	-2.73673	1.09767	-0.01424
H	-3.67327	0.86036	0.03023

Sub-BOD B3LYP/6-311++G structure**

C	0.33115	-1.10078	-0.12832
C	1.18344	-1.02114	1.19532
C	1.32028	-0.90477	-1.26383
C	1.91572	0.34241	1.23765
H	1.89373	-1.85017	1.20972
H	0.52008	-1.14068	2.05466
C	-0.59498	0.10157	-0.08477
H	-0.22324	-2.03447	-0.18948
C	1.95594	0.26608	-1.23293
H	1.50152	-1.68500	-1.99339
C	1.55235	1.15657	-0.06714
H	2.99911	0.21099	1.27489
H	1.62351	0.92239	2.11606
C	0.04597	1.27946	-0.05434
H	2.72205	0.57475	-1.93401
H	2.05289	2.12409	-0.07691
H	-0.45454	2.23705	0.01482
C	-2.05297	-0.07941	-0.02371
O	-2.61829	-1.15100	0.01287
O	-2.74354	1.09379	-0.00980
H	-3.68178	0.85889	0.03152

Sub-BOD CAM-B3LYP/6-311++G structure**

C	0.33213	-1.09743	-0.12139
C	1.17833	-1.01167	1.19270
C	1.31774	-0.90591	-1.25423
C	1.90579	0.34777	1.22930
H	1.88960	-1.83829	1.21180
H	0.51663	-1.12852	2.05226
C	-0.58974	0.10023	-0.08450
H	-0.22324	-2.02990	-0.17949
C	1.94827	0.26057	-1.22803
H	1.49971	-1.68674	-1.98171
C	1.54543	1.15136	-0.06908
H	2.98796	0.21693	1.26973
H	1.61284	0.92912	2.10514
C	0.04304	1.27299	-0.05808
H	2.71285	0.56600	-1.93088
H	2.04474	2.11830	-0.08281
H	-0.46197	2.22784	0.00551
C	-2.04611	-0.07845	-0.02472
O	-2.60874	-1.14466	0.01322
O	-2.73120	1.08628	-0.01205
H	-3.66895	0.85566	0.02917

Sub-BOD CAM-B3LYP-D3/6-311++G structure**

C	0.33096	-1.09660	-0.12449
C	1.17097	-1.01271	1.19342
C	1.32066	-0.90572	-1.25391
C	1.90098	0.34672	1.23282
H	1.88071	-1.84043	1.21633
H	0.50374	-1.12720	2.04899
C	-0.58916	0.10191	-0.08895
H	-0.22619	-2.02795	-0.18523
C	1.95220	0.26038	-1.22492
H	1.50481	-1.68644	-1.98076
C	1.54597	1.15108	-0.06667
H	2.98272	0.21378	1.27606
H	1.60556	0.92817	2.10770
C	0.04344	1.27457	-0.06004
H	2.71985	0.56495	-1.92464
H	2.04626	2.11758	-0.07835
H	-0.46214	2.22892	0.00538
C	-2.04466	-0.07813	-0.02630
O	-2.60390	-1.14617	0.01407
O	-2.73045	1.08630	-0.01414
H	-3.66869	0.85846	0.02932

Sub-BOD CAM-B3LYP-D3BJ/6-311++G structure**

C	0.33141	-1.09679	-0.12399
C	1.17292	-1.01216	1.19258
C	1.31972	-0.90547	-1.25375
C	1.90077	0.34659	1.23191
H	1.88344	-1.83908	1.21407
H	0.50739	-1.12820	2.04905
C	-0.58897	0.10116	-0.08780
H	-0.22485	-2.02834	-0.18406
C	1.95104	0.26053	-1.22501
H	1.50320	-1.68609	-1.98071
C	1.54539	1.15102	-0.06717
H	2.98251	0.21500	1.27537
H	1.60493	0.92785	2.10658
C	0.04351	1.27387	-0.05965
H	2.71789	0.56575	-1.92512
H	2.04560	2.11727	-0.07884
H	-0.46158	2.22835	0.00542
C	-2.04401	-0.07818	-0.02565
O	-2.60535	-1.14496	0.01396
O	-2.72987	1.08603	-0.01390
H	-3.66750	0.85548	0.02889

Sub-BOD M06-2X/6-311++G structure**

C	0.33043	-1.09966	-0.13203
C	1.16516	-1.01580	1.19362
C	1.32992	-0.90596	-1.25380
C	1.89377	0.34417	1.23966
H	1.87593	-1.84277	1.21564
H	0.49046	-1.13100	2.04341
C	-0.58780	0.10001	-0.09615
H	-0.22687	-2.03117	-0.19686
C	1.96184	0.26350	-1.21855
H	1.52139	-1.68620	-1.97978
C	1.54663	1.15498	-0.06267
H	2.97553	0.21144	1.28514
H	1.59068	0.92487	2.11238
C	0.04266	1.27700	-0.06109
H	2.73546	0.56867	-1.91192
H	2.04771	2.12072	-0.06819
H	-0.46657	2.23031	0.00848
C	-2.04840	-0.07934	-0.02923
O	-2.60740	-1.14517	0.01713
O	-2.72793	1.08741	-0.01917
H	-3.66625	0.86381	0.02949

Sub-BOD PBE0-DH/6-311++G structure**

C	0.32644	-1.09336	-0.12295
C	1.16394	-1.00739	1.18824
C	1.31263	-0.90909	-1.24652
C	1.89241	0.34331	1.22648
H	1.87190	-1.83565	1.21105
H	0.49740	-1.12025	2.04353
C	-0.58760	0.10046	-0.08889
H	-0.23318	-2.02257	-0.18082
C	1.94820	0.25773	-1.21833
H	1.49831	-1.69050	-1.97076
C	1.54405	1.14596	-0.06735
H	2.97316	0.20863	1.27035
H	1.59761	0.92612	2.09967
C	0.04920	1.27440	-0.06084
H	2.71767	0.55740	-1.91662
H	2.04779	2.10954	-0.07789
H	-0.45419	2.22905	0.00483
C	-2.03978	-0.07449	-0.02637
O	-2.59895	-1.14057	0.01571
O	-2.71675	1.08548	-0.01701
H	-3.64794	0.85376	0.02625

Sub-BOD PBE0/6-311++G structure**

C	0.32685	-1.09535	-0.12455
C	1.16964	-1.01084	1.19078
C	1.31476	-0.90929	-1.25108
C	1.89962	0.34224	1.22997
H	1.87856	-1.84238	1.21086
H	0.50249	-1.12668	2.04912
C	-0.59009	0.10170	-0.08771
H	-0.23408	-2.02728	-0.18180
C	1.95178	0.25881	-1.22264
H	1.49886	-1.69312	-1.97766
C	1.54800	1.14909	-0.06814
H	2.98376	0.20887	1.27214
H	1.60595	0.92686	2.10620
C	0.05024	1.27704	-0.05943
H	2.72248	0.56155	-1.92297
H	2.05345	2.11523	-0.07766
H	-0.45254	2.23528	0.00715
C	-2.04403	-0.07531	-0.02594
O	-2.60628	-1.14457	0.01524
O	-2.72607	1.08967	-0.01529
H	-3.66071	0.85241	0.02754

Sub-BOD ωB97X-D/6-311++G structure**

C	0.33110	-1.09662	-0.13237
C	1.17083	-1.02064	1.18846
C	1.32163	-0.89931	-1.26040
C	1.90137	0.33746	1.23715
H	1.88047	-1.84994	1.20588
H	0.50091	-1.14010	2.04249
C	-0.58996	0.10242	-0.09019
H	-0.22408	-2.02976	-0.19826
C	1.95548	0.26800	-1.22339
H	1.50484	-1.67591	-1.99278
C	1.54874	1.15136	-0.05942
H	2.98409	0.20383	1.28014
H	1.60423	0.91526	2.11513
C	0.04572	1.27629	-0.05356
H	2.72390	0.57732	-1.92113
H	2.05037	2.11795	-0.06320
H	-0.45602	2.23309	0.01819
C	-2.04835	-0.07672	-0.02640
O	-2.60894	-1.14484	0.01542
O	-2.73133	1.08709	-0.01490
H	-3.66601	0.85684	0.03010

Sub-TCO B2PLYP/6-311++G structure**

C	0.32261	-1.28040	-0.26448
C	-0.51470	-0.00650	0.00026
C	0.34294	1.21433	0.27932
H	-0.27805	2.08319	0.47447
C	1.80993	-1.02670	-0.21210
H	2.37917	-1.93294	-0.40070
C	2.49360	0.24294	-0.67683
H	3.40382	0.37160	-0.08311
H	2.81325	0.12250	-1.71548
C	1.58797	1.48365	-0.53982
H	2.13944	2.30830	-0.07994
H	1.26833	1.83429	-1.52532
C	1.03538	-1.10564	1.07696
H	1.22033	-1.85455	1.83472
C	0.22895	0.18283	1.35151
H	-0.27218	0.38569	2.28856
C	-1.96282	0.11816	-0.15397
O	-2.50414	-0.95794	-0.79055
H	-3.45608	-0.78988	-0.83794
O	-2.64228	1.04742	0.23527
H	-0.10984	-2.18001	-0.67802

Sub-TCO B3LYP/6-311++G structure**

C	0.32194	-1.28595	-0.25104
C	-0.51552	-0.00674	0.00365
C	0.34534	1.21535	0.28473
H	-0.27388	2.08667	0.47429
C	1.80745	-1.03172	-0.21278
H	2.37854	-1.93789	-0.39769
C	2.47976	0.23191	-0.71302
H	3.43063	0.34608	-0.18275
H	2.73037	0.10830	-1.77084
C	1.60317	1.48912	-0.51577
H	2.17174	2.27410	-0.00807
H	1.30462	1.90346	-1.48328
C	1.04086	-1.09980	1.08294
H	1.22989	-1.84336	1.84549
C	0.22908	0.18718	1.35490
H	-0.27002	0.38681	2.29388
C	-1.96321	0.12047	-0.15805
O	-2.51028	-0.96362	-0.77756
H	-3.46246	-0.79513	-0.83435
O	-2.64176	1.05624	0.21023
H	-0.11633	-2.18894	-0.65136

Sub-TCO CAM-B3LYP/6-311++G structure**

C	0.32204	-1.28008	-0.25444
C	-0.51020	-0.00704	0.00607
C	0.34259	1.20999	0.28187
H	-0.27724	2.07949	0.47286
C	1.80094	-1.02604	-0.21183
H	2.37257	-1.92999	-0.39901
C	2.47424	0.23569	-0.69889
H	3.41353	0.35147	-0.15154
H	2.74410	0.11340	-1.75057
C	1.59428	1.48354	-0.51735
H	2.15686	2.27744	-0.02032
H	1.29206	1.88350	-1.48831
C	1.03404	-1.09987	1.07472
H	1.22212	-1.84516	1.83427
C	0.22268	0.18215	1.34625
H	-0.27443	0.38327	2.28483
C	-1.95549	0.11781	-0.15691
O	-2.49934	-0.95165	-0.78133
H	-3.45065	-0.78635	-0.83760
O	-2.62992	1.04612	0.21872
H	-0.11548	-2.17977	-0.66063

Sub-TCO CAM-B3LYP-D3/6-311++G structure**

C	0.32101	-1.27699	-0.26277
C	-0.50929	-0.00468	0.00109
C	0.34219	1.21080	0.28106
H	-0.27781	2.08005	0.47278
C	1.80074	-1.02643	-0.21187
H	2.37176	-1.93030	-0.40100
C	2.48177	0.23840	-0.68060
H	3.40229	0.35740	-0.10291
H	2.78418	0.11864	-1.72348
C	1.59026	1.48138	-0.52461
H	2.14596	2.29187	-0.04747
H	1.27925	1.85476	-1.50333
C	1.02793	-1.10445	1.07048
H	1.21017	-1.85274	1.82851
C	0.21985	0.17974	1.34316
H	-0.28205	0.37848	2.27961
C	-1.95389	0.11904	-0.15678
O	-2.49750	-0.95144	-0.78000
H	-3.44971	-0.79116	-0.83345
O	-2.62603	1.04699	0.22393
H	-0.11924	-2.17230	-0.67557

Sub-TCO CAM-B3LYP-D3BJ/6-311++G structure**

C	0.32171	-1.27815	-0.25827
C	-0.50942	-0.00605	0.00438
C	0.34211	1.20990	0.28231
H	-0.27795	2.07877	0.47414
C	1.80033	-1.02542	-0.21219
H	2.37174	-1.92896	-0.40073
C	2.47580	0.23755	-0.69103
H	3.40704	0.35561	-0.13077
H	2.75939	0.11666	-1.73902
C	1.59060	1.48227	-0.52062
H	2.15037	2.28386	-0.03337
H	1.28338	1.86963	-1.49497
C	1.03165	-1.10166	1.07238
H	1.21764	-1.84847	1.83062
C	0.22220	0.18074	1.34519
H	-0.27671	0.38057	2.28281
C	-1.95359	0.11807	-0.15659
O	-2.49690	-0.95177	-0.78041
H	-3.44841	-0.78763	-0.83517
O	-2.62794	1.04582	0.22049
H	-0.11608	-2.17602	-0.66753

Sub-TCO M06-2X/6-311++G structure**

C	0.32207	-1.27095	-0.28313
C	-0.50600	0.00110	-0.01643
C	0.34314	1.21253	0.27569
H	-0.28018	2.07930	0.47044
C	1.80313	-1.02847	-0.20874
H	2.36838	-1.93560	-0.39781
C	2.50291	0.24295	-0.63852
H	3.38245	0.36959	-0.00157
H	2.86897	0.12903	-1.66107
C	1.59139	1.47696	-0.53655
H	2.13334	2.31393	-0.09117
H	1.27478	1.80129	-1.53091
C	1.01306	-1.11465	1.06099
H	1.17735	-1.87214	1.81327
C	0.21272	0.17488	1.33277
H	-0.30662	0.37010	2.26048
C	-1.95606	0.12289	-0.15674
O	-2.50171	-0.94737	-0.77598
H	-3.45448	-0.79089	-0.81566
O	-2.62427	1.04671	0.23670
H	-0.11413	-2.16288	-0.70775

Sub-TCO PBE0-DH/6-311++G structure**

C	0.32387	-1.27318	-0.26909
C	-0.50801	-0.01045	-0.00161
C	0.33923	1.20169	0.28175
H	-0.28749	2.06399	0.47832
C	1.79862	-1.01590	-0.21418
H	2.36880	-1.91877	-0.40454
C	2.47621	0.24773	-0.67038
H	3.38731	0.37080	-0.08096
H	2.79316	0.13242	-1.70812
C	1.57847	1.47801	-0.52406
H	2.12656	2.29643	-0.05442
H	1.26280	1.84098	-1.50389
C	1.02677	-1.10519	1.06305
H	1.21401	-1.85561	1.81610
C	0.22020	0.17071	1.33923
H	-0.28317	0.36796	2.27409
C	-1.94998	0.11593	-0.15587
O	-2.49192	-0.94388	-0.78044
H	-3.43715	-0.77532	-0.82634
O	-2.61699	1.04267	0.23115
H	-0.10587	-2.16920	-0.68907

Sub-TCO PBE0/6-311++G structure**

C	0.32403	-1.27796	-0.26401
C	-0.51000	-0.00989	-0.00173
C	0.34158	1.20539	0.28388
H	-0.28632	2.07130	0.47757
C	1.80189	-1.02083	-0.21412
H	2.37393	-1.92666	-0.40259
C	2.47652	0.24243	-0.68729
H	3.40834	0.35986	-0.12368
H	2.76486	0.12451	-1.73655
C	1.58917	1.48297	-0.51549
H	2.14613	2.28695	-0.02406
H	1.28199	1.87456	-1.49050
C	1.03129	-1.10401	1.06918
H	1.21865	-1.85438	1.82671
C	0.22181	0.17433	1.34401
H	-0.28411	0.37010	2.28132
C	-1.95413	0.11801	-0.15785
O	-2.50015	-0.95303	-0.77515
H	-3.44909	-0.78004	-0.82316
O	-2.62449	1.05171	0.21931
H	-0.11023	-2.17831	-0.67780

Sub-TCO ωB97X-D/6-311++G structure**

C	0.32253	-1.27895	-0.26062
C	-0.51088	-0.00663	0.00179
C	0.34347	1.21135	0.28085
H	-0.27624	2.08138	0.47441
C	1.80421	-1.02559	-0.21137
H	2.37468	-1.93093	-0.39887
C	2.48331	0.23934	-0.68512
H	3.40770	0.35937	-0.11223
H	2.77873	0.11763	-1.73062
C	1.59197	1.48291	-0.52565
H	2.14835	2.29190	-0.04492
H	1.28030	1.85906	-1.50401
C	1.03073	-1.10359	1.07366
H	1.21470	-1.85132	1.83265
C	0.22168	0.18022	1.34546
H	-0.27875	0.38115	2.28306
C	-1.95853	0.11709	-0.15687
O	-2.49989	-0.94848	-0.78617
H	-3.44874	-0.78477	-0.83694
O	-2.63248	1.04320	0.22828
H	-0.11272	-2.17818	-0.67228

Sub-TS B2PLYP/6-311++G structure**

C	0.24160	-1.15185	-0.26122
C	-0.55114	0.11951	-0.29323
C	0.33240	1.12670	0.42669
H	-0.23079	1.98015	0.79348
C	1.70319	-1.05325	-0.37377
H	2.21589	-1.96429	-0.66659
C	2.24781	0.23876	-0.98060
H	3.33550	0.25234	-0.88235
H	2.01866	0.21998	-2.04910
C	1.62066	1.49071	-0.32263
H	2.32623	1.94618	0.37960
H	1.38314	2.23975	-1.08007
C	1.35479	-1.03773	1.11848
H	1.40570	-1.92203	1.73431
C	0.52862	0.06747	1.44269
H	-0.05298	0.07699	2.36084
C	-1.96081	0.15514	-0.18925
O	-2.55178	-1.05877	-0.53065
H	-3.50101	-0.89079	-0.47490
O	-2.66629	1.11400	0.12583
H	-0.25846	-2.11292	-0.27959

Sub-TS B3LYP/6-311++G structure**

C	0.24283	-1.17108	-0.23489
C	-0.56476	0.09685	-0.22968
C	0.33487	1.12006	0.44164
H	-0.21984	1.97775	0.81270
C	1.69080	-1.05473	-0.40152
H	2.21382	-1.96315	-0.68573
C	2.23358	0.23923	-1.00988
H	3.31865	0.26264	-0.88381
H	2.03844	0.20328	-2.08500
C	1.57858	1.49786	-0.38555
H	2.29513	2.02520	0.25318
H	1.26721	2.19403	-1.16650
C	1.35658	-1.03463	1.10495
H	1.48801	-1.89426	1.74243
C	0.62235	0.10735	1.48556
H	0.15647	0.17020	2.46581
C	-1.96854	0.14712	-0.17310
O	-2.56475	-1.06412	-0.53014
H	-3.51425	-0.88582	-0.51097
O	-2.67937	1.10890	0.12069
H	-0.24831	-2.13634	-0.25165

Sub-TS CAM-B3LYP/6-311++G structure**

C	0.24292	-1.16903	-0.22165
C	-0.55706	0.09884	-0.24112
C	0.33430	1.11608	0.44148
H	-0.22347	1.97158	0.81046
C	1.68355	-1.05212	-0.40103
H	2.20914	-1.95940	-0.67908
C	2.21468	0.23784	-1.01157
H	3.30123	0.25994	-0.91154
H	1.99346	0.20555	-2.08029
C	1.57907	1.48981	-0.37296
H	2.30046	1.99791	0.27394
H	1.27889	2.20018	-1.14351
C	1.33217	-1.03456	1.09471
H	1.47808	-1.88549	1.73960
C	0.61961	0.10692	1.48017
H	0.15673	0.17000	2.46134
C	-1.95397	0.14731	-0.17920
O	-2.55143	-1.05391	-0.52655
H	-3.49921	-0.87606	-0.49728
O	-2.66288	1.10394	0.11889
H	-0.25250	-2.13102	-0.24538

Sub-TS CAM-B3LYP-D3/6-311++G structure**

C	0.24255	-1.16868	-0.22611
C	-0.55318	0.10253	-0.26192
C	0.33217	1.11855	0.43183
H	-0.22996	1.97523	0.79122
C	1.68571	-1.05564	-0.38955
H	2.21235	-1.96447	-0.66015
C	2.22169	0.23161	-1.00192
H	3.30814	0.25076	-0.90234
H	1.99747	0.19687	-2.06977
C	1.58882	1.48650	-0.36590
H	2.30560	1.98511	0.29316
H	1.30339	2.20210	-1.13705
C	1.31752	-1.03339	1.10149
H	1.45192	-1.88363	1.74989
C	0.60011	0.10970	1.47555
H	0.11806	0.17164	2.44727
C	-1.94993	0.14933	-0.18538
O	-2.54908	-1.05305	-0.52562
H	-3.49726	-0.87947	-0.48881
O	-2.65400	1.10690	0.12063
H	-0.25779	-2.12797	-0.25205

Sub-TS CAM-B3LYP-D3BJ/6-311++G structure**

C	0.24268	-1.17118	-0.22100
C	-0.55474	0.10093	-0.25416
C	0.33377	1.11834	0.43319
H	-0.22526	1.97673	0.79290
C	1.68312	-1.05615	-0.39357
H	2.21118	-1.96491	-0.66104
C	2.21948	0.23029	-1.00506
H	3.30535	0.25065	-0.89976
H	2.00259	0.19421	-2.07437
C	1.58371	1.48579	-0.37511
H	2.30265	1.99450	0.27378
H	1.28850	2.19311	-1.15009
C	1.31544	-1.03266	1.09924
H	1.45901	-1.88015	1.74879
C	0.61389	0.11746	1.48134
H	0.15164	0.18945	2.46202
C	-1.95090	0.14829	-0.18282
O	-2.54923	-1.05394	-0.52427
H	-3.49687	-0.87641	-0.49114
O	-2.65852	1.10487	0.11838
H	-0.25546	-2.13135	-0.24636

Sub-TS M06-2X/6-311++G structure**

C	0.23311	-1.13245	-0.25784
C	-0.54377	0.13581	-0.33002
C	0.32766	1.11700	0.43751
H	-0.23764	1.96042	0.82280
C	1.69672	-1.04755	-0.38487
H	2.19968	-1.95732	-0.69357
C	2.22441	0.25162	-0.98613
H	3.31430	0.26061	-0.93856
H	1.94026	0.25579	-2.04071
C	1.63112	1.48646	-0.27772
H	2.34116	1.88535	0.45241
H	1.42345	2.27432	-1.00234
C	1.35305	-1.04919	1.10108
H	1.40954	-1.93860	1.70835
C	0.52009	0.02885	1.42811
H	-0.07656	0.01162	2.33713
C	-1.94923	0.16133	-0.19861
O	-2.53986	-1.04425	-0.52235
H	-3.48843	-0.88762	-0.45003
O	-2.64887	1.10855	0.13334
H	-0.27486	-2.09022	-0.27248

Sub-TS PBE0-DH/6-311++G structure**

C	0.23946	-1.13710	-0.25175
C	-0.54819	0.11940	-0.29244
C	0.32618	1.10708	0.44353
H	-0.23767	1.94799	0.83286
C	1.69319	-1.03508	-0.39455
H	2.20109	-1.93876	-0.70973
C	2.20583	0.26043	-0.99476
H	3.29454	0.27940	-0.94409
H	1.93134	0.25726	-2.05055
C	1.60253	1.48669	-0.29766
H	2.31643	1.91365	0.41101
H	1.36677	2.26034	-1.02725
C	1.36910	-1.04238	1.08942
H	1.44747	-1.92789	1.69785
C	0.54859	0.03790	1.43764
H	-0.01944	0.02737	2.36273
C	-1.94967	0.15066	-0.18823
O	-2.53762	-1.04348	-0.52425
H	-3.47996	-0.87556	-0.46406
O	-2.64823	1.10224	0.13077
H	-0.25592	-2.09949	-0.26814

Sub-TS PBE0/6-311++G structure**

C	0.24003	-1.14265	-0.25197
C	-0.55519	0.11167	-0.26962
C	0.32858	1.10796	0.44921
H	-0.23474	1.95190	0.84146
C	1.69477	-1.03679	-0.40195
H	2.20470	-1.94215	-0.72017
C	2.21307	0.26192	-1.00124
H	3.30389	0.28296	-0.93188
H	1.95911	0.25280	-2.06541
C	1.59395	1.49409	-0.31799
H	2.31071	1.95051	0.37397
H	1.33327	2.25178	-1.06037
C	1.38233	-1.04323	1.09035
H	1.47536	-1.92796	1.70277
C	0.57207	0.04516	1.45009
H	0.02828	0.04645	2.39320
C	-1.95911	0.14895	-0.18205
O	-2.55015	-1.05066	-0.52682
H	-3.49648	-0.87620	-0.47705
O	-2.66150	1.10523	0.12972
H	-0.25390	-2.10924	-0.26874

Sub-TS ωB97X-D/6-311++G structure**

C	0.24017	-1.15096	-0.24776
C	-0.55203	0.11559	-0.28834
C	0.33082	1.11684	0.43580
H	-0.22963	1.96846	0.81112
C	1.69461	-1.04891	-0.38691
H	2.20912	-1.95797	-0.68134
C	2.23272	0.24411	-0.98862
H	3.32063	0.25966	-0.89540
H	1.99934	0.22561	-2.05605
C	1.60558	1.49006	-0.32870
H	2.31674	1.95719	0.36022
H	1.34797	2.23249	-1.08553
C	1.34118	-1.04254	1.10250
H	1.43820	-1.91231	1.73297
C	0.56000	0.06762	1.45295
H	0.01584	0.08833	2.39417
C	-1.95467	0.15203	-0.18956
O	-2.55020	-1.04726	-0.53002
H	-3.49558	-0.87798	-0.47454
O	-2.65674	1.10564	0.13006
H	-0.25736	-2.11360	-0.27414