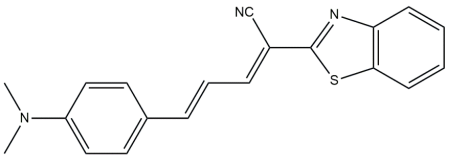
Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplementary Information



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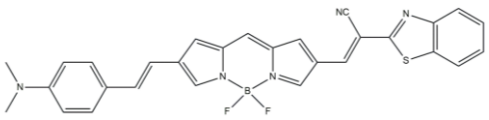

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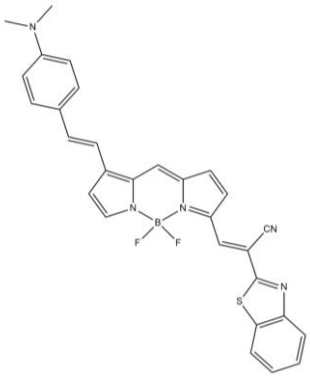

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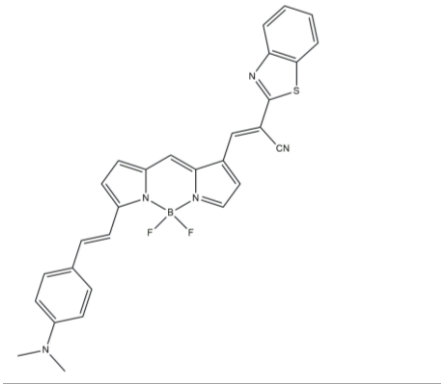

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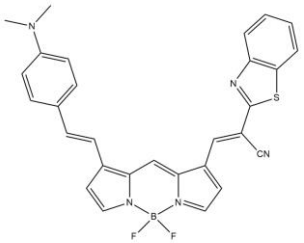

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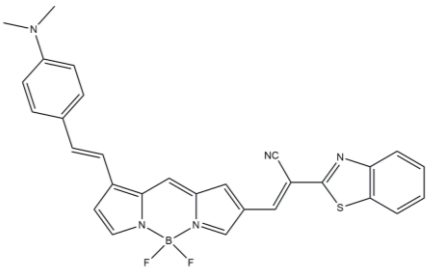

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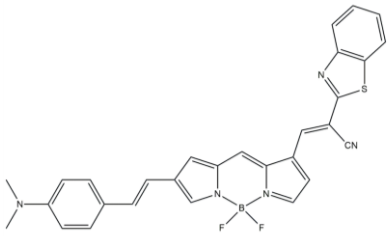

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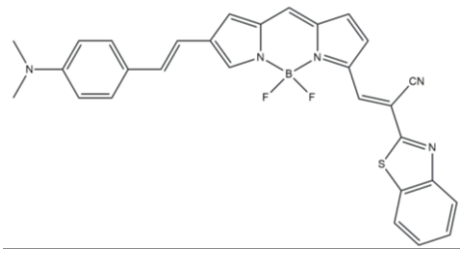

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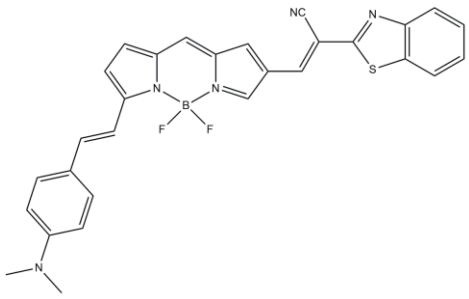

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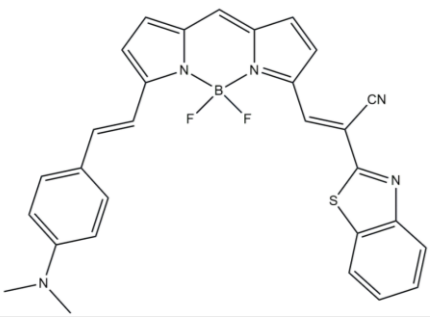


B9

Figure S1. 2D structural representation of B0 and designed B derivatives

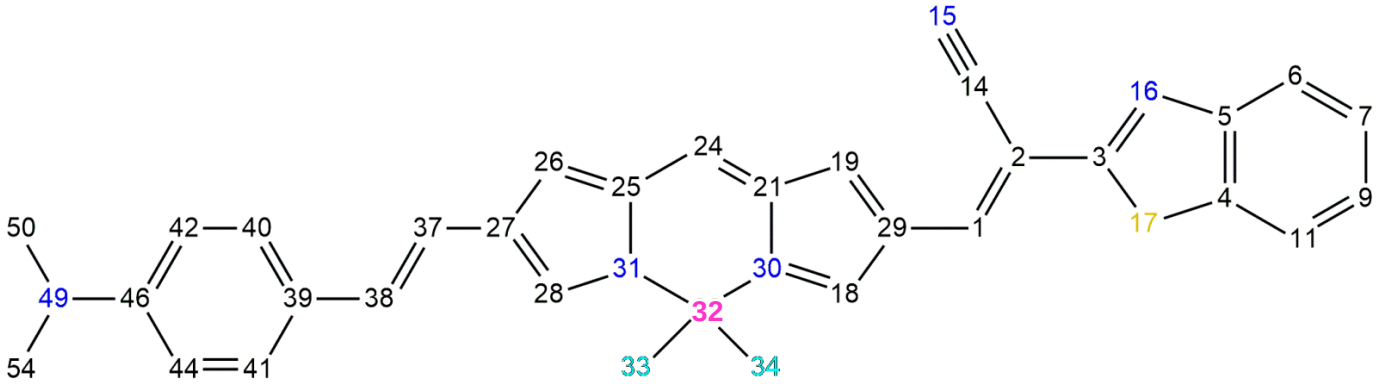


Figure S2. Atom numbering followed in this study.

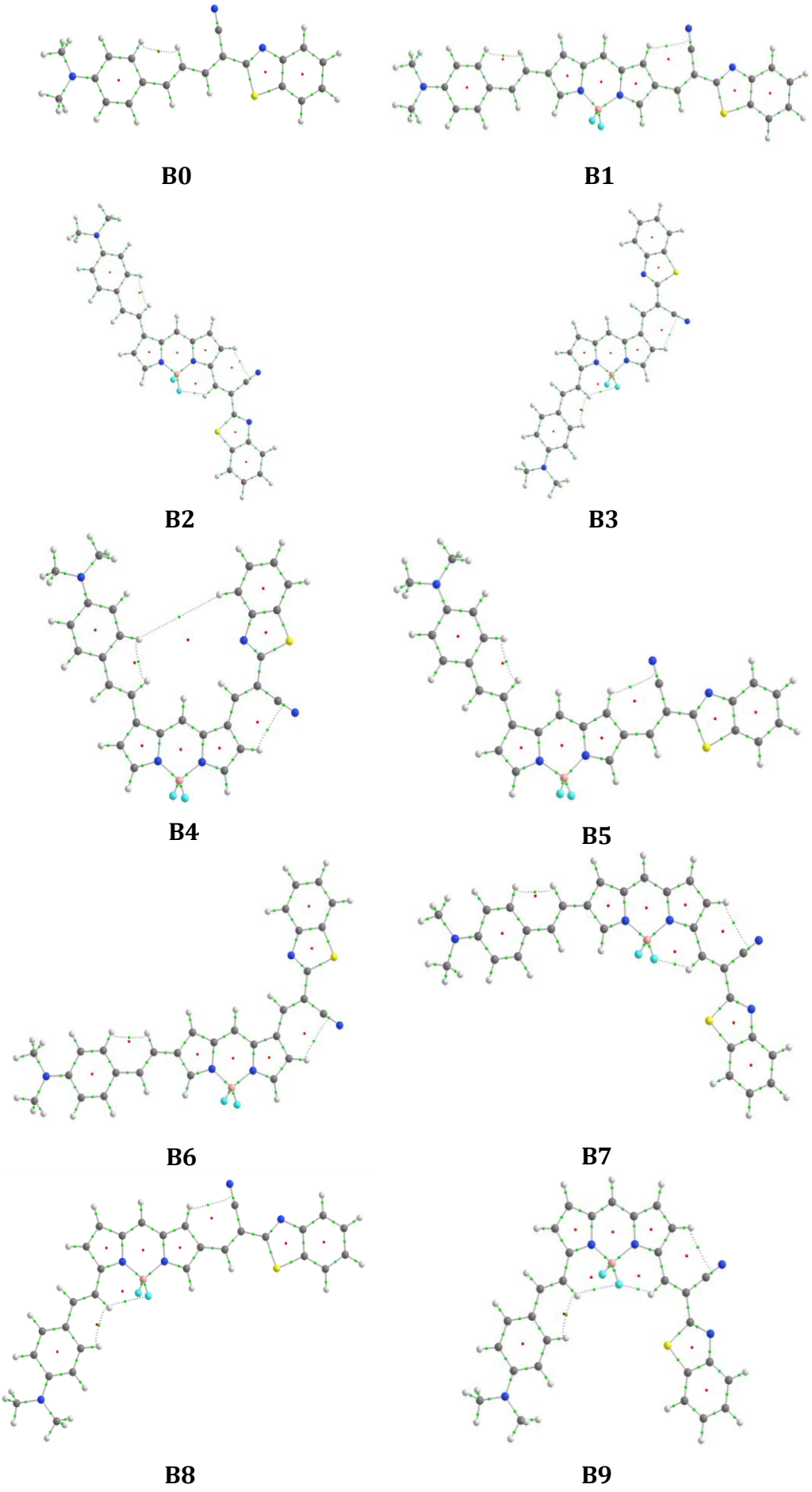
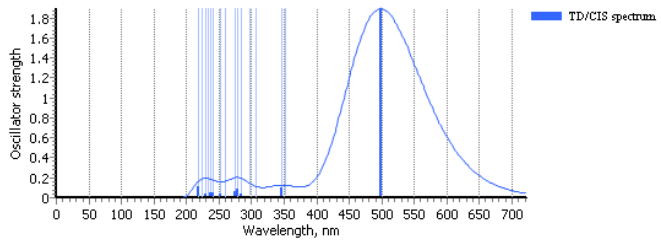


Figure S3. Molecular graphs of B0 and designed B derivatives.



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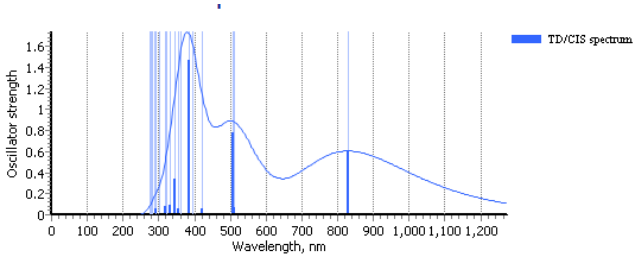

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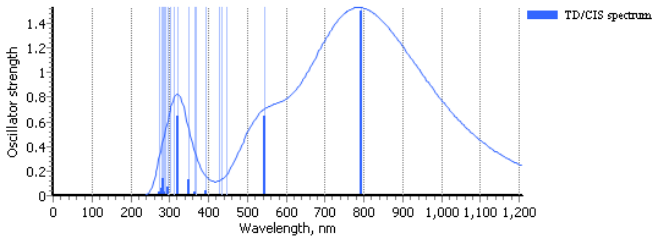

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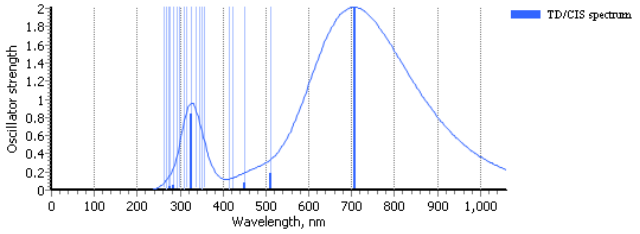

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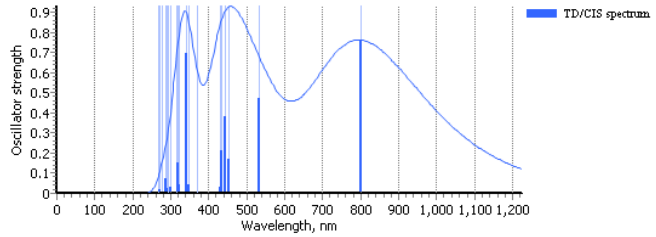

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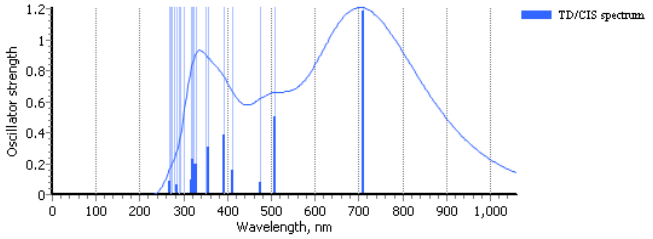

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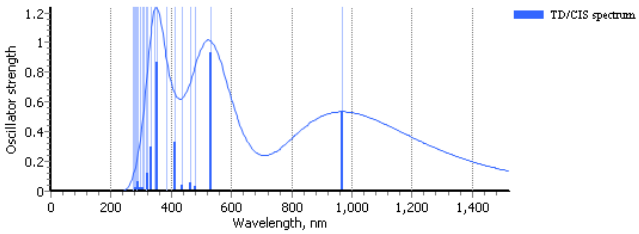

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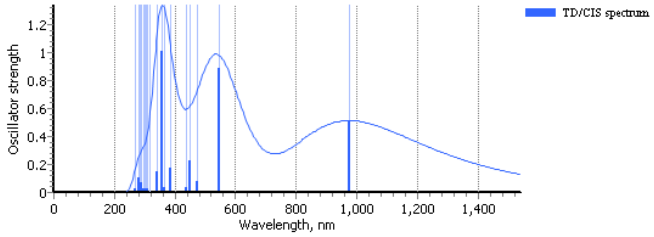

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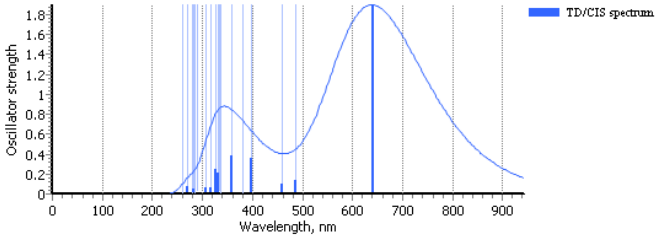

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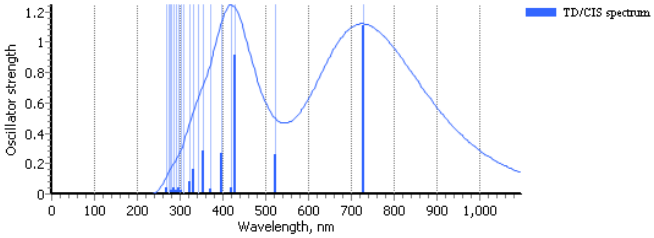

B9

Figure S4. Simulated absorption Spectra of B0 and designed B derivatives at B3PW91/6-31g(d,p) level of theory.

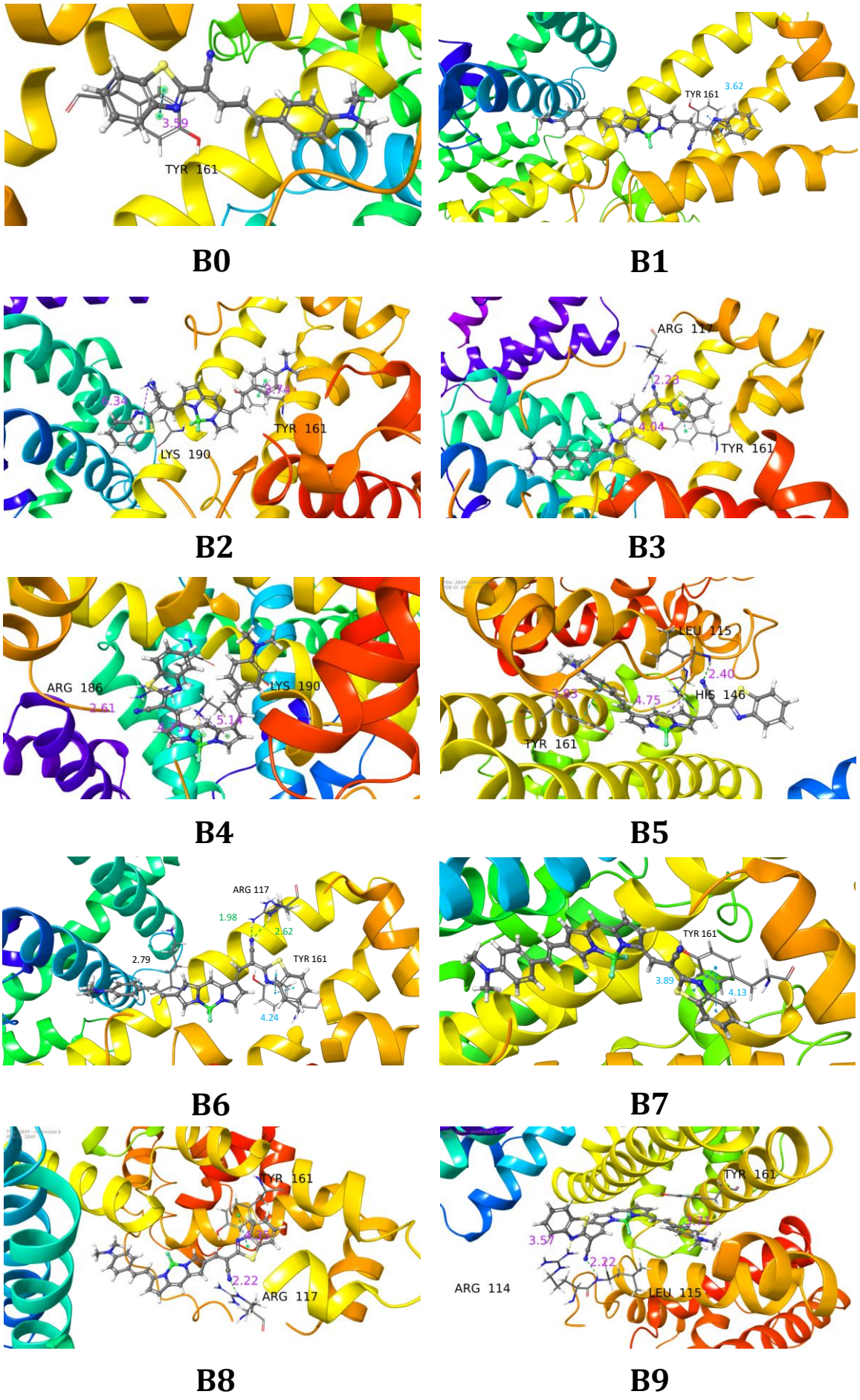

Figure S5. 3D representations of the interactions observed in B0 and designed B derivatives.

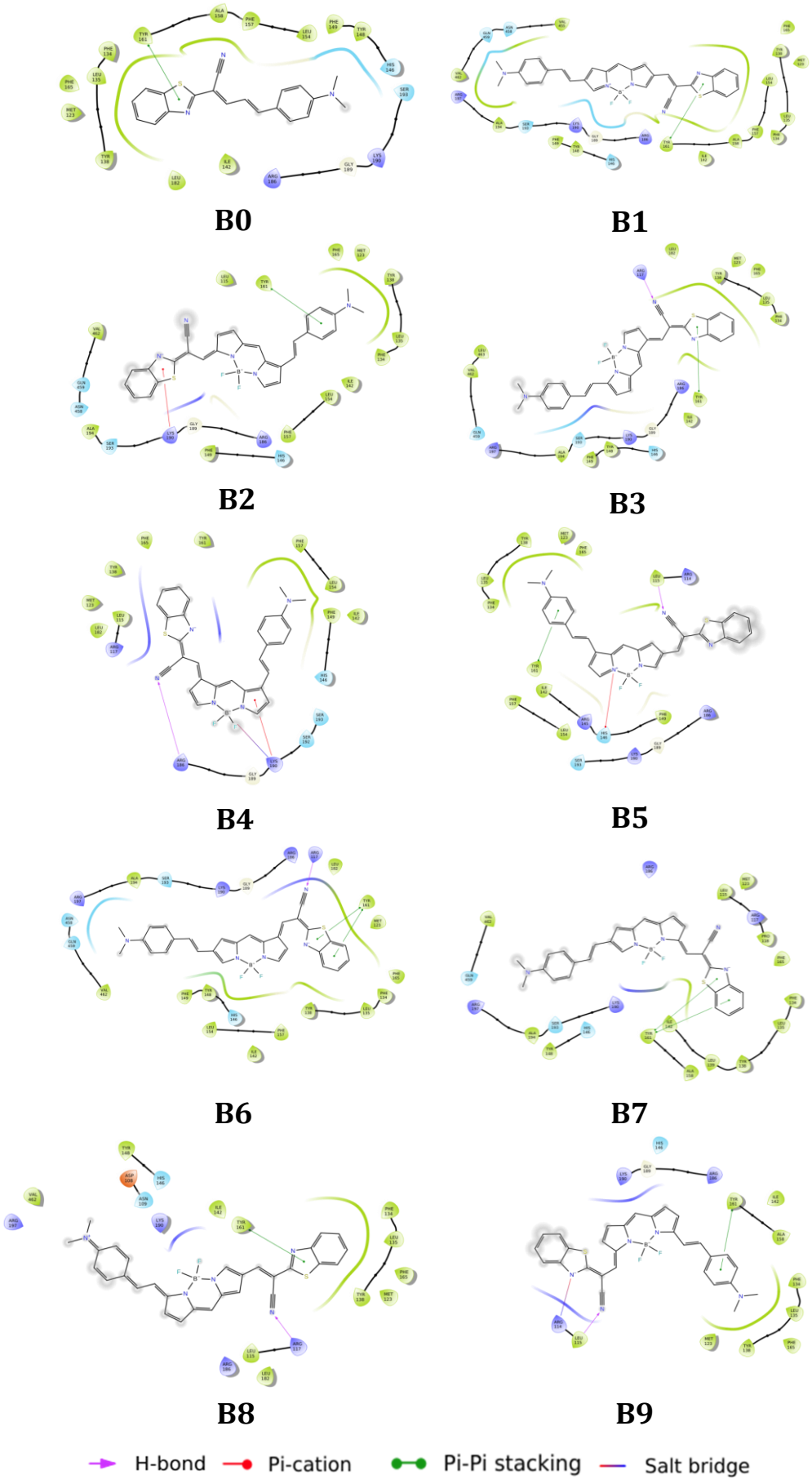

Figure S6. 2D representations of the interactions observed in B0 and designed B derivatives.

Table S1. Selected bond parameters for the molecules obtained from optimized geometries for B0 and designed B derivatives at B3PW91/6-31g(d,p) level of theory.

Bond Parameters		Molecules									
		B0	**B1**	**B2**	**B3**	**B4**	**B5**	**B6**	**B7**	**B8**	**B9**
Bond Length(Å)	C39-C38	1.434	1.452	1.437	1.432	1.437	1.439	1.451	1.451	1.435	1.432
	C38-C37	1.371	1.355	1.366	1.369	1.366	1.365	1.355	1.356	1.367	1.370
	C37-C27	-	1.445	1.426	1.420	1.426	1.428	1.444	1.444	1.423	1.420
	1C-29C	-	1.431	1.425	1.422	1.424	1.429	1.426	1.427	1.428	1.422
	1C-2C	1.379	1.368	1.371	1.374	1.372	1.369	1.370	1.370	1.370	1.374
	2C-14C	1.426	1.428	1.428	1.424	1.424	1.428	1.425	1.429	1.427	1.427
	37C-1C	1.414	-	-	-	-	-	-	-	-	-
	2C-3C	1.452	1.460	1.458	1.462	1.463	1.460	1.464	1.459	1.459	1.457
Bond Angle(^{0})	1C-2C-3C	124.3	114.8	123.0	120.3	120.3	123.5	120.3	122.9	123.5	122.9
	14C-2C-3C	115.8	105.5	114.5	117.0	117.0	114.9	117.0	114.5	114.8	114.5
	39C-38C-37C	128.1	127.5	127.7	127.3	127.5	127.6	127.4	127.5	127.3	127.3
	37C-1C-2C	126.5	-	-	-	-	-	-	-	-	-
	29C-1C-2C	-	129.8	129.3	129.8	129.7	129.9	129.6	129.2	130.0	129.5
Dihedral Angle(^{0})	39C-38C-37C-1C	-180.0	-	-	-	-	-	-	-	-	-
	38C-37C-1C-2C	180.0	-	-	-	-	-	-	-	-	-
	38C-37C-28C-31C	-	-179.7	179.4	176.3	178.7	179.7	180.0	-178.1	-176.0	176.3
	30C-18C-1C-2C	-	-	-173.6	180.0	-179.7	179.7	-180.0	173.7	-179.9	-175.1
	41C-39C-38C-37C	180.0	-179.5	-179.8	-179.8	179.0	179.2	180.0	-179.0	179.8	179.8
	39C-38C-37C-27C	-	179.9	179.6	-179.9	179.7	-179.8	-180.0	-179.9	-179.9	179.8

Table S2. FMO Energies of B0 and designed B derivatives from HOMO-2 to LUMO+2 along with HOMO-LUMO energy gap B3PW91/6-31g(d,p) level of theory.

FMO values (in eV)							
S. No	**HOMO-2**	**HOMO-1**	**HOMO**	**LUMO**	**LUMO+1**	**LUMO+2**	**Energy Gap**
B0	-6.652	-6.394	-5.262	-2.611	-0.799	-0.387	2.651
B1	-6.512	-6.036	-5.015	-3.263	-2.337	-1.223	1.752
B2	-6.712	-5.974	-5.185	-3.465	-2.168	-1.095	1.720
B3	-6.433	-6.049	-5.235	-3.358	-2.085	-1.241	1.877
B4	-6.081	-6.081	-5.198	-3.461	-2.123	-1.106	1.737
B5	-6.577	-6.018	-5.185	-3.236	-2.310	-1.121	1.949
B6	-6.457	-6.094	-5.020	-3.513	-2.080	-1.239	1.507
B7	-6.649	-5.984	-5.017	-3.518	-2.130	-1.243	1.499
B8	-6.505	-5.992	-5.225	-3.130	-2.276	-1.276	2.096
B9	-6.706	-5.974	-5.209	-3.359	-2.133	-1.251	1.850

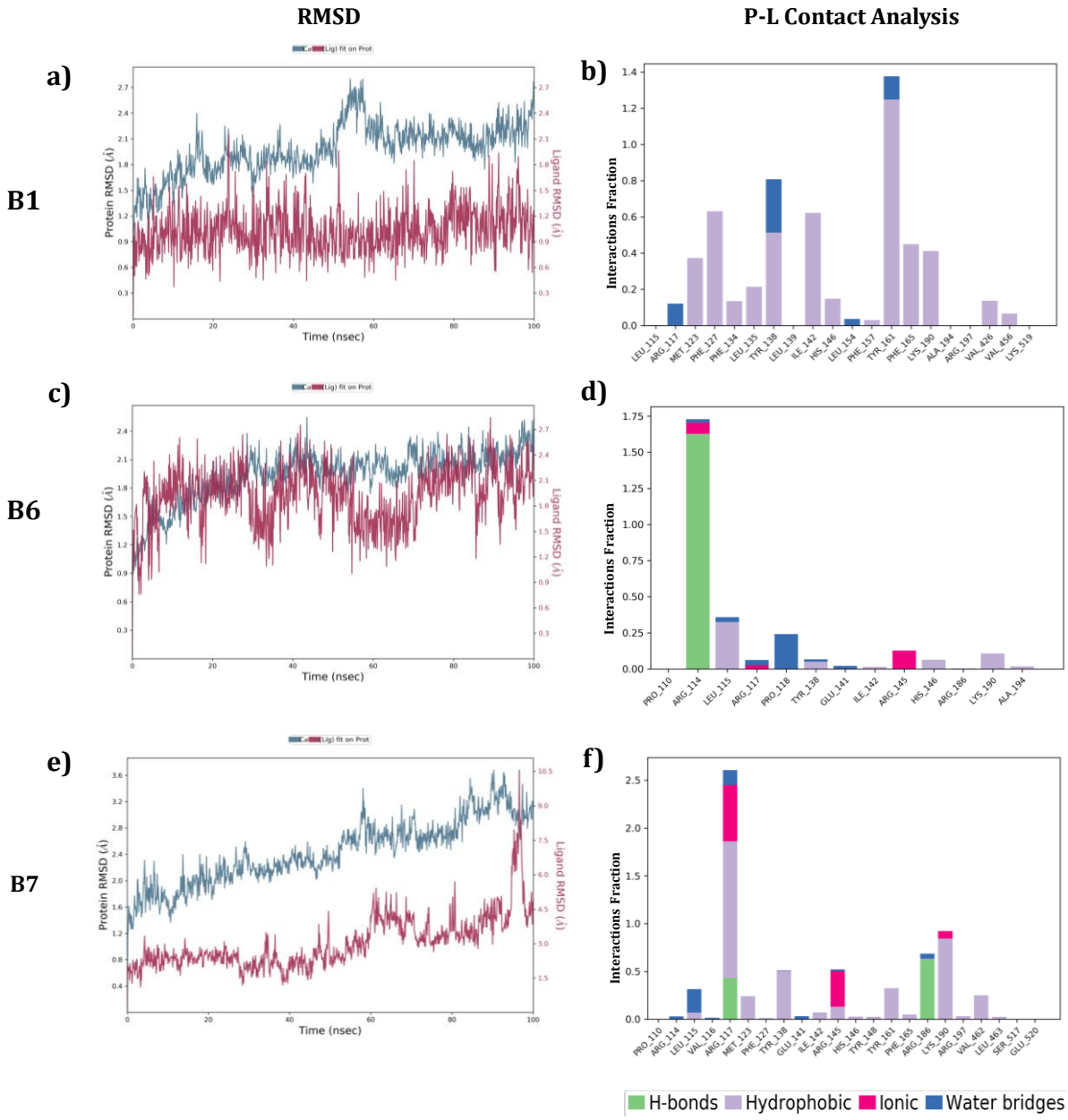

Figure S7. Extended 100 ns plots for MD analysis. (Left) RMSD plots for B1, B6 and B7 with HSA. The blue colour represents the evolution of the backbone Cα atoms of the protein, whereas the red colour indicates the molecule's heavy atoms. (Right) Protein–ligand contacts for the top three B derivatives with HSA.

3D Coordinates of Optimized geometries of B0 and B derivatives at B3PW91/6-31g(d,p) level of theory.

B0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.610348	0.151175	2.165316
2	6	0	-0.255364	0.427571	2.392784
3	6	0	0.395201	1.412864	1.637871
4	6	0	-0.309199	2.121698	0.655255
5	6	0	-1.664283	1.845415	0.427932
6	6	0	-2.314894	0.860284	1.183178
7	1	0	-2.106969	-0.601217	2.741673
8	1	0	0.282515	-0.113538	3.142886
9	1	0	0.187578	2.873689	0.078589
10	1	0	-2.202185	2.386491	-0.322232
11	6	0	1.884146	1.716433	1.888412
12	6	0	2.513933	2.669791	1.159482
13	6	0	4.002775	2.972864	1.411008
14	6	0	4.632828	3.927143	0.683726
15	6	0	6.121568	4.229541	0.936358
16	6	0	8.392656	4.578596	1.955926
17	6	0	8.137356	5.374624	0.910530
18	6	0	9.161298	6.427837	0.468773
19	6	0	10.306269	6.571597	1.195127
20	1	0	11.033141	7.300425	0.903015
21	6	0	10.560668	5.686247	2.446576
22	1	0	11.452532	5.820093	3.022572

23	6	0	9.653510	4.739086	2.810418
24	1	0	9.818875	4.120354	3.667572
25	1	0	2.421482	1.174425	2.638389
26	1	0	1.976775	3.211827	0.409513
27	1	0	4.539973	2.429948	2.160371
28	1	0	8.978685	7.040280	-0.389369
29	6	0	3.860653	4.709217	-0.394695
30	7	0	3.286057	5.292137	-1.198143
31	7	0	-3.736468	0.570729	0.945372
32	7	0	6.806517	5.137961	0.280125
33	16	0	7.106586	3.399468	2.154638
34	6	0	-4.771659	1.377271	1.607769
35	1	0	-4.794429	2.354862	1.173377
36	1	0	-5.724928	0.908206	1.480661
37	1	0	-4.549127	1.455819	2.651421
38	6	0	-4.122730	-0.525343	0.045191
39	1	0	-4.487422	-1.349205	0.622384
40	1	0	-4.890591	-0.187571	-0.619038
41	1	0	-3.271335	-0.837074	-0.523008

B1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.721504	-0.539542	0.190877
2	6	0	-5.570989	0.539214	0.194892
3	6	0	-7.104844	0.320357	0.234786
4	6	0	-9.447934	-0.587846	-0.060725

5	6	0	-9.375877	0.787785	0.019380
6	6	0	-10.522868	1.569852	-0.119528
7	6	0	-11.744998	0.925776	-0.400467
8	1	0	-12.637756	1.504344	-0.511848
9	6	0	-11.796342	-0.482408	-0.539367
10	1	0	-12.722933	-0.962149	-0.773200
11	6	0	-10.631281	-1.252907	-0.367706
12	1	0	-10.654594	-2.317906	-0.466138
13	1	0	-10.475097	2.634115	-0.019772
14	6	0	-5.044955	1.838092	0.163690
15	7	0	-4.615111	2.899551	0.138193
16	7	0	-7.993839	1.299114	0.240317
17	16	0	-7.872939	-1.284790	0.273543
18	6	0	-2.089355	-1.463213	0.130351
19	6	0	-2.538045	0.850402	0.093204
20	1	0	-2.294430	-2.524739	0.141029
21	6	0	-1.054009	0.561796	0.061595
22	1	0	-2.986249	1.810569	0.083598
23	1	0	-5.143980	-1.515703	0.221115
24	6	0	-0.017719	1.458594	0.009693
25	6	0	1.376617	0.822686	-0.251390
26	6	0	2.570441	1.431336	-0.165214
27	6	0	3.656471	0.367295	-0.284434
28	6	0	3.015856	-0.837924	-0.381518
29	6	0	-3.179417	-0.337332	0.136023
30	7	0	-0.891647	-0.902503	0.105485
31	7	0	1.561247	-0.602333	-0.639169
32	5	0	0.565216	-1.554328	0.166230

33	9	0	0.980678	-1.661116	1.557628
34	9	0	0.581334	-2.916608	-0.423567
35	1	0	2.718282	2.477079	-0.058470
36	1	0	3.505621	-1.796568	-0.326465
37	6	0	5.201265	0.607578	-0.206784
38	6	0	6.075204	-0.430789	-0.283035
39	6	0	7.617838	-0.203599	-0.220572
40	6	0	8.146262	1.084567	-0.115365
41	6	0	8.498731	-1.291733	-0.280609
42	6	0	9.542788	1.281259	0.036412
43	1	0	7.485254	1.929527	-0.158121
44	6	0	9.895588	-1.100443	-0.132809
45	1	0	8.107911	-2.275296	-0.447245
46	6	0	10.422442	0.177285	0.147941
47	1	0	9.926595	2.283266	0.064286
48	1	0	10.551535	-1.944272	-0.235273
49	7	0	11.875238	0.355811	0.535975
50	6	0	12.318074	1.716300	0.146313
51	1	0	13.388162	1.796034	0.245426
52	1	0	12.026730	1.858283	-0.865227
53	1	0	11.868840	2.481792	0.769289
54	6	0	12.687102	-0.677704	-0.155433
55	1	0	12.531536	-1.667354	0.260942
56	1	0	12.391541	-0.670101	-1.177987
57	1	0	13.734014	-0.441635	-0.065232
58	1	0	-0.164102	2.524307	0.134364
59	1	0	5.583837	1.609076	-0.103987
60	1	0	5.683646	-1.420748	-0.392295

B2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.165069	-2.646188	-0.775007
2	6	0	-3.000872	-1.200329	-0.467048
3	1	0	-0.636782	-3.570320	-0.964483
4	6	0	-1.682482	-0.463208	-0.395255
5	6	0	-1.471085	0.876071	-0.189145
6	6	0	-0.004440	1.341764	-0.410047
7	6	0	0.517416	2.539807	-0.101084
8	6	0	2.029179	2.462191	-0.286571
9	6	0	2.314146	1.174244	-0.650376
10	6	0	-2.723359	-2.502949	-0.690823
11	7	0	-0.612822	-1.459798	-0.582596
12	7	0	1.043322	0.472651	-1.011691
13	5	0	0.921953	-1.028733	-0.484288
14	9	0	1.351821	-1.114226	0.904202
15	9	0	1.794223	-1.919197	-1.290603
16	1	0	-0.040708	3.392836	0.195007
17	1	0	-2.266204	1.552922	0.097863
18	6	0	3.707629	0.526519	-0.751647
19	6	0	7.614690	-0.918480	0.487788
20	6	0	8.267316	0.359352	0.496758
21	6	0	9.739760	0.630302	0.857444
22	6	0	10.576670	-0.433236	1.221301

23	1	0	11.599731	-0.244978	1.471908
24	6	0	10.078254	-1.742492	1.258060
25	1	0	10.722070	-2.550450	1.536636
26	6	0	8.256356	-2.274145	0.837124
27	6	0	6.108631	0.660553	-0.123132
28	6	0	4.855477	1.303292	-0.544310
29	1	0	3.799263	-0.514823	-0.979926
30	6	0	4.804110	2.827622	-0.757337
31	7	0	4.765864	3.962555	-0.915945
32	1	0	7.816354	-3.249451	0.845841
33	1	0	10.123165	1.628883	0.830285
34	16	0	6.284696	-0.701619	0.101793
35	7	0	7.314051	1.313996	0.115813
36	1	0	2.730627	3.259795	-0.157350
37	1	0	-3.437463	-3.293316	-0.792187
38	6	0	-4.398578	-0.572681	-0.311889
39	6	0	-5.540485	-1.380122	-0.401393
40	6	0	-6.916702	-0.808767	-0.012577
41	6	0	-7.025043	0.510607	0.427863
42	6	0	-8.054880	-1.610210	-0.100825
43	6	0	-8.271225	1.028130	0.780597
44	1	0	-6.127427	1.141955	0.498058
45	6	0	-9.301657	-1.092378	0.251039
46	1	0	-7.969696	-2.650049	-0.448110
47	6	0	-9.409981	0.226524	0.691833
48	1	0	-8.356610	2.067873	1.128362
49	1	0	-10.198945	-1.724389	0.180967
50	7	0	-10.723302	0.772301	1.063607

51	6	0	-10.729276	2.226063	0.845797
52	1	0	-10.085021	2.696229	1.559084
53	1	0	-10.382347	2.439910	-0.143551
54	1	0	-11.724811	2.600230	0.963316
55	6	0	-11.765418	0.148476	0.235513
56	1	0	-11.853534	-0.886375	0.492844
57	1	0	-12.700064	0.639839	0.408424
58	1	0	-11.501200	0.237888	-0.797490
59	1	0	-5.456297	-2.391868	-0.739304
60	1	0	-4.497672	0.478109	-0.136048

B3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.648153	1.388620	-0.020723
2	6	0	-0.997929	3.072762	-0.190615
3	6	0	-0.403018	1.669988	-0.154591
4	6	0	0.897499	1.293105	-0.217235
5	6	0	1.164131	-0.212417	-0.401908
6	6	0	2.334856	-0.839690	-0.344077
7	6	0	2.055083	-2.342265	-0.338913
8	6	0	0.707596	-2.483640	-0.396055
9	6	0	-2.338433	2.910831	-0.107967
10	7	0	-1.511179	0.721882	-0.022743
11	7	0	0.084640	-1.163822	-0.694534
12	5	0	-1.237296	-0.840776	0.118465
13	9	0	-1.045065	-1.159557	1.530647

14	9	0	-2.348825	-1.630270	-0.402719
15	1	0	1.692361	2.005519	-0.146996
16	1	0	2.779920	-3.129847	-0.288468
17	1	0	-3.062860	3.697623	-0.102498
18	1	0	0.179518	-3.401642	-0.246258
19	6	0	3.686683	-0.167129	-0.261684
20	6	0	4.758676	-0.909061	-0.155832
21	6	0	7.870591	1.209141	-0.060276
22	6	0	8.522480	0.048915	0.147430
23	6	0	6.106933	-0.260054	-0.072227
24	1	0	3.799353	0.884197	-0.272741
25	6	0	4.725662	-2.448616	-0.059885
26	7	0	4.700706	-3.609201	0.012439
27	6	0	8.664445	2.513722	-0.140174
28	6	0	10.036399	2.412602	0.009992
29	6	0	9.987048	-0.075121	0.292716
30	6	0	10.725384	1.047577	0.239014
31	7	0	6.393187	1.051301	-0.189335
32	16	0	7.489148	-1.359086	0.264279
33	1	0	8.153968	3.455135	-0.305828
34	1	0	10.612584	3.292215	-0.035353
35	1	0	11.769803	0.946376	0.362407
36	1	0	10.376897	-1.060552	0.445843
37	1	0	-0.463900	3.997409	-0.264815
38	6	0	-4.072962	0.790921	0.063196
39	6	0	-5.161630	1.608849	0.093991
40	6	0	-6.585605	1.012663	0.164056
41	6	0	-6.756708	-0.375940	0.191815

42	6	0	-7.711069	1.856583	0.198821
43	6	0	-8.046040	-0.926431	0.256019
44	1	0	-5.903198	-1.015875	0.161883
45	6	0	-9.002644	1.305489	0.261938
46	1	0	-7.586912	2.918986	0.175545
47	6	0	-9.171967	-0.087724	0.290545
48	1	0	-8.169497	-1.986282	0.273582
49	1	0	-9.856544	1.947797	0.284684
50	7	0	-10.525976	-0.671142	0.339321
51	6	0	-11.452815	0.216175	-0.371471
52	1	0	-12.411432	-0.253985	-0.435005
53	1	0	-11.541352	1.139868	0.161725
54	1	0	-11.082505	0.408081	-1.356477
55	6	0	-10.501303	-1.989907	-0.300304
56	1	0	-10.086336	-1.906521	-1.282070
57	1	0	-9.901892	-2.656893	0.284357
58	1	0	-11.499483	-2.368521	-0.364522
59	1	0	-5.035883	2.669607	0.073623
60	1	0	-4.206289	-0.267800	0.095646

B4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836799	-5.082847	0.110952
2	6	0	-2.430711	-2.804797	-0.103980
3	6	0	-0.921838	-3.016679	-0.066578
4	6	0	0.070939	-2.097559	-0.149779

5	6	0	1.498370	-2.648146	-0.326099
6	6	0	2.639149	-1.966762	-0.284271
7	6	0	3.782986	-2.980229	-0.260787
8	6	0	3.210008	-4.208927	-0.291937
9	6	0	-2.982201	-4.035266	0.004683
10	7	0	-0.679692	-4.451922	0.093907
11	7	0	1.757288	-4.069117	-0.590497
12	5	0	0.801078	-5.019118	0.243769
13	9	0	1.176066	-4.989950	1.654926
14	9	0	0.904269	-6.388791	-0.249973
15	1	0	-0.130162	-1.048087	-0.100399
16	1	0	4.831497	-2.763657	-0.216750
17	1	0	-4.029716	-4.250761	0.016548
18	1	0	3.725166	-5.131199	-0.124421
19	6	0	2.759105	-0.460273	-0.232615
20	6	0	3.947404	0.078427	-0.139956
21	6	0	3.734821	3.837994	-0.120141
22	6	0	5.065476	3.803328	0.085734
23	6	0	4.085714	1.569750	-0.086817
24	1	0	1.915975	0.177484	-0.254963
25	6	0	5.250212	-0.740786	-0.029915
26	7	0	6.232290	-1.358403	0.053035
27	6	0	3.025336	5.188524	-0.226043
28	6	0	3.818950	6.315191	-0.100211
29	6	0	5.926424	4.997459	0.205190
30	6	0	5.344295	6.207275	0.128092
31	7	0	3.108901	2.488026	-0.220663
32	16	0	5.740331	2.195062	0.233885

33	1	0	1.955156	5.232538	-0.390551
34	1	0	3.361677	7.261033	-0.163842
35	1	0	5.969223	7.052675	0.233172
36	1	0	6.972179	4.827150	0.359774
37	1	0	-1.967112	-6.142251	0.185656
38	6	0	-3.175479	-1.463395	-0.236494
39	6	0	-4.576606	-1.441291	-0.253178
40	6	0	-5.324186	-0.099005	-0.148339
41	6	0	-4.606553	1.092244	-0.036988
42	6	0	-6.718696	-0.074139	-0.164811
43	6	0	-5.283369	2.307981	0.058544
44	1	0	-3.507165	1.072236	-0.023256
45	6	0	-7.395857	1.141970	-0.070252
46	1	0	-7.284458	-1.012920	-0.252747
47	6	0	-6.678469	2.332932	0.041553
48	1	0	-4.717799	3.246923	0.146947
49	1	0	-8.495366	1.161303	-0.083680
50	7	0	-7.391527	3.614463	0.142180
51	6	0	-8.859274	3.646751	0.067493
52	1	0	-9.270016	3.071391	0.870706
53	1	0	-9.198120	4.658791	0.144030
54	1	0	-9.178044	3.233572	-0.866621
55	6	0	-6.636839	4.863707	0.317495
56	1	0	-6.046485	4.801823	1.207750
57	1	0	-5.995758	5.014462	-0.525824
58	1	0	-7.318943	5.684150	0.398171
59	1	0	-2.624102	-0.549824	-0.315690
60	1	0	-5.126032	-2.355475	-0.338614

B5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.006057	0.840019	0.173671
2	6	0	4.309421	-0.499131	0.174893
3	6	0	5.787643	-0.961020	0.235890
4	6	0	8.298056	-1.146395	-0.020408
5	6	0	7.640635	-2.357942	0.042216
6	6	0	8.342375	-3.556265	-0.092302
7	6	0	9.727018	-3.498405	-0.350712
8	1	0	10.286226	-4.403873	-0.458312
9	6	0	10.380672	-2.248227	-0.471979
10	1	0	11.427124	-2.211989	-0.688832
11	6	0	9.657120	-1.052770	-0.305070
12	1	0	10.137356	-0.100638	-0.390353
13	1	0	7.840352	-4.497228	-0.005980
14	6	0	3.276898	-1.445615	0.121687
15	7	0	2.433140	-2.219111	0.078207
16	7	0	6.169621	-2.226872	0.240311
17	16	0	7.170184	0.157911	0.303261
18	6	0	2.027504	2.805674	0.092612
19	6	0	1.439083	0.524070	0.032949
20	1	0	2.668597	3.675923	0.118569
21	6	0	0.223753	1.422688	-0.013039
22	1	0	1.431329	-0.535453	0.017152
23	1	0	4.806435	1.539639	0.220772

24	6	0	-1.096352	1.058674	-0.088234
25	6	0	-2.077783	2.233630	-0.358391
26	6	0	-3.418522	2.196705	-0.293947
27	6	0	-3.939922	3.624898	-0.413383
28	6	0	-2.842132	4.438303	-0.488194
29	6	0	2.527796	1.320563	0.097818
30	7	0	0.705640	2.814339	0.046562
31	7	0	-1.625946	3.601856	-0.731138
32	5	0	-0.330572	4.028700	0.097625
33	9	0	-0.682125	4.295725	1.485108
34	9	0	0.249690	5.269007	-0.475839
35	1	0	-2.873287	5.514055	-0.427476
36	1	0	-1.424108	0.032810	0.025320
37	1	0	-4.964895	3.931297	-0.434562
38	6	0	-4.266519	0.918205	-0.160003
39	6	0	-5.663737	1.009846	-0.102504
40	6	0	-6.511733	-0.268653	0.031440
41	6	0	-5.888748	-1.515361	0.095326
42	6	0	-7.902570	-0.180287	0.089000
43	6	0	-6.656537	-2.673438	0.216066
44	1	0	-4.792256	-1.584746	0.049147
45	6	0	-8.670692	-1.338549	0.210768
46	1	0	-8.393735	0.802246	0.038841
47	6	0	-8.047948	-2.585027	0.274168
48	1	0	-6.165594	-3.656189	0.265796
49	1	0	-9.767267	-1.268539	0.256542
50	7	0	-8.856901	-3.805798	0.401504
51	6	0	-8.153165	-4.928557	-0.234945

52	1	0	-7.842983	-4.643551	-1.218539
53	1	0	-7.294668	-5.188196	0.348554
54	1	0	-8.809602	-5.771173	-0.298114
55	6	0	-10.155204	-3.604277	-0.257813
56	1	0	-10.690036	-4.530678	-0.283011
57	1	0	-10.723128	-2.879265	0.286907
58	1	0	-9.997470	-3.256204	-1.257245
59	1	0	-6.140534	1.966484	-0.151583
60	1	0	-3.789722	-0.038433	-0.110924

B6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.955169	-3.631348	0.207206
2	6	0	-3.028621	-1.561968	-0.051988
3	1	0	-1.851519	-4.688800	0.318093
4	6	0	-1.528639	-1.430196	-0.037122
5	6	0	-0.772631	-0.312151	-0.157769
6	6	0	0.744550	-0.523905	-0.339029
7	6	0	1.714862	0.416581	-0.314873
8	6	0	3.057859	-0.323993	-0.297682
9	6	0	2.771056	-1.661279	-0.319485

10	6	0	-3.311339	-2.875200	0.093541
11	7	0	-0.971284	-2.760362	0.150933
12	7	0	1.313268	-1.859988	-0.590820
13	5	0	0.601507	-2.982703	0.282323
14	9	0	0.976372	-2.837685	1.686498
15	9	0	0.995563	-4.306218	-0.184235
16	1	0	1.570589	1.479843	-0.291366
17	1	0	3.481125	-2.443004	-0.156959
18	6	0	4.464795	0.343774	-0.251556
19	6	0	5.601515	-0.414967	-0.227214
20	6	0	7.015185	0.245198	-0.171386
21	6	0	7.161132	1.641457	-0.165350
22	6	0	8.167498	-0.559230	-0.111404
23	6	0	8.437653	2.227679	0.005037
24	1	0	6.299995	2.263448	-0.285889
25	6	0	9.444443	0.023697	0.055598
26	1	0	8.074759	-1.622028	-0.187003
27	6	0	9.578764	1.419052	0.201602
28	1	0	8.537263	3.293131	-0.014470
29	1	0	10.314195	-0.599479	0.074814
30	7	0	10.903960	2.027967	0.554917
31	6	0	10.973790	3.405584	0.046419
32	1	0	11.964424	3.790106	0.193141
33	1	0	10.738893	3.427274	-0.992338
34	1	0	10.273824	4.007626	0.585554
35	6	0	11.989731	1.219854	-0.025416
36	1	0	12.025341	0.276940	0.476447
37	1	0	11.815673	1.065914	-1.065899

38	1	0	12.924393	1.730097	0.104744
39	1	0	-1.201028	0.664816	-0.128850
40	1	0	4.540240	1.411857	-0.233472
41	1	0	5.517075	-1.481822	-0.238982
42	1	0	-4.288809	-3.314156	0.128485
43	6	0	-4.004695	-0.413531	-0.193162
44	6	0	-5.279191	-0.687271	-0.205386
45	6	0	-8.417464	1.738814	0.044069
46	6	0	-7.274457	2.523187	0.062138
47	1	0	-3.704927	0.584330	-0.266814
48	6	0	-6.303685	0.420921	-0.125967
49	6	0	-7.398826	4.009661	0.160356
50	6	0	-8.651239	4.548081	0.222325
51	1	0	-8.737621	5.599180	0.277492
52	6	0	-9.945063	3.640414	0.196651
53	1	0	-10.909528	4.036911	0.257055
54	6	0	-9.786717	2.342359	0.092477
55	6	0	-5.858538	-2.108569	-0.263029
56	7	0	-6.301272	-3.194580	-0.307073
57	7	0	-6.006835	1.747148	-0.039152
58	16	0	-8.077371	-0.018950	-0.054428
59	1	0	-6.524053	4.653636	0.172117
60	1	0	-10.581548	1.678510	0.053729

B7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.937111	-2.073359	0.042212
2	6	0	2.438689	-4.373527	0.037638
3	6	0	1.187342	-3.500722	0.013428
4	1	0	2.482299	-5.439665	0.034933
5	6	0	-0.112032	-3.876934	-0.011583
6	6	0	-1.152349	-2.769533	-0.263911
7	6	0	-2.495660	-2.866187	-0.169983
8	6	0	-3.056886	-1.443040	-0.271088
9	6	0	-1.984109	-0.606707	-0.417520
10	6	0	3.484949	-3.522096	0.045218
11	7	0	1.620578	-2.106236	0.048750
12	7	0	-0.749626	-1.411486	-0.670908
13	5	0	0.552550	-0.922394	0.107634
14	9	0	0.229008	-0.656905	1.505492
15	9	0	1.068688	0.301196	-0.505663
16	1	0	-3.058954	-3.765949	-0.034881
17	1	0	-2.023785	0.459506	-0.359345
18	6	0	-4.562801	-1.053367	-0.199431
19	6	0	-4.958929	0.252014	-0.282399
20	6	0	-6.465383	0.649752	-0.188978
21	6	0	-7.466128	-0.327689	-0.045784
22	6	0	-6.840445	2.005356	-0.251257
23	6	0	-8.811935	0.053399	0.157265
24	1	0	-7.204569	-1.364100	-0.077647
25	6	0	-8.185036	2.386889	-0.051929
26	1	0	-6.098032	2.752455	-0.436737
27	6	0	-9.165656	1.415899	0.223597
28	1	0	-9.565832	-0.697171	0.263122

29	1	0	-8.458040	3.419546	-0.105943
30	7	0	-10.555516	1.824684	0.582335
31	6	0	-11.505909	0.766771	0.219525
32	1	0	-12.504967	1.109837	0.403151
33	1	0	-11.400570	0.522265	-0.817188
34	1	0	-11.310869	-0.100977	0.812881
35	6	0	-10.903685	3.076954	-0.102295
36	1	0	-10.288242	3.867348	0.270526
37	1	0	-10.747882	2.969435	-1.156557
38	1	0	-11.934545	3.307615	0.081526
39	1	0	-0.398082	-4.894628	0.128145
40	1	0	-5.298309	-1.821157	-0.073372
41	1	0	-4.220795	1.015106	-0.412071
42	1	0	4.516699	-3.794619	0.056481
43	6	0	3.863708	-0.848535	0.040816
44	6	0	5.233486	-1.017589	0.040246
45	6	0	6.671138	2.622619	0.008662
46	6	0	7.743187	1.859597	0.016526
47	6	0	6.699377	4.078060	0.004196
48	6	0	7.861827	4.705260	-0.005416
49	1	0	7.879122	5.787060	-0.020751
50	6	0	9.177791	3.884169	0.002474
51	1	0	10.140342	4.401719	0.001810
52	6	0	9.137450	2.545622	0.016674
53	1	0	5.762689	4.627203	-0.005000
54	1	0	10.062639	1.992312	0.025773
55	1	0	3.445025	0.130621	0.030415
56	6	0	6.063982	0.221593	0.011778

57	16	0	5.184124	1.719736	-0.034126
58	7	0	7.380870	0.377524	0.008257
59	6	0	5.884531	-2.393929	0.061302
60	7	0	6.379538	-3.440290	0.077310

B8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.953531	-0.307317	0.060068
2	6	0	-5.101478	0.398998	0.322162
3	6	0	-6.474946	-0.319127	0.313030
4	6	0	-8.417417	-1.862705	-0.183359
5	6	0	-8.785246	-0.595646	0.220664
6	6	0	-10.130062	-0.228082	0.274306
7	6	0	-11.098739	-1.161091	-0.148209
8	1	0	-12.136044	-0.901912	-0.116781
9	6	0	-10.705671	-2.438013	-0.617126
10	1	0	-11.444548	-3.132886	-0.955668
11	6	0	-9.344870	-2.796285	-0.636252
12	1	0	-9.032419	-3.758340	-0.984503
13	1	0	-10.419095	0.741114	0.623604
14	6	0	-5.025362	1.771051	0.598649

15	7	0	-4.963194	2.892297	0.824599
16	7	0	-7.627892	0.282080	0.552974
17	16	0	-6.680341	-2.053883	-0.028149
18	6	0	-1.178227	-0.267758	-0.224823
19	6	0	-2.348434	1.712618	0.289223
20	1	0	-1.029522	-1.311231	-0.465777
21	6	0	-0.858131	1.947189	0.186130
22	1	0	-3.080779	2.446318	0.508891
23	1	0	-4.035788	-1.348985	-0.141058
24	6	0	-0.173027	3.124468	0.345763
25	6	0	1.325710	3.062099	-0.062419
26	6	0	2.263280	3.996681	0.162565
27	6	0	3.620315	3.407981	-0.208576
28	6	0	3.395584	2.112398	-0.587161
29	6	0	-2.568156	0.401613	0.050696
30	7	0	-0.230583	0.648928	-0.119095
31	7	0	1.926632	1.903491	-0.777722
32	5	0	1.358359	0.520933	-0.218582
33	9	0	1.897478	0.250524	1.106647
34	9	0	1.763749	-0.590988	-1.114804
35	1	0	2.075176	4.980522	0.513994
36	1	0	-0.643675	4.025058	0.720120
37	1	0	4.564567	3.910374	-0.178731
38	6	0	4.502458	1.071376	-0.837562
39	6	0	5.847722	1.430596	-0.678982
40	6	0	6.901715	0.347086	-0.384523
41	6	0	6.516585	-0.989471	-0.276072
42	6	0	8.241366	0.701858	-0.226351

43	6	0	7.470857	-1.970884	-0.008839
44	1	0	5.460235	-1.268746	-0.400062
45	6	0	9.196202	-0.279855	0.039991
46	1	0	8.545110	1.755204	-0.311971
47	6	0	8.811167	-1.616053	0.148899
48	1	0	7.167275	-3.024316	0.077279
49	1	0	10.252447	0.000112	0.164247
50	7	0	9.816725	-2.650687	0.430474
51	6	0	11.247654	-2.338659	0.304055
52	1	0	11.516326	-1.597397	1.027412
53	1	0	11.822277	-3.225534	0.471866
54	1	0	11.445918	-1.965922	-0.679133
55	6	0	9.391355	-3.997350	0.838467
56	1	0	8.739044	-3.924617	1.683512
57	1	0	8.874790	-4.468852	0.028686
58	1	0	10.250609	-4.578806	1.100179
59	1	0	6.142037	2.455939	-0.762353
60	1	0	4.244824	0.075503	-1.132115

B9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.437625	-2.904679	0.304608
2	6	0	2.279768	-5.232844	0.690642
3	6	0	0.919893	-4.575247	0.492762
4	1	0	2.473779	-6.269329	0.881469

5	6	0	-0.308360	-5.143994	0.501220
6	6	0	-1.478063	-4.268782	0.026218
7	6	0	-2.794057	-4.553081	0.099485
8	6	0	-3.538678	-3.284884	-0.286212
9	6	0	-2.616207	-2.336514	-0.534829
10	6	0	3.190999	-4.240371	0.574941
11	7	0	1.141892	-3.143393	0.286857
12	7	0	-1.257031	-2.951872	-0.604428
13	5	0	-0.086001	-2.146262	0.115242
14	9	0	-0.518819	-1.708615	1.439618
15	9	0	0.282152	-0.976608	-0.678645
16	1	0	-3.233996	-5.484991	0.384694
17	1	0	-0.458136	-6.151169	0.820286
18	1	0	4.251046	-4.355042	0.655571
19	1	0	-4.599029	-3.154952	-0.324418
20	6	0	3.132412	-1.537554	0.098085
21	6	0	4.493021	-1.444979	0.151904
22	6	0	5.189837	-0.080744	-0.062203
23	6	0	4.422061	1.062599	-0.311456
24	6	0	6.589689	0.022524	-0.009712
25	6	0	5.044576	2.303858	-0.506789
26	1	0	3.355122	0.988480	-0.351349
27	6	0	7.213088	1.265487	-0.206738
28	1	0	7.183413	-0.846850	0.182353
29	6	0	6.440538	2.408634	-0.450553
30	1	0	4.451104	3.173593	-0.698267
31	1	0	8.280868	1.340668	-0.168550
32	7	0	7.092432	3.717409	-0.636020

33	6	0	8.355230	3.737492	0.114404
34	1	0	9.023751	3.009449	-0.295823
35	1	0	8.799465	4.709420	0.041275
36	1	0	8.163954	3.509518	1.140898
37	6	0	6.196516	4.772009	-0.141000
38	1	0	5.309704	4.795298	-0.739460
39	1	0	5.936584	4.570007	0.876121
40	1	0	6.691402	5.719959	-0.201432
41	1	0	2.548346	-0.662329	-0.086672
42	1	0	5.079614	-2.320739	0.341365
43	6	0	-2.984180	-0.866514	-0.684466
44	6	0	-4.292343	-0.497232	-0.662245
45	6	0	-4.257980	3.306565	0.254639
46	6	0	-5.547389	2.973504	0.124182
47	6	0	-3.815657	4.688966	0.609874
48	6	0	-4.726404	5.633178	0.830047
49	1	0	-4.451120	6.614494	1.108675
50	6	0	-6.622176	4.059202	0.337473
51	6	0	-6.218756	5.311748	0.686643
52	1	0	-6.901770	6.100248	0.859712
53	6	0	-4.554134	0.952797	-0.365063
54	7	0	-5.723083	1.545987	-0.266875
55	16	0	-3.202401	1.981583	-0.010571
56	1	0	-2.786457	4.916093	0.687735
57	1	0	-7.664355	3.851075	0.241336
58	1	0	-2.229919	-0.117630	-0.787295
59	6	0	-5.458586	-1.467342	-0.921886
60	7	0	-6.336872	-2.186000	-1.114948