Computational Insights into Intriguing Vibration-Induced Pulsing Diradical Character in Perfluoropentacene

Fengying Zhang, Yiwei Feng, Xinyu Song*, Yuxiang Bu

School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100, P. R. China

Supporting Information

Contents

1. The Diradical Character Spectrum of Pentacene

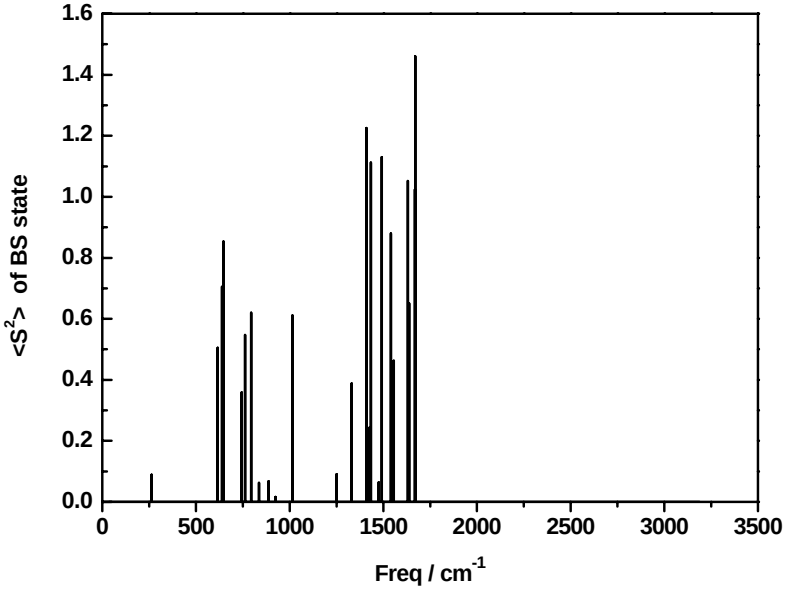


Figure S1. The diradical character spectrum with respect to the vibrational frequencies characterized by the calculated $<S^2>$ values of the ground states of all vibration-distorted configurations in pentacene. 25 vibrational configurations exhibit diradical character among all 102 shift-positive vibrational modes.

2. The Classification of Ground States for All 102 Vibrational Modes with Positively and Negatively Shifted Distorted Configurations and Representatives of the Corresponding Vibrational Modes

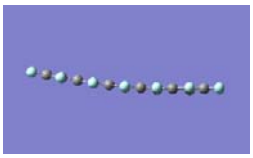
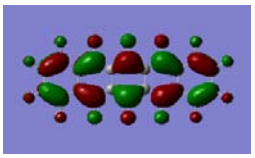
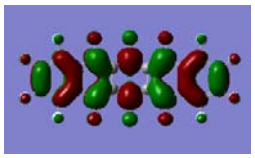
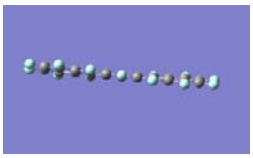
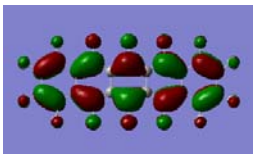
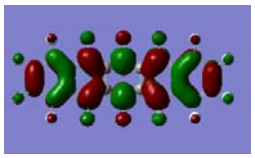
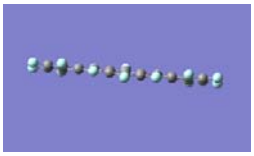
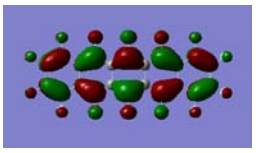
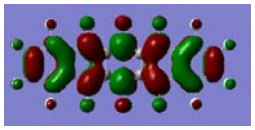
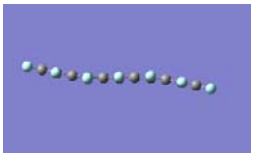
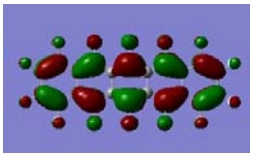
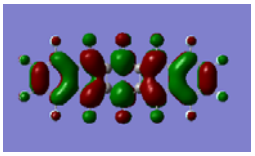
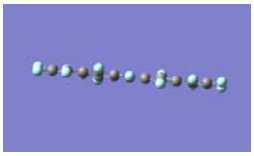
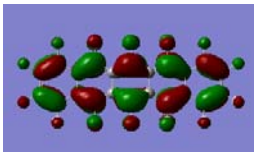
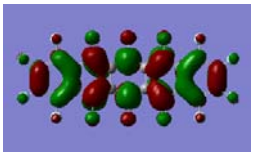
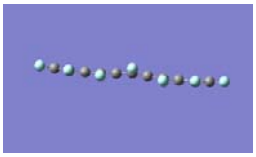
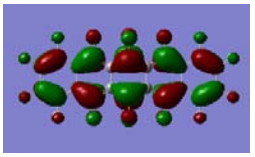
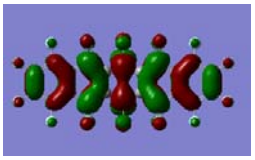
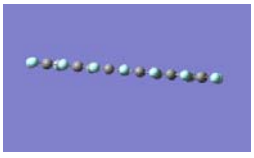
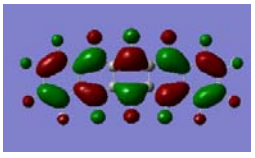
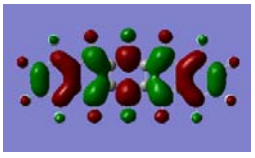
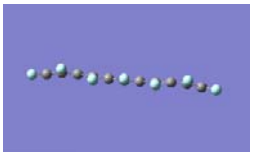
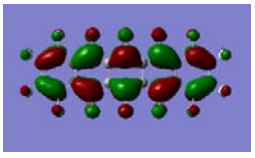
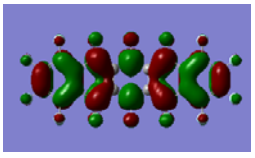
Table S1. All 9 types of the ground states for the negative and positive shifts of the vibrational modes and the representatives of the corresponding vibrational modes. Among them all the diradical vibrations are shown in table.

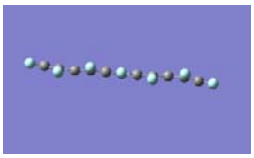
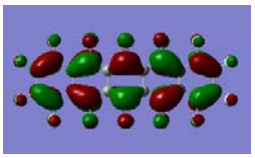
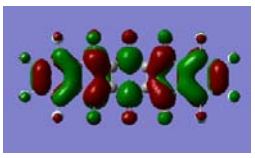
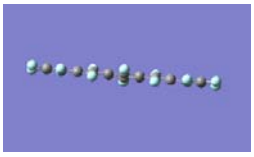
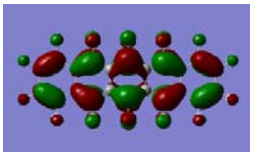
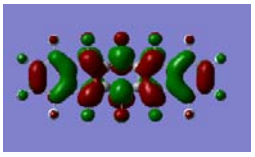
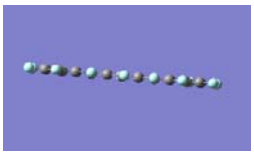
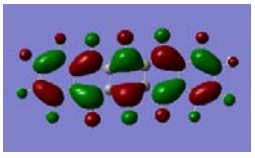
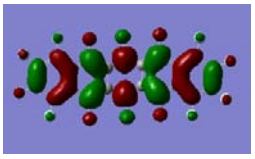
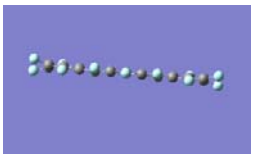
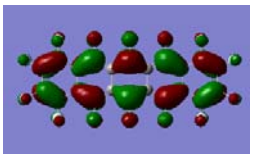
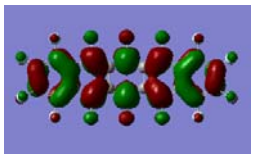
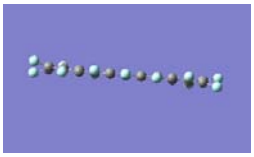
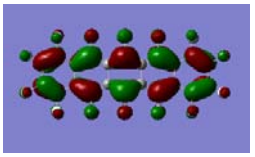
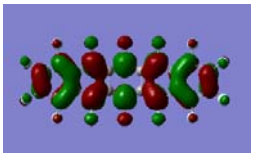
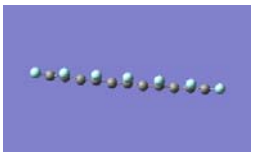
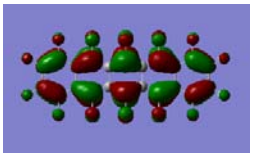
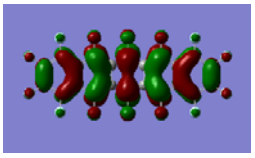
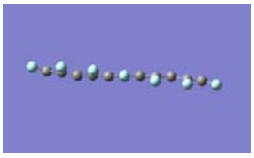
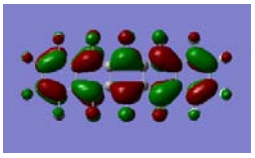
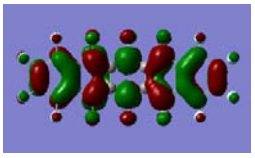
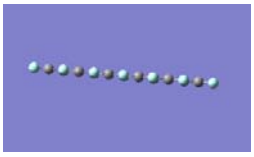
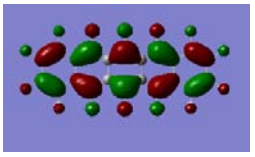
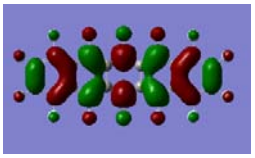
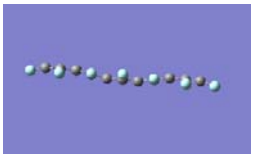
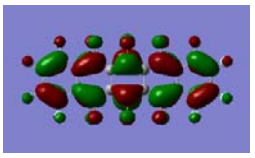
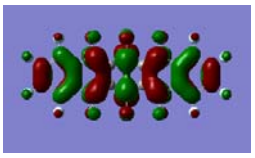
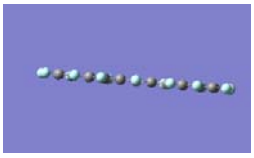
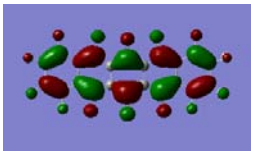
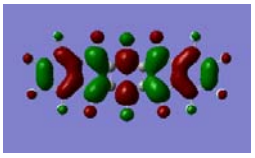
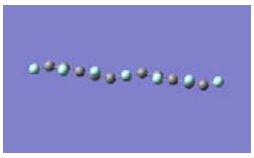
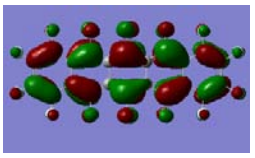
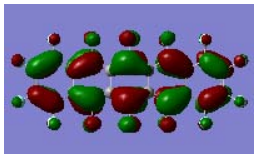
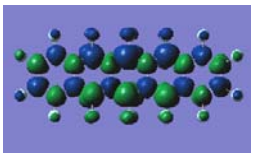
Negative Shifts (ground state)	Positive Shifts (ground state)	Representative Vibrations (modes)
CS	CS	1,2,3,4,5,6,7,8,9,10…
BS	BS	19,31,35,38,39,41,44,49,52,53, 54,56,57,58,60,62,66,70,77,85
T	T	87,89,92,96,100,101,102
BS	CS	16,29,42,73,76
	T	98
CS	BS	22,45,59,68,81,86,93
	T	83
T	BS	94
	CS	99

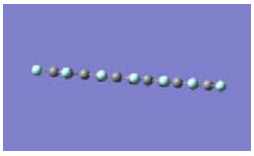
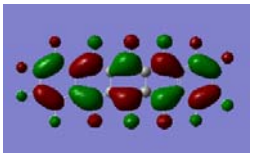
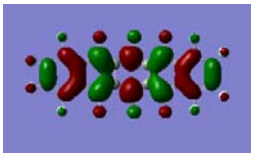
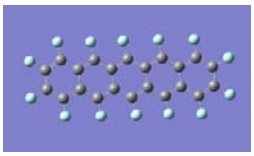
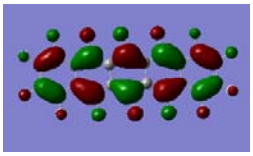
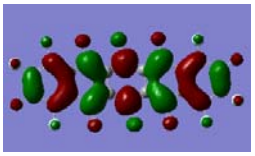
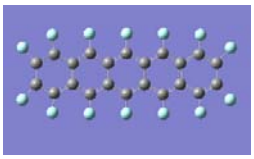
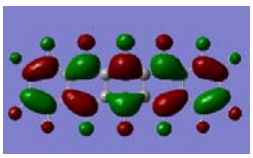
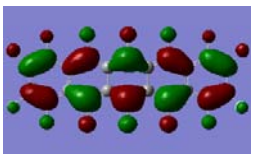
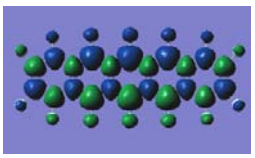
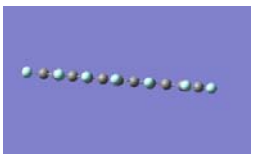
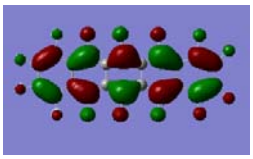
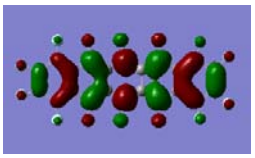
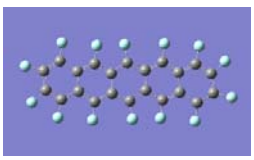
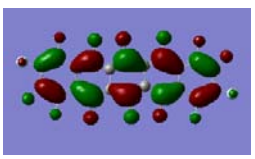
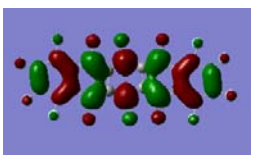
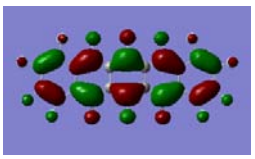
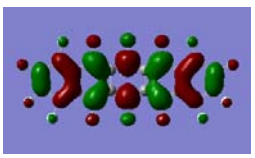
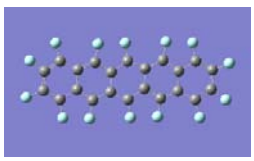
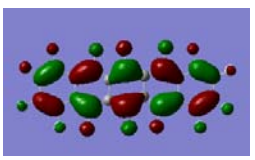
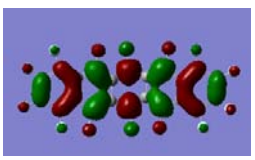
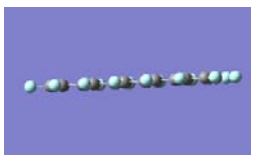
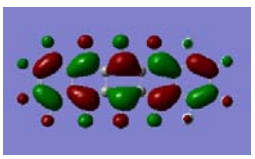
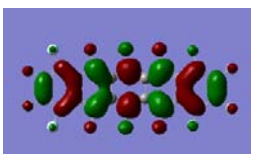
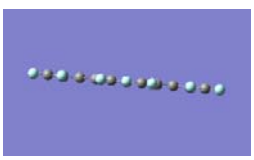
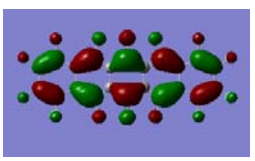
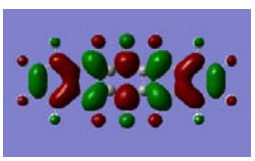
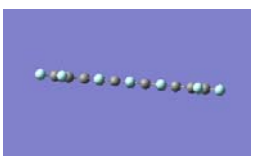
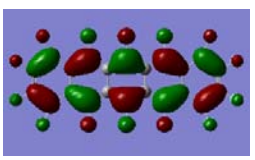
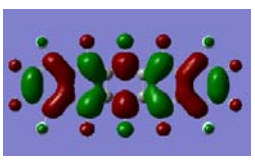
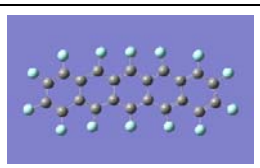
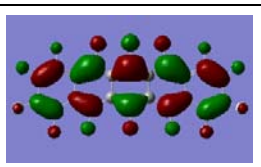
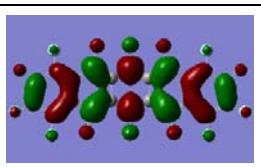
3. Relevant Data of All 102 Positively Shifted Configurations Including the distorted Configurations, HOMO-LUMO gaps, Singlet-Triplet Energy gaps, etc.

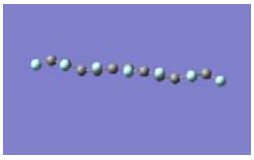
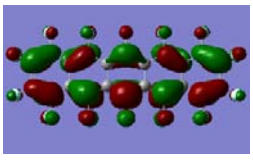
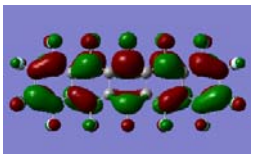
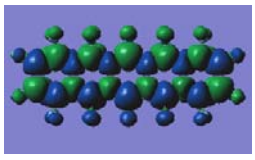
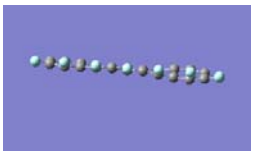
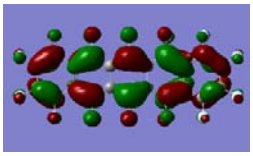
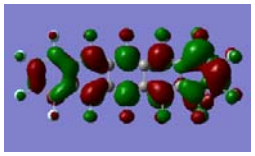
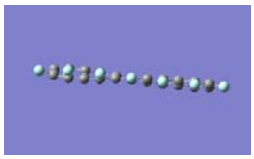
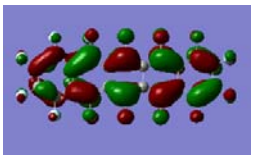
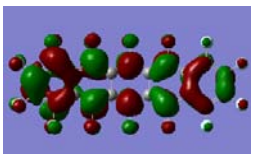
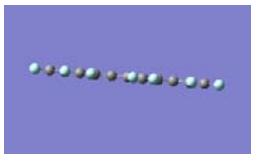
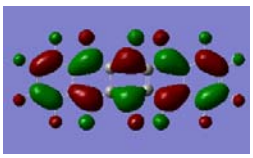
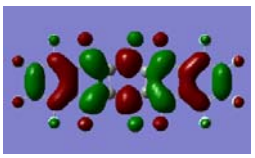
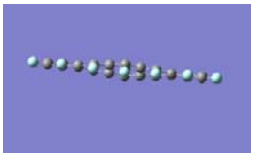
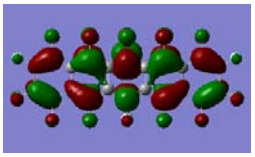
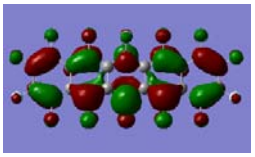
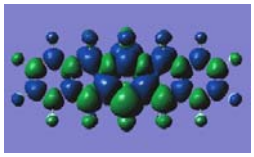
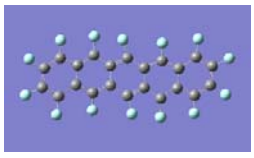
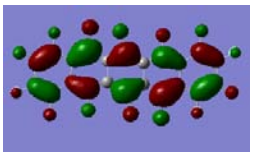
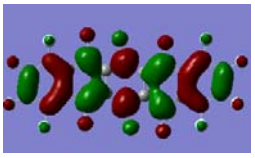
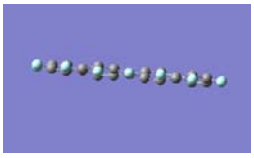
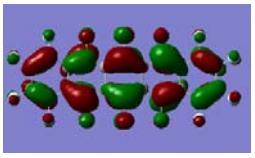
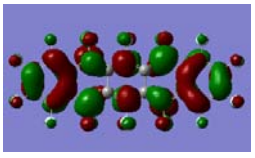
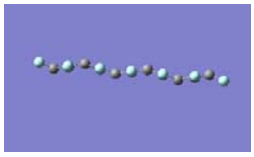
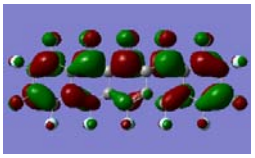
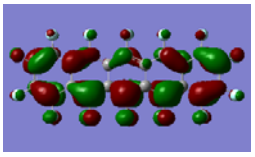
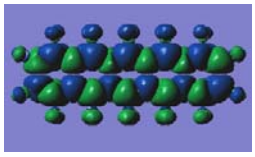
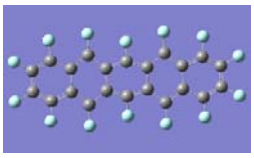
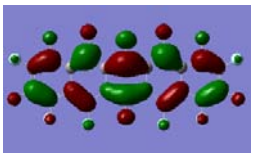
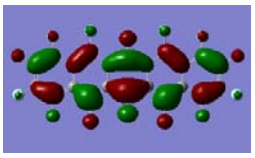
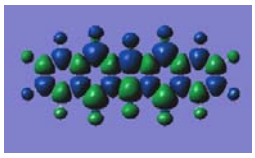
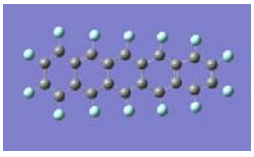
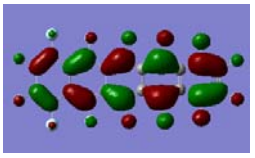
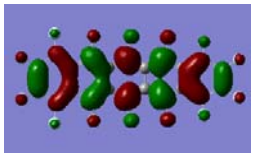
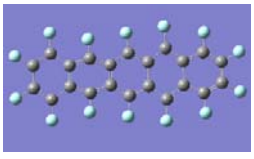
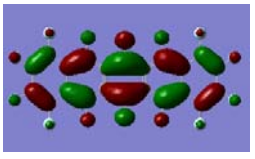
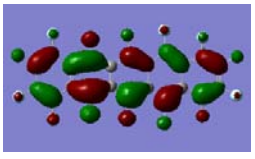
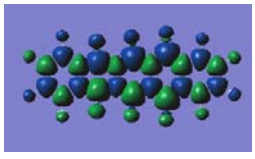
Table S2. All 102 vibration-distorted configurations (positively shifted), HOMO-LUMO gaps of the closed-shell singlet states (H-L gap, eV), T-S gaps between the closed-shell singlet and triplet states ($\Delta E_{(T\text{-}CS)} = E_T - E_{CS}$, kcal/mol) and the $<S^2>$ values, spin density distributions (isovalue = 0.004), two singly occupied molecular orbitals (SOMO(α) or SOMO 1, SOMO(β) or SOMO 2) of the broken symmetry open-shell singlet (BS) or triplet (T) states for 38 diradical vibrational modes.

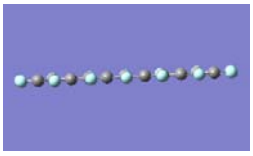
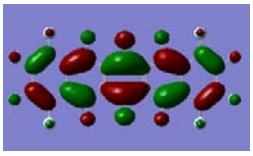
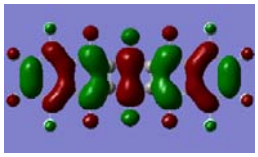
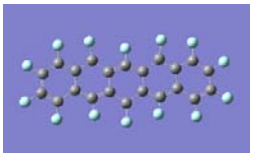
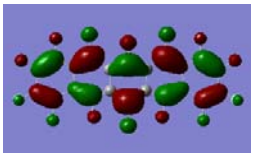
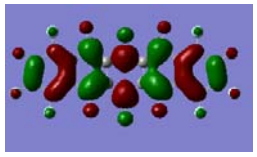
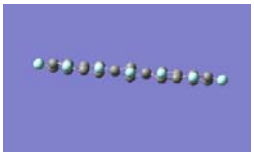
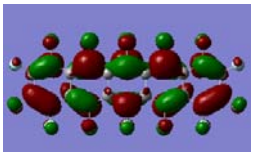
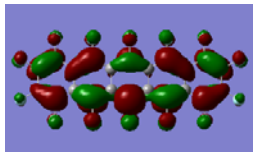
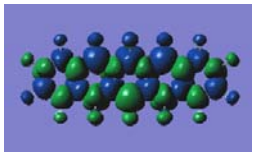
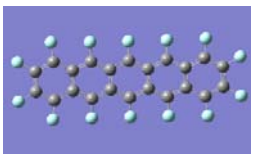
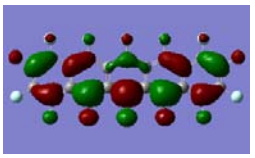
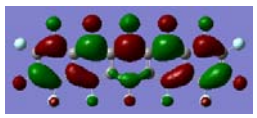
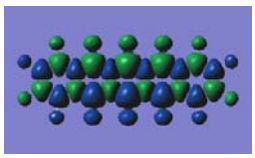
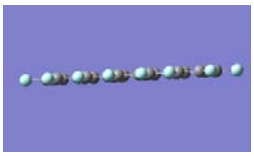
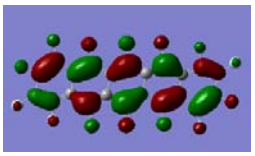
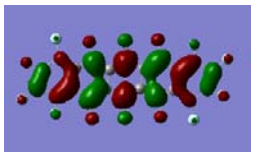
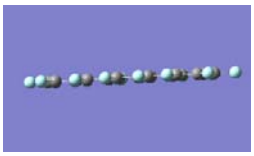
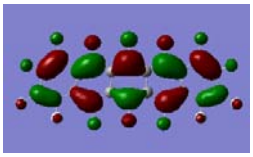
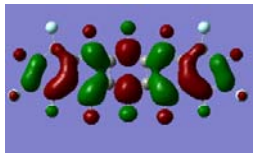
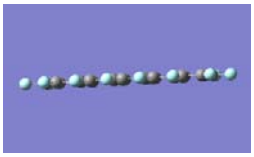
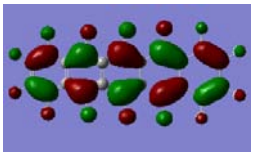
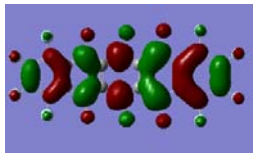
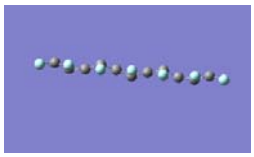
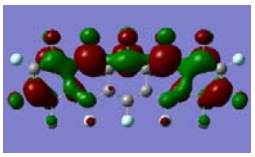
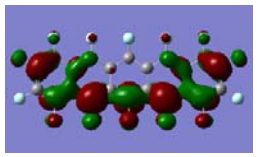
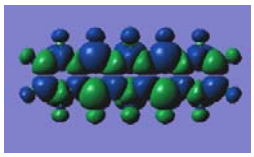
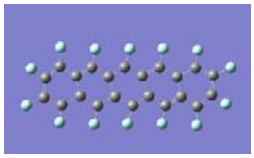
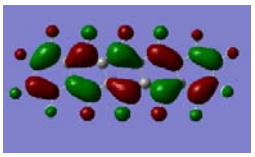
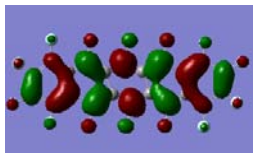
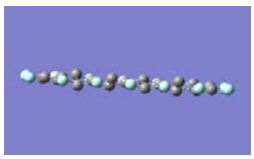
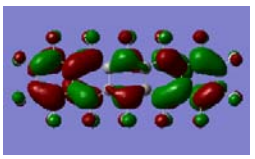
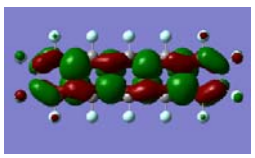
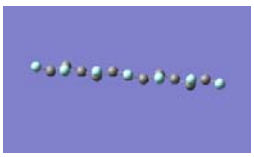
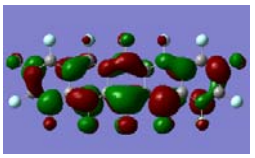
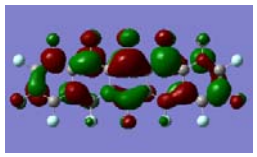
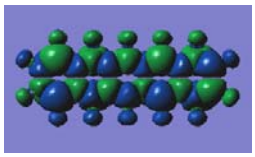
Besides, the shapes of HOMO and LUMO and relevant energies for the vibration-distorted configurations without diradical character are also listed (isovalue = 0.02) (The red data denotes diradical vibrations with BS ground states, and the pink data stands for diradical vibrations with T ground states).

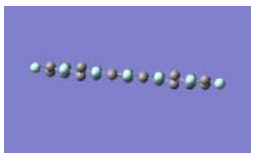
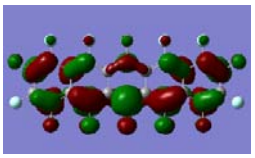
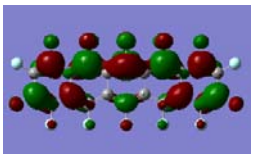
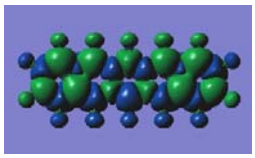
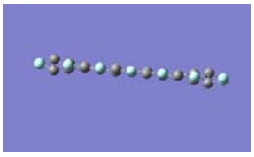
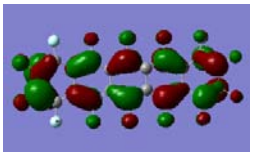
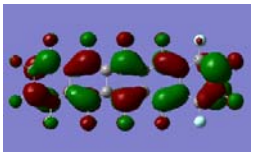
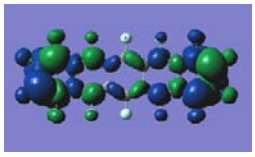
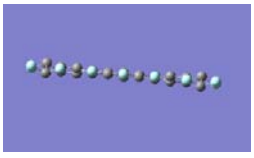
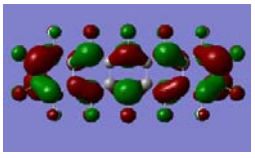
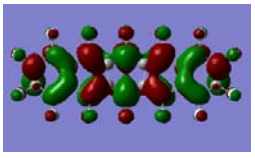
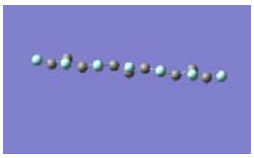
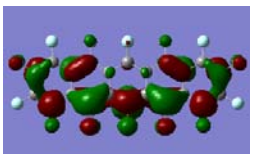
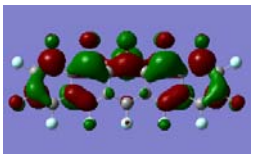
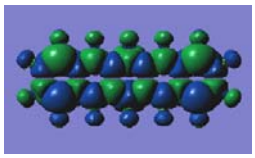
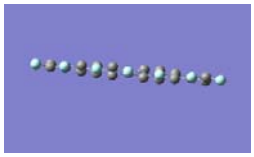
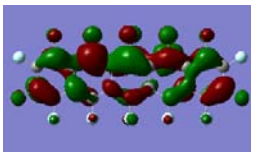
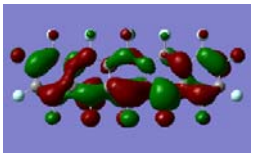
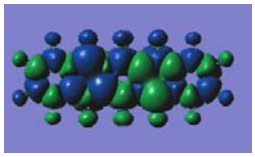
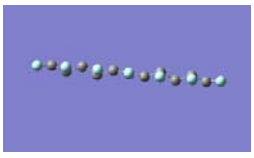
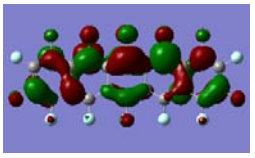
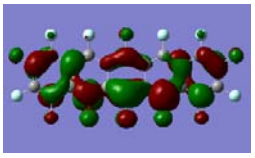
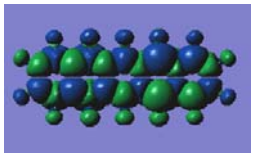
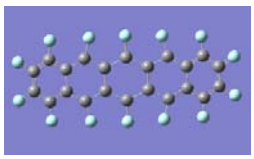
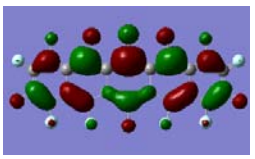
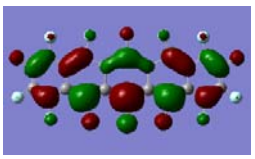
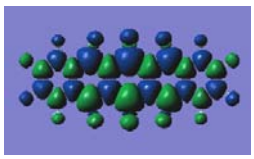
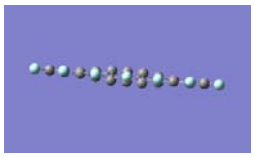
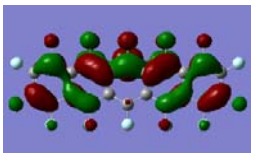
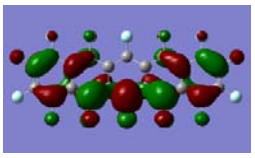
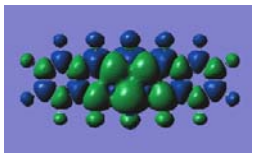
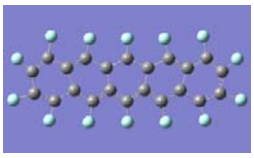
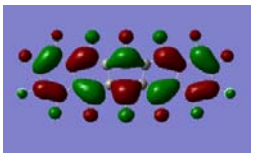
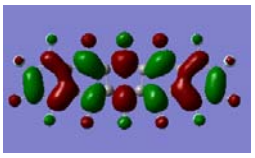
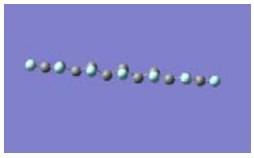
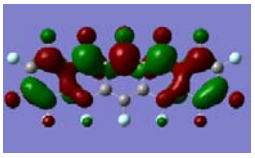
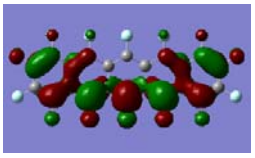
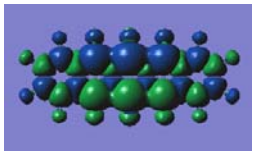
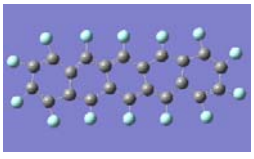
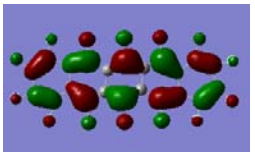
Modes <S^2>	H-L gap T-S gap	Distortion Modes	HOMO or SOMO α (SOMO 1)	LUMO or SOMO β (SOMO 2)	BS or T State Spin density
1 0.00	2.00 19.43				
2 0.00	2.04 20.50				
3 0.00	2.04 20.26				
4 0.00	1.98 19.07				
5 0.00	2.02 19.94				
6 0.00	1.99 18.87				
7 0.00	2.02 19.93				
8 0.00	1.99 19.22				

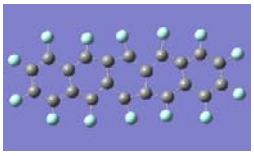
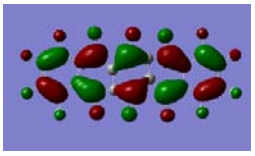
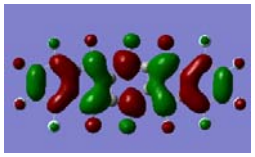
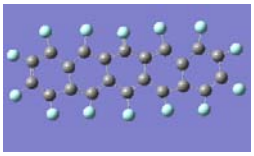
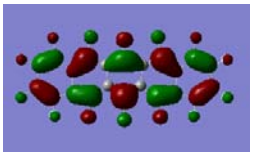
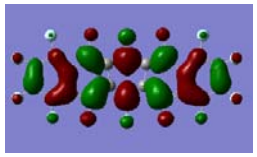
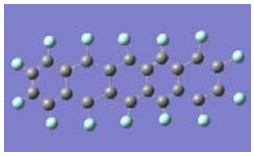
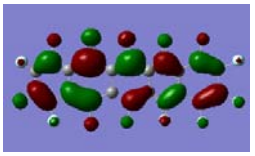
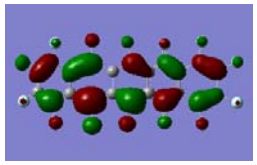
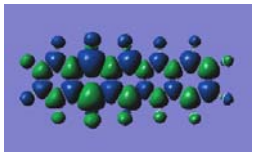
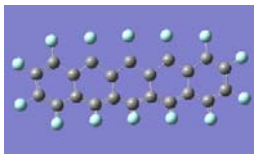
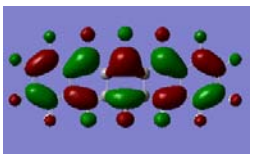
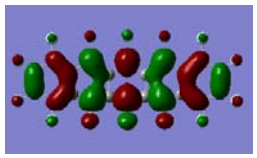
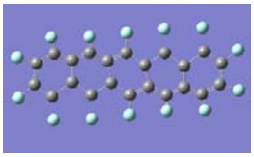
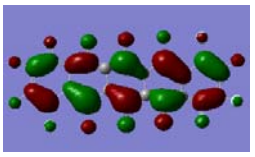
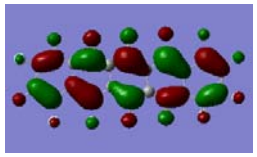
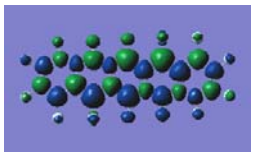
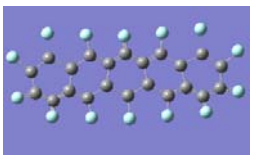
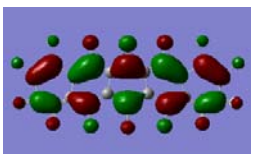
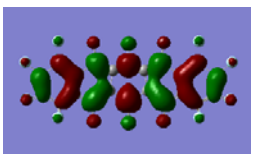
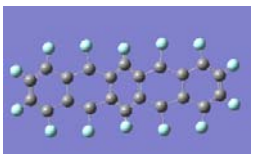
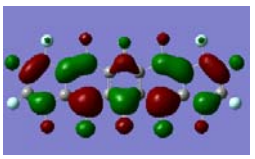
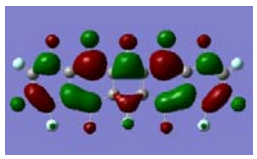
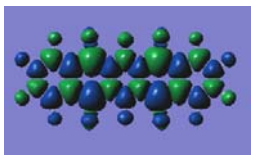
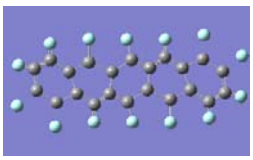
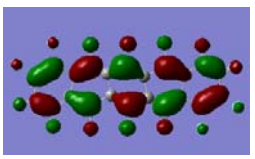
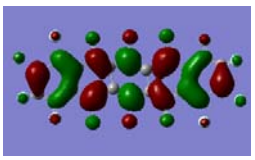
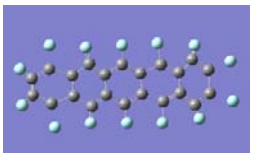
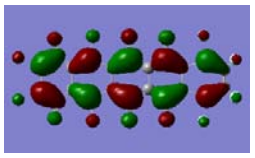
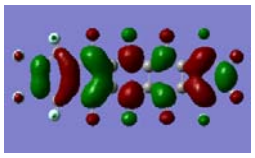
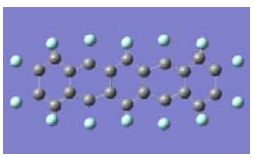
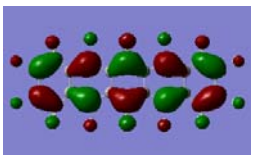
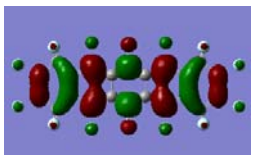
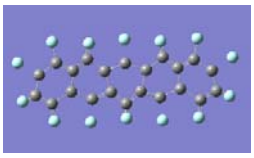
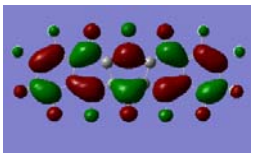
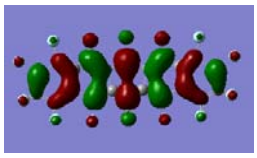
9 **0.00**	**1.99** **19.21**				
10 **0.00**	**1.93** **17.75**				
11 **0.00**	**2.02** **19.76**				
12 **0.00**	**1.99** **19.37**				
13 **0.00**	**2.00** **19.62**				
14 **0.00**	**1.94** **17.78**				
15 **0.00**	**1.99** **19.18**				
16 **0.00**	**2.18** **23.65**				
17 **0.00**	**1.99** **18.98**				
18 **0.00**	**1.99** **19.30**				
19 **0.054**	**1.92** **16.63**				

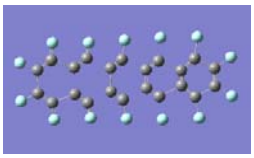
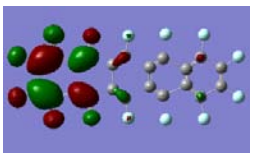
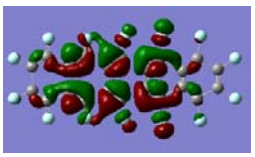
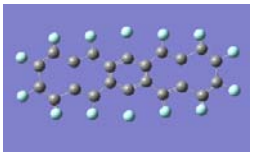
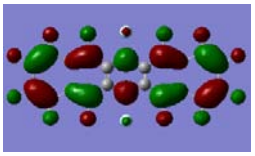
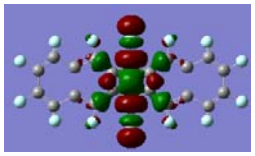
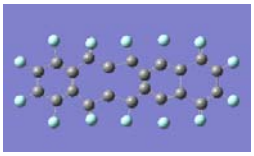
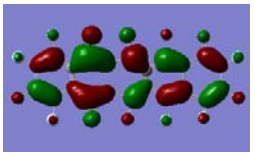
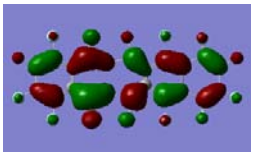
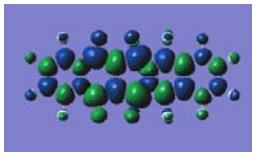
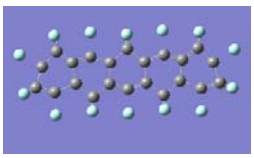
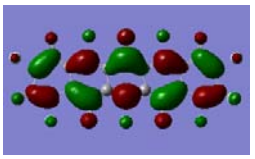
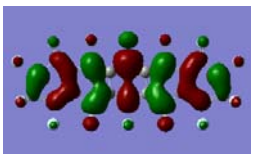
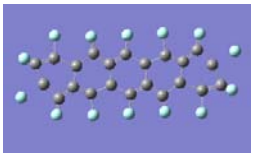
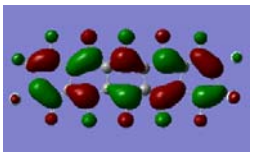
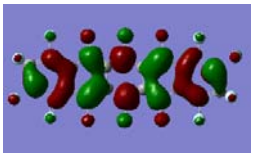
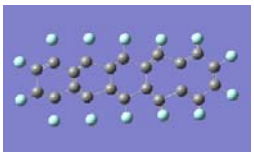
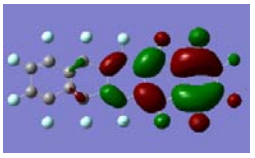
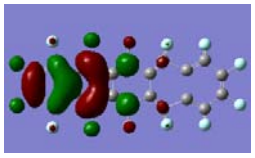
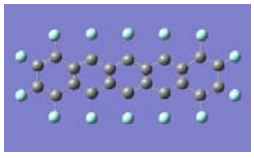
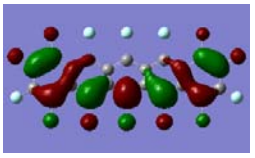
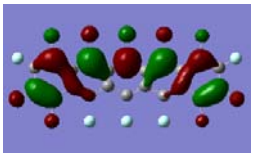
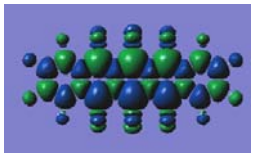
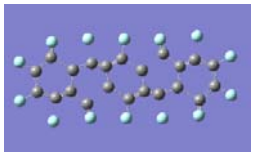
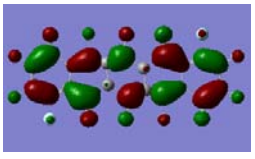
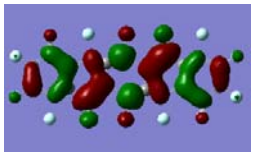
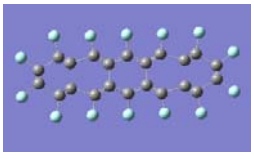
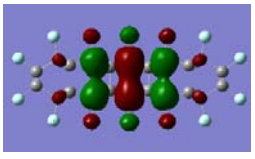
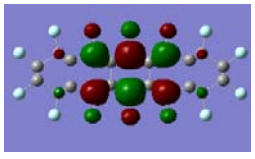
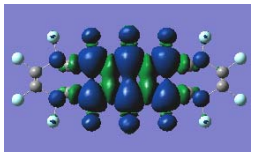
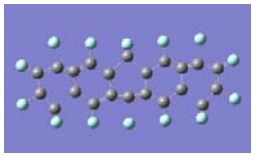
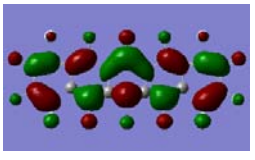
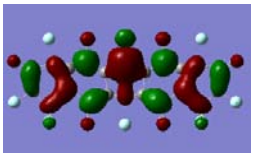
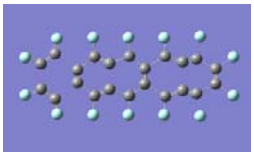
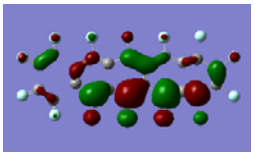
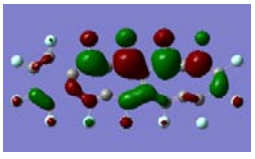
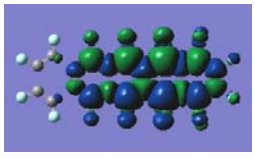
20 **0.00**	**2.00** **19.57**				
21 **0.00**	**2.01** **19.59**				
22 **0.092**	**1.82** **15.41**				
23 **0.00**	**1.98** **18.86**				
24 **0.00**	**1.98** **18.99**				
25 **0.00**	**2.03** **20.26**				
26 **0.00**	**1.97** **18.65**				
27 **0.00**	**2.01** **19.75**				
28 **0.00**	**1.96** **19.23**				
29 **0.00**	**2.17** **25.32**				
30 **0.00**	**2.02** **20.22**				

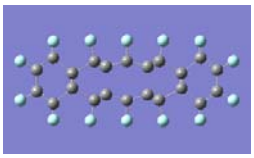
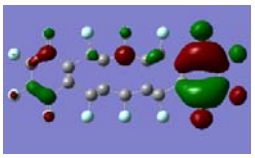
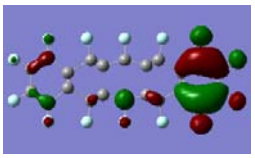
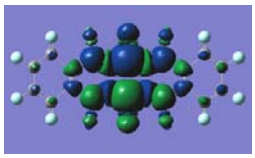
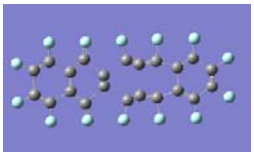
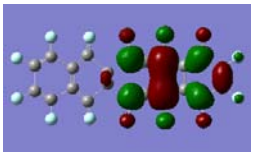
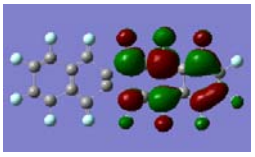
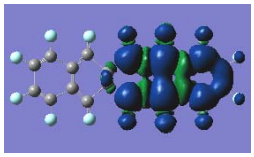
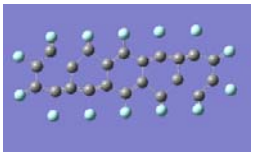
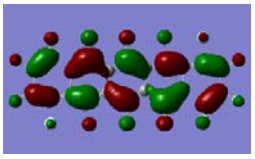
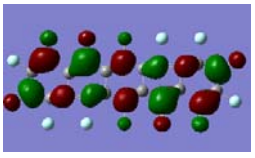
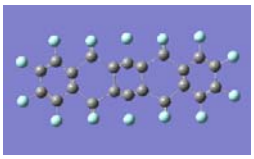
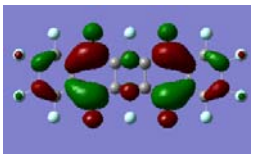
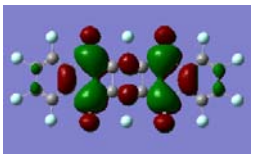
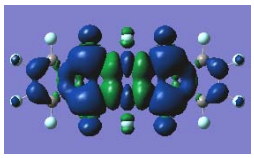
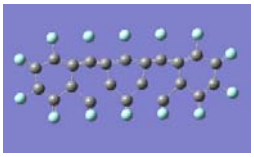
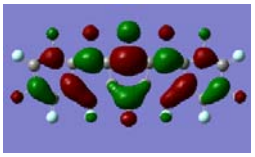
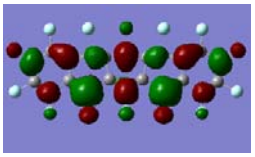
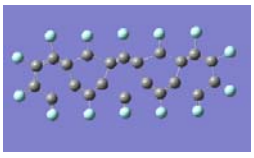
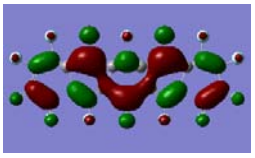
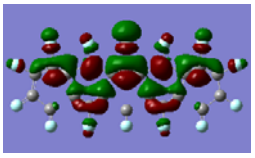
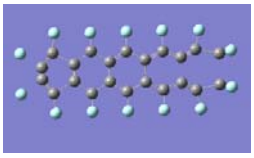
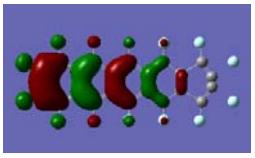
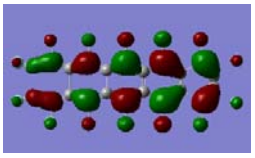
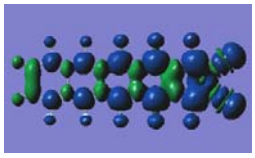
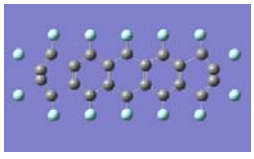
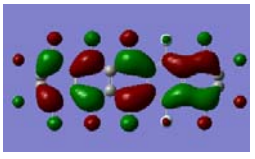
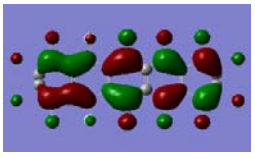
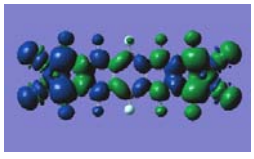
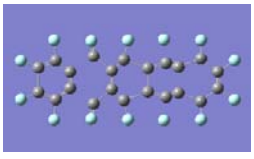
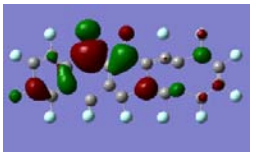
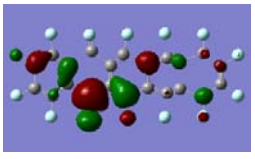
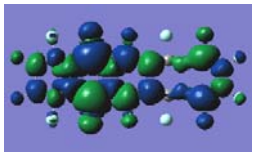
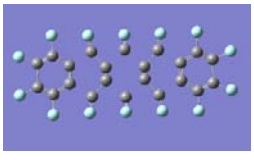
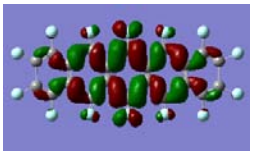
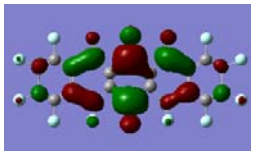
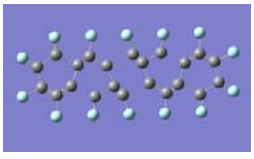
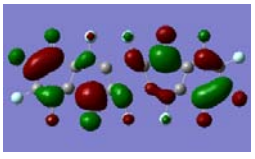
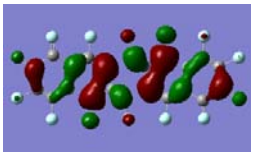
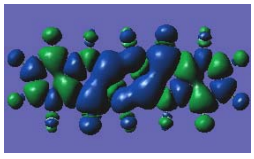
31 0.310	1.70 13.94				
32 0.00	2.11 23.86				
33 0.00	2.13 23.85				
34 0.00	1.99 19.08				
35 0.235	1.91 14.95				
36 0.00	2.05 21.09				
37 0.00	2.08 21.72				
38 0.681	1.52 8.92				
39 0.327	1.68 12.12				
40 0.00	1.87 17.07				
41 0.292	1.68 12.95				

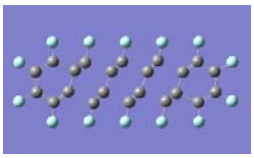
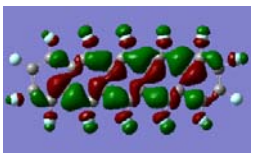
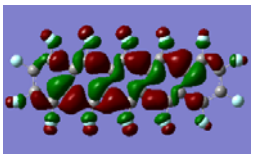
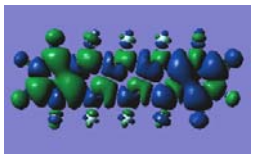
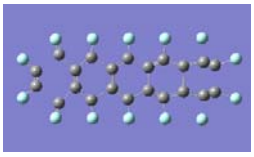
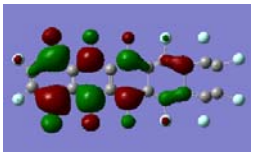
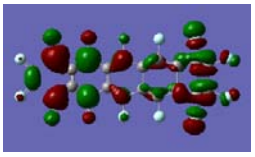
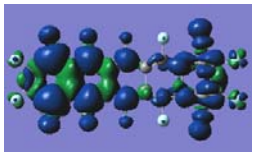
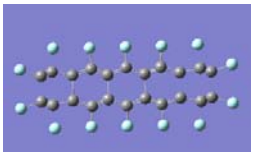
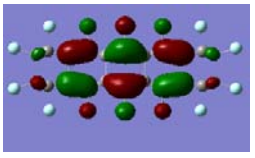
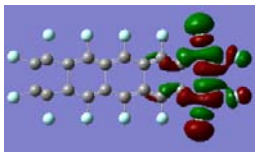
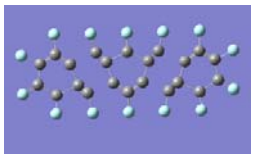
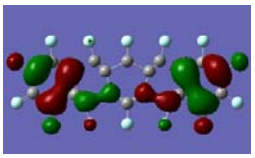
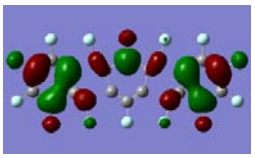
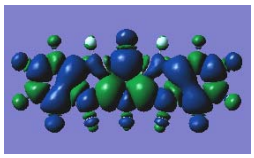
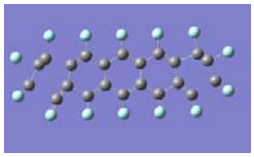
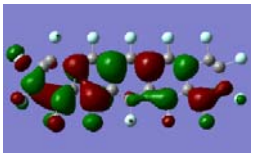
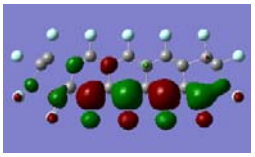
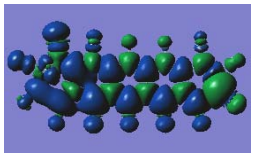
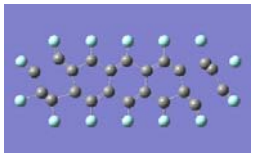
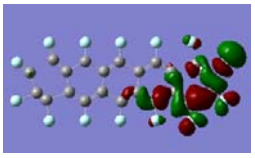
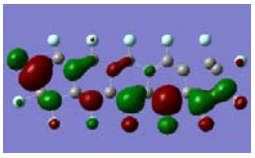
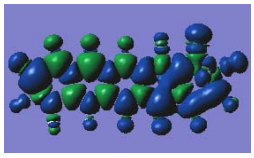
42 0.00	1.94 17.25				
43 0.00	2.08 21.32				
44 0.240	1.91 16.75				
45 0.762	1.38 4.57				
46 0.00	1.99 19.96				
47 0.00	2.10 22.65				
48 0.00	2.02 19.81				
49 1.251	1.22 -0.81				
50 0.00	1.90 17.27				
51 0.00	1.53 13.41				
52 1.449	1.19 3.64				

53 0.947	1.63 11.59				
54 0.407	1.73 16.03				
55 0.00	1.76 15.56				
56 1.560	1.28 1.56				
57 1.170	1.52 4.87				
58 1.409	1.31 1.89				
59 0.642	1.69 8.52				
60 1.121	1.38 -2.41				
61 0.00	1.98 20.05				
62 1.478	1.18 -5.81				
63 0.00	1.92 17.27				

64 0.00	2.01 18.84				
65 0.00	1.94 17.21				
66 0.464	1.87 12.15				
67 0.00	2.06 21.29				
68 0.064	1.84 15.67				
69 0.00	1.97 19.74				
70 0.714	1.70 10.57				
71 0.00	2.01 19.89				
72 0.00	2.00 20.56				
73 0.00	1.98 19.75				
74 0.00	1.89 17.43				

75 0.00	4.96 60.76				
76 0.00	2.05 29.48				
77 0.160	1.95 15.84				
78 0.00	1.90 17.76				
79 0.00	2.02 20.19				
80 0.00	3.16 57.42				
81 1.277	1.02 -9.56				
82 0.00	1.84 15.55				
83 2.027	1.53 -5.24				
84 0.00	1.87 19.70				
85 1.192	0.87 -20.12				

86 0.970	1.44 -18.87				
87 2.017	0.99 -19.43				
88 0.00	1.33 6.10				
89 2.179	1.21 -8.47				
90 0.00	2.04 22.10				
91 0.00	1.73 14.11				
92 2.064	0.68 -17.70				
93 1.905	0.21 -31.74				
94 1.066	1.03 -20.82				
95 0.00	1.76 5.70				
96 2.234	1.19 -12.15				

97 1.179	0.33 -24.90				
98 2.037	0.37 -16.56				
99 0.00	1.49 28.78				
100 2.664	1.03 -27.61				
101 2.518	0.69 -22.54				
102 2.336	0.59 -20.58				

4. Energies of the CS, BS and T States and Corresponding Energy Orders for All Vibrational Modes and the $<S^2>$ Values for the Negatively Shifted Distorted Configurations

Table S3. Energies (in a.u.) for the closed-shell singlet (CS), broken-symmetry open-shell singlet (BS) and triplet (T) of all vibration-distorted snapshot configurations (negatively shifted) with diradical character and the corresponding energy orders calculated at the (U)B3LYP/6-31+G (d) level as well as the $<S^2>$ values

Vibration Mode	$<S^2>$	$E_{(CS)}$	$E_{(BS)}$	$E_{(T)}$	Energy Order
16	0.093	-2236.0587115	-2236.0587483	-2236.0332295	$E_{(BS)} < E_{(CS)} < E_{(T)}$
19	0.056	-2236.0178388	-2236.0178523	-2235.9913210	$E_{(BS)} < E_{(CS)} < E_{(T)}$
29	0.194	-2235.9339193	-2235.9340889	-2235.9105490	$E_{(BS)} < E_{(CS)} < E_{(T)}$
31	0.310	-2235.9646018	-2235.9649967	-2235.9423506	$E_{(BS)} < E_{(CS)} < E_{(T)}$
35	0.204	-2235.9419396	-2235.9421752	-2235.9176272	$E_{(BS)} < E_{(CS)} < E_{(T)}$
38	0.680	-2235.9373558	-2235.9398025	-2235.9230974	$E_{(BS)} < E_{(CS)} < E_{(T)}$
39	0.414	-2235.8737291	-2235.8746688	-2235.8564318	$E_{(BS)} < E_{(CS)} < E_{(T)}$
41	0.290	-2235.8602890	-2235.8606736	-2235.8396095	$E_{(BS)} < E_{(CS)} < E_{(T)}$
42	0.407	-2235.8609972	-2235.8618773	-2235.8436951	$E_{(BS)} < E_{(CS)} < E_{(T)}$
44	0.247	-2235.8677095	-2235.8679875	-2235.8412279	$E_{(BS)} < E_{(CS)} < E_{(T)}$
49	1.251	-2235.8205073	-2235.8341252	-2235.8218020	$E_{(BS)} < E_{(T)} < E_{(CS)}$
52	1.446	-2235.7616539	-2235.7738708	-2235.7558414	$E_{(BS)} < E_{(CS)} < E_{(T)}$
53	0.892	-2235.6241825	-2235.6277384	-2235.6043734	$E_{(BS)} < E_{(CS)} < E_{(T)}$
54	0.404	-2235.6675194	-2235.6680748	-2235.6419440	$E_{(BS)} < E_{(CS)} < E_{(T)}$
56	1.560	-2235.7111462	-2235.7259044	-2235.7086514	$E_{(BS)} < E_{(CS)} < E_{(T)}$
57	1.170	-2235.6275310	-2235.6366556	-2235.6197521	$E_{(BS)} < E_{(CS)} < E_{(T)}$
58	1.433	-2235.6800398	-2235.6958019	-2235.6783697	$E_{(BS)} < E_{(CS)} < E_{(T)}$
60	1.120	-2235.5709646	-2235.5836636	-2235.5747826	$E_{(BS)} < E_{(T)} < E_{(CS)}$
62	1.478	-2235.6437316	-2235.6654025	-2235.6530065	$E_{(BS)} < E_{(T)} < E_{(CS)}$
66	0.464	-2235.3644252	-2235.3659261	-2235.3450315	$E_{(BS)} < E_{(CS)} < E_{(T)}$
70	0.799	-2235.1918275	-2235.1990903	-2235.1879950	$E_{(BS)} < E_{(CS)} < E_{(T)}$
73	0.415	-2234.7085533	-2234.7093851	-2234.6897542	$E_{(BS)} < E_{(CS)} < E_{(T)}$
76	0.989	-2233.5375555	-2233.5467974	-2233.5424792	$E_{(BS)} < E_{(T)} < E_{(CS)}$
77	0.217	-2234.4838420	-2234.4841026	-2234.4598057	$E_{(BS)} < E_{(CS)} < E_{(T)}$
85	1.189	-2233.7527860	-2233.7872634	-2233.7828489	$E_{(BS)} < E_{(T)} < E_{(CS)}$
87	2.018	-2232.9982987		-2233.0283197	$E_{(T)} < E_{(CS)}$
89	2.013	-2234.0988960	-2234.1106849	-2234.1127363	$E_{(T)} < E_{(BS)} < E_{(CS)}$
92	2.034	-2232.8374505		-2232.8668912	$E_{(T)} < E_{(CS)}$
94	2.014	-2233.4746247		-2233.5065568	$E_{(T)} < E_{(CS)}$
96	2.538	-2233.1652417		-2233.1859216	$E_{(T)} < E_{(CS)}$
97	1.188	-2233.2009909	-2233.2416352	-2233.2407263	$E_{(BS)} < E_{(T)} < E_{(CS)}$
98	1.154	-2232.7285707	-2232.7607777	-2232.7563223	$E_{(BS)} < E_{(T)} < E_{(CS)}$
99	2.205	-2234.1181791		-2234.1376367	$E_{(T)} < E_{(CS)}$
100	2.063	-2232.9260215		-2232.9494256	$E_{(T)} < E_{(CS)}$
101	2.208	-2230.9497004	-2230.9510112	-2230.9745305	$E_{(T)} < E_{(BS)} < E_{(CS)}$
102	2.050	-2231.0769920	-2231.0797783	-2231.1008283	$E_{(T)} < E_{(BS)} < E_{(CS)}$

Table S4. Energies (in a.u.) for the closed-shell singlet (CS) and triplet (T) of all vibration-distorted snapshot configurations (negatively shifted) without diradical character and the corresponding energy orders calculated at the (U)B3LYP/6-31+G (d) level

Vibration Mode	$E_{(CS)}$	$E_{(T)}$	Energy Order
1	-2236.0864227	-2236.0554072	$E_{(CS)}<E_{(T)}$
2	-2236.0858787	-2236.0531497	$E_{(CS)}<E_{(T)}$
3	-2236.0835590	-2236.0516400	$E_{(CS)}<E_{(T)}$
4	-2236.0835492	-2236.0531108	$E_{(CS)}<E_{(T)}$
5	-2236.0782406	-2236.0464137	$E_{(CS)}<E_{(T)}$
6	-2236.0764625	-2236.0463421	$E_{(CS)}<E_{(T)}$
7	-2236.0794254	-2236.0476116	$E_{(CS)}<E_{(T)}$
8	-2236.0741374	-2236.0434549	$E_{(CS)}<E_{(T)}$
9	-2236.0734294	-2236.0427241	$E_{(CS)}<E_{(T)}$
10	-2236.0720469	-2236.0438416	$E_{(CS)}<E_{(T)}$
11	-2236.0583299	-2236.0275405	$E_{(CS)}<E_{(T)}$
12	-2236.0531905	-2236.0223392	$E_{(CS)}<E_{(T)}$
13	-2236.0524247	-2236.0210589	$E_{(CS)}<E_{(T)}$
14	-2236.0493336	-2236.0209479	$E_{(CS)}<E_{(T)}$
15	-2236.0493044	-2236.0187701	$E_{(CS)}<E_{(T)}$
17	-2236.0423661	-2236.0120683	$E_{(CS)}<E_{(T)}$
18	-2236.0183330	-2235.9863116	$E_{(CS)}<E_{(T)}$
20	-2235.9774284	-2235.9462747	$E_{(CS)}<E_{(T)}$
21	-2235.9900945	-2235.9594263	$E_{(CS)}<E_{(T)}$
22	-2235.8899892	-2235.8522760	$E_{(CS)}<E_{(T)}$
23	-2235.9672789	-2235.9371637	$E_{(CS)}<E_{(T)}$
24	-2235.9691179	-2235.9366236	$E_{(CS)}<E_{(T)}$
25	-2235.9479681	-2235.9156115	$E_{(CS)}<E_{(T)}$
26	-2235.9316023	-2235.9004161	$E_{(CS)}<E_{(T)}$
27	-2235.9506635	-2235.9192380	$E_{(CS)}<E_{(T)}$
28	-2235.9046746	-2235.8730682	$E_{(CS)}<E_{(T)}$
30	-2235.9457601	-2235.9131714	$E_{(CS)}<E_{(T)}$
32	-2235.9452938	-2235.9057925	$E_{(CS)}<E_{(T)}$
33	-2235.9481764	-2235.9094769	$E_{(CS)}<E_{(T)}$
34	-2235.7925457	-2235.7621807	$E_{(CS)}<E_{(T)}$
36	-2235.8983709	-2235.8677738	$E_{(CS)}<E_{(T)}$
37	-2235.9233141	-2235.8886281	$E_{(CS)}<E_{(T)}$
40	-2235.8785237	-2235.8505877	$E_{(CS)}<E_{(T)}$
43	-2235.8428441	-2235.8087992	$E_{(CS)}<E_{(T)}$

45	-2235.8707889	-2235.8273927	$E_{(CS)}<E_{(T)}$
46	-2235.8120769	-2235.7793411	$E_{(CS)}<E_{(T)}$
47	-2235.7751624	-2235.7395817	$E_{(CS)}<E_{(T)}$
48	-2235.7810916	-2235.7494019	$E_{(CS)}<E_{(T)}$
50	-2235.7376404	-2235.7080472	$E_{(CS)}<E_{(T)}$
51	-2235.7219818	-2235.7007928	$E_{(CS)}<E_{(T)}$
55	-2235.7129519	-2235.6888249	$E_{(CS)}<E_{(T)}$
59	-2235.6419904	-2235.5977611	$E_{(CS)}<E_{(T)}$
61	-2235.6196923	-2235.5876222	$E_{(CS)}<E_{(T)}$
63	-2235.5347178	-2235.5055120	$E_{(CS)}<E_{(T)}$
64	-2235.4824669	-2235.4500160	$E_{(CS)}<E_{(T)}$
65	-2235.4670027	-2235.4396057	$E_{(CS)}<E_{(T)}$
67	-2235.0401440	-2235.0072025	$E_{(CS)}<E_{(T)}$
68	-2235.1261605	-2235.0995616	$E_{(CS)}<E_{(T)}$
69	-2235.0679356	-2235.0364242	$E_{(CS)}<E_{(T)}$
71	-2234.9117407	-2234.8794008	$E_{(CS)}<E_{(T)}$
72	-2234.7861090	-2234.7519159	$E_{(CS)}<E_{(T)}$
74	-2234.6215425	-2234.5937091	$E_{(CS)}<E_{(T)}$
75	-2234.0378811	-2233.9196596	$E_{(CS)}<E_{(T)}$
78	-2234.2044708	-2234.1759915	$E_{(CS)}<E_{(T)}$
79	-2234.0160577	-2233.9839837	$E_{(CS)}<E_{(T)}$
80	-2234.4135840	-2234.3229206	$E_{(CS)}<E_{(T)}$
81	-2233.4161805	-2233.3902387	$E_{(CS)}<E_{(T)}$
82	-2234.2092928	-2234.1832225	$E_{(CS)}<E_{(T)}$
83	-2234.5025742	-2234.3915990	$E_{(CS)}<E_{(T)}$
84	-2233.9544119	-2233.9233609	$E_{(CS)}<E_{(T)}$
86	-2234.2556896	-2234.1893516	$E_{(CS)}<E_{(T)}$
88	-2234.0513713	-2234.0412450	$E_{(CS)}<E_{(T)}$
90	-2233.9959363	-2233.9602172	$E_{(CS)}<E_{(T)}$
91	-2233.8417573	-2233.8193457	$E_{(CS)}<E_{(T)}$
93	-2233.3213149	-2233.3070040	$E_{(CS)}<E_{(T)}$
95	-2233.7189957	-2233.7064755	$E_{(CS)}<E_{(T)}$

Table S5. Energies (in a.u.) for the closed-shell singlet (CS), broken-symmetry open-shell singlet (BS) and triplet (T) of all vibration-distorted snapshot configurations (positively shifted) with diradical character and the corresponding energy orders calculated at the (U)B3LYP/6-31+G (d) level

Vibration Mode	$E_{(CS)}$	$E_{(BS)}$	$E_{(T)}$	Energy Order
19	-2236.0179779	-2236.0179904	-2235.9914243	$E_{(BS)} < E_{(CS)} < E_{(T)}$
22	-2235.9800319	-2235.9800678	-2235.9554244	$E_{(BS)} < E_{(CS)} < E_{(T)}$
31	-2235.9645959	-2235.9649912	-2235.9423452	$E_{(BS)} < E_{(CS)} < E_{(T)}$
35	-2235.9426840	-2235.9430100	-2235.9188188	$E_{(BS)} < E_{(CS)} < E_{(T)}$
38	-2235.9373110	-2235.9397634	-2235.9230644	$E_{(BS)} < E_{(CS)} < E_{(T)}$
39	-2235.8759631	-2235.8764553	-2235.8566144	$E_{(BS)} < E_{(CS)} < E_{(T)}$
41	-2235.8613566	-2235.8617462	-2235.8406789	$E_{(BS)} < E_{(CS)} < E_{(T)}$
44	-2235.8677822	-2235.8680384	-2235.8410404	$E_{(BS)} < E_{(CS)} < E_{(T)}$
45	-2235.7443919	-2235.7482406	-2235.7370894	$E_{(BS)} < E_{(CS)} < E_{(T)}$
49	-2235.8205109	-2235.8341251	-2235.8218038	$E_{(BS)} < E_{(T)} < E_{(CS)}$
52	-2235.7615232	-2235.7738043	-2235.7557117	$E_{(BS)} < E_{(CS)} < E_{(T)}$
53	-2235.6238359	-2235.6279440	-2235.6053300	$E_{(BS)} < E_{(CS)} < E_{(T)}$
54	-2235.6675170	-2235.6680680	-2235.6419264	$E_{(BS)} < E_{(CS)} < E_{(T)}$
56	-2235.7111448	-2235.7259030	-2235.7086503	$E_{(BS)} < E_{(CS)} < E_{(T)}$
57	-2235.6275232	-2235.6366424	-2235.6197398	$E_{(BS)} < E_{(CS)} < E_{(T)}$
58	-2235.6809858	-2235.6958117	-2235.6779657	$E_{(BS)} < E_{(CS)} < E_{(T)}$
59	-2235.5669988	-2235.5699568	-2235.5533993	$E_{(BS)} < E_{(CS)} < E_{(T)}$
60	-2235.5702997	-2235.5830332	-2235.5741482	$E_{(BS)} < E_{(T)} < E_{(CS)}$
62	-2235.6437319	-2235.6654022	-2235.6530060	$E_{(BS)} < E_{(T)} < E_{(CS)}$
66	-2235.3646946	-2235.3661937	-2235.3452967	$E_{(BS)} < E_{(CS)} < E_{(T)}$
68	-2235.1133869	-2235.1134034	-2235.0883642	$E_{(BS)} < E_{(CS)} < E_{(T)}$
70	-2234.9631020	-2234.9663600	-2234.9462283	$E_{(BS)} < E_{(CS)} < E_{(T)}$
77	-2234.4716661	-2234.4718040	-2234.4463636	$E_{(BS)} < E_{(CS)} < E_{(T)}$
81	-2234.3302731	-2234.3559331	-2234.3455425	$E_{(BS)} < E_{(T)} < E_{(CS)}$
83	-2232.6292038		-2232.6375755	$E_{(T)} < E_{(CS)}$
85	-2233.8250736	-2233.8612090	-2233.8572007	$E_{(BS)} < E_{(T)} < E_{(CS)}$
86	-2232.5974032	-2232.6295599	-2232.6275351	$E_{(BS)} < E_{(T)} < E_{(CS)}$
87	-2232.9731270		-2233.0041509	$E_{(T)} < E_{(CS)}$
89	-2233.7329442		-2233.7464699	$E_{(T)} < E_{(CS)}$
92	-2233.1053119		-2233.1335767	$E_{(T)} < E_{(CS)}$
93	-2232.0708900	-2232.1250919	-2232.1229530	$E_{(BS)} < E_{(T)} < E_{(CS)}$
94	-2233.5721661	-2233.6069229	-2233.6053990	$E_{(BS)} < E_{(T)} < E_{(CS)}$
96	-2233.2093191		-2233.2287213	$E_{(T)} < E_{(CS)}$
97	-2233.2745687	-2233.3151679	-2233.3143146	$E_{(BS)} < E_{(T)} < E_{(CS)}$
98	-2232.5839151	-2232.5967574	-2232.6103466	$E_{(T)} < E_{(BS)} < E_{(CS)}$
100	-2232.9032211		-2232.9472928	$E_{(T)} < E_{(CS)}$

101	-2231.0650107		-2231.1009930	$E_{(T)} < E_{(CS)}$
102	-2231.0912443	-2231.1021989	-2231.1240959	$E_{(T)} < E_{(BS)} < E_{(CS)}$

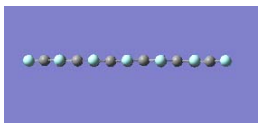
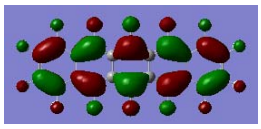
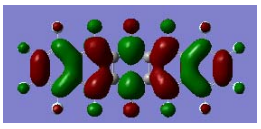
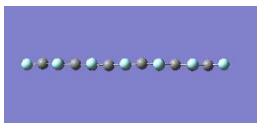
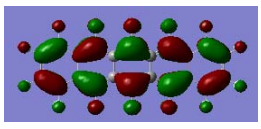
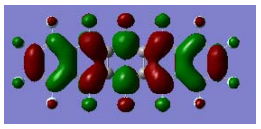
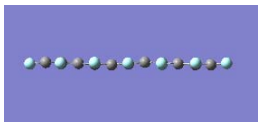
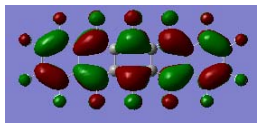
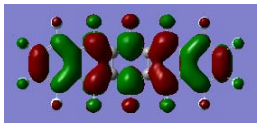
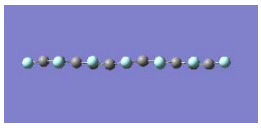
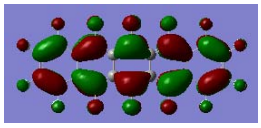
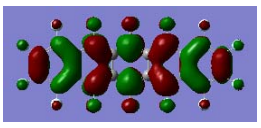
Table S6. Energies (in a.u.) for the closed-shell singlet (CS) and triplet (T) of all vibration-distorted snapshot configurations (positively shifted) without diradical character and the corresponding energy orders calculated at the (U)B3LYP/6-31+G (d) level

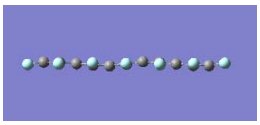
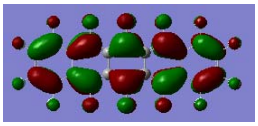
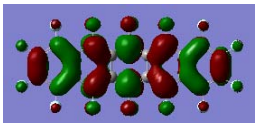
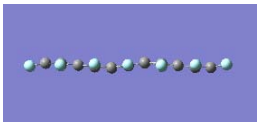
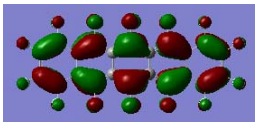
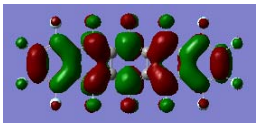
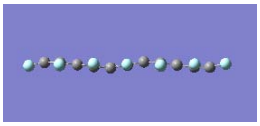
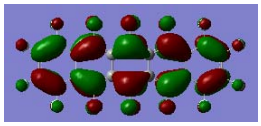
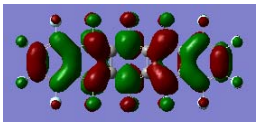
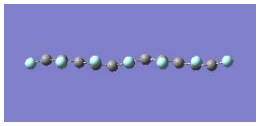
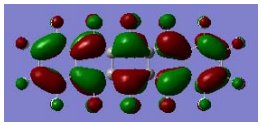
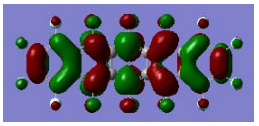
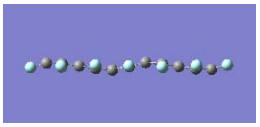
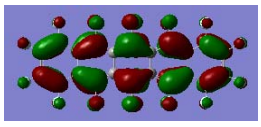
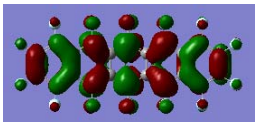
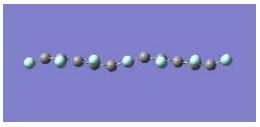
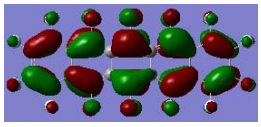
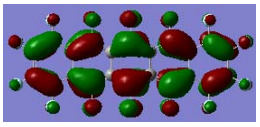
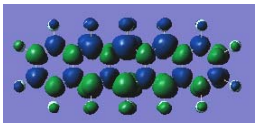
Vibration Mode	$E_{(CS)}$	$E_{(T)}$	Energy Order
1	-2236.0864207	-2236.0554060	$E_{(CS)}<E_{(T)}$
2	-2236.0858773	-2236.0531469	$E_{(CS)}<E_{(T)}$
3	-2236.0830315	-2236.0506797	$E_{(CS)}<E_{(T)}$
4	-2236.0835224	-2236.0530823	$E_{(CS)}<E_{(T)}$
5	-2236.0782507	-2236.0464243	$E_{(CS)}<E_{(T)}$
6	-2236.0764554	-2236.0463345	$E_{(CS)}<E_{(T)}$
7	-2236.0794167	-2236.0476008	$E_{(CS)}<E_{(T)}$
8	-2236.0738701	-2236.0431808	$E_{(CS)}<E_{(T)}$
9	-2236.0734654	-2236.0427975	$E_{(CS)}<E_{(T)}$
10	-2236.0709075	-2236.0425665	$E_{(CS)}<E_{(T)}$
11	-2236.0589382	-2236.0273988	$E_{(CS)}<E_{(T)}$
12	-2236.0521816	-2236.0212579	$E_{(CS)}<E_{(T)}$
13	-2236.0523984	-2236.0210773	$E_{(CS)}<E_{(T)}$
14	-2236.0493543	-2236.0209721	$E_{(CS)}<E_{(T)}$
15	-2236.0493519	-2236.0187236	$E_{(CS)}<E_{(T)}$
16	-2236.0463271	-2236.0085710	$E_{(CS)}<E_{(T)}$
17	-2236.0423663	-2236.0120685	$E_{(CS)}<E_{(T)}$
18	-2236.0183870	-2235.9875723	$E_{(CS)}<E_{(T)}$
20	-2235.9773344	-2235.9460977	$E_{(CS)}<E_{(T)}$
21	-2235.9902060	-2235.9589293	$E_{(CS)}<E_{(T)}$
23	-2235.9672233	-2235.9371116	$E_{(CS)}<E_{(T)}$
24	-2235.9702551	-2235.9399299	$E_{(CS)}<E_{(T)}$
25	-2235.9479747	-2235.9156222	$E_{(CS)}<E_{(T)}$
26	-2235.9305162	-2235.9007443	$E_{(CS)}<E_{(T)}$
27	-2235.9516887	-2235.9201648	$E_{(CS)}<E_{(T)}$
28	-2235.9315778	-2235.9008690	$E_{(CS)}<E_{(T)}$
29	-2235.9464941	-2235.9060715	$E_{(CS)}<E_{(T)}$
30	-2235.9453951	-2235.9131131	$E_{(CS)}<E_{(T)}$
32	-2235.9462368	-2235.9081394	$E_{(CS)}<E_{(T)}$
33	-2235.9490584	-2235.9109759	$E_{(CS)}<E_{(T)}$
34	-2235.7878568	-2235.7573974	$E_{(CS)}<E_{(T)}$
36	-2235.8991532	-2235.8654802	$E_{(CS)}<E_{(T)}$
37	-2235.9233434	-2235.8886695	$E_{(CS)}<E_{(T)}$

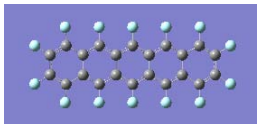
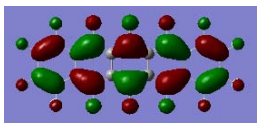
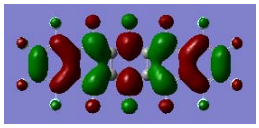
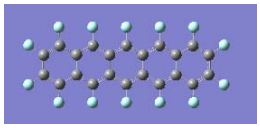
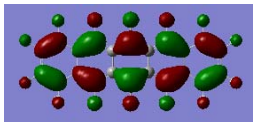
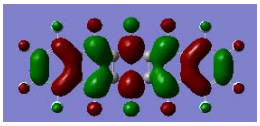
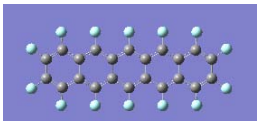
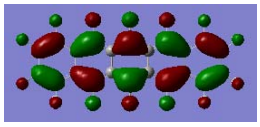
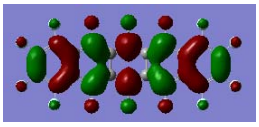
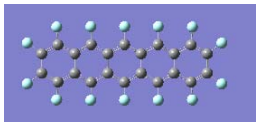
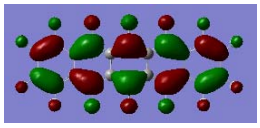
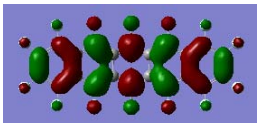
40	-2235.8782167	-2235.8509665	$E_{(CS)}<E_{(T)}$
42	-2235.8569553	-2235.8294037	$E_{(CS)}<E_{(T)}$
43	-2235.8428632	-2235.8088248	$E_{(CS)}<E_{(T)}$
46	-2235.8110071	-2235.7791442	$E_{(CS)}<E_{(T)}$
47	-2235.7751310	-2235.7389737	$E_{(CS)}<E_{(T)}$
48	-2235.7811592	-2235.7495287	$E_{(CS)}<E_{(T)}$
50	-2235.7363180	-2235.7087408	$E_{(CS)}<E_{(T)}$
51	-2235.7219881	-2235.7005721	$E_{(CS)}<E_{(T)}$
55	-2235.7127299	-2235.6878816	$E_{(CS)}<E_{(T)}$
61	-2235.6198165	-2235.5878083	$E_{(CS)}<E_{(T)}$
63	-2235.5336404	-2235.5060668	$E_{(CS)}<E_{(T)}$
64	-2235.4860404	-2235.4559648	$E_{(CS)}<E_{(T)}$
65	-2235.4663516	-2235.4388723	$E_{(CS)}<E_{(T)}$
67	-2235.0271692	-2234.9931845	$E_{(CS)}<E_{(T)}$
69	-2235.0679120	-2235.0363931	$E_{(CS)}<E_{(T)}$
71	-2234.9249777	-2234.8932245	$E_{(CS)}<E_{(T)}$
72	-2234.7815423	-2234.7487187	$E_{(CS)}<E_{(T)}$
73	-2234.6289849	-2234.5974527	$E_{(CS)}<E_{(T)}$
74	-2234.6215415	-2234.5937140	$E_{(CS)}<E_{(T)}$
75	-2234.0393859	-2233.9423859	$E_{(CS)}<E_{(T)}$
76	-2234.5133261	-2234.4662582	$E_{(CS)}<E_{(T)}$
78	-2234.1821923	-2234.1538314	$E_{(CS)}<E_{(T)}$
79	-2234.0240204	-2233.9917853	$E_{(CS)}<E_{(T)}$
80	-2234.3943562	-2234.3026921	$E_{(CS)}<E_{(T)}$
82	-2234.2235578	-2234.1987258	$E_{(CS)}<E_{(T)}$
84	-2233.9609821	-2233.9295385	$E_{(CS)}<E_{(T)}$
88	-2234.0382778	-2234.0285330	$E_{(CS)}<E_{(T)}$
90	-2233.9894067	-2233.9541177	$E_{(CS)}<E_{(T)}$
91	-2233.8375137	-2233.8149858	$E_{(CS)}<E_{(T)}$
95	-2233.4246922	-2233.4155916	$E_{(CS)}<E_{(T)}$
99	-2231.4646959	-2231.4187417	$E_{(CS)}<E_{(T)}$

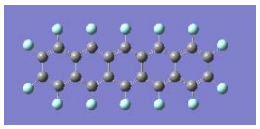
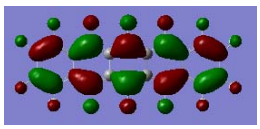
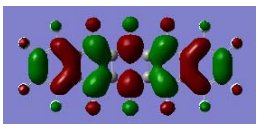
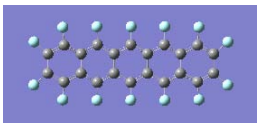
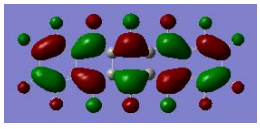
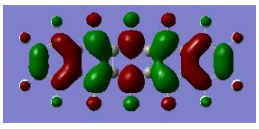
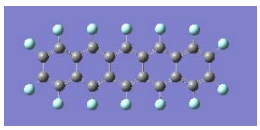
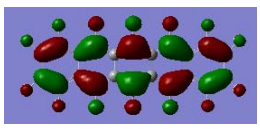
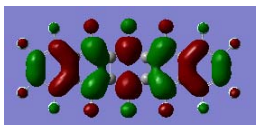
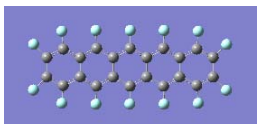
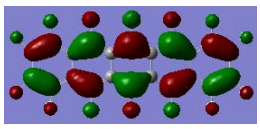
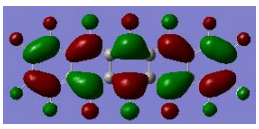
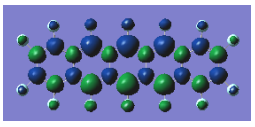
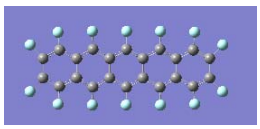
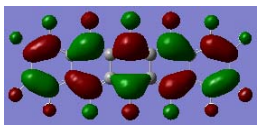
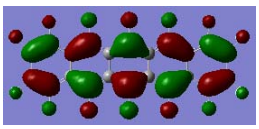
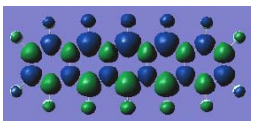
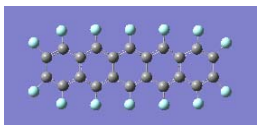
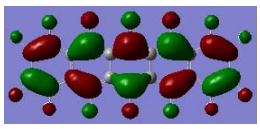
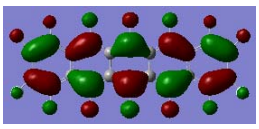
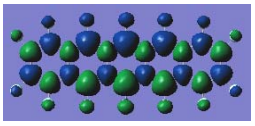
5. The Variational Regularities of the Singlet-Triplet Energy gaps, HOMO-LUMO gaps, $<S^2>$ Values and so on, with the Increase of Vibrational Amplitude for Some Representative Diradical Vibrational Modes (Only the Positive Shift Is Considered for a Vibrational Mode)

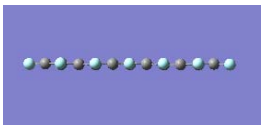
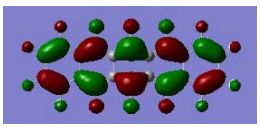
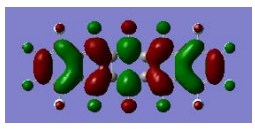
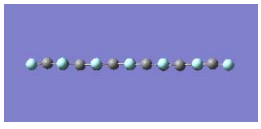
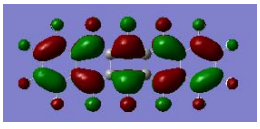
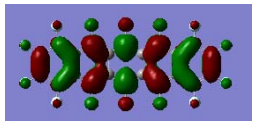
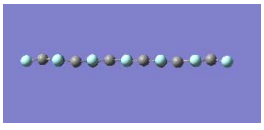
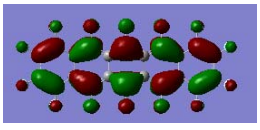
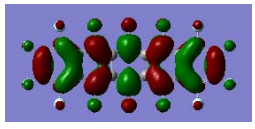
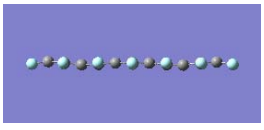
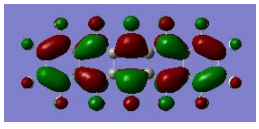
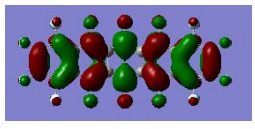
Table S7. The variational regularities of the HOMO-LUMO gaps of the closed-shell singlet states (H-L gap, eV), T-S gaps between the closed-shell singlet and triplet states ($\Delta E_{(T\text{-}CS)} = E_T - E_{CS}$, kcal/mol), T-BS gaps between the broken-symmetry singlet and triplet states ($\Delta E_{(T\text{-}BS)} = E_T - E_{BS}$, kcal/mol), and the $<S^2>$ values with the increase of vibrational amplitude for diradical perturbations in some typical diradical vibrational modes (positively shifted). Two SOMOs and spin densities of the BS or T (only vibrational modes 92 and 98) states for diradical perturbations associated with the shapes of HOMO and LUMO and relevant energies for perturbations not inducing diradical character are also listed.

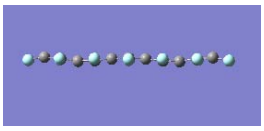
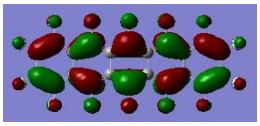
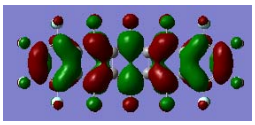
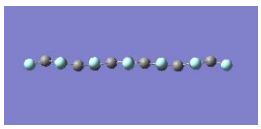
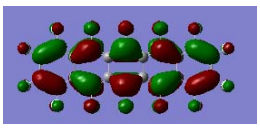
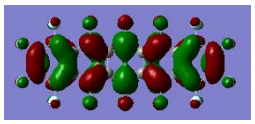
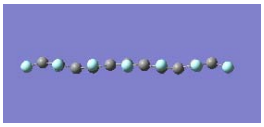
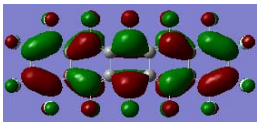
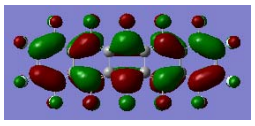
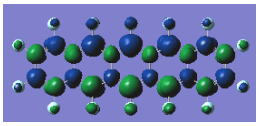
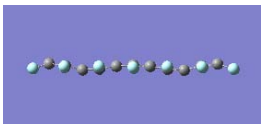
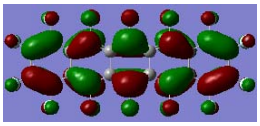
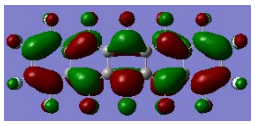
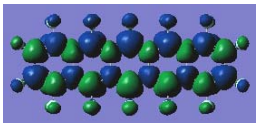
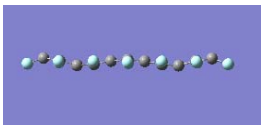
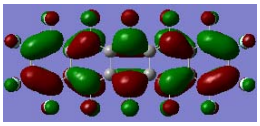
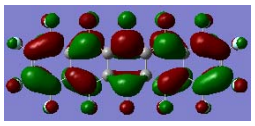
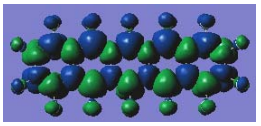
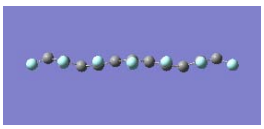
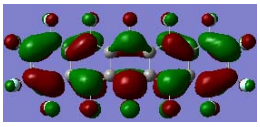
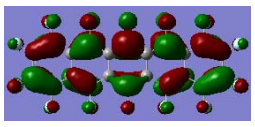
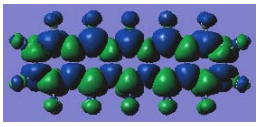
Modes $<S^2>$	H-L gap T-S gap T-BSgap	Distortion Modes	HOMO or SOMO α (SOMO 1)	LUMO or SOMO β (SOMO 2)	BS or T State Spin density
19-1 0.00	2.01 19.76				
19-2 0.00	2.01 19.65				
19-3 0.00	2.00 19.48				
19-4 0.00	2.00 19.27				

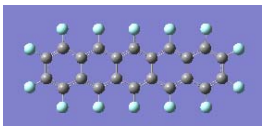
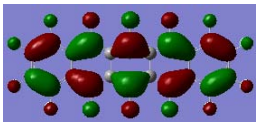
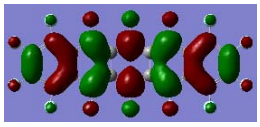
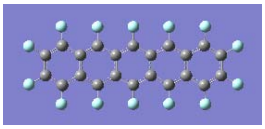
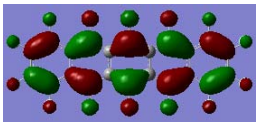
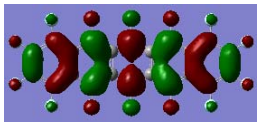
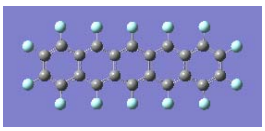
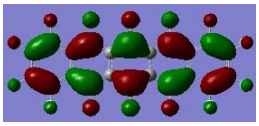
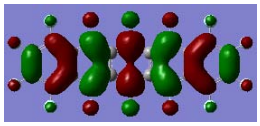
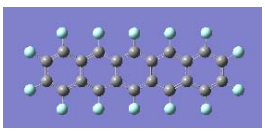
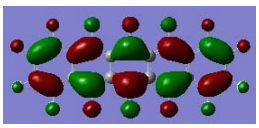
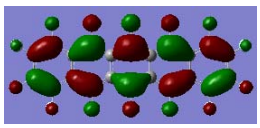
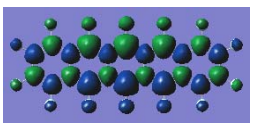
19-5 **0.00**	**1.99** **18.99**				
19-6 **0.00**	**1.98** **18.66**				
19-7 **0.00**	**1.97** **18.26**				
19-8 **0.00**	**1.96** **17.79**				
19-9 **0.00**	**1.94** **17.25**				
19 **0.054**	**1.92** **16.63** **16.64**				

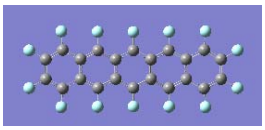
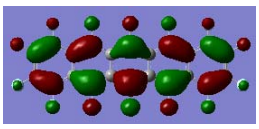
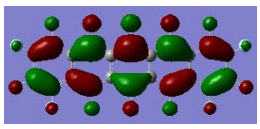
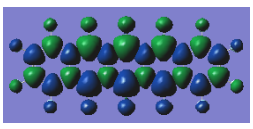
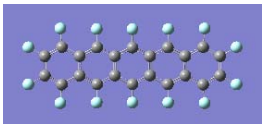
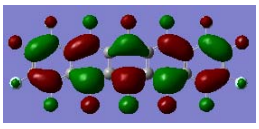
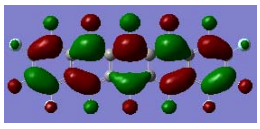
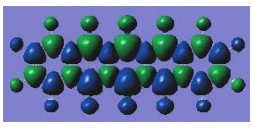
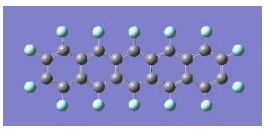
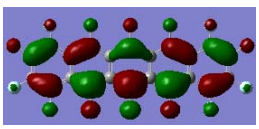
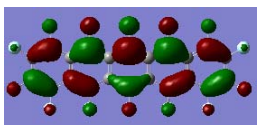
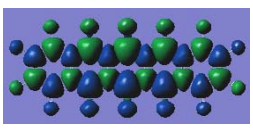
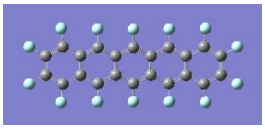
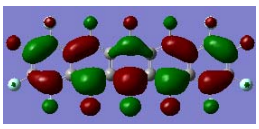
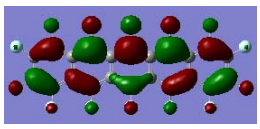
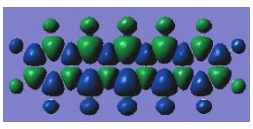
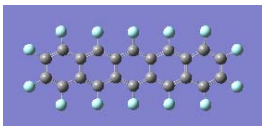
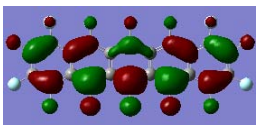
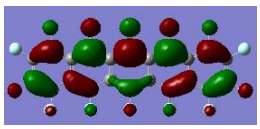
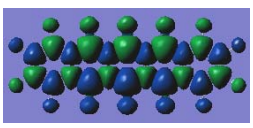
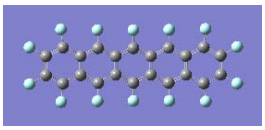
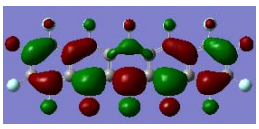
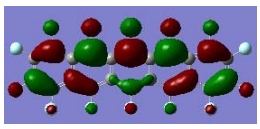
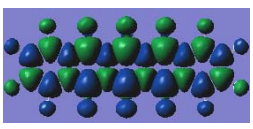
22-1 **0.00**	**1.99** **19.32**				
22-2 **0.00**	**1.97** **18.84**				
22-3 **0.00**	**1.95** **18.36**				
22-4 **0.00**	**1.93** **17.89**				

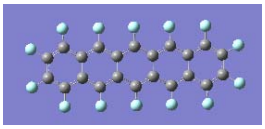
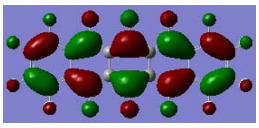
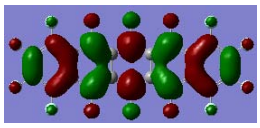
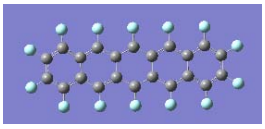
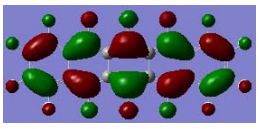
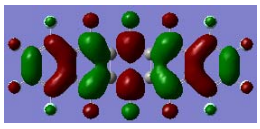
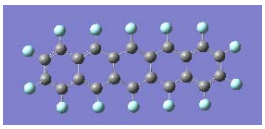
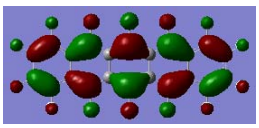
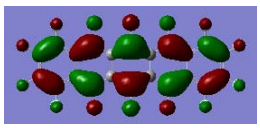
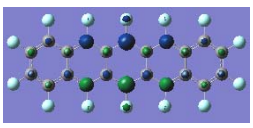
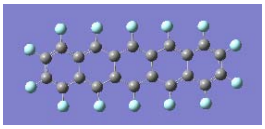
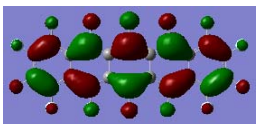
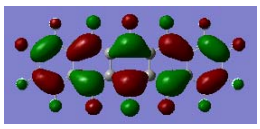
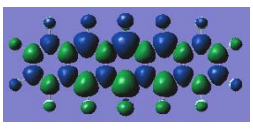
22-5 **0.00**	**1.91** **17.43**				
22-6 **0.00**	**1.89** **16.99**				
22-7 **0.00**	**1.87** **16.56**				
22-8 **0.023**	**1.85** **16.16** **16.16**				
22-9 **0.059**	**1.84** **15.77** **15.78**				
22 **0.092**	**1.82** **15.41** **15.44**				

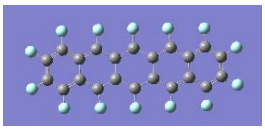
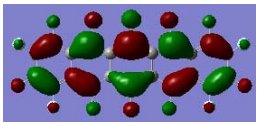
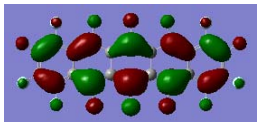
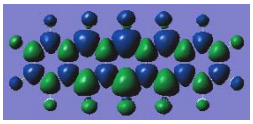
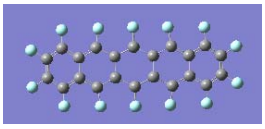
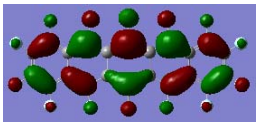
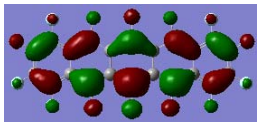
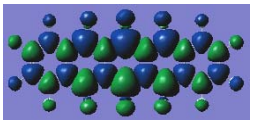
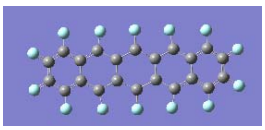
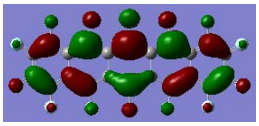
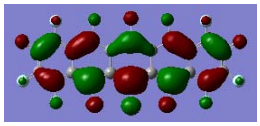
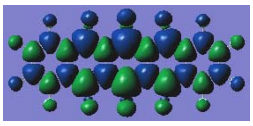
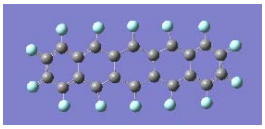
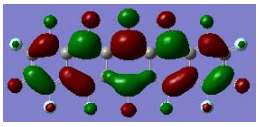
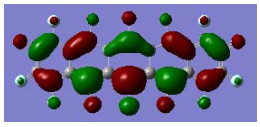
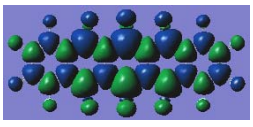
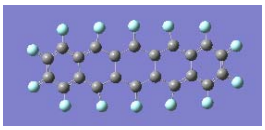
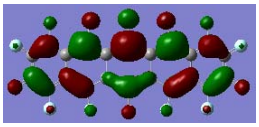
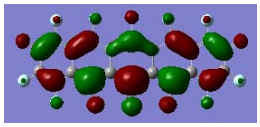
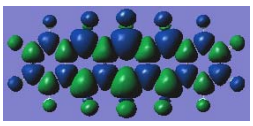
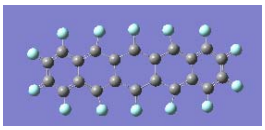
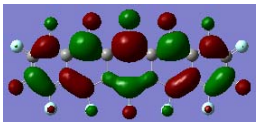
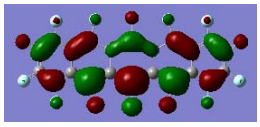
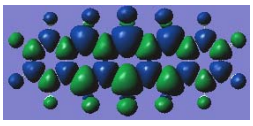
31-1 **0.00**	**2.01** **19.72**				
31-2 **0.00**	**2.00** **19.47**				
31-3 **0.00**	**1.98** **19.09**				
31-4 **0.00**	**1.95** **18.57**				

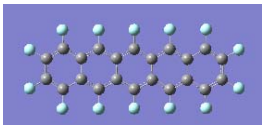
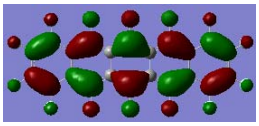
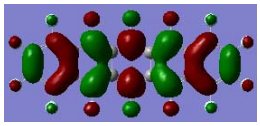
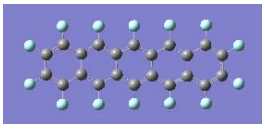
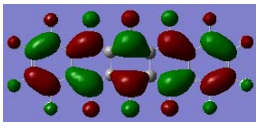
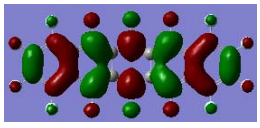
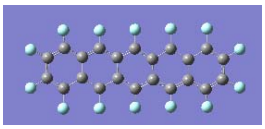
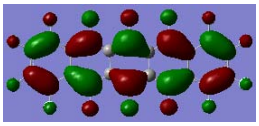
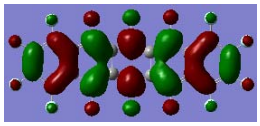
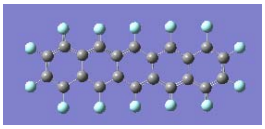
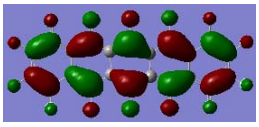
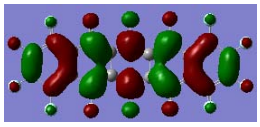
31-5 **0.00**	**1.92** **17.95**				
31-6 **0.00**	**1.88** **17.24**				
31-7 **0.015**	**1.84** **16.47** **16.47**				
31-8 **0.107**	**1.79** **15.65** **15.68**				
31-9 **0.206**	**1.75** **14.80** **14.91**				
31 **0.310**	**1.70** **13.94** **14.18**				

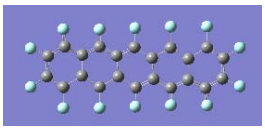
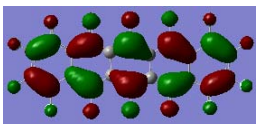
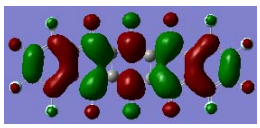
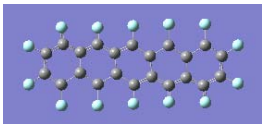
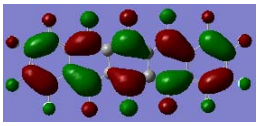
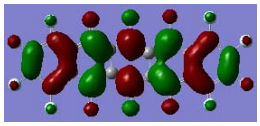
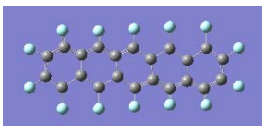
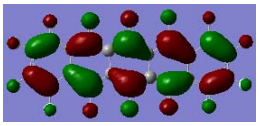
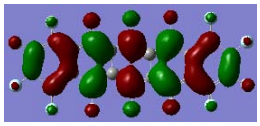
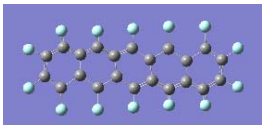
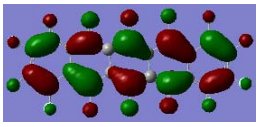
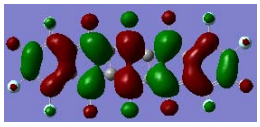
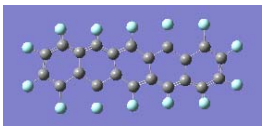
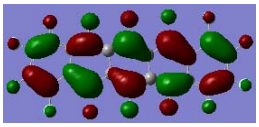
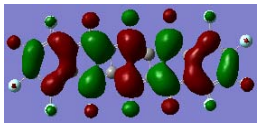
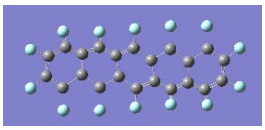
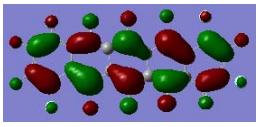
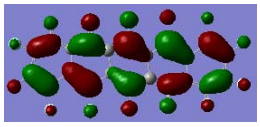
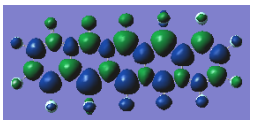
45-1 **0.00**	**1.97** **18.70**				
45-2 **0.00**	**1.92** **17.51**				
45-3 **0.00**	**1.87** **16.24**				
45-4 **0.074**	**1.81** **14.88** **14.90**				

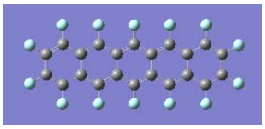
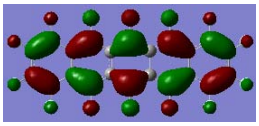
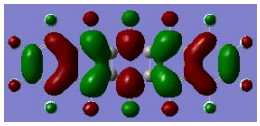
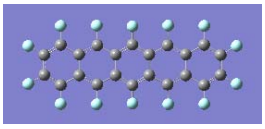
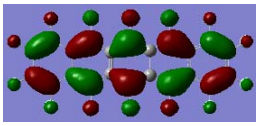
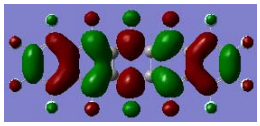
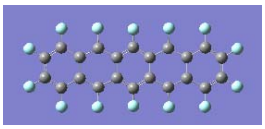
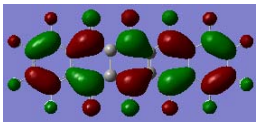
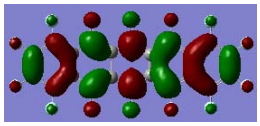
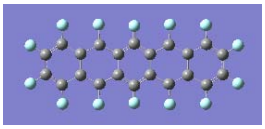
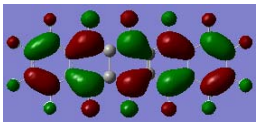
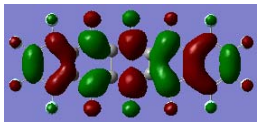
45-5 0.189	1.75 13.43 13.53				
45-6 0.307	1.68 11.88 12.16				
45-7 0.424	1.61 10.22 10.80				
45-8 0.541	1.54 8.46 9.47				
45-9 0.654	1.46 6.58 8.19				
45 0.762	1.38 4.57 6.98				

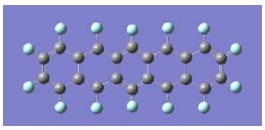
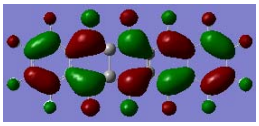
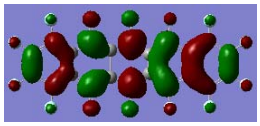
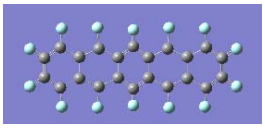
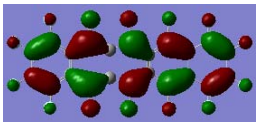
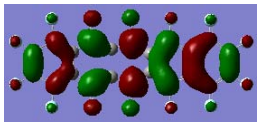
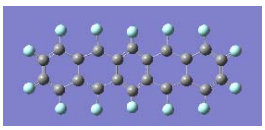
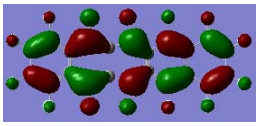
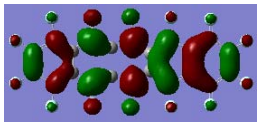
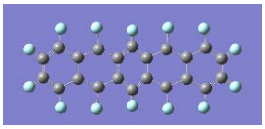
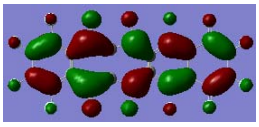
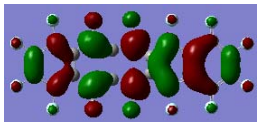
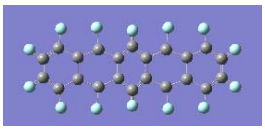
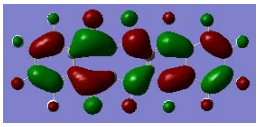
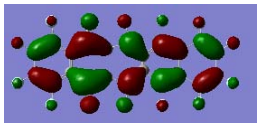
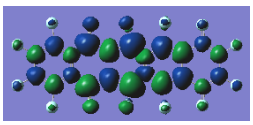
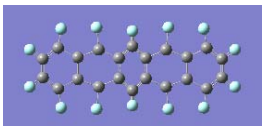
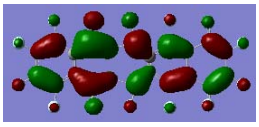
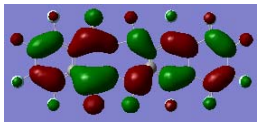
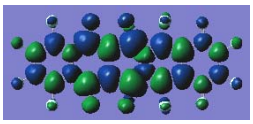
59-1 0.00	1.98 18.83				
59-2 0.00	1.95 17.82				
59-3 0.001	1.92 16.78 16.78				
59-4 0.109	1.89 15.70 15.73				

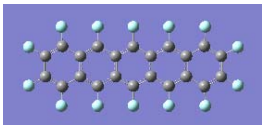
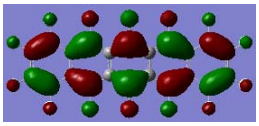
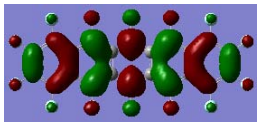
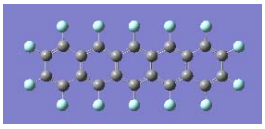
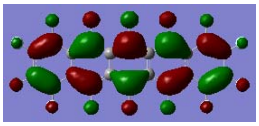
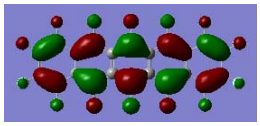
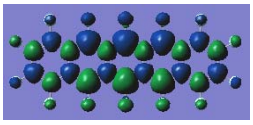
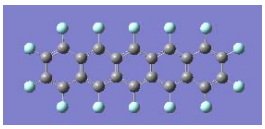
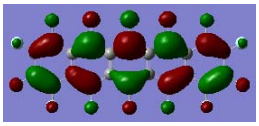
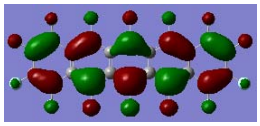
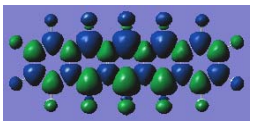
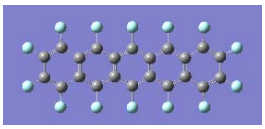
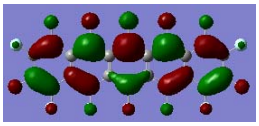
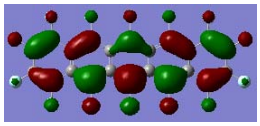
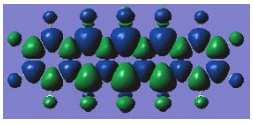
59-5 0.212	1.86 14.59 14.73				
59-6 0.310	1.83 13.44 13.76				
59-7 0.402	1.79 12.26 12.84				
59-8 0.488	1.76 11.05 11.97				
59-9 0.568	1.73 9.80 11.14				
59 0.642	1.69 8.52 10.37				

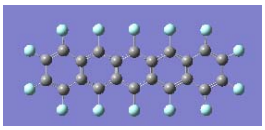
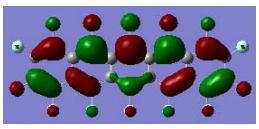
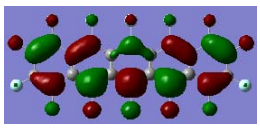
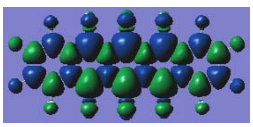
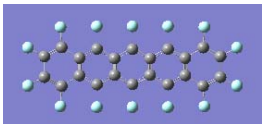
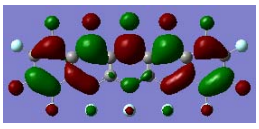
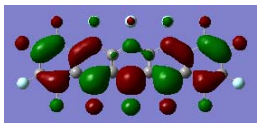
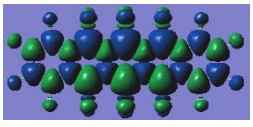
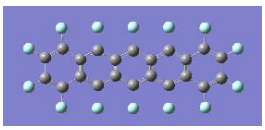
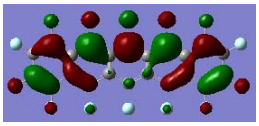
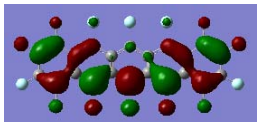
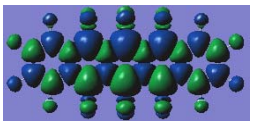
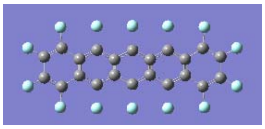
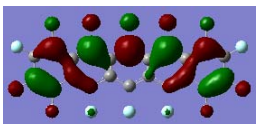
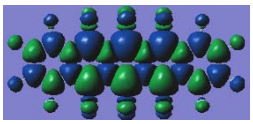
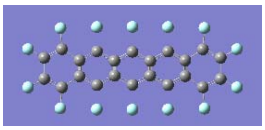
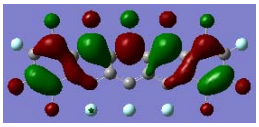
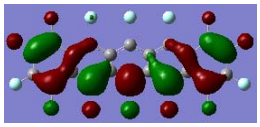
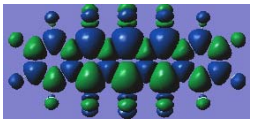
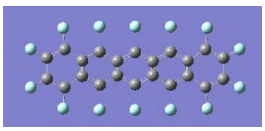
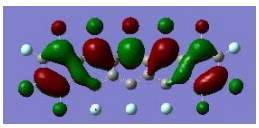
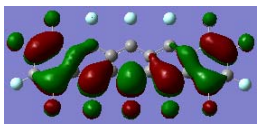
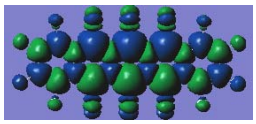
68-1 0.00	2.01 19.71				
68-2 0.00	2.00 19.55				
68-3 0.00	2.00 19.32				
68-4 0.00	1.98 19.03				

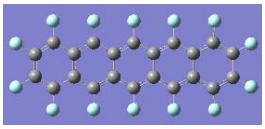
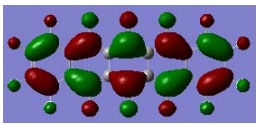
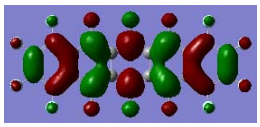
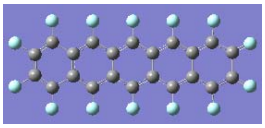
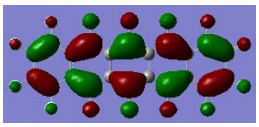
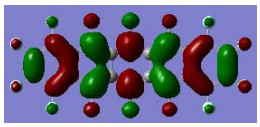
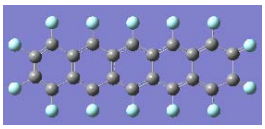
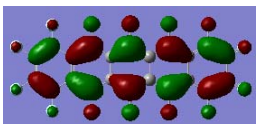
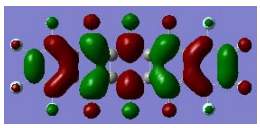
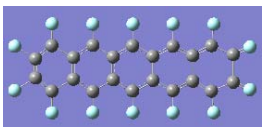
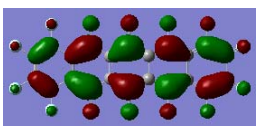
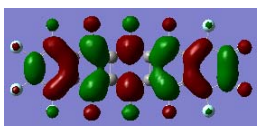
68-5 **0.00**	**1.97** **18.67**				
68-6 **0.00**	**1.95** **18.23**				
68-7 **0.00**	**1.93** **17.72**				
68-8 **0.00**	**1.90** **17.13**				
68-9 **0.00**	**1.87** **16.45**				
68 **0.064**	**1.84** **15.67** **15.68**				

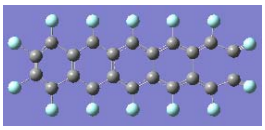
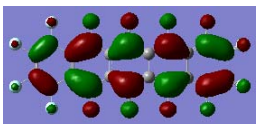
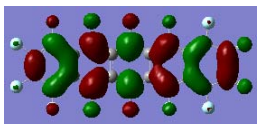
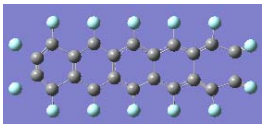
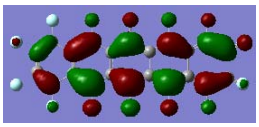
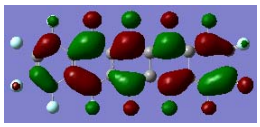
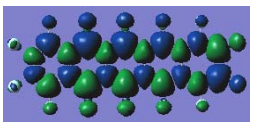
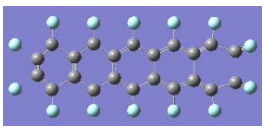
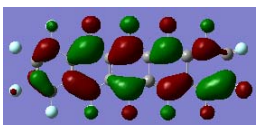
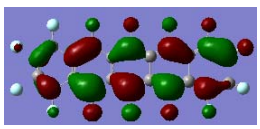
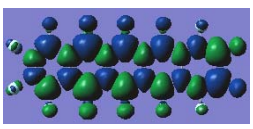
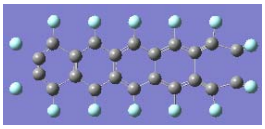
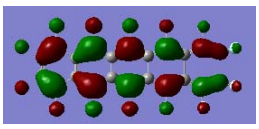
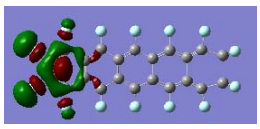
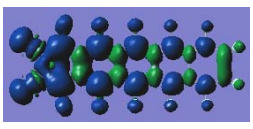
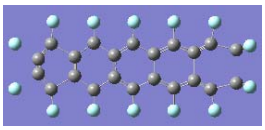
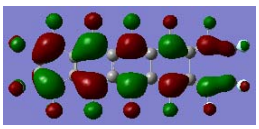
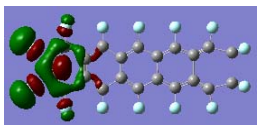
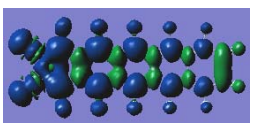
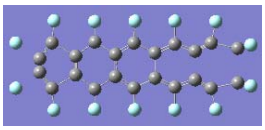
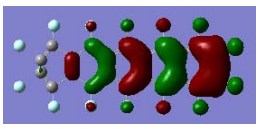
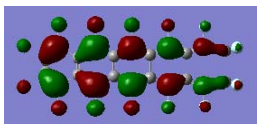
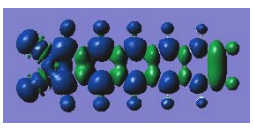
77-1 **0.00**	**2.02** **19.84**				
77-2 **0.00**	**2.02** **19.85**				
77-3 **0.00**	**2.02** **19.81**				
77-4 **0.00**	**2.02** **19.70**				

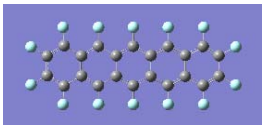
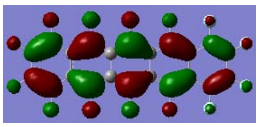
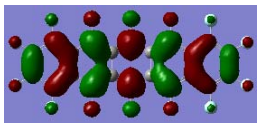
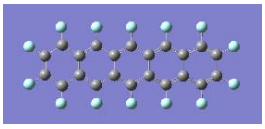
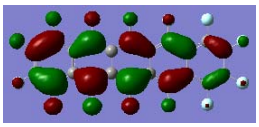
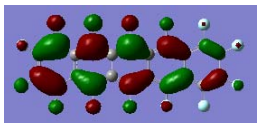
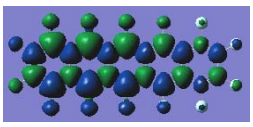
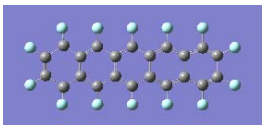
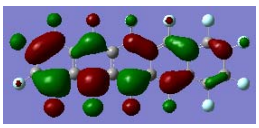
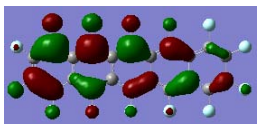
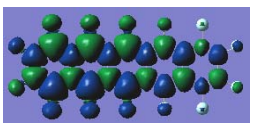
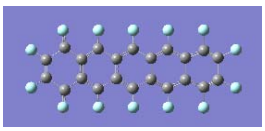
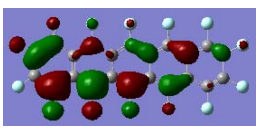
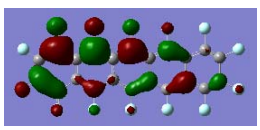
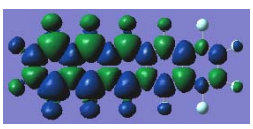
77-5 **0.00**	**2.03** **19.50**				
77-6 **0.00**	**2.02** **19.19**				
77-7 **0.00**	**2.02** **18.72**				
77-8 **0.00**	**2.00** **18.04**				
77-9 **0.052**	**1.98** **17.11** **17.12**				
77 **0.160**	**1.95** **15.85** **15.94**				

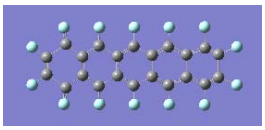
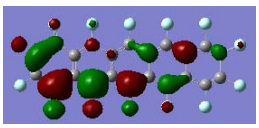
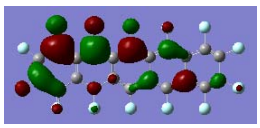
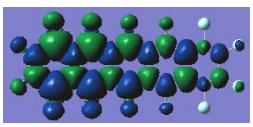
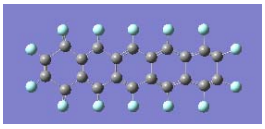
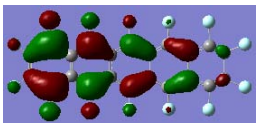
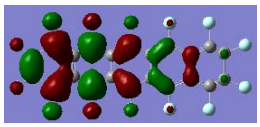
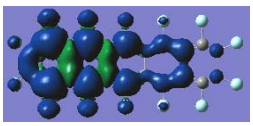
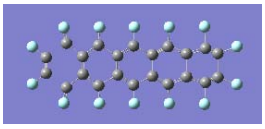
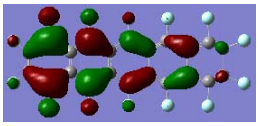
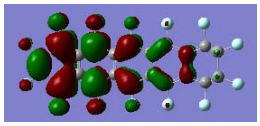
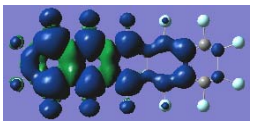
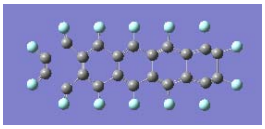
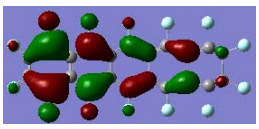
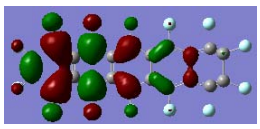
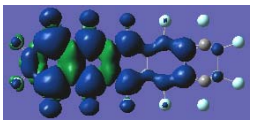
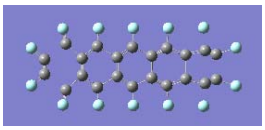
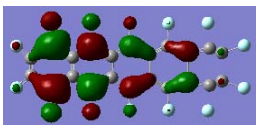
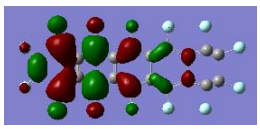
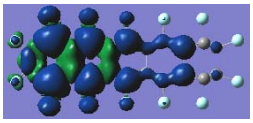
81-1 **0.00**	**1.96** **18.13**				
81-2 **0.080**	**1.90** **16.27** **16.29**				
81-3 **0.277**	**1.83** **14.20** **14.44**				
81-4 **0.463**	**1.75** **11.87** **12.66**				

81-5 0.637	1.66 9.25 10.97				
81-6 0.795	1.56 6.31 9.45				
81-7 0.938	1.45 3.00 8.16				
81-8 1.064	1.32 -0.72 7.17				
81-9 1.176	1.18 -4.89 6.58				
81 1.277	1.02 -9.56 6.51				

92-1 0.00	2.00 19.55				
92-2 0.00	1.98 18.98				
92-3 0.00	1.94 18.13				
92-4 0.00	1.90 17.06				

92-5 **0.00**	**1.85** **15.84**				
92-6 **0.251**	**1.33** **14.57** **14.75**				
92-7 **0.362**	**0.59** **10.07** **10.46**				
92-8 **2.031**	**0.60** **-2.52** **-2.37**				
92-9 **2.044**	**0.64** **-12.20** **-0.50**				
92 **2.064**	**0.68** **-17.70**				

98-1 **0.00**	**1.97** **18.52**				
98-2 **0.198**	**1.86** **14.94** **15.06**				
98-3 **0.551**	**1.69** **9.87** **11.14**				
98-4 **0.804**	**1.51** **4.22** **7.89**				

98-5 **0.962**	**1.33** **-1.33** **5.62**				
98-6 **2.030**	**1.16** **-6.40**				
98-7 **2.029**	**1.00** **-10.82**				
98-8 **2.028**	**0.87** **-14.57**				
98-9 **2.027**	**0.40** **-16.95** **-16.87**				
98 **2.036**	**0.37** **-16.56** **-8.51**