Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters

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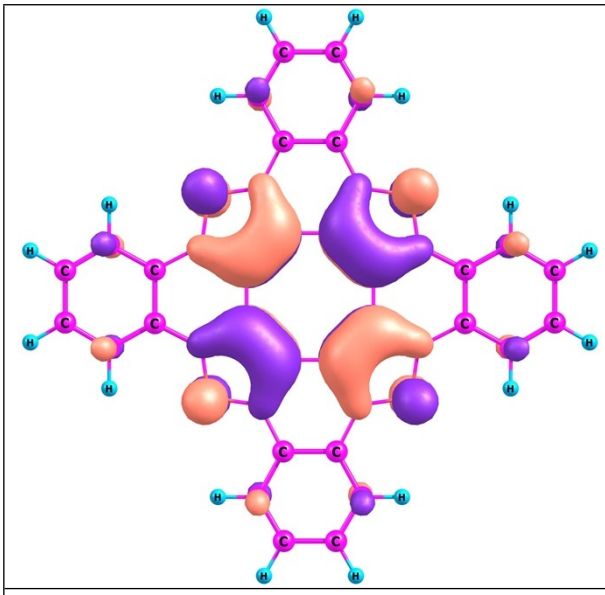
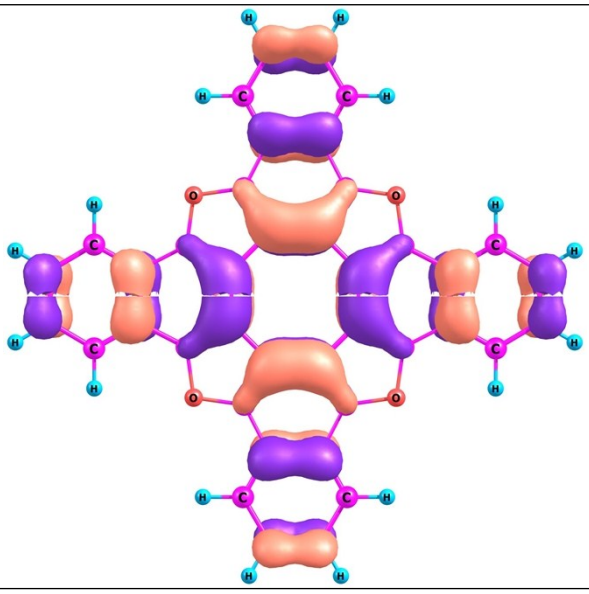
Electronic Supplementary Information

List of Content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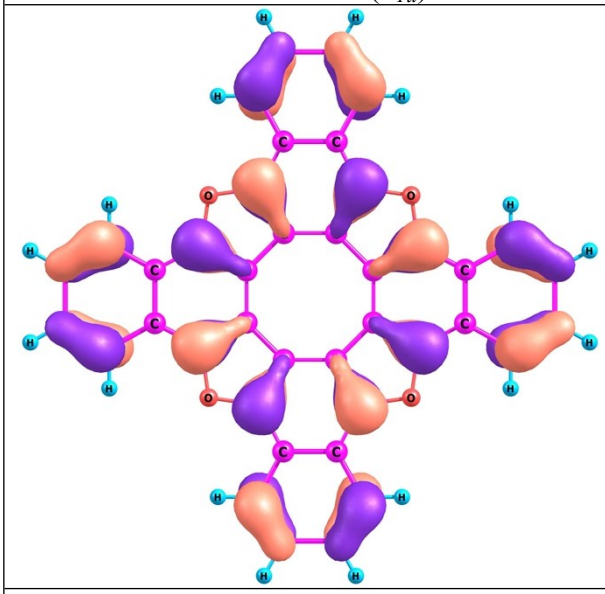	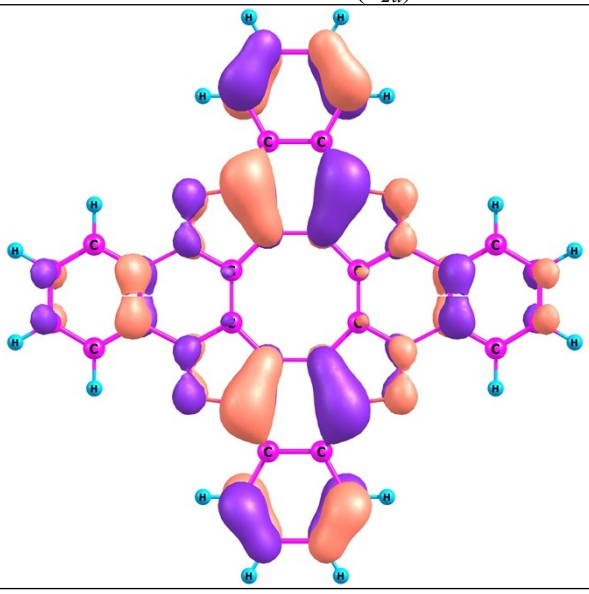
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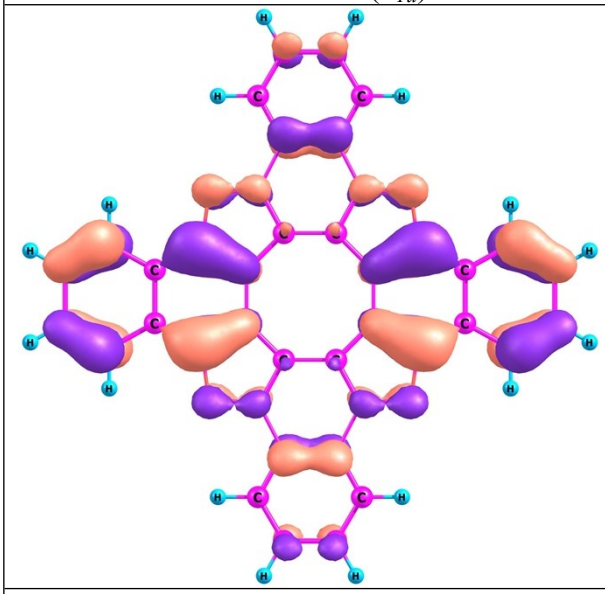	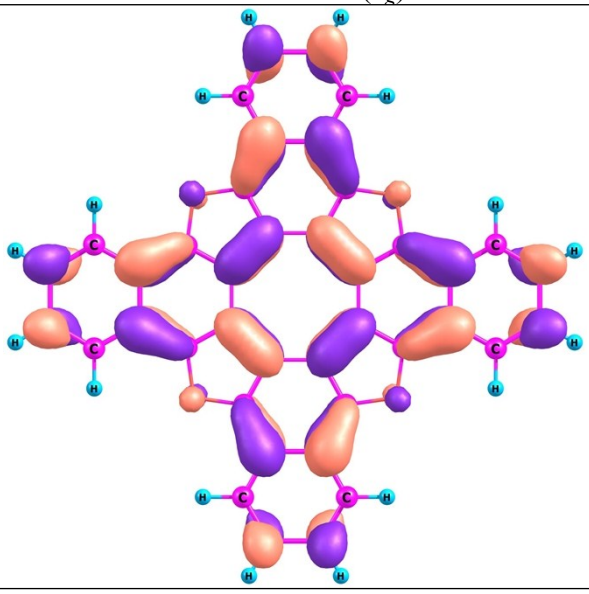
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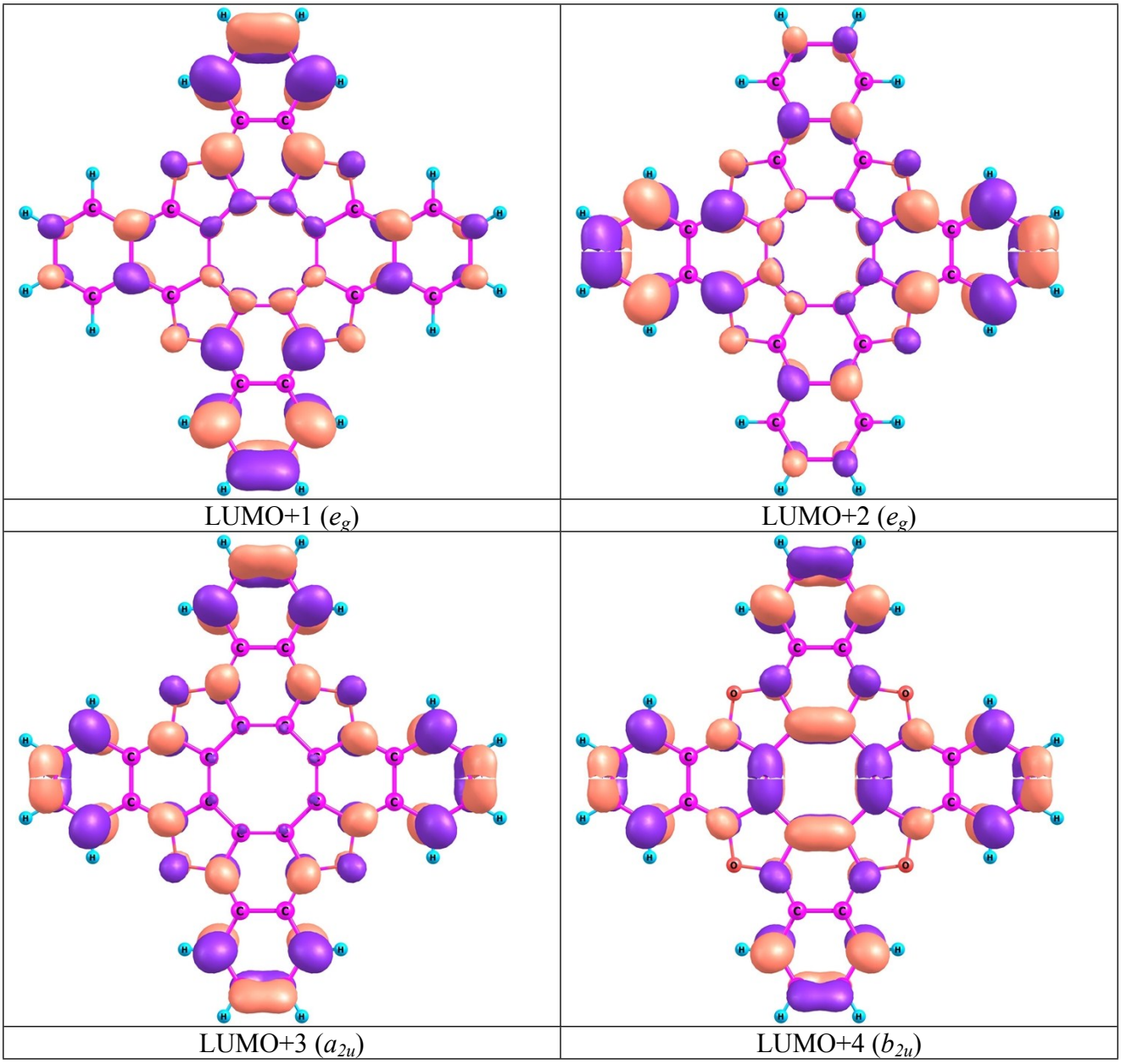
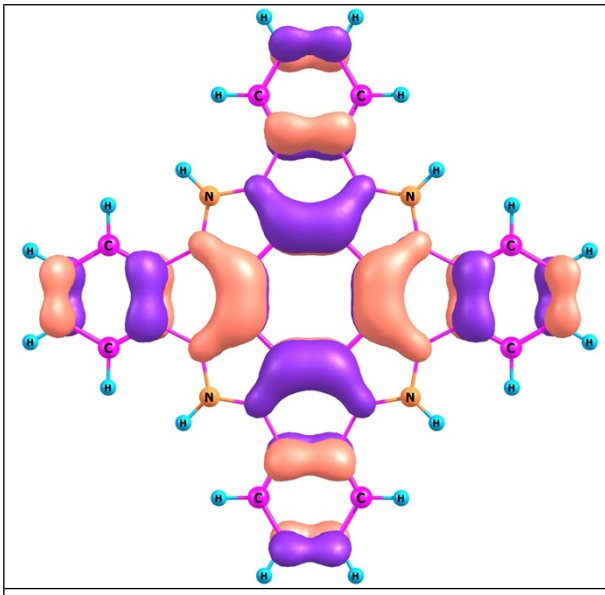
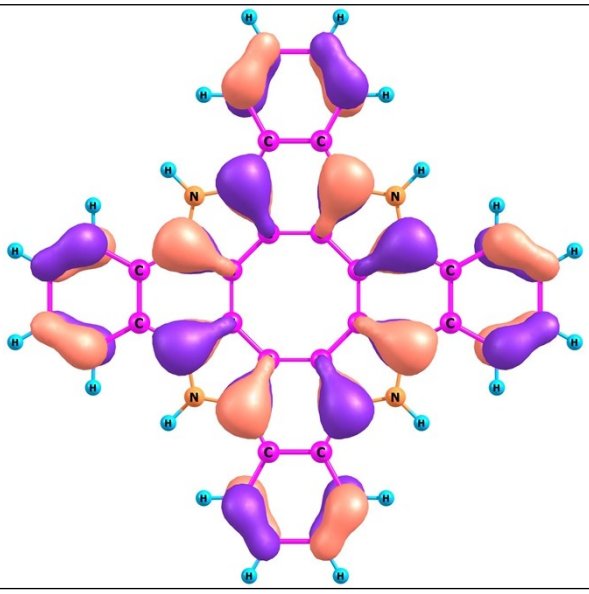


Figure S1. The shapes of molecular orbitals of tetrabenzotetraoxa[8]circulene calculated by the XMC-QDPT2/6-311(d,p) method.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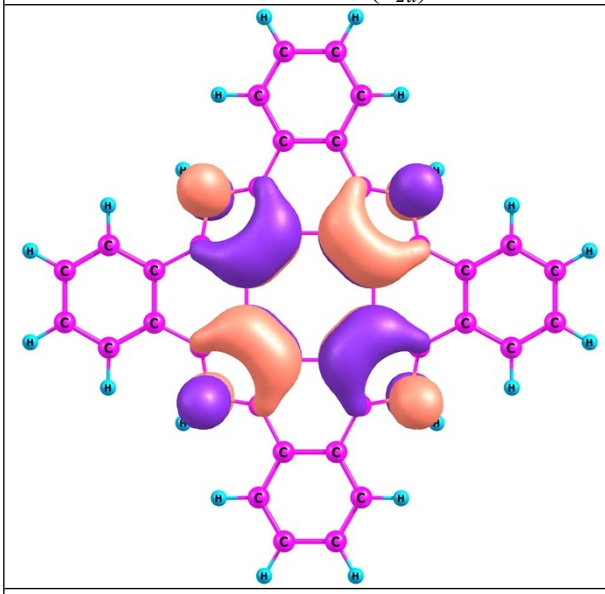	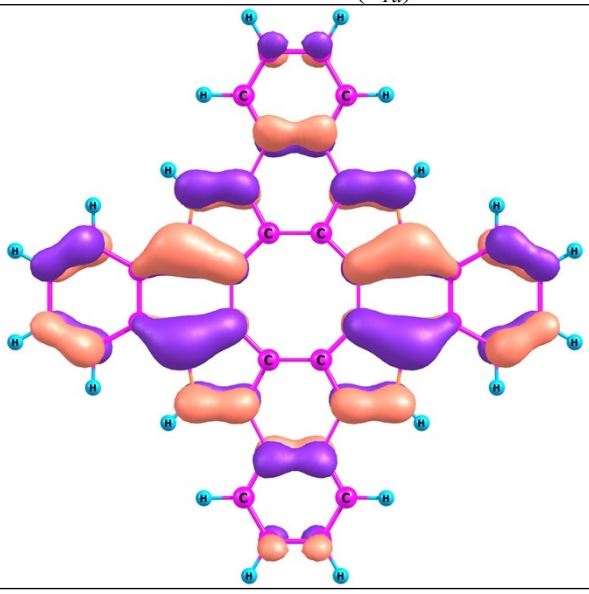
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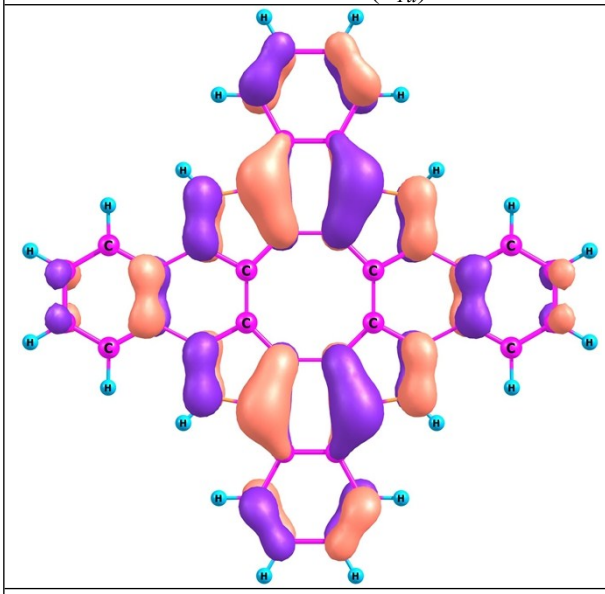	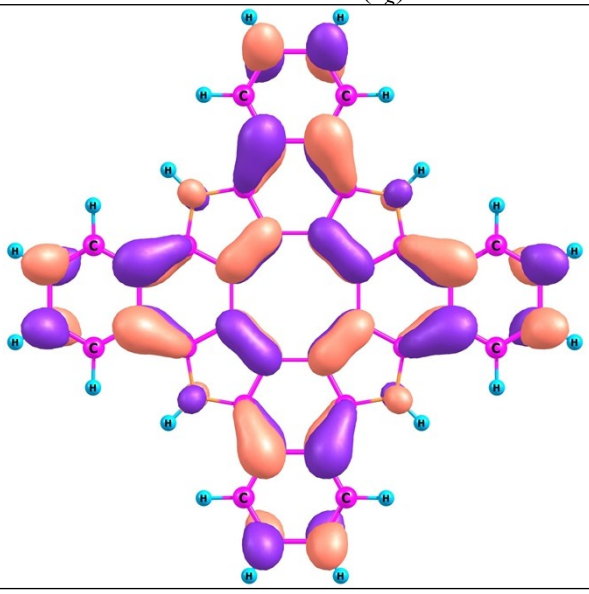
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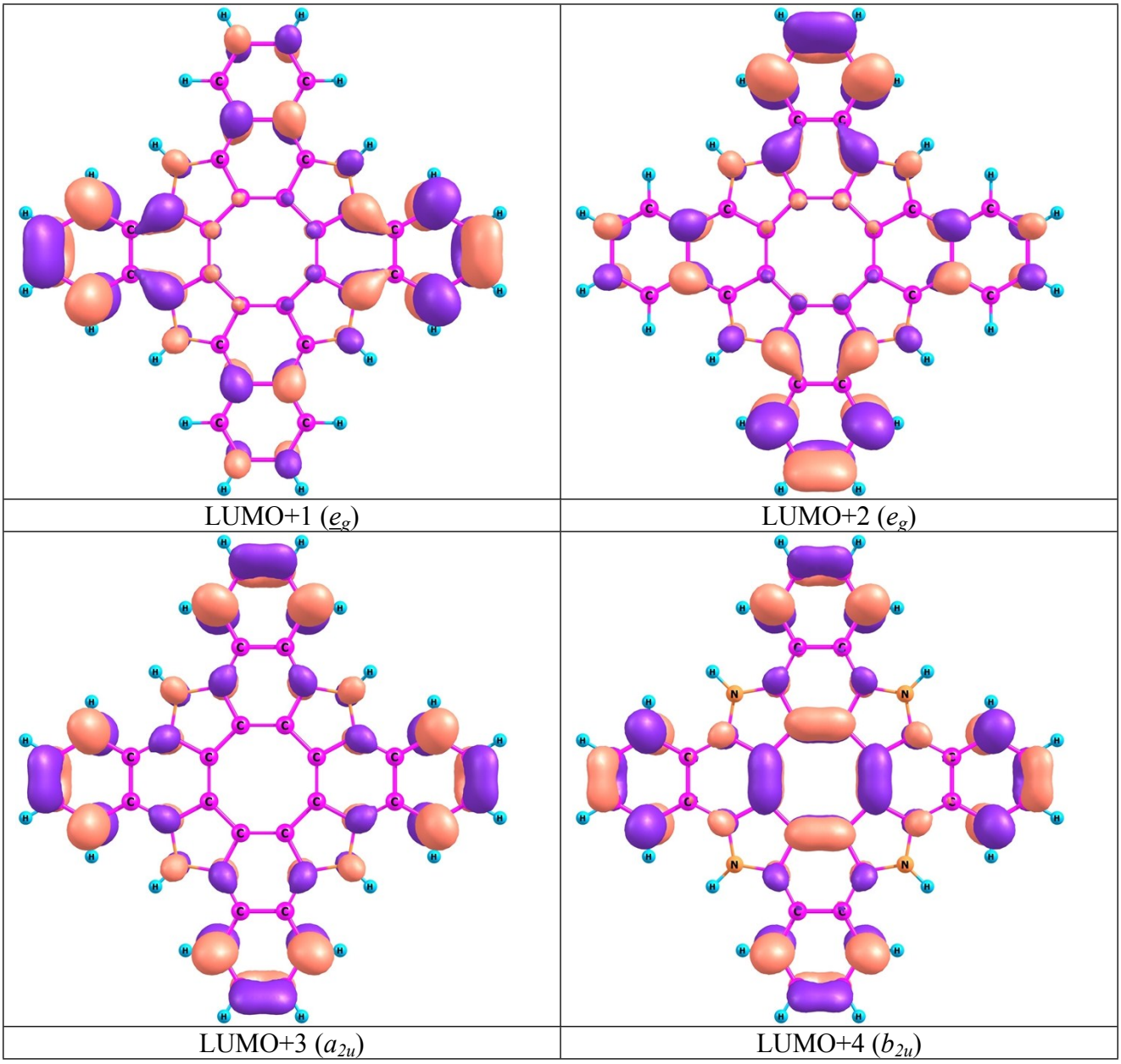
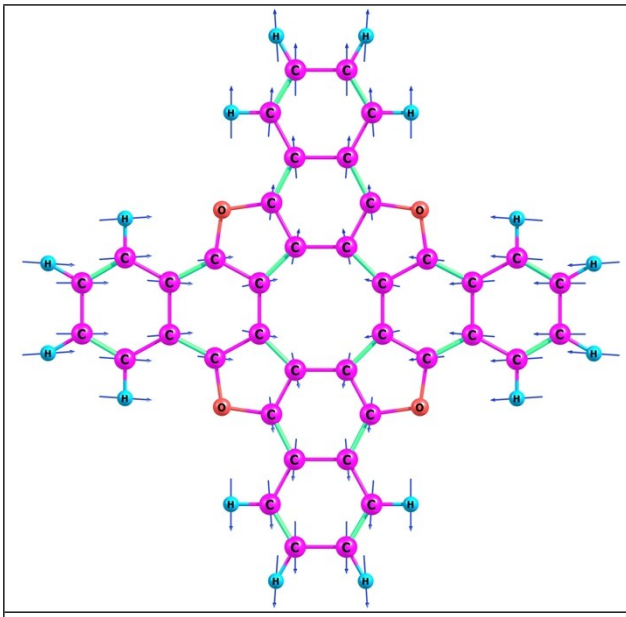
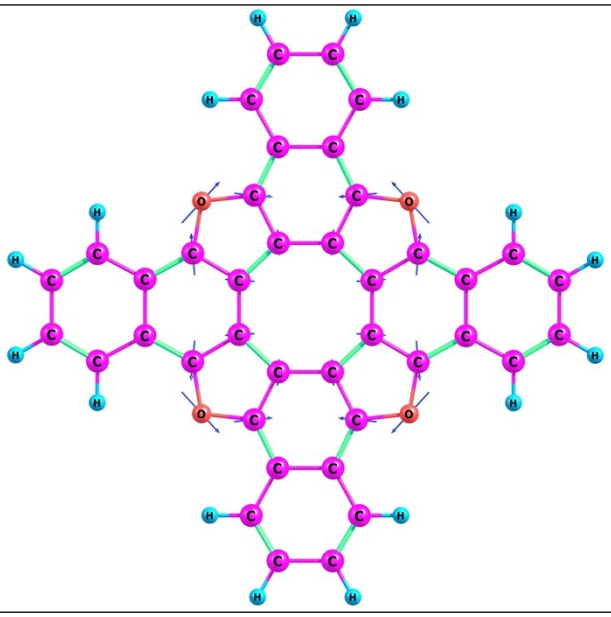


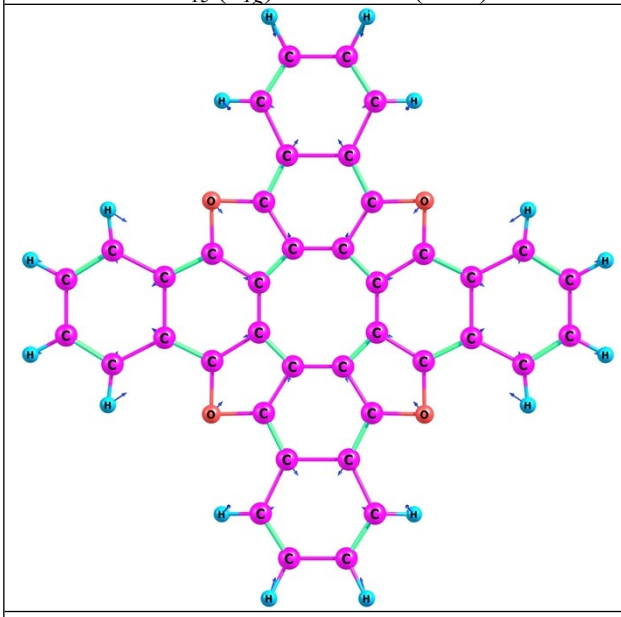
Figure S2. The shapes of molecular orbitals of tetrabenzotetraaza[8]circulene calculated by the XMC-QDPT2/6-311(d,p) method.



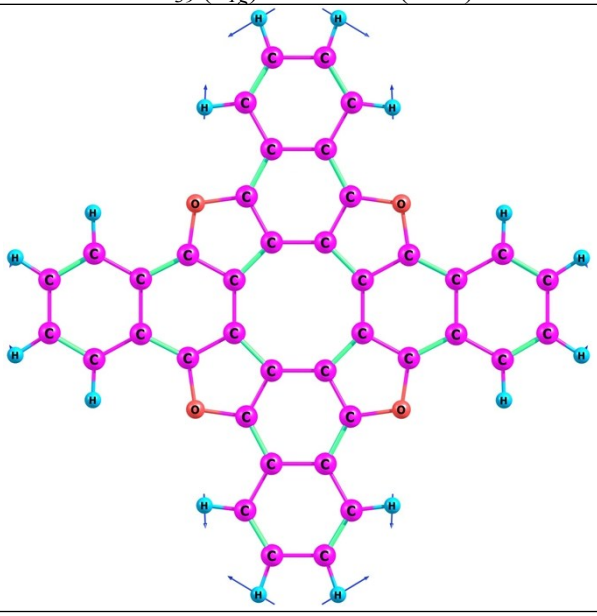
ν_{15} (b_{1g}): 221 cm^{-1} (0.12)



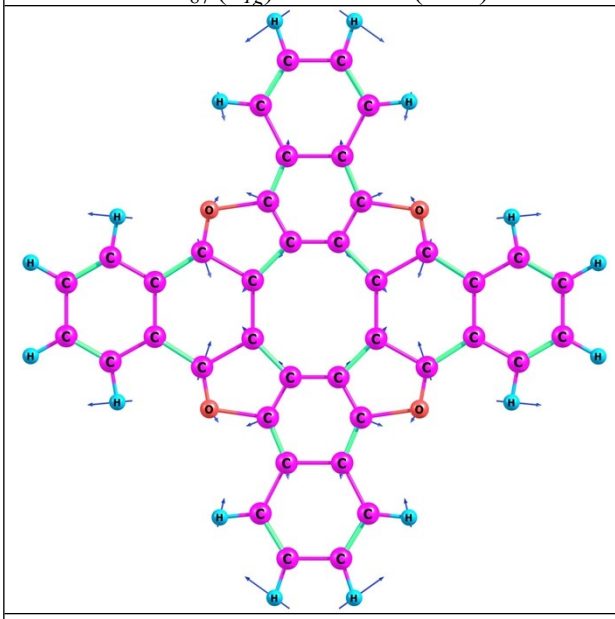
ν_{39} (b_{1g}): 518 cm^{-1} (0.05)



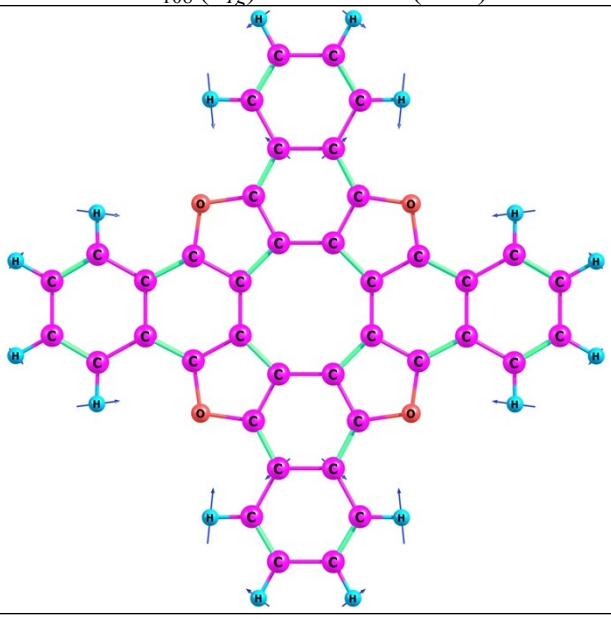
ν_{87} (a_{1g}): 963 cm^{-1} (0.16)



ν_{108} (b_{1g}): 1188 cm^{-1} (0.04)



ν_{115} (b_{1g}): 1275 cm^{-1} (0.08)



ν_{119} (b_{1g}): 1326 cm^{-1} (0.07)

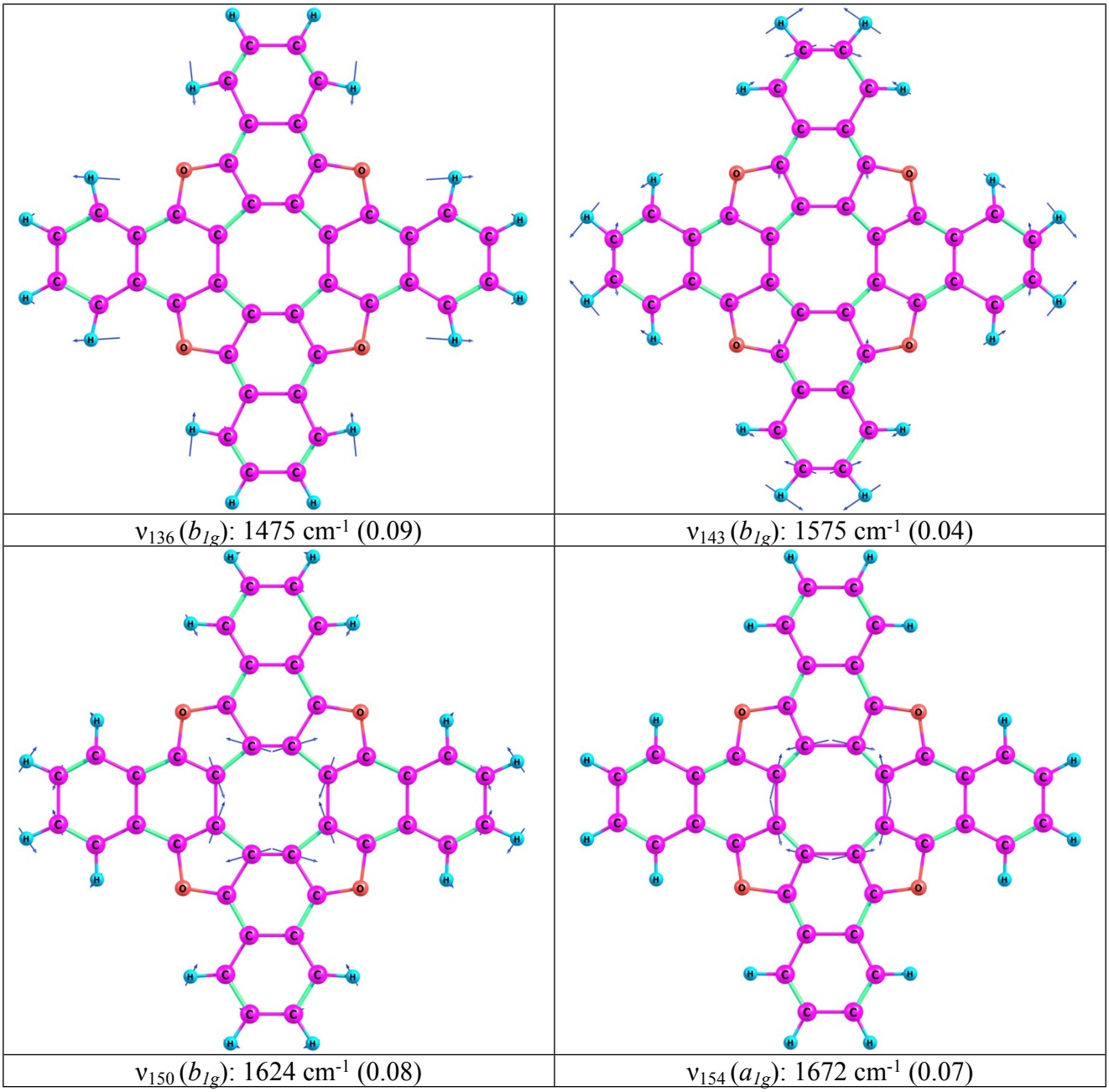
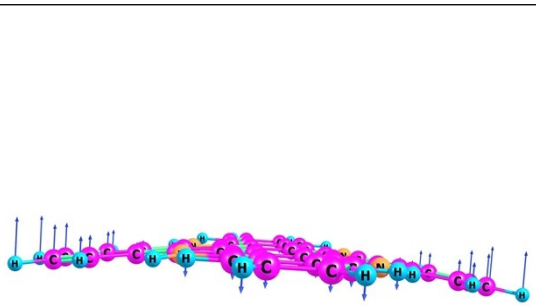
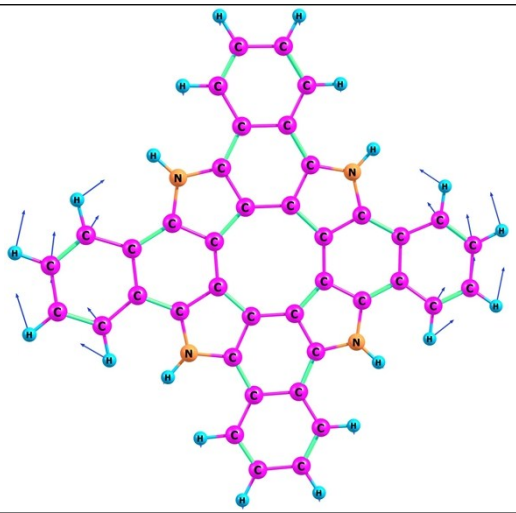


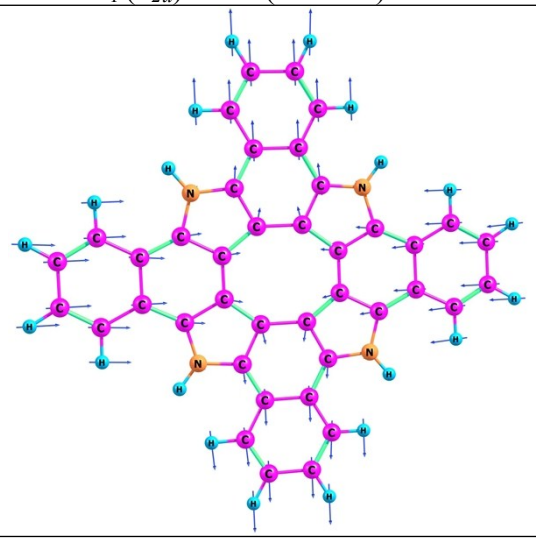
Figure S3. The displacement vectors for the FC active modes which produce the vibronic progression of the $S_0 \rightarrow S_1$ electronic transition in the absorption spectrum of TBTOC **46** compound.



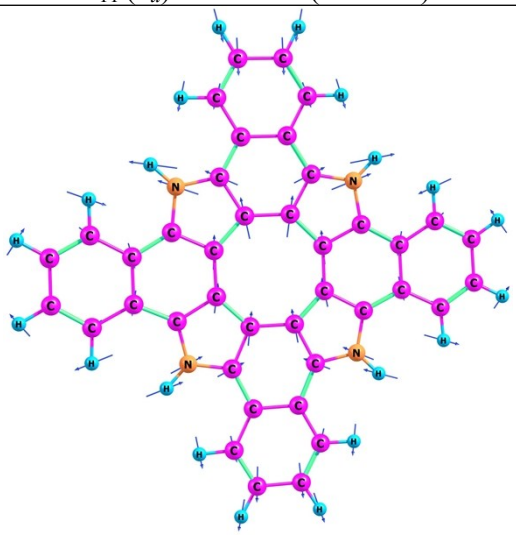
ν_1 (b_{2u}): 39.4 ($3.5 \cdot 10^{-4}$) $\times 2$



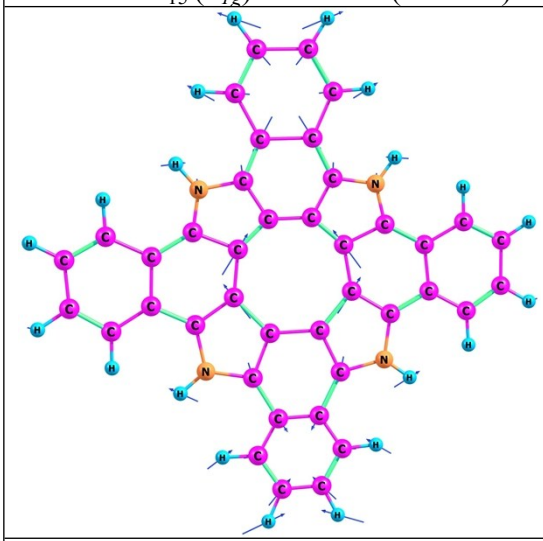
ν_{11} (e_u): 148 cm^{-1} ($3.1 \cdot 10^{-4}$)



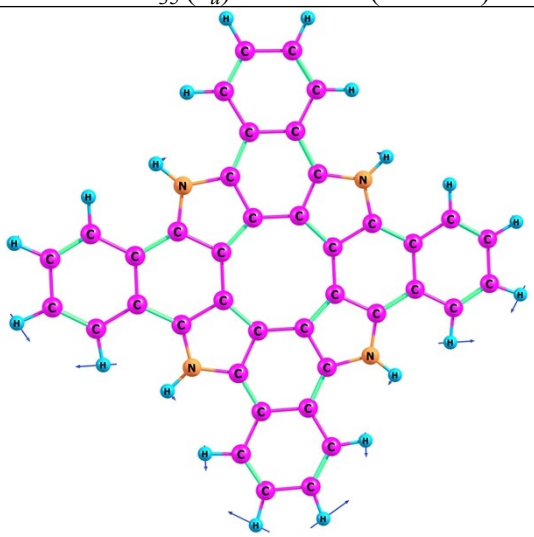
ν_{15} (b_{1g}): 220 cm^{-1} ($1.6 \cdot 10^{-4}$)



ν_{35} (e_u): 461 cm^{-1} ($2.9 \cdot 10^{-4}$)

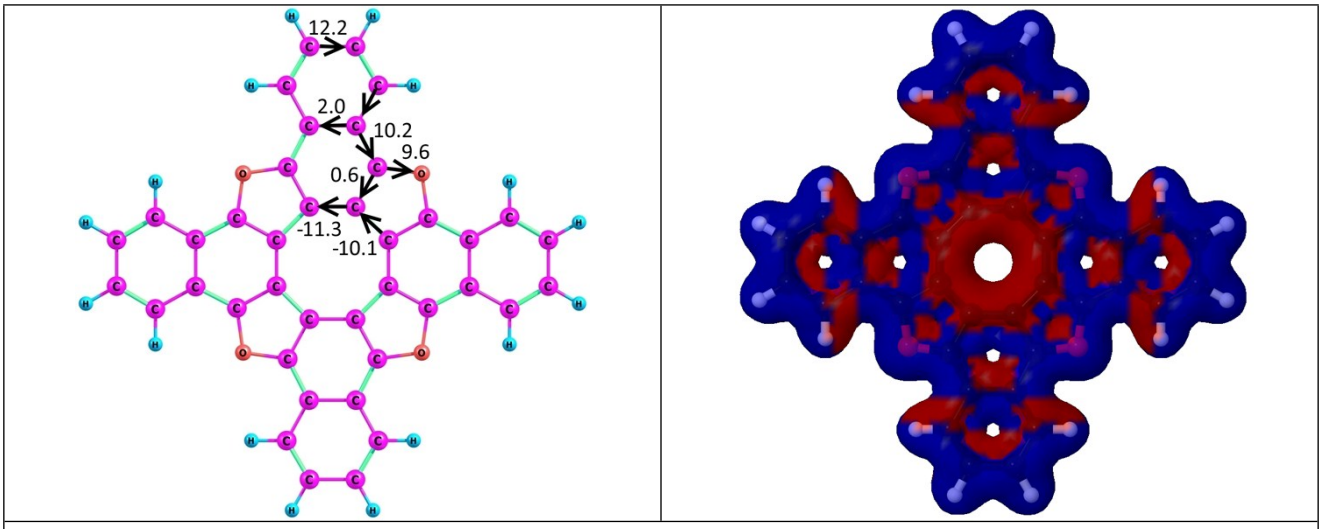


ν_{97} (e_u): 1029 cm^{-1} ($1.2 \cdot 10^{-4}$)

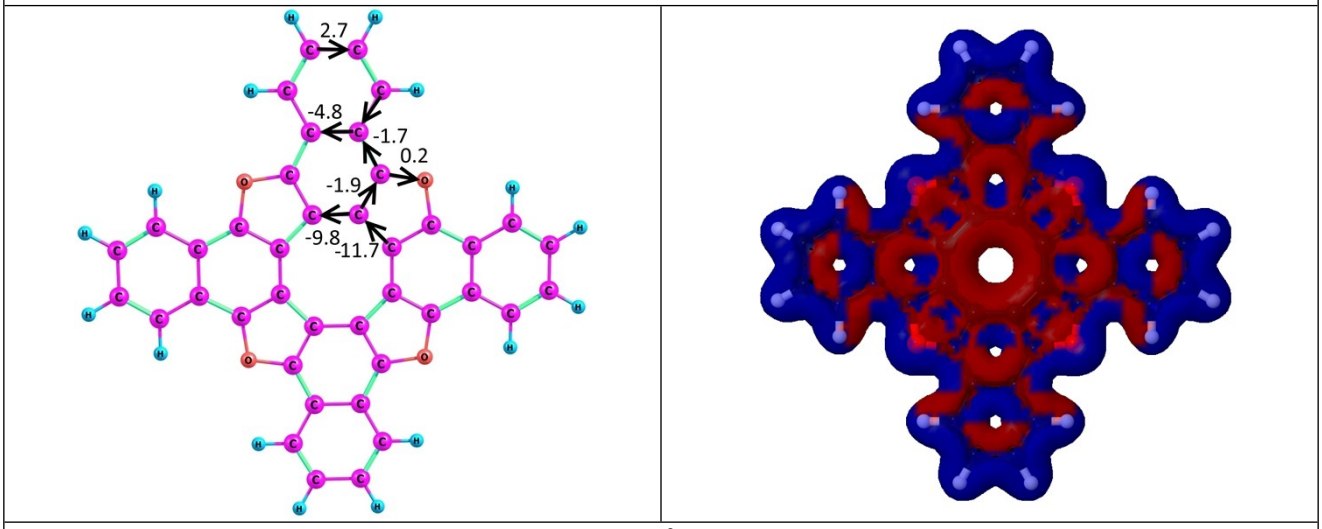


ν_{113} (e_u): 1195 ($1.1 \cdot 10^{-4}$)

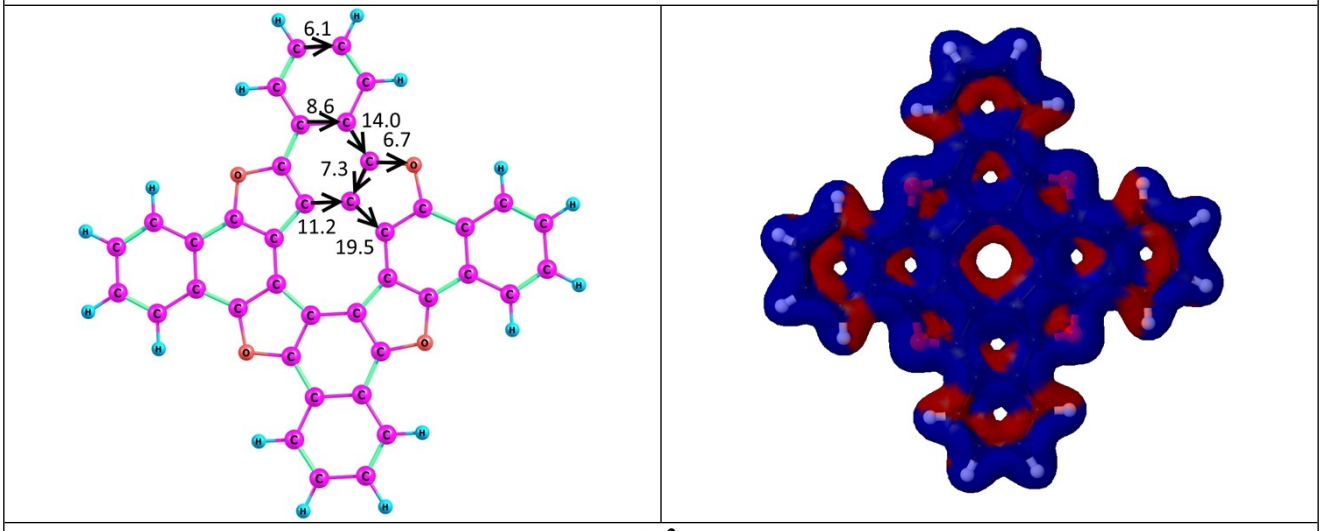
Figure S4. The displacement vectors for the FC active modes which produce the vibronic progression of the $S_0 \rightarrow S_1$ electronic transition in the absorption spectrum of TBTAC **51** compound.



46



46^{2+}



46^{2-}

Figure S5. The signed modulus of the magnetically induced current densities, current strengths and current pathways for the neutral and doubly charged circulene **46**. Paratropic current densities are shown in red and the diatropic ones in blue.

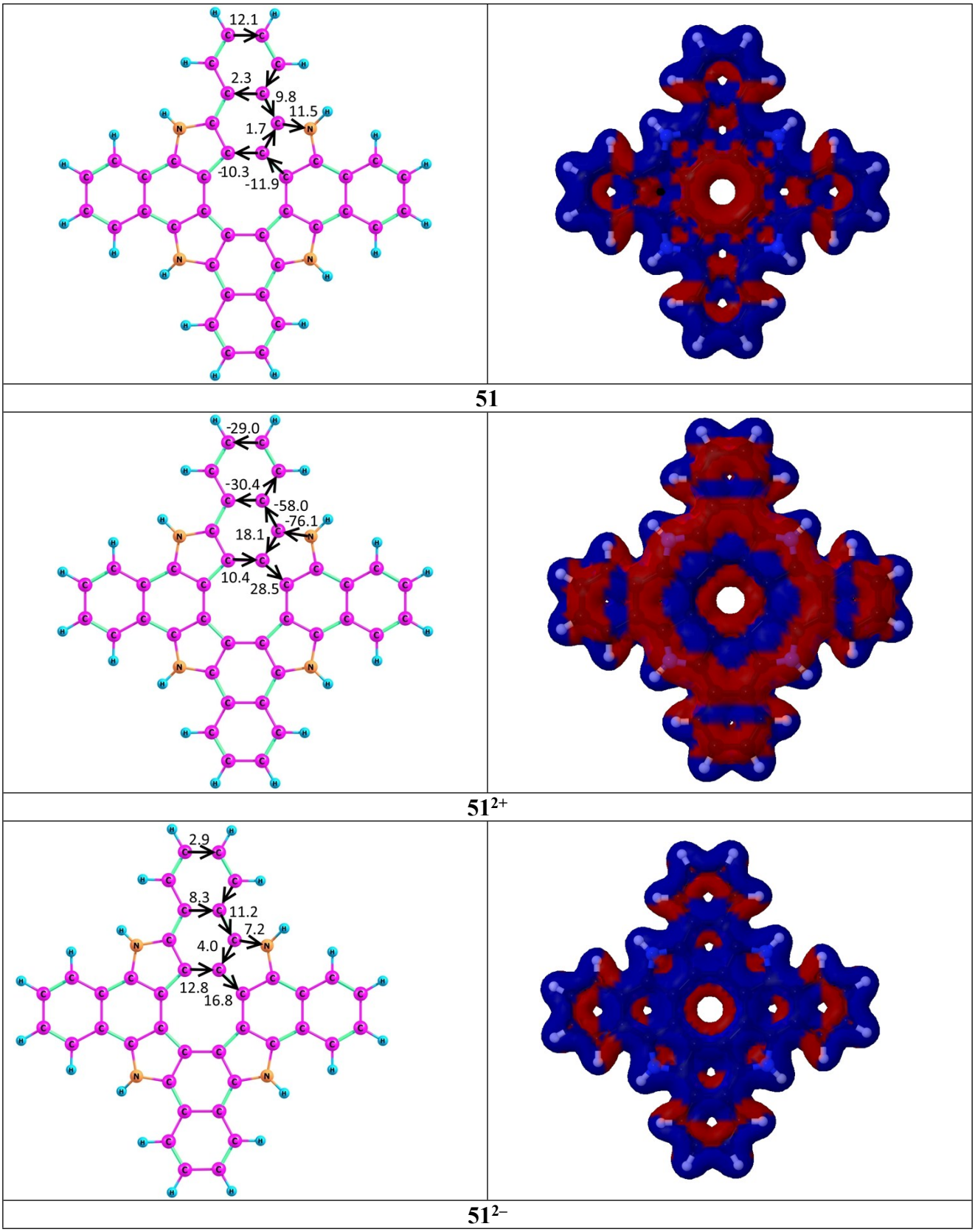


Figure S6. The signed modulus of the magnetically induced current densities, current strengths and current pathways for the neutral and doubly charged circulene **51**. Paratropic current densities are shown in red and the diatropic ones in blue.

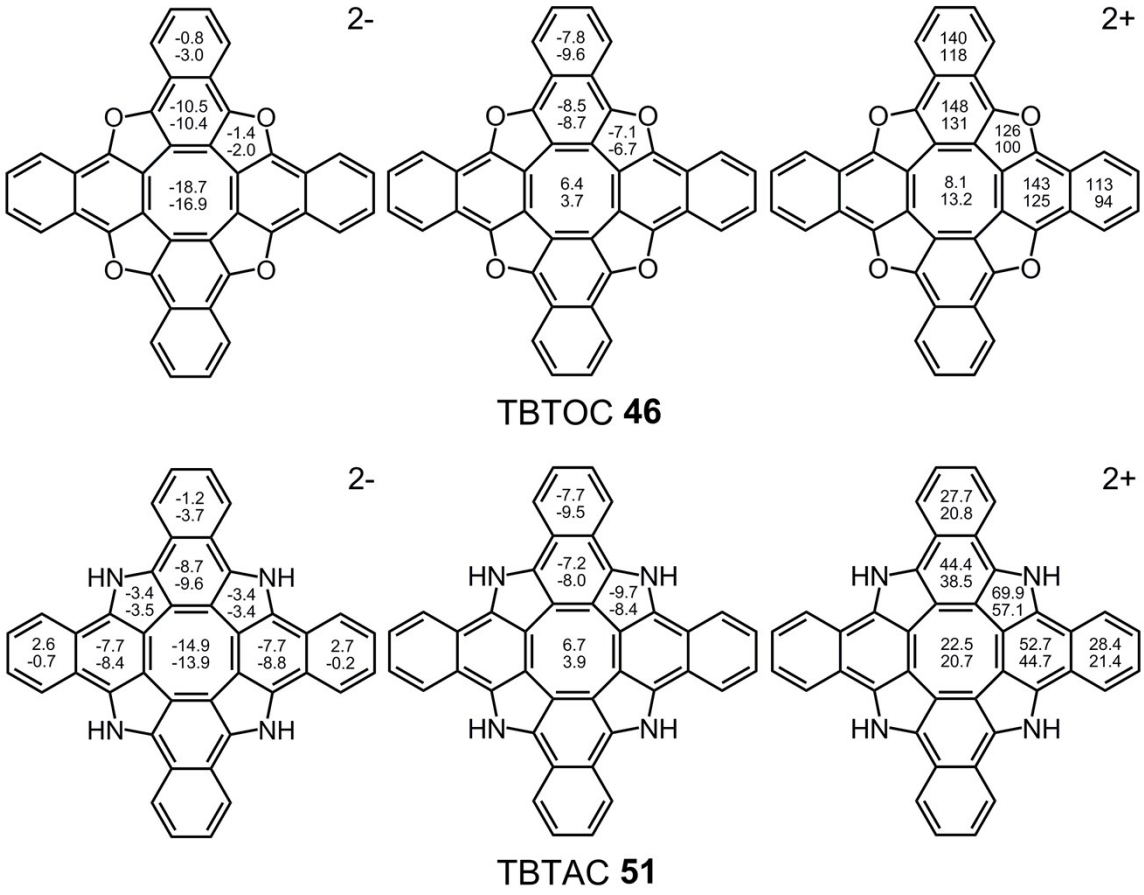


Figure S7. The NICS(0) (top value) and NICS(1) (bottom value) indices for the neutral and doubly charged circulenes **46** and **51**.

Table S1. The TDDFT/B3LYP/6-311G(d,p) calculated photophysical parameters for the hetero[8]circuelens **1**–**51** and the main characteristics of their ground electronic singlet state including the total energy values (E0) and the wavenumber for the first vibrational frequency calculated by the DFT/B3LYP/6-311G(d,p) method.

Molecule (Sym.)	ν_1, cm^{-1} (Sym.)	E_0, a.u.	$\lambda(S_0 \rightarrow S_1)$, nm	$f(S_0 \rightarrow S_1)$	$\lambda(S_0 \rightarrow T_1)$, nm	λ/ν (S_1T_1), nm/cm^{-1}
1 (D_{4h})	73.6 (b_{1u})	–1141.1390428	436	0	512	76/3404.53
2 (C_{2v})	80.2 (a_2)	–1161.0017796	421	1.1×10^{-3}	525	104/4705.35
3 (C_{2v})	82.9 (b_1)	–1180.8629314	420	8.0×10^{-4}	526	106/4798.12
4 (D_{2h})	83.0 (a_u)	–1180.8636638	420	0	526	106/4798.12
5 (C_{2v})	85.6 (a_2)	–1200.7232483	420	2.0×10^{-4}	528	108/4870.13
6 (D_{4h})	78.7 (a_{2u})	–1220.5819783	419	0	529	110/4962.76
7 (C_s)	46.3 (a'')	–1314.6801542	420	0.139	521	101/4615.67
8 (C_{2v})	43.9 (a_2)	–1468.3587633	408	0.236	519	111/5241.98
9 (C_s)	30.7 (a'')	–1622.0374621	408	0.288	519	111/5241.98
10 (C_s)	47.0 (a'')	–1314.6808787	411	0.183	519	108/5063.08
11 (C_{2v})	45.3 (a_2)	–1468.3599890	408	0.242	512	104/4978.55
12 (C_s)	42.7 (a'')	–1468.3593887	411	0.137	512	101/4799.65
13 (C_s)	30.9 (a'')	–1622.0379689	409	0.288	512	103/4918.63
14 (C_s)	34.0 (a'')	–1468.3592209	421	0.344	530	109/4885.04
15 (C_{2v})	29.3 (a_2)	–1775.7166500	396	0.257	505	109/5450.55
16 (C_s)	46.6 (a'')	–1354.4031082	398	0.027	508	110/5440.59
17 (C_{2v})	48.8 (a_2)	–1508.0829457	390	0.212	501	111/5680.95
18 (C_s)	32.1 (a'')	–1661.7615197	398	0.329	505	107/5323.65
19 (C_s)	46.6 (a'')	–1354.4025636	405	0.182	509	104/5044.99
20 (C_{2v})	47.3 (a_2)	–1508.0820921	390	0.212	504	114/5799.76
21 (C_s)	46.8 (a'')	–1508.0823078	402	0.233	507	105/5151.76
22 (C_s)	32.1 (a'')	–1661.7612126	397	0.326	507	110/5465.05
23 (C_s)	34.1 (a'')	–1508.0823331	409	0.379	513	104/4956.70
24 (C_{2v})	32.0 (a_2)	–1815.4407885	387	0.271	500	113/5839.79
25 (C_{2v})	48.8 (b_1)	–1334.5414993	420	0.183	521	101/4615.67
26 (C_s)	43.7 (a'')	–1488.2206580	409	0.169	512	103/4918.63
27 (C_s)	32.0 (a'')	–1641.8998006	408	0.285	514	106/5054.55
28 (C_{2v})	29.1 (b_1)	–1795.5789059	395	0.213	503	108/5435.74
29 (C_{2v})	49.7 (b_1)	–1334.5427739	410	0.235	518	108/5085.22
30 (C_s)	45.9 (a'')	–1488.2217438	405	0.203	507	102/4967.49
31 (C_{2v})	34.2 (b_1)	–1641.9005732	401	0.318	504	103/5096.39
32 (C_s)	47.0 (a'')	–1334.5421335	407	0.119	510	103/4962.18
33 (C_{2v})	35.3 (b_1)	–1488.2213018	413	0.369	519	106/4945.25
34 (C_{2v})	33.3 (b_1)	–1641.8997477	399	0.330	512	113/5531.41
35 (C_{2v})	35.4 (b_1)	–1488.2210078	421	0.336	527	106/4777.64
36 (C_s)	47.0 (a'')	–1334.5428516	406	0.230	514	108/5175.29
37 (C_{2h})	34.3 (a_u)	–1488.2219896	413	0.395	522	109/5055.99
38 (C_{2v})	46.7 (a_2)	–1488.2223053	392	0.255	504	112/5668.93
39 (C_{2v})	46.3 (a_2)	–1488.2220077	407	0.259	514	107/5114.77
40 (C_s)	31.6 (a'')	–1641.9007787	402	0.340	511	109/5306.15
41 (D_{2h})	30.7 (a_u)	–1795.5799897	394	0.297	503	109/5499.99
42 (C_{2v})	48.1 (b_1)	–1374.2622091	397	5.0×10^{-3}	507	110/5465.05
43 (C_{2v})	48.9 (b_1)	–1527.9420292	390	0.237	501	111/5680.95
44 (D_{2h})	34.6 (b_{3u})	–1527.9420309	400	0.408	504	104/5158.73

45 (C_{2v})	34.5 (b_1)	–1681.6215524	388	0.359	501	113/5813.12
46 (D_{4h})	32.2 (b_{2u})	–1835.3009317	376	0.276×2	497	121/6475.02
47 (C_{2v})	47.7 (b_1)	–1294.8175408	424	0.016	522	98/4427.82
48 (C_{2v})	42.8 (a_2)	–1448.4960351	413	6.2×10^{-3}	517	104/4870.72
49 (D_{2h})	34.1 (b_{3u})	–1448.4957600	423	0.380	534	111/4914.07
50 (C_{2v})	31.2 (b_1)	–1602.1741801	411	0.311	520	109/5100.13
51 (D_{4h})	25.8 (b_{2u})	–1755.8520700	399	0.219×2	505	106/5260.68

Table S2. The rate constants of electronic transitions (in s^{-1}) and fluorescence quantum yield for the HCs **1–47**.

Molecules	k_r	k_{IC}	$\sum_i k_{S_1T_i}$	$\varphi_{fl,theory}$	$\varphi_{fl,exp}$
1	0.00D+00	2.80D+06	1.52D+08		
2	4.38D+05	1.63D+06	1.26D+08	0.0034	
3	3.20D+05	1.42D+06	3.27D+08	0.001	
4	0	3.4D+5	1.1D+8	0	0.1-0.2
5	1.82D+04	2.95D+5	7.13D+5	0.018	0.3
6	0	2.53D+5	0	0	0
7	5.55D+07	4.63D+05	9.46D+07	0.3688	
8	1.00D+08	3.97D+05	4.70D+06	0.9516	
9	1.22D+08	5.01D+05	1.93D+07	0.8605	
10	7.68D+07	6.24D+05	1.18D+08	0.3934	
11	1.03D+08	3.05D+05	1.50D+06	0.9827	
12	5.73D+07	4.32D+05	3.56D+07	0.6139	
13	1.22D+08	4.69D+05	4.57D+07	0.7251	
14	1.37D+08	6.07D+05	7.23D+06	0.9458	
15	1.15D+08	2.68D+05	6.06D+05	0.9925	
16	1.21D+07	7.21D+05	2.31D+07	0.337	
16	4.84D+6	3.92D+03	4.74D+05	0.91	0.91
18	1.47D+08	1.63D+05	5.48D+06	0.9631	
19	7.83D+07	5.28D+05	1.33D+08	0.3698	
20	9.85D+07	1.35D+05	1.18D+07	0.892	
21	1.02D+08	2.03D+05	7.80D+07	0.5671	
22	1.47D+08	1.99D+05	4.67D+07	0.7581	
23	1.60D+08	2.50D+05	7.80D+06	0.9521	
24	1.28D+08	1.23D+05	4.22D+06	0.9671	
25	7.36D+07	4.12D+05	1.50D+05	0.9924	
26	7.13D+07	3.68D+05	4.95D+07	0.5886	
27	1.21D+08	4.22D+05	3.13D+07	0.7928	
28	9.65D+07	2.64D+05	8.76D+05	0.9883	
29	9.87D+07	1.23D+06	1.42D+08	0.4079	
30	8.78D+07	2.81D+05	1.55D+08	0.3611	
31	1.40D+08	2.23D+05	1.32D+07	0.9121	
32	5.07D+07	5.66D+05	1.00D+08	0.3354	
33	1.53D+08	3.10D+05	1.60D+06	0.9877	
34	1.47D+08	2.96D+05	1.16D+07	0.925	
35	1.34D+08	5.45D+05	1.60D+06	0.9842	
36	9.89D+07	6.43D+05	5.53D+08	0.1516	
37	1.63D+08	3.56D+05	2.14D+07	0.8824	
38	1.17D+08	1.49D+05	1.16D+07	0.9092	
39	1.10D+08	1.80D+05	1.22D+07	0.8992	
40	1.48D+08	2.44D+05	4.25D+07	0.7759	
41	9.21D+07	1.84D+05	3.40D+07	0.7292	
42	6.52D+06	4.53D+06	1.2D+05	0.58	0.55
43	1.52D+07	1.1D+07	6.86D+05	0.57	0.51
44	1.64D+08	1.92D+07	3.12D+06	0.88	0.83
45	2.22D+06	1.92D+06	6.1D+06	0.27	0.36
46	1.38D+08	4.40D+03	1.50D+05	0.9989	0.16
47	6.32D+06	5.77D+05	3.62D+07	0.1468	
48	2.58D+06	5.34D+05	4.22D+07	0.0568	
49	1.50D+08	7.45D+05	1.60D+06	0.9846	
50	1.30D+08	6.20D+05	5.25D+06	0.9569	
51	9.77D+07	4.51D+05	2.50D+06	0.9707	0.55

Table S3. The Cartesian coordinates for the compound **1** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.721556	0.705259	0.000000
2	6	1.721556	-0.705259	0.000000
3	6	0.705259	1.721556	0.000000
4	6	-0.705259	1.721556	0.000000
5	6	-1.721556	0.705259	0.000000
6	6	-1.721556	-0.705259	0.000000
7	6	-0.705259	-1.721556	0.000000
8	6	0.705259	-1.721556	0.000000
9	6	2.971504	1.372379	0.000000
10	6	4.200363	0.693266	0.000000
11	6	4.200363	-0.693266	0.000000
12	6	2.971504	-1.372379	0.000000
13	7	2.737708	-2.737708	0.000000
14	6	1.372379	-2.971504	0.000000
15	6	0.693266	-4.200363	0.000000
16	6	-1.372379	-2.971504	0.000000
17	6	1.372379	2.971504	0.000000
18	7	2.737708	2.737708	0.000000
19	6	0.693266	4.200363	0.000000
20	6	-0.693266	4.200363	0.000000
21	6	-1.372379	2.971504	0.000000
22	7	-2.737708	2.737708	0.000000
23	6	-2.971504	1.372379	0.000000
24	6	-4.200363	0.693266	0.000000
25	6	-4.200363	-0.693266	0.000000
26	6	-2.971504	-1.372379	0.000000
27	7	-2.737708	-2.737708	0.000000
28	6	-0.693266	-4.200363	0.000000
29	1	3.448271	3.448271	0.000000
30	1	-3.448271	-3.448271	0.000000
31	1	5.136527	1.240298	0.000000
32	1	5.136527	-1.240298	0.000000
33	1	1.240298	-5.136527	0.000000
34	1	1.240298	5.136527	0.000000
35	1	-1.240298	5.136527	0.000000
36	1	-5.136527	1.240298	0.000000
37	1	-5.136527	-1.240298	0.000000
38	1	-1.240298	-5.136527	0.000000
39	1	3.448271	-3.448271	0.000000
40	1	-3.448271	3.448271	0.000000

Table S4. The Cartesian coordinates for the compound **2** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	-0.717421	1.690143
2	6	0.000000	-1.716202	0.705418
3	6	0.000000	0.717421	1.690143
4	6	0.000000	1.716202	0.705418
5	6	0.000000	1.719026	-0.729067
6	6	0.000000	0.719390	-1.723449
7	6	0.000000	-0.719390	-1.723449
8	6	0.000000	-1.719026	-0.729067
9	6	0.000000	-1.100324	3.036694
10	6	0.000000	-2.430299	3.461042

11	6	0.000000	-3.428913	2.490921
12	6	0.000000	-3.066675	1.133939
13	7	0.000000	-3.871333	0.005911
14	6	0.000000	-3.075589	-1.132018
15	6	0.000000	-3.463840	-2.481880
16	6	0.000000	-1.131364	-3.078301
17	6	0.000000	1.100324	3.036694
18	8	0.000000	0.000000	3.868059
19	6	0.000000	2.430299	3.461042
20	6	0.000000	3.428913	2.490921
21	6	0.000000	3.066675	1.133939
22	7	0.000000	3.871333	0.005911
23	6	0.000000	3.075589	-1.132018
24	6	0.000000	3.463840	-2.481880
25	6	0.000000	2.482616	-3.462540
26	6	0.000000	1.131364	-3.078301
27	7	0.000000	0.000000	-3.878468
28	6	0.000000	-2.482616	-3.462540
29	1	0.000000	0.000000	-4.883614
30	1	0.000000	-2.672807	4.515977
31	1	0.000000	-4.471787	2.786890
32	1	0.000000	-4.511965	-2.759056
33	1	0.000000	2.672807	4.515977
34	1	0.000000	4.471787	2.786890
35	1	0.000000	4.511965	-2.759056
36	1	0.000000	2.760209	-4.510646
37	1	0.000000	-2.760209	-4.510646
38	1	0.000000	-4.876404	0.009627
39	1	0.000000	4.876404	0.009627

Table S5. The Cartesian coordinates for the compound **3** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.697537	1.692819
2	6	0.000000	-0.697537	1.692819
3	6	0.000000	1.711987	0.682590
4	6	0.000000	1.718140	-0.719404
5	6	0.000000	0.704729	-1.736649
6	6	0.000000	-0.704729	-1.736649
7	6	0.000000	-1.718140	-0.719404
8	6	0.000000	-1.711987	0.682590
9	6	0.000000	1.363736	2.924023
10	6	0.000000	0.699186	4.152047
11	6	0.000000	-0.699186	4.152047
12	6	0.000000	-1.363736	2.924023
13	8	0.000000	-2.730610	2.739157
14	6	0.000000	-2.929619	1.370852
15	6	0.000000	-4.170399	0.729853
16	6	0.000000	-2.975492	-1.370838
17	6	0.000000	2.929619	1.370852
18	8	0.000000	2.730610	2.739157
19	6	0.000000	4.170399	0.729853
20	6	0.000000	4.189724	-0.662982
21	6	0.000000	2.975492	-1.370838
22	7	0.000000	2.746395	-2.738015
23	6	0.000000	1.378506	-2.980310
24	6	0.000000	0.693978	-4.207788
25	6	0.000000	-0.693978	-4.207788
26	6	0.000000	-1.378506	-2.980310
27	7	0.000000	-2.746395	-2.738015
28	6	0.000000	-4.189724	-0.662982
29	1	0.000000	-3.459845	-3.446286
30	1	0.000000	1.254674	5.080956

31	1	0.000000	-1.254674	5.080956
32	1	0.000000	-5.089120	1.302113
33	1	0.000000	5.089120	1.302113
34	1	0.000000	5.137429	-1.189183
35	1	0.000000	1.236965	-5.146092
36	1	0.000000	-1.236965	-5.146092
37	1	0.000000	-5.137429	-1.189183
38	1	0.000000	3.459845	-3.446286

Table S6. The Cartesian coordinates for the compound **4** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.719178	-0.715859	0.000000
2	6	0.718124	-1.697551	0.000000
3	6	1.719178	0.715859	0.000000
4	6	0.718124	1.697551	0.000000
5	6	-0.718124	1.697551	0.000000
6	6	-1.719178	0.715859	0.000000
7	6	-1.719178	-0.715859	0.000000
8	6	-0.718124	-1.697551	0.000000
9	6	3.070673	-1.135296	0.000000
10	6	3.432538	-2.493020	0.000000
11	6	2.433193	-3.463469	0.000000
12	6	1.101026	-3.043417	0.000000
13	8	0.000000	-3.874698	0.000000
14	6	-1.101026	-3.043417	0.000000
15	6	-2.433193	-3.463469	0.000000
16	6	-3.070673	-1.135296	0.000000
17	6	3.070673	1.135296	0.000000
18	7	3.871010	0.000000	0.000000
19	6	3.432538	2.493020	0.000000
20	6	2.433193	3.463469	0.000000
21	6	1.101026	3.043417	0.000000
22	8	0.000000	3.874698	0.000000
23	6	-1.101026	3.043417	0.000000
24	6	-2.433193	3.463469	0.000000
25	6	-3.432538	2.493020	0.000000
26	6	-3.070673	1.135296	0.000000
27	7	-3.871010	0.000000	0.000000
28	6	-3.432538	-2.493020	0.000000
29	1	-4.876353	0.000000	0.000000
30	1	4.474733	-2.790905	0.000000
31	1	2.678292	-4.517801	0.000000
32	1	-2.678292	-4.517801	0.000000
33	1	4.474733	2.790905	0.000000
34	1	2.678292	4.517801	0.000000
35	1	-2.678292	4.517801	0.000000
36	1	-4.474733	2.790905	0.000000
37	1	-4.474733	-2.790905	0.000000
38	1	4.876353	0.000000	0.000000

Table S7. The Cartesian coordinates for the compound **5** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	-0.716657	1.726612
2	6	0.000000	-1.700560	0.728356

3	6	0.000000	0.716657	1.726612
4	6	0.000000	1.700560	0.728356
5	6	0.000000	1.697699	-0.704570
6	6	0.000000	0.714281	-1.693420
7	6	0.000000	-0.714281	-1.693420
8	6	0.000000	-1.697699	-0.704570
9	6	0.000000	-1.135811	3.077484
10	6	0.000000	-2.495610	3.435225
11	6	0.000000	-3.467319	2.435416
12	6	0.000000	-3.047560	1.102721
13	8	0.000000	-3.874544	-0.006113
14	6	0.000000	-3.038732	-1.104058
15	6	0.000000	-3.433033	-2.444229
16	6	0.000000	-1.105115	-3.036352
17	6	0.000000	1.135811	3.077484
18	7	0.000000	0.000000	3.878120
19	6	0.000000	2.495610	3.435225
20	6	0.000000	3.467319	2.435416
21	6	0.000000	3.047560	1.102721
22	8	0.000000	3.874544	-0.006113
23	6	0.000000	3.038732	-1.104058
24	6	0.000000	3.433033	-2.444229
25	6	0.000000	2.443811	-3.434449
26	6	0.000000	1.105115	-3.036352
27	8	0.000000	0.000000	-3.867797
28	6	0.000000	-2.443811	-3.434449
29	1	0.000000	-2.795904	4.476563
30	1	0.000000	-4.520946	2.682845
31	1	0.000000	-4.481923	-2.710881
32	1	0.000000	2.795904	4.476563
33	1	0.000000	4.520946	2.682845
34	1	0.000000	4.481923	-2.710881
35	1	0.000000	2.710541	-4.483242
36	1	0.000000	-2.710541	-4.483242
37	1	0.000000	0.000000	4.884064

Table S8. The Cartesian coordinates for the compound **6** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.700839	-0.714892	0.000000
2	6	0.714892	-1.700839	0.000000
3	6	1.700839	0.714892	0.000000
4	6	0.714892	1.700839	0.000000
5	6	-0.714892	1.700839	0.000000
6	6	-1.700839	0.714892	0.000000
7	6	-1.700839	-0.714892	0.000000
8	6	-0.714892	-1.700839	0.000000
9	6	3.042868	-1.105853	0.000000
10	6	3.436969	-2.446930	0.000000
11	6	2.446930	-3.436969	0.000000
12	6	1.105853	-3.042868	0.000000
13	8	0.000000	-3.874017	0.000000
14	6	-1.105853	-3.042868	0.000000
15	6	-2.446930	-3.436969	0.000000
16	6	-3.042868	-1.105853	0.000000
17	6	3.042868	1.105853	0.000000
18	8	3.874017	0.000000	0.000000
19	6	3.436969	2.446930	0.000000
20	6	2.446930	3.436969	0.000000
21	6	1.105853	3.042868	0.000000
22	8	0.000000	3.874017	0.000000
23	6	-1.105853	3.042868	0.000000
24	6	-2.446930	3.436969	0.000000

25	6	-3.436969	2.446930	0.000000
26	6	-3.042868	1.105853	0.000000
27	8	-3.874017	0.000000	0.000000
28	6	-3.436969	-2.446930	0.000000
29	1	4.485185	-2.715899	0.000000
30	1	2.715899	-4.485185	0.000000
31	1	-2.715899	-4.485185	0.000000
32	1	4.485185	2.715899	0.000000
33	1	2.715899	4.485185	0.000000
34	1	-2.715899	4.485185	0.000000
35	1	-4.485185	2.715899	0.000000
36	1	-4.485185	-2.715899	0.000000

Table S9. The Cartesian coordinates for the compound **7** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.034835	-1.726244	0.000000
2	6	-1.446645	-1.736528	0.000000
3	6	0.984084	-0.712760	0.000000
4	6	0.980839	0.712178	0.000000
5	6	-0.047104	1.710500	0.000000
6	6	-1.451464	1.692665	0.000000
7	6	-2.461134	0.674958	0.000000
8	6	-2.464128	-0.727145	0.000000
9	6	0.631565	-2.976952	0.000000
10	6	-0.045215	-4.207024	0.000000
11	6	-1.431821	-4.212428	0.000000
12	6	-2.114479	-2.984594	0.000000
13	7	-3.482722	-2.750294	0.000000
14	6	-3.719522	-1.385002	0.000000
15	6	-4.938196	-0.688641	0.000000
16	6	-3.688173	1.349899	0.000000
17	6	2.222250	-1.374043	0.000000
18	7	1.994962	-2.737617	0.000000
19	6	3.482300	-0.699301	0.000000
20	6	3.475291	0.735307	0.000000
21	6	2.206971	1.393363	0.000000
22	7	1.958440	2.756187	0.000000
23	6	0.591862	2.976116	0.000000
24	6	-0.116896	4.187796	0.000000
25	6	-1.508048	4.158474	0.000000
26	6	-2.138711	2.912672	0.000000
27	8	-3.503232	2.716652	0.000000
28	6	-4.924945	0.704269	0.000000
29	6	4.725673	-1.369019	0.000000
30	6	4.711029	1.418779	0.000000
31	1	0.406839	5.136949	0.000000
32	1	-2.090030	5.071061	0.000000
33	1	2.657386	3.478382	0.000000
34	1	0.504782	-5.141397	0.000000
35	1	-1.975152	-5.150500	0.000000
36	6	5.908515	0.734605	0.000000
37	6	5.915752	-0.671938	0.000000
38	1	-5.881928	-1.221960	0.000000
39	1	-5.845102	1.274344	0.000000
40	1	4.750695	-2.453796	0.000000
41	1	4.723600	2.503725	0.000000
42	1	6.845039	1.280230	0.000000
43	1	6.857963	-1.207746	0.000000
44	1	-4.191544	-3.462608	0.000000
45	1	2.703802	-3.450059	0.000000

Table S10. The Cartesian coordinates for the compound **8** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.717862	-0.758797
2	6	0.000000	1.729312	0.247613
3	6	0.000000	-0.717862	-0.758797
4	6	0.000000	-1.729312	0.247613
5	6	0.000000	-1.716841	1.679985
6	6	0.000000	-0.716390	2.665157
7	6	0.000000	0.716390	2.665157
8	6	0.000000	1.716841	1.679985
9	6	0.000000	1.126923	-2.103063
10	6	0.000000	2.492123	-2.523166
11	6	0.000000	3.504362	-1.507553
12	6	0.000000	3.076248	-0.144232
13	7	0.000000	3.870273	0.990342
14	6	0.000000	3.065876	2.116465
15	6	0.000000	3.428510	3.472079
16	6	0.000000	1.100131	4.011913
17	6	0.000000	-1.126923	-2.103063
18	7	0.000000	0.000000	-2.900309
19	6	0.000000	-2.492123	-2.523166
20	6	0.000000	-3.504362	-1.507553
21	6	0.000000	-3.076248	-0.144232
22	7	0.000000	-3.870273	0.990342
23	6	0.000000	-3.065876	2.116465
24	6	0.000000	-3.428510	3.472079
25	6	0.000000	-2.428387	4.440409
26	6	0.000000	-1.100131	4.011913
27	8	0.000000	0.000000	4.842706
28	6	0.000000	2.428387	4.440409
29	1	0.000000	-4.875440	1.000574
30	6	0.000000	2.893462	-3.877775
31	6	0.000000	4.860753	-1.901393
32	1	0.000000	4.875440	1.000574
33	1	0.000000	0.000000	-3.904879
34	6	0.000000	-4.860753	-1.901393
35	6	0.000000	-5.219587	-3.232833
36	6	0.000000	-4.226710	-4.229644
37	1	0.000000	4.471363	3.767749
38	1	0.000000	2.667184	5.496019
39	1	0.000000	-5.639196	-1.145638
40	1	0.000000	-6.266519	-3.513094
41	1	0.000000	-4.511592	-5.275394
42	6	0.000000	-2.893462	-3.877775
43	1	0.000000	-2.142442	-4.660898
44	6	0.000000	4.226710	-4.229644
45	6	0.000000	5.219587	-3.232833
46	1	0.000000	-4.471363	3.767749
47	1	0.000000	-2.667184	5.496019
48	1	0.000000	2.142442	-4.660898
49	1	0.000000	5.639196	-1.145638
50	1	0.000000	4.511592	-5.275394
51	1	0.000000	6.266519	-3.513094

Table S11. The Cartesian coordinates for the compound **9** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.400652	1.012701	0.000000

2	6	2.167532	-0.190082	0.000000
3	6	0.000000	1.325988	0.000000
4	6	-1.209192	0.565398	0.000000
5	6	-1.520821	-0.830611	0.000000
6	6	-0.750710	-2.023002	0.000000
7	6	0.649514	-2.328139	0.000000
8	6	1.841569	-1.584323	0.000000
9	6	2.094580	2.234766	0.000000
10	6	3.518066	2.346502	0.000000
11	6	4.283786	1.134125	0.000000
12	6	3.567648	-0.101809	0.000000
13	7	4.093700	-1.382908	0.000000
14	6	3.062821	-2.305329	0.000000
15	6	3.123509	-3.707710	0.000000
16	6	0.735840	-3.726415	0.000000
17	6	-0.104752	2.727342	0.000000
18	7	1.168946	3.258701	0.000000
19	6	-1.343036	3.440465	0.000000
20	6	-2.554152	2.673985	0.000000
21	6	-2.435159	1.250776	0.000000
22	7	-3.456903	0.318567	0.000000
23	6	-2.921012	-0.953041	0.000000
24	6	-3.608780	-2.205724	0.000000
25	6	-2.816502	-3.403407	0.000000
26	6	-1.406544	-3.243646	0.000000
27	8	-0.519594	-4.294408	0.000000
28	6	1.937606	-4.435266	0.000000
29	1	-4.438106	0.534660	0.000000
30	6	4.206287	3.580498	0.000000
31	6	5.693491	1.221709	0.000000
32	1	5.072192	-1.613062	0.000000
33	1	1.388071	4.239034	0.000000
34	1	4.077759	-4.221701	0.000000
35	1	1.940265	-5.517536	0.000000
36	6	5.584091	3.632178	0.000000
37	6	6.335006	2.442227	0.000000
38	6	-5.015972	-2.335047	0.000000
39	6	-3.458813	-4.661251	0.000000
40	1	3.644615	4.508880	0.000000
41	1	6.287235	0.313639	0.000000
42	1	6.090649	4.590368	0.000000
43	1	7.417880	2.486556	0.000000
44	6	-4.833935	-4.746811	0.000000
45	6	-5.617385	-3.575739	0.000000
46	6	-1.433914	4.849837	0.000000
47	6	-3.789541	3.358437	0.000000
48	1	-5.637809	-1.445746	0.000000
49	1	-2.847656	-5.555589	0.000000
50	1	-5.316890	-5.717139	0.000000
51	1	-6.698699	-3.651625	0.000000
52	6	-3.844514	4.736492	0.000000
53	6	-2.656097	5.488950	0.000000
54	1	-0.527803	5.446700	0.000000
55	1	-4.716460	2.794368	0.000000
56	1	-4.803726	5.241018	0.000000
57	1	-2.701972	6.571786	0.000000

Table S12. The Cartesian coordinates for the compound **10** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.490286	-1.711535	0.000000
2	6	-0.078667	-1.741133	0.000000
3	6	-2.489801	-0.677956	0.000000

4	6	-2.469650	0.731619	0.000000
5	6	-1.436180	1.725178	0.000000
6	6	-0.032991	1.692083	0.000000
7	6	0.969899	0.666209	0.000000
8	6	0.957251	-0.751924	0.000000
9	6	-2.178670	-2.949399	0.000000
10	6	-1.520287	-4.190854	0.000000
11	6	-0.133965	-4.217922	0.000000
12	6	0.567188	-3.001757	0.000000
13	7	1.937276	-2.784654	0.000000
14	6	2.189107	-1.425844	0.000000
15	6	3.453300	-0.756834	0.000000
16	6	2.188168	1.325565	0.000000
17	6	-3.751441	-1.322449	0.000000
18	7	-3.539798	-2.692014	0.000000
19	6	-4.966104	-0.618565	0.000000
20	6	-4.942798	0.769201	0.000000
21	6	-3.702797	1.426886	0.000000
22	7	-3.436478	2.789860	0.000000
23	6	-2.066510	2.994823	0.000000
24	6	-1.345313	4.199897	0.000000
25	6	0.046136	4.157950	0.000000
26	6	0.664093	2.907371	0.000000
27	8	2.025880	2.691354	0.000000
28	6	3.452346	0.679929	0.000000
29	1	-1.859620	5.154092	0.000000
30	1	0.635821	5.065675	0.000000
31	1	-4.131558	3.515544	0.000000
32	1	-2.084721	-5.116449	0.000000
33	1	0.394576	-5.164551	0.000000
34	6	4.698678	-1.423856	0.000000
35	6	4.681339	1.374863	0.000000
36	1	2.633799	-3.509518	0.000000
37	1	-4.262117	-3.390935	0.000000
38	6	5.876309	0.688367	0.000000
39	6	5.884718	-0.720138	0.000000
40	1	-5.912476	-1.147647	0.000000
41	1	-5.870085	1.330814	0.000000
42	1	4.727400	-2.508643	0.000000
43	1	4.664177	2.458041	0.000000
44	1	6.813948	1.232270	0.000000
45	1	6.828686	-1.253125	0.000000

Table S13. The Cartesian coordinates for the compound **11** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.718611	-2.688975
2	6	0.000000	1.720484	-1.694408
3	6	0.000000	-0.718611	-2.688975
4	6	0.000000	-1.720484	-1.694408
5	6	0.000000	-1.727930	-0.262378
6	6	0.000000	-0.717381	0.734149
7	6	0.000000	0.717381	0.734149
8	6	0.000000	1.727930	-0.262378
9	6	0.000000	1.131255	-4.044243
10	6	0.000000	2.480920	-4.433176
11	6	0.000000	3.463816	-3.454658
12	6	0.000000	3.076010	-2.106046
13	7	0.000000	3.871284	-0.969688
14	6	0.000000	3.069097	0.155124
15	6	0.000000	3.469529	1.527878
16	6	0.000000	1.096461	2.068070
17	6	0.000000	-1.131255	-4.044243
18	7	0.000000	0.000000	-4.843621

19	6	0.000000	-2.480920	-4.433176
20	6	0.000000	-3.463816	-3.454658
21	6	0.000000	-3.076010	-2.106046
22	7	0.000000	-3.871284	-0.969688
23	6	0.000000	-3.069097	0.155124
24	6	0.000000	-3.469529	1.527878
25	6	0.000000	-2.438361	2.527998
26	6	0.000000	-1.096461	2.068070
27	8	0.000000	0.000000	2.897353
28	6	0.000000	2.438361	2.527998
29	6	0.000000	-4.816108	1.955415
30	6	0.000000	-2.797327	3.893923
31	1	0.000000	-4.876365	-0.971917
32	1	0.000000	2.754678	-5.482195
33	1	0.000000	4.511885	-3.732116
34	6	0.000000	4.816108	1.955415
35	6	0.000000	2.797327	3.893923
36	1	0.000000	4.876365	-0.971917
37	1	0.000000	0.000000	-5.848761
38	6	0.000000	4.122496	4.271704
39	6	0.000000	5.138646	3.296108
40	1	0.000000	-2.754678	-5.482195
41	1	0.000000	-4.511885	-3.732116
42	1	0.000000	5.613919	1.219824
43	1	0.000000	2.010222	4.638221
44	1	0.000000	4.386116	5.323156
45	1	0.000000	6.178741	3.601575
46	6	0.000000	-5.138646	3.296108
47	6	0.000000	-4.122496	4.271704
48	1	0.000000	-5.613919	1.219824
49	1	0.000000	-2.010222	4.638221
50	1	0.000000	-6.178741	3.601575
51	1	0.000000	-4.386116	5.323156

Table S14. The Cartesian coordinates for the compound **12** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.131327	-2.396919	0.000000
2	6	-1.278863	-2.460264	0.000000
3	6	1.110773	-1.345814	0.000000
4	6	1.055736	0.079746	0.000000
5	6	0.000000	1.045894	0.000000
6	6	-1.418024	0.973462	0.000000
7	6	-2.383016	-0.087156	0.000000
8	6	-2.332567	-1.489382	0.000000
9	6	0.843759	-3.622289	0.000000
10	6	0.213931	-4.876509	0.000000
11	6	-1.171783	-4.933891	0.000000
12	6	-1.899380	-3.732832	0.000000
13	7	-3.275348	-3.549130	0.000000
14	6	-3.562705	-2.194146	0.000000
15	6	-4.808268	-1.546615	0.000000
16	6	-3.637983	0.536110	0.000000
17	6	2.373094	-1.960822	0.000000
18	7	2.196908	-3.331572	0.000000
19	6	3.609417	-1.243067	0.000000
20	6	3.552056	0.189820	0.000000
21	6	2.261246	0.800110	0.000000
22	7	1.962583	2.151072	0.000000
23	6	0.592846	2.320350	0.000000
24	6	-0.149916	3.541627	0.000000
25	6	-1.583049	3.452698	0.000000
26	6	-2.148824	2.150739	0.000000
27	8	-3.502235	1.908123	0.000000

28	6	-4.849250	-0.154796	0.000000
29	6	0.439579	4.825606	0.000000
30	6	-2.352789	4.636263	0.000000
31	1	2.638691	2.894040	0.000000
32	1	0.798507	-5.789669	0.000000
33	1	-1.679544	-5.891652	0.000000
34	1	-3.957817	-4.287315	0.000000
35	1	2.932186	-4.016647	0.000000
36	6	4.875257	-1.869210	0.000000
37	6	4.763110	0.916439	0.000000
38	6	-0.335964	5.965992	0.000000
39	6	-1.741265	5.871304	0.000000
40	1	1.520541	4.921690	0.000000
41	1	-3.432801	4.552195	0.000000
42	1	0.138106	6.940882	0.000000
43	1	-2.341806	6.773682	0.000000
44	6	5.983676	0.274339	0.000000
45	6	6.040390	-1.131047	0.000000
46	1	-5.730091	-2.116888	0.000000
47	1	-5.790500	0.379718	0.000000
48	1	4.938474	-2.952420	0.000000
49	1	4.738401	2.001270	0.000000
50	1	6.900462	0.852580	0.000000
51	1	7.000776	-1.633468	0.000000

Table S15. The Cartesian coordinates for the compound **13** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.658073	-2.355070	0.000000
2	6	1.852851	-1.599528	0.000000
3	6	-0.746407	-2.054961	0.000000
4	6	-1.517263	-0.854690	0.000000
5	6	-1.204278	0.541358	0.000000
6	6	0.000000	1.295729	0.000000
7	6	1.400291	0.986785	0.000000
8	6	2.171335	-0.204107	0.000000
9	6	0.775214	-3.767332	0.000000
10	6	2.008359	-4.439740	0.000000
11	6	3.177811	-3.696077	0.000000
12	6	3.086875	-2.294857	0.000000
13	7	4.109650	-1.358839	0.000000
14	6	3.570994	-0.086629	0.000000
15	6	4.259063	1.166422	0.000000
16	6	2.059436	2.206844	0.000000
17	6	-1.429564	-3.281693	0.000000
18	7	-0.499854	-4.304114	0.000000
19	6	-2.853481	-3.401328	0.000000
20	6	-3.626790	-2.193702	0.000000
21	6	-2.917993	-0.954693	0.000000
22	7	-3.446306	0.323948	0.000000
23	6	-2.420522	1.246569	0.000000
24	6	-2.514253	2.672934	0.000000
25	6	-1.290368	3.423114	0.000000
26	6	-0.081616	2.680042	0.000000
27	8	1.167625	3.252994	0.000000
28	6	3.468535	2.365767	0.000000
29	1	-4.426130	0.546360	0.000000
30	1	5.090465	-1.579714	0.000000
31	1	-0.709893	-5.287151	0.000000
32	6	5.666650	1.292636	0.000000
33	6	4.114733	3.622143	0.000000
34	6	-3.735016	3.384594	0.000000
35	6	-1.341042	4.834414	0.000000

36	6	-2.551283	5.493246	0.000000
37	6	-3.756142	4.763278	0.000000
38	6	-3.533057	-4.639894	0.000000
39	6	-5.036093	-2.291188	0.000000
40	1	-4.674462	2.841481	0.000000
41	1	-0.409909	5.387785	0.000000
42	1	-2.578723	6.576777	0.000000
43	1	-4.704099	5.288933	0.000000
44	6	-5.668915	-3.516187	0.000000
45	6	-4.910530	-4.701394	0.000000
46	1	-2.964542	-5.564007	0.000000
47	1	-5.636635	-1.387506	0.000000
48	1	-6.751525	-3.567608	0.000000
49	1	-5.410823	-5.662826	0.000000
50	6	6.271262	2.531490	0.000000
51	6	5.489827	3.704183	0.000000
52	1	2.047676	-5.523070	0.000000
53	1	4.142535	-4.190346	0.000000
54	1	6.285703	0.401497	0.000000
55	1	3.507077	4.518854	0.000000
56	1	7.352681	2.605300	0.000000
57	1	5.975000	4.673449	0.000000

Table S16. The Cartesian coordinates for the compound **14** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.321372	-1.323418	0.000000
2	6	1.867777	-0.007506	0.000000
3	6	-0.009295	-1.865182	0.000000
4	6	-1.318545	-1.331034	0.000000
5	6	-1.878122	-0.013200	0.000000
6	6	-1.327305	1.293203	0.000000
7	6	0.000000	1.835402	0.000000
8	6	1.303474	1.309323	0.000000
9	6	2.209568	-2.410653	0.000000
10	6	3.631471	-2.273662	0.000000
11	6	4.177999	-0.947045	0.000000
12	6	3.261788	0.148387	0.000000
13	7	3.557368	1.501902	0.000000
14	6	2.381306	2.230847	0.000000
15	6	2.197583	3.622822	0.000000
16	6	-0.157647	3.227504	0.000000
17	6	0.124061	-3.275897	0.000000
18	7	1.473667	-3.580935	0.000000
19	6	-0.972334	-4.154409	0.000000
20	6	-2.254185	-3.627696	0.000000
21	6	-2.411323	-2.231964	0.000000
22	7	-3.583156	-1.490571	0.000000
23	6	-3.276434	-0.143104	0.000000
24	6	-4.171026	0.971965	0.000000
25	6	-3.600106	2.290609	0.000000
26	6	-2.184503	2.381629	0.000000
27	8	-1.492414	3.570415	0.000000
28	6	0.903547	4.133790	0.000000
29	1	-4.509480	-1.881108	0.000000
30	6	4.521465	-3.371264	0.000000
31	6	5.582322	-0.792112	0.000000
32	1	4.480475	1.899395	0.000000
33	1	1.852489	-4.511936	0.000000
34	1	3.048180	4.294635	0.000000
35	1	0.718759	5.200194	0.000000
36	6	5.887510	-3.186016	0.000000
37	6	6.423156	-1.884521	0.000000
38	6	-5.579473	0.853532	0.000000

39	6	-4.453313	3.416543	0.000000
40	1	4.126635	-4.381825	0.000000
41	1	6.011239	0.204428	0.000000
42	1	6.551344	-4.042802	0.000000
43	1	7.497678	-1.742890	0.000000
44	6	-5.821833	3.259981	0.000000
45	6	-6.388597	1.969581	0.000000
46	1	-0.821099	-5.227861	0.000000
47	1	-3.116929	-4.284017	0.000000
48	1	-6.035312	-0.131126	0.000000
49	1	-4.007960	4.403966	0.000000
50	1	-6.467454	4.130648	0.000000
51	1	-7.466556	1.855593	0.000000

Table S17. The Cartesian coordinates for the compound **15** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.717503	-1.732418
2	6	0.000000	1.730762	-0.726106
3	6	0.000000	-0.717503	-1.732418
4	6	0.000000	-1.730762	-0.726106
5	6	0.000000	-1.728683	0.704125
6	6	0.000000	-0.716779	1.700917
7	6	0.000000	0.716779	1.700917
8	6	0.000000	1.728683	0.704125
9	6	0.000000	1.126779	-3.076931
10	6	0.000000	2.490571	-3.502042
11	6	0.000000	3.504717	-2.489173
12	6	0.000000	3.076914	-1.126904
13	7	0.000000	3.869411	0.006351
14	6	0.000000	3.068655	1.129493
15	6	0.000000	3.469256	2.501328
16	6	0.000000	1.096228	3.034777
17	6	0.000000	-1.126779	-3.076931
18	7	0.000000	0.000000	-3.873259
19	6	0.000000	-2.490571	-3.502042
20	6	0.000000	-3.504717	-2.489173
21	6	0.000000	-3.076914	-1.126904
22	7	0.000000	-3.869411	0.006351
23	6	0.000000	-3.068655	1.129493
24	6	0.000000	-3.469256	2.501328
25	6	0.000000	-2.436785	3.498839
26	6	0.000000	-1.096228	3.034777
27	8	0.000000	0.000000	3.863307
28	6	0.000000	2.436785	3.498839
29	1	0.000000	-4.874035	0.010486
30	1	0.000000	4.874035	0.010486
31	1	0.000000	0.000000	-4.877685
32	6	0.000000	4.815205	2.931359
33	6	0.000000	2.792130	4.865706
34	6	0.000000	-4.815205	2.931359
35	6	0.000000	-2.792130	4.865706
36	6	0.000000	-4.116427	5.246404
37	6	0.000000	-5.134542	4.272726
38	6	0.000000	-2.887828	-4.857488
39	6	0.000000	-4.860041	-2.886380
40	1	0.000000	-5.614926	2.197839
41	1	0.000000	-2.003291	5.608025
42	1	0.000000	-4.378009	6.298261
43	1	0.000000	-6.173901	4.580453
44	6	0.000000	-5.215308	-4.218971
45	6	0.000000	-4.220293	-5.213299
46	1	0.000000	-2.134873	-5.638803
47	1	0.000000	-5.641194	-2.133258

48	1	0.000000	-6.261690	-4.501362
49	1	0.000000	-4.502072	-6.259856
50	6	0.000000	5.134542	4.272726
51	6	0.000000	4.116427	5.246404
52	6	0.000000	2.887828	-4.857488
53	6	0.000000	4.860041	-2.886380
54	1	0.000000	5.614926	2.197839
55	1	0.000000	2.003291	5.608025
56	1	0.000000	6.173901	4.580453
57	1	0.000000	4.378009	6.298261
58	6	0.000000	5.215308	-4.218971
59	6	0.000000	4.220293	-5.213299
60	1	0.000000	2.134873	-5.638803
61	1	0.000000	5.641194	-2.133258
62	1	0.000000	6.261690	-4.501362
63	1	0.000000	4.502072	-6.259856

Table S18. The Cartesian coordinates for the compound **16** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.455271	1.690141	0.000000
2	6	0.059495	1.703307	0.000000
3	6	2.464705	0.674155	0.000000
4	6	2.467573	-0.727425	0.000000
5	6	1.449268	-1.735149	0.000000
6	6	0.046560	-1.719238	0.000000
7	6	-0.965321	-0.705774	0.000000
8	6	-0.961915	0.705681	0.000000
9	6	2.128189	2.917734	0.000000
10	6	1.469889	4.149721	0.000000
11	6	0.070409	4.160835	0.000000
12	6	-0.601073	2.937495	0.000000
13	8	-1.971017	2.749185	0.000000
14	6	-2.167574	1.384145	0.000000
15	6	-3.435209	0.739632	0.000000
16	6	-2.182878	-1.363949	0.000000
17	6	3.686638	1.354915	0.000000
18	8	3.494076	2.724875	0.000000
19	6	4.921705	0.703826	0.000000
20	6	4.934328	-0.691088	0.000000
21	6	3.716792	-1.392237	0.000000
22	7	3.472194	-2.760231	0.000000
23	6	2.102123	-2.990606	0.000000
24	6	1.391184	-4.203509	0.000000
25	6	-0.002787	-4.179006	0.000000
26	6	-0.641574	-2.937725	0.000000
27	8	-2.008916	-2.728817	0.000000
28	6	-3.442206	-0.702099	0.000000
29	6	-4.667319	1.430162	0.000000
30	6	-4.681866	-1.379136	0.000000
31	6	-5.857878	0.736926	0.000000
32	6	-5.865077	-0.673313	0.000000
33	1	5.844527	1.269284	0.000000
34	1	5.879945	-1.220498	0.000000
35	1	-4.655558	2.513316	0.000000
36	1	-4.681981	-2.462355	0.000000
37	1	-6.797214	1.277654	0.000000
38	1	-6.809980	-1.204307	0.000000
39	1	1.913408	-5.153053	0.000000
40	1	-0.576811	-5.096555	0.000000
41	1	4.179558	-3.475384	0.000000
42	1	2.031160	5.074950	0.000000
43	1	-0.476671	5.094576	0.000000

Table S19. The Cartesian coordinates for the compound **17** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.708140	-0.233186
2	6	0.000000	0.713705	0.770144
3	6	0.000000	1.701927	-1.665135
4	6	0.000000	0.716176	-2.663250
5	6	0.000000	-0.716176	-2.663250
6	6	0.000000	-1.701927	-1.665135
7	6	0.000000	-1.708140	-0.233186
8	6	0.000000	-0.713705	0.770144
9	6	0.000000	3.037394	0.154767
10	6	0.000000	3.470865	1.509300
11	6	0.000000	2.454792	2.531879
12	6	0.000000	1.101121	2.099888
13	8	0.000000	0.000000	2.929280
14	6	0.000000	-1.101121	2.099888
15	6	0.000000	-2.454792	2.531879
16	6	0.000000	-3.037394	0.154767
17	6	0.000000	3.048357	-2.047868
18	8	0.000000	3.873160	-0.937789
19	6	0.000000	3.467451	-3.378819
20	6	0.000000	2.493662	-4.377032
21	6	0.000000	1.135904	-4.015029
22	7	0.000000	0.000000	-4.814781
23	6	0.000000	-1.135904	-4.015029
24	6	0.000000	-2.493662	-4.377032
25	6	0.000000	-3.467451	-3.378819
26	6	0.000000	-3.048357	-2.047868
27	8	0.000000	-3.873160	-0.937789
28	6	0.000000	-3.470865	1.509300
29	6	0.000000	-2.849860	3.888267
30	6	0.000000	-4.829858	1.895101
31	6	0.000000	4.829858	1.895101
32	6	0.000000	2.849860	3.888267
33	6	0.000000	-4.184883	4.228055
34	6	0.000000	-5.179136	3.227631
35	1	0.000000	4.520895	-3.627142
36	1	0.000000	2.790570	-5.419264
37	1	0.000000	-2.083634	4.653920
38	1	0.000000	-5.589110	1.122538
39	1	0.000000	-4.475691	5.272228
40	1	0.000000	-6.225133	3.511632
41	6	0.000000	4.184883	4.228055
42	6	0.000000	5.179136	3.227631
43	1	0.000000	-2.790570	-5.419264
44	1	0.000000	-4.520895	-3.627142
45	1	0.000000	5.589110	1.122538
46	1	0.000000	2.083634	4.653920
47	1	0.000000	4.475691	5.272228
48	1	0.000000	6.225133	3.511632
49	1	0.000000	0.000000	-5.820653

Table S20. The Cartesian coordinates for the compound **18** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.727632	-2.038857	0.000000
2	6	-1.496305	-0.854142	0.000000
3	6	0.672385	-2.337124	0.000000
4	6	1.859426	-1.586013	0.000000
5	6	2.174462	-0.190843	0.000000
6	6	1.399799	0.997607	0.000000
7	6	0.000000	1.299800	0.000000

8	6	-1.191990	0.539972	0.000000
9	6	-1.390607	-3.255020	0.000000
10	6	-2.805793	-3.390913	0.000000
11	6	-3.588921	-2.180207	0.000000
12	6	-2.878238	-0.950289	0.000000
13	8	-3.453708	0.302404	0.000000
14	6	-2.409403	1.201638	0.000000
15	6	-2.547422	2.615745	0.000000
16	6	-0.103269	2.681925	0.000000
17	6	0.759321	-3.734039	0.000000
18	8	-0.500154	-4.303459	0.000000
19	6	1.969063	-4.431327	0.000000
20	6	3.151508	-3.695096	0.000000
21	6	3.087554	-2.291683	0.000000
22	7	4.110340	-1.353802	0.000000
23	6	3.572118	-0.076826	0.000000
24	6	4.253137	1.182075	0.000000
25	6	3.457799	2.381426	0.000000
26	6	2.047321	2.222132	0.000000
27	8	1.142882	3.263098	0.000000
28	6	-1.333866	3.393592	0.000000
29	1	5.091411	-1.573752	0.000000
30	6	5.659480	1.313151	0.000000
31	6	4.101511	3.638278	0.000000
32	6	-3.790032	3.286963	0.000000
33	6	-1.425628	4.802874	0.000000
34	6	-2.655146	5.424889	0.000000
35	6	-3.842039	4.663855	0.000000
36	6	-3.472488	-4.636142	0.000000
37	6	-4.997928	-2.277345	0.000000
38	1	-4.699944	2.699070	0.000000
39	1	-0.511612	5.384311	0.000000
40	1	-2.711844	6.507353	0.000000
41	1	-4.802071	5.167125	0.000000
42	6	6.260930	2.554001	0.000000
43	6	5.476780	3.723786	0.000000
44	1	6.281513	0.424107	0.000000
45	1	3.492241	4.533961	0.000000
46	1	7.342139	2.629924	0.000000
47	1	5.958643	4.694642	0.000000
48	6	-4.849037	-4.693602	0.000000
49	6	-5.614671	-3.509403	0.000000
50	1	-2.880044	-5.543103	0.000000
51	1	-5.583096	-1.365681	0.000000
52	1	-5.348724	-5.655495	0.000000
53	1	-6.696927	-3.570411	0.000000
54	1	1.984001	-5.513517	0.000000
55	1	4.106691	-4.207319	0.000000

Table S21. The Cartesian coordinates for the compound **19** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.015673	-1.688422	0.000000
2	6	-1.411257	-1.715219	0.000000
3	6	0.987882	-0.666046	0.000000
4	6	0.975143	0.751614	0.000000
5	6	-0.061550	1.737674	0.000000
6	6	-1.464803	1.702121	0.000000
7	6	-2.458084	0.670666	0.000000
8	6	-2.438308	-0.723757	0.000000
9	6	0.665627	-2.911759	0.000000
10	6	0.018597	-4.148800	0.000000
11	6	-1.380229	-4.171364	0.000000

12	6	-2.063452	-2.953248	0.000000
13	8	-3.435327	-2.783351	0.000000
14	6	-3.653348	-1.417602	0.000000
15	6	-4.892256	-0.774364	0.000000
16	6	-3.701040	1.314511	0.000000
17	6	2.200370	-1.331793	0.000000
18	8	2.029005	-2.700618	0.000000
19	6	3.464068	-0.681290	0.000000
20	6	3.464367	0.757827	0.000000
21	6	2.200461	1.431870	0.000000
22	7	1.940272	2.793191	0.000000
23	6	0.568145	3.005572	0.000000
24	6	-0.161430	4.206463	0.000000
25	6	-1.553785	4.160144	0.000000
26	6	-2.173740	2.907556	0.000000
27	8	-3.538357	2.684632	0.000000
28	6	-4.915399	0.625248	0.000000
29	6	4.693332	-1.374548	0.000000
30	6	4.709301	1.424315	0.000000
31	1	0.346111	5.164236	0.000000
32	1	-2.142833	5.068066	0.000000
33	1	2.634383	3.520631	0.000000
34	1	0.587328	-5.069662	0.000000
35	1	-1.919855	-5.109421	0.000000
36	6	5.895730	0.720728	0.000000
37	6	5.888019	-0.687028	0.000000
38	1	-5.812605	-1.343730	0.000000
39	1	-5.854769	1.162853	0.000000
40	1	4.677604	-2.457690	0.000000
41	1	4.737856	2.508962	0.000000
42	1	6.839218	1.254261	0.000000
43	1	6.825676	-1.230596	0.000000

Table S22. The Cartesian coordinates for the compound **20** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.698252	0.000000	1.631124
2	6	0.713508	0.000000	2.620222
3	6	1.709163	0.000000	0.199137
4	6	0.714519	0.000000	-0.813699
5	6	-0.714519	0.000000	-0.813699
6	6	-1.709163	0.000000	0.199137
7	6	-1.698252	0.000000	1.631124
8	6	-0.713508	0.000000	2.620222
9	6	3.038415	0.000000	2.038191
10	6	3.432689	0.000000	3.376686
11	6	2.441972	0.000000	4.365418
12	6	1.105097	0.000000	3.963899
13	8	0.000000	0.000000	4.794394
14	6	-1.105097	0.000000	3.963899
15	6	-2.441972	0.000000	4.365418
16	6	-3.038415	0.000000	2.038191
17	6	3.044259	0.000000	-0.164264
18	8	3.871714	0.000000	0.938989
19	6	3.505080	0.000000	-1.508665
20	6	2.507864	0.000000	-2.545463
21	6	1.131453	0.000000	-2.153348
22	7	0.000000	0.000000	-2.950921
23	6	-1.131453	0.000000	-2.153348
24	6	-2.507864	0.000000	-2.545463
25	6	-3.505080	0.000000	-1.508665
26	6	-3.044259	0.000000	-0.164264
27	8	-3.871714	0.000000	0.938989

28	6	-3.432689	0.000000	3.376686
29	1	0.000000	0.000000	-3.955943
30	6	-2.943243	0.000000	-3.889229
31	6	-4.872136	0.000000	-1.860655
32	6	-4.285900	0.000000	-4.204049
33	6	-5.256718	0.000000	-3.184021
34	1	-2.212321	0.000000	-4.691171
35	1	-5.611257	0.000000	-1.068827
36	1	-4.596404	0.000000	-5.242504
37	1	-6.309141	0.000000	-3.442701
38	1	-2.705832	0.000000	5.414858
39	1	-4.481450	0.000000	3.643889
40	6	4.872136	0.000000	-1.860655
41	6	5.256718	0.000000	-3.184021
42	6	4.285900	0.000000	-4.204049
43	6	2.943243	0.000000	-3.889229
44	1	5.611257	0.000000	-1.068827
45	1	6.309141	0.000000	-3.442701
46	1	4.596404	0.000000	-5.242504
47	1	2.212321	0.000000	-4.691171
48	1	4.481450	0.000000	3.643889
49	1	2.705832	0.000000	5.414858

Table S23. The Cartesian coordinates for the compound **21** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.784659	-2.619038	0.000000
2	6	1.743701	-1.604836	0.000000
3	6	-0.646173	-2.667543	0.000000
4	6	-1.677663	-1.715503	0.000000
5	6	-1.734544	-0.286092	0.000000
6	6	-0.757512	0.742757	0.000000
7	6	0.674091	0.786440	0.000000
8	6	1.706108	-0.178018	0.000000
9	6	1.227521	-3.947379	0.000000
10	6	2.578162	-4.302374	0.000000
11	6	3.537969	-3.284225	0.000000
12	6	3.097940	-1.960201	0.000000
13	8	3.890987	-0.827771	0.000000
14	6	3.024296	0.244465	0.000000
15	6	3.417448	1.610650	0.000000
16	6	1.026767	2.126375	0.000000
17	6	-0.977676	-4.026530	0.000000
18	8	0.156931	-4.816789	0.000000
19	6	-2.294279	-4.493365	0.000000
20	6	-3.325821	-3.556552	0.000000
21	6	-3.012818	-2.187354	0.000000
22	7	-3.849363	-1.079555	0.000000
23	6	-3.088428	0.078507	0.000000
24	6	-3.529928	1.440610	0.000000
25	6	-2.530576	2.476226	0.000000
26	6	-1.171550	2.064271	0.000000
27	8	-0.093524	2.924288	0.000000
28	6	2.367529	2.598981	0.000000
29	1	-4.853853	-1.118007	0.000000
30	6	-4.889001	1.824052	0.000000
31	6	-2.935669	3.828535	0.000000
32	6	-5.255765	3.153666	0.000000
33	6	-4.273060	4.161832	0.000000
34	1	-5.662240	1.062826	0.000000
35	1	-2.174360	4.599156	0.000000
36	1	-6.305430	3.423866	0.000000
37	1	-4.570859	5.203984	0.000000

38	6	4.762541	2.039862	0.000000
39	6	2.718596	3.966837	0.000000
40	1	2.874618	-5.343251	0.000000
41	1	4.594698	-3.518033	0.000000
42	6	5.068433	3.383547	0.000000
43	6	4.042318	4.350268	0.000000
44	1	-2.504064	-5.555120	0.000000
45	1	-4.357137	-3.890256	0.000000
46	1	5.547080	1.292831	0.000000
47	1	1.928643	4.708121	0.000000
48	1	6.104897	3.700784	0.000000
49	1	4.297839	5.403721	0.000000

Table S24. The Cartesian coordinates for the compound **22** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.144634	-0.206893	0.000000
2	6	-1.394524	0.989585	0.000000
3	6	-1.814180	-1.594864	0.000000
4	6	-0.626678	-2.330277	0.000000
5	6	0.770650	-2.017914	0.000000
6	6	1.533158	-0.820833	0.000000
7	6	1.210810	0.571258	0.000000
8	6	0.000000	1.314057	0.000000
9	6	-3.527173	-0.136406	0.000000
10	6	-4.257942	1.082287	0.000000
11	6	-3.496713	2.306918	0.000000
12	6	-2.080133	2.193927	0.000000
13	8	-1.201843	3.252186	0.000000
14	6	0.060544	2.697819	0.000000
15	6	1.265910	3.449143	0.000000
16	6	2.422656	1.279205	0.000000
17	6	-3.032171	-2.286029	0.000000
18	8	-4.089030	-1.395737	0.000000
19	6	-3.121157	-3.678591	0.000000
20	6	-1.933783	-4.417875	0.000000
21	6	-0.720308	-3.727983	0.000000
22	6	1.426753	-3.236597	0.000000
23	6	2.839695	-3.382978	0.000000
24	6	3.625177	-2.177582	0.000000
25	6	2.932390	-0.925764	0.000000
26	6	2.498856	2.708336	0.000000
27	6	3.491263	-4.635267	0.000000
28	6	5.032350	-2.298520	0.000000
29	6	1.305536	4.860100	0.000000
30	6	3.711927	3.431482	0.000000
31	6	3.720812	4.810731	0.000000
32	6	2.510364	5.529619	0.000000
33	6	-5.668398	1.151918	0.000000
34	6	-4.187510	3.539053	0.000000
35	1	0.370111	5.406288	0.000000
36	1	4.656367	2.897187	0.000000
37	1	4.664446	5.343983	0.000000
38	1	2.527505	6.613291	0.000000
39	6	4.867351	-4.711313	0.000000
40	6	5.642158	-3.535592	0.000000
41	1	2.887190	-5.534433	0.000000
42	1	5.648737	-1.405518	0.000000
43	1	5.356283	-5.678554	0.000000
44	1	6.723953	-3.603297	0.000000
45	6	-6.308857	2.371817	0.000000
46	6	-5.565041	3.569759	0.000000
47	1	-6.234699	0.228453	0.000000

48	1	-3.614353	4.458286	0.000000
49	1	-7.391992	2.412493	0.000000
50	1	-6.082462	4.522268	0.000000
51	1	-4.083702	-4.173214	0.000000
52	1	-1.953818	-5.499936	0.000000
53	8	0.537984	-4.291481	0.000000
54	7	3.454444	0.356497	0.000000
55	1	4.433495	0.583065	0.000000

Table S25. The Cartesian coordinates for the compound **23** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.714928	0.705770	0.000000
2	6	1.707167	-0.705396	0.000000
3	6	0.706527	1.722063	0.000000
4	6	-0.698203	1.743625	0.000000
5	6	-1.726047	0.748674	0.000000
6	6	-1.726563	-0.668994	0.000000
7	6	-0.714340	-1.682425	0.000000
8	6	0.682670	-1.699032	0.000000
9	6	2.935602	1.359366	0.000000
10	6	4.192223	0.694266	0.000000
11	6	4.180645	-0.748045	0.000000
12	6	2.911420	-1.387505	0.000000
13	8	2.709465	-2.751864	0.000000
14	6	1.339704	-2.935558	0.000000
15	6	0.666884	-4.158458	0.000000
16	6	-1.385890	-2.911654	0.000000
17	6	1.399294	2.937986	0.000000
18	8	2.765086	2.724706	0.000000
19	6	0.768288	4.184036	0.000000
20	6	-0.624148	4.215513	0.000000
21	6	-1.339829	3.006075	0.000000
22	7	-2.709446	2.781302	0.000000
23	6	-2.958038	1.417713	0.000000
24	6	-4.215293	0.733353	0.000000
25	6	-4.202527	-0.706065	0.000000
26	6	-2.934077	-1.344762	0.000000
27	8	-2.750318	-2.712206	0.000000
28	6	-0.731647	-4.145144	0.000000
29	1	-3.409733	3.502806	0.000000
30	6	-5.466276	1.389158	0.000000
31	6	-5.426428	-1.409791	0.000000
32	6	5.434149	1.366911	0.000000
33	6	5.410362	-1.442448	0.000000
34	6	-6.646329	0.675588	0.000000
35	6	-6.626488	-0.732564	0.000000
36	1	-5.503894	2.473517	0.000000
37	1	-5.401610	-2.492756	0.000000
38	1	-7.594444	1.200877	0.000000
39	1	-7.559579	-1.283982	0.000000
40	6	6.615048	0.657046	0.000000
41	6	6.603311	-0.753059	0.000000
42	1	5.438796	2.450198	0.000000
43	1	5.395861	-2.525658	0.000000
44	1	7.561572	1.185354	0.000000
45	1	7.540748	-1.297257	0.000000
46	1	1.348016	5.097980	0.000000
47	1	-1.142563	5.167374	0.000000
48	1	1.213315	-5.092609	0.000000
49	1	-1.295031	-5.069209	0.000000

Table S26. The Cartesian coordinates for the compound **24** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.709223	0.704642
2	6	0.000000	0.713404	1.707476
3	6	0.000000	1.711186	-0.727145
4	6	0.000000	0.714478	-1.739058
5	6	0.000000	-0.714478	-1.739058
6	6	0.000000	-1.711186	-0.727145
7	6	0.000000	-1.709223	0.704642
8	6	0.000000	-0.713404	1.707476
9	6	0.000000	3.037662	1.100108
10	6	0.000000	3.471118	2.453527
11	6	0.000000	2.452905	3.473629
12	6	0.000000	1.101007	3.037693
13	8	0.000000	0.000000	3.866244
14	6	0.000000	-1.101007	3.037693
15	6	0.000000	-2.452905	3.473629
16	6	0.000000	-3.037662	1.100108
17	6	0.000000	3.045602	-1.098713
18	8	0.000000	3.870027	0.006030
19	6	0.000000	3.505694	-2.442042
20	6	0.000000	2.505971	-3.475985
21	6	0.000000	1.131310	-3.079365
22	7	0.000000	0.000000	-3.876209
23	6	0.000000	-1.131310	-3.079365
24	6	0.000000	-2.505971	-3.475985
25	6	0.000000	-3.505694	-2.442042
26	6	0.000000	-3.045602	-1.098713
27	8	0.000000	-3.870027	0.006030
28	6	0.000000	-3.471118	2.453527
29	6	0.000000	4.871845	-2.799080
30	6	0.000000	2.936761	-4.821366
31	6	0.000000	5.251878	-4.123584
32	6	0.000000	4.278079	-5.141010
33	1	0.000000	5.614747	-2.010809
34	1	0.000000	2.203073	-5.620814
35	1	0.000000	6.303555	-4.385434
36	1	0.000000	4.585302	-6.180406
37	1	0.000000	0.000000	-4.881252
38	6	0.000000	-2.936761	-4.821366
39	6	0.000000	-4.871845	-2.799080
40	6	0.000000	-2.843868	4.831111
41	6	0.000000	-4.829002	2.843544
42	6	0.000000	-5.174421	4.177077
43	6	0.000000	-4.177771	5.175041
44	6	0.000000	4.829002	2.843544
45	6	0.000000	2.843868	4.831111
46	1	0.000000	-2.075382	5.594532
47	1	0.000000	-5.591790	2.074446
48	1	0.000000	-6.219772	4.463599
49	1	0.000000	-4.465571	6.220033
50	6	0.000000	-4.278079	-5.141010
51	6	0.000000	-5.251878	-4.123584
52	1	0.000000	-2.203073	-5.620814
53	1	0.000000	-5.614747	-2.010809
54	1	0.000000	-4.585302	-6.180406
55	1	0.000000	-6.303555	-4.385434
56	6	0.000000	5.174421	4.177077
57	6	0.000000	4.177771	5.175041
58	1	0.000000	5.591790	2.074446
59	1	0.000000	2.075382	5.594532
60	1	0.000000	6.219772	4.463599
61	1	0.000000	4.465571	6.220033

Table S27. The Cartesian coordinates for the compound **25** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.716937	0.000000	-0.032453
2	6	-1.710006	0.000000	-1.436434
3	6	-0.712411	0.000000	0.991551
4	6	0.712411	0.000000	0.991551
5	6	1.716937	0.000000	-0.032453
6	6	1.710006	0.000000	-1.436434
7	6	0.697316	0.000000	-2.446674
8	6	-0.697316	0.000000	-2.446674
9	6	-2.978741	0.000000	0.612460
10	6	-4.192321	0.000000	-0.094669
11	6	-4.170778	0.000000	-1.487134
12	6	-2.928068	0.000000	-2.124536
13	8	-2.730123	0.000000	-3.492489
14	6	-1.363282	0.000000	-3.678710
15	6	-0.699781	0.000000	-4.905945
16	6	1.363282	0.000000	-3.678710
17	6	-1.387087	0.000000	2.220179
18	7	-2.751603	0.000000	1.978555
19	6	-0.717717	0.000000	3.484008
20	6	0.717717	0.000000	3.484008
21	6	1.387087	0.000000	2.220179
22	7	2.751603	0.000000	1.978555
23	6	2.978741	0.000000	0.612460
24	6	4.192321	0.000000	-0.094669
25	6	4.170778	0.000000	-1.487134
26	6	2.928068	0.000000	-2.124536
27	8	2.730123	0.000000	-3.492489
28	6	0.699781	0.000000	-4.905945
29	1	-3.470347	0.000000	2.681631
30	1	3.470347	0.000000	2.681631
31	6	-1.394255	0.000000	4.723814
32	6	1.394255	0.000000	4.723814
33	6	0.703348	0.000000	5.917116
34	6	-0.703348	0.000000	5.917116
35	1	-5.139983	0.000000	0.431489
36	1	-5.087513	0.000000	-2.062282
37	1	5.139983	0.000000	0.431489
38	1	5.087513	0.000000	-2.062282
39	1	-2.478980	0.000000	4.742297
40	1	2.478980	0.000000	4.742297
41	1	1.243262	0.000000	6.856820
42	1	-1.243262	0.000000	6.856820
43	1	-1.255098	0.000000	-5.834857
44	1	1.255098	0.000000	-5.834857

Table S28. The Cartesian coordinates for the compound **26** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.682762	-1.688588	0.000000
2	6	0.659243	-2.649348	0.000000
3	6	1.734363	-0.255794	0.000000
4	6	0.754479	0.780740	0.000000
5	6	-0.677471	0.816789	0.000000
6	6	-1.702216	-0.165484	0.000000

7	6	-1.730870	-1.595813	0.000000
8	6	-0.770074	-2.608322	0.000000
9	6	3.018870	-2.161798	0.000000
10	6	3.340312	-3.528605	0.000000
11	6	2.314856	-4.470828	0.000000
12	6	0.997953	-4.007113	0.000000
13	8	-0.131894	-4.803356	0.000000
14	6	-1.206253	-3.939464	0.000000
15	6	-2.553088	-4.305104	0.000000
16	6	-3.082211	-1.966140	0.000000
17	6	3.091024	0.099673	0.000000
18	7	3.853476	-1.057105	0.000000
19	6	3.552579	1.453286	0.000000
20	6	2.567876	2.497392	0.000000
21	6	1.191211	2.114639	0.000000
22	7	0.078406	2.937873	0.000000
23	6	-1.066876	2.166539	0.000000
24	6	-2.431317	2.596569	0.000000
25	6	-3.455563	1.588342	0.000000
26	6	-3.027685	0.234294	0.000000
27	8	-3.885179	-0.845200	0.000000
28	6	-3.516590	-3.291510	0.000000
29	1	0.100869	3.942283	0.000000
30	1	4.857943	-1.094827	0.000000
31	6	-2.830236	3.951694	0.000000
32	6	-4.812767	1.976161	0.000000
33	6	-5.162028	3.309407	0.000000
34	6	-4.164022	4.302813	0.000000
35	6	4.918361	1.811305	0.000000
36	6	3.005897	3.839906	0.000000
37	1	-2.078211	4.734007	0.000000
38	1	-5.572541	1.204027	0.000000
39	1	-6.207326	3.595924	0.000000
40	1	-4.446021	5.349466	0.000000
41	6	4.348429	4.155895	0.000000
42	6	5.313313	3.132878	0.000000
43	1	5.676564	1.035203	0.000000
44	1	2.275896	4.642667	0.000000
45	1	4.660704	5.193781	0.000000
46	1	6.367654	3.383765	0.000000
47	1	4.374211	-3.854418	0.000000
48	1	2.528092	-5.531883	0.000000
49	1	-2.842430	-5.347964	0.000000
50	1	-4.572772	-3.527880	0.000000

Table S29. The Cartesian coordinates for the compound **27** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.644917	-2.348478	0.000000
2	6	1.829346	-1.592947	0.000000
3	6	-0.756381	-2.046766	0.000000
4	6	-1.520246	-0.842256	0.000000
5	6	-1.203492	0.554525	0.000000
6	6	0.000000	1.309328	0.000000
7	6	1.395226	0.994630	0.000000
8	6	2.149194	-0.199445	0.000000
9	6	0.774931	-3.760206	0.000000
10	6	2.019422	-4.411292	0.000000
11	6	3.185522	-3.651134	0.000000
12	6	3.059768	-2.261224	0.000000
13	8	4.107277	-1.360461	0.000000
14	6	3.532049	-0.111547	0.000000
15	6	4.254866	1.111340	0.000000

16	6	2.072909	2.204212	0.000000
17	6	-1.434857	-3.274419	0.000000
18	7	-0.500562	-4.297480	0.000000
19	6	-2.859563	-3.389756	0.000000
20	6	-3.629825	-2.178664	0.000000
21	6	-2.920682	-0.938810	0.000000
22	7	-3.445440	0.342031	0.000000
23	6	-2.417089	1.262910	0.000000
24	6	-2.503331	2.690905	0.000000
25	6	-1.276735	3.439617	0.000000
26	6	-0.069490	2.693401	0.000000
27	8	1.188316	3.256391	0.000000
28	6	3.487266	2.330349	0.000000
29	1	-4.424592	0.566912	0.000000
30	1	-0.710691	-5.280416	0.000000
31	6	5.665196	1.189597	0.000000
32	6	4.169564	3.567444	0.000000
33	6	-3.721580	3.405896	0.000000
34	6	-1.324840	4.850475	0.000000
35	6	-2.533874	5.512093	0.000000
36	6	-3.739749	4.784939	0.000000
37	6	-3.542256	-4.625992	0.000000
38	6	-5.038934	-2.273528	0.000000
39	1	-4.662610	2.865448	0.000000
40	1	-0.392645	5.402225	0.000000
41	1	-2.558422	6.595683	0.000000
42	1	-4.686906	5.312042	0.000000
43	6	-5.674913	-3.497181	0.000000
44	6	-4.920128	-4.684070	0.000000
45	1	-2.976170	-5.551635	0.000000
46	1	-5.637808	-1.368709	0.000000
47	1	-6.757692	-3.545035	0.000000
48	1	-5.422391	-5.644450	0.000000
49	6	6.298005	2.413327	0.000000
50	6	5.546702	3.607037	0.000000
51	1	6.236938	0.269446	0.000000
52	1	3.589967	4.482690	0.000000
53	1	7.380942	2.460946	0.000000
54	1	6.058440	4.562681	0.000000
55	1	2.078120	-5.493640	0.000000
56	1	4.161285	-4.119346	0.000000

Table S30. The Cartesian coordinates for the compound **28** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.725070	0.728166
2	6	0.000000	1.719230	-0.692077
3	6	0.000000	0.713957	1.742199
4	6	0.000000	-0.713957	1.742199
5	6	0.000000	-1.725070	0.728166
6	6	0.000000	-1.719230	-0.692077
7	6	0.000000	-0.706589	-1.701991
8	6	0.000000	0.706589	-1.701991
9	6	0.000000	2.972866	1.374490
10	6	0.000000	4.225479	0.683955
11	6	0.000000	4.201999	-0.752735
12	6	0.000000	2.925951	-1.373310
13	8	0.000000	2.728463	-2.737052
14	6	0.000000	1.366701	-2.921435
15	6	0.000000	0.719931	-4.185635
16	6	0.000000	-1.366701	-2.921435
17	6	0.000000	1.381942	2.977026
18	7	0.000000	2.744226	2.735502

19	6	0.000000	0.717234	4.241978
20	6	0.000000	-0.717234	4.241978
21	6	0.000000	-1.381942	2.977026
22	7	0.000000	-2.744226	2.735502
23	6	0.000000	-2.972866	1.374490
24	6	0.000000	-4.225479	0.683955
25	6	0.000000	-4.201999	-0.752735
26	6	0.000000	-2.925951	-1.373310
27	8	0.000000	-2.728463	-2.737052
28	6	0.000000	-0.719931	-4.185635
29	1	0.000000	-3.457587	3.443076
30	1	0.000000	3.457587	3.443076
31	6	0.000000	1.404499	-5.421627
32	6	0.000000	-1.404499	-5.421627
33	6	0.000000	-5.481485	1.331019
34	6	0.000000	-5.420049	-1.467040
35	6	0.000000	-6.625453	-0.799413
36	6	0.000000	-6.656063	0.608742
37	6	0.000000	1.394049	5.481491
38	6	0.000000	-1.394049	5.481491
39	1	0.000000	-5.528030	2.415132
40	1	0.000000	-5.387262	-2.549725
41	1	0.000000	-7.554314	-1.357891
42	1	0.000000	-7.608207	1.126682
43	6	0.000000	-0.703244	6.675112
44	6	0.000000	0.703244	6.675112
45	1	0.000000	2.478892	5.501023
46	1	0.000000	-2.478892	5.501023
47	1	0.000000	-1.243843	7.614417
48	1	0.000000	1.243843	7.614417
49	6	0.000000	0.705318	-6.608457
50	6	0.000000	-0.705318	-6.608457
51	6	0.000000	5.481485	1.331019
52	6	0.000000	5.420049	-1.467040
53	1	0.000000	2.487720	-5.416975
54	1	0.000000	-2.487720	-5.416975
55	1	0.000000	1.241367	-7.550583
56	1	0.000000	-1.241367	-7.550583
57	6	0.000000	6.625453	-0.799413
58	6	0.000000	6.656063	0.608742
59	1	0.000000	5.528030	2.415132
60	1	0.000000	5.387262	-2.549725
61	1	0.000000	7.554314	-1.357891
62	1	0.000000	7.608207	1.126682

Table S31. The Cartesian coordinates for the compound **29** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.717742	-1.464956
2	6	0.000000	1.713462	-0.061718
3	6	0.000000	0.704747	-2.481863
4	6	0.000000	-0.704747	-2.481863
5	6	0.000000	-1.717742	-1.464956
6	6	0.000000	-1.713462	-0.061718
7	6	0.000000	-0.705862	0.954483
8	6	0.000000	0.705862	0.954483
9	6	0.000000	2.975466	-2.117182
10	6	0.000000	4.191712	-1.412980
11	6	0.000000	4.175211	-0.020209
12	6	0.000000	2.935760	0.620797
13	8	0.000000	2.734494	1.988505
14	6	0.000000	1.371028	2.169219
15	6	0.000000	0.720297	3.432985

16	6	0.000000	-1.371028	2.169219
17	6	0.000000	1.378058	-3.726531
18	7	0.000000	2.745952	-3.483817
19	6	0.000000	0.694343	-4.953241
20	6	0.000000	-0.694343	-4.953241
21	6	0.000000	-1.378058	-3.726531
22	7	0.000000	-2.745952	-3.483817
23	6	0.000000	-2.975466	-2.117182
24	6	0.000000	-4.191712	-1.412980
25	6	0.000000	-4.175211	-0.020209
26	6	0.000000	-2.935760	0.620797
27	8	0.000000	-2.734494	1.988505
28	6	0.000000	-0.720297	3.432985
29	1	0.000000	-3.459539	-4.191951
30	1	0.000000	3.459539	-4.191951
31	6	0.000000	1.404530	4.668460
32	6	0.000000	-1.404530	4.668460
33	1	0.000000	1.237458	-5.891472
34	1	0.000000	-1.237458	-5.891472
35	6	0.000000	0.705074	5.855706
36	6	0.000000	-0.705074	5.855706
37	1	0.000000	5.137798	-1.941942
38	1	0.000000	5.094728	0.550827
39	1	0.000000	2.487845	4.662831
40	1	0.000000	-2.487845	4.662831
41	1	0.000000	1.241371	6.797783
42	1	0.000000	-1.241371	6.797783
43	1	0.000000	-5.137798	-1.941942
44	1	0.000000	-5.094728	0.550827

Table S32. The Cartesian coordinates for the compound **30** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.786032	2.647227	0.000000
2	6	1.742970	1.621268	0.000000
3	6	-0.647811	2.694958	0.000000
4	6	-1.677732	1.729976	0.000000
5	6	-1.731431	0.297384	0.000000
6	6	-0.756661	-0.733658	0.000000
7	6	0.673756	-0.776628	0.000000
8	6	1.702789	0.191256	0.000000
9	6	1.257614	3.983598	0.000000
10	6	2.625639	4.302595	0.000000
11	6	3.566939	3.275442	0.000000
12	6	3.101517	1.960529	0.000000
13	8	3.890166	0.825141	0.000000
14	6	3.019710	-0.239275	0.000000
15	6	3.413308	-1.604752	0.000000
16	6	1.026933	-2.117258	0.000000
17	6	-1.008333	4.063487	0.000000
18	7	0.154651	4.822492	0.000000
19	6	-2.345562	4.494692	0.000000
20	6	-3.359182	3.546864	0.000000
21	6	-3.018828	2.184851	0.000000
22	7	-3.850272	1.073830	0.000000
23	6	-3.084576	-0.076933	0.000000
24	6	-3.525313	-1.438750	0.000000
25	6	-2.526418	-2.472695	0.000000
26	6	-1.169915	-2.056138	0.000000
27	8	-0.092285	-2.915794	0.000000
28	6	2.365408	-2.592829	0.000000
29	1	-4.854924	1.108418	0.000000
30	1	0.189754	5.827437	0.000000

31	6	-4.884434	-1.823906	0.000000
32	6	-2.929150	-3.826016	0.000000
33	6	-4.265784	-4.161247	0.000000
34	6	-5.249726	-3.153693	0.000000
35	1	-5.658396	-1.063352	0.000000
36	1	-2.166055	-4.594895	0.000000
37	1	-4.562793	-5.203695	0.000000
38	1	-6.299070	-3.425428	0.000000
39	6	4.759206	-2.033134	0.000000
40	6	2.716464	-3.961158	0.000000
41	1	-2.588010	5.551242	0.000000
42	1	-4.397215	3.859708	0.000000
43	6	5.065924	-3.376306	0.000000
44	6	4.040022	-4.344020	0.000000
45	1	2.953284	5.335823	0.000000
46	1	4.628230	3.488078	0.000000
47	1	5.542703	-1.284989	0.000000
48	1	1.926129	-4.702089	0.000000
49	1	6.102546	-3.693315	0.000000
50	1	4.296561	-5.397282	0.000000

Table S33. The Cartesian coordinates for the compound **31** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.726340	-1.342848
2	6	0.000000	1.720871	0.075756
3	6	0.000000	0.706661	-2.349966
4	6	0.000000	-0.706661	-2.349966
5	6	0.000000	-1.726340	-1.342848
6	6	0.000000	-1.720871	0.075756
7	6	0.000000	-0.706902	1.085106
8	6	0.000000	0.706902	1.085106
9	6	0.000000	2.969405	-1.995595
10	6	0.000000	4.222247	-1.304636
11	6	0.000000	4.201297	0.132853
12	6	0.000000	2.927473	0.756973
13	8	0.000000	2.729390	2.121179
14	6	0.000000	1.367247	2.304404
15	6	0.000000	0.719864	3.568616
16	6	0.000000	-1.367247	2.304404
17	6	0.000000	1.373522	-3.598965
18	7	0.000000	2.739550	-3.358415
19	6	0.000000	0.693374	-4.828263
20	6	0.000000	-0.693374	-4.828263
21	6	0.000000	-1.373522	-3.598965
22	7	0.000000	-2.739550	-3.358415
23	6	0.000000	-2.969405	-1.995595
24	6	0.000000	-4.222247	-1.304636
25	6	0.000000	-4.201297	0.132853
26	6	0.000000	-2.927473	0.756973
27	8	0.000000	-2.729390	2.121179
28	6	0.000000	-0.719864	3.568616
29	6	0.000000	5.477363	-1.954103
30	6	0.000000	5.421532	0.844373
31	6	0.000000	1.404496	4.804607
32	6	0.000000	-1.404496	4.804607
33	6	0.000000	-5.477363	-1.954103
34	6	0.000000	-5.421532	0.844373
35	6	0.000000	6.653177	-1.234456
36	6	0.000000	6.625112	0.174171
37	1	0.000000	3.448104	-4.071919
38	1	0.000000	-3.448104	-4.071919
39	1	0.000000	5.520780	-3.038253

40	1	0.000000	5.391073	1.927123
41	1	0.000000	7.604537	-1.753804
42	1	0.000000	7.555290	0.730507
43	6	0.000000	-6.653177	-1.234456
44	6	0.000000	-6.625112	0.174171
45	1	0.000000	-5.520780	-3.038253
46	1	0.000000	-5.391073	1.927123
47	1	0.000000	-7.604537	-1.753804
48	1	0.000000	-7.555290	0.730507
49	6	0.000000	0.705316	5.991460
50	6	0.000000	-0.705316	5.991460
51	1	0.000000	1.239611	-5.764522
52	1	0.000000	-1.239611	-5.764522
53	1	0.000000	2.487689	4.799793
54	1	0.000000	-2.487689	4.799793
55	1	0.000000	1.241275	6.933631
56	1	0.000000	-1.241275	6.933631

Table S34. The Cartesian coordinates for the compound **32** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.475741	0.700371	0.000000
2	6	2.452930	-0.701263	0.000000
3	6	1.475025	1.728728	0.000000
4	6	0.063699	1.747240	0.000000
5	6	-0.968242	0.751938	0.000000
6	6	-0.977617	-0.665851	0.000000
7	6	0.030378	-1.682157	0.000000
8	6	1.426482	-1.697936	0.000000
9	6	3.741940	1.335891	0.000000
10	6	4.946864	0.614271	0.000000
11	6	4.910786	-0.778986	0.000000
12	6	3.662991	-1.403986	0.000000
13	8	3.446415	-2.769878	0.000000
14	6	2.077942	-2.937781	0.000000
15	6	1.401563	-4.159111	0.000000
16	6	-0.645358	-2.909372	0.000000
17	6	2.164173	2.964359	0.000000
18	7	3.528592	2.705636	0.000000
19	6	1.498828	4.202606	0.000000
20	6	0.111528	4.222071	0.000000
21	6	-0.587938	3.004132	0.000000
22	7	-1.957573	2.779645	0.000000
23	6	-2.202870	1.419054	0.000000
24	6	-3.462732	0.739129	0.000000
25	6	-3.455104	-0.698743	0.000000
26	6	-2.187180	-1.338356	0.000000
27	8	-2.009336	-2.705906	0.000000
28	6	0.003430	-4.144483	0.000000
29	1	-2.657757	3.500972	0.000000
30	1	4.250199	3.405742	0.000000
31	1	2.056659	5.132043	0.000000
32	1	-0.419699	5.167159	0.000000
33	1	5.900641	1.129401	0.000000
34	1	5.822365	-1.362505	0.000000
35	6	-4.711646	1.399086	0.000000
36	6	-4.680382	-1.399590	0.000000
37	6	-5.894079	0.689144	0.000000
38	6	-5.878797	-0.718967	0.000000
39	1	1.948166	-5.093210	0.000000
40	1	-0.562676	-5.066957	0.000000
41	1	-4.746225	2.483629	0.000000
42	1	-4.658023	-2.482651	0.000000

43	1	-6.840632	1.217398	0.000000
44	1	-6.813638	-1.267507	0.000000

Table S35. The Cartesian coordinates for the compound **33** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	-1.726609	-0.748672
2	6	0.000000	-1.719156	0.668934
3	6	0.000000	-0.706748	-1.755802
4	6	0.000000	0.706748	-1.755802
5	6	0.000000	1.726609	-0.748672
6	6	0.000000	1.719156	0.668934
7	6	0.000000	0.698677	1.671985
8	6	0.000000	-0.698677	1.671985
9	6	0.000000	-2.969740	-1.400484
10	6	0.000000	-4.220433	-0.705706
11	6	0.000000	-4.195696	0.732037
12	6	0.000000	-2.920946	1.355832
13	8	0.000000	-2.725633	2.721242
14	6	0.000000	-1.359790	2.907620
15	6	0.000000	-0.699016	4.136403
16	6	0.000000	1.359790	2.907620
17	6	0.000000	-1.374068	-3.004315
18	7	0.000000	-2.740322	-2.763755
19	6	0.000000	-0.693334	-4.233752
20	6	0.000000	0.693334	-4.233752
21	6	0.000000	1.374068	-3.004315
22	7	0.000000	2.740322	-2.763755
23	6	0.000000	2.969740	-1.400484
24	6	0.000000	4.220433	-0.705706
25	6	0.000000	4.195696	0.732037
26	6	0.000000	2.920946	1.355832
27	8	0.000000	2.725633	2.721242
28	6	0.000000	0.699016	4.136403
29	6	0.000000	-5.477784	-1.351018
30	6	0.000000	-5.413379	1.447648
31	6	0.000000	5.477784	-1.351018
32	6	0.000000	5.413379	1.447648
33	6	0.000000	-6.651082	-0.627262
34	6	0.000000	-6.619110	0.781359
35	1	0.000000	-3.448843	-3.477327
36	1	0.000000	3.448843	-3.477327
37	1	0.000000	-5.524708	-2.435019
38	1	0.000000	-5.377922	2.530264
39	1	0.000000	-7.604104	-1.143626
40	1	0.000000	-7.547685	1.340324
41	6	0.000000	6.651082	-0.627262
42	6	0.000000	6.619110	0.781359
43	1	0.000000	5.524708	-2.435019
44	1	0.000000	5.377922	2.530264
45	1	0.000000	7.604104	-1.143626
46	1	0.000000	7.547685	1.340324
47	1	0.000000	-1.239316	-5.170169
48	1	0.000000	1.239316	-5.170169
49	1	0.000000	-1.256204	5.064141
50	1	0.000000	1.256204	5.064141

Table S36. The Cartesian coordinates for the compound **34** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.725283	0.119390
2	6	0.000000	1.717431	-1.299862
3	6	0.000000	0.714063	1.133380
4	6	0.000000	-0.714063	1.133380
5	6	0.000000	-1.725283	0.119390
6	6	0.000000	-1.717431	-1.299862
7	6	0.000000	-0.698435	-2.303453
8	6	0.000000	0.698435	-2.303453
9	6	0.000000	2.973240	0.764765
10	6	0.000000	4.223552	0.070470
11	6	0.000000	4.196296	-1.366531
12	6	0.000000	2.919484	-1.986753
13	8	0.000000	2.724743	-3.351709
14	6	0.000000	1.359345	-3.539193
15	6	0.000000	0.699035	-4.767959
16	6	0.000000	-1.359345	-3.539193
17	6	0.000000	1.382556	2.367788
18	7	0.000000	2.744999	2.126236
19	6	0.000000	0.717272	3.632879
20	6	0.000000	-0.717272	3.632879
21	6	0.000000	-1.382556	2.367788
22	7	0.000000	-2.744999	2.126236
23	6	0.000000	-2.973240	0.764765
24	6	0.000000	-4.223552	0.070470
25	6	0.000000	-4.196296	-1.366531
26	6	0.000000	-2.919484	-1.986753
27	8	0.000000	-2.724743	-3.351709
28	6	0.000000	-0.699035	-4.767959
29	6	0.000000	1.393988	4.872310
30	6	0.000000	-1.393988	4.872310
31	6	0.000000	0.703175	6.066037
32	6	0.000000	-0.703175	6.066037
33	1	0.000000	2.478824	4.891808
34	1	0.000000	-2.478824	4.891808
35	1	0.000000	1.243785	7.005334
36	1	0.000000	-1.243785	7.005334
37	6	0.000000	5.481867	0.713381
38	6	0.000000	5.411874	-2.084929
39	1	0.000000	1.256303	-5.695633
40	1	0.000000	-1.256303	-5.695633
41	6	0.000000	-5.481867	0.713381
42	6	0.000000	-5.411874	-2.084929
43	6	0.000000	6.653848	-0.012988
44	6	0.000000	6.619342	-1.421214
45	1	0.000000	3.458366	2.833862
46	1	0.000000	-3.458366	2.833862
47	1	0.000000	5.531958	1.797333
48	1	0.000000	5.374100	-3.167465
49	1	0.000000	7.607655	0.501954
50	1	0.000000	7.546611	-1.982285
51	6	0.000000	-6.653848	-0.012988
52	6	0.000000	-6.619342	-1.421214
53	1	0.000000	-5.531958	1.797333
54	1	0.000000	-5.374100	-3.167465
55	1	0.000000	-7.607655	0.501954
56	1	0.000000	-7.546611	-1.982285

Table S37. The Cartesian coordinates for the compound **35** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.716752	0.714046
2	6	0.000000	1.711608	-0.691137
3	6	0.000000	0.712376	1.737888
4	6	0.000000	-0.712376	1.737888
5	6	0.000000	-1.716752	0.714046
6	6	0.000000	-1.711608	-0.691137
7	6	0.000000	-0.705594	-1.707658
8	6	0.000000	0.705594	-1.707658
9	6	0.000000	2.978548	1.359754
10	6	0.000000	4.194554	0.656083
11	6	0.000000	4.175825	-0.735908
12	6	0.000000	2.934018	-1.373477
13	8	0.000000	2.733969	-2.740752
14	6	0.000000	1.370546	-2.922865
15	6	0.000000	0.720334	-4.185809
16	6	0.000000	-1.370546	-2.922865
17	6	0.000000	1.386540	2.967295
18	7	0.000000	2.751123	2.725242
19	6	0.000000	0.717842	4.230367
20	6	0.000000	-0.717842	4.230367
21	6	0.000000	-1.386540	2.967295
22	7	0.000000	-2.751123	2.725242
23	6	0.000000	-2.978548	1.359754
24	6	0.000000	-4.194554	0.656083
25	6	0.000000	-4.175825	-0.735908
26	6	0.000000	-2.934018	-1.373477
27	8	0.000000	-2.733969	-2.740752
28	6	0.000000	-0.720334	-4.185809
29	1	0.000000	3.470013	3.428144
30	1	0.000000	-3.470013	3.428144
31	6	0.000000	1.394390	5.470642
32	6	0.000000	-1.394390	5.470642
33	6	0.000000	-0.703564	6.663622
34	6	0.000000	0.703564	6.663622
35	6	0.000000	1.404844	-5.422067
36	6	0.000000	0.705502	-6.608629
37	6	0.000000	-0.705502	-6.608629
38	6	0.000000	-1.404844	-5.422067
39	1	0.000000	5.140479	1.185200
40	1	0.000000	5.093201	-1.310082
41	1	0.000000	-5.140479	1.185200
42	1	0.000000	-5.093201	-1.310082
43	1	0.000000	2.479133	5.489187
44	1	0.000000	-2.479133	5.489187
45	1	0.000000	-1.243410	7.603374
46	1	0.000000	1.243410	7.603374
47	1	0.000000	2.488073	-5.416099
48	1	0.000000	1.241197	-7.550973
49	1	0.000000	-1.241197	-7.550973
50	1	0.000000	-2.488073	-5.416099

Table S38. The Cartesian coordinates for the compound **36** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.076405	1.731377	0.000000

2	6	1.479691	1.684636	0.000000
3	6	-0.964435	0.751442	0.000000
4	6	-0.980371	-0.666406	0.000000
5	6	0.018225	-1.698252	0.000000
6	6	1.420620	-1.742361	0.000000
7	6	2.455083	-0.753904	0.000000
8	6	2.472149	0.647825	0.000000
9	6	-0.547455	3.002892	0.000000
10	6	0.183759	4.201770	0.000000
11	6	1.575013	4.147372	0.000000
12	6	2.187912	2.891819	0.000000
13	8	3.549209	2.670981	0.000000
14	6	3.710472	1.300762	0.000000
15	6	4.934193	0.629295	0.000000
16	6	3.693156	-1.440388	0.000000
17	6	-2.186773	1.438514	0.000000
18	7	-1.920078	2.798057	0.000000
19	6	-3.454897	0.775348	0.000000
20	6	-3.461262	-0.662458	0.000000
21	6	-2.201432	-1.319029	0.000000
22	8	-2.045604	-2.686058	0.000000
23	6	-0.684411	-2.909659	0.000000
24	6	-0.068242	-4.161859	0.000000
25	6	1.323847	-4.211290	0.000000
26	6	2.051784	-3.009718	0.000000
27	7	3.425096	-2.803474	0.000000
28	6	4.923855	-0.764425	0.000000
29	1	-2.610366	3.528983	0.000000
30	6	-4.696336	1.449032	0.000000
31	6	-4.694298	-1.349899	0.000000
32	6	-5.885363	-0.656526	0.000000
33	6	-5.886202	0.751717	0.000000
34	1	-0.320917	5.161085	0.000000
35	1	2.171003	5.050855	0.000000
36	1	-0.660315	-5.068032	0.000000
37	1	1.831435	-5.168935	0.000000
38	1	-4.718817	2.533891	0.000000
39	1	-4.683681	-2.433127	0.000000
40	1	-6.825913	-1.195257	0.000000
41	1	-6.827205	1.289765	0.000000
42	1	5.865383	1.181182	0.000000
43	1	5.859221	-1.312049	0.000000
44	1	4.119547	-3.530401	0.000000

Table S39. The Cartesian coordinates for the compound **37** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.052111	-1.537273	0.000000
2	6	0.325728	-1.813254	0.000000
3	6	-1.842017	-0.346142	0.000000
4	6	-1.533421	1.037615	0.000000
5	6	-0.325728	1.813254	0.000000
6	6	1.052111	1.537273	0.000000
7	6	1.842017	0.346142	0.000000
8	6	1.533421	-1.037615	0.000000
9	6	-1.950290	-2.632775	0.000000
10	6	-1.515431	-3.968231	0.000000
11	6	-0.149021	-4.234904	0.000000
12	6	0.733515	-3.152948	0.000000
13	8	2.109105	-3.246584	0.000000
14	6	2.573973	-1.951459	0.000000
15	6	3.949422	-1.600250	0.000000
16	6	3.189197	0.735839	0.000000

17	6	-3.189197	-0.735839	0.000000
18	7	-3.239520	-2.120427	0.000000
19	6	-4.271735	0.198846	0.000000
20	6	-3.949422	1.600250	0.000000
21	6	-2.573973	1.951459	0.000000
22	8	-2.109105	3.246584	0.000000
23	6	-0.733515	3.152948	0.000000
24	6	0.149021	4.234904	0.000000
25	6	1.515431	3.968231	0.000000
26	6	1.950290	2.632775	0.000000
27	7	3.239520	2.120427	0.000000
28	6	4.271735	-0.198846	0.000000
29	1	-4.078289	-2.675146	0.000000
30	6	-5.634819	-0.173856	0.000000
31	6	-4.993830	2.551378	0.000000
32	6	-6.310933	2.148002	0.000000
33	6	-6.633543	0.776301	0.000000
34	1	-2.227708	-4.785110	0.000000
35	1	0.224377	-5.250741	0.000000
36	1	-0.224377	5.250741	0.000000
37	1	2.227708	4.785110	0.000000
38	1	-5.903436	-1.225061	0.000000
39	1	-4.736198	3.603467	0.000000
40	1	-7.104166	2.886614	0.000000
41	1	-7.672695	0.468100	0.000000
42	6	4.993830	-2.551378	0.000000
43	6	5.634819	0.173856	0.000000
44	1	4.078289	2.675146	0.000000
45	6	6.310933	-2.148002	0.000000
46	6	6.633543	-0.776301	0.000000
47	1	4.736198	-3.603467	0.000000
48	1	5.903436	1.225061	0.000000
49	1	7.104166	-2.886614	0.000000
50	1	7.672695	-0.468100	0.000000

Table S40. The Cartesian coordinates for the compound **38** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	-0.713937	0.804396
2	6	0.000000	-1.705901	-0.211515
3	6	0.000000	0.713937	0.804396
4	6	0.000000	1.705901	-0.211515
5	6	0.000000	1.697851	-1.646855
6	6	0.000000	0.715324	-2.648359
7	6	0.000000	-0.715324	-2.648359
8	6	0.000000	-1.697851	-1.646855
9	6	0.000000	-1.130680	2.144880
10	6	0.000000	-2.504799	2.540745
11	6	0.000000	-3.500508	1.504405
12	6	0.000000	-3.039816	0.160494
13	8	0.000000	-3.871803	-0.934894
14	6	0.000000	-3.043047	-2.037399
15	6	0.000000	-3.463210	-3.367565
16	6	0.000000	-1.135166	-4.000693
17	6	0.000000	1.130680	2.144880
18	7	0.000000	0.000000	2.942484
19	6	0.000000	2.504799	2.540745
20	6	0.000000	3.500508	1.504405
21	6	0.000000	3.039816	0.160494
22	8	0.000000	3.871803	-0.934894
23	6	0.000000	3.043047	-2.037399
24	6	0.000000	3.463210	-3.367565
25	6	0.000000	2.491045	-4.366204

26	6	0.000000	1.135166	-4.000693
27	7	0.000000	0.000000	-4.800491
28	6	0.000000	-2.491045	-4.366204
29	1	0.000000	0.000000	3.947638
30	6	0.000000	2.939459	3.885125
31	6	0.000000	4.868128	1.856115
32	6	0.000000	5.252773	3.179278
33	6	0.000000	4.281929	4.199911
34	6	0.000000	-2.939459	3.885125
35	6	0.000000	-4.868128	1.856115
36	1	0.000000	4.517413	-3.612890
37	1	0.000000	2.786336	-5.408926
38	1	0.000000	2.208150	4.686738
39	1	0.000000	5.606952	1.064043
40	1	0.000000	6.305246	3.438022
41	1	0.000000	4.592903	5.238254
42	1	0.000000	0.000000	-5.806033
43	6	0.000000	-4.281929	4.199911
44	6	0.000000	-5.252773	3.179278
45	1	0.000000	-4.517413	-3.612890
46	1	0.000000	-2.786336	-5.408926
47	1	0.000000	-2.208150	4.686738
48	1	0.000000	-5.606952	1.064043
49	1	0.000000	-4.592903	5.238254
50	1	0.000000	-6.305246	3.438022

Table S41. The Cartesian coordinates for the compound **39** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.720843	0.000000	-1.671050
2	6	0.717282	0.000000	-2.652729
3	6	1.731364	0.000000	-0.241680
4	6	0.717935	0.000000	0.751668
5	6	-0.717935	0.000000	0.751668
6	6	-1.731364	0.000000	-0.241680
7	6	-1.720843	0.000000	-1.671050
8	6	-0.717282	0.000000	-2.652729
9	6	3.071102	0.000000	-2.099194
10	6	3.432568	0.000000	-3.455590
11	6	2.431135	0.000000	-4.423828
12	6	1.100939	0.000000	-3.998977
13	8	0.000000	0.000000	-4.829587
14	6	-1.100939	0.000000	-3.998977
15	6	-2.431135	0.000000	-4.423828
16	6	-3.071102	0.000000	-2.099194
17	6	3.073325	0.000000	0.166236
18	7	3.871459	0.000000	-0.965689
19	6	3.473551	0.000000	1.539757
20	6	2.441554	0.000000	2.540455
21	6	1.097179	0.000000	2.084728
22	8	0.000000	0.000000	2.914041
23	6	-1.097179	0.000000	2.084728
24	6	-2.441554	0.000000	2.540455
25	6	-3.473551	0.000000	1.539757
26	6	-3.073325	0.000000	0.166236
27	7	-3.871459	0.000000	-0.965689
28	6	-3.432568	0.000000	-3.455590
29	1	4.877007	0.000000	-0.971676
30	6	4.820334	0.000000	1.966938
31	6	2.801778	0.000000	3.906329
32	6	4.126934	0.000000	4.283158
33	6	5.143023	0.000000	3.307276
34	6	-2.801778	0.000000	3.906329

35	6	-4.820334	0.000000	1.966938
36	1	5.617267	0.000000	1.230630
37	1	2.015141	0.000000	4.650936
38	1	4.391368	0.000000	5.334282
39	1	6.182871	0.000000	3.613038
40	1	-4.877007	0.000000	-0.971676
41	1	-2.671938	0.000000	-5.478982
42	1	-4.474583	0.000000	-3.753854
43	6	-4.126934	0.000000	4.283158
44	6	-5.143023	0.000000	3.307276
45	1	4.474583	0.000000	-3.753854
46	1	2.671938	0.000000	-5.478982
47	1	-2.015141	0.000000	4.650936
48	1	-5.617267	0.000000	1.230630
49	1	-4.391368	0.000000	5.334282
50	1	-6.182871	0.000000	3.613038

Table S42. The Cartesian coordinates for the compound **40** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.837067	-1.602527	0.000000
2	6	0.639525	-2.337086	0.000000
3	6	2.166312	-0.212158	0.000000
4	6	1.399502	0.981457	0.000000
5	6	0.000000	1.300697	0.000000
6	6	-1.211598	0.558575	0.000000
7	6	-1.530393	-0.832781	0.000000
8	6	-0.761107	-2.025704	0.000000
9	6	3.058286	-2.320864	0.000000
10	6	3.111839	-3.723921	0.000000
11	6	1.921483	-4.446035	0.000000
12	6	0.720104	-3.735229	0.000000
13	8	-0.538584	-4.297562	0.000000
14	6	-1.421865	-3.243031	0.000000
15	6	-2.833956	-3.393078	0.000000
16	6	-2.930119	-0.940821	0.000000
17	6	3.565527	-0.112992	0.000000
18	7	4.090793	-1.394650	0.000000
19	6	4.261916	1.136110	0.000000
20	6	3.478546	2.341501	0.000000
21	6	2.067015	2.196316	0.000000
22	8	1.181781	3.248718	0.000000
23	6	-0.072276	2.684866	0.000000
24	6	-1.278982	3.433232	0.000000
25	6	-2.509314	2.691163	0.000000
26	6	-2.425994	1.263665	0.000000
27	7	-3.455311	0.339358	0.000000
28	6	-3.622510	-2.191521	0.000000
29	1	5.069667	-1.624935	0.000000
30	6	5.670089	1.252583	0.000000
31	6	4.134311	3.592864	0.000000
32	6	5.509954	3.664978	0.000000
33	6	6.283298	2.487169	0.000000
34	6	-1.320970	4.844735	0.000000
35	6	-3.724811	3.411347	0.000000
36	1	6.282574	0.356987	0.000000
37	1	3.533402	4.494080	0.000000
38	1	6.001799	4.630823	0.000000
39	1	7.365127	2.553509	0.000000
40	1	-4.434994	0.563686	0.000000
41	6	-3.482056	-4.647910	0.000000
42	6	-5.029995	-2.315483	0.000000
43	6	-2.526774	5.511687	0.000000

44	6	-3.736441	4.790141	0.000000
45	1	4.062498	-4.244324	0.000000
46	1	1.921509	-5.528315	0.000000
47	1	-0.386339	5.392161	0.000000
48	1	-4.667720	2.874376	0.000000
49	1	-2.546722	6.595329	0.000000
50	1	-4.680745	5.322214	0.000000
51	6	-4.857525	-4.727786	0.000000
52	6	-5.636259	-3.553792	0.000000
53	1	-2.874841	-5.544897	0.000000
54	1	-5.648012	-1.423598	0.000000
55	1	-5.344314	-5.696137	0.000000
56	1	-6.717808	-3.625374	0.000000

Table S43. The Cartesian coordinates for the compound **41** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.713627	1.732995
2	6	0.000000	1.706862	0.717613
3	6	0.000000	-0.713627	1.732995
4	6	0.000000	-1.706862	0.717613
5	6	0.000000	-1.706862	-0.717613
6	6	0.000000	-0.713627	-1.732995
7	6	0.000000	0.713627	-1.732995
8	6	0.000000	1.706862	-0.717613
9	6	0.000000	1.130507	3.073963
10	6	0.000000	2.503042	3.473774
11	6	0.000000	3.500827	2.439820
12	6	0.000000	3.040126	1.097065
13	8	0.000000	3.868492	0.000000
14	6	0.000000	3.040126	-1.097065
15	6	0.000000	3.500827	-2.439820
16	6	0.000000	1.130507	-3.073963
17	6	0.000000	-1.130507	3.073963
18	7	0.000000	0.000000	3.870837
19	6	0.000000	-2.503042	3.473774
20	6	0.000000	-3.500827	2.439820
21	6	0.000000	-3.040126	1.097065
22	8	0.000000	-3.868492	0.000000
23	6	0.000000	-3.040126	-1.097065
24	6	0.000000	-3.500827	-2.439820
25	6	0.000000	-2.503042	-3.473774
26	6	0.000000	-1.130507	-3.073963
27	7	0.000000	0.000000	-3.870837
28	6	0.000000	2.503042	-3.473774
29	1	0.000000	0.000000	4.875772
30	6	0.000000	-2.933658	4.819343
31	6	0.000000	-4.867499	2.795767
32	6	0.000000	2.933658	4.819343
33	6	0.000000	4.867499	2.795767
34	6	0.000000	-4.867499	-2.795767
35	6	0.000000	-2.933658	-4.819343
36	6	0.000000	-5.248340	-4.120010
37	6	0.000000	-4.275091	-5.138294
38	6	0.000000	4.867499	-2.795767
39	6	0.000000	2.933658	-4.819343
40	1	0.000000	-5.609933	-2.007058
41	1	0.000000	-2.200116	-5.618978
42	1	0.000000	-6.300223	-4.381287
43	1	0.000000	-4.583077	-6.177516
44	6	0.000000	5.248340	-4.120010
45	6	0.000000	4.275091	-5.138294
46	6	0.000000	-4.275091	5.138294

47	6	0.000000	-5.248340	4.120010
48	1	0.000000	0.000000	-4.875772
49	1	0.000000	-2.200116	5.618978
50	1	0.000000	-5.609933	2.007058
51	1	0.000000	5.609933	-2.007058
52	1	0.000000	2.200116	-5.618978
53	1	0.000000	6.300223	-4.381287
54	1	0.000000	4.583077	-6.177516
55	1	0.000000	-4.583077	6.177516
56	1	0.000000	-6.300223	4.381287
57	6	0.000000	4.275091	5.138294
58	6	0.000000	5.248340	4.120010
59	1	0.000000	2.200116	5.618978
60	1	0.000000	5.609933	2.007058
61	1	0.000000	4.583077	6.177516
62	1	0.000000	6.300223	4.381287

Table S44. The Cartesian coordinates for the compound **42** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.709576	0.000000	0.044422
2	6	1.707754	0.000000	1.440077
3	6	0.705688	0.000000	-0.972494
4	6	-0.705688	0.000000	-0.972494
5	6	-1.709576	0.000000	0.044422
6	6	-1.707754	0.000000	1.440077
7	6	-0.697215	0.000000	2.450532
8	6	0.697215	0.000000	2.450532
9	6	2.939748	0.000000	-0.622052
10	6	4.165194	0.000000	0.047550
11	6	4.162329	0.000000	1.447717
12	6	2.933595	0.000000	2.113391
13	8	2.738928	0.000000	3.482560
14	6	1.369231	0.000000	3.677098
15	6	0.700466	0.000000	4.903262
16	6	-1.369231	0.000000	3.677098
17	6	1.377118	0.000000	-2.181269
18	8	2.743427	0.000000	-1.991419
19	6	0.721565	0.000000	-3.444728
20	6	-0.721565	0.000000	-3.444728
21	6	-1.377118	0.000000	-2.181269
22	8	-2.743427	0.000000	-1.991419
23	6	-2.939748	0.000000	-0.622052
24	6	-4.165194	0.000000	0.047550
25	6	-4.162329	0.000000	1.447717
26	6	-2.933595	0.000000	2.113391
27	8	-2.738928	0.000000	3.482560
28	6	-0.700466	0.000000	4.903262
29	6	1.404661	0.000000	-4.680365
30	6	-1.404661	0.000000	-4.680365
31	6	0.704822	0.000000	-5.867479
32	6	-0.704822	0.000000	-5.867479
33	1	2.487851	0.000000	-4.675197
34	1	-2.487851	0.000000	-4.675197
35	1	1.240803	0.000000	-6.809494
36	1	-1.240803	0.000000	-6.809494
37	1	5.097343	0.000000	-0.502253
38	1	5.091910	0.000000	2.001628
39	1	1.251566	0.000000	5.834597
40	1	-1.251566	0.000000	5.834597
41	1	-5.097343	0.000000	-0.502253
42	1	-5.091910	0.000000	2.001628

Table S45. The Cartesian coordinates for the compound **43** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.702334	0.000000	1.649800
2	6	0.714319	0.000000	2.635551
3	6	1.711451	0.000000	0.221171
4	6	0.714277	0.000000	-0.779213
5	6	-0.714277	0.000000	-0.779213
6	6	-1.711451	0.000000	0.221171
7	6	-1.702334	0.000000	1.649800
8	6	-0.714319	0.000000	2.635551
9	6	3.043718	0.000000	2.049130
10	6	3.436946	0.000000	3.388430
11	6	2.444658	0.000000	4.376799
12	6	1.105848	0.000000	3.978658
13	8	0.000000	0.000000	4.809042
14	6	-1.105848	0.000000	3.978658
15	6	-2.444658	0.000000	4.376799
16	6	-3.043718	0.000000	2.049130
17	6	3.041861	0.000000	-0.158237
18	8	3.873067	0.000000	0.942278
19	6	3.475598	0.000000	-1.513323
20	6	2.458035	0.000000	-2.536556
21	6	1.101964	0.000000	-2.108120
22	8	0.000000	0.000000	-2.937263
23	6	-1.101964	0.000000	-2.108120
24	6	-2.458035	0.000000	-2.536556
25	6	-3.475598	0.000000	-1.513323
26	6	-3.041861	0.000000	-0.158237
27	8	-3.873067	0.000000	0.942278
28	6	-3.436946	0.000000	3.388430
29	6	4.833974	0.000000	-1.899299
30	6	2.853969	0.000000	-3.892242
31	6	5.183309	0.000000	-3.232045
32	6	4.189269	0.000000	-4.231948
33	1	5.593543	0.000000	-1.127027
34	1	2.088279	0.000000	-4.658434
35	1	6.229290	0.000000	-3.515871
36	1	4.479773	0.000000	-5.276163
37	1	4.484899	0.000000	3.658551
38	1	2.710247	0.000000	5.425800
39	6	-2.853969	0.000000	-3.892242
40	6	-4.833974	0.000000	-1.899299
41	6	-5.183309	0.000000	-3.232045
42	6	-4.189269	0.000000	-4.231948
43	1	-2.710247	0.000000	5.425800
44	1	-4.484899	0.000000	3.658551
45	1	-2.088279	0.000000	-4.658434
46	1	-5.593543	0.000000	-1.127027
47	1	-6.229290	0.000000	-3.515871
48	1	-4.479773	0.000000	-5.276163

Table S46. The Cartesian coordinates for the compound **44** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.709376	-0.698435
2	6	0.000000	1.709376	0.698435

3	6	0.000000	0.705640	-1.715060
4	6	0.000000	-0.705640	-1.715060
5	6	0.000000	-1.709376	-0.698435
6	6	0.000000	-1.709376	0.698435
7	6	0.000000	-0.705640	1.715060
8	6	0.000000	0.705640	1.715060
9	6	0.000000	2.939579	-1.365776
10	6	0.000000	4.167204	-0.699897
11	6	0.000000	4.167204	0.699897
12	6	0.000000	2.939579	1.365776
13	8	0.000000	2.742984	2.734537
14	6	0.000000	1.376537	2.924755
15	6	0.000000	0.721703	4.187410
16	6	0.000000	-1.376537	2.924755
17	6	0.000000	1.376537	-2.924755
18	8	0.000000	2.742984	-2.734537
19	6	0.000000	0.721703	-4.187410
20	6	0.000000	-0.721703	-4.187410
21	6	0.000000	-1.376537	-2.924755
22	8	0.000000	-2.742984	-2.734537
23	6	0.000000	-2.939579	-1.365776
24	6	0.000000	-4.167204	-0.699897
25	6	0.000000	-4.167204	0.699897
26	6	0.000000	-2.939579	1.365776
27	8	0.000000	-2.742984	2.734537
28	6	0.000000	-0.721703	4.187410
29	6	0.000000	1.404799	5.423621
30	6	0.000000	1.404799	-5.423621
31	6	0.000000	-1.404799	-5.423621
32	6	0.000000	-1.404799	5.423621
33	6	0.000000	0.705078	6.610338
34	6	0.000000	-0.705078	6.610338
35	6	0.000000	0.705078	-6.610338
36	6	0.000000	-0.705078	-6.610338
37	1	0.000000	2.488001	5.418468
38	1	0.000000	2.488001	-5.418468
39	1	0.000000	-2.488001	-5.418468
40	1	0.000000	-2.488001	5.418468
41	1	0.000000	1.240962	7.552424
42	1	0.000000	-1.240962	7.552424
43	1	0.000000	1.240962	-7.552424
44	1	0.000000	-1.240962	-7.552424
45	1	0.000000	5.097501	-1.252678
46	1	0.000000	5.097501	1.252678
47	1	0.000000	-5.097501	-1.252678
48	1	0.000000	-5.097501	1.252678

Table S47. The Cartesian coordinates for the compound **45** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.698363	-2.318870
2	6	0.000000	-0.698363	-2.318870
3	6	0.000000	1.714800	-1.315215
4	6	0.000000	1.716844	0.097060
5	6	0.000000	0.706739	1.107087
6	6	0.000000	-0.706739	1.107087
7	6	0.000000	-1.716844	0.097060
8	6	0.000000	-1.714800	-1.315215
9	6	0.000000	1.365240	-3.549609
10	6	0.000000	0.699959	-4.777084
11	6	0.000000	-0.699959	-4.777084
12	6	0.000000	-1.365240	-3.549609
13	8	0.000000	-2.733796	-3.353124

14	6	0.000000	-2.924475	-1.987069
15	6	0.000000	-4.188958	-1.336225
16	6	0.000000	-2.931294	0.762083
17	6	0.000000	2.924475	-1.987069
18	8	0.000000	2.733796	-3.353124
19	6	0.000000	4.188958	-1.336225
20	6	0.000000	4.192837	0.106854
21	6	0.000000	2.931294	0.762083
22	8	0.000000	2.738413	2.127556
23	6	0.000000	1.373237	2.320895
24	6	0.000000	0.721368	3.584658
25	6	0.000000	-0.721368	3.584658
26	6	0.000000	-1.373237	2.320895
27	8	0.000000	-2.738413	2.127556
28	6	0.000000	-4.192837	0.106854
29	6	0.000000	-5.422846	-2.023620
30	6	0.000000	5.422846	-2.023620
31	6	0.000000	5.431644	0.785675
32	6	0.000000	1.404405	4.820894
33	6	0.000000	-1.404405	4.820894
34	6	0.000000	-5.431644	0.785675
35	6	0.000000	-6.611955	-1.328191
36	6	0.000000	-6.615959	0.081996
37	6	0.000000	6.611955	-1.328191
38	6	0.000000	6.615959	0.081996
39	6	0.000000	0.704969	6.007854
40	6	0.000000	-0.704969	6.007854
41	1	0.000000	-5.413764	-3.106796
42	1	0.000000	5.413764	-3.106796
43	1	0.000000	5.431476	1.868883
44	1	0.000000	2.487600	4.816794
45	1	0.000000	-2.487600	4.816794
46	1	0.000000	-5.431476	1.868883
47	1	0.000000	-7.552318	-1.867039
48	1	0.000000	-7.559657	0.615105
49	1	0.000000	7.552318	-1.867039
50	1	0.000000	7.559657	0.615105
51	1	0.000000	1.241112	6.949793
52	1	0.000000	-1.241112	6.949793
53	1	0.000000	1.252996	-5.707221
54	1	0.000000	-1.252996	-5.707221

Table S48. The Cartesian coordinates for the compound **46** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.706638	1.716654	0.000000
2	6	-0.706638	1.716654	0.000000
3	6	1.716654	0.706638	0.000000
4	6	1.716654	-0.706638	0.000000
5	6	0.706638	-1.716654	0.000000
6	6	-0.706638	-1.716654	0.000000
7	6	-1.716654	-0.706638	0.000000
8	6	-1.716654	0.706638	0.000000
9	6	1.372636	2.930937	0.000000
10	6	0.721334	4.194522	0.000000
11	6	-0.721334	4.194522	0.000000
12	6	-1.372636	2.930937	0.000000
13	8	-2.737664	2.737664	0.000000
14	6	-2.930937	1.372636	0.000000
15	6	-4.194522	0.721334	0.000000
16	6	-2.930937	-1.372636	0.000000
17	6	2.930937	1.372636	0.000000
18	8	2.737664	2.737664	0.000000

19	6	4.194522	0.721334	0.000000
20	6	4.194522	-0.721334	0.000000
21	6	2.930937	-1.372636	0.000000
22	8	2.737664	-2.737664	0.000000
23	6	1.372636	-2.930937	0.000000
24	6	0.721334	-4.194522	0.000000
25	6	-0.721334	-4.194522	0.000000
26	6	-1.372636	-2.930937	0.000000
27	8	-2.737664	-2.737664	0.000000
28	6	-4.194522	-0.721334	0.000000
29	6	1.404465	5.430886	0.000000
30	6	-1.404465	5.430886	0.000000
31	6	-5.430886	1.404465	0.000000
32	6	5.430886	1.404465	0.000000
33	6	5.430886	-1.404465	0.000000
34	6	1.404465	-5.430886	0.000000
35	6	-1.404465	-5.430886	0.000000
36	6	-5.430886	-1.404465	0.000000
37	6	-6.617714	0.705056	0.000000
38	6	-6.617714	-0.705056	0.000000
39	6	-0.705056	6.617714	0.000000
40	6	0.705056	6.617714	0.000000
41	6	6.617714	0.705056	0.000000
42	6	6.617714	-0.705056	0.000000
43	6	0.705056	-6.617714	0.000000
44	6	-0.705056	-6.617714	0.000000
45	1	2.487663	5.426785	0.000000
46	1	-2.487663	5.426785	0.000000
47	1	-5.426785	2.487663	0.000000
48	1	5.426785	2.487663	0.000000
49	1	5.426785	-2.487663	0.000000
50	1	2.487663	-5.426785	0.000000
51	1	-2.487663	-5.426785	0.000000
52	1	-5.426785	-2.487663	0.000000
53	1	-7.559675	1.241169	0.000000
54	1	-7.559675	-1.241169	0.000000
55	1	-1.241169	7.559675	0.000000
56	1	1.241169	7.559675	0.000000
57	1	7.559675	1.241169	0.000000
58	1	7.559675	-1.241169	0.000000
59	1	1.241169	-7.559675	0.000000
60	1	-1.241169	-7.559675	0.000000

Table S49. The Cartesian coordinates for the compound **47** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.720198	0.000000	0.049341
2	6	1.719557	0.000000	1.461869
3	6	0.712661	0.000000	-0.973575
4	6	-0.712661	0.000000	-0.973575
5	6	-1.720198	0.000000	0.049341
6	6	-1.719557	0.000000	1.461869
7	6	-0.705070	0.000000	2.478375
8	6	0.705070	0.000000	2.478375
9	6	2.974564	0.000000	-0.611434
10	6	4.202990	0.000000	0.067129
11	6	4.200927	0.000000	1.452875
12	6	2.969838	0.000000	2.128816
13	7	2.737094	0.000000	3.493805
14	6	1.371934	0.000000	3.728932
15	6	0.693601	0.000000	4.957243
16	6	-1.371934	0.000000	3.728932
17	6	1.380673	0.000000	-2.209042

18	7	2.742623	0.000000	-1.975422
19	6	0.716842	0.000000	-3.473499
20	6	-0.716842	0.000000	-3.473499
21	6	-1.380673	0.000000	-2.209042
22	7	-2.742623	0.000000	-1.975422
23	6	-2.974564	0.000000	-0.611434
24	6	-4.202990	0.000000	0.067129
25	6	-4.200927	0.000000	1.452875
26	6	-2.969838	0.000000	2.128816
27	7	-2.737094	0.000000	3.493805
28	6	-0.693601	0.000000	4.957243
29	6	1.393981	0.000000	-4.713035
30	6	-1.393981	0.000000	-4.713035
31	6	0.703392	0.000000	-5.906914
32	6	-0.703392	0.000000	-5.906914
33	1	2.478919	0.000000	-4.732023
34	1	-2.478919	0.000000	-4.732023
35	1	1.244167	0.000000	-6.846353
36	1	-1.244167	0.000000	-6.846353
37	1	3.448771	0.000000	4.203732
38	1	3.458404	0.000000	-2.680544
39	1	-3.458404	0.000000	-2.680544
40	1	-3.448771	0.000000	4.203732
41	1	-5.138989	0.000000	-0.480178
42	1	-5.135293	0.000000	2.002780
43	1	1.240963	0.000000	5.893187
44	1	-1.240963	0.000000	5.893187
45	1	5.138989	0.000000	-0.480178
46	1	5.135293	0.000000	2.002780

Table S50. The Cartesian coordinates for the compound **48** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.717214	-0.759972
2	6	0.000000	1.725880	0.249534
3	6	0.000000	-0.717214	-0.759972
4	6	0.000000	-1.725880	0.249534
5	6	0.000000	-1.716493	1.684545
6	6	0.000000	-0.717632	2.682619
7	6	0.000000	0.717632	2.682619
8	6	0.000000	1.716493	1.684545
9	6	0.000000	1.126259	-2.105117
10	6	0.000000	2.488908	-2.529595
11	6	0.000000	3.500404	-1.514530
12	6	0.000000	3.072155	-0.151980
13	7	0.000000	3.870156	0.975600
14	6	0.000000	3.070782	2.104593
15	6	0.000000	3.459806	3.452428
16	6	0.000000	1.130476	4.038440
17	6	0.000000	-1.126259	-2.105117
18	7	0.000000	0.000000	-2.902304
19	6	0.000000	-2.488908	-2.529595
20	6	0.000000	-3.500404	-1.514530
21	6	0.000000	-3.072155	-0.151980
22	7	0.000000	-3.870156	0.975600
23	6	0.000000	-3.070782	2.104593
24	6	0.000000	-3.459806	3.452428
25	6	0.000000	-2.478245	4.431123
26	6	0.000000	-1.130476	4.038440
27	7	0.000000	0.000000	4.837879
28	6	0.000000	2.478245	4.431123
29	6	0.000000	-2.888895	-3.884364
30	6	0.000000	-4.856595	-1.909005

31	6	0.000000	-4.222122	-4.237322
32	6	0.000000	-5.215155	-3.240805
33	1	0.000000	-2.137368	-4.667212
34	1	0.000000	-5.635961	-1.153994
35	1	0.000000	-4.506066	-5.283443
36	1	0.000000	-6.262284	-3.520868
37	1	0.000000	4.874914	0.982182
38	1	0.000000	0.000000	-3.906539
39	1	0.000000	-4.874914	0.982182
40	1	0.000000	0.000000	5.842906
41	6	0.000000	2.888895	-3.884364
42	6	0.000000	4.856595	-1.909005
43	1	0.000000	-4.508672	3.727231
44	1	0.000000	-2.750130	5.480658
45	1	0.000000	4.508672	3.727231
46	1	0.000000	2.750130	5.480658
47	6	0.000000	4.222122	-4.237322
48	6	0.000000	5.215155	-3.240805
49	1	0.000000	2.137368	-4.667212
50	1	0.000000	5.635961	-1.153994
51	1	0.000000	4.506066	-5.283443
52	1	0.000000	6.262284	-3.520868

Table S51. The Cartesian coordinates for the compound **49** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.718497	0.707286
2	6	0.000000	1.718497	-0.707286
3	6	0.000000	0.712512	1.730757
4	6	0.000000	-0.712512	1.730757
5	6	0.000000	-1.718497	0.707286
6	6	0.000000	-1.718497	-0.707286
7	6	0.000000	-0.712512	-1.730757
8	6	0.000000	0.712512	-1.730757
9	6	0.000000	2.972887	1.367991
10	6	0.000000	4.203967	0.692453
11	6	0.000000	4.203967	-0.692453
12	6	0.000000	2.972887	-1.367991
13	7	0.000000	2.742323	-2.731661
14	6	0.000000	1.380529	-2.966371
15	6	0.000000	0.716903	-4.230206
16	6	0.000000	-1.380529	-2.966371
17	6	0.000000	1.380529	2.966371
18	7	0.000000	2.742323	2.731661
19	6	0.000000	0.716903	4.230206
20	6	0.000000	-0.716903	4.230206
21	6	0.000000	-1.380529	2.966371
22	7	0.000000	-2.742323	2.731661
23	6	0.000000	-2.972887	1.367991
24	6	0.000000	-4.203967	0.692453
25	6	0.000000	-4.203967	-0.692453
26	6	0.000000	-2.972887	-1.367991
27	7	0.000000	-2.742323	-2.731661
28	6	0.000000	-0.716903	-4.230206
29	6	0.000000	1.394323	5.470367
30	6	0.000000	-1.394323	5.470367
31	6	0.000000	0.703791	6.663546
32	6	0.000000	-0.703791	6.663546
33	1	0.000000	2.479220	5.488844
34	1	0.000000	-2.479220	5.488844
35	1	0.000000	1.243768	7.603372
36	1	0.000000	-1.243768	7.603372
37	1	0.000000	3.459038	-3.435813

38	1	0.000000	3.459038	3.435813
39	1	0.000000	-3.459038	3.435813
40	1	0.000000	-3.459038	-3.435813
41	1	0.000000	-5.138142	1.242563
42	1	0.000000	-5.138142	-1.242563
43	6	0.000000	1.394323	-5.470367
44	6	0.000000	-1.394323	-5.470367
45	6	0.000000	-0.703791	-6.663546
46	6	0.000000	0.703791	-6.663546
47	1	0.000000	5.138142	1.242563
48	1	0.000000	5.138142	-1.242563
49	1	0.000000	2.479220	-5.488844
50	1	0.000000	-2.479220	-5.488844
51	1	0.000000	-1.243768	-7.603372
52	1	0.000000	1.243768	-7.603372

Table S52. The Cartesian coordinates for the compound **50** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.707017	-2.334597
2	6	0.000000	-0.707017	-2.334597
3	6	0.000000	1.728762	-1.328156
4	6	0.000000	1.729258	0.098382
5	6	0.000000	0.714387	1.111142
6	6	0.000000	-0.714387	1.111142
7	6	0.000000	-1.729258	0.098382
8	6	0.000000	-1.728762	-1.328156
9	6	0.000000	1.367416	-3.589118
10	6	0.000000	0.692388	-4.820065
11	6	0.000000	-0.692388	-4.820065
12	6	0.000000	-1.367416	-3.589118
13	7	0.000000	-2.730478	-3.357239
14	6	0.000000	-2.964840	-1.996000
15	6	0.000000	-4.230922	-1.335925
16	6	0.000000	-2.969759	0.760037
17	6	0.000000	2.964840	-1.996000
18	7	0.000000	2.730478	-3.357239
19	6	0.000000	4.230922	-1.335925
20	6	0.000000	4.233400	0.097153
21	6	0.000000	2.969759	0.760037
22	7	0.000000	2.735993	2.119729
23	6	0.000000	1.376296	2.351750
24	6	0.000000	0.716114	3.617767
25	6	0.000000	-0.716114	3.617767
26	6	0.000000	-1.376296	2.351750
27	7	0.000000	-2.735993	2.119729
28	6	0.000000	-4.233400	0.097153
29	6	0.000000	-5.469108	-2.015892
30	6	0.000000	5.469108	-2.015892
31	6	0.000000	5.474374	0.772311
32	6	0.000000	1.393926	4.856849
33	6	0.000000	-1.393926	4.856849
34	6	0.000000	-5.474374	0.772311
35	6	0.000000	-6.664153	-1.327733
36	6	0.000000	-6.666575	0.079321
37	6	0.000000	6.664153	-1.327733
38	6	0.000000	6.666575	0.079321
39	6	0.000000	0.703329	6.050793
40	6	0.000000	-0.703329	6.050793
41	1	0.000000	-5.485950	-3.100803
42	1	0.000000	5.485950	-3.100803
43	1	0.000000	5.496048	1.857220
44	1	0.000000	2.478847	4.876469

45	1	0.000000	-2.478847	4.876469
46	1	0.000000	-5.496048	1.857220
47	1	0.000000	-7.602609	-1.870013
48	1	0.000000	-7.607007	0.618225
49	1	0.000000	7.602609	-1.870013
50	1	0.000000	7.607007	0.618225
51	1	0.000000	1.244099	6.990119
52	1	0.000000	-1.244099	6.990119
53	1	0.000000	-3.435407	-4.073223
54	1	0.000000	3.435407	-4.073223
55	1	0.000000	3.445488	2.830547
56	1	0.000000	-3.445488	2.830547
57	1	0.000000	1.242761	-5.754074
58	1	0.000000	-1.242761	-5.754074

Table S53. The Cartesian coordinates for the compound **51** optimized by the DFT/B3LYP/6-311G(d,p) method.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.714069	1.727446	0.000000
2	6	-0.714069	1.727446	0.000000
3	6	1.727446	0.714069	0.000000
4	6	1.727446	-0.714069	0.000000
5	6	0.714069	-1.727446	0.000000
6	6	-0.714069	-1.727446	0.000000
7	6	-1.727446	-0.714069	0.000000
8	6	-1.727446	0.714069	0.000000
9	6	1.375705	2.968132	0.000000
10	6	0.716070	4.234120	0.000000
11	6	-0.716070	4.234120	0.000000
12	6	-1.375705	2.968132	0.000000
13	7	-2.735098	2.735098	0.000000
14	6	-2.968132	1.375705	0.000000
15	6	-4.234120	0.716070	0.000000
16	6	-2.968132	-1.375705	0.000000
17	6	2.968132	1.375705	0.000000
18	7	2.735098	2.735098	0.000000
19	6	4.234120	0.716070	0.000000
20	6	4.234120	-0.716070	0.000000
21	6	2.968132	-1.375705	0.000000
22	7	2.735098	-2.735098	0.000000
23	6	1.375705	-2.968132	0.000000
24	6	0.716070	-4.234120	0.000000
25	6	-0.716070	-4.234120	0.000000
26	6	-1.375705	-2.968132	0.000000
27	7	-2.735098	-2.735098	0.000000
28	6	-4.234120	-0.716070	0.000000
29	6	1.394055	5.473209	0.000000
30	6	-1.394055	5.473209	0.000000
31	6	-5.473209	1.394055	0.000000
32	6	5.473209	1.394055	0.000000
33	6	5.473209	-1.394055	0.000000
34	6	1.394055	-5.473209	0.000000
35	6	-1.394055	-5.473209	0.000000
36	6	-5.473209	-1.394055	0.000000
37	6	-6.667014	0.703385	0.000000
38	6	-6.667014	-0.703385	0.000000
39	6	-0.703385	6.667014	0.000000
40	6	0.703385	6.667014	0.000000
41	6	6.667014	0.703385	0.000000
42	6	6.667014	-0.703385	0.000000
43	6	0.703385	-6.667014	0.000000
44	6	-0.703385	-6.667014	0.000000
45	1	2.478979	5.492851	0.000000

46	1	-2.478979	5.492851	0.000000
47	1	-5.492851	2.478979	0.000000
48	1	5.492851	2.478979	0.000000
49	1	5.492851	-2.478979	0.000000
50	1	2.478979	-5.492851	0.000000
51	1	-2.478979	-5.492851	0.000000
52	1	-5.492851	-2.478979	0.000000
53	1	-7.606397	1.244060	0.000000
54	1	-7.606397	-1.244060	0.000000
55	1	-1.244060	7.606397	0.000000
56	1	1.244060	7.606397	0.000000
57	1	7.606397	1.244060	0.000000
58	1	7.606397	-1.244060	0.000000
59	1	1.244060	-7.606397	0.000000
60	1	-1.244060	-7.606397	0.000000
61	1	-3.445247	3.445247	0.000000
62	1	3.445247	3.445247	0.000000
63	1	3.445247	-3.445247	0.000000
64	1	-3.445247	-3.445247	0.000000