Supporting Information

Mesomerism Induced Temperature-Dependent Multicomponent Phosphorescence Emissions in ClBDBT

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States	M062X		LR-CC2
	ΔE	*f*	ΔE
T_1	3.24	-	3.43
T_2	3.56	-	3.74
S_1	3.73	0.0012	3.88
S_2	4.47	0.0086	4.29
S_3	4.63	0.1663	4.68
S_4	4.94	0.3619	4.87
S_5	5.17	0.4497	5.06

Table S2. The vertical excitation energies (ΔE in eV) and oscillator strengths (*f*) for several low-lying singlet and triplet excited states for $\mathbf{2_{FBDBT}}$ calculated at the M062x/6-311++G** and CC2/cc-pVDZ levels of theory, respectively.

States	M062X		CC2
	ΔE	*f*	ΔE
T_1	3.27	-	3.48
T_2	3.59	-	3.75
S_1	3.77	0.0016	3.92
S_2	4.47	0.0272	4.31
S_3	4.68	0.1505	4.72
S_4	4.95	0.2441	4.89
S_5	5.12	0.4172	5.07

Table S3. The vertical excitation energies (ΔE in eV) and oscillator strengths (*f*) for several low-lying singlet and triplet excited states for $\mathbf{4_{BrBDBT}}$ calculated at the M062x/6-311++G** and CC2/cc-pVDZ levels of theory, respectively.

States	M062X		CC2
	ΔE	*f*	ΔE
T_1	3.23	-	3.43

T_2	3.57	-	3.74
S_1	3.73	0.0017	3.87
S_2	4.46	0.0368	4.30
S_3	4.62	0.2075	4.65
S_4	4.91	0.2331	4.85
S_5	5.08	0.3890	4.97

Table S4. The vertical excitation energies (ΔE in eV) and oscillator strengths (*f*) for several low-lying singlet and triplet excited states for $\mathbf{5_{FBDBF}}$ calculated at the M062x/6-311++G** and CC2/cc-pVDZ levels of theory, respectively.

States	M062X		CC2
	ΔE	*f*	ΔE
T_1	3.30	-	3.52
T_2	3.65	-	3.81
S_1	3.79	0.0014	3.97
S_2	4.72	0.0293	4.55
S_3	4.93	0.1074	4.87
S_4	5.12	0.5554	5.09
S_5	5.32	0.1189	5.17

Table S5. The vertical excitation energies (ΔE in eV) and oscillator strengths (*f*) for several low-lying singlet and triplet excited states for $\mathbf{6_{ClBDBF}}$ calculated at the M062x/6-311++G** and CC2/cc-pVDZ levels of theory, respectively.

States	M062X		CC2
	ΔE	*f*	ΔE
T_1	3.27	-	3.48
T_2	3.65	-	3.81
S_1	3.76	0.0015	3.93
S_2	4.70	0.0318	4.55
S_3	4.92	0.0602	4.85
S_4	5.06	0.6702	5.01
S_5	5.23	0.0311	5.09

Table S6. The emission energies (ΔE, eV) and wavelength (λ, nm) of $\mathbf{1}_{\mathbf{BDBT}}$, $\mathbf{2}_{\mathbf{FBDBT}}$, $\mathbf{3}_{\mathbf{ClBDBT}}$, $\mathbf{4}_{\mathbf{BrBDBT}}$, $\mathbf{5}_{\mathbf{FBDBF}}$, and $\mathbf{6}_{\mathbf{ClBDBF}}$ with S_1, T_1, and T_2 states at the M062x/6-311G** and CC2/cc-pVDZ levels, respectively.

Systems	Method	S_1^{emi}	λ	T_1^{emi}	λ	T_2^{emi}	λ
$\mathbf{1}_{\mathbf{BDBT}}$	M062X	3.149	394	2.495	497	3.160	392
	CC2	3.173	391	2.512	494	3.333	372
$\mathbf{2}_{\mathbf{FBDBT}}$	M062X	3.189	389	2.508	494	2.565	483
	CC2	3.225	384	2.684	461	3.141	395
$\mathbf{3}_{\mathbf{ClBDBT}}$	M062X	3.136	395	2.495	497	2.690	461
	CC2	3.173	391	2.513	493	3.144	372
$\mathbf{4}_{\mathbf{BrBDBT}}$	M062X	3.137	395	2.480	500	2.690	461
	CC2	3.167	392	2.504	495	3.142	372
$\mathbf{5}_{\mathbf{FBDBF}}$	M062X	3.193	388	2.542	488	2.566	483
	CC2	3.229	384	2.72	456	3.14	395
$\mathbf{6}_{\mathbf{ClBDBF}}$	M062X	3.123	397	2.506	495	2.569	483
	CC2	3.163	392	2.675	463	3.071	404

II. Figs. S1-S27

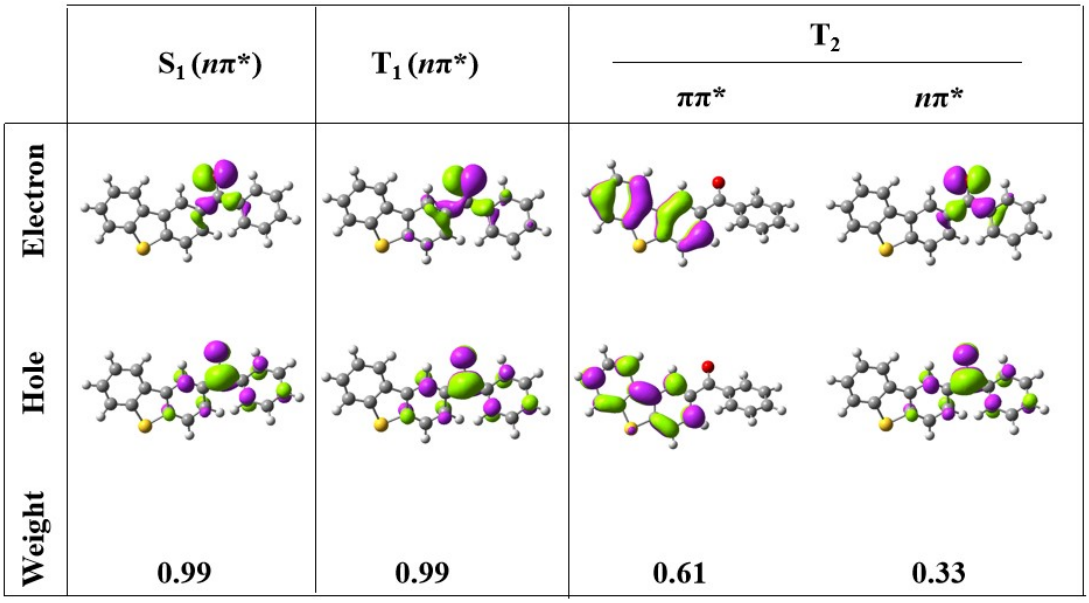


Fig. S1. Leading NTOs involved in S_1, T_1, and T_2 at their optimized structures for $\mathbf{1}_{\mathbf{BDBT}}$ with isovalue=0.04.

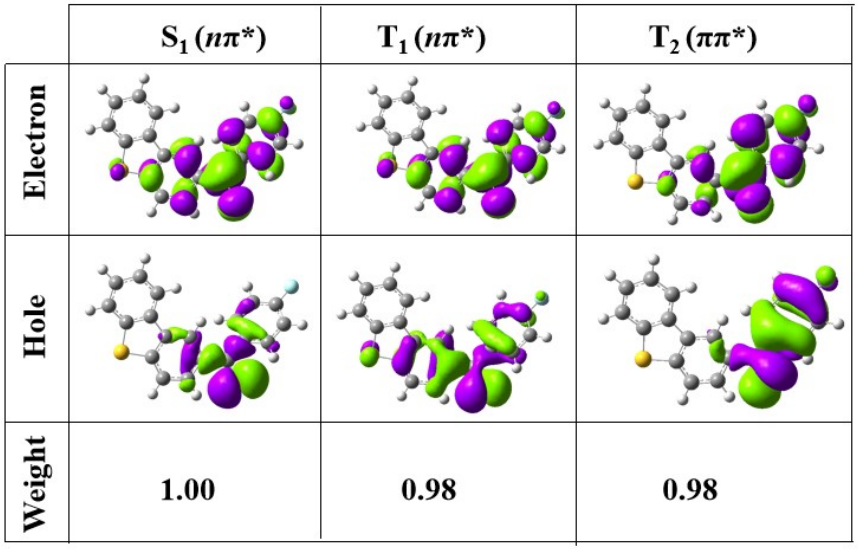


Fig. S2. Leading NTOs involved in S_1, T_1, and T_2 at their respective optimized structures for $\mathbf{2}_{\mathbf{FBDBT}}$ with isovalue=0.02.

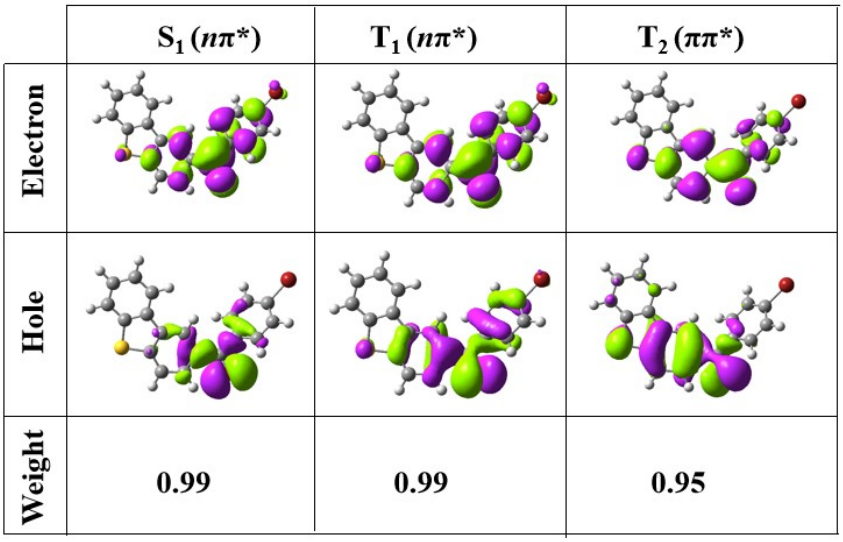


Fig. S3. Leading NTOs involved in S_1, T_1, and T_2 at their respective optimized structures for $\mathbf{4}_{\mathbf{BrBDBT}}$ with isovalue=0.02.

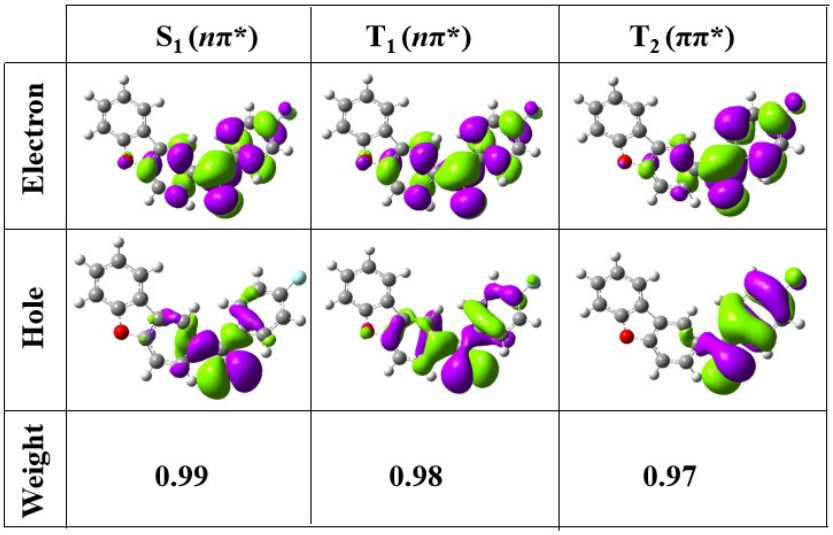


Fig. S4. Leading NTOs involved in S_1, T_1, and T_2 at their respective optimized structures for $\mathbf{5}_{\mathbf{FBDBF}}$ with isovalue=0.02.

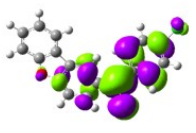
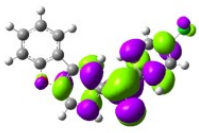
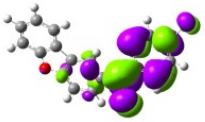
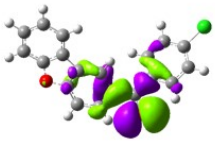
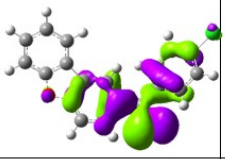
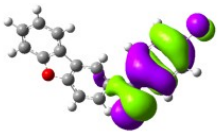
	S_1 ($n\pi^*$)	T_1 ($n\pi^*$)	T_2 ($\pi\pi^*$)
Electron			
Hole			
Weight	0.99	0.98	0.97

Fig. S5. Leading NTOs involved in S_1, T_1, and T_2 at their respective optimized structures for $\mathbf{6}_{\mathbf{ClBDBF}}$ with isovalue=0.02.

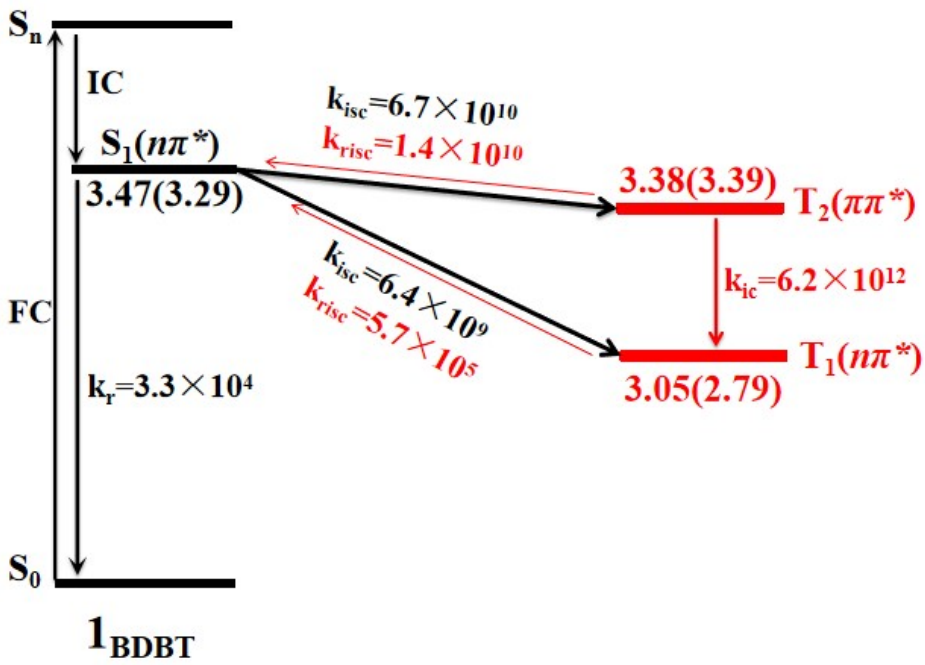


Fig. S6. The adiabatic energy levels, radiative (k_r) and nonradiative (k_{ic} and k_{isc}) rates for $\mathbf{1}_{\mathbf{BDBT}}$. The ground state energy of $\mathbf{1}_{\mathbf{BDBT}}$ is set to the zero-reference point, whose absolute energy at the CC2/cc-pVDZ level is -1201.70298913 a.u., respectively.

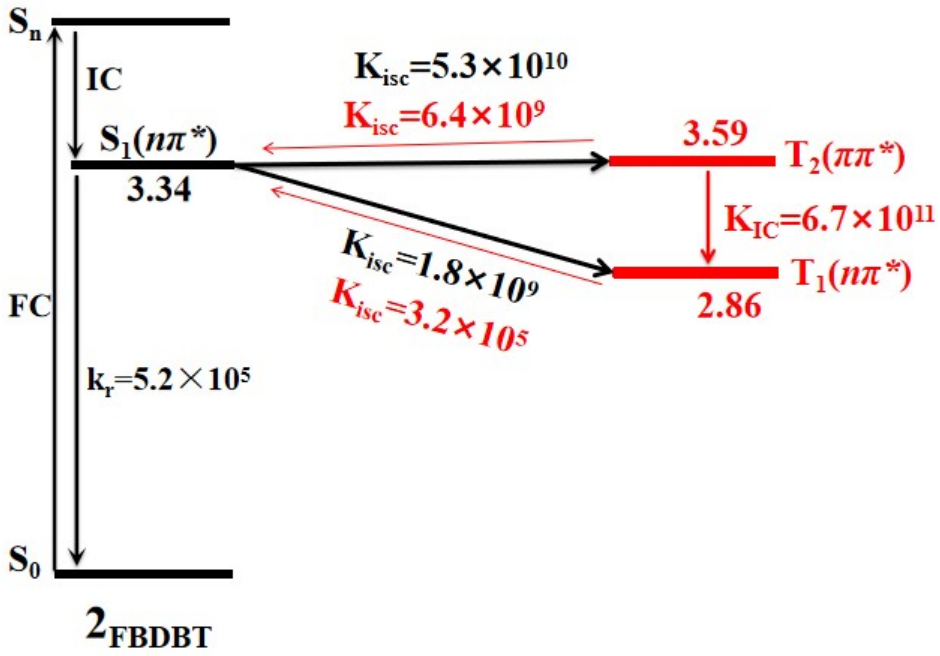


Fig. S7. The adiabatic energy levels, radiative (k_r) and nonradiative (k_{ic} and k_{isc}) rates for $\mathbf{2}_{\mathbf{FBDBT}}$. The ground state energy of $\mathbf{2}_{\mathbf{FBDBT}}$ is set to the zero-reference point, whose absolute energy CC2/cc-pVDZ level is -1300.73841865 a.u., respectively.

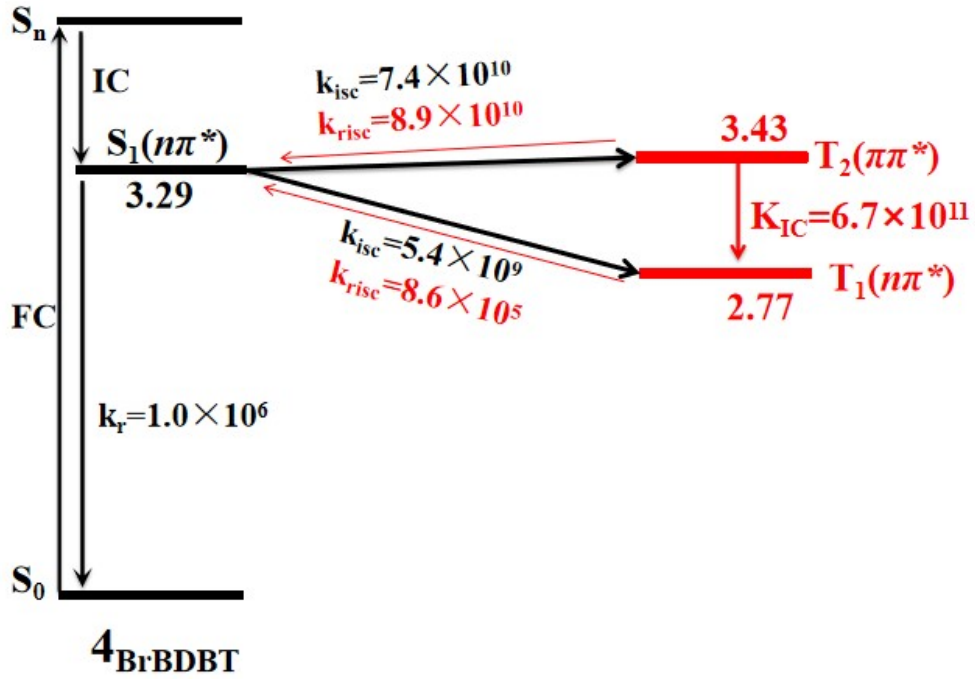


Fig. S8. The adiabatic energy levels, radiative (k_r) and nonradiative (k_{ic} and k_{isc}) rates for $\mathbf{4}_{\mathbf{BrBDBT}}$. The ground state energy of $\mathbf{4}_{\mathbf{BrBDBT}}$ is set to the zero-reference point, whose absolute energy CC2/cc-pVDZ level is -3772.94197071 a.u., respectively.

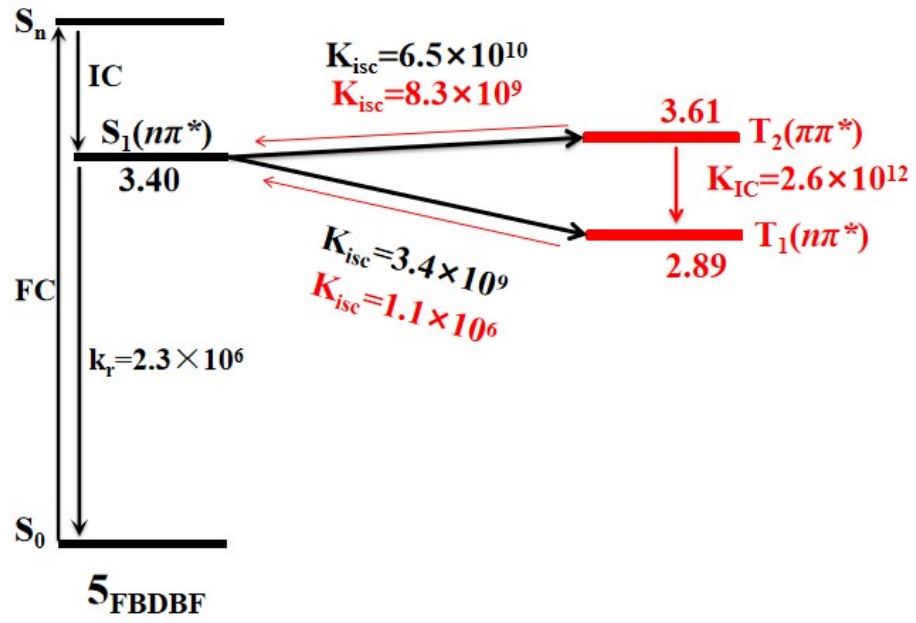


Fig. S9. The adiabatic energy levels, radiative (k_r) and nonradiative (k_{ic} and k_{isc}) rates for $\mathbf{5}_{\mathbf{FBDBF}}$. The ground state energy of $\mathbf{5}_{\mathbf{FBDBF}}$ is set to the zero-reference point, whose absolute energy CC2/cc-pVDZ level is -978.10881207 a.u., respectively.

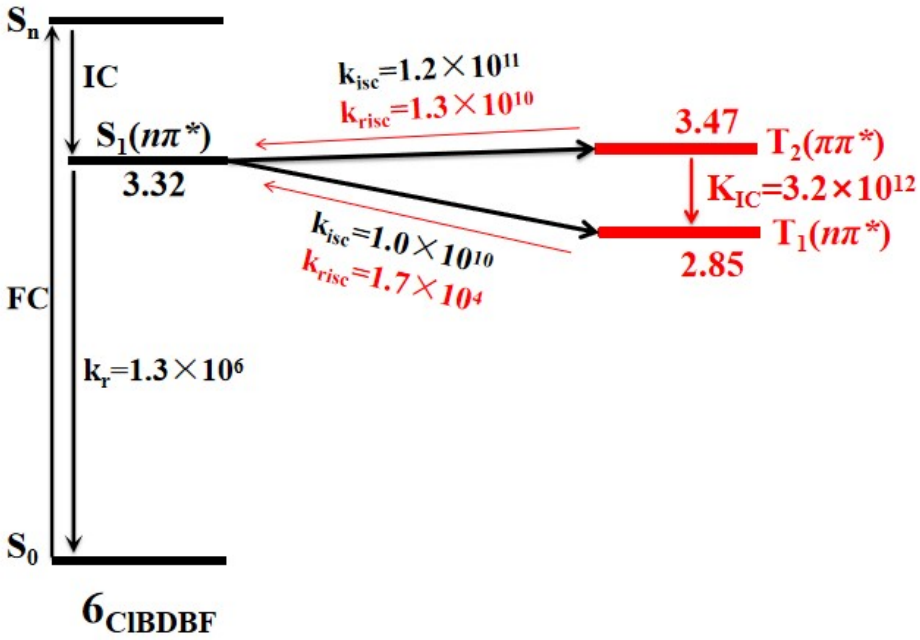


Fig. S10. The adiabatic energy levels, radiative (k_r) and nonradiative (k_{ic} and k_{isc}) rates for $\mathbf{6}_{\mathbf{ClBDBF}}$. The ground state energy of $\mathbf{6}_{\mathbf{ClBDBF}}$ is set to the zero-reference point, whose absolute energy CC2/cc-pVDZ level is -1338.12363822 a.u., respectively.

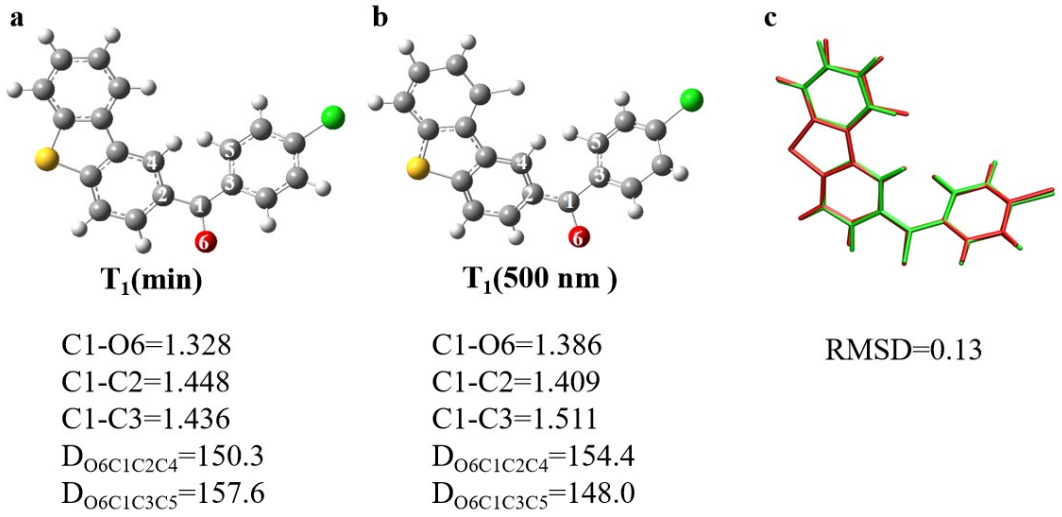


Fig. S11. A comparison of structures between T_1(min) and T_1(500 nm) for $\mathbf{3_{ClBDBT}}$: the minimum structure with the T_1 state in gas and b the structure with the emission wavelength of 500 nm at 0 K, and **c** a superposition between the two structures.

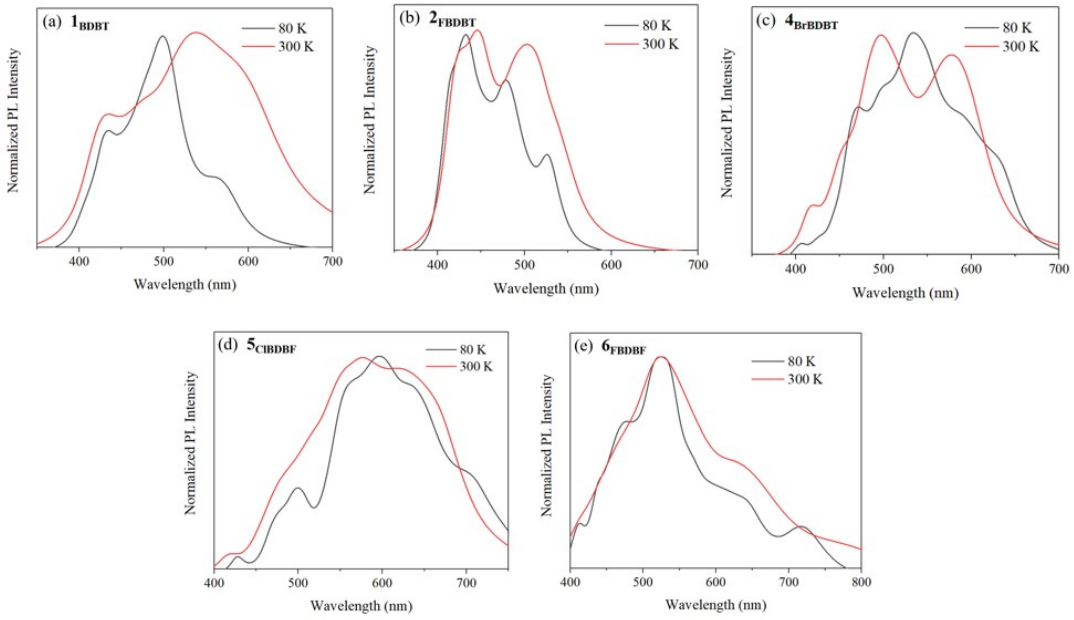


Fig. S12. The simulated phosphorescence spectra for (a) $\mathbf{1_{BDBT}}$, (b) $\mathbf{2_{FBDBT}}$, (c) $\mathbf{4_{BrBDBT}}$, (d) $\mathbf{5_{ClBDBF}}$ and (e) $\mathbf{6_{FBDBF}}$ with the temperature of 80 K (black line) and 300 K (red line).

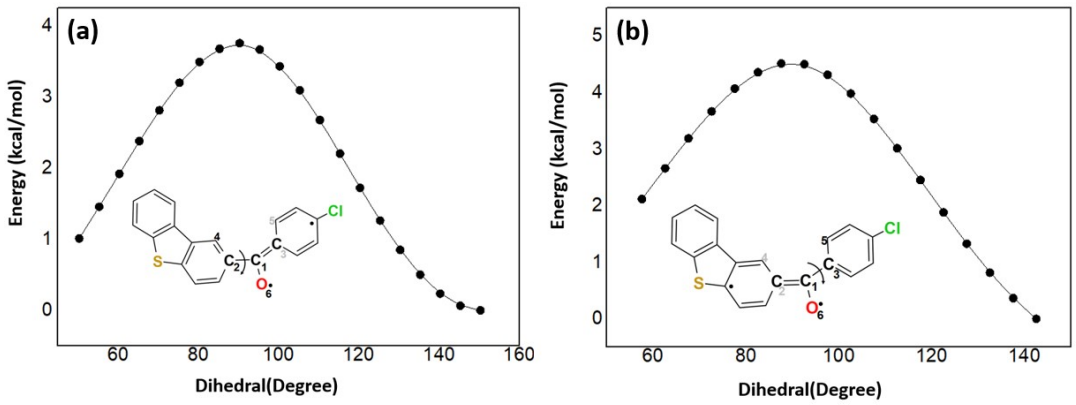


Fig. S13. The potential energy curves of $\mathbf{3_{ClBDBT}}$ by rotation of the dihedral of (a) $\angle C_4C_2C_1O_6$ and (b) $\angle C_5C_3C_1O_6$.

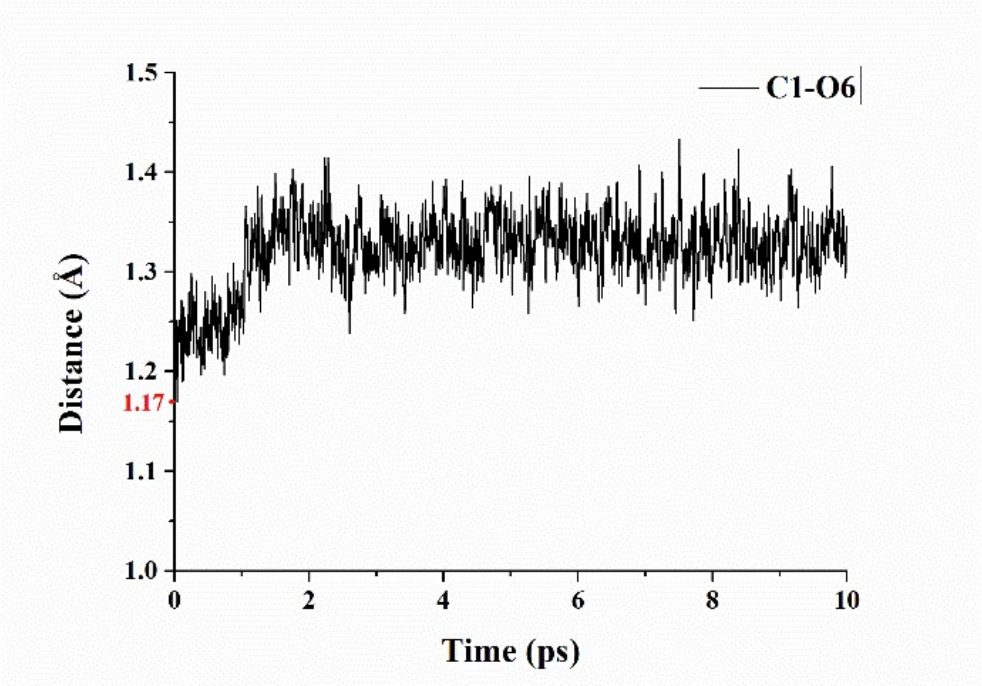


Fig. S14. Change curve of the distance between C1 and O6 atoms of $\mathbf{3_{ClBDBT}}$ in the QM/MM MD simulation. The red number indicates the initial value.

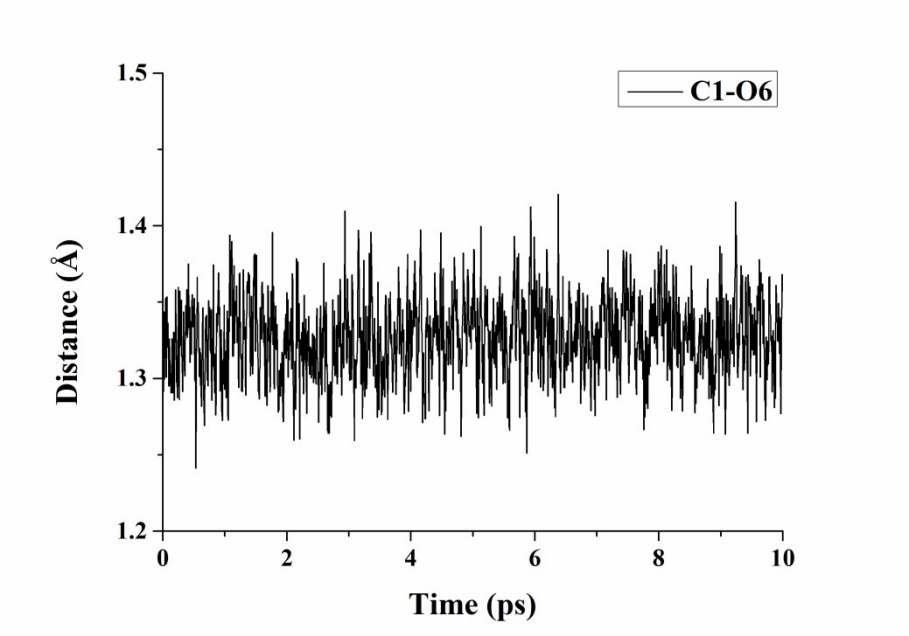


Fig. S15. Change curve of the distance between C1 and O6 atoms of $\mathbf{1_{BDBT}}$ in the QM/MM MD simulation.

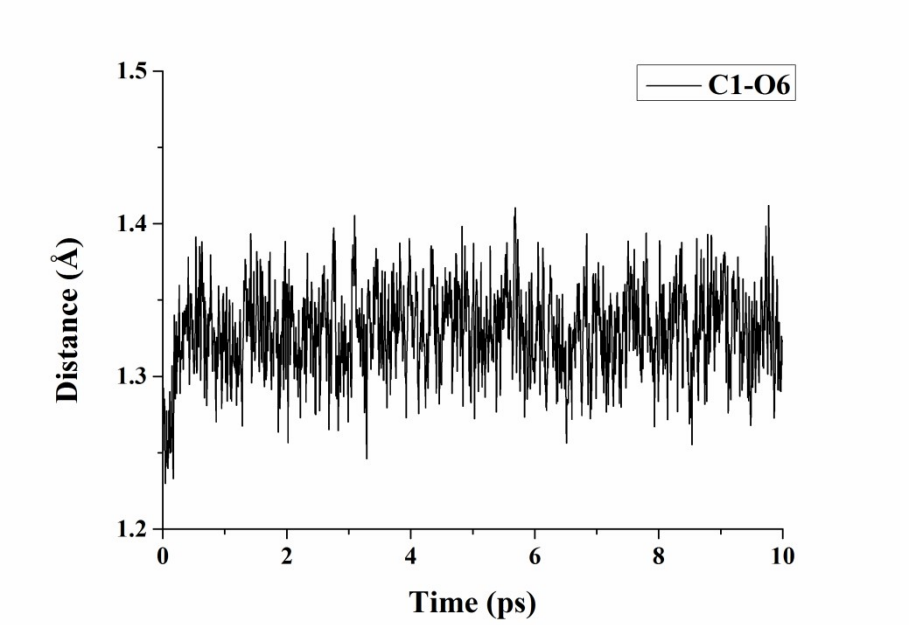


Fig. S16. Change curve of the distance between C1 and O6 atoms of $\mathbf{2_{FBDBT}}$ in the QM/MM MD simulation.

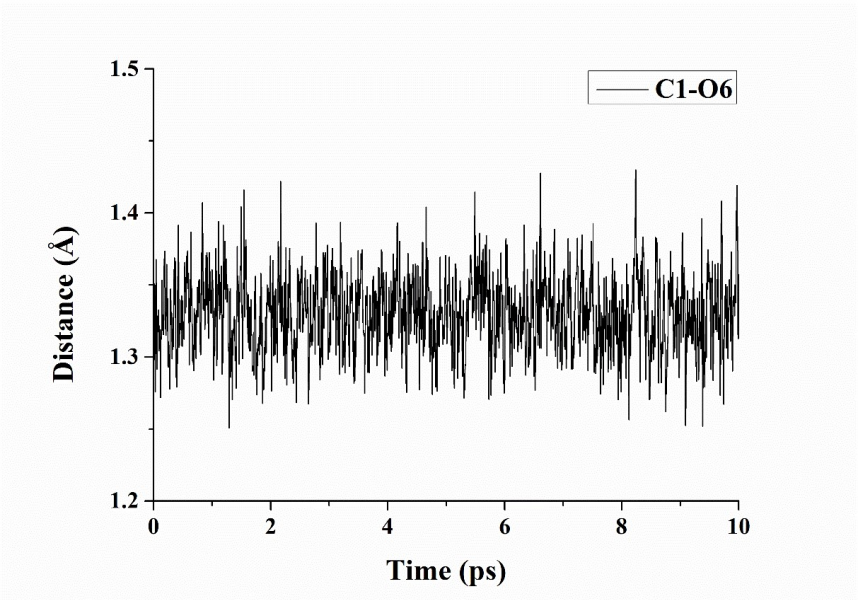


Fig. S17. Change curve of the distance between C1 and O6 atoms of $\mathbf{4_{BrBDBT}}$ in the QM/MM MD simulation.

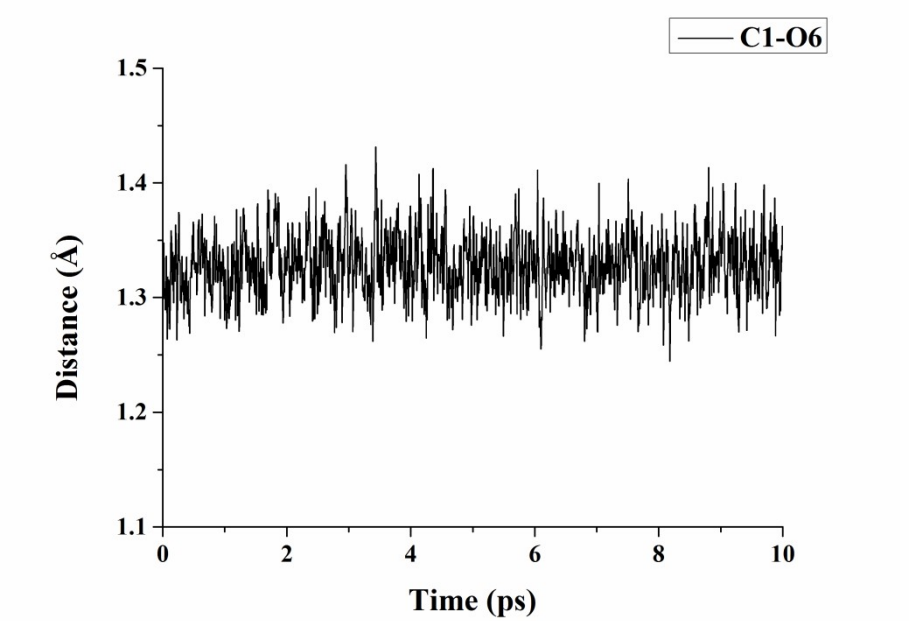


Fig. S18. Change curve of the distance between C1 and O6 atoms of $\mathbf{5_{FBDBF}}$ in the QM/MM MD simulation.

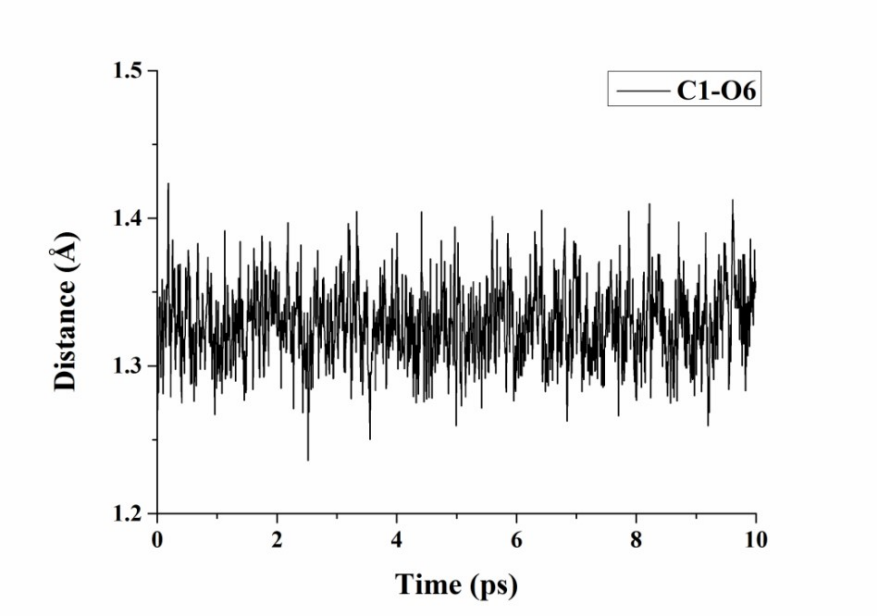


Fig. S19. Change curve of the distance between C1 and O6 atoms of $\mathbf{6}_{\mathbf{ClBDBF}}$ in the QM/MM MD simulation.

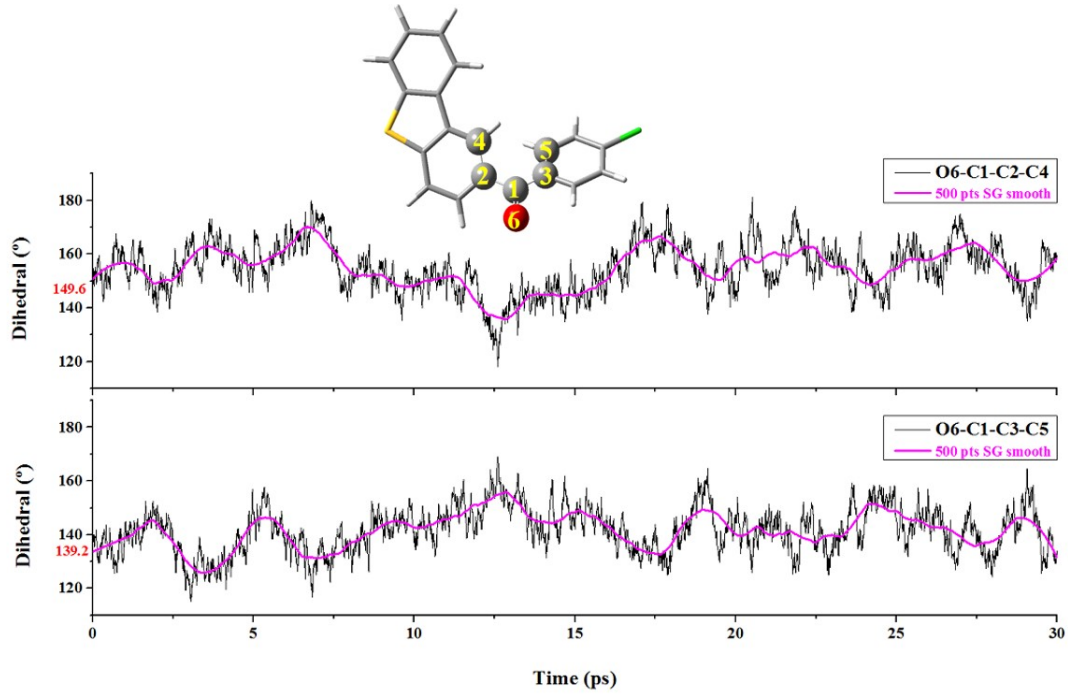


Fig. S20. Change curves of two dihedrals of $\mathbf{3}_{\mathbf{ClBDBT}}$ in the QM/MM MD simulation. Here we performed a total of 30 ps MD simulation for ClBDBT in order to evaluate the effect of simulation duration on the conformational sampling and determine the optimal step number of MD simulation for our research. The result shows that 10 ps MD simulation is enough for the sampling and thus the other molecules are subjected to 10ps simulation.

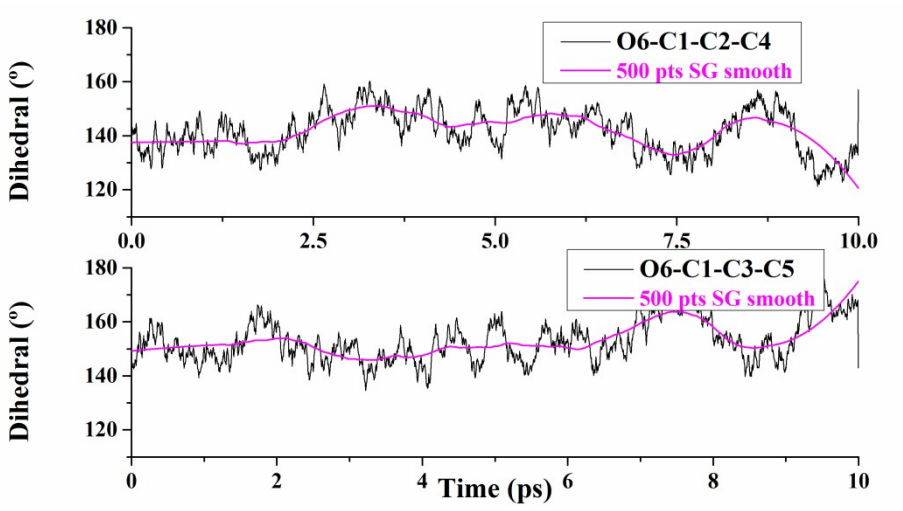


Fig. S21. Change curves of two dihedrals of $\mathbf{1}_{\mathbf{BDBT}}$ in the QM/MM MD simulation.

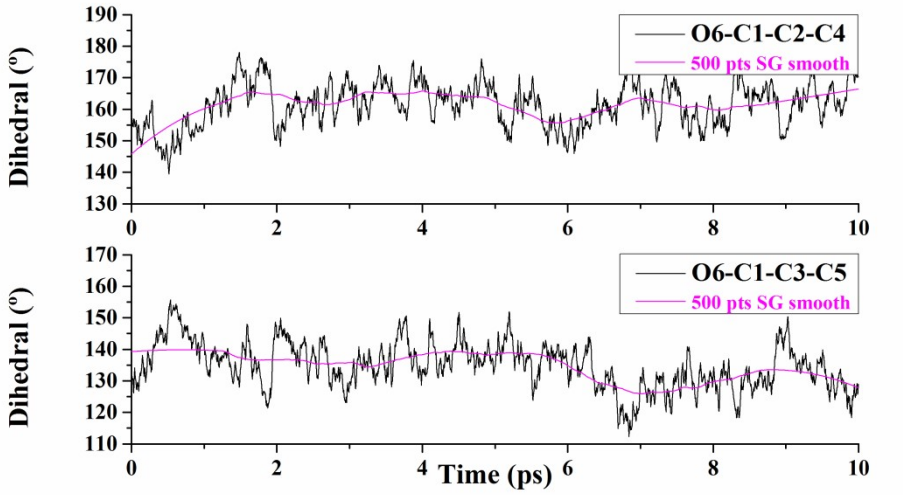


Fig. S22. Change curves of two dihedrals of $\mathbf{2}_{\mathbf{FBDBT}}$ in the QM/MM MD simulation.

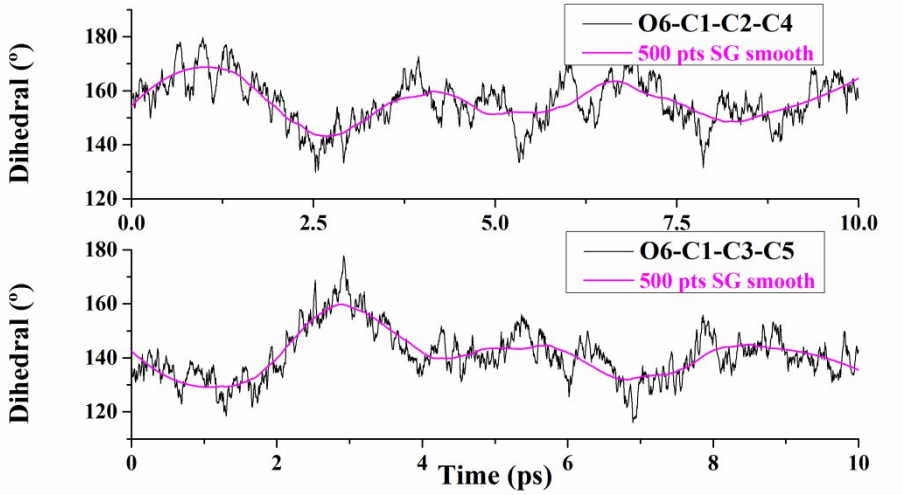


Fig. S23. Change curves of two dihedrals of $\mathbf{4}_{\mathbf{BrBDBT}}$ in the QM/MM MD simulation.

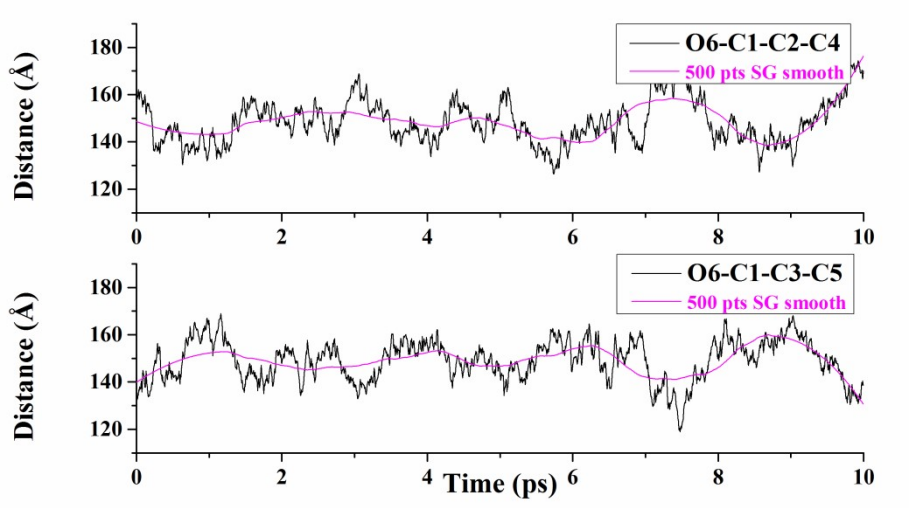


Fig. S24. Change curves of two dihedrals of $\mathbf{5}_{\mathbf{FBDBF}}$ in the QM/MM MD simulation.

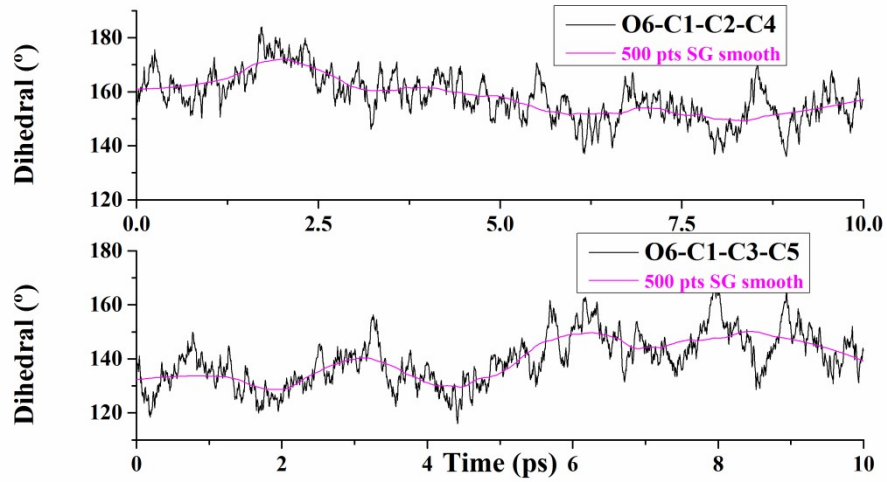


Fig. S25. Change curves of two dihedrals of $\mathbf{6}_{\mathbf{ClBDBF}}$ in the QM/MM MD simulation.

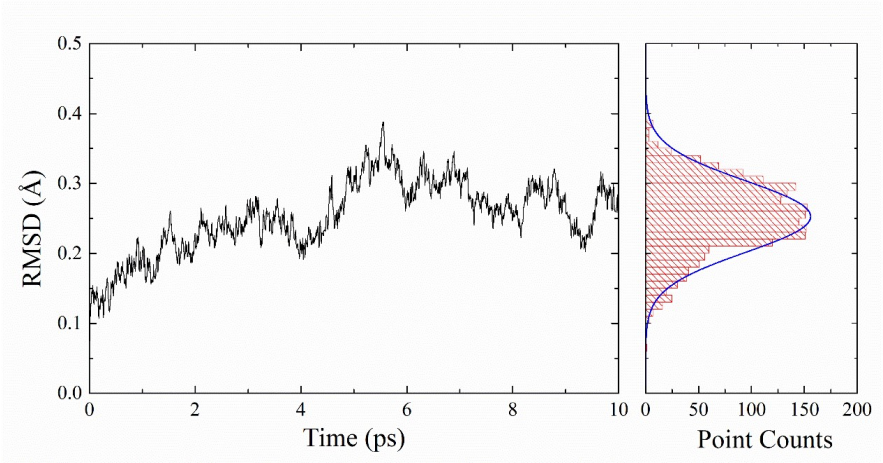


Fig. S26. Changes of $\mathbf{3}_{\mathbf{ClBDBT}}$'s RMSD values with the simulation time, as well as the corresponding distribution, in the QM/MM MD simulation.

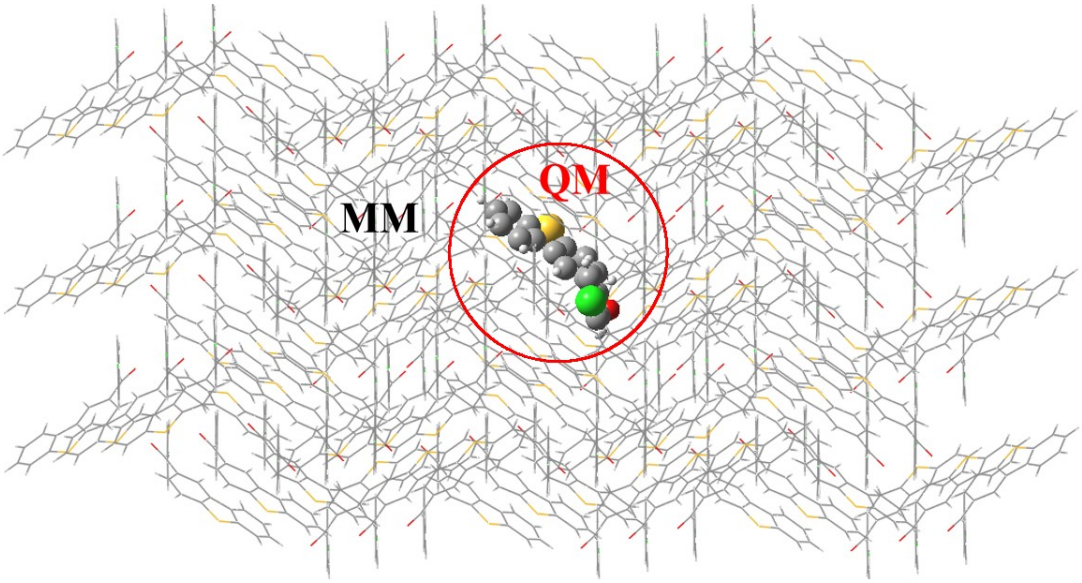


Fig. S27. A schematic QM/MM model for BDBTs.

III. Cartesian Coordinates of All Optimized Structures

In xyz format (unit: Ångstrom)

$3_{ClBDBT}(S_0)$

Cl	5.76672500	2.09896500	-0.42651600
S	-4.34376400	-0.96329100	-0.51052500
O	1.85014600	-3.15328800	0.73884700
C	-3.99482900	0.70374600	-0.07803900
C	-4.92001900	1.74319500	-0.01463000
H	-5.96458600	1.57039400	-0.24287700
C	-4.47114500	3.00219200	0.34973000
H	-5.17542800	3.82309600	0.40691000
C	-3.12118700	3.22492700	0.64590800
H	-2.79200800	4.21643400	0.93060200
C	-2.20650700	2.18876100	0.57973200
H	-1.16188400	2.36477900	0.81047200
C	-2.63793700	0.91042900	0.21447300
C	-1.86420500	-0.31253000	0.08072900
C	-0.49590500	-0.50650400	0.27477000
H	0.12910200	0.32370100	0.58393500
C	0.05342000	-1.77124600	0.10119400
C	-0.76913300	-2.85399200	-0.25359600
H	-0.31461700	-3.83224300	-0.35126400
C	-2.12142000	-2.67886100	-0.46974700
H	-2.74916700	-3.51351900	-0.75641300
C	-2.66313900	-1.40280800	-0.30190800
C	1.49841800	-2.05671600	0.36752500
C	2.51508000	-0.97091700	0.17122700
C	2.37710200	0.01809600	-0.80317300
H	1.49584300	0.04123900	-1.43317800
C	3.37905200	0.96041400	-0.99801000
H	3.28682200	1.72252800	-1.76065900

C	4.51316300	0.91200800	-0.19945000
C	4.67566000	-0.06996700	0.77153700
H	5.57429100	-0.08844000	1.37427200
C	3.67835100	-1.01713400	0.94097900
H	3.78745300	-1.80998700	1.67109000

$3_{ClBDBT}(S_1)$

Cl	5.90063642	2.04653815	-0.47217403
S	-4.34750631	-1.00802307	-0.60049604
O	1.79646113	-3.06206022	0.89558106
C	-4.05784629	0.65446505	-0.11106201
C	-5.01347536	1.66582012	-0.04869100
H	-6.04552844	1.47032810	-0.31298802
C	-4.61205433	2.92667021	0.36258903
H	-5.34110440	3.72573127	0.41994603
C	-3.27879524	3.17920023	0.70562005
H	-2.98614222	4.17180330	1.02431308
C	-2.33349617	2.17047516	0.64112905
H	-1.30120609	2.36909017	0.90660106
C	-2.71734120	0.89109106	0.23046102
C	-1.90426414	-0.30677502	0.09306501
C	-0.54589604	-0.46631503	0.35379403
H	0.03873300	0.36159303	0.73716505
C	0.05801800	-1.70668212	0.13815501
C	-0.72337205	-2.80318420	-0.28631502
H	-0.24578002	-3.76216727	-0.44179703
C	-2.07603315	-2.65939119	-0.52776004
H	-2.66596619	-3.50493025	-0.85970806
C	-2.66229419	-1.40784410	-0.34548902
C	1.49395311	-1.90284114	0.40496803
C	2.54703518	-0.92850806	0.19851601
C	2.37076517	0.17077801	-0.66282505
H	1.43906411	0.29388602	-1.20016708
C	3.39429125	1.07990708	-0.86216106

H	3.25942423	1.91984114	-1.53150111
C	4.61313533	0.89944906	-0.21593402
C	4.81964435	-0.18760801	0.62255805
H	5.77645144	-0.31582302	1.11219208
C	3.79462827	-1.09548408	0.82953306
H	3.95003928	-1.93499214	1.49529011

$3_{ClBDBT}(T_1)$

Cl	5.96915144	2.01293915	-0.38084303
S	-4.38478532	-1.03748608	-0.49100704
O	1.83138713	-3.07683022	0.71855105
C	-4.08809229	0.64559905	-0.08380901
C	-5.04824136	1.65291912	-0.02452800
H	-6.08825542	1.44080510	-0.24062402
C	-4.64082233	2.93154321	0.32042002
H	-5.37320038	3.72778127	0.37489803
C	-3.29715324	3.20557123	0.60091304
H	-3.00044421	4.21175730	0.86963406
C	-2.34732717	2.20090916	0.53854204
H	-1.30715209	2.41605117	0.75621805
C	-2.73683320	0.90386506	0.19402701
C	-1.91962914	-0.29328302	0.07105901
C	-0.55217404	-0.43285103	0.27986202
H	0.03841200	0.41411003	0.60861804
C	0.05897600	-1.68135512	0.09854301
C	-0.74012805	-2.80048420	-0.24558102
H	-0.26453302	-3.76385827	-0.38117503
C	-2.09975015	-2.67300319	-0.43793403
H	-2.69677919	-3.53445425	-0.71150005
C	-2.68818919	-1.41621310	-0.28824002
C	1.47913111	-1.86101313	0.31589502
C	2.53995418	-0.90597707	0.15927601
C	2.40281917	0.22540002	-0.67368305
H	1.48256811	0.38132703	-1.22237809

C	3.44632125	1.11738108	-0.82978806
H	3.34042024	1.98225914	-1.47211810
C	4.65463233	0.88713906	-0.17634601
C	4.82892035	-0.23343002	0.62726505
H	5.77711640	-0.39689003	1.12306208
C	3.78291827	-1.12263708	0.79415506
H	3.90974728	-1.98492414	1.43709810

$3_{ClBDBT}(T_2)$

Cl	-5.90247045	2.04818215	-0.02656200
S	4.42491832	-1.00994907	0.01092000
O	-1.84978713	-3.22862623	0.17939601
C	4.04351229	0.71042605	-0.05150500
C	4.96771736	1.74715613	-0.09406501
H	6.03156043	1.54458711	-0.08914601
C	4.49132733	3.05076622	-0.14406901
H	5.19477137	3.87347428	-0.17941301
C	3.11890823	3.31087124	-0.15020901
H	2.76745220	4.33417131	-0.19150901
C	2.20396716	2.26952016	-0.10453501
H	1.13962208	2.47472918	-0.11067001
C	2.66174319	0.95290807	-0.05363700
C	1.88895013	-0.28241002	0.00567100
C	0.52125504	-0.43530803	0.02955900
H	-0.11821301	0.43511803	-0.02356700
C	-0.05388000	-1.74692413	0.04500200
C	0.84209306	-2.88169221	0.04540000
H	0.40480803	-3.87012528	0.01769100
C	2.19870616	-2.72467520	0.04719800
H	2.85133421	-3.58898926	0.03152200
C	2.74013020	-1.42178210	0.04049000
C	-1.45448810	-1.99356414	0.06375700
C	-2.51604918	-0.95815407	0.04278400
C	-2.48352018	0.17317501	0.86581306

H	-1.66108212	0.31607602	1.55608511
C	-3.51805025	1.09871808	0.84467106
H	-3.49544825	1.97053814	1.48562711
C	-4.60273533	0.88573406	0.00525600
C	-4.67499034	-0.24271202	-0.79989506
H	-5.53522339	-0.39605003	-1.43840311
C	-3.63404026	-1.15899508	-0.77401606
H	-3.68133526	-2.04279615	-1.39858010

$1_{BDBT}(S_0)$

S	6.43369679	2.25553031	13.60610570
O	1.98291639	1.03192831	18.37096645
C	5.22329402	1.29239732	12.77123766
C	5.21293645	0.99352371	11.41083749
H	5.99222795	1.36305883	10.75567630
C	4.18046633	0.21229781	10.91730680
H	4.15463536	-0.03160021	9.86222556
C	3.17331651	-0.26486001	11.76398829
H	2.37610361	-0.87429474	11.35696881
C	3.18888953	0.03600640	13.11485986
H	2.40882220	-0.33445782	13.77003082
C	4.22106359	0.82244694	13.63329746
C	4.43785377	1.25644314	15.00384492
C	3.66594859	1.00233907	16.13407740
H	2.74909678	0.42711529	16.07266607
C	4.06253920	1.49535798	17.37168904
C	5.22134778	2.28243863	17.47613214
H	5.50457467	2.69602432	18.43638214
C	5.99033858	2.56558512	16.36016760
H	6.87402980	3.18616263	16.44185727
C	5.59983320	2.03939228	15.13044376
C	3.16569215	1.22569104	18.54162344
C	3.73956850	1.19272955	19.92694442
C	2.90003054	1.53927010	20.98693008

H	1.88693005	1.85084376	20.76302994
C	3.36253514	1.47759124	22.29301565
H	2.71204036	1.76000970	23.11186508
C	4.66015781	1.04260022	22.55112806
H	5.01954789	0.98691662	23.57184288
C	5.49206815	0.66954316	21.50156090
H	6.49460392	0.31240340	21.70411198
C	5.03714169	0.75054085	20.19018509
H	5.68175272	0.44602505	19.37400095

$1_{BDBT}(S_1)$

S	6.47173859	2.18863903	13.56348275
O	2.01402075	1.16288226	18.33427258
C	5.22432917	1.26070069	12.74703549
C	5.18972432	0.95599325	11.38794164
H	5.97248867	1.30005130	10.72308261
C	4.13002124	0.20344341	10.90873907
H	4.08602092	-0.04415667	9.85513349
C	3.11843890	-0.24047987	11.76849755
H	2.29963724	-0.82849433	11.37297324
C	3.15739949	0.06619153	13.11741511
H	2.37282081	-0.27914620	13.78094044
C	4.21734324	0.82444197	13.62236761
C	4.46081505	1.25929977	14.98831658
C	3.69555075	1.01618575	16.12784320
H	2.79095247	0.42410130	16.06244915
C	4.11124825	1.51498524	17.36596883
C	5.28961559	2.29203097	17.44528518
H	5.57834260	2.72533138	18.39432670
C	6.05857817	2.52643781	16.32403968
H	6.96054242	3.12187770	16.39648451
C	5.64420621	2.00599678	15.09604115
C	3.28406058	1.28872695	18.55599567
C	3.74987322	1.20764124	19.93455736

C	2.85271716	1.44304301	20.99151903
H	1.82899808	1.71783344	20.77035696
C	3.28122878	1.34837943	22.30669175
H	2.57936792	1.53811274	23.11012081
C	4.60155206	1.02149670	22.59831835
H	4.93366917	0.95286296	23.62663497
C	5.49180089	0.77283717	21.55546811
H	6.51661860	0.49549415	21.77248275
C	5.07673950	0.85233410	20.23615070
H	5.76553922	0.61192508	19.43606697

$1_{BDBT}(T_1)$

S	6.45343731	2.20781663	13.55885114
O	2.06393982	1.00990306	18.32107640
C	5.20764052	1.28274118	12.73494159
C	5.16394287	1.00373029	11.37113018
H	5.93912121	1.36400545	10.70608477
C	4.10360936	0.25435160	10.88697115
H	4.05121578	0.02675306	9.82933412
C	3.10190537	-0.21016987	11.74709087
H	2.28195172	-0.79392139	11.34772838
C	3.15109100	0.07086278	13.10169935
H	2.37381326	-0.28918402	13.76580940
C	4.21137859	0.82464983	13.61144153
C	4.46288897	1.23767493	14.98358795
C	3.71272945	0.96852570	16.12183348
H	2.81083146	0.37260772	16.06329216
C	4.14221358	1.44421446	17.37954111
C	5.31548154	2.24517243	17.44933316
H	5.60760868	2.66840326	18.40226526
C	6.06864138	2.50094800	16.32845015
H	6.96597529	3.10384274	16.39716759
C	5.64469126	1.99258066	15.09062227
C	3.33844936	1.18733145	18.55294086

C	3.77599159	1.16806117	19.93697428
C	2.85893957	1.45336246	20.96845736
H	1.84249839	1.71960653	20.70834064
C	3.26324531	1.42037722	22.29301377
H	2.55052474	1.65472918	23.07478667
C	4.57728884	1.09854720	22.62374532
H	4.89003413	1.07686199	23.66024226
C	5.48648679	0.79163415	21.61014270
H	6.50473937	0.51961771	21.86172563
C	5.09278541	0.80746008	20.28358530
H	5.79090807	0.52390236	19.50479325

$1_{BDBT}(T_2)$

S	3.02376100	2.07840100	-0.26012800
O	-2.09618700	-2.21278400	-0.65898700
C	3.78287400	0.51765900	0.03974900
C	5.12295900	0.27867300	0.21144300
H	5.84492500	1.08434000	0.16632700
C	5.54876200	-1.05140000	0.44966800
H	6.60276600	-1.25419200	0.58768200
C	4.61873800	-2.10569900	0.50881100
H	4.97306400	-3.11263700	0.69241300
C	3.27350800	-1.87717600	0.33666600
H	2.56004400	-2.69043300	0.38181100
C	2.81229700	-0.54041600	0.09489400
C	1.50200100	-0.08454900	-0.10489300
C	0.28812200	-0.83728000	-0.11785600
H	0.30189000	-1.91012400	0.02619700
C	-0.92083600	-0.19061400	-0.32155700
C	-0.95740200	1.20072700	-0.53895600
H	-1.89994400	1.68916300	-0.74749900
C	0.23416800	1.96583200	-0.53706500
H	0.19106800	3.03284300	-0.71519500
C	1.43085000	1.33124000	-0.31667400

C	-2.16059500	-1.01574400	-0.36486300
C	-3.49081200	-0.43859200	-0.02855100
C	-4.62714800	-1.00018700	-0.62295500
H	-4.49881700	-1.80585100	-1.33505200
C	-5.88916200	-0.52043300	-0.30689900
H	-6.76279700	-0.95087200	-0.78134900
C	-6.03434900	0.50867200	0.61955800
H	-7.02095600	0.88061100	0.86820000
C	-4.90977100	1.05222500	1.23410600
H	-5.02113100	1.83953700	1.96902600
C	-3.64238000	0.58264100	0.91650500
H	-2.77173800	0.99198400	1.41458000

$2_{FBDBT}(S_0)$

S	3.94432000	-1.24031400	0.45332200
O	-2.44530200	-2.78288000	-0.75491000
C	3.75638500	0.46201800	0.06334200
C	4.77888700	1.40677100	0.00942100
H	5.80420400	1.12647700	0.21697200
C	4.45169600	2.71272100	-0.31711800
H	5.23286500	3.46144600	-0.36510500
C	3.12637800	3.07492800	-0.58593100
H	2.89294600	4.10131500	-0.84003000
C	2.11476000	2.13235600	-0.53024700
H	1.08949500	2.41563700	-0.73967000
C	2.42256500	0.80866600	-0.20296500
C	1.53324100	-0.33445600	-0.08481200
C	0.14976600	-0.38804100	-0.26244100
H	-0.39326300	0.50632400	-0.54615800
C	-0.51982500	-1.59574600	-0.10789600
C	0.19679500	-2.76254500	0.20957200
H	-0.35130100	-3.69303300	0.29040900
C	1.56253400	-2.72701800	0.40815500

H	2.10862400	-3.62623000	0.66506900
C	2.22529800	-1.50693100	0.26095000
C	-1.98964800	-1.73333000	-0.35955700
C	-2.89676400	-0.56393400	-0.12119100
C	-2.64868000	0.39497000	0.86303500
H	-1.75495200	0.32980800	1.47167000
C	-3.55848900	1.41877800	1.09426000
H	-3.39883000	2.16632400	1.86030600
C	-4.70515600	1.47080900	0.32108600
C	-4.98554800	0.52939600	-0.65715400
H	-5.90163700	0.61194600	-1.22753000
C	-4.07858300	-0.49716000	-0.86327500
H	-4.27093000	-1.26809600	-1.59923100
F	-5.57973400	2.46251400	0.53066900

$2_{FBDBT}(S_1)$

S	3.97692400	-1.25542300	0.41300600
O	-2.43346200	-2.79253900	-0.67751800
C	3.78787300	0.45367400	0.05544800
C	4.81244200	1.39638200	0.00501900
H	5.83950000	1.10878600	0.19318400
C	4.48580200	2.70957200	-0.29235100
H	5.26920500	3.45625500	-0.33657200
C	3.15852500	3.08161400	-0.53588600
H	2.92513800	4.11356300	-0.76640300
C	2.14464900	2.14097100	-0.48403100
H	1.11730300	2.43161300	-0.67221000
C	2.45202500	0.81039900	-0.18696700
C	1.55778200	-0.33156000	-0.07948100
C	0.17845700	-0.36994200	-0.26402500
H	-0.35490700	0.52561000	-0.55903400
C	-0.51091700	-1.57543600	-0.09914800
C	0.21041200	-2.75313300	0.20627200
H	-0.32784200	-3.68412000	0.33003700
C	1.58110000	-2.72651900	0.37083000

H	2.12031200	-3.63508700	0.60925300
C	2.25285700	-1.51238000	0.23681500
C	-1.95996600	-1.64999900	-0.28672000
C	-2.91795800	-0.56449300	-0.09632600
C	-2.65363000	0.49574900	0.78918300
H	-1.73242600	0.50719600	1.35753600
C	-3.57901100	1.51014300	0.96685300
H	-3.39291300	2.33251600	1.64583700
C	-4.78152300	1.45518500	0.27878900
C	-5.08642200	0.41279200	-0.57813600
H	-6.03964500	0.40684200	-1.09100700
C	-4.15393700	-0.59567100	-0.76609300
H	-4.37127600	-1.40704300	-1.44874300
F	-5.67632400	2.43854000	0.45665500

$2_{FBDBT}(T_1)$

S	3.97670900	-1.26248600	0.39224400
O	-2.42255400	-2.79103900	-0.65228100
C	3.79454700	0.45252300	0.04970600
C	4.82349600	1.38895700	0.00009100
H	5.85038000	1.09460600	0.17840900
C	4.50120000	2.70706700	-0.28423400
H	5.28808000	3.45008800	-0.32771000
C	3.17476800	3.08724600	-0.51497600
H	2.94462600	4.12220400	-0.73498200
C	2.15597100	2.15074100	-0.46368400
H	1.12866200	2.44789700	-0.64127100
C	2.45891600	0.81689700	-0.18041500
C	1.55869200	-0.32184700	-0.07653400
C	0.18366400	-0.35629800	-0.25661200
H	-0.35205500	0.54057800	-0.54520500
C	-0.51926500	-1.56445700	-0.08418200
C	0.21223800	-2.75352700	0.19655700
H	-0.33263400	-3.68118400	0.31075200

C	1.57930200	-2.72926400	0.35356600
H	2.12024600	-3.63894500	0.58380400
C	2.25524400	-1.51103900	0.22684600
C	-1.95243600	-1.63511000	-0.25167100
C	-2.91341600	-0.56193900	-0.08083400
C	-2.68553800	0.49150600	0.82844500
H	-1.77952800	0.49796500	1.42235200
C	-3.61544600	1.50245400	0.98540000
H	-3.45468700	2.32133600	1.67496500
C	-4.79858400	1.44746100	0.25970900
C	-5.07632000	0.40822200	-0.61385500
H	-6.01416900	0.40569100	-1.15443800
C	-4.13788400	-0.59532800	-0.78083800
H	-4.32726200	-1.40785800	-1.46981100
F	-5.70149600	2.42556900	0.41895200

$2_{FBDBT}(T_2)$

S	3.92876200	-1.32607700	0.62064500
O	-2.41389300	-2.52089600	-1.17931600
C	3.86556500	0.35945200	0.13414800
C	4.94554800	1.23874900	0.08932800
H	5.93911700	0.90990800	0.36809700
C	4.71821100	2.54205200	-0.32144400
H	5.54590100	3.23944500	-0.36360200
C	3.43405100	2.96677400	-0.68253000
H	3.27842100	3.98961500	-1.00218400
C	2.36466500	2.08971400	-0.63455000
H	1.37159300	2.42157600	-0.91568500
C	2.57111900	0.76973900	-0.22320100
C	1.60642000	-0.31028000	-0.09589000
C	0.23590900	-0.29044200	-0.36139300
H	-0.22026600	0.61052000	-0.75461200
C	-0.53066600	-1.43831300	-0.17477600
C	0.10315800	-2.62539900	0.24447700

H	-0.49265600	-3.52200200	0.36582900
C	1.45931400	-2.66594400	0.50518700
H	1.92990800	-3.58593400	0.82938300
C	2.20652800	-1.49988500	0.34421900
C	-1.97742700	-1.48306300	-0.47000000
C	-2.93732300	-0.49717400	-0.15434800
C	-2.63102300	0.73075800	0.53149300
H	-1.62749700	0.90572600	0.89194800
C	-3.61134900	1.64808600	0.79913800
H	-3.40161600	2.55974600	1.34447000
C	-4.92653100	1.40166000	0.37373800
C	-5.28194600	0.21975400	-0.27512600
H	-6.31731800	0.05752000	-0.54649400
C	-4.31404000	-0.72006800	-0.52836800
H	-4.57079500	-1.66004600	-0.99530900
F	-5.86499300	2.31570100	0.63130600

$4_{BrBDBT}(S_0)$

Br	-5.50163210	-1.38553478	-0.24477370
S	5.03204294	0.63559715	-0.52539062
O	-0.87408531	3.51399547	0.69087360
C	4.50416589	-0.97850306	-0.07764033
C	5.31142725	-2.11154705	-0.00574435
H	6.36863316	-2.05459729	-0.23397970
C	4.72819934	-3.31223164	0.36447411
H	5.33910597	-4.20470392	0.42482116
C	3.36164309	-3.38577293	0.65856621
H	2.92631636	-4.33463188	0.94625151
C	2.56462069	-2.25673899	0.58521874
H	1.50671045	-2.31713391	0.81447993
C	3.13247286	-1.03464001	0.21429430
C	2.49639596	0.26429873	0.07079435
C	1.15826207	0.60991537	0.26648147
H	0.44911921	-0.14300859	0.59157306

C	0.75098060	1.92539649	0.08005618
C	1.68673256	2.90731771	-0.28841159
H	1.34111647	3.92822697	-0.39371788
C	3.01129096	2.58262846	-0.50248282
H	3.72671492	3.34052087	-0.79685481
C	3.40913238	1.25679758	-0.32242224
C	-0.65056524	2.37462148	0.34972529
C	-1.78680712	1.40518998	0.19913359
C	-1.78330651	0.37617077	-0.74280818
H	-0.92386577	0.23001350	-1.38630344
C	-2.89164577	-0.44949737	-0.88943736
H	-2.89943668	-1.24136329	-1.62683082
C	-3.99670449	-0.24337756	-0.07462122
C	-4.02637381	0.78331623	0.86307812
H	-4.90237935	0.93005146	1.48113379
C	-2.92211327	1.61219102	0.98350800
H	-2.92434573	2.43687805	1.68588469

$4_{BrBDBT}(S_1)$

Br	-5.57756700	-1.38063900	-0.23051400
S	5.07193000	0.69013000	-0.51864300
O	-0.84593500	3.45491200	0.73911600
C	4.57457100	-0.93607500	-0.07939000
C	5.40434200	-2.05287400	-0.01190300
H	6.46093800	-1.97253700	-0.23589800
C	4.84472400	-3.26806800	0.34786600
H	5.47389900	-4.14808500	0.40375500
C	3.47912200	-3.37223000	0.63603800
H	3.06212800	-4.33216400	0.91383400
C	2.65957600	-2.25884200	0.56798700
H	1.60187400	-2.34295800	0.79058400
C	3.20359700	-1.02288700	0.20869100
C	2.53940500	0.26401800	0.07282800
C	1.20020600	0.57583500	0.29301400

H	0.51542900	-0.18503200	0.64799700
C	0.75062400	1.88167800	0.08322200
C	1.66895000	2.88540200	-0.29797700
H	1.31121800	3.89553100	-0.45131700
C	3.00385700	2.58973400	-0.49384300
H	3.69826600	3.36674300	-0.78882800
C	3.43494100	1.27659500	-0.31623500
C	-0.65423000	2.24580800	0.31607700
C	-1.81094700	1.37860500	0.17014900
C	-1.77963300	0.23797700	-0.65392900
H	-0.88816000	0.00436400	-1.22223200
C	-2.89361700	-0.57477000	-0.77412500
H	-2.86433600	-1.45015300	-1.41037000
C	-4.06059800	-0.25095300	-0.08795200
C	-4.12758900	0.88787000	0.70476400
H	-5.04350600	1.13337700	1.22630500
C	-3.01066900	1.69651900	0.83319000
H	-3.05610100	2.57186900	1.46868100

$4_{BrBDBT}(T_1)$

Br	11.38914425	3.85430103	5.94922108
S	1.68128995	8.69925847	6.73971915
O	4.96540463	3.78880371	3.68392675
C	2.74924057	8.77389247	8.13475774
C	2.56806850	9.57592720	9.25797608
H	1.70916880	10.23066731	9.33930241
C	3.51485624	9.51618397	10.26874183
H	3.39264781	10.13438432	11.14980333
C	4.62488768	8.67165104	10.16232478
H	5.35422099	8.64212694	10.96216747
C	4.79853579	7.87592689	9.04217524
H	5.66097516	7.22398399	8.96177349
C	3.85549400	7.91919059	8.01291340
C	3.83698057	7.18202804	6.75786374

C	4.73992195	6.23521109	6.29590201
H	5.57423680	5.92901221	6.91640042
C	4.56046007	5.65229105	5.02757492
C	3.40385369	5.98949620	4.26966420
H	3.26456225	5.52289209	3.30353626
C	2.49051374	6.90830936	4.73456095
H	1.62144418	7.16485342	4.14124861
C	2.70998113	7.51322801	5.97590834
C	5.48150067	4.66360987	4.51154210
C	6.87731485	4.49289247	4.85569175
C	7.67823785	5.57682821	5.27178508
H	7.25136038	6.57158128	5.31992344
C	9.00781950	5.38938861	5.59992480
H	9.61593394	6.22273623	5.92764439
C	9.57161184	4.11859855	5.48433834
C	8.81728108	3.04017195	5.03213530
H	9.27139633	2.06208539	4.94076065
C	7.48378877	3.22631584	4.71644009
H	6.88486602	2.38917221	4.38235186

$4_{BrBDBT}(T_2)$

Br	5.58341500	-1.35589000	-0.01391700
S	-5.12304200	0.69024700	0.01486900
O	0.88011600	3.56839400	0.16725300
C	-4.55948700	-0.97922000	-0.04987100
C	-5.36755300	-2.10884800	-0.09318300
H	-6.44698400	-2.02128400	-0.08660900
C	-4.75447500	-3.35385300	-0.14630200
H	-5.36585900	-4.24707200	-0.18244900
C	-3.36206900	-3.46552300	-0.15466000
H	-2.90315800	-4.44525000	-0.19834700
C	-2.56372000	-2.33230100	-0.10818700
H	-1.48353100	-2.42249500	-0.11623900
C	-3.15969300	-1.07228800	-0.05432400

C	-2.52379500	0.23881300	0.00530800
C	-1.18042500	0.53777600	0.02659000
H	-0.45124800	-0.25891000	-0.02870300
C	-0.74946200	1.90363500	0.04152500
C	-1.76191500	2.93565000	0.04408600
H	-1.43334900	3.96535200	0.01574100
C	-3.09383200	2.63369100	0.04888200
H	-3.83558300	3.42290000	0.03502900
C	-3.49216500	1.28027400	0.04261800
C	0.61685100	2.29816500	0.05706500
C	1.78137600	1.37965100	0.04194200
C	1.86546900	0.25714700	0.87304600
H	1.06161800	0.03488100	1.56437400
C	2.98979600	-0.55799600	0.85839500
H	3.05188400	-1.42215200	1.50690800
C	4.04698900	-0.24043300	0.01601400
C	4.00298900	0.88432700	-0.79735600
H	4.84000000	1.12443100	-1.43974400
C	2.87270500	1.68902000	-0.77675900
H	2.82894700	2.56852000	-1.40777400

$5_{FBDBF}(S_0)$

O	2.30318000	2.75797100	-0.64385800
C	-3.88936400	-0.07835000	0.13657900
C	-5.11929800	-0.71276800	0.15045500
H	-6.02088500	-0.17637500	0.41457600
C	-5.12668100	-2.05932300	-0.19097500
H	-6.06609200	-2.59819200	-0.19493200
C	-3.94686700	-2.73377000	-0.53051100
H	-3.99358800	-3.78342700	-0.79201300
C	-2.72421300	-2.07825200	-0.53725900
H	-1.81423700	-2.60342100	-0.80159600

C	-2.69505800	-0.72641900	-0.19719200
C	-1.66625400	0.29173400	-0.08195700
C	-0.28604200	0.33116000	-0.25843600
H	0.25553900	-0.55237400	-0.57484300
C	0.37812200	1.53905900	-0.05386700
C	-0.33606900	2.69593400	0.30710500
H	0.22064700	3.61760200	0.42174500
C	-1.70559300	2.67227900	0.50522200
H	-2.26390500	3.55275500	0.79384400
C	-2.34210700	1.45626400	0.30455400
C	1.84773900	1.69139400	-0.29616800
C	2.75889700	0.51559200	-0.10764600
C	2.51686100	-0.48472100	0.83589900
H	1.62395400	-0.44882400	1.44814900
C	3.43177500	-1.51315500	1.02266500
H	3.27682200	-2.29286500	1.75696000
C	4.57730300	-1.52763600	0.24626600
C	4.85178400	-0.54482500	-0.69209000
H	5.76726800	-0.59935800	-1.26680500
C	3.93978400	0.48521700	-0.85352800
H	4.12766400	1.28729300	-1.55656600
F	5.45674300	-2.52328000	0.41319700
O	-3.67970300	1.24080600	0.44110900

$5_{FBDBF}(S_1)$

O	2.25072400	2.72911700	-0.71744100
C	-3.92338700	-0.06197300	0.15803300
C	-5.15906100	-0.68546000	0.17953600
H	-6.05186300	-0.14419700	0.46292100
C	-5.18455900	-2.02701600	-0.18026900
H	-6.12946800	-2.55629100	-0.17858300
C	-4.01661500	-2.70887700	-0.54520500
H	-4.07738700	-3.75447300	-0.81968000
C	-2.78791200	-2.06493300	-0.55972300

H	-1.88639300	-2.59510500	-0.84252100
C	-2.74085600	-0.71831100	-0.20206400
C	-1.69840500	0.28688300	-0.09007900
C	-0.32700500	0.30946100	-0.31011200
H	0.19381600	-0.56700000	-0.67546600
C	0.36858600	1.50157100	-0.07215200
C	-0.32914800	2.66300600	0.33207900
H	0.23059800	3.57296900	0.50554400
C	-1.69989400	2.65376900	0.53228100
H	-2.23784000	3.53813600	0.84677500
C	-2.35750000	1.45352400	0.32302900
C	1.82017900	1.58199100	-0.29169800
C	2.78406400	0.50908500	-0.10939500
C	2.51062800	-0.58746700	0.73004700
H	1.57345100	-0.63377800	1.26964600
C	3.44623600	-1.59308800	0.90114400
H	3.25267000	-2.44074200	1.54613100
C	4.66721200	-1.49889600	0.25081300
C	4.98001600	-0.42372400	-0.56188900
H	5.94716600	-0.38707900	-1.04675300
C	4.03927600	0.57771600	-0.74295400
H	4.26563700	1.41470400	-1.39089000
F	5.57164400	-2.47564500	0.42163500
O	-3.69776300	1.24964200	0.47739500

$5_{FBDBF}(T_1)$

O	2.27509000	2.74543500	-0.60566400
C	-3.92951900	-0.06414000	0.13081400
C	-5.16478000	-0.68744700	0.14510500
H	-6.06344400	-0.13907100	0.39417900
C	-5.18233100	-2.03947500	-0.17598600
H	-6.12693000	-2.56929300	-0.17834500
C	-4.00714400	-2.73016700	-0.49660500
H	-4.06157000	-3.78335900	-0.74178700

C	-2.77839500	-2.08525700	-0.50433600
H	-1.87088000	-2.62232000	-0.75282300
C	-2.73933700	-0.72903000	-0.18531300
C	-1.69850000	0.27931800	-0.08102900
C	-0.32653700	0.29847800	-0.27546400
H	0.20351000	-0.58661800	-0.60639600
C	0.37240400	1.50052300	-0.05274600
C	-0.34564000	2.67775100	0.29662100
H	0.21187100	3.59211900	0.45014200
C	-1.71668000	2.66919500	0.46954200
H	-2.26404000	3.55985100	0.74824000
C	-2.36917200	1.45879700	0.28447800
C	1.80889100	1.57769600	-0.23533800
C	2.77561300	0.51006700	-0.08581600
C	2.54880900	-0.56992000	0.79388900
H	1.63782000	-0.59938900	1.37916000
C	3.48454500	-1.57772800	0.93028400
H	3.32379500	-2.41673000	1.59526300
C	4.67368300	-1.49512300	0.21621500
C	4.95030300	-0.43114700	-0.62747300
H	5.89197500	-0.40791900	-1.16088200
C	4.00598600	0.56949000	-0.77620700
H	4.19458200	1.39928700	-1.44448100
F	5.58213500	-2.47123000	0.35646700
O	-3.71122800	1.25747000	0.41637700

$5_{FBDBF}(T_2)$

O	2.24493500	2.51129800	-1.11327700
C	-3.97098300	0.00090700	0.24330100
C	-5.23291900	-0.56664200	0.28803600
H	-6.08237200	-0.00753900	0.65720000
C	-5.34279100	-1.87562300	-0.16374000
H	-6.31118900	-2.36035500	-0.14832200
C	-4.22954500	-2.58056500	-0.63892300

H	-4.35516500	-3.59921900	-0.98384800
C	-2.97319700	-1.99321000	-0.67449500
H	-2.11491500	-2.54163300	-1.04393100
C	-2.84116800	-0.67982100	-0.22535000
C	-1.74717600	0.26654800	-0.09708700
C	-0.38396300	0.24715300	-0.38119700
H	0.06988900	-0.62501500	-0.83658600
C	0.37858800	1.38575000	-0.11584200
C	-0.24527700	2.54061200	0.39753500
H	0.36119800	3.42021100	0.57634900
C	-1.60176100	2.58076000	0.67847000
H	-2.08100000	3.46636600	1.07400700
C	-2.32544600	1.42650600	0.42971100
C	1.82430200	1.45425800	-0.42664600
C	2.78931200	0.46593500	-0.14863200
C	2.49045600	-0.78936600	0.49476200
H	1.48717300	-0.98197100	0.84723500
C	3.47538900	-1.70968600	0.72616300
H	3.27261300	-2.64227500	1.23774000
C	4.78953500	-1.44137400	0.30490800
C	5.13765300	-0.23562100	-0.30516700
H	6.17139200	-0.06044800	-0.57482800
C	4.16580600	0.70757200	-0.52273000
H	4.41423700	1.66418900	-0.95918000
F	5.73266700	-2.35943200	0.52784000
O	-3.66577900	1.27345400	0.64142000

$6_{ClBDBF}(S_0)$

O	-1.70817200	3.12132300	0.60924400
C	4.17558400	-0.32284200	-0.14793600
C	5.33687100	-1.07560600	-0.15826300
H	6.28517500	-0.63477200	-0.43519500
C	5.21355200	-2.41110200	0.20379100
H	6.09514600	-3.04007400	0.21110800

C	3.97526500	-2.96068900	0.55958000
H	3.91976900	-4.00587300	0.83676800
C	2.82331700	-2.18767800	0.56269800
H	1.86773500	-2.61657700	0.83949800
C	2.92559700	-0.84471500	0.20210900
C	2.00158900	0.26827300	0.07651100
C	0.63356300	0.44642600	0.26039000
H	0.00981200	-0.37452900	0.59364300
C	0.09044700	1.71108000	0.04054600
C	0.91227400	2.78617600	-0.34350800
H	0.44816500	3.75618300	-0.47096600
C	2.27127500	2.62416200	-0.54906500
H	2.91160500	3.44036000	-0.85572100
C	2.78622000	1.35440000	-0.33224300
C	-1.35478700	2.00915300	0.28826700
C	-2.37452600	0.91784500	0.13765800
C	-2.24428200	-0.11151200	-0.79507700
H	-1.36584700	-0.16477200	-1.42698000
C	-3.25064100	-1.05739500	-0.94592900
H	-3.16565300	-1.85133300	-1.67616300
C	-4.38102800	-0.97120300	-0.14535900
C	-4.53663300	0.05183900	0.78313400
H	-5.43309300	0.09951600	1.38718600
C	-3.53493800	1.00097300	0.90873300
H	-3.63782000	1.82468600	1.60453800
O	4.09484600	1.00590700	-0.47244700
Cl	-5.63768900	-2.16565700	-0.31401800

$6_{ClBDBF}(S_1)$

O	-1.61930600	3.01559500	0.84556100
C	4.22622800	-0.27739600	-0.22072700
C	5.40798200	-0.99680400	-0.25608900
H	6.32401100	-0.54755200	-0.61574300
C	5.34855400	-2.31037800	0.19221400

H	6.24860700	-2.91267200	0.18339600
C	4.15173200	-2.87205100	0.65508200
H	4.14595600	-3.89947200	0.99653200
C	2.97819800	-2.13291100	0.68188600
H	2.05419700	-2.57052200	1.04021500
C	3.01669000	-0.81233200	0.23621400
C	2.05091600	0.26420600	0.10367900
C	0.69797700	0.41310900	0.38192900
H	0.12483800	-0.39210400	0.82512900
C	0.08880900	1.63754900	0.08682300
C	0.85059000	2.71181700	-0.42303400
H	0.35292600	3.65013100	-0.63103900
C	2.20526200	2.57921000	-0.68250100
H	2.79501700	3.39392500	-1.08083800
C	2.77626800	1.34578300	-0.41856800
C	-1.34863600	1.84608800	0.36113700
C	-2.40648000	0.87854300	0.18043800
C	-2.22754900	-0.26813600	-0.61863200
H	-1.28830300	-0.42961200	-1.13184100
C	-3.25631400	-1.17698600	-0.78655600
H	-3.11785400	-2.05427500	-1.40533200
C	-4.48438700	-0.95217500	-0.17228400
C	-4.69432000	0.18082900	0.60297700
H	-5.65770500	0.34333000	1.06887600
C	-3.66470700	1.08917300	0.77934200
H	-3.82469500	1.96478100	1.39550500
O	4.08572700	1.02563000	-0.61832400
Cl	-5.77583800	-2.10344600	-0.38604400

$6_{ClBDBF}(T_1)$

O	-1.68139100	3.07174400	0.62062700
C	4.23123800	-0.28954300	-0.15475900
C	5.40661700	-1.01925000	-0.17068200
H	6.34540700	-0.55876800	-0.44806800

C	5.31083000	-2.35883800	0.18661000
H	6.20497300	-2.96994200	0.18897900
C	4.08521800	-2.93464900	0.54330200
H	4.05098700	-3.98197900	0.81568100
C	2.91820900	-2.18395500	0.55237300
H	1.97151300	-2.63251000	0.82857500
C	2.99308400	-0.83806400	0.19752200
C	2.04369600	0.25555100	0.08119600
C	0.68258000	0.40242200	0.29668500
H	0.08197400	-0.42232100	0.66131100
C	0.09016100	1.65494700	0.05055100
C	0.90134700	2.75413900	-0.34227100
H	0.42376700	3.71002000	-0.51174900
C	2.26309100	2.61925100	-0.53671900
H	2.88217700	3.44978400	-0.84886600
C	2.80889800	1.36100700	-0.32771600
C	-1.33266500	1.86365000	0.25507800
C	-2.39139500	0.88923300	0.12535100
C	-2.26586800	-0.22732600	-0.72949200
H	-1.36263600	-0.35552200	-1.31354700
C	-3.28971600	-1.14651500	-0.84575600
H	-3.18988400	-2.00605600	-1.49607100
C	-4.47518300	-0.95072200	-0.13730100
C	-4.64271700	0.16073400	0.68176900
H	-5.57176500	0.29554800	1.22044500
C	-3.61305100	1.07489900	0.81001600
H	-3.72814200	1.93204700	1.46043700
O	4.12481600	1.03847200	-0.47390100
Cl	-5.76482400	-2.10963900	-0.29090900

$6_{ClBDBF}(T_2)$

O	-1.67353400	2.81425700	1.14073200
C	4.28082700	-0.20262100	-0.28661300
C	5.49337200	-0.86853700	-0.33838800

H	6.37084700	-0.39646300	-0.75981300
C	5.51671300	-2.15883000	0.17567100
H	6.44383400	-2.71837100	0.15698800
C	4.36851100	-2.75054300	0.71766300
H	4.42655200	-3.75811000	1.10989600
C	3.16282500	-2.06566800	0.75925700
H	2.27743500	-2.52655300	1.18060800
C	3.11778900	-0.76918300	0.24792500
C	2.09632600	0.25254600	0.10242100
C	0.74454600	0.35354300	0.42193700
H	0.23600200	-0.45850500	0.92835900
C	0.06619200	1.53376800	0.11760400
C	0.75789300	2.60999300	-0.47096000
H	0.21399600	3.52386300	-0.67697900
C	2.10430500	2.52973200	-0.79064800
H	2.63774600	3.35377900	-1.24534900
C	2.74461100	1.33678900	-0.49985900
C	-1.36318100	1.73126100	0.46681000
C	-2.40598000	0.81978900	0.20913100
C	-2.21653400	-0.46775500	-0.41729800
H	-1.23572200	-0.74665000	-0.77619600
C	-3.27116100	-1.30852900	-0.61937300
H	-3.13411400	-2.25928000	-1.11878400
C	-4.57017900	-0.94060600	-0.18645200
C	-4.80092000	0.31065300	0.40965200
H	-5.80817700	0.58510300	0.69582100
C	-3.75788600	1.17547600	0.59784800
H	-3.92258300	2.15579400	1.02177100
O	4.06147000	1.06913300	-0.74050300
Cl	-5.88339600	-2.03231800	-0.43624200