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Effect of connectivity variation in Azulene-BODIPY triads and their optoelectronic properties

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Experimental section

Materials

All reagents were obtained from commercial sources (Sigma Aldrich, Spectrochem, Merck and Alfa Aesar) and used as received without further purification unless otherwise specified. Toluene was dried over sodium/benzophenone before use. Triethylamine was distilled using potassium hydroxide flakes. Dry reactions were conducted in oven-dried glassware using a standard Schlenk line under an inert atmosphere of dry nitrogen.

General instrumentation

^{1}H and ^{13}C NMR spectra of the monomers and precursors were recorded at room temperature on a Jeol JNM-ECS 400 spectrometer (400 MHz ^{1}H, 100 MHz ^{13}C) or Bruker Avance 500 (500 MHz ^{1}H, 125 MHz ^{13}C) spectrometer with tetramethylsilane as the internal reference; chemical shifts (δ) are given in parts per million (ppm). Spectra were processed using MestReNova v5 and referenced to residual protonated solvent signals ($CDCl_3$: ^{1}H 7.26 ppm, ^{13}C 77.16 ppm). Thermogravimetric analysis (TGA) was performed under nitrogen on a Mettler Toledo TGA/SDTA 851 thermogravimetric analyzer at a heating rate of 10 °C min^{-1}.UV–vis–absorption spectra were recorded on an Agilent Cary–60 UV–vis spectrophotometer. Solid-state UV-vis spectra were recorded by drop-casting the compounds from dichloromethane solution on ITO glass plates and then drying the films under vacuum. Cyclic voltammetry was performed on a computer-controlled Princeton Applied Research 263A electrochemical workstation using a three-electrode arrangement. A Pt wire was used as the counter electrode, a platinum electrode as the working electrode and Ag/AgCl was used as the reference electrode. Ferrocene was used as an internal standard. $TBAPF_6$ (0.1 M) dissolved in dry DCM was used as the supporting electrolyte. The half-wave potential of the ferrocene/ferrocenium couple was calculated to be 0.36 V. All electrochemical experiments were performed under a nitrogen atmosphere. DFT calculation was performed using Gaussian 09 program[1] with B3LYP functional and the 6-31G(d) basis set. Fourier transform infrared spectroscopy (FTIR) spectra were recorded in the range of 4000-400 cm^{-1} using the KBR pellet technique on a Perkin-Elmer RX1 IR Spectrometer.

Synthesis of precursors and azulene-BODIPY triads

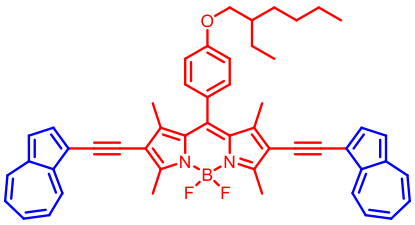
2-bromoazulene (**2**), 6-bromoazulene (**3**), 1-iodoazulene (**1**) and 1,3-diiodoazulene (**4**) was synthesized starting from tropolone by following the procedures reported in literature.[2] Ethynyl-BODIPY derivatives **7** and **8** were synthesized from 4-hydroxy benzaldehyde by following the literature method.[3]

General procedure for Sonogashira coupling of bromo azulenes with ethynyl substituted BODIPY.

An oven-dried three-neck round-bottomed flask fitted with a reflux condenser is flushed with N_2 gas for few minutes, and then it is charged with bromoazulene (1 equivalent), $Pd(PPh_3)_2Cl_2$ (5 mol%) and CuI (10 mol%). A separate single neck round-bottomed flask fitted with a rubber septum is charged with 5 mL dry toluene and 5 mL dry triethylamine. This mixture is purged with N_2 for 10 minutes and then transferred to the three-necked round-bottomed flask using a metal syringe. The three-necked round-bottomed flask is further flushed with N_2 for 10 minutes. In a single-neck round-bottomed flask is taken ethynyl substituted BODPIY (0.5 equivalents, with respect to bromoazulene) and this is followed by addition of 5 mL of toluene to it. This round-bottomed flask is flushed with N_2, and then the solvent mixture is transferred to the three-necked round-bottomed flask, and the temperature of the oil bath is raised to 65 ^oC. After addition of acetylene compound, an immediate change of colour is observed in the reaction mixture. The progress of the reaction was monitored by thin-layer chromatography. The reaction was completed in less than 1 hour, and prolonged heating led to decomposition of the products formed. After the completion of the reaction, the mixture was allowed to cool to room temperature, and then the contents were transferred to single-necked round-bottomed flask, and the solvents evaporated using rotavapor. Further purification of the compound was done by column chromatography using dicholoromethane/hexane mixture. The solid product obtained after column chromatography was further washed with methanol and then dried under vacuum. All the products were obtained in more than 70% yield.

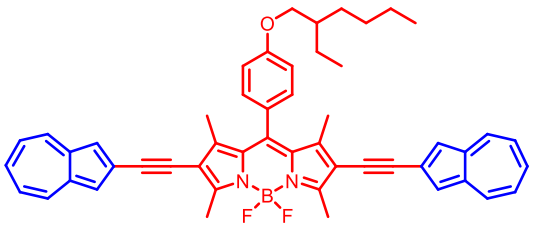
** For the synthesis of compound **D**, 1 equivalent of 1,3-diiodoazulene (**4**) was used with and 2 equivalents of the BODIPY counterpart (**7**).

Purification procedure and characterization



A (1AZBDP1AZ)

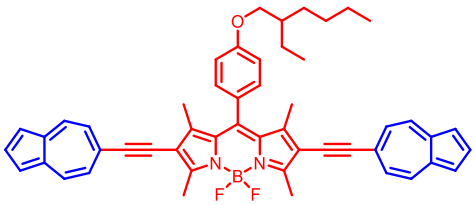
Reaction time: 30 minutes; Purification by column chromatography (silica gel, 35% DCM/Hexane) first and then the obtained solid is washed with methanol; Yield: 72%; dark green solid with magenta metallic lustre; Melting point: > 300 ^{o}C; ^{1}H NMR (400 MHz, Jeol, $CDCl_3$): δ 0.84-0.99 (m, 6H); 1.34-1.80 (m, 15H); 2.82 (s, 6H); 3.94 (d, 2H, J = 5 Hz); 7.06-7.26 (m, 10 H); 7.63 (t, 2H, J = 10 Hz); 7.97 (d, 2H, J = 5 Hz); 8.28 (d, 2H, J = 10 Hz); 8.53 (d, 2H, J = 10 Hz); ^{13}C NMR (100 MHz, Jeol, $CDCl_3$): δ. 11.32, 13.96, 14.01, 14.24, 23.13, 24.05, 29.31, 30.62, 39.58, 71.10, 86.37, 92.94, 111.06, 115.47, 117.14, 117.95, 124.08, 124.77, 126.57, 129.39, 131.96, 136.4, 137.32, 138.80, 139.30, 140.89, 141.61, 142.37, 142.97, 158.12, 160.43. HRMS, $(M+Na)^+$: m/z calculated for $(C_{51}H_{47}BF_2N_2ONa)^+$: 775.3647, found: 775.3628. IR (KBr pellet) ν^{-1}: 2954, 2922, 2871, 2855, 2187, 1610, 1530, 1472, 1395, 1326, 1308, 1246, 1221, 1212, 1186, 1089, 1007, 835, 767, 736, 710, 585, 529 cm^{-1}, Analysis calculated for $C_{51}H_{47}BF_2N_2O$: C, 81.38; H, 6.29; B, 1.44; F, 5.05; N, 3.72; O, 2.13. Found: C, 81.33; H, 6.20; N, 3.68.



B (2AzBDP2Az)

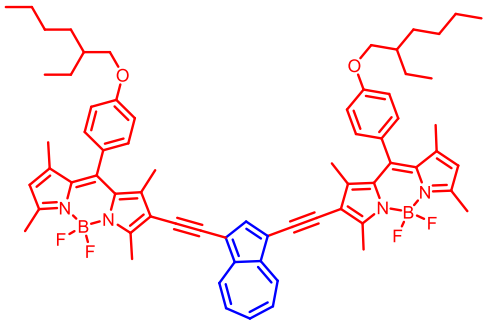
Reaction time: 45 minutes; Purification by column chromatography (silica gel, 30% DCM/Hexane) first and then the obtained solid is washed with methanol; Yield: 72%; dark magenta solid with metallic lustre; Melting point: > 300 ^{o}C; ^{1}H NMR (400 MHz, Jeol, $CDCl_3$): δ 0.93-1.00 (m, 6H); 1.37-1.39 (m, 4H); 1.45-1.57 (m, 4H); 1.67 (s, 6H); 1.79-1.82 (m, 1H); 2.79 (s, 6H); 3.94 (d, 2H, J = 4 Hz); 7.07 (d, 2H, J = 8 Hz); 7.15-7.18 (m, 6H); 7.41 (s, 4H); 7.53 (t, 2H, J = 4 Hz); 8.22 (d, 4H, J = 8 Hz); ^{13}C NMR (100 MHz, Jeol, $CDCl_3$): δ11.33, 13.91, 14.26,

23.21, 24.06, 29.32, 29.86, 30.73, 39.59, 71.14, 88.55, 95.33, 115.58, 116.68, 120.39, 124.23, 129.28, 130.76, 136.35, 140.52, 142.98, 144.44, 159.10, 160.53. HRMS $(M+H)^+$: m/z calculated for $(C_{51}H_{48}BF_2N_2O)^+$: 753.3828, found: 753.3865; IR (KBr pellet) ν^{-1}: 2957, 2922, 2871, 2853, 2189, 1609, 1535, 1482, 1395, 1328, 1309, 1260, 1245, 1222, 1209, 1173, 1071, 1009, 890, 802, 764, 724, 705, 587, 570 cm^{-1}, Analysis calculated for $C_{51}H_{47}BF_2N_2O$: C, 81.38; H, 6.29; B, 1.44; F, 5.05; N, 3.72; O, 2.13. Found: C, 81.29; H, 6.24; N, 3.67.



C (6AzBDP6Az)

Reaction time: 45 minutes; Purification by column chromatography (silica gel, 30% DCM/Hexane) first and then the obtained solid is washed with methanol; Yield: 75%; dark magenta solid with metallic lustre; Melting point: > 300 ^oC; ^1H NMR (400 MHz, Jeol, $CDCl_3$): δ 0.93-1.01 (m, 6H); 1.34-1.39 (m, 4H); 1.46-1.57 (m, 4H); 1.66 (s, 6H); 1.78-1.82 (m, 1H); 2.78 (s, 6H); 3.95 (d, 2H, J = 4 Hz), 7.09 (d, 2H, J = 8 Hz); 7.19 (d, 2H, J = 8 Hz); 7.31-7.37 (m, 8H); 7.85 (t, 2H, J = 4 Hz); 8.21 (d, 4H, J = 8 Hz). ^{13}C NMR (100 MHz, Jeol, $CDCl_3$): δ 11.33, 13.94, 14.26, 23.20, 24.05, 29.31, 30.71, 39.58, 71.15, 84.95, 101.85, 115.62, 116.02, 119.24, 125.58, 126.04, 129.20, 132.15, 135.13, 137.51, 143.47, 144.93, 158.95, 160.62. HRMS $(M+H)^+$: m/z calculated for $(C_{51}H_{48}BF_2N_2O)^+$: 753.3828, found: 753.3811; (IR (KBr pellet) ν^{-1}: 2995, 2924, 2870, 2857, 2188, 1609, 1528, 1443, 1393, 1318, 1270, 1246, 1219, 1180, 1125, 1067, 1011, 837, 768, 749, 705, 592, 568, 468 cm^{-1}, Analysis calculated for $C_{51}H_{47}BF_2N_2O$: C, 81.38; H, 6.29; B, 1.44; F, 5.05; N, 3.72; O, 2.13. Found: C, 81.35; H, 6.22; N, 3.70.



D (BDPAzBDP)

Reaction time: 30 minutes; Purification by column chromatography (silica gel, 80% DCM/Hexane) first and then the obtained solid is washed with methanol; Yield: 85%; dark magenta solid with metallic lustre; Melting point: 272 ^{o}C; ^{1}H NMR (100 MHz, Jeol, $CDCl_3$): δ 0.91-0.98 (m, 12H); 1.31-1.35 (m, 6H); 1.50 (6H, s); 1.52-1.55 (10H, m); 1.64-1.79 (m, 8H); 2.58 (s, 6H); 2.77 (s, 6H); 3.91 (d, 4H, J = 4 Hz); 6.01 (s, 2H); 7.03 (d, 4H, J = 8 Hz); 7.17-7.23 (m, 6H); 7.62 (t, 1H, J = 8 Hz); 8.01 (s, 1H); 8.44 (d, 2H, J = 8 Hz); ^{13}C NMR (100 MHz, Jeol, $CDCl_3$): δ 11.51, 13.59, 13.70, 14.09, 23.03, 23.41, 23.88, 29.15, 29.69, 30.55, 39.42, 70.92, 86.60, 91.09, 111.07, 115.26, 115.84, 121.80, 125.03, 125.33, 126.43, 129.13, 130.89, 132.81, 135.19, 136.83, 139.91, 141.01, 141.36, 142.19, 144.44, 156.41, 156.99, 160.15. HRMS $(M+Na)^+$: m/z calculated for $(C_{68}H_{74}B_2F_4N_4O_2Na)^+$: 1099.5832, found: 1099.8521, IR (KBr pellet) ν^{-1}: 2957, 2923, 2870, 2854, 2193, 1609, 1539, 1515, 1467, 1402, 1360, 1313, 1246, 1222, 1187, 1163, 1074, 1004, 981, 832, 763, 732, 704, 651, 566, 555, 487, 434 cm^{-1}, Analysis calculated for $C_{68}H_{74}B_2F_4N_4O_2$: C, 75.84; H, 6.93; B, 2.01; F, 7.06; N, 5.20; O, 2.97. Found: C, 75.79; H, 6.88; N, 5.14.

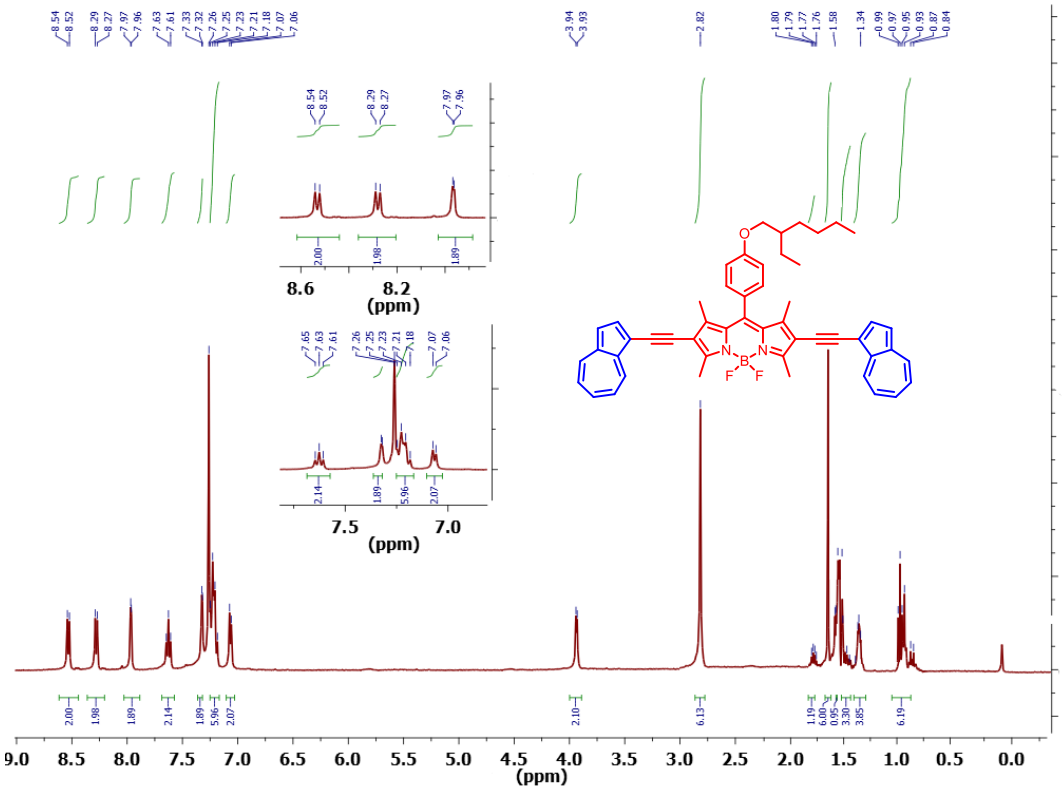


Figure S1: ^{1}H NMR Spectra of **A** (**1AzBDP1Az)**

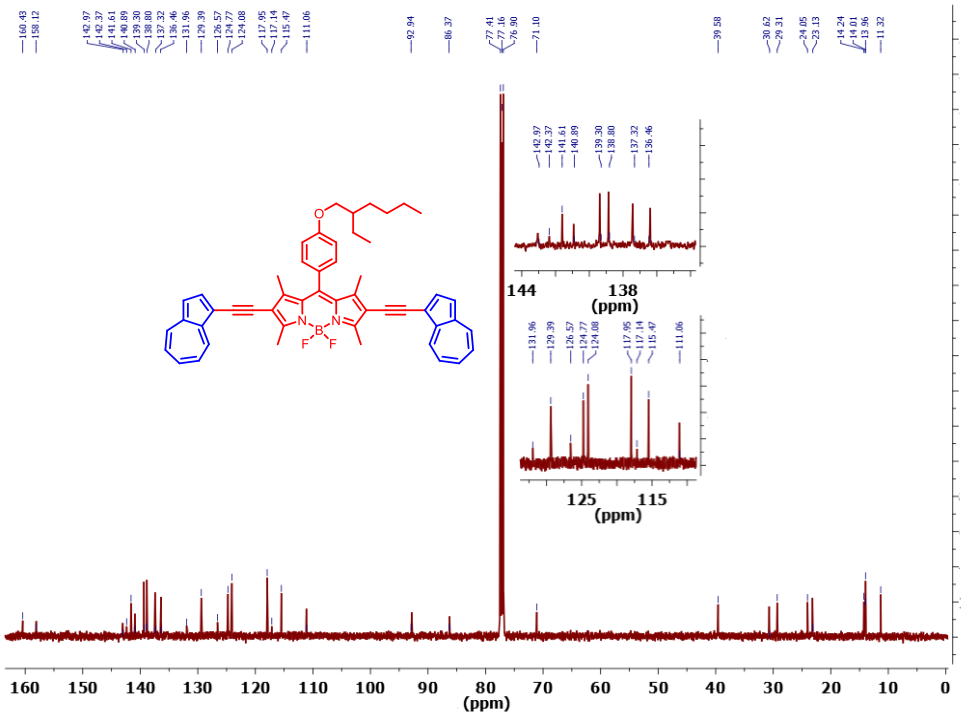


Figure S2: ^{13}C NMR Spectra of **A** (**1AzBDP1Az)**

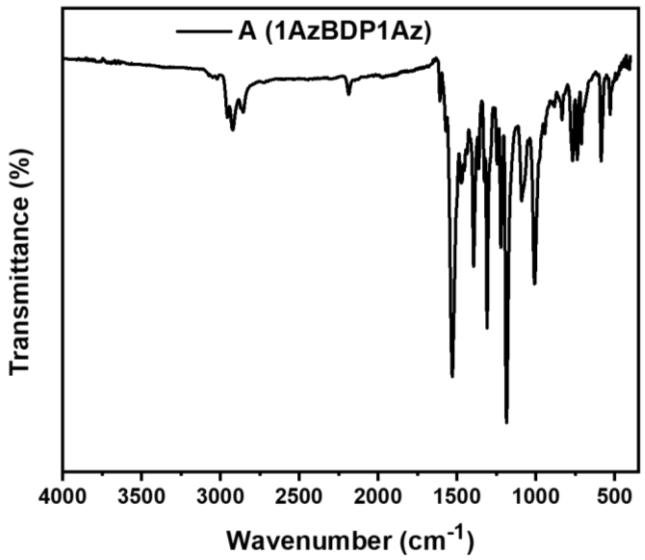


Figure S3: IR Spectra of **A** (**1AzBDP1Az)**

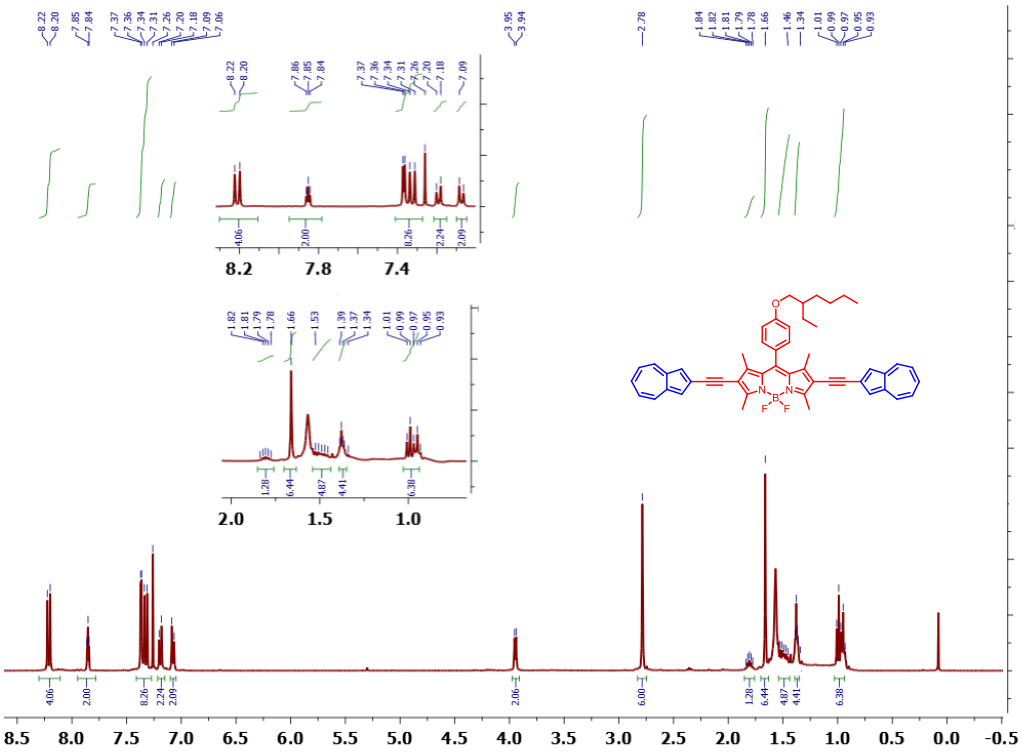


Figure S4: ^{1}H NMR Spectra of **B** (**2AzBDP2Az)**

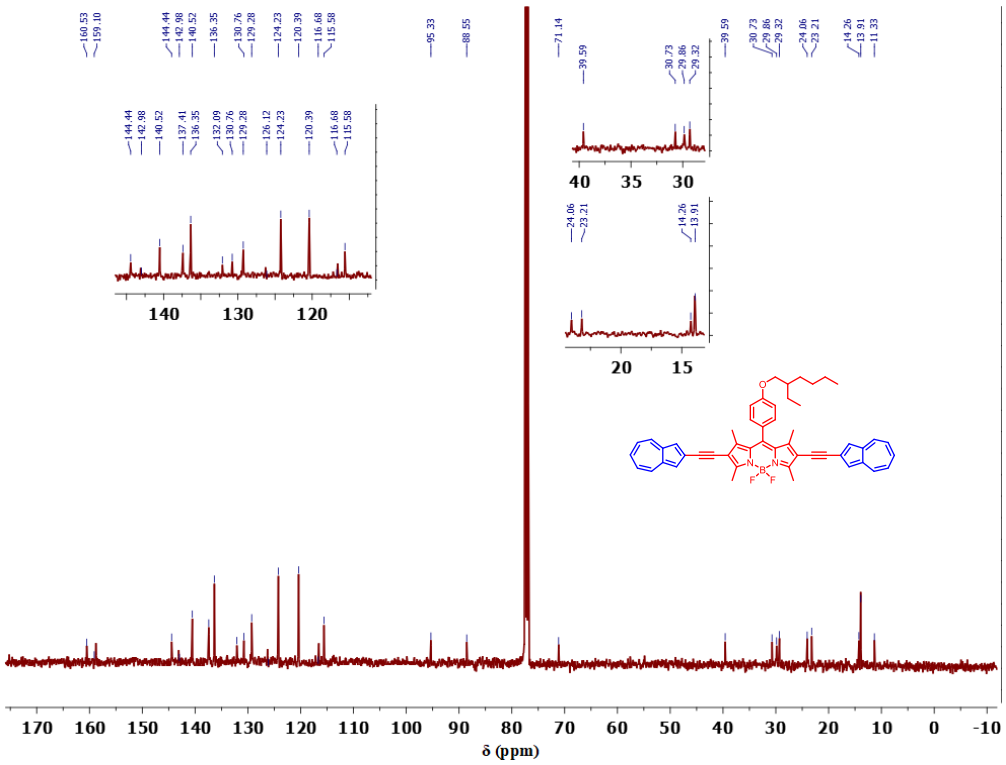


Figure S5: ^{13}C NMR Spectra of **B** (**2AzBDP2Az)**

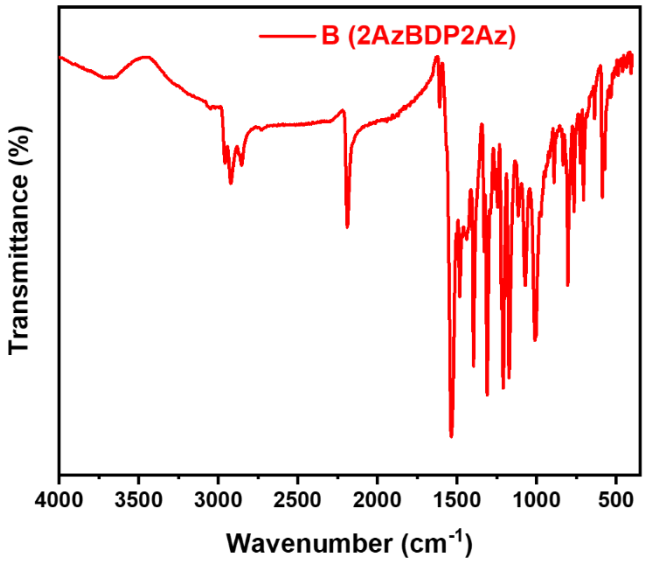


Figure S6: IR Spectra of **B** (**2AzBDP2Az)**

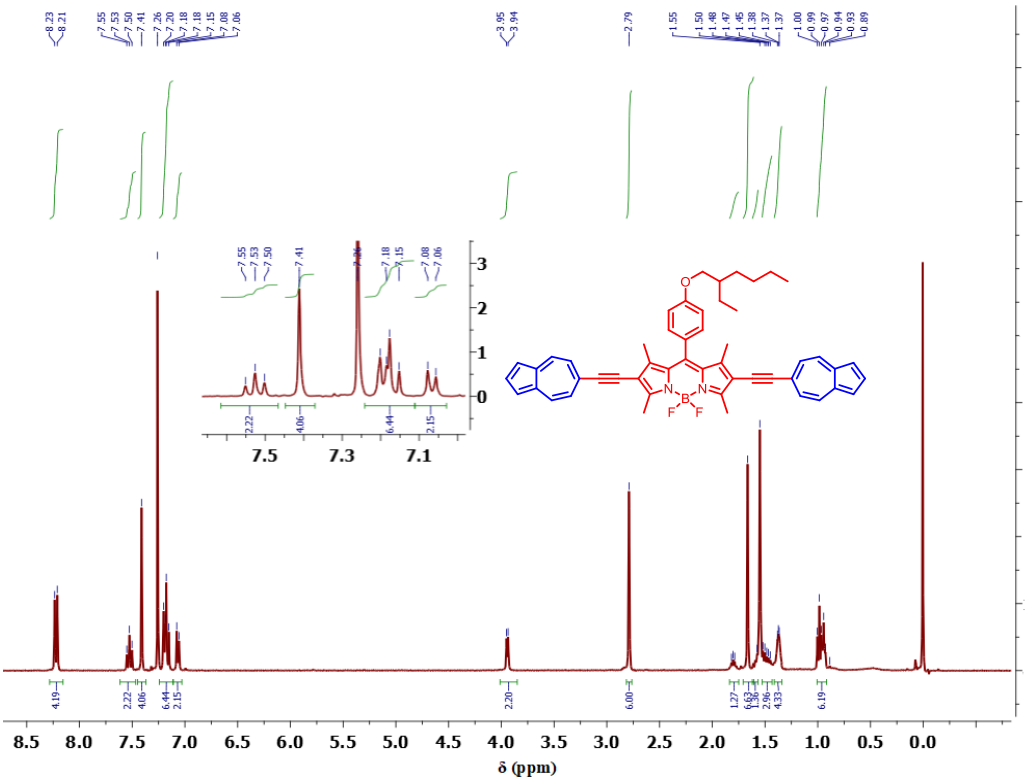


Figure S7: ^{1}H NMR Spectra of **C** (**6AzBDP6Az)**

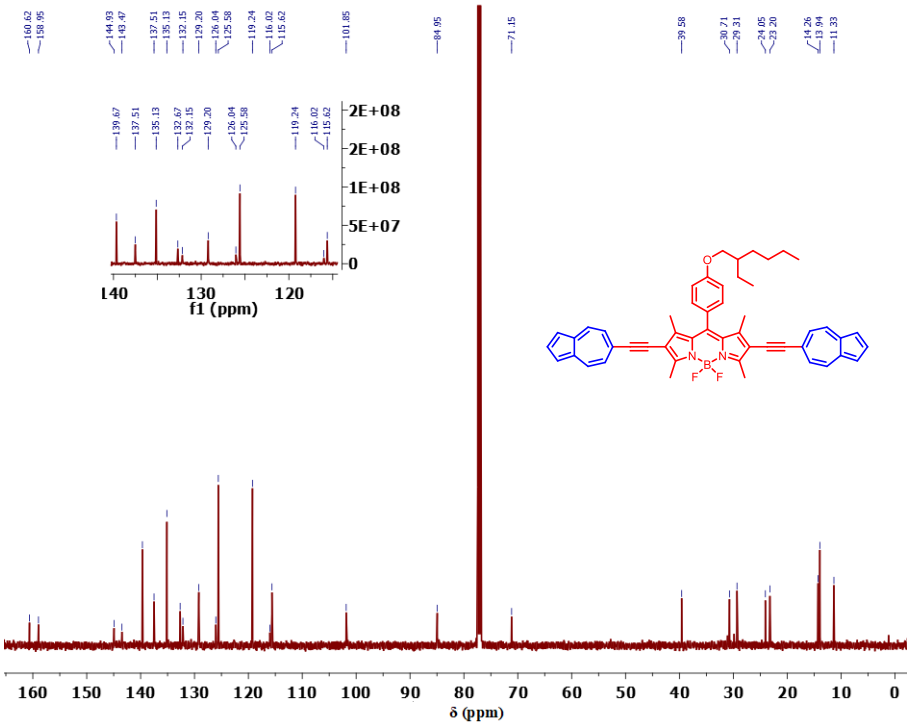


Figure S8: ^{13}C NMR Spectra of **C** (**6AzBDP6Az)**

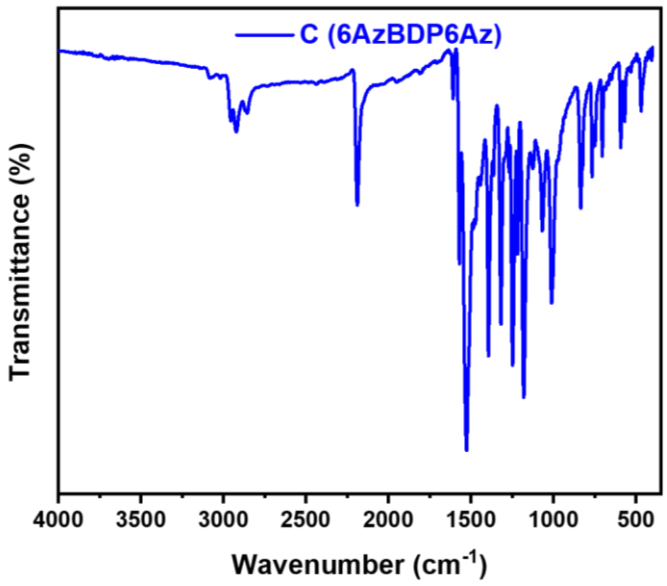


Figure S9: IR Spectra of **C** (**6AzBDP6Az)**

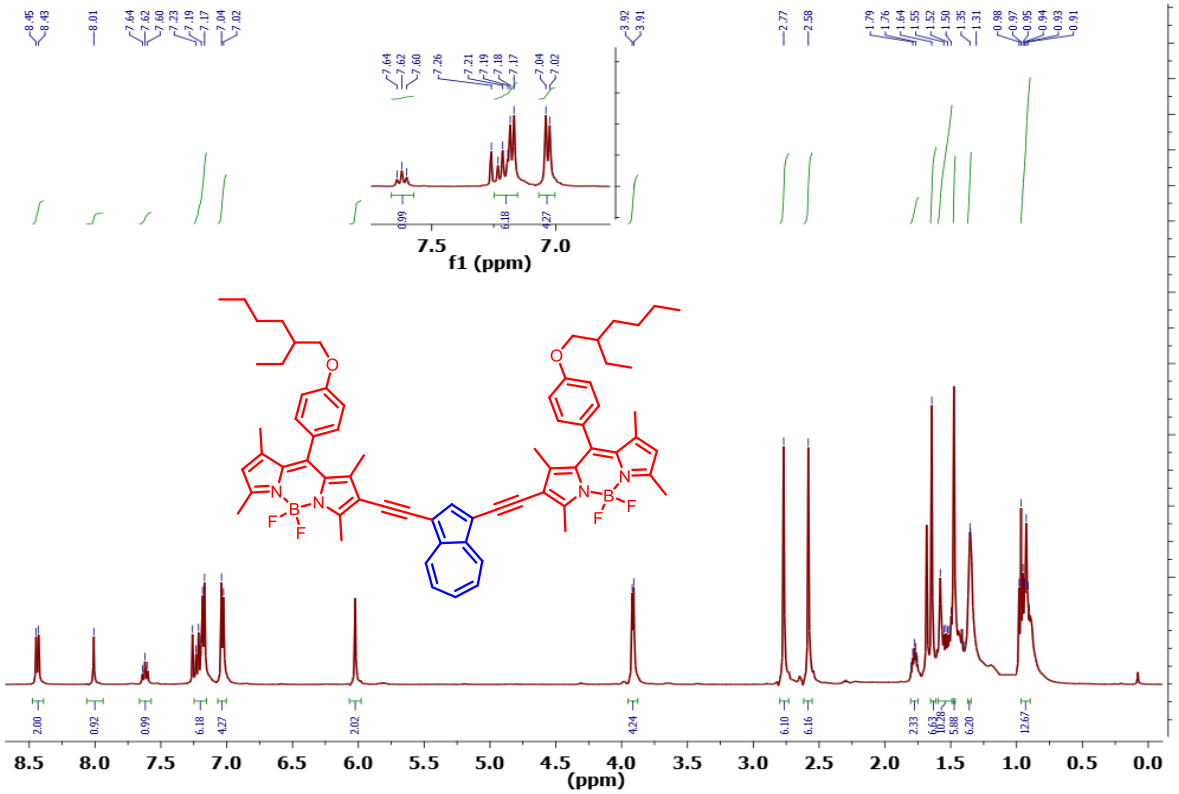


Figure S10: ^{1}H NMR Spectra of **D** (**BDPAzBDP**)

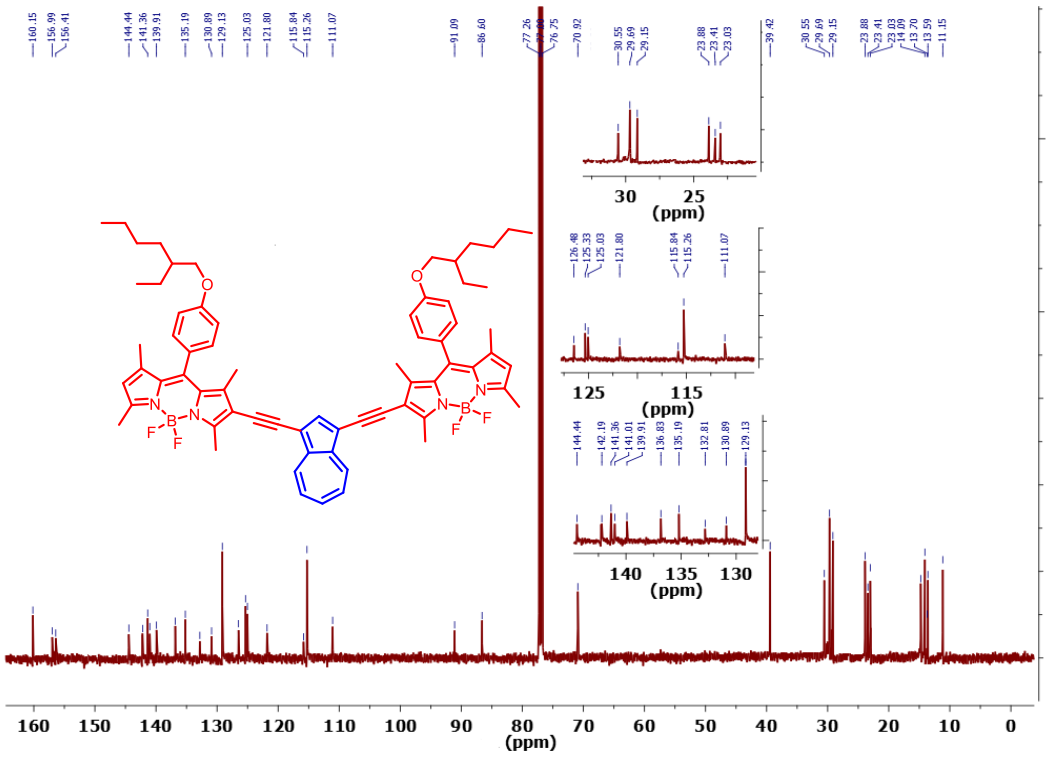


Figure S11: ^{13}C NMR Spectra of **D** (**BDPAzBDP**)

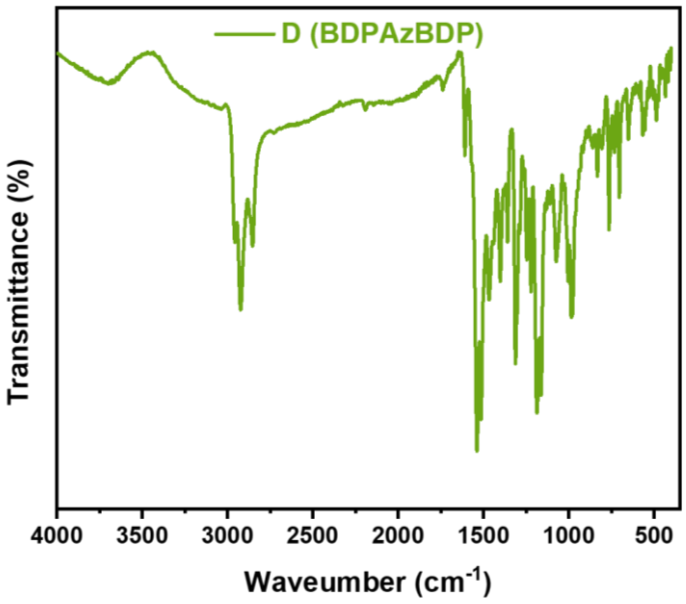
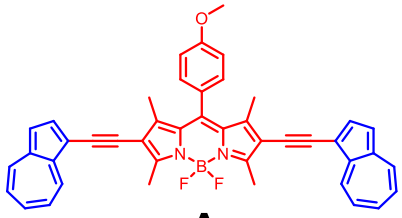
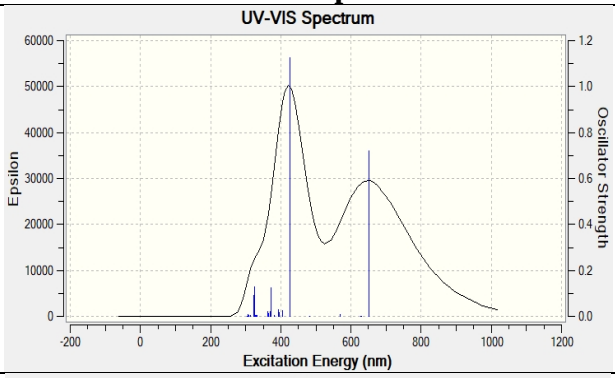
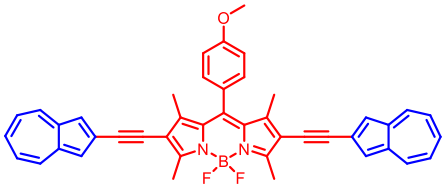
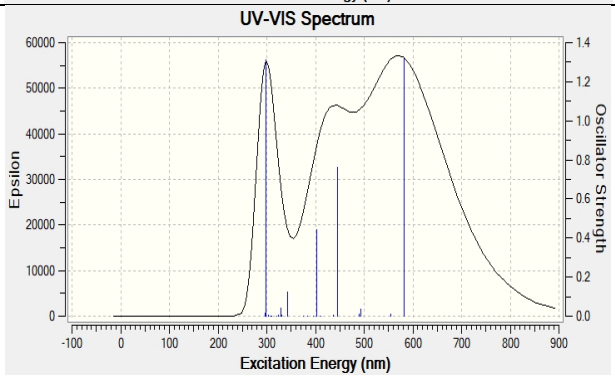
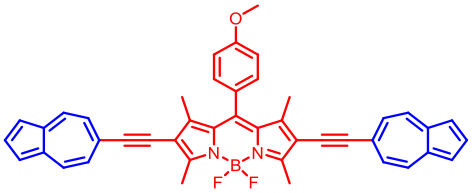
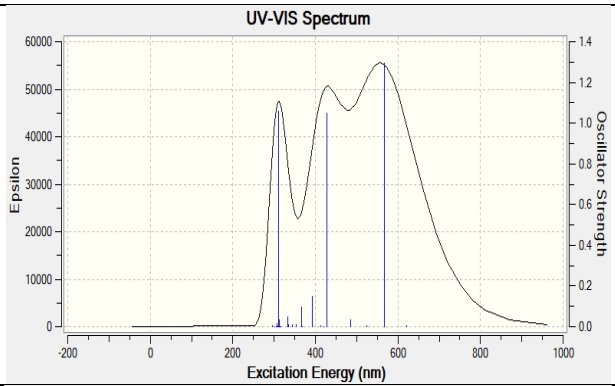
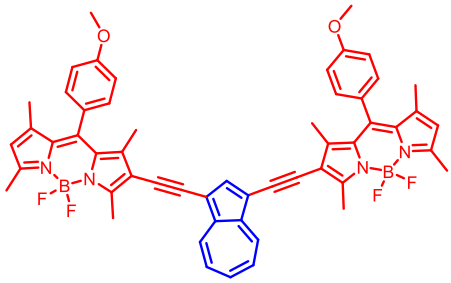
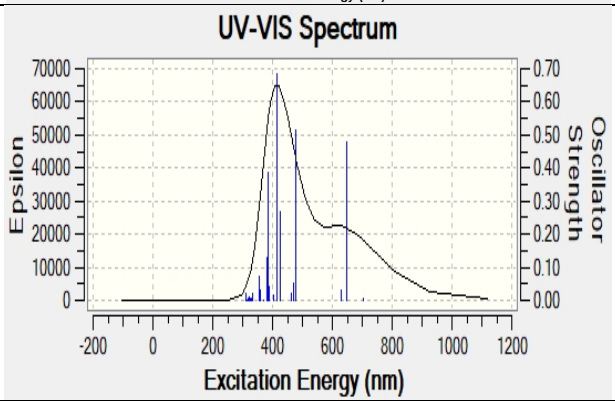


Figure S12: IR Spectra of **D** (**BDPAzBDP**)

Table S1: TD-DFT spectra of azulene-BODIPY triads

Compound	TD-DFT spectra
 **A**	
 **B**	
 **C**	
 **D**	

References

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision E.01, Gaussian, Inc.: Wallingford CT, 2009.

[2] (a) J. Dubovik, A. Bredihhin, *Synthesis*, 2015**,** *47*, 2663–2669. (b) R. N. McDonald, Richmond, J. R. Curtis, H. E. Petty, T. L. Hoskinsl, *J. Org. Chem.*, 1976, **41**, 1811-1821. (c) T. Nozoe, S. Matsumura, Y. Murase, S. Seto, *Bull. Chem. Soc. Jpn*., 1962, **35**, 1179-1188.

[3] (a) C. P. Sen, R. G. Shrestha, L. K. Shrestha, K. Ariga, S. Valiyaveettil, *Chem.Eur.J.*, 2015, **21**, 17344-17354. (b) C. Lambert, T. Scherpf, H. Ceymann, A. Schmiedel, M. Holzapfel, *J. Am. Chem. Soc.*, 2015, **137**, 3547-3557.

Coordinates for optimised geometries

A (1AzBDP1Az)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.081238	3.923605	-0.791227
2	6	0	-0.076964	2.528058	-0.870636
3	6	0	-0.003412	1.735076	0.277122
4	6	0	0.064476	2.372988	1.526680
5	6	0	0.057227	3.758609	1.621448
6	6	0	-0.015187	4.545498	0.461358
7	8	0	-0.014526	5.893688	0.660307
8	6	0	-0.089906	6.742154	-0.475506
9	6	0	0.000258	0.244000	0.175991
10	6	0	1.226882	-0.441728	0.126486
11	7	0	1.250799	-1.841515	0.028123
12	5	0	0.006153	-2.777772	-0.058195

13	7	0	-1.242150	-1.845541	0.014606
14	6	0	-1.223719	-0.446700	0.126861
15	6	0	-2.513175	-2.267181	-0.013615
16	6	0	-3.381825	-1.139465	0.084064
17	6	0	-2.575770	0.009524	0.176041
18	6	0	2.577220	0.021803	0.151207
19	6	0	3.387839	-1.124600	0.068540
20	6	0	2.523365	-2.257545	-0.006814
21	9	0	0.001114	-3.662692	1.015210
22	9	0	0.014633	-3.467282	-1.266998
23	6	0	-3.115199	1.401138	0.306458
24	6	0	-2.896447	-3.703751	-0.127710
25	6	0	3.109286	1.419329	0.243243
26	6	0	2.912130	-3.693259	-0.112605
27	6	0	-4.792372	-1.207367	0.084361
28	6	0	4.798456	-1.188609	0.055796
29	6	0	-6.010316	-1.289349	0.082335
30	6	0	6.016265	-1.271918	0.043439
31	6	0	-7.416238	-1.394511	0.084364
32	6	0	7.421633	-1.383296	0.033779
33	6	0	-8.341301	-0.332498	-0.118435
34	6	0	-9.705112	-0.926974	-0.021670
35	6	0	-9.532597	-2.303862	0.228014
36	6	0	-8.167882	-2.581735	0.291471
37	6	0	8.166901	-2.583551	0.180535
38	6	0	9.532962	-2.311321	0.123424
39	6	0	9.712970	-0.925293	-0.062164
40	6	0	8.352406	-0.318446	-0.122929
41	6	0	-8.008394	0.993017	-0.364776
42	6	0	-8.854125	2.087968	-0.572827
43	6	0	-10.251862	2.121076	-0.584248
44	6	0	-11.172075	1.085624	-0.397865
45	6	0	-10.923843	-0.268862	-0.149670
46	6	0	10.935238	-0.269614	-0.166831
47	6	0	11.191060	1.093394	-0.352949
48	6	0	10.276685	2.142405	-0.483685
49	6	0	8.878888	2.117798	-0.463761
50	6	0	8.027195	1.019575	-0.302704
51	1	0	-0.136013	4.506559	-1.703439
52	1	0	-0.129970	2.052404	-1.846282
53	1	0	0.121335	1.773594	2.431293
54	1	0	0.107253	4.257405	2.584250
55	1	0	-0.078151	7.762062	-0.087463
56	1	0	0.769129	6.598371	-1.143937
57	1	0	-1.017591	6.579050	-1.039549
58	1	0	-4.201758	1.357948	0.425967
59	1	0	-2.695917	1.928271	1.169033
60	1	0	-2.894519	2.014244	-0.574949
61	1	0	-2.462806	-4.143697	-1.031848
62	1	0	-2.501744	-4.272922	0.720786
63	1	0	-3.983653	-3.801128	-0.158294
64	1	0	2.806806	1.916503	1.170994
65	1	0	4.202417	1.393185	0.213551
66	1	0	2.757988	2.050405	-0.580179

67	1	0	3.999917	-3.788061	-0.123105
68	1	0	2.502063	-4.263211	0.727818
69	1	0	2.497371	-4.134239	-1.025271
70	1	0	-10.337003	-3.019200	0.350901
71	1	0	-7.725994	-3.554823	0.473111
72	1	0	7.719766	-3.561509	0.317778
73	1	0	10.333378	-3.036633	0.207894
74	1	0	-6.939655	1.200510	-0.401539
75	1	0	-8.357508	3.039437	-0.748763
76	1	0	-10.689891	3.101188	-0.767089
77	1	0	-12.220525	1.369183	-0.454968
78	1	0	-11.806247	-0.899199	-0.041249
79	1	0	11.814033	-0.910008	-0.093760
80	1	0	12.241017	1.372530	-0.403804
81	1	0	10.720079	3.127252	-0.622953
82	1	0	8.387486	3.079765	-0.590264
83	1	0	6.959778	1.236044	-0.321486

B (2AZBDP2AZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000879	4.435385	-1.057471
2	6	0	-0.000698	3.038042	-1.087900
3	6	0	-0.000357	2.286247	0.089734
4	6	0	-0.000221	2.966879	1.318324
5	6	0	-0.000463	4.354961	1.363625
6	6	0	-0.000773	5.100836	0.174483
7	8	0	-0.000939	6.454311	0.325877
8	6	0	-0.001369	7.263688	-0.841257
9	6	0	-0.000112	0.792722	0.041182
10	6	0	1.224722	0.102691	0.017913
11	7	0	1.246769	-1.300839	-0.036377
12	5	0	0.000406	-2.238512	-0.084477
13	7	0	-1.246282	-1.301205	-0.038061
14	6	0	-1.224704	0.102334	0.016259
15	6	0	-2.516917	-1.720999	-0.051684
16	6	0	-3.382554	-0.586946	-0.004763
17	6	0	-2.574791	0.564500	0.037658
18	6	0	2.574659	0.565255	0.040731
19	6	0	3.382795	-0.585958	-0.000785
20	6	0	2.517542	-1.720262	-0.048602
21	9	0	-0.000192	-3.083759	1.019609
22	9	0	0.001284	-2.968384	-1.268228
23	6	0	-3.112875	1.961162	0.095040
24	6	0	-2.904545	-3.159521	-0.108153
25	6	0	3.112273	1.962077	0.098573
26	6	0	2.905651	-3.158677	-0.104590
27	6	0	-4.791336	-0.646716	-0.001622

28	6	0	4.791604	-0.645318	0.003750
29	6	0	-6.009862	-0.708928	0.001987
30	6	0	6.010151	-0.707056	0.007790
31	6	0	-7.418390	-0.790998	0.009329
32	6	0	7.418668	-0.789666	0.013083
33	6	0	-8.171469	-1.992107	-0.040938
34	6	0	-9.532088	-1.671196	-0.013606
35	6	0	-9.624003	-0.177188	0.057743
36	6	0	-8.312428	0.308696	0.068931
37	6	0	8.171187	-1.991135	-0.036977
38	6	0	9.531974	-1.670730	-0.012286
39	6	0	9.624609	-0.176677	0.057197
40	6	0	8.313244	0.309743	0.069971
41	6	0	-10.587649	-2.584024	-0.046599
42	6	0	-11.961898	-2.340069	-0.021663
43	6	0	-12.633425	-1.114507	0.042587
44	6	0	-12.117970	0.184705	0.098459
45	6	0	-10.784132	0.597542	0.104979
46	6	0	10.587109	-2.584027	-0.045946
47	6	0	11.961495	-2.340597	-0.023587
48	6	0	12.633627	-1.115223	0.038058
49	6	0	12.118786	0.184270	0.093257
50	6	0	10.785123	0.597646	0.101568
51	1	0	-0.001110	4.986387	-1.990874
52	1	0	-0.000800	2.528918	-2.047993
53	1	0	0.000062	2.400141	2.245505
54	1	0	-0.000401	4.887250	2.309600
55	1	0	-0.001500	8.296132	-0.488004
56	1	0	0.893663	7.089121	-1.452443
57	1	0	-0.896606	7.088748	-1.452038
58	1	0	-4.205957	1.928662	0.099651
59	1	0	-2.781128	2.493072	0.992946
60	1	0	-2.790476	2.561654	-0.762205
61	1	0	-3.992201	-3.255502	-0.114007
62	1	0	-2.489682	-3.630857	-1.005429
63	1	0	-2.493167	-3.699401	0.751221
64	1	0	2.780695	2.493433	0.996875
65	1	0	4.205367	1.929962	0.102808
66	1	0	2.789329	2.562876	-0.758245
67	1	0	2.493873	-3.698527	0.754625
68	1	0	2.491501	-3.630300	-1.002033
69	1	0	3.993339	-3.254328	-0.109675
70	1	0	-7.754471	-2.990115	-0.091456
71	1	0	-8.020683	1.350422	0.116110
72	1	0	7.753710	-2.989039	-0.085633
73	1	0	8.021979	1.351642	0.116373
74	1	0	-10.293728	-3.632119	-0.098624
75	1	0	-12.596530	-3.222918	-0.056948
76	1	0	-13.720152	-1.182011	0.050117
77	1	0	-12.856556	0.982187	0.142999
78	1	0	-10.622219	1.674123	0.154079
79	1	0	10.292676	-3.632064	-0.096243
80	1	0	12.595722	-3.223738	-0.058863
81	1	0	13.720338	-1.183155	0.043833

82	1	0	12.857774	0.981502	0.135591
83	1	0	10.623715	1.674349	0.149677

C (6AZBDP6AZ)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000551	4.426784	-1.056276
2	6	0	0.000555	3.029462	-1.085189
3	6	0	-0.000012	2.279271	0.093559
4	6	0	-0.000560	2.961093	1.321599
5	6	0	-0.000527	4.349144	1.365148
6	6	0	0.000019	5.093849	0.175011
7	8	0	-0.000028	6.446675	0.324936
8	6	0	0.000606	7.256023	-0.842769
9	6	0	-0.000019	0.785825	0.046995
10	6	0	1.224458	0.095009	0.023794
11	7	0	1.246560	-1.308591	-0.028437
12	5	0	-0.000021	-2.246868	-0.073745
13	7	0	-1.246597	-1.308600	-0.028173
14	6	0	-1.224498	0.095004	0.023949
15	6	0	-2.516766	-1.728584	-0.040861
16	6	0	-3.381841	-0.593905	0.004447
17	6	0	-2.574215	0.557838	0.044982
18	6	0	2.574175	0.557842	0.044905
19	6	0	3.381803	-0.593893	0.004239
20	6	0	2.516729	-1.728572	-0.041169
21	6	0	-4.790892	-0.652809	0.007272
22	6	0	4.790854	-0.652801	0.007102
23	9	0	0.000107	-3.088818	1.032102
24	9	0	-0.000149	-2.977874	-1.256082
25	6	0	-6.008901	-0.713363	0.009468
26	6	0	6.008863	-0.713362	0.009349
27	6	0	3.110151	1.955224	0.100384
28	6	0	2.902798	-3.167586	-0.095345
29	6	0	-3.110195	1.955227	0.100209
30	6	0	-2.902834	-3.167602	-0.094960
31	6	0	-7.431693	-0.795830	0.012138
32	6	0	7.431653	-0.795852	0.012084
33	6	0	-7.979063	-2.099397	-0.047359
34	6	0	-9.312913	-2.497336	-0.060136
35	6	0	-10.474174	-1.727053	-0.018198
36	6	0	-10.563645	-0.236242	0.053854
37	6	0	-9.502769	0.667647	0.092042
38	6	0	-8.130797	0.432899	0.074059
39	6	0	8.130780	0.432885	0.073576
40	6	0	9.502756	0.667613	0.091519
41	6	0	10.563616	-0.236309	0.053680
42	6	0	10.474116	-1.727144	-0.017843

43	6	0	9.312841	-2.497420	-0.059538
44	6	0	7.978999	-2.099451	-0.046926
45	6	0	-11.793191	-2.209148	-0.035422
46	6	0	-12.668314	-1.110898	0.021348
47	6	0	-11.930865	0.084282	0.075526
48	6	0	11.930843	0.084193	0.075278
49	6	0	12.668267	-1.111021	0.021547
50	6	0	11.793123	-2.209274	-0.034857
51	1	0	0.000962	4.976752	-1.990257
52	1	0	0.000981	2.519419	-2.044828
53	1	0	-0.000995	2.395619	2.249579
54	1	0	-0.000926	4.882548	2.310465
55	1	0	0.896124	7.080886	-1.452927
56	1	0	-0.894362	7.081051	-1.453784
57	1	0	2.777098	2.487547	0.997439
58	1	0	4.203251	1.925688	0.105247
59	1	0	2.786586	2.553646	-0.757732
60	1	0	3.990170	-3.266177	-0.100707
61	1	0	2.490482	-3.705524	0.764738
62	1	0	2.487711	-3.639635	-0.992078
63	1	0	-4.203301	1.925737	0.103873
64	1	0	-2.778138	2.487293	0.997794
65	1	0	-2.785629	2.553867	-0.757368
66	1	0	-2.487995	-3.639625	-0.991823
67	1	0	-2.490273	-3.705556	0.764993
68	1	0	-3.990207	-3.266203	-0.100029
69	1	0	-7.246623	-2.900643	-0.088834
70	1	0	-9.472384	-3.574335	-0.110733
71	1	0	-9.790394	1.717731	0.143788
72	1	0	-7.499266	1.316027	0.113563
73	1	0	7.499266	1.316041	0.112732
74	1	0	9.790399	1.717711	0.142898
75	1	0	9.472294	-3.574439	-0.109746
76	1	0	7.246544	-2.900698	-0.088114
77	1	0	-12.076814	-3.253912	-0.084294
78	1	0	-13.751338	-1.176019	0.023168
79	1	0	-12.337508	1.087547	0.125516
80	1	0	12.337506	1.087467	0.124924
81	1	0	13.751290	-1.176165	0.023423
82	1	0	12.076724	-3.254061	-0.083348
83	1	0	0.000530	8.288369	-0.489523

D (BDPAZBDP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.965027	2.403532	1.999212
2	6	0	-9.413634	1.167356	1.650254
3	6	0	-9.187854	0.823269	0.315078

4	6	0	-9.529575	1.752168	-0.681315
5	6	0	-10.080363	2.983393	-0.349800
6	6	0	-10.302187	3.318952	0.994849
7	8	0	-10.845645	4.548975	1.214847
8	6	0	-11.096665	4.945611	2.554887
9	6	0	-8.599372	-0.502389	-0.044496
10	6	0	-9.447175	-1.605798	-0.232713
11	7	0	-8.919585	-2.858891	-0.568113
12	5	0	-7.413551	-3.194677	-0.767973
13	7	0	-6.636747	-1.861074	-0.528437
14	6	0	-7.205100	-0.623701	-0.189921
15	6	0	-5.306481	-1.726629	-0.605833
16	6	0	-4.956619	-0.374539	-0.314202
17	6	0	-6.148163	0.324817	-0.049943
18	6	0	-10.875430	-1.739094	-0.155404
19	6	0	-11.150908	-3.069621	-0.446267
20	6	0	-9.933419	-3.735937	-0.696188
21	9	0	-7.190941	-3.644538	-2.066287
22	9	0	-7.008890	-4.150520	0.160084
23	6	0	-6.205463	1.779405	0.305044
24	6	0	-4.388935	-2.850906	-0.949608
25	6	0	-11.916441	-0.706114	0.162302
26	6	0	-9.719941	-5.171211	-1.051582
27	6	0	-3.637520	0.130590	-0.300820
28	6	0	-2.488981	0.542562	-0.292177
29	6	0	-1.155592	1.003973	-0.275715
30	6	0	-0.733943	2.362866	-0.378353
31	6	0	0.746984	2.364133	-0.307041
32	6	0	1.159527	1.005206	-0.172032
33	6	0	-0.000927	0.204137	-0.154382
34	6	0	-1.577483	3.455231	-0.525286
35	6	0	-1.248839	4.812045	-0.632063
36	6	0	0.016370	5.405970	-0.613314
37	6	0	1.277773	4.816299	-0.489345
38	6	0	1.597432	3.459921	-0.355303
39	6	0	2.488578	0.542823	-0.071750
40	6	0	3.632287	0.126083	0.014193
41	6	0	10.126325	2.907380	0.477520
42	6	0	9.537238	1.675972	0.778997
43	6	0	9.220456	0.757314	-0.224648
44	6	0	9.507645	1.097628	-1.556788
45	6	0	10.092332	2.317483	-1.871496
46	6	0	10.407203	3.232724	-0.854857
47	8	0	10.978813	4.399342	-1.266156
48	6	0	11.323476	5.364563	-0.283621
49	6	0	8.593920	-0.557953	0.108316
50	6	0	7.191653	-0.663559	0.155620
51	7	0	6.587545	-1.891802	0.463513
52	5	0	7.330840	-3.229355	0.776025
53	7	0	8.850612	-2.912018	0.676428
54	6	0	9.414279	-1.668517	0.364759
55	6	0	9.843038	-3.799794	0.878053
56	6	0	11.082242	-3.150441	0.701398
57	6	0	10.842662	-1.819703	0.380781

58	6	0	6.157400	0.295046	-0.064073
59	6	0	4.942621	-0.389887	0.120722
60	6	0	5.256880	-1.743384	0.445957
61	9	0	6.980201	-4.194825	-0.163458
62	9	0	7.012568	-3.656561	2.062733
63	6	0	11.914851	-0.802953	0.119406
64	6	0	9.588283	-5.229239	1.229317
65	6	0	6.256749	1.746986	-0.420095
66	6	0	4.306331	-2.856745	0.730082
67	1	0	-10.124675	2.636808	3.045670
68	1	0	-9.155417	0.461413	2.435125
69	1	0	-9.362212	1.502931	-1.725679
70	1	0	-10.348367	3.704928	-1.115221
71	1	0	-11.525734	5.947169	2.494086
72	1	0	-11.812220	4.273836	3.046883
73	1	0	-10.171412	4.982619	3.144686
74	1	0	-12.130802	-3.528833	-0.480606
75	1	0	-5.188056	2.171212	0.395199
76	1	0	-6.732073	2.368724	-0.454115
77	1	0	-6.724214	1.953845	1.253069
78	1	0	-4.521361	-3.679584	-0.246389
79	1	0	-4.621142	-3.242368	-1.945871
80	1	0	-3.351453	-2.511070	-0.925763
81	1	0	-11.881061	0.143491	-0.527608
82	1	0	-12.912622	-1.154958	0.096612
83	1	0	-11.796999	-0.294709	1.170423
84	1	0	-10.675353	-5.699784	-1.099680
85	1	0	-9.211280	-5.256583	-2.017733
86	1	0	-9.074917	-5.659040	-0.312919
87	1	0	-0.004679	-0.874969	-0.059944
88	1	0	-2.638979	3.214574	-0.564570
89	1	0	-2.089860	5.492433	-0.743366
90	1	0	0.020023	6.490635	-0.710133
91	1	0	2.123372	5.500016	-0.501223
92	1	0	2.657620	3.223170	-0.277064
93	1	0	10.358458	3.595198	1.282454
94	1	0	9.322918	1.430652	1.815810
95	1	0	9.268319	0.396443	-2.351700
96	1	0	10.316298	2.586272	-2.899058
97	1	0	11.761193	6.202288	-0.829091
98	1	0	10.439909	5.712558	0.267399
99	1	0	12.060699	4.970107	0.427921
100	1	0	12.052043	-3.621231	0.801949
101	1	0	12.898933	-1.271992	0.218034
102	1	0	11.843569	-0.374304	-0.885821
103	1	0	11.868179	0.036802	0.820936
104	1	0	8.996384	-5.299403	2.148027
105	1	0	9.006500	-5.721600	0.442550
106	1	0	10.531549	-5.764074	1.366251
107	1	0	6.818260	1.908827	-1.345846
108	1	0	5.251627	2.157194	-0.554412
109	1	0	6.761515	2.328555	0.359345
110	1	0	3.276633	-2.499416	0.664129
111	1	0	4.456224	-3.676635	0.019726

112	1	0	4.488645	-3.267958	1.728452