Electronic Supplementary Material (ESI) for RSC Advances.

Support information for

Franck-Condon simulation for unraveling vibronic origin in solvent enhanced absorption and fluorescence spectra of rubrene

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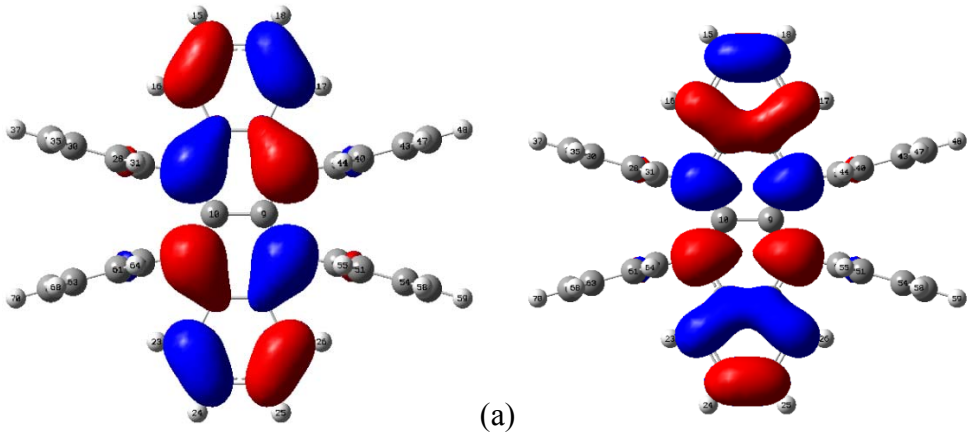
Table S1 Optimized bond lengths (in Å), bond angles and dihedral angles (in degree) for ground S_0 (first excited S_1) state under group symmetries D_2, C_{2H}, and D_{2H} by (TD)-BHandHLYP/6-31G plus PCM model in benzene solvent. The parameters are listed for optimized representative geometries and the atom numbering is showed in Fig. 1.

parameters	S0(S1)-D_2(1)	S0(S1)-D_2(2)	S0(S1)-C_{2H}(1)	S0(S1)-C_{2H}(2)	S0(S1)-D_{2H}
B(1,2)	1.3578(1.3863)	1.3578(1.3863)	1.3571(1.3859)	1.3571(1.3859)	1.3564(1.3868)
B(1,6)	1.4262(1.3947)	1.4262(1.3947)	1.4243(1.3936)	1.4243(1.3936)	1.4235(1.3916)
B(1,15)	1.0735(1.0731)	1.0735(1.0731)	1.073(1.0731)	1.073(1.0731)	1.0733(1.0731)
B(2,3)	1.4413(1.4109)	1.4413(1.4109)	1.4424(1.1448)	1.4424(1.1448)	1.4451(1.4142)
B(2,16)	1.0690(1.0690)	1.0690(1.0690)	1.068(1.0681)	1.068(1.0681)	1.067(1.0671)
B(3,4)	1.4443(1.4371)	1.4443(1.4371)	1.4397(1.4328)	1.4397(1.4328)	1.4356(1.427)
B(3.7)	1.3993(1.4380)	1.3993(1.4380)	1.4012(1.4379)	1.4012(1.4379)	1.4015(1.4361)
B(7,10)	1.4305(1.4132)	1.4305(1.4132)	1.4301(1.4206)	1.4301(1.4206)	1.4336(1.4238)
B(7,27)	1.4994(1.4910)	1.4994(1.4910)	1.5044(1.4968)	1.5044(1.4968)	1.5062(1.5025)
B(8,38)	1.4994(1.4910)	1.4994(1.4910)	1.5044(1.4968)	1.5044(1.4968)	1.5068(1.5025)
B(9,10)	1.4052(1.4690)	1.4052(1.4690)	1.4691(1.47)	1.4691(1.47)	1.4777(1.4911)
B(39,42)	1.0726(1.0724)	1.073(1.073)	1.0736(1.0733)	1.0736(1.0733)	1.0735(1.0734)
A(1,2,3)	121.64(121.77)	121.64(121.77)	121.97(121.95)	121.97(121.95)	122.06(122.05)
A(2,3,4)	117.75(118.15)	117.75(118.15)	117.86(118.26)	117.86(118.26)	117.82(118.25)
A(2,1,6)	120.25(119.83)	120.25(119.83)	120.15(119.76)	120.15(119.76)	120.11(119.75)
A(3,7,10)	119.76(120.01)	119.76(120.01)	120.43(120.73)	120.43(120.73)	120.84(121.70)
A(4,3,7)	119.86(119.30)	119.86(119.30)	120.20(119.26)	120.20(119.26)	120.45(119.75)
A(7,10,9)	118.26(117.86)	118.26(117.86)	118.84(118.79)	118.84(118.79)	118.72(118.5)
D(3,7,27,29)	104.96(113.11)	69.68(63.54)	92.5(102.01)	80.25(72.35)	84.57(84.57)
D(4,8,38,39)	-69.68(-63.5)	-104.96(-113.11)	-92.55(-102.01)	-80.25(-72.35)	-84.57(-84.57)
D(2,3,4,8)	-168.53(-169.92)	168.53(169.91)	-175.90(-175.92)	175.90(175.91)	180.0(180.0)
D(3,7,10,11)	165.65(161.74)	-165.65(-161.74)	171.61(167.35)	-171.61(-167.34)	180.0(180.0)
D(1,2,3,4)	-6.78(-5.75)	6.75(5.78)	-1.63(-2.09)	1.63(2.09)	0.0(0.0)
D(7,10,9,8)	23.37(28.15)	-23.37(-28.15)	0.0(0.0)	0.0(0.0)	0.0(0.0)

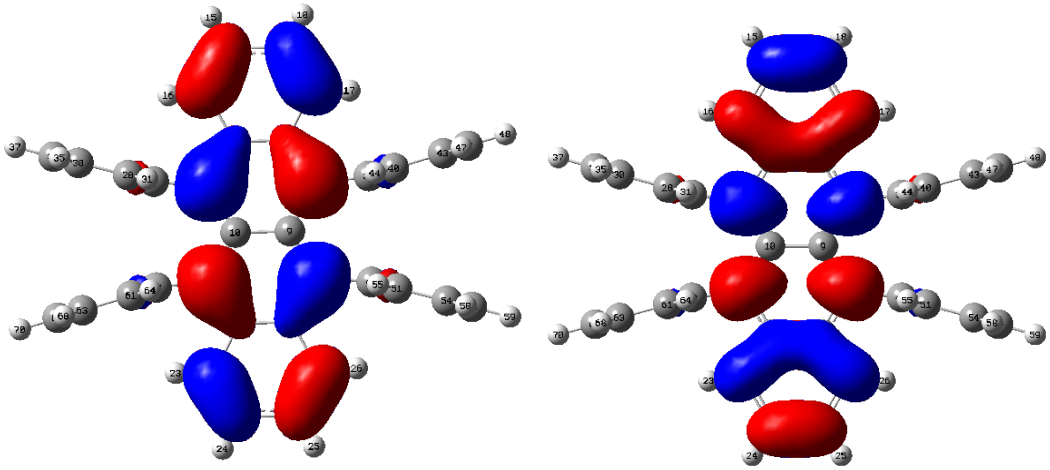
Table S2 Optimized bond lengths (in Å), bond angles and dihedral angles (in degree) for ground S_0 (first excited S_1) state under group symmetries D_2, C_{2H}, and D_{2H} by (TD)-BHandHLYP/6-31G plus PCM model in cyclohexane solvent. The parameters are listed for optimized representative geometries and the atom numbering is showed in Fig. 1.

parameters	S0(S1)-D_2(1)	S0(S1)-D_2(2)	S0(S1)- C_{2H}(1)	S0(S1)- C_{2H}(2)	S0(S1)-D_{2H}
B(1,2)	1.3577(1.3863)	1.3577(1.3863)	1.357(1.3859)	1.357(1.3859)	1.3563(1.3967)
B(1,6)	1.4261(1.3947)	1.4261(1.3947)	1.4242(1.3936)	1.4242(1.3936)	1.4235(1.3916
B(1,15)	1.0734(1.0731)	1.0734(1.0731)	1.0733(1.0731)	1.0733(1.0731)	1.0733(1.0731)
B(2,3)	1.4413(1.4108)	1.4413(1.4108)	1.4424(1.4118)	1.4424(1.4118)	1.4415(1.4142)
B(2,16)	1.069(1.069)	1.069(1.069)	1.068(1.0682)	1.068(1.0682)	1.0669(1.0671)
B(3,4)	1.4443(1.4372)	1.4443(1.4372)	1.4396(1.4328)	1.4396(1.4328)	1.4356(1.427)
B(3.7)	1.3992(1.4379)	1.3992(1.4379)	1.4012(1.4377)	1.4012(1.4377)	1.4015(1.4361)
B(7,10)	1.4305(1.4161)	1.4305(1.4161)	1.4301(1.4206)	1.4301(1.4206)	1.4336(1.4239)
B(7,27)	1.4994(1.491)	1.4994(1.491)	1.5044(1.4969)	1.5044(1.4969)	1.5062(1.5024)
B(8,38)	1.4994(1.491)	1.4994(1.491)	1.5044(1.4969)	1.5044(1.4969)	1.5062(1.5024)
B(9,10)	1.4501(1.4669)	1.4501(1.4669)	1.4691(1.4701)	1.4691(1.4701)	1.4778(1.4912)
B(39,42)	1.0726(1.0724)	1.0726(1.0724)	1.0736(1.0733)	1.0736(1.0733)	1.0734(1.0734)
A(1,2,3)	121.63(121.76)	121.63(121.76)	121.96(121.94)	121.96(121.94)	122.06(122.05)
A(2,3,4)	117.76(148.15)	117.76(148.15)	117.86(118.26)	117.86(118.26)	117.82(118.25)
A(2,1,6)	120.26(119.29)	120.26(119.29)	120.16(119.77)	120.16(119.77)	120.12(119.70)
A(3,7,10)	119.76(120.02)	119.76(120.02)	120.44(120.76)	120.44(120.76)	120.85(121.71)
A(4,3,7)	119.86(119.29)	119.86(119.29)	120.19(119.26)	120.19(119.26)	120.44(119.74)
A(7,10,9)	118.26(117.85)	118.26(117.85)	118.84(118.89)	118.84(118.89)	118.72(118.54)
D(3,7,27,29)	104.85(113.01)	69.84(63.66)	92.50(101.79)	80.31(72.60)	84.61(84.61)
D(4,8,38,39)	-69.8(-63.6)	-104.85(-113.01)	-92.50(-101.79)	-80.31(-72.60)	-84.61(-84.61)
D(2,3,4,8)	-168.57(-169.93)	168.57(169.93)	-175.91(-175.93)	175.90(175.90)	180.0(180.0)
D(3,7,10,11)	165.66(161.76)	-165.6(-151.76)	171.63(167.41)	-171.63(-167.41)	180.0(180.0)
D(1,2,3,4)	-6.76(-5.77)	6.76(5.77)	-1.63(-2.09)	1.63(2.09)	0.0(0.0)
D(7,10,9,8)	23.35(28.13)	-23.35(-28.11)	0.0(0.0)	0.0(0.0)	0.0(0.0)



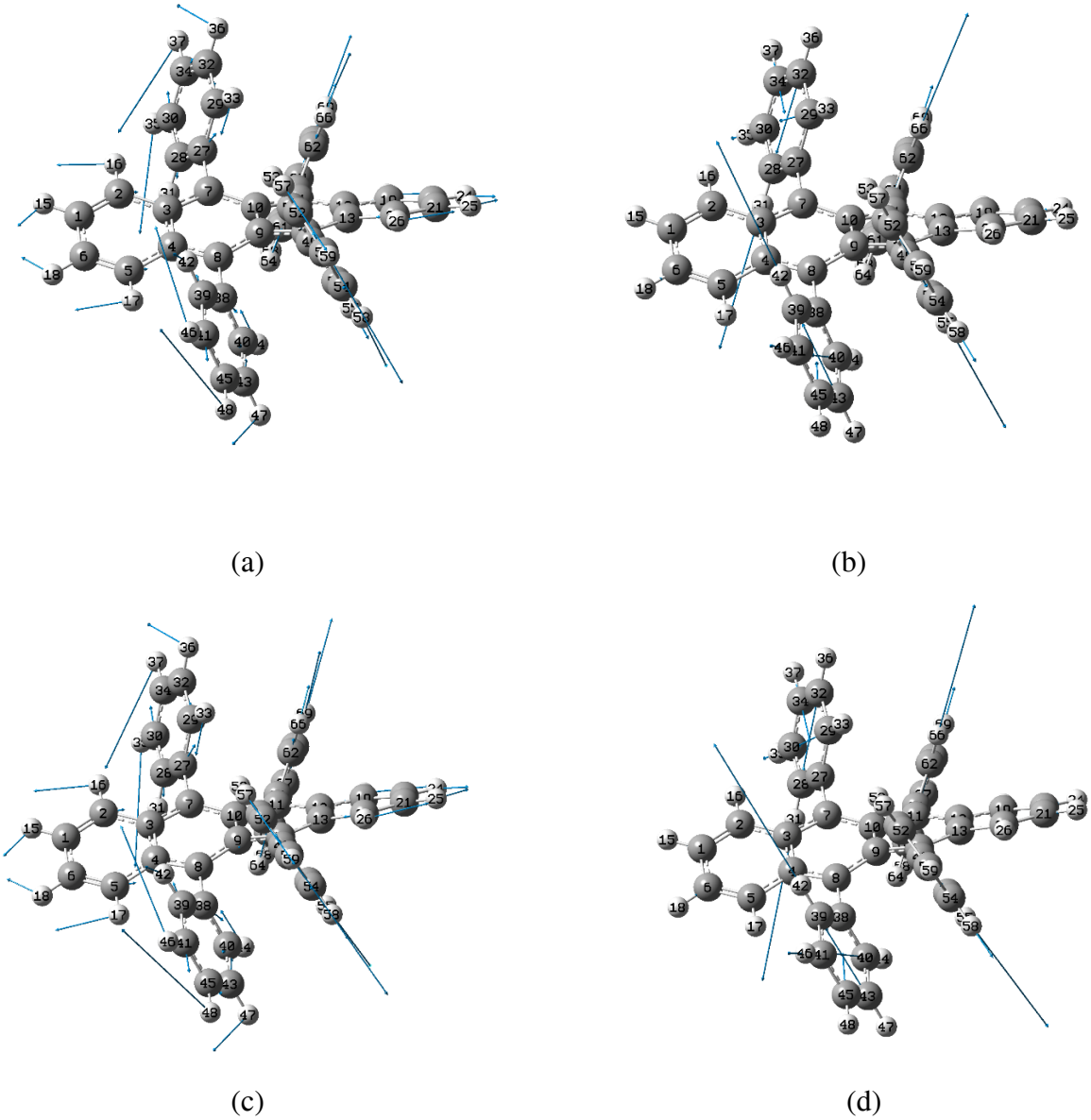
(a)

HOMO LUMO



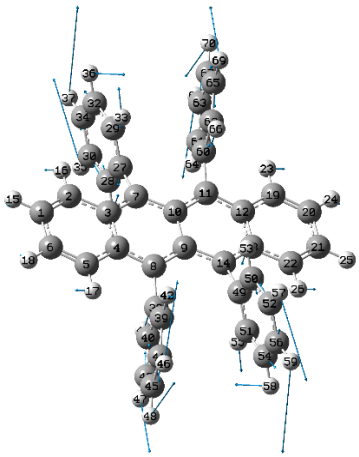
HOMO (b) LUMO

Fig. S1 Frontier molecular orbitals involved in $S_0(1Ag) \rightarrow S_1(1B3u)$ excitation calculated by BHandHLYP/6-31G plus PCM model (a) in benzene solvent and (b) in cyclohexane solvent.

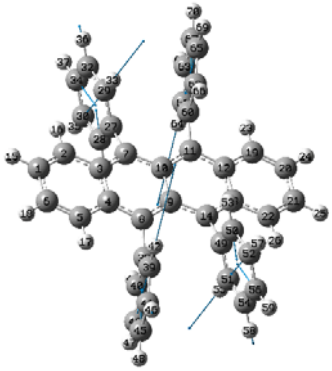


(a) (b) (c) (d)

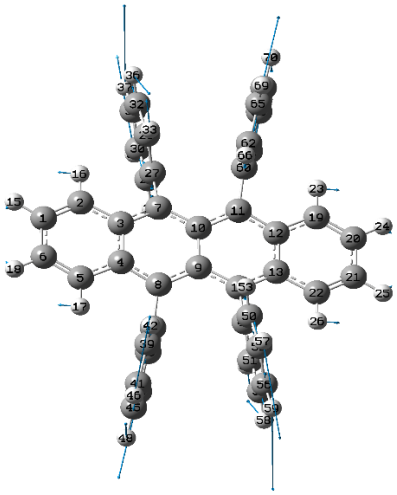
Fig. S2 Vibrational normal-mode motions coressponding large Huang–Rhys factor *S* and associated frequency due to large difference of dihedral angles in phenyl group between S_0 and S_1 states for absorption spectra at $D_2(1)$ group symmetry. (a) *S*= 15.5 and *v*=1565.66cm^{-1} and (b) *S*=12.8 and *v*=3331.35cm^{-1} in benzene slovent. (c) *S*= 15.4 and *v*=1565.77cm^{-1} and (d) *S*=12.6 and *v*=3331.38cm^{-1} in cyclohexane slovent.



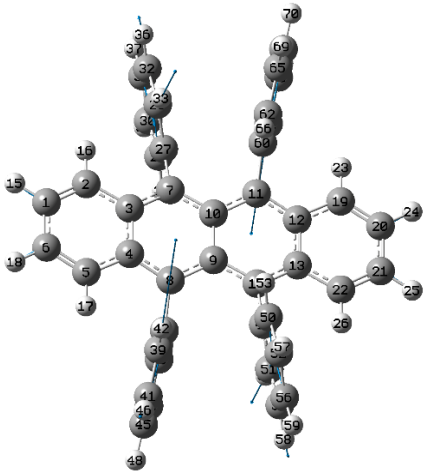
(a)



(b)

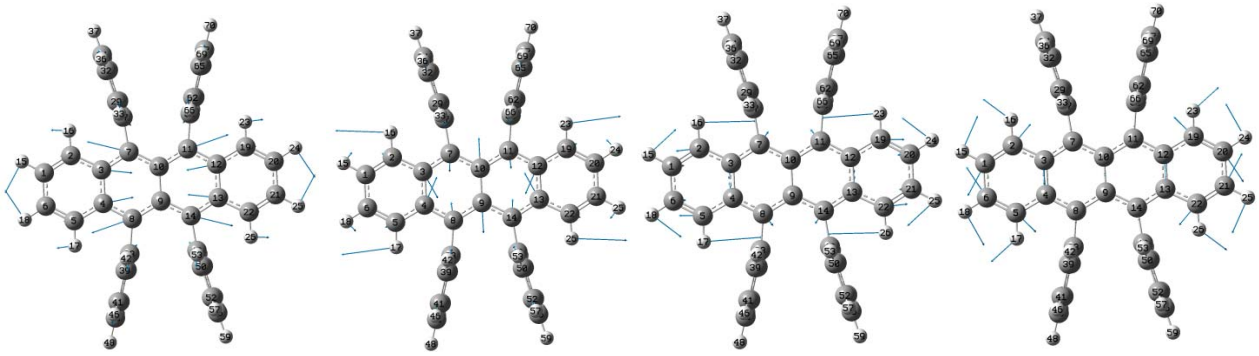


(c)



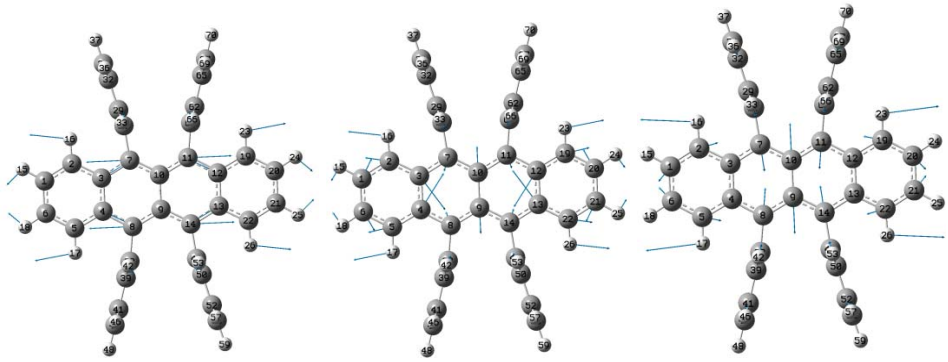
(d)

Fig. S3 Vibrational normal-mode motions coressponding large Huang–Rhys factor *S* and associated frequency due to large difference of dihedral angles in phenyl group between S_0 and S_1 states for absorption spectra at $C_{2H}(1)$ group symmetry. (a) *S*= 23.5 and *v*=1563.47cm^{-1} and (b) *S*=12.7 and *v*=3330.68cm^{-1} in benzene slovent. (c) *S*= 22.6 and *v*=1563.58cm^{-1} and (d) *S*=13.1 and *v*=3330.66cm^{-1} in cyclohexane slovent.



15ag 16ag 17ag 20ag

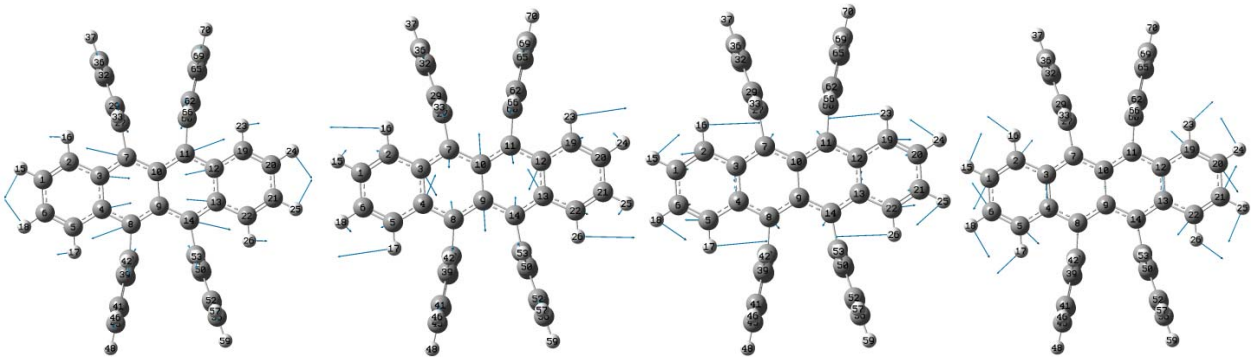
(a)



13ag 14ag 15ag

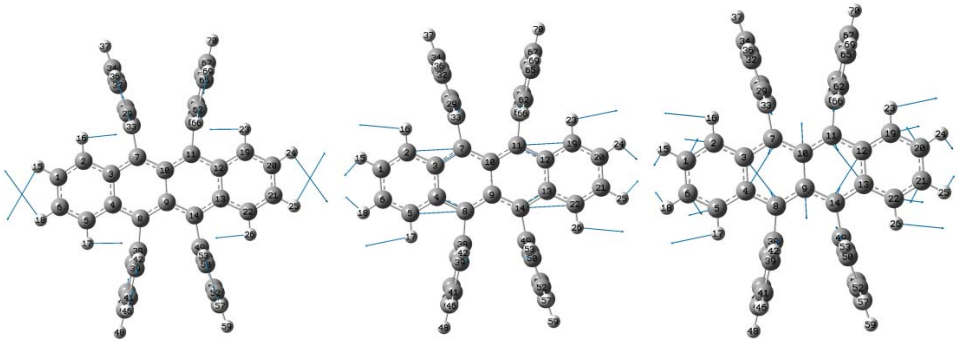
(b)

Fig. S4 Active vibrational normal-mode motions for vibronic spectra calculated by BHandHLYP/6-31G plus PCM model in benzene solvent. (a) Four modes for S_0 state and (b) three modes for S_1 state.



13ag 14ag 15ag 17ag

(a)



12ag 14ag 15ag

(b)

Fig. S5 Active vibrational normal-mode motions for vibronic spectra calculated by BHandHLYP/6-31G plus PCM model in cyclohexane solvent. (a) Four modes for S_0 state and (b) three modes for S_1 state.

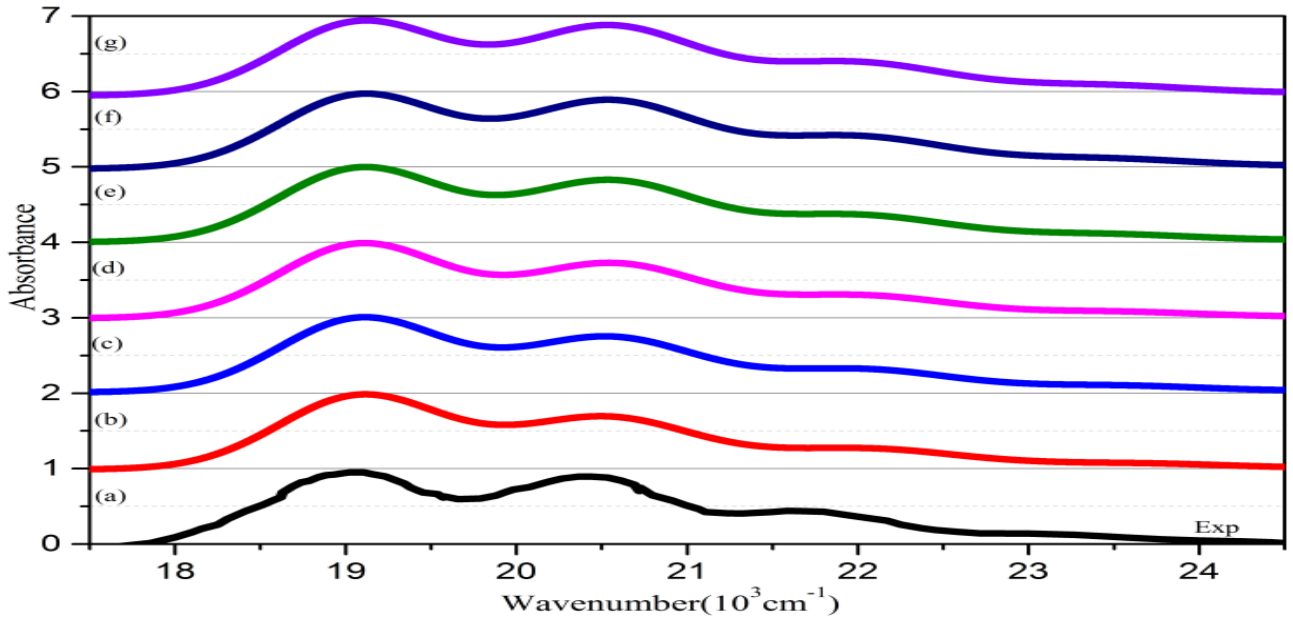


Fig. S6 Simulated absorption spectra from $S_0(1Ag) \rightarrow S_1(1B3u)$ for D_{2H} in benzene solvent at temperature T = 298K. (a) Experimental data from Ref. 43. The scaling parameters ζ for 8 backbone-H atoms 15, 16, 17, 18 and 23, 24, 25, and 26 (see Fig. 1) are varied equally as (b) ζ_H=1.0, (c) ζ_H=1.2, (d) ζ_H=1.4, (e) ζ_H=1.6, (f) ζ_H=1.8 and (g) ζ_H=2.0. For the rest of hydrogen atoms and all carbon atoms are fixed as ζ_H=1.0 and ζ_C=1.0 (no scaling).

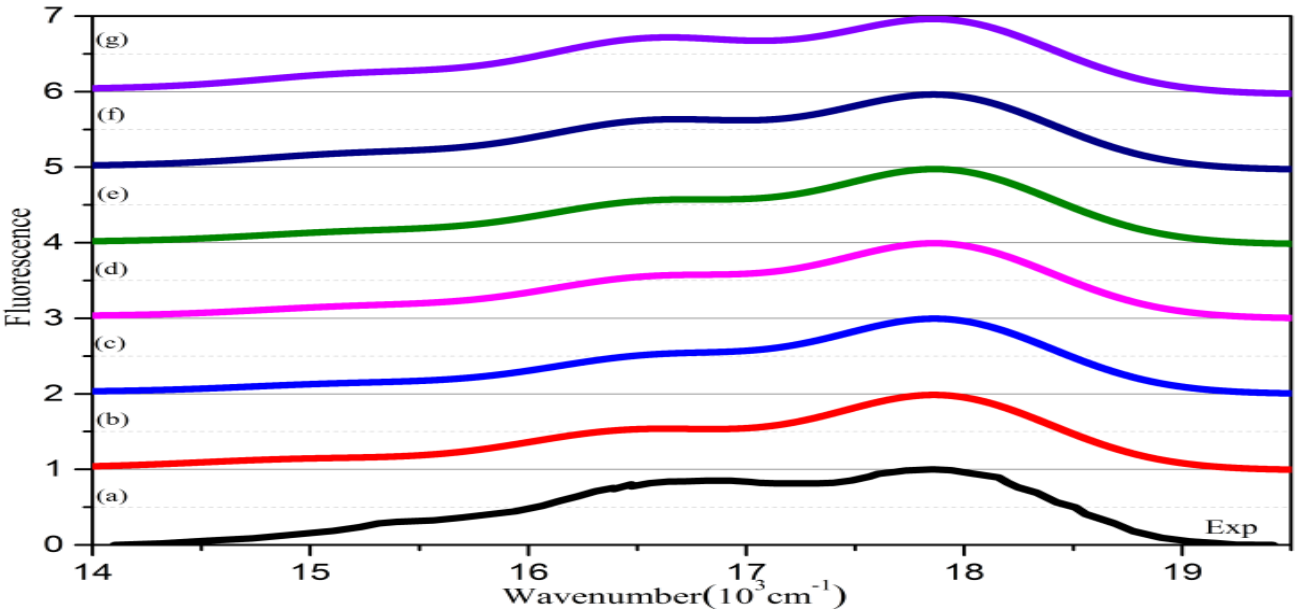


Fig. S7 Simulated fluorescence spectra from $S_0(1Ag) \leftarrow S_1(1B3u)$ for D_{2H} in benzene solvent at temperature T=298K. (a) Experimental data from Ref. 43. The scaling parameters ζ for 8 backbone-H atoms 15, 16, 17, 18 and 23, 24, 25, and 26 and for 12 backbone-C atoms 1, 2, 3, 4, 5, and 6, and 12, 13, 19, 20, 21, and 22 (see Fig. 1) are varied equally as (b) ζ_H=1.0 and ζ_C=1.0, (c) ζ_H=1.4 and ζ_C=1.2, (d) ζ_H=1.6 and ζ_C=1.2, (e) ζ_H=1.8 and ζ_C=1.2, (f) ζ_H=2.0 and ζ_C=1.2, and (g) ζ_H=2.3 and ζ_C=1.2. For the rest of hydrogen atoms and the rest carbon atoms are fixed as ζ_H=1.0 and ζ_C=1.0 (no scaling).

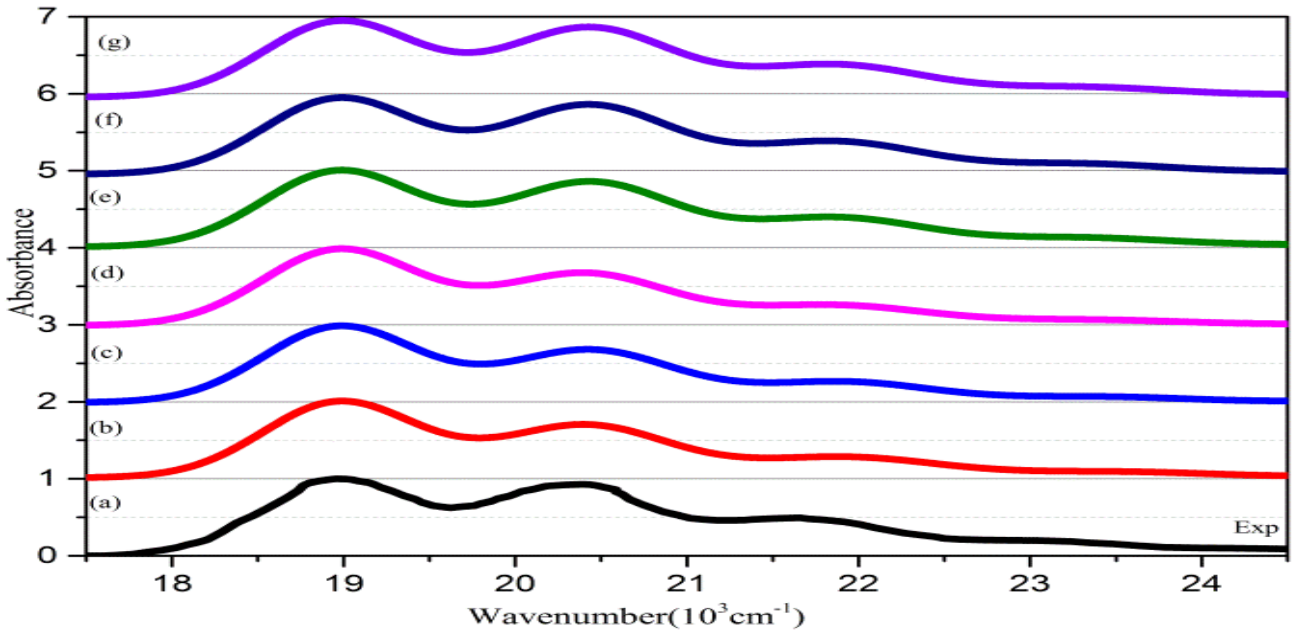


Fig. S8 Simulated absorption spectra from $S_0(1Ag) \rightarrow S_1(1B3u)$ for D_{2H} in cyclohexane solvent at temperature T = 298K. (a) Experimental data from Ref. 42. The scaling parameters ζ for 8 backbone-H atoms 15, 16, 17, 18 and 23, 24, 25, and 26 (see Fig. 1) are varied equally as (b) ζ_H=1.0, (c) ζ_H=1.2, (d) ζ_H=1.4, (e) ζ_H=1.6, (f) ζ_H=1.8 and (g) ζ_H=2.0. For the rest of hydrogen atoms and all carbon atoms are fixed as ζ_H=1.0 and ζ_C=1.0 (no scaling).

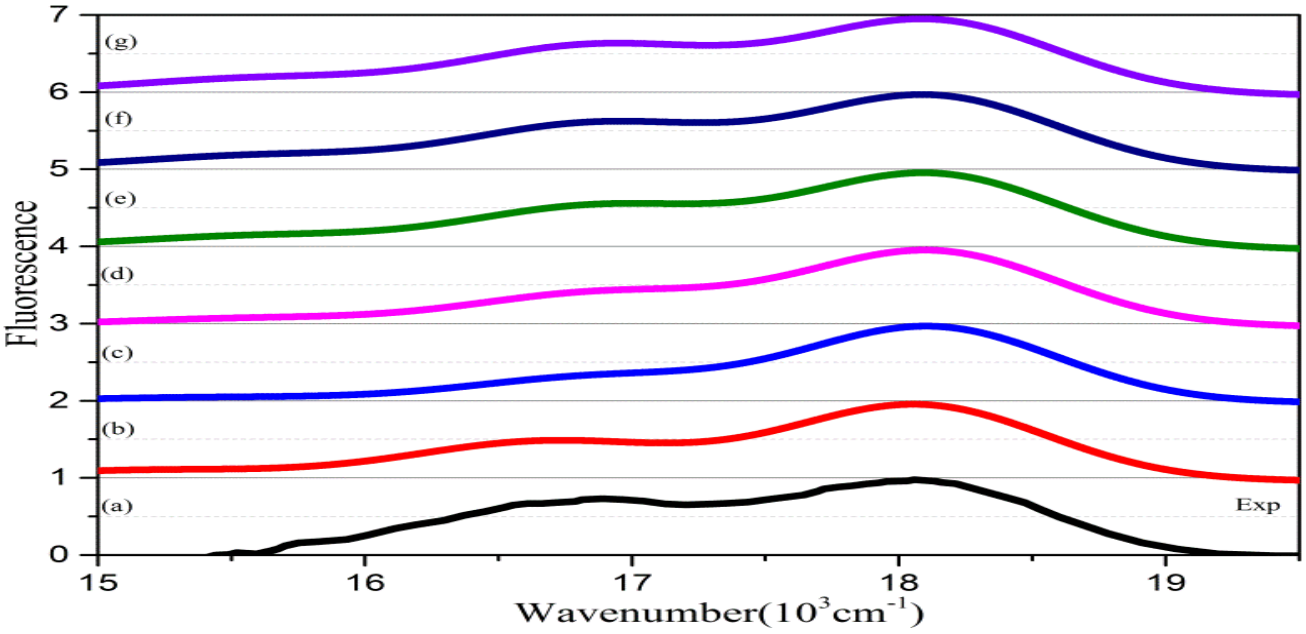


Fig. S9 Simulated fluorescence spectra from $S_0(1Ag) \leftarrow S_1(1B3u)$ for D_{2H} in cyclohexane solvent at temperature T=298K. (a) Experimental data from Ref. 42. The scaling parameters ζ for 8 backbone-H atoms 15, 16, 17, 18 and 23, 24, 25, and 26 and for 12 backbone-C atoms 1, 2, 3, 4, 5, and 6, and 12, 13, 19, 20, 21, and 22 (see Fig. 1) are varied equally as (b) ζ_H=1.0 and ζ_C=1.0, (c) ζ_H=1.2 and ζ_C=1.4, (d) ζ_H=1.4 and ζ_C=1.4, (e) ζ_H=1.6 and ζ_C=1.4, (f) ζ_H=1.8 and ζ_C=1.4, and (g) ζ_H=1.9 and ζ_C=1.4. For the rest of hydrogen atoms and the rest of carbon atoms are fixed as ζ_H=1.0 and ζ_C=1.0 (no scaling).

Table S3: Cartesian coordinates (in angstrom) for all optimized geometries of S_0 and S_1 states at the (TD)-BHandHLYP/6-31G level plus PCM model. X, Y and Z stand for S_0 state, and X', Y' and Z' correspond related S_1 state.

Table S3-1: Second-order transition state points with D_{2H} symmetry in benzene solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-0.711754	4.916848	0.000000	-0.695809	4.948043	0.000000
C2	-1.392277	3.743543	0.000000	-1.382821	3.743392	0.000000
C3	-0.717814	2.465512	0.000000	-0.713505	2.497598	0.000000
C4	0.717814	2.465512	0.000000	0.713505	2.497598	0.000000
C5	1.392277	3.743543	0.000000	1.382821	3.743392	0.000000
C6	0.711754	4.916848	0.000000	0.695809	4.948043	0.000000
C7	-1.427774	1.257196	0.000000	-1.426059	1.250689	0.000000
C8	1.427774	1.257196	0.000000	1.426059	1.250689	0.000000
C9	0.738856	0.000000	0.000000	0.745560	0.000000	0.000000
C10	-0.738856	0.000000	0.000000	-0.745560	0.000000	0.000000
C11	-1.427774	-1.257196	0.000000	-1.426059	-1.250689	0.000000
C12	-0.717814	-2.465512	0.000000	-0.713505	-2.497598	0.000000
C13	0.717814	-2.465512	0.000000	0.713505	-2.497598	0.000000
C14	1.427774	-1.257196	0.000000	1.426059	-1.250689	0.000000
H15	-1.244385	5.848675	0.000000	-1.242363	5.871482	0.000000
H16	-2.459020	3.765074	0.000000	-2.449643	3.769329	0.000000
H17	2.459020	3.765074	0.000000	2.449643	3.769329	0.000000
H18	1.244385	5.848675	0.000000	1.242363	5.871482	0.000000
C19	-1.392277	-3.743543	0.000000	-1.382821	-3.743392	0.000000
C20	-0.711754	-4.916848	0.000000	-0.695809	-4.948043	0.000000
C21	0.711754	-4.916848	0.000000	0.695809	-4.948043	0.000000
C22	1.392277	-3.743543	0.000000	1.382821	-3.743392	0.000000
H23	-2.459020	-3.765074	0.000000	-2.449643	-3.769329	0.000000
H24	-1.244385	-5.848675	0.000000	-1.242363	-5.871482	0.000000
H25	1.244385	-5.848675	0.000000	1.242363	-5.871482	0.000000
H26	2.459020	-3.765074	0.000000	2.449643	-3.769329	0.000000
C27	-2.923401	1.435359	0.000000	-2.917046	1.435990	0.000000
C28	-3.611157	1.632176	1.200084	-3.604963	1.636400	1.200419
C29	-3.611157	1.632176	-1.200084	-3.604963	1.636400	-1.200419
C30	-4.952034	2.001938	1.202192	-4.945022	2.009134	1.202131
H31	-3.090954	1.510582	2.131163	-3.085348	1.513142	2.131559
C32	-4.952034	2.001938	-1.202192	-4.945022	2.009134	-1.202131
H33	-3.090954	1.510582	-2.131163	-3.085348	1.513142	-2.131559
C34	-5.627643	2.190066	0.000000	-5.620370	2.198523	0.000000
H35	-5.462167	2.149714	2.135345	-5.454886	2.157510	2.135393
H36	-5.462167	2.149714	-2.135345	-5.454886	2.157510	-2.135393
H37	-6.660546	2.482435	0.000000	-6.652787	2.492631	0.000000
C38	2.923401	1.435359	0.000000	2.917046	1.435990	0.000000
C39	3.611157	1.632176	-1.200084	3.604963	1.636400	-1.200419
C40	3.611157	1.632176	1.200084	3.604963	1.636400	1.200419
C41	4.952034	2.001938	-1.202192	4.945022	2.009134	-1.202131
H42	3.090954	1.510582	-2.131163	3.085348	1.513142	-2.131559
C43	4.952034	2.001938	1.202192	4.945022	2.009134	1.202131
H44	3.090954	1.510582	2.131163	3.085348	1.513142	2.131559
C45	5.627643	2.190066	0.000000	5.620370	2.198523	0.000000

H46	5.462167	2.149714	-2.135345	5.454886	2.157510	-2.135393
H47	5.462167	2.149714	2.135345	5.454886	2.157510	2.135393
H48	6.660546	2.482435	0.000000	6.652787	2.492631	0.000000
C49	2.923401	-1.435359	0.000000	2.917046	-1.435990	0.000000
C50	3.611157	-1.632176	-1.200084	3.604963	-1.636400	-1.200419
C51	3.611157	-1.632176	1.200084	3.604963	-1.636400	1.200419
C52	4.952034	-2.001938	-1.202192	4.945022	-2.009134	-1.202131
H53	3.090954	-1.510582	-2.131163	3.085348	-1.513142	-2.131559
C54	4.952034	-2.001938	1.202192	4.945022	-2.009134	1.202131
H55	3.090954	-1.510582	2.131163	3.085348	-1.513142	2.131559
C56	5.627643	-2.190066	0.000000	5.620370	-2.198523	0.000000
H57	5.462167	-2.149714	-2.135345	5.454886	-2.157510	-2.135393
H58	5.462167	-2.149714	2.135345	5.454886	-2.157510	2.135393
H59	6.660546	-2.482435	0.000000	6.652787	-2.492631	0.000000
C60	-2.923401	-1.435359	0.000000	-2.917046	-1.435990	0.000000
C61	-3.611157	-1.632176	1.200084	-3.604963	-1.636400	1.200419
C62	-3.611157	-1.632176	-1.200084	-3.604963	-1.636400	-1.200419
C63	-4.952034	-2.001938	1.202192	-4.945022	-2.009134	1.202131
H64	-3.090954	-1.510582	2.131163	-3.085348	-1.513142	2.131559
C65	-4.952034	-2.001938	-1.202192	-4.945022	-2.009134	-1.202131
H66	-3.090954	-1.510582	-2.131163	-3.085348	-1.513142	-2.131559
C67	-5.627643	-2.190066	0.000000	-5.620370	-2.198523	0.000000
H68	-5.462167	-2.149714	2.135345	-5.454886	-2.157510	2.135393
H69	-5.462167	-2.149714	-2.135345	-5.454886	-2.157510	-2.135393
H70	-6.660546	-2.482435	0.000000	-6.652787	-2.492631	0.000000

Table S3-2: Second-order transition state points with D_{2H} symmetry in cyclohexane solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-0.711743	4.916834	0.000000	-0.695823	4.948032	0.000000
C2	-1.392275	3.743586	0.000000	-1.382834	3.743454	0.000000
C3	-0.717804	2.465583	0.000000	-0.713509	2.497640	0.000000
C4	0.717804	2.465583	0.000000	0.713509	2.497640	0.000000
C5	1.392275	3.743586	0.000000	1.382834	3.743454	0.000000
C6	0.711743	4.916834	0.000000	0.695823	4.948032	0.000000
C7	-1.427724	1.257244	0.000000	-1.425968	1.250755	0.000000
C8	1.427724	1.257244	0.000000	1.425968	1.250755	0.000000
C9	0.738916	0.000000	0.000000	0.745611	0.000000	0.000000
C10	-0.738916	0.000000	0.000000	-0.745611	0.000000	0.000000
C11	-1.427724	-1.257244	0.000000	-1.425968	-1.250755	0.000000
C12	-0.717804	-2.465583	0.000000	-0.713509	-2.497640	0.000000
C13	0.717804	-2.465583	0.000000	0.713509	-2.497640	0.000000
C14	1.427724	-1.257244	0.000000	1.425968	-1.250755	0.000000
H15	-1.244392	5.848653	0.000000	-1.242369	5.871477	0.000000
H16	-2.458999	3.765142	0.000000	-2.449636	3.769387	0.000000
H17	2.458999	3.765142	0.000000	2.449636	3.769387	0.000000
H18	1.244392	5.848653	0.000000	1.242369	5.871477	0.000000
C19	-1.392275	-3.743586	0.000000	-1.382834	-3.743454	0.000000
C20	-0.711743	-4.916834	0.000000	-0.695823	-4.948032	0.000000
C21	0.711743	-4.916834	0.000000	0.695823	-4.948032	0.000000
C22	1.392275	-3.743586	0.000000	1.382834	-3.743454	0.000000
H23	-2.458999	-3.765142	0.000000	-2.449636	-3.769387	0.000000
H24	-1.244392	-5.848653	0.000000	-1.242369	-5.871477	0.000000
H25	1.244392	-5.848653	0.000000	1.242369	-5.871477	0.000000
H26	2.458999	-3.765142	0.000000	2.449636	-3.769387	0.000000
C27	-2.923305	1.435366	0.000000	-2.916921	1.436053	0.000000
C28	-3.611313	1.631330	1.200064	-3.605038	1.635772	1.200396
C29	-3.611313	1.631330	-1.200064	-3.605038	1.635772	-1.200396
C30	-4.952953	1.998249	1.202145	-4.945736	2.006159	1.202084
H31	-3.090582	1.511243	2.131028	-3.084914	1.513884	2.131420
C32	-4.952953	1.998249	-1.202145	-4.945736	2.006159	-1.202084
H33	-3.090582	1.511243	-2.131028	-3.084914	1.513884	-2.131420
C34	-5.628997	2.184334	0.000000	-5.621443	2.193801	0.000000
H35	-5.463412	2.145213	2.135241	-5.455874	2.153903	2.135291
H36	-5.463412	2.145213	-2.135241	-5.455874	2.153903	-2.135291
H37	-6.662673	2.473970	0.000000	-6.654517	2.485608	0.000000
C38	2.923305	1.435366	0.000000	2.916921	1.436053	0.000000
C39	3.611313	1.631330	-1.200064	3.605038	1.635772	-1.200396
C40	3.611313	1.631330	1.200064	3.605038	1.635772	1.200396
C41	4.952953	1.998249	-1.202145	4.945736	2.006159	-1.202084
H42	3.090582	1.511243	-2.131028	3.084914	1.513884	-2.131420
C43	4.952953	1.998249	1.202145	4.945736	2.006159	1.202084
H44	3.090582	1.511243	2.131028	3.084914	1.513884	2.131420
C45	5.628997	2.184334	0.000000	5.621443	2.193801	0.000000
H46	5.463412	2.145213	-2.135241	5.455874	2.153903	-2.135291
H47	5.463412	2.145213	2.135241	5.455874	2.153903	2.135291
H48	6.662673	2.473970	0.000000	6.654517	2.485608	0.000000
C49	2.923305	-1.435366	0.000000	2.916921	-1.436053	0.000000
C50	3.611313	-1.631330	-1.200064	3.605038	-1.635772	-1.200396
C51	3.611313	-1.631330	1.200064	3.605038	-1.635772	1.200396

C52	4.952953	-1.998249	-1.202145	4.945736	-2.006159	-1.202084
H53	3.090582	-1.511243	-2.131028	3.084914	-1.513884	-2.131420
C54	4.952953	-1.998249	1.202145	4.945736	-2.006159	1.202084
H55	3.090582	-1.511243	2.131028	3.084914	-1.513884	2.131420
C56	5.628997	-2.184334	0.000000	5.621443	-2.193801	0.000000
H57	5.463412	-2.145213	-2.135241	5.455874	-2.153903	-2.135291
H58	5.463412	-2.145213	2.135241	5.455874	-2.153903	2.135291
H59	6.662673	-2.473970	0.000000	6.654517	-2.485608	0.000000
C60	-2.923305	-1.435366	0.000000	-2.916921	-1.436053	0.000000
C61	-3.611313	-1.631330	1.200064	-3.605038	-1.635772	1.200396
C62	-3.611313	-1.631330	-1.200064	-3.605038	-1.635772	-1.200396
C63	-4.952953	-1.998249	1.202145	-4.945736	-2.006159	1.202084
H64	-3.090582	-1.511243	2.131028	-3.084914	-1.513884	2.131420
C65	-4.952953	-1.998249	-1.202145	-4.945736	-2.006159	-1.202084
H66	-3.090582	-1.511243	-2.131028	-3.084914	-1.513884	-2.131420
C67	-5.628997	-2.184334	0.000000	-5.621443	-2.193801	0.000000
H68	-5.463412	-2.145213	2.135241	-5.455874	-2.153903	2.135291
H69	-5.463412	-2.145213	-2.135241	-5.455874	-2.153903	-2.135291
H70	-6.662673	-2.473970	0.000000	-6.654517	-2.485608	0.000000

Table S3-3: Local minima with $D_2(1)$ symmetry in benzene solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-0.266059	4.882592	0.661591	-0.268055	4.904944	0.643784
C2	-0.486643	3.710336	1.310199	-0.502721	3.702716	1.292990
C3	-0.197137	2.439575	0.694711	-0.215231	2.462153	0.685629
C4	0.197137	2.439575	-0.694711	0.215231	2.462153	-0.685629
C5	0.486643	3.710336	-1.310199	0.502721	3.702716	-1.292990
C6	0.266059	4.882592	-0.661591	0.268055	4.904944	-0.643784
C7	-0.255216	1.233905	1.402468	-0.304542	1.214525	1.395110
C8	0.255216	1.233905	-1.402468	0.304542	1.214525	-1.395110
C9	0.000000	0.000000	-0.725110	0.000000	0.000000	-0.733458
C10	0.000000	0.000000	0.725110	0.000000	0.000000	0.733458
C11	0.255216	-1.233905	1.402468	0.304542	-1.214525	1.395110
C12	0.197137	-2.439575	0.694711	0.215231	-2.462153	0.685629
C13	-0.197137	-2.439575	-0.694711	-0.215231	-2.462153	-0.685629
C14	-0.255216	-1.233905	-1.402468	-0.304542	-1.214525	-1.395110
H15	-0.481193	5.816057	1.145783	-0.488397	5.830294	1.140530
H16	-0.871554	3.723287	2.307397	-0.895955	3.721957	2.286803
H17	0.871554	3.723287	-2.307397	0.895955	3.721957	-2.286803
H18	0.481193	5.816057	-1.145783	0.488397	5.830294	-1.140530
C19	0.486643	-3.710336	1.310199	0.502721	-3.702716	1.292990
C20	0.266059	-4.882592	0.661591	0.268055	-4.904944	0.643784
C21	-0.266059	-4.882592	-0.661591	-0.268055	-4.904944	-0.643784
C22	-0.486643	-3.710336	-1.310199	-0.502721	-3.702716	-1.292990
H23	0.871554	-3.723287	2.307397	0.895955	-3.721957	2.286803
H24	0.481193	-5.816057	1.145783	0.488397	-5.830294	1.140530
H25	-0.481193	-5.816057	-1.145783	-0.488397	-5.830294	-1.140530
H26	-0.871554	-3.723287	-2.307397	-0.895955	-3.721957	-2.286803
C27	-0.753625	1.266303	2.816274	-0.879227	1.202708	2.770836
C28	-0.025634	1.848789	3.858156	-0.286537	1.875158	3.847761
C29	-2.042696	0.794571	3.088381	-2.100422	0.550095	2.992174
C30	-0.565572	1.948408	5.135818	-0.888687	1.887883	5.100628
H31	0.964228	2.215743	3.668585	0.655170	2.368714	3.707539
C32	-2.586071	0.896372	4.365035	-2.707036	0.569304	4.242908
H33	-2.621061	0.357879	2.296536	-2.575711	0.038045	2.177748
C34	-1.848711	1.473821	5.394023	-2.103170	1.238085	5.303719
H35	0.012255	2.392908	5.923880	-0.409593	2.398778	5.914361
H36	-3.579195	0.533305	4.551624	-3.646578	0.069469	4.385780
H37	-2.266527	1.554686	6.379565	-2.569366	1.252674	6.270537
C38	0.753625	1.266303	-2.816274	0.879227	1.202708	-2.770836
C39	0.025634	1.848789	-3.858156	0.286537	1.875158	-3.847761
C40	2.042696	0.794571	-3.088381	2.100422	0.550095	-2.992174
C41	0.565572	1.948408	-5.135818	0.888687	1.887883	-5.100628
H42	-0.964228	2.215743	-3.668585	-0.655170	2.368714	-3.707539
C43	2.586071	0.896372	-4.365035	2.707036	0.569304	-4.242908
H44	2.621061	0.357879	-2.296536	2.575711	0.038045	-2.177748
C45	1.848711	1.473821	-5.394023	2.103170	1.238085	-5.303719
H46	-0.012255	2.392908	-5.923880	0.409593	2.398778	-5.914361
H47	3.579195	0.533305	-4.551624	3.646578	0.069469	-4.385780
H48	2.266527	1.554686	-6.379565	2.569366	1.252674	-6.270537
C49	-0.753625	-1.266303	-2.816274	-0.879227	-1.202708	-2.770836
C50	-2.042696	-0.794571	-3.088381	-2.100422	-0.550095	-2.992174
C51	-0.025634	-1.848789	-3.858156	-0.286537	-1.875158	-3.847761

C52	-2.586071	-0.896372	-4.365035	-2.707036	-0.569304	-4.242908
H53	-2.621061	-0.357879	-2.296536	-2.575711	-0.038045	-2.177748
C54	-0.565572	-1.948408	-5.135818	-0.888687	-1.887883	-5.100628
H55	0.964228	-2.215743	-3.668585	0.655170	-2.368714	-3.707539
C56	-1.848711	-1.473821	-5.394023	-2.103170	-1.238085	-5.303719
H57	-3.579195	-0.533305	-4.551624	-3.646578	-0.069469	-4.385780
H58	0.012255	-2.392908	-5.923880	-0.409593	-2.398778	-5.914361
H59	-2.266527	-1.554686	-6.379565	-2.569366	-1.252674	-6.270537
C60	0.753625	-1.266303	2.816274	0.879227	-1.202708	2.770836
C61	2.042696	-0.794571	3.088381	2.100422	-0.550095	2.992174
C62	0.025634	-1.848789	3.858156	0.286537	-1.875158	3.847761
C63	2.586071	-0.896372	4.365035	2.707036	-0.569304	4.242908
H64	2.621061	-0.357879	2.296536	2.575711	-0.038045	2.177748
C65	0.565572	-1.948408	5.135818	0.888687	-1.887883	5.100628
H66	-0.964228	-2.215743	3.668585	-0.655170	-2.368714	3.707539
C67	1.848711	-1.473821	5.394023	2.103170	-1.238085	5.303719
H68	3.579195	-0.533305	4.551624	3.646578	-0.069469	4.385780
H69	-0.012255	-2.392908	5.923880	0.409593	-2.398778	5.914361
H70	2.266527	-1.554686	6.379565	2.569366	-1.252674	6.270537

Table S3-4: Local minima with $D_2(2)$ symmetry in benzene solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-0.266060	4.882591	-0.661591	-0.268048	4.904940	-0.643786
C2	-0.486644	3.710336	-1.310199	-0.502704	3.702712	-1.292997
C3	-0.197137	2.439575	-0.694710	-0.215223	2.462148	-0.685634
C4	0.197137	2.439575	0.694710	0.215223	2.462148	0.685634
C5	0.486644	3.710336	1.310199	0.502704	3.702712	1.292997
C6	0.266060	4.882591	0.661591	0.268048	4.904940	0.643786
C7	-0.255216	1.233905	-1.402468	-0.304542	1.214526	-1.395108
C8	0.255216	1.233905	1.402468	0.304542	1.214526	1.395108
C9	0.000000	0.000000	0.725110	0.000000	0.000000	0.733460
C10	0.000000	0.000000	-0.725110	0.000000	0.000000	-0.733460
C11	0.255216	-1.233905	-1.402468	0.304542	-1.214526	-1.395108
C12	0.197137	-2.439575	-0.694710	0.215223	-2.462148	-0.685634
C13	-0.197137	-2.439575	0.694710	-0.215223	-2.462148	0.685634
C14	-0.255216	-1.233905	1.402468	-0.304542	-1.214526	1.395108
H15	-0.481194	5.816057	-1.145783	-0.488382	5.830289	-1.140537
H16	-0.871555	3.723286	-2.307397	-0.895930	3.721952	-2.286813
H17	0.871555	3.723286	2.307397	0.895930	3.721952	2.286813
H18	0.481194	5.816057	1.145783	0.488382	5.830289	1.140537
C19	0.486644	-3.710336	-1.310199	0.502704	-3.702712	-1.292997
C20	0.266060	-4.882591	-0.661591	0.268048	-4.904940	-0.643786
C21	-0.266060	-4.882591	0.661591	-0.268048	-4.904940	0.643786
C22	-0.486644	-3.710336	1.310199	-0.502704	-3.702712	1.292997
H23	0.871555	-3.723286	-2.307397	0.895930	-3.721952	-2.286813
H24	0.481194	-5.816057	-1.145783	0.488382	-5.830289	-1.140537
H25	-0.481194	-5.816057	1.145783	-0.488382	-5.830289	1.140537
H26	-0.871555	-3.723286	2.307397	-0.895930	-3.721952	2.286813
C27	-0.753624	1.266304	-2.816274	-0.879237	1.202685	-2.770834
C28	-2.042696	0.794573	-3.088382	-2.100433	0.550068	-2.992146
C29	-0.025632	1.848789	-3.858155	-0.286571	1.875139	-3.847770
C30	-2.586070	0.896374	-4.365037	-2.707063	0.569257	-4.242875
H31	-2.621062	0.357881	-2.296538	-2.575713	0.038028	-2.177710
C32	-0.565569	1.948410	-5.135817	-0.888726	1.887825	-5.100633
H33	0.964229	2.215744	-3.668583	0.655134	2.368702	-3.707565
C34	-1.848708	1.473824	-5.394024	-2.103207	1.238013	-5.303704
H35	-3.579194	0.533308	-4.551627	-3.646602	0.069409	-4.385724
H36	0.012259	2.392910	-5.923879	-0.409646	2.398711	-5.914381
H37	-2.266524	1.554690	-6.379566	-2.569407	1.252585	-6.270520
C38	0.753624	1.266304	2.816274	0.879237	1.202685	2.770834
C39	2.042696	0.794573	3.088382	2.100433	0.550068	2.992146
C40	0.025632	1.848789	3.858155	0.286571	1.875139	3.847770
C41	2.586070	0.896374	4.365037	2.707063	0.569257	4.242875
H42	2.621062	0.357881	2.296538	2.575713	0.038028	2.177710
C43	0.565569	1.948410	5.135817	0.888726	1.887825	5.100633
H44	-0.964229	2.215744	3.668583	-0.655134	2.368702	3.707565
C45	1.848708	1.473824	5.394024	2.103207	1.238013	5.303704
H46	3.579194	0.533308	4.551627	3.646602	0.069409	4.385724
H47	-0.012259	2.392910	5.923879	0.409646	2.398711	5.914381
H48	2.266524	1.554690	6.379566	2.569407	1.252585	6.270520
C49	-0.753624	-1.266304	2.816274	-0.879237	-1.202685	2.770834
C50	-0.025632	-1.848789	3.858155	-0.286571	-1.875139	3.847770
C51	-2.042696	-0.794573	3.088382	-2.100433	-0.550068	2.992146

C52	-0.565569	-1.948410	5.135817	-0.888726	-1.887825	5.100633
H53	0.964229	-2.215744	3.668583	0.655134	-2.368702	3.707565
C54	-2.586070	-0.896374	4.365037	-2.707063	-0.569257	4.242875
H55	-2.621062	-0.357881	2.296538	-2.575713	-0.038028	2.177710
C56	-1.848708	-1.473824	5.394024	-2.103207	-1.238013	5.303704
H57	0.012259	-2.392910	5.923879	-0.409646	-2.398711	5.914381
H58	-3.579194	-0.533308	4.551627	-3.646602	-0.069409	4.385724
H59	-2.266524	-1.554690	6.379566	-2.569407	-1.252585	6.270520
C60	0.753624	-1.266304	-2.816274	0.879237	-1.202685	-2.770834
C61	0.025632	-1.848789	-3.858155	0.286571	-1.875139	-3.847770
C62	2.042696	-0.794573	-3.088382	2.100433	-0.550068	-2.992146
C63	0.565569	-1.948410	-5.135817	0.888726	-1.887825	-5.100633
H64	-0.964229	-2.215744	-3.668583	-0.655134	-2.368702	-3.707565
C65	2.586070	-0.896374	-4.365037	2.707063	-0.569257	-4.242875
H66	2.621062	-0.357881	-2.296538	2.575713	-0.038028	-2.177710
C67	1.848708	-1.473824	-5.394024	2.103207	-1.238013	-5.303704
H68	-0.012259	-2.392910	-5.923879	0.409646	-2.398711	-5.914381
H69	3.579194	-0.533308	-4.551627	3.646602	-0.069409	-4.385724
H70	2.266524	-1.554690	-6.379566	2.569407	-1.252585	-6.270520

Table S3-5: Local minima with $D_2(1)$ symmetry in cyclohexane solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-0.265462	4.882474	0.661819	-0.267810	4.904821	0.643891
C2	-0.485678	3.710291	1.310597	-0.502295	3.702669	1.293194
C3	-0.196849	2.439593	0.694779	-0.215055	2.462141	0.685676
C4	0.196849	2.439593	-0.694779	0.215055	2.462141	-0.685676
C5	0.485678	3.710291	-1.310597	0.502295	3.702669	-1.293194
C6	0.265462	4.882474	-0.661819	0.267810	4.904821	-0.643891
C7	-0.254956	1.233929	1.402416	-0.304300	1.214578	1.395028
C8	0.254956	1.233929	-1.402416	0.304300	1.214578	-1.395028
C9	0.000000	0.000000	-0.725067	0.000000	0.000000	-0.733454
C10	0.000000	0.000000	0.725067	0.000000	0.000000	0.733454
C11	0.254956	-1.233929	1.402416	0.304300	-1.214578	1.395028
C12	0.196849	-2.439593	0.694779	0.215055	-2.462141	0.685676
C13	-0.196849	-2.439593	-0.694779	-0.215055	-2.462141	-0.685676
C14	-0.254956	-1.233929	-1.402416	-0.304300	-1.214578	-1.395028
H15	-0.480059	5.815962	1.146232	-0.487970	5.830198	1.140690
H16	-0.869804	3.723108	2.308115	-0.895259	3.721758	2.287130
H17	0.869804	3.723108	-2.308115	0.895259	3.721758	-2.287130
H18	0.480059	5.815962	-1.146232	0.487970	5.830198	-1.140690
C19	0.485678	-3.710291	1.310597	0.502295	-3.702669	1.293194
C20	0.265462	-4.882474	0.661819	0.267810	-4.904821	0.643891
C21	-0.265462	-4.882474	-0.661819	-0.267810	-4.904821	-0.643891
C22	-0.485678	-3.710291	-1.310597	-0.502295	-3.702669	-1.293194
H23	0.869804	-3.723108	2.308115	0.895259	-3.721758	2.287130
H24	0.480059	-5.815962	1.146232	0.487970	-5.830198	1.140690
H25	-0.480059	-5.815962	-1.146232	-0.487970	-5.830198	-1.140690
H26	-0.869804	-3.723108	-2.308115	-0.895259	-3.721758	-2.287130
C27	-0.753346	1.266014	2.816236	-0.878846	1.202904	2.770886
C28	-0.024193	1.845423	3.858944	-0.284770	1.873552	3.848078
C29	-2.043261	0.796278	3.087687	-2.101130	0.552384	2.991932
C30	-0.563630	1.943440	5.136889	-0.886743	1.886660	5.100983
H31	0.966323	2.210789	3.669795	0.657845	2.365382	3.707897
C32	-2.586225	0.896776	4.364568	-2.707532	0.571948	4.242734
H33	-2.622448	0.362075	2.295076	-2.577349	0.041713	2.177177
C34	-1.847537	1.470779	5.394465	-2.102365	1.239029	5.303798
H35	0.015244	2.385225	5.925712	-0.406569	2.396100	5.914997
H36	-3.580033	0.535303	4.550670	-3.647983	0.073755	4.385442
H37	-2.264950	1.550477	6.380283	-2.568439	1.253915	6.270682
C38	0.753346	1.266014	-2.816236	0.878846	1.202904	-2.770886
C39	0.024193	1.845423	-3.858944	0.284770	1.873552	-3.848078
C40	2.043261	0.796278	-3.087687	2.101130	0.552384	-2.991932
C41	0.563630	1.943440	-5.136889	0.886743	1.886660	-5.100983
H42	-0.966323	2.210789	-3.669795	-0.657845	2.365382	-3.707897
C43	2.586225	0.896776	-4.364568	2.707532	0.571948	-4.242734
H44	2.622448	0.362075	-2.295076	2.577349	0.041713	-2.177177
C45	1.847537	1.470779	-5.394465	2.102365	1.239029	-5.303798
H46	-0.015244	2.385225	-5.925712	0.406569	2.396100	-5.914997
H47	3.580033	0.535303	-4.550670	3.647983	0.073755	-4.385442
H48	2.264950	1.550477	-6.380283	2.568439	1.253915	-6.270682
C49	-0.753346	-1.266014	-2.816236	-0.878846	-1.202904	-2.770886
C50	-2.043261	-0.796278	-3.087687	-2.101130	-0.552384	-2.991932
C51	-0.024193	-1.845423	-3.858944	-0.284770	-1.873552	-3.848078

C52	-2.586225	-0.896776	-4.364568	-2.707532	-0.571948	-4.242734
H53	-2.622448	-0.362075	-2.295076	-2.577349	-0.041713	-2.177177
C54	-0.563630	-1.943440	-5.136889	-0.886743	-1.886660	-5.100983
H55	0.966323	-2.210789	-3.669795	0.657845	-2.365382	-3.707897
C56	-1.847537	-1.470779	-5.394465	-2.102365	-1.239029	-5.303798
H57	-3.580033	-0.535303	-4.550670	-3.647983	-0.073755	-4.385442
H58	0.015244	-2.385225	-5.925712	-0.406569	-2.396100	-5.914997
H59	-2.264950	-1.550477	-6.380283	-2.568439	-1.253915	-6.270682
C60	0.753346	-1.266014	2.816236	0.878846	-1.202904	2.770886
C61	2.043261	-0.796278	3.087687	2.101130	-0.552384	2.991932
C62	0.024193	-1.845423	3.858944	0.284770	-1.873552	3.848078
C63	2.586225	-0.896776	4.364568	2.707532	-0.571948	4.242734
H64	2.622448	-0.362075	2.295076	2.577349	-0.041713	2.177177
C65	0.563630	-1.943440	5.136889	0.886743	-1.886660	5.100983
H66	-0.966323	-2.210789	3.669795	-0.657845	-2.365382	3.707897
C67	1.847537	-1.470779	5.394465	2.102365	-1.239029	5.303798
H68	3.580033	-0.535303	4.550670	3.647983	-0.073755	4.385442
H69	-0.015244	-2.385225	5.925712	0.406569	-2.396100	5.914997
H70	2.264950	-1.550477	6.380283	2.568439	-1.253915	6.270682

Table S3-6: Local minima with $D_2(2)$ symmetry in cyclohexane solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-0.265458	4.882471	-0.661820	-0.267810	4.904821	-0.643891
C2	-0.485675	3.710288	-1.310599	-0.502295	3.702669	-1.293194
C3	-0.196851	2.439591	-0.694779	-0.215055	2.462141	-0.685676
C4	0.196851	2.439591	0.694779	0.215055	2.462141	0.685676
C5	0.485675	3.710288	1.310599	0.502295	3.702669	1.293194
C6	0.265458	4.882471	0.661820	0.267810	4.904821	0.643891
C7	-0.254957	1.233928	-1.402416	-0.304300	1.214578	-1.395028
C8	0.254957	1.233928	1.402416	0.304300	1.214578	1.395028
C9	0.000000	0.000000	0.725067	0.000000	0.000000	0.733454
C10	0.000000	0.000000	-0.725067	0.000000	0.000000	-0.733454
C11	0.254957	-1.233928	-1.402416	0.304300	-1.214578	-1.395028
C12	0.196851	-2.439591	-0.694779	0.215055	-2.462141	-0.685676
C13	-0.196851	-2.439591	0.694779	-0.215055	-2.462141	0.685676
C14	-0.254957	-1.233928	1.402416	-0.304300	-1.214578	1.395028
H15	-0.480055	5.815959	-1.146234	-0.487970	5.830198	-1.140690
H16	-0.869798	3.723104	-2.308119	-0.895259	3.721758	-2.287130
H17	0.869798	3.723104	2.308119	0.895259	3.721758	2.287130
H18	0.480055	5.815959	1.146234	0.487970	5.830198	1.140690
C19	0.485675	-3.710288	-1.310599	0.502295	-3.702669	-1.293194
C20	0.265458	-4.882471	-0.661820	0.267810	-4.904821	-0.643891
C21	-0.265458	-4.882471	0.661820	-0.267810	-4.904821	0.643891
C22	-0.485675	-3.710288	1.310599	-0.502295	-3.702669	1.293194
H23	0.869798	-3.723104	-2.308119	0.895259	-3.721758	-2.287130
H24	0.480055	-5.815959	-1.146234	0.487970	-5.830198	-1.140690
H25	-0.480055	-5.815959	1.146234	-0.487970	-5.830198	1.140690
H26	-0.869798	-3.723104	2.308119	-0.895259	-3.721758	2.287130
C27	-0.753346	1.266013	-2.816235	-0.878846	1.202904	-2.770886
C28	-2.043264	0.796283	-3.087685	-2.101130	0.552384	-2.991932
C29	-0.024190	1.845415	-3.858944	-0.284770	1.873552	-3.848078
C30	-2.586225	0.896778	-4.364567	-2.707532	0.571948	-4.242734
H31	-2.622454	0.362087	-2.295072	-2.577349	0.041713	-2.177177
C32	-0.563626	1.943429	-5.136890	-0.886743	1.886660	-5.100983
H33	0.966327	2.210779	-3.669795	0.657845	2.365382	-3.707897
C34	-1.847534	1.470774	-5.394466	-2.102365	1.239029	-5.303798
H35	-3.580038	0.535313	-4.550669	-3.647983	0.073755	-4.385442
H36	0.015251	2.385207	-5.925715	-0.406569	2.396100	-5.914997
H37	-2.264946	1.550468	-6.380284	-2.568439	1.253915	-6.270682
C38	0.753346	1.266013	2.816235	0.878846	1.202904	2.770886
C39	2.043264	0.796283	3.087685	2.101130	0.552384	2.991932
C40	0.024190	1.845415	3.858944	0.284770	1.873552	3.848078
C41	2.586225	0.896778	4.364567	2.707532	0.571948	4.242734
H42	2.622454	0.362087	2.295072	2.577349	0.041713	2.177177
C43	0.563626	1.943429	5.136890	0.886743	1.886660	5.100983
H44	-0.966327	2.210779	3.669795	-0.657845	2.365382	3.707897
C45	1.847534	1.470774	5.394466	2.102365	1.239029	5.303798
H46	3.580038	0.535313	4.550669	3.647983	0.073755	4.385442
H47	-0.015251	2.385207	5.925715	0.406569	2.396100	5.914997
H48	2.264946	1.550468	6.380284	2.568439	1.253915	6.270682
C49	-0.753346	-1.266013	2.816235	-0.878846	-1.202904	2.770886
C50	-0.024190	-1.845415	3.858944	-0.284770	-1.873552	3.848078
C51	-2.043264	-0.796283	3.087685	-2.101130	-0.552384	2.991932

C52	-0.563626	-1.943429	5.136890	-0.886743	-1.886660	5.100983
H53	0.966327	-2.210779	3.669795	0.657845	-2.365382	3.707897
C54	-2.586225	-0.896778	4.364567	-2.707532	-0.571948	4.242734
H55	-2.622454	-0.362087	2.295072	-2.577349	-0.041713	2.177177
C56	-1.847534	-1.470774	5.394466	-2.102365	-1.239029	5.303798
H57	0.015251	-2.385207	5.925715	-0.406569	-2.396100	5.914997
H58	-3.580038	-0.535313	4.550669	-3.647983	-0.073755	4.385442
H59	-2.264946	-1.550468	6.380284	-2.568439	-1.253915	6.270682
C60	0.753346	-1.266013	-2.816235	0.878846	-1.202904	-2.770886
C61	0.024190	-1.845415	-3.858944	0.284770	-1.873552	-3.848078
C62	2.043264	-0.796283	-3.087685	2.101130	-0.552384	-2.991932
C63	0.563626	-1.943429	-5.136890	0.886743	-1.886660	-5.100983
H64	-0.966327	-2.210779	-3.669795	-0.657845	-2.365382	-3.707897
C65	2.586225	-0.896778	-4.364567	2.707532	-0.571948	-4.242734
H66	2.622454	-0.362087	-2.295072	2.577349	-0.041713	-2.177177
C67	1.847534	-1.470774	-5.394466	2.102365	-1.239029	-5.303798
H68	-0.015251	-2.385207	-5.925715	0.406569	-2.396100	-5.914997
H69	3.580038	-0.535313	-4.550669	3.647983	-0.073755	-4.385442
H70	2.264946	-1.550468	-6.380284	2.568439	-1.253915	-6.270682

Table S3-7: Local minima with $C_{2H}(1)$ symmetry in benzene solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-4.842524	0.783778	0.712127	-4.836723	0.949675	0.696798
C2	-3.688696	0.570183	1.393828	-3.667966	0.664243	1.384765
C3	-2.428744	0.373105	0.719839	-2.450152	0.412456	0.716425
C4	-2.428744	0.373105	-0.719839	-2.450152	0.412456	-0.716425
C5	-3.688696	0.570183	-1.393828	-3.667966	0.664243	-1.384765
C6	-4.842524	0.783778	-0.712127	-4.836723	0.949675	-0.696798
C7	-1.248583	0.100930	1.424449	-1.242875	0.071644	1.419273
C8	-1.248583	0.100930	-1.424449	-1.242875	0.071644	-1.419273
C9	0.000000	0.000000	-0.734574	0.000000	0.000000	-0.735018
C10	0.000000	0.000000	0.734574	0.000000	0.000000	0.735018
C11	1.248583	-0.100930	1.424449	1.242875	-0.071644	1.419273
C12	2.428744	-0.373105	0.719839	2.450152	-0.412456	0.716425
C13	2.428744	-0.373105	-0.719839	2.450152	-0.412456	-0.716425
C14	1.248583	-0.100930	-1.424449	1.242875	-0.071644	-1.419273
H15	-5.761161	0.944239	1.243505	-5.739672	1.149375	1.241198
H16	-3.707845	0.557415	2.461556	-3.698824	0.627963	2.451839
H17	-3.707845	0.557415	-2.461556	-3.698824	0.627963	-2.451839
H18	-5.761161	0.944239	-1.243505	-5.739672	1.149375	-1.241198
C19	3.688696	-0.570183	1.393828	3.667966	-0.664243	1.384765
C20	4.842524	-0.783778	0.712127	4.836723	-0.949675	0.696798
C21	4.842524	-0.783778	-0.712127	4.836723	-0.949675	-0.696798
C22	3.688696	-0.570183	-1.393828	3.667966	-0.664243	-1.384765
H23	3.707845	-0.557415	2.461556	3.698824	-0.627963	2.451839
H24	5.761161	-0.944239	1.243505	5.739672	-1.149375	1.241198
H25	5.761161	-0.944239	-1.243505	5.739672	-1.149375	-1.241198
H26	3.707845	-0.557415	-2.461556	3.698824	-0.627963	-2.451839
C27	-1.420638	-0.264679	2.873609	-1.395894	-0.394886	2.833266
C28	-1.620870	0.685537	3.877888	-1.736472	0.449803	3.895512
C29	-1.530911	-1.618557	3.206878	-1.304732	-1.770332	3.085129
C30	-1.907067	0.294014	5.181304	-1.970339	-0.061487	5.167209
H31	-1.548678	1.728702	3.639460	-1.799246	1.507657	3.730094
C32	-1.816743	-2.013001	4.510155	-1.543920	-2.283525	4.355406
H33	-1.401445	-2.360738	2.441942	-1.057702	-2.435325	2.279711
C34	-2.006286	-1.056920	5.502805	-1.878382	-1.430483	5.402518
H35	-2.052458	1.039422	5.940073	-2.220148	0.606336	5.969886
H36	-1.899212	-3.057641	4.744620	-1.475536	-3.341993	4.522971
H37	-2.231066	-1.357861	6.508464	-2.064207	-1.824206	6.383752
C38	-1.420638	-0.264679	-2.873609	-1.395894	-0.394886	-2.833266
C39	-1.530911	-1.618557	-3.206878	-1.304732	-1.770332	-3.085129
C40	-1.620870	0.685537	-3.877888	-1.736472	0.449803	-3.895512
C41	-1.816743	-2.013001	-4.510155	-1.543920	-2.283525	-4.355406
H42	-1.401445	-2.360738	-2.441942	-1.057702	-2.435325	-2.279711
C43	-1.907067	0.294014	-5.181304	-1.970339	-0.061487	-5.167209
H44	-1.548678	1.728702	-3.639460	-1.799246	1.507657	-3.730094
C45	-2.006286	-1.056920	-5.502805	-1.878382	-1.430483	-5.402518
H46	-1.899212	-3.057641	-4.744620	-1.475536	-3.341993	-4.522971
H47	-2.052458	1.039422	-5.940073	-2.220148	0.606336	-5.969886
H48	-2.231066	-1.357861	-6.508464	-2.064207	-1.824206	-6.383752
C49	1.420638	0.264679	-2.873609	1.395894	0.394886	-2.833266
C50	1.620870	-0.685537	-3.877888	1.736472	-0.449803	-3.895512
C51	1.530911	1.618557	-3.206878	1.304732	1.770332	-3.085129

C52	1.907067	-0.294014	-5.181304	1.970339	0.061487	-5.167209
H53	1.548678	-1.728702	-3.639460	1.799246	-1.507657	-3.730094
C54	1.816743	2.013001	-4.510155	1.543920	2.283525	-4.355406
H55	1.401445	2.360738	-2.441942	1.057702	2.435325	-2.279711
C56	2.006286	1.056920	-5.502805	1.878382	1.430483	-5.402518
H57	2.052458	-1.039422	-5.940073	2.220148	-0.606336	-5.969886
H58	1.899212	3.057641	-4.744620	1.475536	3.341993	-4.522971
H59	2.231066	1.357861	-6.508464	2.064207	1.824206	-6.383752
C60	1.420638	0.264679	2.873609	1.395894	0.394886	2.833266
C61	1.530911	1.618557	3.206878	1.304732	1.770332	3.085129
C62	1.620870	-0.685537	3.877888	1.736472	-0.449803	3.895512
C63	1.816743	2.013001	4.510155	1.543920	2.283525	4.355406
H64	1.401445	2.360738	2.441942	1.057702	2.435325	2.279711
C65	1.907067	-0.294014	5.181304	1.970339	0.061487	5.167209
H66	1.548678	-1.728702	3.639460	1.799246	-1.507657	3.730094
C67	2.006286	1.056920	5.502805	1.878382	1.430483	5.402518
H68	1.899212	3.057641	4.744620	1.475536	3.341993	4.522971
H69	2.052458	-1.039422	5.940073	2.220148	-0.606336	5.969886
H70	2.231066	1.357861	6.508464	2.064207	1.824206	6.383752

Table S3-8: Local minima with $C_{2H}(2)$ symmetry in benzene solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	4.842522	0.783777	0.712127	4.836723	0.949675	0.696798
C2	3.688694	0.570182	1.393829	3.667966	0.664243	1.384765
C3	2.428744	0.373102	0.719840	2.450152	0.412456	0.716425
C4	2.428744	0.373102	-0.719840	2.450152	0.412456	-0.716425
C5	3.688694	0.570182	-1.393829	3.667966	0.664243	-1.384765
C6	4.842522	0.783777	-0.712127	4.836723	0.949675	-0.696798
C7	1.248583	0.100926	1.424449	1.242875	0.071644	1.419273
C8	1.248583	0.100926	-1.424449	1.242875	0.071644	-1.419273
C9	0.000000	0.000000	-0.734575	0.000000	0.000000	-0.735018
C10	0.000000	0.000000	0.734575	0.000000	0.000000	0.735018
C11	-1.248583	-0.100926	1.424449	-1.242875	-0.071644	1.419273
C12	-2.428744	-0.373102	0.719840	-2.450152	-0.412456	0.716425
C13	-2.428744	-0.373102	-0.719840	-2.450152	-0.412456	-0.716425
C14	-1.248583	-0.100926	-1.424449	-1.242875	-0.071644	-1.419273
H15	5.761159	0.944239	1.243503	5.739672	1.149375	1.241198
H16	3.707847	0.557416	2.461557	3.698824	0.627963	2.451839
H17	3.707847	0.557416	-2.461557	3.698824	0.627963	-2.451839
H18	5.761159	0.944239	-1.243503	5.739672	1.149375	-1.241198
C19	-3.688694	-0.570182	1.393829	-3.667966	-0.664243	1.384765
C20	-4.842522	-0.783777	0.712127	-4.836723	-0.949675	0.696798
C21	-4.842522	-0.783777	-0.712127	-4.836723	-0.949675	-0.696798
C22	-3.688694	-0.570182	-1.393829	-3.667966	-0.664243	-1.384765
H23	-3.707847	-0.557416	2.461557	-3.698824	-0.627963	2.451839
H24	-5.761159	-0.944239	1.243503	-5.739672	-1.149375	1.241198
H25	-5.761159	-0.944239	-1.243503	-5.739672	-1.149375	-1.241198
H26	-3.707847	-0.557416	-2.461557	-3.698824	-0.627963	-2.451839
C27	1.420638	-0.264682	2.873610	1.395894	-0.394886	2.833266
C28	1.530914	-1.618556	3.206882	1.304732	-1.770332	3.085129
C29	1.620868	0.685539	3.877888	1.736472	0.449803	3.895512
C30	1.816748	-2.012997	4.510163	1.543920	-2.283525	4.355406
H31	1.401449	-2.360742	2.441950	1.057702	-2.435325	2.279711
C32	1.907072	0.294021	5.181301	1.970339	-0.061487	5.167209
H33	1.548674	1.728703	3.639454	1.799246	1.507657	3.730094
C34	2.006293	-1.056914	5.502807	1.878382	-1.430483	5.402518
H35	1.899217	-3.057637	4.744627	1.475536	-3.341993	4.522971
H36	2.052464	1.039430	5.940070	2.220148	0.606336	5.969886
H37	2.231073	-1.357848	6.508468	2.064207	-1.824206	6.383752
C38	1.420638	-0.264682	-2.873610	1.395894	-0.394886	-2.833266
C39	1.620868	0.685539	-3.877888	1.736472	0.449803	-3.895512
C40	1.530914	-1.618556	-3.206882	1.304732	-1.770332	-3.085129
C41	1.907072	0.294021	-5.181301	1.970339	-0.061487	-5.167209
H42	1.548674	1.728703	-3.639454	1.799246	1.507657	-3.730094
C43	1.816748	-2.012997	-4.510163	1.543920	-2.283525	-4.355406
H44	1.401449	-2.360742	-2.441950	1.057702	-2.435325	-2.279711
C45	2.006293	-1.056914	-5.502807	1.878382	-1.430483	-5.402518
H46	2.052464	1.039430	-5.940070	2.220148	0.606336	-5.969886
H47	1.899217	-3.057637	-4.744627	1.475536	-3.341993	-4.522971
H48	2.231073	-1.357848	-6.508468	2.064207	-1.824206	-6.383752
C49	-1.420638	0.264682	-2.873610	-1.395894	0.394886	-2.833266
C50	-1.530914	1.618556	-3.206882	-1.304732	1.770332	-3.085129
C51	-1.620868	-0.685539	-3.877888	-1.736472	-0.449803	-3.895512

C52	-1.816748	2.012997	-4.510163	-1.543920	2.283525	-4.355406
H53	-1.401449	2.360742	-2.441950	-1.057702	2.435325	-2.279711
C54	-1.907072	-0.294021	-5.181301	-1.970339	0.061487	-5.167209
H55	-1.548674	-1.728703	-3.639454	-1.799246	-1.507657	-3.730094
C56	-2.006293	1.056914	-5.502807	-1.878382	1.430483	-5.402518
H57	-1.899217	3.057637	-4.744627	-1.475536	3.341993	-4.522971
H58	-2.052464	-1.039430	-5.940070	-2.220148	-0.606336	-5.969886
H59	-2.231073	1.357848	-6.508468	-2.064207	1.824206	-6.383752
C60	-1.420638	0.264682	2.873610	-1.395894	0.394886	2.833266
C61	-1.620868	-0.685539	3.877888	-1.736472	-0.449803	3.895512
C62	-1.530914	1.618556	3.206882	-1.304732	1.770332	3.085129
C63	-1.907072	-0.294021	5.181301	-1.970339	0.061487	5.167209
H64	-1.548674	-1.728703	3.639454	-1.799246	-1.507657	3.730094
C65	-1.816748	2.012997	4.510163	-1.543920	2.283525	4.355406
H66	-1.401449	2.360742	2.441950	-1.057702	2.435325	2.279711
C67	-2.006293	1.056914	5.502807	-1.878382	1.430483	5.402518
H68	-2.052464	-1.039430	5.940070	-2.220148	-0.606336	5.969886
H69	-1.899217	3.057637	4.744627	-1.475536	3.341993	4.522971
H70	-2.231073	1.357848	6.508468	-2.064207	1.824206	6.383752

Table S3-9: Local minima with $C_{2H}(1)$ symmetry in cyclohexane solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	-4.842561	0.783002	0.712105	-4.837590	0.945056	0.696802
C2	-3.688763	0.569614	1.393830	-3.668560	0.661032	1.384829
C3	-2.428828	0.372787	0.719817	-2.450533	0.410616	0.716393
C4	-2.428828	0.372787	-0.719817	-2.450533	0.410616	-0.716393
C5	-3.688763	0.569614	-1.393830	-3.668560	0.661032	-1.384829
C6	-4.842561	0.783002	-0.712105	-4.837590	0.945056	-0.696802
C7	-1.248608	0.100926	1.424378	-1.242975	0.071461	1.419146
C8	-1.248608	0.100926	-1.424378	-1.242975	0.071461	-1.419146
C9	0.000000	0.000000	-0.734564	0.000000	0.000000	-0.735045
C10	0.000000	0.000000	0.734564	0.000000	0.000000	0.735045
C11	1.248608	-0.100926	1.424378	1.242975	-0.071461	1.419146
C12	2.428828	-0.372787	0.719817	2.450533	-0.410616	0.716393
C13	2.428828	-0.372787	-0.719817	2.450533	-0.410616	-0.716393
C14	1.248608	-0.100926	-1.424378	1.242975	-0.071461	-1.419146
H15	-5.761242	0.943239	1.243498	-5.740816	1.143655	1.241163
H16	-3.707882	0.556665	2.461557	-3.699187	0.624638	2.451934
H17	-3.707882	0.556665	-2.461557	-3.699187	0.624638	-2.451934
H18	-5.761242	0.943239	-1.243498	-5.740816	1.143655	-1.241163
C19	3.688763	-0.569614	1.393830	3.668560	-0.661032	1.384829
C20	4.842561	-0.783002	0.712105	4.837590	-0.945056	0.696802
C21	4.842561	-0.783002	-0.712105	4.837590	-0.945056	-0.696802
C22	3.688763	-0.569614	-1.393830	3.668560	-0.661032	-1.384829
H23	3.707882	-0.556665	2.461557	3.699187	-0.624638	2.451934
H24	5.761242	-0.943239	1.243498	5.740816	-1.143655	1.241163
H25	5.761242	-0.943239	-1.243498	5.740816	-1.143655	-1.241163
H26	3.707882	-0.556665	-2.461557	3.699187	-0.624638	-2.451934
C27	-1.420631	-0.264208	2.873648	-1.395969	-0.392579	2.834034
C28	-1.619662	0.686386	3.877778	-1.731686	0.455176	3.895270
C29	-1.531901	-1.617879	3.207327	-1.309350	-1.767829	3.087988
C30	-1.905396	0.295428	5.181428	-1.964065	-0.052920	5.168465
H31	-1.546683	1.729409	3.638998	-1.791457	1.512870	3.727767
C32	-1.817302	-2.011748	4.510831	-1.547374	-2.277866	4.359735
H33	-1.403552	-2.360265	2.442408	-1.066495	-2.435020	2.283109
C34	-2.005429	-1.055302	5.503333	-1.876084	-1.421730	5.406065
H35	-2.049608	1.041144	5.940117	-2.209632	0.617214	5.970523
H36	-1.900568	-3.056264	4.745604	-1.482429	-3.336278	4.529086
H37	-2.229802	-1.355808	6.509217	-2.060733	-1.812991	6.388515
C38	-1.420631	-0.264208	-2.873648	-1.395969	-0.392579	-2.834034
C39	-1.531901	-1.617879	-3.207327	-1.309350	-1.767829	-3.087988
C40	-1.619662	0.686386	-3.877778	-1.731686	0.455176	-3.895270
C41	-1.817302	-2.011748	-4.510831	-1.547374	-2.277866	-4.359735
H42	-1.403552	-2.360265	-2.442408	-1.066495	-2.435020	-2.283109
C43	-1.905396	0.295428	-5.181428	-1.964065	-0.052920	-5.168465
H44	-1.546683	1.729409	-3.638998	-1.791457	1.512870	-3.727767
C45	-2.005429	-1.055302	-5.503333	-1.876084	-1.421730	-5.406065
H46	-1.900568	-3.056264	-4.745604	-1.482429	-3.336278	-4.529086
H47	-2.049608	1.041144	-5.940117	-2.209632	0.617214	-5.970523
H48	-2.229802	-1.355808	-6.509217	-2.060733	-1.812991	-6.388515
C49	1.420631	0.264208	-2.873648	1.395969	0.392579	-2.834034
C50	1.619662	-0.686386	-3.877778	1.731686	-0.455176	-3.895270
C51	1.531901	1.617879	-3.207327	1.309350	1.767829	-3.087988

C52	1.905396	-0.295428	-5.181428	1.964065	0.052920	-5.168465
H53	1.546683	-1.729409	-3.638998	1.791457	-1.512870	-3.727767
C54	1.817302	2.011748	-4.510831	1.547374	2.277866	-4.359735
H55	1.403552	2.360265	-2.442408	1.066495	2.435020	-2.283109
C56	2.005429	1.055302	-5.503333	1.876084	1.421730	-5.406065
H57	2.049608	-1.041144	-5.940117	2.209632	-0.617214	-5.970523
H58	1.900568	3.056264	-4.745604	1.482429	3.336278	-4.529086
H59	2.229802	1.355808	-6.509217	2.060733	1.812991	-6.388515
C60	1.420631	0.264208	2.873648	1.395969	0.392579	2.834034
C61	1.531901	1.617879	3.207327	1.309350	1.767829	3.087988
C62	1.619662	-0.686386	3.877778	1.731686	-0.455176	3.895270
C63	1.817302	2.011748	4.510831	1.547374	2.277866	4.359735
H64	1.403552	2.360265	2.442408	1.066495	2.435020	2.283109
C65	1.905396	-0.295428	5.181428	1.964065	0.052920	5.168465
H66	1.546683	-1.729409	3.638998	1.791457	-1.512870	3.727767
C67	2.005429	1.055302	5.503333	1.876084	1.421730	5.406065
H68	1.900568	3.056264	4.745604	1.482429	3.336278	4.529086
H69	2.049608	-1.041144	5.940117	2.209632	-0.617214	5.970523
H70	2.229802	1.355808	6.509217	2.060733	1.812991	6.388515

Table S3-10: Local minima with $C_{2H}(2)$ symmetry in cyclohexane solvent.

Center Number	Coordinates X	Y	Z	X'	Y'	Z'
C1	4.842555	0.783006	0.712106	4.837590	0.945056	0.696802
C2	3.688756	0.569624	1.393834	3.668560	0.661032	1.384829
C3	2.428825	0.372788	0.719818	2.450533	0.410616	0.716393
C4	2.428825	0.372788	-0.719818	2.450533	0.410616	-0.716393
C5	3.688756	0.569624	-1.393834	3.668560	0.661032	-1.384829
C6	4.842555	0.783006	-0.712106	4.837590	0.945056	-0.696802
C7	1.248607	0.100913	1.424378	1.242975	0.071461	1.419146
C8	1.248607	0.100913	-1.424378	1.242975	0.071461	-1.419146
C9	0.000000	0.000000	-0.734564	0.000000	0.000000	-0.735045
C10	0.000000	0.000000	0.734564	0.000000	0.000000	0.735045
C11	-1.248607	-0.100913	1.424378	-1.242975	-0.071461	1.419146
C12	-2.428825	-0.372788	0.719818	-2.450533	-0.410616	0.716393
C13	-2.428825	-0.372788	-0.719818	-2.450533	-0.410616	-0.716393
C14	-1.248607	-0.100913	-1.424378	-1.242975	-0.071461	-1.419146
H15	5.761239	0.943237	1.243495	5.740816	1.143655	1.241163
H16	3.707871	0.556672	2.461563	3.699187	0.624638	2.451934
H17	3.707871	0.556672	-2.461563	3.699187	0.624638	-2.451934
H18	5.761239	0.943237	-1.243495	5.740816	1.143655	-1.241163
C19	-3.688756	-0.569624	1.393834	-3.668560	-0.661032	1.384829
C20	-4.842555	-0.783006	0.712106	-4.837590	-0.945056	0.696802
C21	-4.842555	-0.783006	-0.712106	-4.837590	-0.945056	-0.696802
C22	-3.688756	-0.569624	-1.393834	-3.668560	-0.661032	-1.384829
H23	-3.707871	-0.556672	2.461563	-3.699187	-0.624638	2.451934
H24	-5.761239	-0.943237	1.243495	-5.740816	-1.143655	1.241163
H25	-5.761239	-0.943237	-1.243495	-5.740816	-1.143655	-1.241163
H26	-3.707871	-0.556672	-2.461563	-3.699187	-0.624638	-2.451934
C27	1.420623	-0.264219	2.873650	1.395969	-0.392579	2.834034
C28	1.531890	-1.617886	3.207335	1.309350	-1.767829	3.087988
C29	1.619656	0.686381	3.877779	1.731686	0.455176	3.895270
C30	1.817302	-2.011750	4.510842	1.547374	-2.277866	4.359735
H31	1.403542	-2.360279	2.442422	1.066495	-2.435020	2.283109
C32	1.905402	0.295429	5.181425	1.964065	-0.052920	5.168465
H33	1.546677	1.729402	3.638991	1.791457	1.512870	3.727767
C34	2.005440	-1.055301	5.503336	1.876084	-1.421730	5.406065
H35	1.900569	-3.056266	4.745616	1.482429	-3.336278	4.529086
H36	2.049622	1.041146	5.940112	2.209632	0.617214	5.970523
H37	2.229819	-1.355800	6.509220	2.060733	-1.812991	6.388515
C38	1.420623	-0.264219	-2.873650	1.395969	-0.392579	-2.834034
C39	1.619656	0.686381	-3.877779	1.731686	0.455176	-3.895270
C40	1.531890	-1.617886	-3.207335	1.309350	-1.767829	-3.087988
C41	1.905402	0.295429	-5.181425	1.964065	-0.052920	-5.168465
H42	1.546677	1.729402	-3.638991	1.791457	1.512870	-3.727767
C43	1.817302	-2.011750	-4.510842	1.547374	-2.277866	-4.359735
H44	1.403542	-2.360279	-2.442422	1.066495	-2.435020	-2.283109
C45	2.005440	-1.055301	-5.503336	1.876084	-1.421730	-5.406065
H46	2.049622	1.041146	-5.940112	2.209632	0.617214	-5.970523
H47	1.900569	-3.056266	-4.745616	1.482429	-3.336278	-4.529086
H48	2.229819	-1.355800	-6.509220	2.060733	-1.812991	-6.388515
C49	-1.420623	0.264219	-2.873650	-1.395969	0.392579	-2.834034
C50	-1.531890	1.617886	-3.207335	-1.309350	1.767829	-3.087988
C51	-1.619656	-0.686381	-3.877779	-1.731686	-0.455176	-3.895270

C52	-1.817302	2.011750	-4.510842	-1.547374	2.277866	-4.359735
H53	-1.403542	2.360279	-2.442422	-1.066495	2.435020	-2.283109
C54	-1.905402	-0.295429	-5.181425	-1.964065	0.052920	-5.168465
H55	-1.546677	-1.729402	-3.638991	-1.791457	-1.512870	-3.727767
C56	-2.005440	1.055301	-5.503336	-1.876084	1.421730	-5.406065
H57	-1.900569	3.056266	-4.745616	-1.482429	3.336278	-4.529086
H58	-2.049622	-1.041146	-5.940112	-2.209632	-0.617214	-5.970523
H59	-2.229819	1.355800	-6.509220	-2.060733	1.812991	-6.388515
C60	-1.420623	0.264219	2.873650	-1.395969	0.392579	2.834034
C61	-1.619656	-0.686381	3.877779	-1.731686	-0.455176	3.895270
C62	-1.531890	1.617886	3.207335	-1.309350	1.767829	3.087988
C63	-1.905402	-0.295429	5.181425	-1.964065	0.052920	5.168465
H64	-1.546677	-1.729402	3.638991	-1.791457	-1.512870	3.727767
C65	-1.817302	2.011750	4.510842	-1.547374	2.277866	4.359735
H66	-1.403542	2.360279	2.442422	-1.066495	2.435020	2.283109
C67	-2.005440	1.055301	5.503336	-1.876084	1.421730	5.406065
H68	-2.049622	-1.041146	5.940112	-2.209632	-0.617214	5.970523
H69	-1.900569	3.056266	4.745616	-1.482429	3.336278	4.529086
H70	-2.229819	1.355800	6.509220	-2.060733	1.812991	6.388515
