Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information-2

Effect of Alkyl Substituents in BODIPYs: A Comparative DFT Computational Investigation

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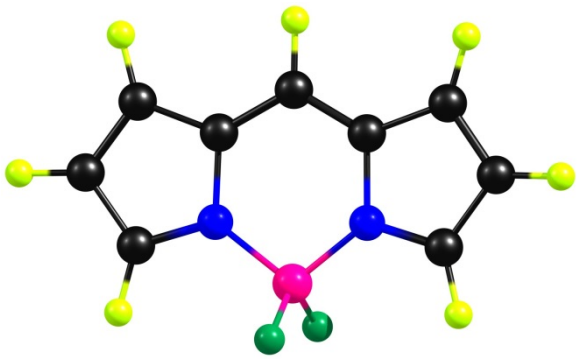

Figure S2-1: DFT B3LYP/6-31G(d) optimised ground-state structure of **BODIPY**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.129105	4.183757	2.060494
2	9	0	5.198934	4.314698	1.049648
3	9	0	5.598052	3.556089	3.170572
4	7	0	6.687936	5.598928	2.466738
5	7	0	7.379793	3.379059	1.542542
6	6	0	5.969459	6.652221	2.877364
7	6	0	6.820486	7.725940	3.222565
8	1	0	6.500529	8.694918	3.580019
9	6	0	8.119702	7.288968	3.006527
10	1	0	9.037729	7.842329	3.155905
11	6	0	8.035086	5.954046	2.530025
12	6	0	9.019865	5.058217	2.124119
13	6	0	8.708106	3.794614	1.630991
14	6	0	9.532069	2.757285	1.119849
15	1	0	10.611726	2.792041	1.053315
16	6	0	8.690038	1.727339	0.725164
17	1	0	8.967431	0.779672	0.284661
18	6	0	7.371833	2.152601	1.004036
19	1	0	6.438290	1.630682	0.840247
20	1	0	4.889140	6.601244	2.909643
21	1	0	10.061564	5.360449	2.177996

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.131143	4.214420	1.988349
2	9	0	5.277510	4.399851	0.903943
3	9	0	5.473053	3.573590	3.034896
4	7	0	6.690055	5.597869	2.473476
5	7	0	7.382456	3.376292	1.548557
6	6	0	5.974794	6.629811	2.939158
7	6	0	6.826587	7.702634	3.277015
8	1	0	6.511177	8.654206	3.674872
9	6	0	8.120327	7.288817	2.997948
10	1	0	9.034780	7.847197	3.130602
11	6	0	8.033654	5.966131	2.493064
12	6	0	9.015888	5.083388	2.060702
13	6	0	8.705279	3.811213	1.595891
14	6	0	9.530791	2.763321	1.113843
15	1	0	10.606466	2.804415	1.031129
16	6	0	8.694927	1.708033	0.781297
17	1	0	8.975897	0.746108	0.382526
18	6	0	7.378008	2.127579	1.064757
19	1	0	6.451526	1.587055	0.940127
20	1	0	4.899326	6.567310	3.013534

21	*1*	*0*	*10.053228*	*5.395858*	*2.086735*

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	*5*	*0*	*6.137368*	*4.215826*	*1.989660*
2	*9*	*0*	*5.287237*	*4.399995*	*0.910926*
3	*9*	*0*	*5.486258*	*3.578240*	*3.033673*
4	*7*	*0*	*6.695257*	*5.593964*	*2.471049*
5	*7*	*0*	*7.384429*	*3.382668*	*1.550417*
6	*6*	*0*	*5.981232*	*6.620402*	*2.933005*
7	*6*	*0*	*6.827935*	*7.691716*	*3.271277*
8	*1*	*0*	*6.510869*	*8.642754*	*3.668065*
9	*6*	*0*	*8.118347*	*7.279300*	*2.995027*
10	*1*	*0*	*9.032784*	*7.836932*	*3.128177*
11	*6*	*0*	*8.030704*	*5.960866*	*2.492430*
12	*6*	*0*	*9.011600*	*5.081352*	*2.062360*
13	*6*	*0*	*8.700044*	*3.813201*	*1.598262*
14	*6*	*0*	*9.523826*	*2.769719*	*1.117548*
15	*1*	*0*	*10.599221*	*2.810916*	*1.035671*
16	*6*	*0*	*8.689520*	*1.718709*	*0.784571*
17	*1*	*0*	*8.968602*	*0.756974*	*0.385040*
18	*6*	*0*	*7.377569*	*2.140161*	*1.067783*
19	*1*	*0*	*6.449594*	*1.602657*	*0.943114*
20	*1*	*0*	*4.905972*	*6.555465*	*3.005049*
21	*1*	*0*	*10.048503*	*5.393281*	*2.089320*

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	*5*	*0*	*6.135835*	*4.216066*	*1.987933*
2	*9*	*0*	*5.285433*	*4.402315*	*0.903926*
3	*9*	*0*	*5.479981*	*3.576314*	*3.033644*
4	*7*	*0*	*6.694260*	*5.594551*	*2.471561*
5	*7*	*0*	*7.383986*	*3.381508*	*1.550232*
6	*6*	*0*	*5.979036*	*6.620987*	*2.935014*
7	*6*	*0*	*6.825806*	*7.695306*	*3.274342*
8	*1*	*0*	*6.507589*	*8.647391*	*3.672681*
9	*6*	*0*	*8.119066*	*7.283902*	*2.996622*
10	*1*	*0*	*9.034647*	*7.843618*	*3.130069*
11	*6*	*0*	*8.033217*	*5.964366*	*2.492672*
12	*6*	*0*	*9.015462*	*5.083063*	*2.061141*
13	*6*	*0*	*8.703958*	*3.812236*	*1.596720*
14	*6*	*0*	*9.527016*	*2.766357*	*1.115862*
15	*1*	*0*	*10.604465*	*2.806696*	*1.033090*
16	*6*	*0*	*8.690081*	*1.713599*	*0.783984*
17	*1*	*0*	*8.969006*	*0.749690*	*0.384630*
18	*6*	*0*	*7.376389*	*2.137450*	*1.068392*
19	*1*	*0*	*6.444875*	*1.602066*	*0.945825*
20	*1*	*0*	*4.902252*	*6.551718*	*3.006523*
21	*1*	*0*	*10.054514*	*5.395900*	*2.087557*

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	*5*	*0*	*6.191626*	*4.144471*	*2.229562*
2	*9*	*0*	*5.120560*	*4.124221*	*1.359342*

3	9	0	5.903936	3.501241	3.422333
4	7	0	6.719206	5.574582	2.447324
5	7	0	7.406035	3.374321	1.570148
6	6	0	5.963942	6.665763	2.710751
7	6	0	6.788964	7.747403	3.073523
8	1	0	6.443702	8.739805	3.330996
9	6	0	8.104971	7.300836	3.030683
10	1	0	9.004020	7.869409	3.225623
11	6	0	8.075355	5.930271	2.619536
12	6	0	9.084404	5.040654	2.332337
13	6	0	8.750153	3.756315	1.715405
14	6	0	9.511003	2.802824	1.126603
15	1	0	10.589696	2.782886	1.046230
16	6	0	8.575048	1.765953	0.576977
17	1	0	8.866756	0.860883	0.062222
18	6	0	7.311334	2.188857	0.870943
19	1	0	6.345959	1.751315	0.670987
20	1	0	4.886129	6.615092	2.644845
21	1	0	10.124074	5.307994	2.466051

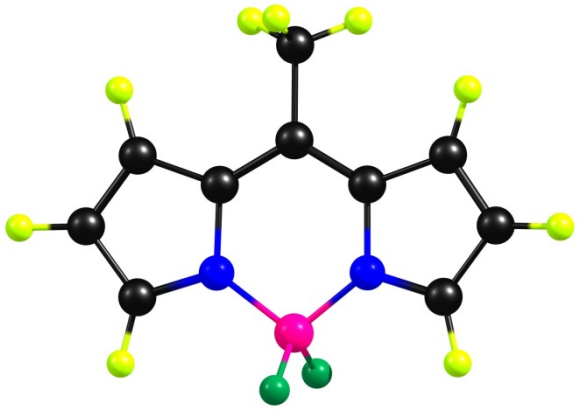

Figure S2-2: DFT B3LYP/6-31G(d) optimised ground-state structure of **1.01**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138771	4.180886	2.076855
2	9	0	5.189869	4.299938	1.080784
3	9	0	5.628401	3.552087	3.197694
4	7	0	6.695735	5.594575	2.466646
5	7	0	7.386308	3.392190	1.545550
6	6	0	5.965046	6.651516	2.844986
7	6	0	6.805771	7.722193	3.213938
8	1	0	6.479510	8.695650	3.553140
9	6	0	8.110653	7.277419	3.049106
10	1	0	9.016603	7.839897	3.229332
11	6	0	8.042637	5.940009	2.574808
12	6	0	9.054218	5.045922	2.194305
13	6	0	8.717616	3.787357	1.674517
14	6	0	9.531556	2.745850	1.153923
15	1	0	10.611761	2.752595	1.101734
16	6	0	8.681222	1.740975	0.712487
17	1	0	8.954686	0.801774	0.251790
18	6	0	7.366986	2.180429	0.975089
19	1	0	6.426924	1.680859	0.782187
20	1	0	4.884374	6.600383	2.839632
21	6	0	10.498990	5.463071	2.280078
22	1	0	10.810938	5.950821	1.347772
23	1	0	10.661184	6.171035	3.095986
24	1	0	11.152913	4.602834	2.440090

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.141479	4.211096	2.006689
2	9	0	5.258011	4.379157	0.942491
3	9	0	5.512728	3.568135	3.072673
4	7	0	6.698464	5.595116	2.471606
5	7	0	7.389882	3.389974	1.549368
6	6	0	5.968350	6.636640	2.890330
7	6	0	6.810578	7.700134	3.268274
8	1	0	6.486926	8.658967	3.641386
9	6	0	8.113612	7.267972	3.066856
10	1	0	9.016615	7.828958	3.249887
11	6	0	8.044895	5.943466	2.562730
12	6	0	9.055738	5.058185	2.166102
13	6	0	8.718724	3.794420	1.663950
14	6	0	9.533026	2.741029	1.173582
15	1	0	10.610581	2.745320	1.123788
16	6	0	8.685562	1.720243	0.767345
17	1	0	8.960998	0.768401	0.341369
18	6	0	7.371749	2.160773	1.018422
19	1	0	6.436544	1.650488	0.842881
20	1	0	4.890082	6.582628	2.905610
21	6	0	10.497075	5.481869	2.233637
22	1	0	10.788760	5.965634	1.295577
23	1	0	10.665727	6.193549	3.041280
24	1	0	11.156565	4.628113	2.386595

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.151439	4.204630	2.029632
2	9	0	5.244732	4.353956	0.991792
3	9	0	5.563088	3.567230	3.113135
4	7	0	6.704833	5.592341	2.467435
5	7	0	7.393150	3.397141	1.549979
6	6	0	5.976348	6.633303	2.870706
7	6	0	6.814202	7.696453	3.244382
8	1	0	6.489360	8.658919	3.605829
9	6	0	8.113882	7.260812	3.056181
10	1	0	9.017622	7.820761	3.238075
11	6	0	8.042931	5.937253	2.564346
12	6	0	9.052141	5.053272	2.174644
13	6	0	8.714558	3.795458	1.669159
14	6	0	9.527502	2.751263	1.171375
15	1	0	10.604919	2.756756	1.121516
16	6	0	8.681649	1.738888	0.754422
17	1	0	8.955261	0.791810	0.317759
18	6	0	7.372660	2.179081	1.008957
19	1	0	6.435986	1.673639	0.828659
20	1	0	4.898234	6.579170	2.879110
21	6	0	10.485636	5.472030	2.249452
22	1	0	10.777712	5.964505	1.317225
23	1	0	10.651901	6.175294	3.063968
24	1	0	11.142927	4.616303	2.394686

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.146829	4.213695	2.004648
2	9	0	5.274816	4.387814	0.934719
3	9	0	5.511161	3.571504	3.063558
4	7	0	6.703857	5.591138	2.474123
5	7	0	7.392905	3.393311	1.554863
6	6	0	5.974171	6.627968	2.890231
7	6	0	6.811932	7.693113	3.267103
8	1	0	6.486059	8.653471	3.638497
9	6	0	8.114272	7.262772	3.066152
10	1	0	9.018382	7.826261	3.248677
11	6	0	8.045052	5.940760	2.565791
12	6	0	9.054583	5.056626	2.168870
13	6	0	8.718084	3.794020	1.667889
14	6	0	9.530732	2.744752	1.176453
15	1	0	10.610348	2.748436	1.124830
16	6	0	8.682790	1.725719	0.771202
17	1	0	8.956676	0.773048	0.342460
18	6	0	7.372195	2.168745	1.025138
19	1	0	6.432377	1.663213	0.851062
20	1	0	4.894641	6.568069	2.902534
21	6	0	10.492243	5.480955	2.231983
22	1	0	10.772662	5.963107	1.289413
23	1	0	10.662222	6.194676	3.038943
24	1	0	11.153682	4.627093	2.383290

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.210562	4.121020	2.296396
2	9	0	5.084206	4.062787	1.500351
3	9	0	6.020357	3.488390	3.514795
4	7	0	6.718484	5.563015	2.455454
5	7	0	7.399754	3.382116	1.569212
6	6	0	5.945069	6.643000	2.711819
7	6	0	6.753394	7.744935	3.042237
8	1	0	6.394341	8.735906	3.286510
9	6	0	8.077909	7.323300	2.987712
10	1	0	8.960665	7.924765	3.152717
11	6	0	8.072754	5.944868	2.599303
12	6	0	9.101315	5.070499	2.304589
13	6	0	8.741394	3.784858	1.673508
14	6	0	9.494446	2.860727	1.029875
15	1	0	10.568390	2.859503	0.904185
16	6	0	8.554766	1.822639	0.489070
17	1	0	8.840518	0.933818	-0.056506
18	6	0	7.296514	2.217132	0.842428
19	1	0	6.331114	1.768568	0.668431
20	1	0	4.867733	6.567238	2.666979
21	6	0	10.549417	5.400394	2.476063
22	1	0	11.072080	5.490010	1.510452
23	1	0	10.684657	6.342557	3.012358
24	1	0	11.072834	4.618223	3.044486

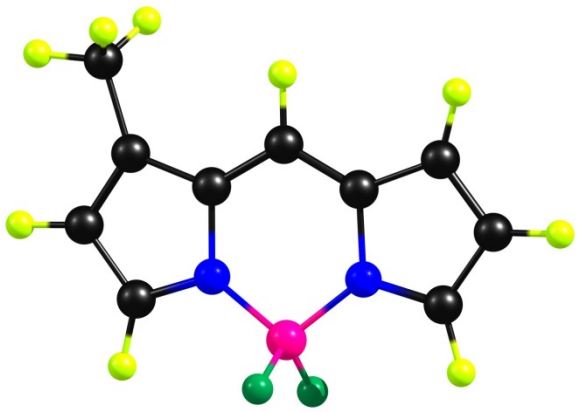

Figure S2-3: DFT B3LYP/6-31G(d) optimised ground-state structure of **1.02**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.132239	4.186009	2.059859
2	9	0	5.200336	4.318953	1.049950
3	9	0	5.598345	3.560325	3.170695
4	7	0	6.691666	5.600932	2.465895
5	7	0	7.380711	3.381364	1.543130
6	6	0	5.974958	6.653601	2.873510
7	6	0	6.826580	7.724181	3.222892
8	1	0	6.507832	8.694442	3.580304
9	6	0	8.134198	7.299590	3.016916
10	6	0	8.040564	5.956105	2.536078
11	6	0	9.020982	5.059088	2.134021
12	6	0	8.708324	3.794254	1.636967
13	6	0	9.532218	2.758530	1.126951
14	1	0	10.612178	2.791958	1.064073
15	6	0	8.689612	1.729300	0.726263
16	1	0	8.968220	0.782554	0.284433
17	6	0	7.372365	2.154756	1.001031
18	1	0	6.438339	1.635117	0.833323
19	1	0	4.894288	6.605443	2.901914
20	1	0	10.064570	5.354779	2.190674
21	6	0	9.396065	8.078153	3.235226
22	1	0	10.065114	7.577089	3.945876
23	1	0	9.956553	8.213268	2.301513
24	1	0	9.173119	9.071958	3.633818

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134541	4.219633	1.982379
2	9	0	5.285722	4.413267	0.894280
3	9	0	5.464935	3.579223	3.023272
4	7	0	6.694785	5.599154	2.475658
5	7	0	7.383541	3.379478	1.548111
6	6	0	5.981701	6.629592	2.939322
7	6	0	6.834158	7.698437	3.286325
8	1	0	6.517748	8.650005	3.685721
9	6	0	8.136631	7.296201	3.019178
10	6	0	8.041694	5.966251	2.506156
11	6	0	9.018671	5.082249	2.077645
12	6	0	8.706157	3.809709	1.605395
13	6	0	9.531486	2.763046	1.125904

14	1	0	10.607825	2.801350	1.050355
15	6	0	8.694209	1.709519	0.783595
16	1	0	8.976225	0.748466	0.383350
17	6	0	7.378198	2.130657	1.059304
18	1	0	6.450732	1.593874	0.927031
19	1	0	4.905399	6.570905	3.006878
20	1	0	10.058827	5.385365	2.108886
21	6	0	9.394865	8.081576	3.220997
22	1	0	10.074251	7.581512	3.918318
23	1	0	9.936474	8.223112	2.280510
24	1	0	9.170600	9.069166	3.626744

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.141699	4.223722	1.982580
2	9	0	5.299060	4.417405	0.898267
3	9	0	5.475989	3.586358	3.018870
4	7	0	6.700654	5.597197	2.474192
5	7	0	7.386956	3.388061	1.551141
6	6	0	5.989032	6.621841	2.935653
7	6	0	6.836460	7.689281	3.282718
8	1	0	6.518905	8.640039	3.682081
9	6	0	8.135323	7.288596	3.016388
10	6	0	8.039088	5.963404	2.505115
11	6	0	9.015231	5.083602	2.078425
12	6	0	8.702285	3.814579	1.607689
13	6	0	9.526035	2.772163	1.130285
14	1	0	10.602050	2.810887	1.055109
15	6	0	8.690566	1.722129	0.789277
16	1	0	8.970907	0.760883	0.389335
17	6	0	7.379523	2.144908	1.064945
18	1	0	6.450757	1.610584	0.933705
19	1	0	4.913041	6.560331	3.002071
20	1	0	10.054660	5.387537	2.110142
21	6	0	9.388955	8.068308	3.216523
22	1	0	10.066416	7.566576	3.912807
23	1	0	9.928763	8.208023	2.275999
24	1	0	9.167020	9.055334	3.621995

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139953	4.218281	1.990446
2	9	0	5.286455	4.409729	0.908597
3	9	0	5.481981	3.576941	3.035132
4	7	0	6.697143	5.595551	2.479094
5	7	0	7.386535	3.387152	1.550480
6	6	0	5.985388	6.619359	2.944197
7	6	0	6.833203	7.691821	3.288169
8	1	0	6.515861	8.644336	3.688684
9	6	0	8.132739	7.292909	3.015611
10	6	0	8.038893	5.967179	2.503521
11	6	0	9.016314	5.091141	2.067847
12	6	0	8.704963	3.817999	1.597071
13	6	0	9.527955	2.777739	1.111589
14	1	0	10.605374	2.819662	1.027660
15	6	0	8.690859	1.723301	0.775144
16	1	0	8.971591	0.761869	0.371183
17	6	0	7.379101	2.143157	1.062095
18	1	0	6.447632	1.608297	0.938012
19	1	0	4.908074	6.552880	3.013689
20	1	0	10.056660	5.401194	2.091980

21	6	0	9.394670	8.067426	3.225313
22	1	0	9.980960	7.647121	4.049376
23	1	0	10.024767	8.058599	2.330550
24	1	0	9.172305	9.108107	3.469869

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.198796	4.140220	2.248672
2	9	0	5.112857	4.109906	1.396654
3	9	0	5.931785	3.505176	3.451251
4	7	0	6.725869	5.572209	2.445420
5	7	0	7.405502	3.371077	1.574946
6	6	0	5.976255	6.668049	2.702657
7	6	0	6.806815	7.748195	3.053014
8	1	0	6.467217	8.745078	3.304005
9	6	0	8.128505	7.310170	3.013618
10	6	0	8.083136	5.927996	2.609306
11	6	0	9.090466	5.040371	2.322136
12	6	0	8.752640	3.754108	1.707408
13	6	0	9.508330	2.804901	1.107086
14	1	0	10.585955	2.787312	1.013928
15	6	0	8.567431	1.769657	0.563409
16	1	0	8.853802	0.865754	0.043518
17	6	0	7.305236	2.190557	0.872663
18	1	0	6.338815	1.751459	0.681262
19	1	0	4.897860	6.621296	2.643493
20	1	0	10.131279	5.306736	2.448419
21	6	0	9.375558	8.090887	3.279721
22	1	0	9.960664	7.657863	4.102726
23	1	0	10.035153	8.117966	2.401058
24	1	0	9.139449	9.124805	3.548941

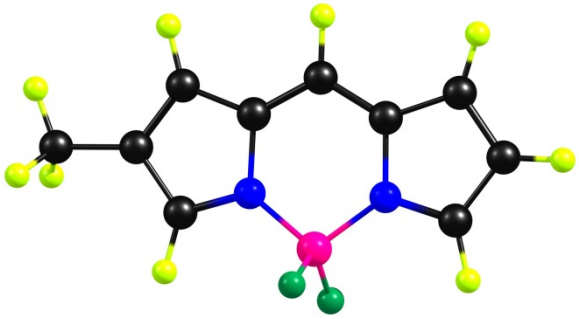

Figure S2-4: DFT B3LYP/6-31G(d) optimised ground-state structure of **1.03**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.133555	4.208920	2.024287
2	9	0	5.225246	4.346380	0.993900
3	9	0	5.569018	3.599768	3.128636
4	7	0	6.700846	5.621543	2.432009
5	7	0	7.382939	3.385894	1.539594
6	6	0	5.988456	6.681625	2.828683
7	6	0	6.837729	7.765148	3.178943
8	6	0	8.132682	7.307210	2.973750
9	6	0	8.049621	5.968580	2.504974

10	6	0	9.029283	5.062076	2.118454
11	6	0	8.712426	3.793029	1.636398
12	6	0	9.533979	2.743630	1.150631
13	1	0	10.614569	2.769769	1.096072
14	6	0	8.688557	1.712130	0.762248
15	1	0	8.964819	0.755849	0.339965
16	6	0	7.371777	2.149836	1.019511
17	1	0	6.436193	1.632287	0.853839
18	1	0	4.906720	6.638147	2.852078
19	1	0	10.073042	5.355844	2.179277
20	1	0	9.051180	7.859429	3.129787
21	6	0	6.394979	9.115110	3.662591
22	1	0	5.767871	9.625900	2.921401
23	1	0	5.808388	9.042514	4.586744
24	1	0	7.256724	9.757837	3.866761

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.137223	4.241051	1.948803
2	9	0	5.301428	4.418066	0.848319
3	9	0	5.453103	3.629122	2.996883
4	7	0	6.701578	5.628747	2.418519
5	7	0	7.385079	3.384069	1.546030
6	6	0	5.990414	6.674551	2.852744
7	6	0	6.840441	7.758937	3.190914
8	6	0	8.131513	7.318739	2.938123
9	6	0	8.047482	5.985973	2.454665
10	6	0	9.025689	5.087289	2.055612
11	6	0	8.710041	3.807256	1.607879
12	6	0	9.533121	2.744866	1.159675
13	1	0	10.610383	2.774804	1.094613
14	6	0	8.692469	1.689568	0.831533
15	1	0	8.971978	0.718234	0.455140
16	6	0	7.376563	2.125018	1.084324
17	1	0	6.446934	1.591465	0.954039
18	1	0	4.912352	6.621860	2.909509
19	1	0	10.065883	5.389064	2.092984
20	1	0	9.047959	7.873871	3.077262
21	6	0	6.399403	9.093792	3.712211
22	1	0	5.737518	9.602246	3.004583
23	1	0	5.854135	8.995912	4.655852
24	1	0	7.257912	9.743958	3.890317

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142879	4.246310	1.949233
2	9	0	5.313413	4.424188	0.852610
3	9	0	5.462427	3.637704	2.992679
4	7	0	6.706902	5.627572	2.417499
5	7	0	7.386366	3.393055	1.549036
6	6	0	5.997390	6.667353	2.849547
7	6	0	6.842569	7.750176	3.187820
8	6	0	8.130159	7.311872	2.936024
9	6	0	8.044749	5.983671	2.454041
10	6	0	9.021159	5.088224	2.056394
11	6	0	8.704170	3.811999	1.610078
12	6	0	9.525203	2.753548	1.163843
13	1	0	10.602156	2.783420	1.099075
14	6	0	8.685946	1.702123	0.837025
15	1	0	8.963388	0.730495	0.460931
16	6	0	7.375194	2.139730	1.089842

17	1	0	6.444048	1.609024	0.960569
18	1	0	4.919645	6.612202	2.905266
19	1	0	10.060928	5.389447	2.093819
20	1	0	9.046459	7.866511	3.075308
21	6	0	6.401345	9.078070	3.706698
22	1	0	5.741286	9.585270	2.998230
23	1	0	5.854785	8.978324	4.648056
24	1	0	7.258038	9.728165	3.886909

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142351	4.242192	1.955946
2	9	0	5.304371	4.418015	0.859813
3	9	0	5.465851	3.633772	3.007994
4	7	0	6.707257	5.626655	2.418923
5	7	0	7.385847	3.389530	1.551060
6	6	0	5.997451	6.665093	2.856046
7	6	0	6.842566	7.751799	3.189900
8	6	0	8.131711	7.318438	2.930452
9	6	0	8.048416	5.988064	2.447535
10	6	0	9.024840	5.092085	2.045651
11	6	0	8.707261	3.811230	1.602721
12	6	0	9.527401	2.751997	1.154514
13	1	0	10.605975	2.783558	1.083136
14	6	0	8.686045	1.695970	0.835355
15	1	0	8.964323	0.722193	0.460153
16	6	0	7.374266	2.133347	1.095292
17	1	0	6.440324	1.602030	0.974180
18	1	0	4.918607	6.604774	2.919575
19	1	0	10.066427	5.395936	2.076884
20	1	0	9.047847	7.878362	3.066878
21	6	0	6.397383	9.084816	3.709278
22	1	0	5.822886	9.635093	2.957144
23	1	0	5.763469	8.975313	4.594526
24	1	0	7.257726	9.698193	3.987579

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.222537	4.119084	2.310536
2	9	0	5.090384	4.155895	1.519737
3	9	0	5.967003	3.552008	3.549129
4	7	0	6.733480	5.592527	2.555311
5	7	0	7.393278	3.423175	1.584960
6	6	0	5.933648	6.673289	2.838723
7	6	0	6.731143	7.754674	3.114206
8	6	0	8.145267	7.264652	2.951654
9	6	0	8.084796	5.952716	2.611386
10	6	0	9.123698	4.992334	2.235686
11	6	0	8.753694	3.791023	1.680243
12	6	0	9.518421	2.755879	1.050146
13	1	0	10.594946	2.757901	0.946350
14	6	0	8.618443	1.812449	0.571937
15	1	0	8.848311	0.905145	0.029240
16	6	0	7.323943	2.250681	0.916690
17	1	0	6.368208	1.779128	0.735222
18	1	0	4.859081	6.573091	2.841254
19	1	0	10.163873	5.278998	2.315437
20	1	0	9.034398	7.870122	3.074630
21	6	0	6.345364	9.129616	3.506652
22	1	0	6.751169	9.870274	2.800363
23	1	0	5.260085	9.251147	3.551366

24	1	0	6.765431	9.392648	4.489676

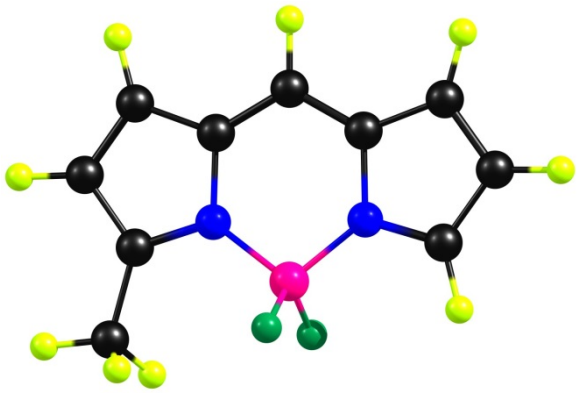

Figure S2-5: DFT B3LYP/6-31G(d) optimised ground-state structure of **1.04**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.123455	4.246824	1.914412
2	9	0	5.319340	4.438106	0.802543
3	9	0	5.429885	3.619657	2.936696
4	7	0	6.681852	5.630327	2.416061
5	7	0	7.382937	3.396082	1.522915
6	6	0	5.955883	6.675521	2.854500
7	6	0	6.829446	7.736287	3.216059
8	6	0	8.123152	7.304924	2.983619
9	6	0	8.032817	5.979705	2.480072
10	6	0	9.018144	5.085630	2.086159
11	6	0	8.709753	3.810146	1.612985
12	6	0	9.536664	2.750224	1.163686
13	1	0	10.617643	2.776724	1.117859
14	6	0	8.696327	1.702524	0.805426
15	1	0	8.978635	0.732930	0.418974
16	6	0	7.377789	2.142689	1.042517
17	1	0	6.444671	1.617130	0.889299
18	1	0	10.059258	5.388035	2.148205
19	1	0	9.044113	7.850104	3.144991
20	1	0	6.511095	8.696011	3.600607
21	6	0	4.464827	6.641360	2.918633
22	1	0	4.044340	6.450507	1.925257
23	1	0	4.129213	5.822131	3.563811
24	1	0	4.071858	7.586376	3.301395

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134586	4.242544	1.912981
2	9	0	5.316109	4.427024	0.796544
3	9	0	5.427829	3.607535	2.936508
4	7	0	6.678055	5.626735	2.414672
5	7	0	7.386939	3.392497	1.522079
6	6	0	5.951800	6.671597	2.852712
7	6	0	6.826988	7.730221	3.212425
8	6	0	8.118989	7.298708	2.979733
9	6	0	8.029369	5.974643	2.477363

10	6	0	9.016065	5.085264	2.085274
11	6	0	8.710625	3.810516	1.613061
12	6	0	9.538599	2.753370	1.165043
13	1	0	10.616897	2.781147	1.119393
14	6	0	8.700784	1.704181	0.807012
15	1	0	8.985276	0.737636	0.422051
16	6	0	7.382493	2.138882	1.042276
17	1	0	6.453737	1.610382	0.888372
18	1	0	10.053995	5.390257	2.147888
19	1	0	9.037757	7.842763	3.140116
20	1	0	6.511168	8.688284	3.595799
21	6	0	4.463510	6.652121	2.922940
22	1	0	4.033696	6.469685	1.934428
23	1	0	4.119172	5.842582	3.571982
24	1	0	4.088655	7.601377	3.306025

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138012	4.248418	1.914557
2	9	0	5.324992	4.433802	0.802659
3	9	0	5.435561	3.616902	2.934011
4	7	0	6.682435	5.625289	2.413990
5	7	0	7.385694	3.401523	1.525224
6	6	0	5.957851	6.663913	2.849703
7	6	0	6.827764	7.721294	3.209575
8	6	0	8.116254	7.291679	2.977846
9	6	0	8.025324	5.971933	2.476888
10	6	0	9.009965	5.085645	2.085978
11	6	0	8.702463	3.814817	1.615010
12	6	0	9.527783	2.761233	1.168586
13	1	0	10.605762	2.788487	1.122946
14	6	0	8.690812	1.716340	0.811967
15	1	0	8.972676	0.749449	0.427004
16	6	0	7.377906	2.153726	1.047761
17	1	0	6.447416	1.628396	0.894906
18	1	0	10.047576	5.389753	2.148470
19	1	0	9.035031	7.835014	3.138252
20	1	0	6.510206	8.678412	3.592838
21	6	0	4.476496	6.638667	2.917115
22	1	0	4.051734	6.454254	1.927882
23	1	0	4.136836	5.826364	3.563493
24	1	0	4.096543	7.584642	3.300020

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138230	4.237605	1.936302
2	9	0	5.301515	4.411482	0.835568
3	9	0	5.457723	3.605671	2.976727
4	7	0	6.682119	5.623707	2.418815
5	7	0	7.385488	3.396596	1.531088
6	6	0	5.958214	6.664268	2.848344
7	6	0	6.827115	7.727510	3.203984
8	6	0	8.117852	7.298808	2.974441
9	6	0	8.029671	5.973770	2.479440
10	6	0	9.014174	5.086260	2.087916
11	6	0	8.705958	3.811115	1.616941
12	6	0	9.530680	2.759020	1.165258
13	1	0	10.610479	2.786978	1.114567
14	6	0	8.691352	1.711516	0.808782
15	1	0	8.974810	0.744714	0.419706
16	6	0	7.377405	2.147775	1.050880

17	1	0	6.444591	1.621954	0.901399
18	1	0	10.053988	5.391626	2.147025
19	1	0	9.036721	7.846776	3.132645
20	1	0	6.506153	8.687462	3.582804
21	6	0	4.469865	6.644156	2.903133
22	1	0	4.054776	6.597441	1.891926
23	1	0	4.114833	5.760962	3.440081
24	1	0	4.099383	7.542778	3.398909

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.155968	4.262965	1.957989
2	9	0	5.327382	4.385334	0.851055
3	9	0	5.512320	3.590877	2.988354
4	7	0	6.714896	5.622790	2.415124
5	7	0	7.408966	3.402789	1.528755
6	6	0	5.959459	6.673102	2.838193
7	6	0	6.813985	7.738407	3.205885
8	6	0	8.123586	7.330546	3.005268
9	6	0	8.076325	5.989883	2.502913
10	6	0	9.085536	5.133655	2.138012
11	6	0	8.755052	3.806133	1.626945
12	6	0	9.522726	2.786606	1.174979
13	1	0	10.602127	2.759793	1.110208
14	6	0	8.594767	1.681241	0.769522
15	1	0	8.889867	0.721914	0.367064
16	6	0	7.326282	2.129769	1.011165
17	1	0	6.365984	1.660571	0.865758
18	1	0	10.123641	5.428675	2.211696
19	1	0	9.030735	7.892661	3.180311
20	1	0	6.475115	8.696837	3.577756
21	6	0	4.470442	6.615747	2.879261
22	1	0	4.058614	6.415575	1.882521
23	1	0	4.129794	5.796801	3.525265
24	1	0	4.059523	7.557282	3.252682

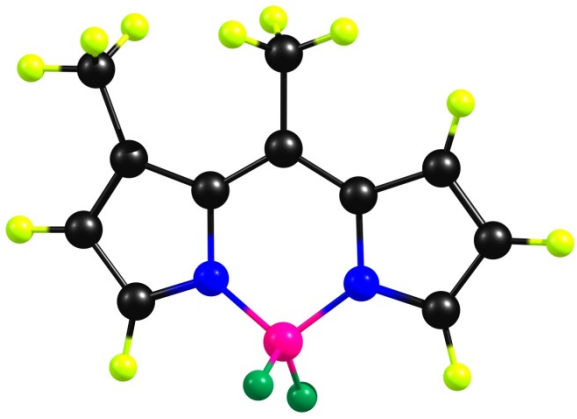

Figure S2-6: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.01**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.160039	4.183323	2.113346
2	9	0	5.168511	4.278924	1.155707

3	9	0	5.694727	3.581383	3.269820
4	7	0	6.727975	5.604603	2.445874
5	7	0	7.384196	3.389491	1.554046
6	6	0	5.989597	6.662128	2.797668
7	6	0	6.821581	7.739470	3.148483
8	6	0	8.140139	7.316834	3.005169
9	6	0	8.077221	5.955603	2.552783
10	6	0	9.073596	5.037253	2.183014
11	6	0	8.717998	3.775146	1.671884
12	6	0	9.516106	2.723252	1.145742
13	1	0	10.594988	2.712755	1.077742
14	6	0	8.652410	1.724329	0.714437
15	1	0	8.914734	0.782755	0.252085
16	6	0	7.346386	2.175694	0.987188
17	1	0	6.398926	1.686135	0.805461
18	1	0	6.492632	8.720286	3.465621
19	1	0	4.909363	6.603472	2.786767
20	6	0	10.531974	5.397666	2.296788
21	1	0	10.779629	6.244069	1.646499
22	1	0	10.781996	5.693925	3.320687
23	1	0	11.176721	4.562569	2.022959
24	6	0	9.345231	8.169472	3.271198
25	1	0	9.991572	7.746522	4.049934
26	1	0	9.966398	8.305216	2.377334
27	1	0	9.032330	9.162449	3.607223

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.153952	4.236509	1.977538
2	9	0	5.309006	4.425451	0.883191
3	9	0	5.466407	3.618159	3.023189
4	7	0	6.730811	5.606278	2.452900
5	7	0	7.389326	3.383434	1.566193
6	6	0	5.996000	6.637692	2.878542
7	6	0	6.829745	7.707182	3.241850
8	6	0	8.144675	7.307999	3.027343
9	6	0	8.080250	5.966602	2.523236
10	6	0	9.074531	5.061086	2.126937
11	6	0	8.719192	3.785814	1.653377
12	6	0	9.520784	2.709647	1.191181
13	1	0	10.597102	2.697353	1.128635
14	6	0	8.663082	1.677967	0.833087
15	1	0	8.930304	0.709716	0.440150
16	6	0	7.356619	2.134707	1.080405
17	1	0	6.415471	1.626913	0.932197
18	1	0	6.502513	8.664206	3.618810
19	1	0	4.918570	6.571803	2.906690
20	6	0	10.529541	5.435811	2.198530
21	1	0	10.736268	6.312432	1.580022
22	1	0	10.816340	5.685881	3.222706
23	1	0	11.169563	4.625598	1.858409
24	6	0	9.347781	8.161479	3.290566
25	1	0	10.018418	7.713489	4.029690
26	1	0	9.935414	8.337883	2.384811
27	1	0	9.035312	9.133630	3.675273

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.166756	4.220992	2.031026
2	9	0	5.256381	4.369026	0.994147
3	9	0	5.567921	3.608182	3.124814

4	7	0	6.737253	5.606318	2.446524
5	7	0	7.392997	3.394653	1.562454
6	6	0	6.002907	6.642525	2.841788
7	6	0	6.832146	7.712504	3.199213
8	6	0	8.144402	7.303583	3.013492
9	6	0	8.078284	5.960204	2.531586
10	6	0	9.071476	5.054558	2.148243
11	6	0	8.715764	3.788602	1.662163
12	6	0	9.515768	2.727524	1.178698
13	1	0	10.592002	2.716928	1.115381
14	6	0	8.659282	1.709990	0.793378
15	1	0	8.924482	0.752264	0.375182
16	6	0	7.357638	2.163616	1.049277
17	1	0	6.414990	1.662694	0.889200
18	1	0	6.503542	8.677515	3.552846
19	1	0	4.925309	6.578793	2.854974
20	6	0	10.518622	5.420630	2.238536
21	1	0	10.737437	6.293406	1.620123
22	1	0	10.789297	5.673681	3.265499
23	1	0	11.158858	4.605802	1.911934
24	6	0	9.344393	8.148768	3.276735
25	1	0	10.004443	7.704542	4.026147
26	1	0	9.939957	8.311315	2.374639
27	1	0	9.034671	9.126109	3.647461

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.163902	4.217606	2.032453
2	9	0	5.252649	4.370348	0.990876
3	9	0	5.561068	3.600401	3.127164
4	7	0	6.734151	5.603184	2.453438
5	7	0	7.391170	3.391600	1.562060
6	6	0	5.999778	6.639907	2.850253
7	6	0	6.830486	7.712755	3.207546
8	6	0	8.143997	7.303212	3.021026
9	6	0	8.079091	5.959031	2.539153
10	6	0	9.072563	5.053460	2.151350
11	6	0	8.717819	3.785388	1.661111
12	6	0	9.516830	2.725949	1.170373
13	1	0	10.595157	2.715088	1.103695
14	6	0	8.657690	1.708286	0.780840
15	1	0	8.924049	0.751757	0.355984
16	6	0	7.354851	2.161321	1.042762
17	1	0	6.409141	1.661878	0.884015
18	1	0	6.501610	8.680175	3.560226
19	1	0	4.920479	6.575056	2.862846
20	6	0	10.523375	5.428712	2.231269
21	1	0	10.743428	6.240660	1.531598
22	1	0	10.778873	5.779062	3.233775
23	1	0	11.172270	4.588784	1.989520
24	6	0	9.350250	8.148359	3.289023
25	1	0	9.963693	7.734596	4.096392
26	1	0	9.989914	8.247176	2.406936
27	1	0	9.038694	9.150974	3.589774

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.243243	4.109254	2.362143
2	9	0	5.074315	4.049306	1.628656
3	9	0	6.115647	3.493975	3.597882
4	7	0	6.760161	5.552436	2.474200

5	7	0	7.392676	3.376638	1.581437
6	6	0	5.981857	6.633664	2.692636
7	6	0	6.784304	7.740307	3.006994
8	6	0	8.119495	7.338948	2.985907
9	6	0	8.118448	5.937931	2.623852
10	6	0	9.128751	5.036949	2.339015
11	6	0	8.740821	3.771648	1.674269
12	6	0	9.476294	2.875956	0.973629
13	1	0	10.546451	2.878941	0.820911
14	6	0	8.522697	1.867640	0.410823
15	1	0	8.791699	0.996841	-0.171330
16	6	0	7.269487	2.251957	0.808208
17	1	0	6.299920	1.811852	0.634979
18	1	0	6.424544	8.738385	3.223377
19	1	0	4.905398	6.552352	2.640024
20	6	0	10.594246	5.270181	2.536699
21	1	0	11.127355	5.398946	1.580487
22	1	0	10.795138	6.150628	3.145815
23	1	0	11.059224	4.408895	3.036971
24	6	0	9.295127	8.235547	3.228877
25	1	0	9.862845	7.951438	4.125460
26	1	0	10.001237	8.238151	2.388450
27	1	0	8.955600	9.265955	3.375087

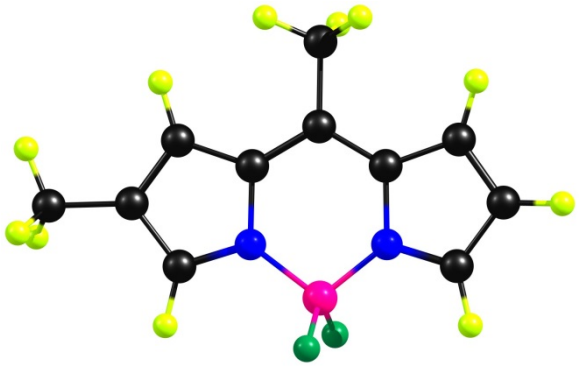

Figure S2-7: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.02**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.137227	4.317813	1.761526
2	9	0	5.527307	4.594567	0.551246
3	9	0	5.261949	3.720996	2.648147
4	7	0	6.710754	5.642059	2.379935
5	7	0	7.389555	3.404889	1.534501
6	6	0	5.988229	6.675120	2.826316
7	6	0	6.827681	7.740071	3.240305
8	6	0	8.126700	7.298748	3.021137
9	6	0	8.058948	5.984057	2.483433
10	6	0	9.063546	5.079892	2.118297
11	6	0	8.721472	3.796763	1.658464
12	6	0	9.534350	2.695139	1.285338
13	1	0	10.615718	2.679193	1.279984
14	6	0	8.682339	1.652032	0.941959
15	1	0	8.956372	0.658566	0.614685
16	6	0	7.368984	2.132682	1.110357
17	1	0	6.427732	1.624871	0.947350
18	1	0	4.906779	6.622691	2.836321
19	6	0	10.511697	5.486548	2.193232
20	1	0	10.851208	5.859696	1.218574
21	1	0	10.669832	6.279472	2.926998
22	1	0	11.148953	4.640587	2.462535

23	1	0	9.032455	7.853265	3.228992
24	6	0	6.378483	9.057119	3.802578
25	1	0	7.236676	9.695798	4.033299
26	1	0	5.738926	9.602523	3.097602
27	1	0	5.802529	8.928466	4.727427

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.145103	4.263941	1.910398
2	9	0	5.321480	4.457501	0.802252
3	9	0	5.441318	3.643907	2.943153
4	7	0	6.712750	5.635642	2.403165
5	7	0	7.391256	3.410896	1.519449
6	6	0	5.989110	6.687853	2.798912
7	6	0	6.829867	7.752204	3.205410
8	6	0	8.128160	7.290745	3.038918
9	6	0	8.060650	5.963917	2.533762
10	6	0	9.064603	5.059661	2.176286
11	6	0	8.721084	3.794447	1.673558
12	6	0	9.533418	2.723047	1.227205
13	1	0	10.612111	2.709795	1.215842
14	6	0	8.682634	1.708210	0.806258
15	1	0	8.957380	0.745715	0.404410
16	6	0	7.370137	2.172499	1.005012
17	1	0	6.432849	1.675508	0.804790
18	1	0	4.909190	6.649327	2.781892
19	6	0	10.512599	5.451120	2.286009
20	1	0	10.878703	5.808009	1.317756
21	1	0	10.659372	6.248102	3.013480
22	1	0	11.129965	4.601682	2.579827
23	1	0	9.032459	7.841189	3.249957
24	6	0	6.379211	9.091041	3.708252
25	1	0	7.235183	9.717998	3.965057
26	1	0	5.789340	9.624589	2.956662
27	1	0	5.756466	8.995079	4.602866

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.153055	4.257348	1.942444
2	9	0	5.296490	4.433217	0.865835
3	9	0	5.497387	3.638747	2.998429
4	7	0	6.718979	5.633043	2.407084
5	7	0	7.393020	3.421266	1.519241
6	6	0	5.997721	6.683577	2.790500
7	6	0	6.834540	7.746702	3.194660
8	6	0	8.128994	7.282118	3.039774
9	6	0	8.058583	5.957534	2.543361
10	6	0	9.059987	5.055495	2.189151
11	6	0	8.715268	3.798351	1.678010
12	6	0	9.526316	2.738595	1.217895
13	1	0	10.604897	2.727373	1.204813
14	6	0	8.677325	1.733896	0.782228
15	1	0	8.950376	0.778203	0.364330
16	6	0	7.369685	2.196403	0.988656
17	1	0	6.431062	1.704885	0.782491
18	1	0	4.918167	6.645142	2.767145
19	6	0	10.500302	5.440346	2.306547
20	1	0	10.871520	5.793364	1.339971
21	1	0	10.644516	6.237660	3.032986
22	1	0	11.111618	4.589062	2.604815
23	1	0	9.033790	7.831526	3.250693

24	6	0	6.384945	9.083598	3.682627
25	1	0	7.239275	9.709154	3.943533
26	1	0	5.804427	9.612931	2.922481
27	1	0	5.754156	8.994085	4.570839

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.151256	4.261577	1.926660
2	9	0	5.317912	4.451286	0.828206
3	9	0	5.464013	3.643646	2.968381
4	7	0	6.718847	5.632578	2.408507
5	7	0	7.393161	3.416033	1.525474
6	6	0	5.996003	6.679990	2.800609
7	6	0	6.832267	7.746347	3.203294
8	6	0	8.129247	7.288760	3.038253
9	6	0	8.062025	5.963021	2.537933
10	6	0	9.063214	5.060588	2.179594
11	6	0	8.718973	3.796496	1.676085
12	6	0	9.530045	2.733450	1.221538
13	1	0	10.610845	2.722705	1.205010
14	6	0	8.679012	1.720924	0.798429
15	1	0	8.953072	0.760301	0.387833
16	6	0	7.369825	2.184408	1.006073
17	1	0	6.428129	1.691618	0.807866
18	1	0	4.914709	6.636219	2.783871
19	6	0	10.508899	5.448010	2.286250
20	1	0	10.871563	5.788579	1.310728
21	1	0	10.658639	6.253964	3.004927
22	1	0	11.120675	4.597510	2.592418
23	1	0	9.033222	7.844450	3.248543
24	6	0	6.377010	9.085443	3.697822
25	1	0	7.227663	9.685303	4.030490
26	1	0	5.858055	9.646065	2.913600
27	1	0	5.688120	8.984355	4.542144

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.224231	4.113026	2.325502
2	9	0	5.073392	4.129935	1.560735
3	9	0	6.008744	3.540644	3.569970
4	7	0	6.722912	5.588258	2.554000
5	7	0	7.389553	3.443914	1.572169
6	6	0	5.922676	6.675043	2.799279
7	6	0	6.718193	7.760169	3.067939
8	6	0	8.133156	7.263326	2.939910
9	6	0	8.074780	5.944529	2.626191
10	6	0	9.140417	4.982080	2.279471
11	6	0	8.754516	3.794342	1.691339
12	6	0	9.508648	2.763889	1.038950
13	1	0	10.583896	2.747796	0.929750
14	6	0	8.599727	1.846752	0.525907
15	1	0	8.824389	0.953376	-0.041670
16	6	0	7.309624	2.291549	0.871083
17	1	0	6.348730	1.837770	0.672819
18	1	0	4.847891	6.577305	2.784977
19	6	0	10.566005	5.388744	2.475425
20	1	0	10.844690	6.244498	1.840376
21	1	0	10.755529	5.694324	3.514406
22	1	0	11.251062	4.569828	2.243634
23	1	0	9.018987	7.872086	3.065036
24	6	0	6.329268	9.142292	3.431176

25	1	0	6.732694	9.420555	4.416983
26	1	0	6.749024	9.870533	2.720122
27	1	0	5.243668	9.267061	3.455061

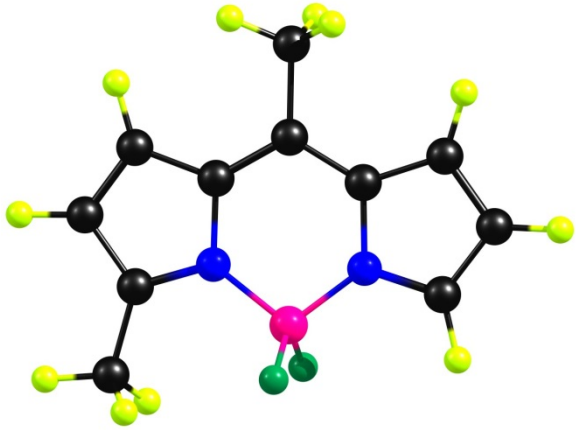

Figure S2-8: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.03**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.130407	4.256069	1.914153
2	9	0	5.338545	4.464639	0.794899
3	9	0	5.418296	3.620938	2.920421
4	7	0	6.691987	5.624756	2.437142
5	7	0	7.387194	3.410142	1.529832
6	6	0	5.954837	6.665508	2.866977
7	6	0	6.818206	7.719419	3.261091
8	6	0	8.117062	7.287485	3.059415
9	6	0	8.043884	5.966517	2.538267
10	6	0	9.052251	5.077953	2.154906
11	6	0	8.715928	3.807296	1.655015
12	6	0	9.533205	2.742509	1.199221
13	1	0	10.614368	2.743695	1.168635
14	6	0	8.685486	1.713967	0.801290
15	1	0	8.963914	0.749266	0.399941
16	6	0	7.371357	2.166998	1.022773
17	1	0	6.432798	1.659942	0.843282
18	6	0	10.500709	5.484258	2.233429
19	1	0	10.863248	5.795920	1.245772
20	1	0	10.652987	6.315316	2.924220
21	1	0	11.124841	4.649151	2.563429
22	1	0	9.024127	7.842882	3.254431
23	1	0	6.493585	8.676439	3.647246
24	6	0	4.462077	6.631880	2.893738
25	1	0	4.065914	6.454818	1.888091
26	1	0	4.110125	5.804767	3.519608
27	1	0	4.061555	7.572594	3.279462

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142041	4.257887	1.900829
2	9	0	5.343822	4.470128	0.772746

3	9	0	5.407282	3.611540	2.899256
4	7	0	6.689612	5.622671	2.435334
5	7	0	7.390964	3.410689	1.521385
6	6	0	5.951509	6.658391	2.873638
7	6	0	6.815301	7.709684	3.269970
8	6	0	8.112660	7.282399	3.060206
9	6	0	8.042136	5.965405	2.532350
10	6	0	9.051212	5.083441	2.144356
11	6	0	8.716573	3.813016	1.644981
12	6	0	9.535115	2.751401	1.192168
13	1	0	10.613731	2.754033	1.162356
14	6	0	8.690199	1.719096	0.798303
15	1	0	8.971110	0.756406	0.401088
16	6	0	7.376188	2.166033	1.018047
17	1	0	6.442201	1.654931	0.839834
18	6	0	10.498869	5.482417	2.232509
19	1	0	10.910825	5.632151	1.229850
20	1	0	10.634955	6.404291	2.794069
21	1	0	11.087249	4.699094	2.714908
22	1	0	9.015563	7.838410	3.256927
23	1	0	6.492455	8.661607	3.662761
24	6	0	4.461373	6.635958	2.910337
25	1	0	4.054145	6.469844	1.909666
26	1	0	4.103998	5.815470	3.537884
27	1	0	4.077803	7.578728	3.300927

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.146747	4.263635	1.902370
2	9	0	5.354219	4.476749	0.779014
3	9	0	5.416619	3.620876	2.896904
4	7	0	6.695348	5.621623	2.434766
5	7	0	7.391472	3.419452	1.524473
6	6	0	5.959484	6.651299	2.871322
7	6	0	6.818631	7.701029	3.267691
8	6	0	8.112308	7.275098	3.058088
9	6	0	8.039147	5.962930	2.531401
10	6	0	9.045745	5.084215	2.144515
11	6	0	8.709683	3.817886	1.646429
12	6	0	9.526824	2.761399	1.195101
13	1	0	10.605298	2.765471	1.165115
14	6	0	8.683670	1.732473	0.802453
15	1	0	8.962817	0.769866	0.404826
16	6	0	7.374572	2.180622	1.023140
17	1	0	6.439282	1.671971	0.846041
18	6	0	10.485456	5.479661	2.232551
19	1	0	10.898591	5.617746	1.229809
20	1	0	10.621036	6.406301	2.784907
21	1	0	11.069740	4.699713	2.723471
22	1	0	9.015788	7.830089	3.254408
23	1	0	6.494533	8.651977	3.660775
24	6	0	4.476415	6.623612	2.905714
25	1	0	4.073801	6.455144	1.904614
26	1	0	4.123617	5.800878	3.531236
27	1	0	4.088048	7.563405	3.295554

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.147008	4.246068	1.941127
2	9	0	5.310977	4.435839	0.840885
3	9	0	5.459773	3.602561	2.971937

4	7	0	6.693452	5.620257	2.442426
5	7	0	7.391073	3.415365	1.531161
6	6	0	5.957638	6.654365	2.866418
7	6	0	6.815474	7.711584	3.255884
8	6	0	8.111524	7.284731	3.054056
9	6	0	8.041854	5.964574	2.539408
10	6	0	9.047461	5.083763	2.154734
11	6	0	8.712208	3.814184	1.652589
12	6	0	9.529808	2.764023	1.187443
13	1	0	10.610443	2.771438	1.151810
14	6	0	8.684705	1.735014	0.786335
15	1	0	8.964729	0.776078	0.375691
16	6	0	7.374448	2.179338	1.017087
17	1	0	6.436153	1.672741	0.839331
18	6	0	10.494057	5.474205	2.240459
19	1	0	10.905962	5.590445	1.233179
20	1	0	10.638056	6.409886	2.779252
21	1	0	11.069469	4.694511	2.745988
22	1	0	9.015224	7.844922	3.247174
23	1	0	6.487418	8.667611	3.638494
24	6	0	4.467747	6.631349	2.883364
25	1	0	4.079531	6.611206	1.860753
26	1	0	4.100652	5.733450	3.386356
27	1	0	4.082049	7.515614	3.393342

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.163545	4.219957	2.080451
2	9	0	5.215783	4.274153	1.067795
3	9	0	5.665238	3.553514	3.192570
4	7	0	6.713740	5.611100	2.434896
5	7	0	7.399576	3.408701	1.538232
6	6	0	5.947299	6.671415	2.811106
7	6	0	6.791211	7.741967	3.179191
8	6	0	8.106321	7.327242	3.033387
9	6	0	8.076728	5.975359	2.557986
10	6	0	9.102520	5.114803	2.226171
11	6	0	8.744900	3.806029	1.653718
12	6	0	9.508944	2.822722	1.120274
13	1	0	10.586549	2.799818	1.038120
14	6	0	8.577322	1.751321	0.641069
15	1	0	8.868318	0.820895	0.173134
16	6	0	7.310495	2.184177	0.921105
17	1	0	6.348033	1.729394	0.746862
18	6	0	10.552985	5.455469	2.359999
19	1	0	11.060120	5.486356	1.383039
20	1	0	10.695712	6.428645	2.834729
21	1	0	11.087822	4.710485	2.967479
22	1	0	8.999113	7.907507	3.217669
23	1	0	6.444457	8.710623	3.515857
24	6	0	4.457067	6.616158	2.827308
25	1	0	4.055905	6.413296	1.827513
26	1	0	4.104221	5.803316	3.474822
27	1	0	4.044967	7.560701	3.192202

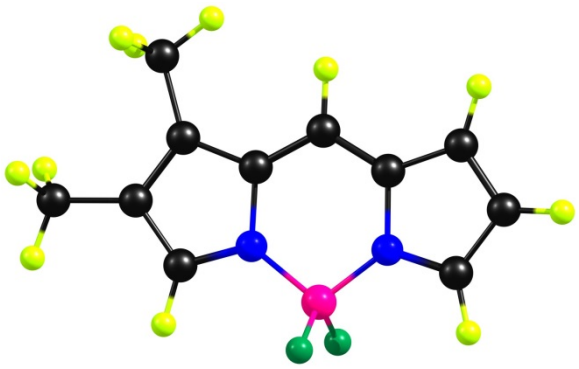

Figure S2-9: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.04**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.121964	4.266940	1.863989
2	9	0	5.419141	4.480719	0.692593
3	9	0	5.331753	3.678168	2.832042
4	7	0	6.698510	5.629952	2.396155
5	7	0	7.381328	3.370306	1.574818
6	6	0	5.990269	6.676427	2.836136
7	6	0	6.833914	7.757179	3.180326
8	6	0	8.140134	7.330775	2.928441
9	6	0	8.045030	5.992991	2.438018
10	6	0	9.022470	5.083187	2.057427
11	6	0	8.708224	3.790531	1.638414
12	6	0	9.535966	2.705907	1.251409
13	1	0	10.617127	2.729070	1.206696
14	6	0	8.696507	1.637999	0.959372
15	1	0	8.979043	0.645925	0.635103
16	6	0	7.377126	2.091233	1.171493
17	1	0	6.444219	1.556817	1.050455
18	1	0	4.909793	6.626274	2.889726
19	1	0	10.067137	5.376500	2.097520
20	6	0	9.397421	8.114939	3.145181
21	1	0	10.277609	7.604677	2.742477
22	1	0	9.337326	9.099270	2.664433
23	1	0	9.579243	8.293637	4.213319
24	6	0	6.392290	9.087339	3.716099
25	1	0	6.749394	9.254104	4.740834
26	1	0	6.771830	9.916764	3.105715
27	1	0	5.300524	9.163207	3.732490

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134990	4.246313	1.933186
2	9	0	5.324163	4.420981	0.812150
3	9	0	5.419084	3.644758	2.967729
4	7	0	6.701400	5.627869	2.405741
5	7	0	7.382828	3.374501	1.564297
6	6	0	5.990503	6.683557	2.817203
7	6	0	6.835359	7.759365	3.167392
8	6	0	8.142308	7.320559	2.951818
9	6	0	8.049351	5.979088	2.472850
10	6	0	9.025791	5.068654	2.101999
11	6	0	8.708686	3.787567	1.654648
12	6	0	9.533546	2.716467	1.232618

13	1	0	10.612300	2.737277	1.192602
14	6	0	8.692291	1.665209	0.891113
15	1	0	8.973176	0.689425	0.527364
16	6	0	7.374591	2.112405	1.110181
17	1	0	6.443821	1.585756	0.961529
18	1	0	4.910871	6.642634	2.850014
19	1	0	10.069489	5.353725	2.158687
20	6	0	9.396014	8.104026	3.178731
21	1	0	10.290981	7.530172	2.932657
22	1	0	9.407897	9.014044	2.569813
23	1	0	9.480774	8.418256	4.224261
24	6	0	6.394314	9.101107	3.669978
25	1	0	6.798818	9.312065	4.665387
26	1	0	6.725873	9.908572	3.008891
27	1	0	5.306075	9.156483	3.737840

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.844672	-1.335643	-0.000002
2	9	0	0.994935	-2.110386	-1.142007
3	9	0	0.994936	-2.110394	1.141998
4	7	0	-0.556798	-0.651740	0.000001
5	7	0	1.885379	-0.174222	0.000002
6	6	0	-1.738515	-1.265233	0.000002
7	6	0	-2.793859	-0.333277	0.000001
8	6	0	-2.202743	0.925964	-0.000001
9	6	0	-0.796387	0.714039	-0.000001
10	6	0	0.259431	1.605063	-0.000002
11	6	0	1.581269	1.175773	0.000000
12	6	0	2.792017	1.900915	0.000001
13	1	0	2.875750	2.977019	0.000000
14	6	0	3.819174	0.971899	0.000003
15	1	0	4.880219	1.163555	0.000004
16	6	0	3.214948	-0.295800	0.000004
17	1	0	3.678377	-1.270777	0.000006
18	1	0	-1.798564	-2.344265	0.000003
19	1	0	0.059411	2.669501	-0.000003
20	6	0	-2.905420	2.238318	-0.000001
21	1	0	-2.209831	3.077873	-0.000017
22	1	0	-3.548011	2.339097	-0.879425
23	1	0	-3.547987	2.339111	0.879439
24	6	0	-4.251567	-0.652593	0.000003
25	1	0	-4.753057	-0.240798	0.880522
26	1	0	-4.753060	-0.240789	-0.880511
27	1	0	-4.416963	-1.730626	-0.000002

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.849485	-1.338690	-0.000003
2	9	0	0.999200	-2.114911	-1.145862
3	9	0	0.999199	-2.114919	1.145851
4	7	0	-0.554062	-0.654033	-0.000001
5	7	0	1.889929	-0.175221	0.000001
6	6	0	-1.735978	-1.268488	0.000001
7	6	0	-2.792881	-0.334858	0.000000
8	6	0	-2.203256	0.924790	-0.000003
9	6	0	-0.795034	0.716116	-0.000002
10	6	0	0.261340	1.608519	-0.000002
11	6	0	1.587140	1.178706	0.000000
12	6	0	2.799324	1.902987	0.000004
13	1	0	2.885689	2.981029	0.000004

14	6	0	3.827683	0.970590	0.000002
15	1	0	4.890617	1.162005	0.000002
16	6	0	3.221000	-0.298114	0.000007
17	1	0	3.682706	-1.275712	0.000009
18	1	0	-1.795358	-2.349438	0.000003
19	1	0	0.061024	2.675316	-0.000004
20	6	0	-2.919054	2.236048	-0.000002
21	1	0	-2.230137	3.083834	-0.000030
22	1	0	-3.562482	2.326340	-0.881741
23	1	0	-3.562437	2.326363	0.881769
24	6	0	-4.257831	-0.645851	0.000003
25	1	0	-4.753505	-0.228029	0.883007
26	1	0	-4.753509	-0.228022	-0.882997
27	1	0	-4.431054	-1.724775	-0.000002

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.200907	4.161908	2.178024
2	9	0	5.141171	4.255853	1.296254
3	9	0	5.813765	3.609456	3.389162
4	7	0	6.741387	5.619855	2.483646
5	7	0	7.396773	3.420701	1.553527
6	6	0	5.944509	6.708447	2.742608
7	6	0	6.743477	7.765410	3.086457
8	6	0	8.170590	7.254204	3.000280
9	6	0	8.091394	5.946324	2.627563
10	6	0	9.118124	4.954823	2.307385
11	6	0	8.752389	3.756453	1.736661
12	6	0	9.531966	2.693918	1.178361
13	1	0	10.612909	2.668001	1.149925
14	6	0	8.643281	1.758779	0.658236
15	1	0	8.888264	0.836086	0.149164
16	6	0	7.342624	2.232696	0.905056
17	1	0	6.389584	1.782298	0.665274
18	1	0	4.870342	6.627981	2.676560
19	1	0	10.161657	5.202499	2.448445
20	6	0	9.376982	8.080617	3.268733
21	1	0	10.298758	7.509931	3.134293
22	1	0	9.416466	8.953241	2.601287
23	1	0	9.368099	8.476317	4.294239
24	6	0	6.348435	9.140432	3.476830
25	1	0	6.706146	9.387942	4.487436
26	1	0	6.792610	9.891151	2.806242
27	1	0	5.262687	9.265514	3.459033

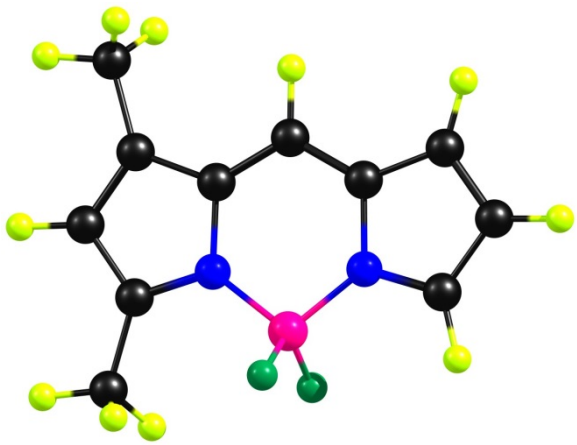

Figure S2-10: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.05**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.121968	4.244795	1.912054
2	9	0	5.318221	4.439381	0.799454
3	9	0	5.423300	3.618253	2.932376
4	7	0	6.679696	5.627517	2.416896
5	7	0	7.380115	3.394807	1.522841
6	6	0	5.954077	6.670529	2.854169
7	6	0	6.826554	7.729552	3.218887
8	6	0	8.129135	7.313298	2.994478
9	6	0	8.031817	5.979553	2.485818
10	6	0	9.013640	5.086142	2.093505
11	6	0	8.705552	3.808848	1.616946
12	6	0	9.533858	2.751444	1.169043
13	1	0	10.615005	2.778433	1.126173
14	6	0	8.694450	1.702400	0.806521
15	1	0	8.979139	0.733663	0.419536
16	6	0	7.376385	2.140583	1.040154
17	1	0	6.443599	1.615458	0.883940
18	1	0	10.056334	5.383281	2.156534
19	1	0	6.508185	8.689857	3.604258
20	6	0	9.393413	8.082878	3.228471
21	1	0	10.048830	7.577286	3.948697
22	1	0	9.967723	8.211099	2.302379
23	1	0	9.173061	9.078988	3.622817
24	6	0	4.462927	6.637634	2.914959
25	1	0	4.045527	6.447454	1.920190
26	1	0	4.126194	5.817035	3.557755
27	1	0	4.069077	7.582166	3.297980

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134154	4.241660	1.910840
2	9	0	5.315836	4.429312	0.793398
3	9	0	5.421574	3.606747	2.931942
4	7	0	6.677057	5.624515	2.415895
5	7	0	7.384835	3.392059	1.522213
6	6	0	5.951874	6.666882	2.852682
7	6	0	6.825780	7.724445	3.216244
8	6	0	8.126533	7.307918	2.991715
9	6	0	8.030636	5.975221	2.483857
10	6	0	9.012822	5.086358	2.093401
11	6	0	8.707070	3.809525	1.617404
12	6	0	9.536229	2.754990	1.170790
13	1	0	10.614713	2.782963	1.128221
14	6	0	8.698911	1.704490	0.808134
15	1	0	8.985546	0.738796	0.422519
16	6	0	7.381420	2.137426	1.039806
17	1	0	6.452850	1.609743	0.882757
18	1	0	10.052944	5.384128	2.156502
19	1	0	6.508016	8.682516	3.600462
20	6	0	9.388292	8.078215	3.225608
21	1	0	10.040320	7.573083	3.945007
22	1	0	9.959006	8.205625	2.300468
23	1	0	9.165784	9.071388	3.618617
24	6	0	4.463370	6.649425	2.919568
25	1	0	4.036543	6.468002	1.929590
26	1	0	4.117462	5.838540	3.566070
27	1	0	4.088208	7.598358	3.303120

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138547	4.248692	1.913112
2	9	0	5.325642	4.436633	0.800252
3	9	0	5.430785	3.617089	2.930361
4	7	0	6.681780	5.624606	2.415688
5	7	0	7.385143	3.402888	1.526162
6	6	0	5.958401	6.661071	2.850160
7	6	0	6.827114	7.717439	3.213712
8	6	0	8.124236	7.302214	2.989942
9	6	0	8.026690	5.974030	2.483750
10	6	0	9.007590	5.089113	2.094864
11	6	0	8.700478	3.815938	1.620166
12	6	0	9.527194	2.765297	1.175051
13	1	0	10.605337	2.792989	1.132496
14	6	0	8.690927	1.718913	0.813676
15	1	0	8.975196	0.752992	0.427946
16	6	0	7.378743	2.154153	1.045938
17	1	0	6.448552	1.629441	0.889952
18	1	0	10.047062	5.387388	2.158324
19	1	0	6.507902	8.674669	3.597751
20	6	0	9.381779	8.066203	3.221823
21	1	0	10.031672	7.558944	3.939987
22	1	0	9.950572	8.191265	2.296476
23	1	0	9.162330	9.058946	3.614597
24	6	0	4.476889	6.638138	2.914466
25	1	0	4.054853	6.454059	1.924011
26	1	0	4.135564	5.825075	3.559004
27	1	0	4.096807	7.584150	3.297163

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.136129	4.246796	1.908090
2	9	0	5.325697	4.437565	0.788475
3	9	0	5.421721	3.615267	2.926600
4	7	0	6.678525	5.625340	2.413633
5	7	0	7.384305	3.400543	1.526502
6	6	0	5.957043	6.662552	2.846361
7	6	0	6.826043	7.721682	3.214647
8	6	0	8.123639	7.305211	2.994333
9	6	0	8.028634	5.975134	2.487158
10	6	0	9.010379	5.088671	2.104788
11	6	0	8.703460	3.811255	1.626940
12	6	0	9.530759	2.759377	1.187516
13	1	0	10.611301	2.785378	1.150785
14	6	0	8.692657	1.710946	0.821510
15	1	0	8.979958	0.743110	0.437699
16	6	0	7.378751	2.149077	1.046747
17	1	0	6.446133	1.626105	0.887037
18	1	0	10.051859	5.387180	2.175243
19	1	0	6.504593	8.680047	3.599805
20	6	0	9.388294	8.071088	3.215937
21	1	0	10.106021	7.494983	3.808184
22	1	0	9.867996	8.322795	2.264184
23	1	0	9.185336	9.003922	3.746048
24	6	0	4.469144	6.640619	2.907878
25	1	0	4.050099	6.451406	1.915775
26	1	0	4.127516	5.833258	3.561524
27	1	0	4.091796	7.593025	3.283429

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.149524	4.260813	1.946153
2	9	0	5.329080	4.390479	0.833127
3	9	0	5.492177	3.588646	2.968645
4	7	0	6.710226	5.616057	2.411950
5	7	0	7.403168	3.398111	1.525775
6	6	0	5.958933	6.666791	2.839213
7	6	0	6.816435	7.728734	3.206219
8	6	0	8.131933	7.332695	3.005639
9	6	0	8.071514	5.983897	2.497819
10	6	0	9.081086	5.132587	2.131890
11	6	0	8.751711	3.802690	1.623593
12	6	0	9.520910	2.782563	1.177538
13	1	0	10.600319	2.756449	1.114524
14	6	0	8.594566	1.675962	0.776851
15	1	0	8.889287	0.714602	0.378871
16	6	0	7.323375	2.125446	1.015849
17	1	0	6.364504	1.652904	0.871157
18	1	0	10.119443	5.427153	2.203341
19	1	0	6.481434	8.688097	3.581507
20	6	0	9.388197	8.105892	3.246571
21	1	0	10.042126	7.606694	3.975397
22	1	0	9.975989	8.228100	2.325918
23	1	0	9.164338	9.105217	3.632052
24	6	0	4.470341	6.612315	2.883383
25	1	0	4.056755	6.412371	1.887144
26	1	0	4.129740	5.792957	3.529048
27	1	0	4.060672	7.554111	3.257651

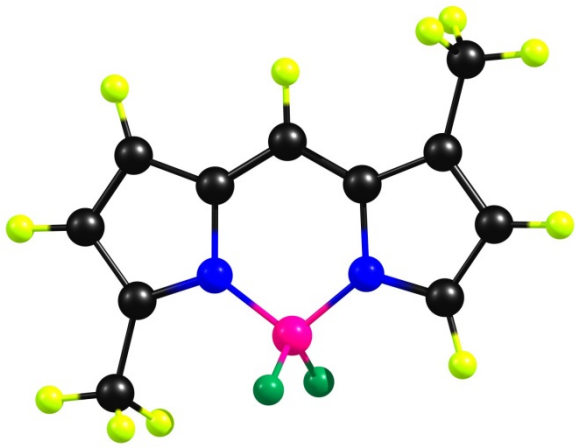

Figure S-11: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.06**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.117956	4.258488	1.911848
2	9	0	5.303249	4.480284	0.812509
3	9	0	5.427616	3.615651	2.927580
4	7	0	6.688983	5.623514	2.435881
5	7	0	7.369317	3.405769	1.489774
6	6	0	5.974618	6.657709	2.900116
7	6	0	6.829093	7.711151	3.282221
8	6	0	8.135816	7.297093	3.037104
9	6	0	8.036613	5.977205	2.503302
10	6	0	9.015201	5.081617	2.083127

11	6	0	8.697921	3.822753	1.586012
12	6	0	9.526150	2.773257	1.110600
13	1	0	10.607021	2.803336	1.062178
14	6	0	8.687608	1.737333	0.733871
15	1	0	8.967288	0.775630	0.324881
16	6	0	7.355089	2.158252	0.980759
17	1	0	10.060091	5.371267	2.144017
18	1	0	6.516381	8.663002	3.690876
19	6	0	9.399648	8.069941	3.266448
20	1	0	10.131550	7.493581	3.845296
21	1	0	9.881563	8.349450	2.320474
22	1	0	9.194531	8.993199	3.816149
23	1	0	4.894718	6.605599	2.942624
24	6	0	6.085610	1.408017	0.745994
25	1	0	5.528522	1.297965	1.682772
26	1	0	5.436636	1.961405	0.058548
27	1	0	6.291437	0.418603	0.330237

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.125371	4.267408	1.917021
2	9	0	5.292820	4.488861	0.816593
3	9	0	5.420839	3.621409	2.936586
4	7	0	6.690664	5.627992	2.439265
5	7	0	7.364224	3.407348	1.490458
6	6	0	5.977294	6.661406	2.904559
7	6	0	6.834072	7.711766	3.284297
8	6	0	8.139143	7.296218	3.036820
9	6	0	8.038710	5.978125	2.503530
10	6	0	9.013392	5.082508	2.082100
11	6	0	8.691926	3.826499	1.586063
12	6	0	9.518744	2.778929	1.109362
13	1	0	10.596962	2.809530	1.059775
14	6	0	8.681686	1.743179	0.732965
15	1	0	8.962664	0.784814	0.324031
16	6	0	7.349596	2.160121	0.980504
17	1	0	10.057329	5.367676	2.139630
18	1	0	6.522691	8.661164	3.692747
19	6	0	9.401569	8.068010	3.266399
20	1	0	10.120820	7.500225	3.864180
21	1	0	9.892008	8.326063	2.321975
22	1	0	9.192411	8.999635	3.794601
23	1	0	4.899483	6.613195	2.949668
24	6	0	6.090774	1.398573	0.741582
25	1	0	5.532007	1.275984	1.673182
26	1	0	5.438789	1.939088	0.050294
27	1	0	6.314241	0.415346	0.327010

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.132420	4.267068	1.915680
2	9	0	5.306452	4.487185	0.818671
3	9	0	5.432000	3.624340	2.930896
4	7	0	6.695611	5.622644	2.435460
5	7	0	7.368423	3.412689	1.493485
6	6	0	5.982949	6.650769	2.896289
7	6	0	6.833959	7.699939	3.276753
8	6	0	8.135913	7.285606	3.032821
9	6	0	8.035115	5.971796	2.502340
10	6	0	9.009918	5.079638	2.085911
11	6	0	8.688647	3.827277	1.591058

12	6	0	9.514287	2.783042	1.118338
13	1	0	10.592287	2.813276	1.071452
14	6	0	8.679024	1.751373	0.741573
15	1	0	8.958145	0.792480	0.333546
16	6	0	7.351811	2.171365	0.986435
17	1	0	10.053094	5.365212	2.146293
18	1	0	6.520603	8.648759	3.684000
19	6	0	9.393033	8.053621	3.257925
20	1	0	10.133338	7.466646	3.807070
21	1	0	9.850303	8.356105	2.311159
22	1	0	9.193631	8.958914	3.831600
23	1	0	4.905372	6.599820	2.938592
24	6	0	6.095474	1.419257	0.747837
25	1	0	5.534064	1.306961	1.677948
26	1	0	5.450801	1.961737	0.052758
27	1	0	6.313557	0.433554	0.339307

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.131349	4.254167	1.945660
2	9	0	5.273514	4.464375	0.866291
3	9	0	5.461978	3.604273	2.983617
4	7	0	6.692720	5.616876	2.451661
5	7	0	7.367696	3.411711	1.493945
6	6	0	5.979702	6.642659	2.920463
7	6	0	6.830787	7.698951	3.291248
8	6	0	8.133503	7.289298	3.033303
9	6	0	8.034428	5.975370	2.503633
10	6	0	9.011052	5.090209	2.067923
11	6	0	8.691379	3.835379	1.573194
12	6	0	9.516183	2.798232	1.079384
13	1	0	10.595200	2.835101	1.015510
14	6	0	8.679849	1.762537	0.708249
15	1	0	8.959114	0.806588	0.288457
16	6	0	7.352580	2.174531	0.977041
17	1	0	10.054503	5.386649	2.112549
18	1	0	6.517483	8.649785	3.698851
19	6	0	9.399773	8.049742	3.270803
20	1	0	9.971108	7.617090	4.099052
21	1	0	10.042821	8.045797	2.385198
22	1	0	9.182144	9.089704	3.523229
23	1	0	4.901097	6.585325	2.971835
24	6	0	6.090030	1.420199	0.737615
25	1	0	5.478215	1.395392	1.642937
26	1	0	5.497888	1.911728	-0.040078
27	1	0	6.314133	0.399402	0.423630

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.179415	4.238760	1.934548
2	9	0	5.316725	4.532490	0.888061
3	9	0	5.504130	3.634231	2.985370
4	7	0	6.748786	5.618682	2.474704
5	7	0	7.396820	3.422124	1.476008
6	6	0	5.949179	6.626069	2.976916
7	6	0	6.756801	7.657793	3.347222
8	6	0	8.176178	7.239686	3.042444
9	6	0	8.099910	5.989473	2.513769
10	6	0	9.114871	5.058120	2.024841
11	6	0	8.743690	3.829696	1.531315
12	6	0	9.532811	2.759507	1.002579

13	1	0	10.610534	2.772571	0.912573
14	6	0	8.657971	1.742320	0.644120
15	1	0	8.909856	0.783051	0.210574
16	6	0	7.346944	2.167150	0.942516
17	1	0	10.157532	5.344329	2.055139
18	1	0	6.464511	8.605915	3.779144
19	6	0	9.367351	8.088362	3.300338
20	1	0	9.438353	8.350572	4.366058
21	1	0	10.296236	7.594128	3.006489
22	1	0	9.295669	9.040506	2.754588
23	1	0	4.878546	6.502604	3.018903
24	6	0	6.059730	1.439748	0.745053
25	1	0	5.530898	1.314083	1.697759
26	1	0	5.387645	2.004578	0.087523
27	1	0	6.239138	0.454524	0.306644

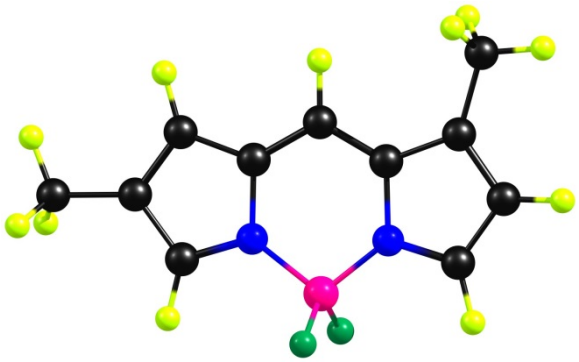

Figure S-12: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.07**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.125667	4.223315	1.979315
2	9	0	5.254707	4.410620	0.923378
3	9	0	5.516212	3.569699	3.033755
4	7	0	6.691372	5.609119	2.462800
5	7	0	7.382337	3.405893	1.500128
6	6	0	5.976108	6.641687	2.925891
7	6	0	6.827567	7.704273	3.292772
8	6	0	8.133857	7.297268	3.038908
9	6	0	8.038273	5.972069	2.514642
10	6	0	9.019061	5.086908	2.081194
11	6	0	8.708508	3.826428	1.578404
12	6	0	9.529126	2.785256	1.071634
13	1	0	10.609372	2.817909	1.000975
14	6	0	8.697754	1.739283	0.687565
15	6	0	7.378247	2.174333	0.974324
16	1	0	10.061571	5.387651	2.129817
17	1	0	6.511711	8.657352	3.696087
18	6	0	9.393930	8.081381	3.248816
19	1	0	10.140902	7.510857	3.813840
20	1	0	9.856955	8.367986	2.295531
21	1	0	9.188996	9.001289	3.804111
22	1	0	4.896979	6.583067	2.979734
23	1	0	6.445374	1.646345	0.821507
24	6	0	9.084087	0.417561	0.090183
25	1	0	8.741454	-0.422460	0.706951
26	1	0	8.652048	0.281300	-0.909066
27	1	0	10.171170	0.335873	-0.005805

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.135568	4.239615	1.947744
2	9	0	5.285244	4.449576	0.862932
3	9	0	5.467379	3.574543	2.974971
4	7	0	6.694516	5.607679	2.466097
5	7	0	7.384851	3.408004	1.495492
6	6	0	5.980208	6.629646	2.951508
7	6	0	6.832239	7.689381	3.318819
8	6	0	8.135956	7.291614	3.041664
9	6	0	8.040607	5.973849	2.503518
10	6	0	9.019306	5.095251	2.059129
11	6	0	8.707640	3.834757	1.562355
12	6	0	9.527966	2.791478	1.061369
13	1	0	10.605244	2.827302	0.986253
14	6	0	8.697897	1.739878	0.694297
15	6	0	7.379753	2.170813	0.983085
16	1	0	10.059451	5.397300	2.098566
17	1	0	6.517477	8.632487	3.739064
18	6	0	9.392263	8.079857	3.246223
19	1	0	10.146871	7.506911	3.792942
20	1	0	9.836921	8.380581	2.291699
21	1	0	9.187764	8.988332	3.814996
22	1	0	4.904179	6.568241	3.019649
23	1	0	6.450157	1.638459	0.840438
24	6	0	9.083727	0.412839	0.111889
25	1	0	8.763951	-0.415214	0.751832
26	1	0	8.629748	0.258189	-0.871698
27	1	0	10.166465	0.340894	-0.007442

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.143811	4.240849	1.947291
2	9	0	5.299066	4.449786	0.866630
3	9	0	5.480714	3.578691	2.970521
4	7	0	6.700934	5.603490	2.463144
5	7	0	7.389637	3.414165	1.497520
6	6	0	5.987835	6.620146	2.944901
7	6	0	6.834746	7.678424	3.312543
8	6	0	8.135046	7.281630	3.037908
9	6	0	8.038615	5.968377	2.502220
10	6	0	9.016835	5.093751	2.060789
11	6	0	8.705245	3.836977	1.564973
12	6	0	9.524219	2.798075	1.066204
13	1	0	10.601209	2.833775	0.992124
14	6	0	8.695933	1.750359	0.699107
15	6	0	7.382554	2.182994	0.987095
16	1	0	10.056187	5.396691	2.101661
17	1	0	6.518606	8.621073	3.731759
18	6	0	9.386743	8.064266	3.240639
19	1	0	10.143000	7.486914	3.778109
20	1	0	9.824323	8.370789	2.285940
21	1	0	9.186054	8.967836	3.816461
22	1	0	4.912018	6.556463	3.010832
23	1	0	6.451806	1.653187	0.844287
24	6	0	9.077961	0.429025	0.119181
25	1	0	8.758601	-0.397158	0.759793
26	1	0	8.622305	0.275330	-0.862489
27	1	0	10.159344	0.356360	-0.001753

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.141638	4.234671	1.960616
2	9	0	5.285537	4.441625	0.882921
3	9	0	5.486908	3.568935	2.992792
4	7	0	6.697870	5.600673	2.473032
5	7	0	7.388150	3.412250	1.501495
6	6	0	5.985046	6.615406	2.961479
7	6	0	6.832331	7.679943	3.321557
8	6	0	8.132750	7.287054	3.035162
9	6	0	8.038154	5.973618	2.499027
10	6	0	9.017152	5.104538	2.042157
11	6	0	8.706339	3.843107	1.550403
12	6	0	9.524160	2.806808	1.040846
13	1	0	10.602085	2.845846	0.950966
14	6	0	8.694629	1.753484	0.686318
15	6	0	7.381607	2.179371	0.991431
16	1	0	10.056862	5.416428	2.068459
17	1	0	6.517444	8.624746	3.741865
18	6	0	9.393104	8.061876	3.255358
19	1	0	9.986519	7.628237	4.067388
20	1	0	10.018643	8.077720	2.357394
21	1	0	9.164877	9.095452	3.523954
22	1	0	4.908224	6.547109	3.034707
23	1	0	6.450652	1.643337	0.860355
24	6	0	9.078345	0.428604	0.100181
25	1	0	8.776138	-0.398418	0.750394
26	1	0	8.607478	0.272201	-0.875460
27	1	0	10.160705	0.367641	-0.037406

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.224050	4.103282	2.326311
2	9	0	5.114136	4.046982	1.504947
3	9	0	5.990221	3.492850	3.549119
4	7	0	6.731742	5.550116	2.487614
5	7	0	7.423388	3.346010	1.634036
6	6	0	5.971087	6.635644	2.747625
7	6	0	6.791390	7.738850	3.054006
8	6	0	8.117760	7.325359	2.982994
9	6	0	8.086311	5.933609	2.604342
10	6	0	9.098384	5.058876	2.301111
11	6	0	8.760615	3.756413	1.720109
12	6	0	9.519297	2.813943	1.108502
13	1	0	10.594462	2.817635	0.981831
14	6	0	8.588414	1.743945	0.603705
15	6	0	7.327435	2.158014	0.954109
16	1	0	10.138300	5.343634	2.390409
17	1	0	6.439566	8.733637	3.296689
18	6	0	9.357813	8.132736	3.196601
19	1	0	9.974681	7.727096	4.010467
20	1	0	9.991226	8.153265	2.298564
21	1	0	9.111331	9.167805	3.452003
22	1	0	4.892398	6.568378	2.721362
23	1	0	6.366108	1.693674	0.795891
24	6	0	9.007851	0.512779	-0.104299
25	1	0	8.153292	-0.111279	-0.377934
26	1	0	9.570439	0.755648	-1.019050
27	1	0	9.691649	-0.086638	0.516328

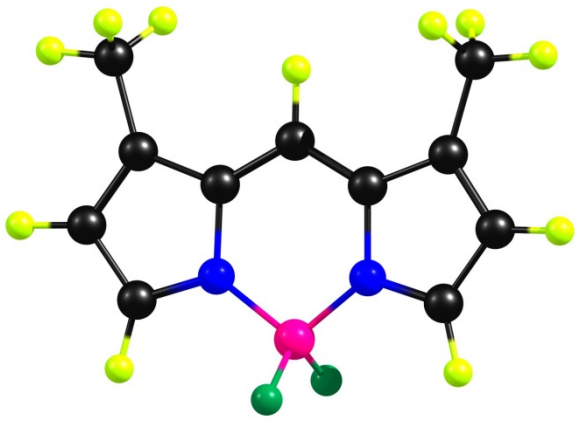

Figure S-13: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.08**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.136093	4.184600	2.061034
2	9	0	5.196238	4.307370	1.056530
3	9	0	5.611306	3.560977	3.178345
4	7	0	6.694260	5.600961	2.455611
5	7	0	7.383057	3.380444	1.539757
6	6	0	5.977308	6.661207	2.847665
7	6	0	6.830500	7.725876	3.205022
8	6	0	8.139313	7.290227	3.020715
9	6	0	8.043325	5.946882	2.545212
10	6	0	9.025321	5.041189	2.157145
11	6	0	8.714682	3.782588	1.652549
12	6	0	9.550286	2.741589	1.144630
13	6	0	8.691044	1.727930	0.731171
14	6	0	7.373708	2.159551	0.990956
15	1	0	10.068639	5.333951	2.231995
16	1	0	6.514172	8.700340	3.553137
17	6	0	9.402605	8.065189	3.245422
18	1	0	10.105699	7.522362	3.888943
19	1	0	9.922483	8.276454	2.301928
20	1	0	9.187652	9.024882	3.724315
21	1	0	4.896150	6.619337	2.860800
22	1	0	6.438994	1.645580	0.809375
23	1	0	8.970531	0.781629	0.287065
24	6	0	11.046666	2.765133	1.059416
25	1	0	11.400397	3.512042	0.336860
26	1	0	11.507007	3.004862	2.025718
27	1	0	11.431309	1.791870	0.741038

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139418	4.216959	1.985063
2	9	0	5.275799	4.394555	0.904956
3	9	0	5.483449	3.579165	3.038056
4	7	0	6.697562	5.600792	2.461576
5	7	0	7.386992	3.378272	1.544891
6	6	0	5.982709	6.641481	2.904264
7	6	0	6.836888	7.702989	3.262096
8	6	0	8.142383	7.285930	3.025038
9	6	0	8.045668	5.955527	2.519253

10	6	0	9.025833	5.060135	2.111603
11	6	0	8.715668	3.795643	1.628398
12	6	0	9.551672	2.742780	1.151197
13	6	0	8.696801	1.707151	0.789095
14	6	0	7.380078	2.136756	1.046280
15	1	0	10.066037	5.359509	2.168096
16	1	0	6.522038	8.660280	3.648918
17	6	0	9.402153	8.067033	3.236558
18	1	0	10.123102	7.516518	3.848333
19	1	0	9.891883	8.304107	2.286338
20	1	0	9.189403	9.010302	3.742128
21	1	0	4.904930	6.591754	2.950588
22	1	0	6.451090	1.607368	0.894772
23	1	0	8.976956	0.746314	0.384778
24	6	0	11.045407	2.769641	1.051622
25	1	0	11.384847	3.491188	0.301216
26	1	0	11.510710	3.043287	2.003312
27	1	0	11.429270	1.789589	0.763928

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.150860	4.208763	2.013583
2	9	0	5.252195	4.361221	0.968130
3	9	0	5.548037	3.576567	3.092891
4	7	0	6.704846	5.599081	2.454719
5	7	0	7.390928	3.387290	1.542454
6	6	0	5.990561	6.641793	2.874837
7	6	0	6.839919	7.701374	3.233604
8	6	0	8.142977	7.276786	3.020533
9	6	0	8.045319	5.946859	2.528090
10	6	0	9.024827	5.051222	2.132425
11	6	0	8.712901	3.794715	1.640483
12	6	0	9.546793	2.751183	1.154236
13	6	0	8.692838	1.728020	0.770191
14	6	0	7.380931	2.159533	1.026284
15	1	0	10.065250	5.346411	2.199164
16	1	0	6.523271	8.663718	3.605029
17	6	0	9.398815	8.049764	3.235277
18	1	0	10.126625	7.484609	3.822820
19	1	0	9.874283	8.310276	2.285075
20	1	0	9.192398	8.979238	3.766133
21	1	0	4.912362	6.594568	2.906289
22	1	0	6.449807	1.638193	0.862129
23	1	0	8.970845	0.773392	0.350999
24	6	0	11.033916	2.778464	1.062189
25	1	0	11.373549	3.484155	0.298368
26	1	0	11.492703	3.073366	2.009251
27	1	0	11.420990	1.794461	0.797173

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142635	4.219247	1.981994
2	9	0	5.284049	4.398742	0.901156
3	9	0	5.487753	3.582538	3.033138
4	7	0	6.700634	5.598085	2.458153
5	7	0	7.387542	3.383608	1.544735
6	6	0	5.987843	6.634809	2.898841
7	6	0	6.839182	7.695964	3.259598
8	6	0	8.142216	7.277119	3.024676
9	6	0	8.044429	5.952084	2.519631
10	6	0	9.024928	5.058557	2.114724

11	6	0	8.712979	3.796788	1.630628
12	6	0	9.547087	2.748043	1.156552
13	6	0	8.694721	1.714006	0.792194
14	6	0	7.380001	2.146720	1.047616
15	1	0	10.067560	5.357048	2.175145
16	1	0	6.524890	8.654879	3.647261
17	6	0	9.406514	8.049592	3.231221
18	1	0	10.148923	7.464776	3.783290
19	1	0	9.854221	8.338781	2.274364
20	1	0	9.211745	8.963286	3.796755
21	1	0	4.908592	6.580785	2.941653
22	1	0	6.446936	1.621413	0.896031
23	1	0	8.976289	0.751960	0.387513
24	6	0	11.039428	2.785341	1.059858
25	1	0	11.367424	3.460462	0.262188
26	1	0	11.494077	3.128212	1.994574
27	1	0	11.436147	1.792176	0.838864

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.203492	4.172710	2.166585
2	9	0	5.168138	4.167203	1.252791
3	9	0	5.867887	3.498286	3.330282
4	7	0	6.726569	5.590743	2.434671
5	7	0	7.436665	3.393411	1.536231
6	6	0	5.971665	6.673144	2.745539
7	6	0	6.798267	7.739006	3.133475
8	6	0	8.122290	7.306554	3.063927
9	6	0	8.078618	5.941691	2.608379
10	6	0	9.092428	5.064627	2.302233
11	6	0	8.776048	3.774841	1.684233
12	6	0	9.550470	2.810777	1.118790
13	6	0	8.600308	1.764943	0.582852
14	6	0	7.338436	2.193129	0.861633
15	1	0	10.127793	5.345007	2.441986
16	1	0	6.457793	8.723960	3.426632
17	6	0	9.368536	8.079078	3.357529
18	1	0	9.958541	7.614257	4.159724
19	1	0	10.025303	8.145818	2.478626
20	1	0	9.131076	9.100272	3.671061
21	1	0	4.893340	6.625100	2.686431
22	1	0	6.371347	1.758630	0.663563
23	1	0	8.895374	0.853960	0.078867
24	6	0	11.028485	2.731761	0.997267
25	1	0	11.329998	2.654195	-0.057555
26	1	0	11.524665	3.602069	1.432994
27	1	0	11.415213	1.829852	1.493609

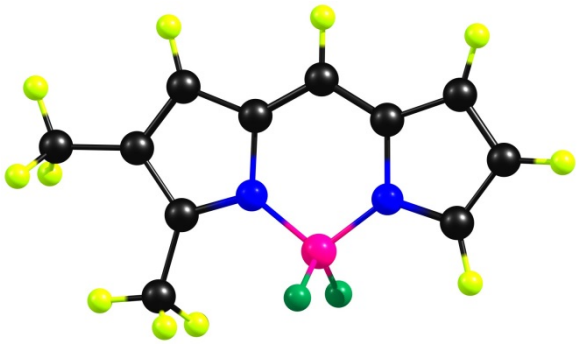

Figure S-14: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.09**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.133855	4.244621	1.896647
2	9	0	5.334078	4.426998	0.779435
3	9	0	5.431765	3.633953	2.923887
4	7	0	6.692126	5.634229	2.385111
5	7	0	7.391407	3.387415	1.522355
6	6	0	5.966741	6.684212	2.806455
7	6	0	6.835907	7.762514	3.165633
8	6	0	8.126343	7.313866	2.940931
9	6	0	8.042754	5.982390	2.452340
10	6	0	9.026399	5.082703	2.074814
11	6	0	8.717655	3.800118	1.614561
12	6	0	9.544797	2.734934	1.182956
13	6	0	8.704246	1.682907	0.832191
14	6	0	7.386419	2.126844	1.056400
15	1	0	10.068112	5.382828	2.138350
16	1	0	6.453186	1.601160	0.904509
17	1	0	8.987985	0.708542	0.458928
18	1	0	10.626106	2.759076	1.142624
19	1	0	9.045763	7.863049	3.102145
20	6	0	6.404717	9.104158	3.681432
21	1	0	5.763713	9.632291	2.964209
22	1	0	5.839033	9.020674	4.618050
23	1	0	7.273607	9.739882	3.876961
24	6	0	4.475012	6.644101	2.859576
25	1	0	4.064754	6.437719	1.864975
26	1	0	4.139714	5.829201	3.510460
27	1	0	4.068347	7.588847	3.227479

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.144990	4.241926	1.895907
2	9	0	5.330324	4.418133	0.774334
3	9	0	5.429162	3.623674	2.924504
4	7	0	6.688474	5.631963	2.384525
5	7	0	7.394943	3.385195	1.521900
6	6	0	5.962756	6.681761	2.805774
7	6	0	6.833927	7.757750	3.163297
8	6	0	8.122462	7.309458	2.938427
9	6	0	8.039039	5.978517	2.450493
10	6	0	9.023801	5.083781	2.074632
11	6	0	8.717912	3.801634	1.614955
12	6	0	9.546047	2.739543	1.184459
13	6	0	8.707791	1.685840	0.833659
14	6	0	7.390475	2.124190	1.056178
15	1	0	10.062415	5.386245	2.138647
16	1	0	6.461529	1.595760	0.903631
17	1	0	8.993691	0.714625	0.461665
18	1	0	10.624681	2.764894	1.144245
19	1	0	9.040958	7.855687	3.098031
20	6	0	6.405256	9.098917	3.678552
21	1	0	5.766550	9.624397	2.961543
22	1	0	5.842464	9.013983	4.613553
23	1	0	7.273871	9.730926	3.872162
24	6	0	4.473698	6.654373	2.864099
25	1	0	4.054931	6.455701	1.873844
26	1	0	4.130507	5.848152	3.518063
27	1	0	4.081888	7.602208	3.232338

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.148596	4.249915	1.897992
2	9	0	5.339383	4.427595	0.781130
3	9	0	5.436946	3.635789	2.922764
4	7	0	6.693720	5.632392	2.384273
5	7	0	7.393564	3.395978	1.525578
6	6	0	5.970241	6.676019	2.803190
7	6	0	6.836034	7.750350	3.160923
8	6	0	8.121217	7.304223	2.937279
9	6	0	8.036212	5.977515	2.450635
10	6	0	9.018413	5.085411	2.076008
11	6	0	8.709808	3.807229	1.617537
12	6	0	9.534894	2.748495	1.188538
13	6	0	8.697071	1.699399	0.838980
14	6	0	7.385328	2.140889	1.062022
15	1	0	10.056876	5.386397	2.139887
16	1	0	6.454429	1.616054	0.910477
17	1	0	8.979954	0.727750	0.466927
18	1	0	10.613211	2.772934	1.148397
19	1	0	9.039635	7.849806	3.097060
20	6	0	6.403065	9.083131	3.673488
21	1	0	5.764591	9.604919	2.955139
22	1	0	5.838961	8.994116	4.606108
23	1	0	7.267484	9.718262	3.869518
24	6	0	4.488426	6.646371	2.859877
25	1	0	4.073090	6.445932	1.869613
26	1	0	4.148114	5.839379	3.512787
27	1	0	4.095276	7.592981	3.227289

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.150875	4.235723	1.927653
2	9	0	5.313234	4.405115	0.826052
3	9	0	5.464980	3.617751	2.974404
4	7	0	6.695760	5.626718	2.398045
5	7	0	7.394857	3.390295	1.533769
6	6	0	5.974159	6.673443	2.807852
7	6	0	6.839437	7.754127	3.156857
8	6	0	8.125678	7.309089	2.937894
9	6	0	8.043556	5.975005	2.460377
10	6	0	9.024825	5.082920	2.084169
11	6	0	8.715203	3.800320	1.623073
12	6	0	9.538037	2.743512	1.185612
13	6	0	8.695993	1.693744	0.832831
14	6	0	7.384196	2.135488	1.063564
15	1	0	10.065725	5.384507	2.144174
16	1	0	6.449426	1.613446	0.913958
17	1	0	8.977728	0.722672	0.453168
18	1	0	10.618339	2.766980	1.140157
19	1	0	9.044435	7.859714	3.093356
20	6	0	6.394628	9.093640	3.657486
21	1	0	5.744212	9.596889	2.934484
22	1	0	5.838161	9.006952	4.596847
23	1	0	7.255726	9.741045	3.839137
24	6	0	4.485493	6.653079	2.849235
25	1	0	4.080250	6.692577	1.833031
26	1	0	4.125619	5.727498	3.304422
27	1	0	4.104009	7.506983	3.411810

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.173647	4.222319	2.015757
2	9	0	5.257115	4.363699	0.983050
3	9	0	5.579068	3.649587	3.132955
4	7	0	6.713603	5.650147	2.422110
5	7	0	7.407907	3.420527	1.552707
6	6	0	5.915177	6.703951	2.830987
7	6	0	6.741991	7.765779	3.134207
8	6	0	8.143188	7.296528	2.880217
9	6	0	8.071483	6.012110	2.452619
10	6	0	9.109881	5.074823	2.052327
11	6	0	8.759504	3.822331	1.607578
12	6	0	9.549375	2.733749	1.118197
13	6	0	8.673612	1.711646	0.774785
14	6	0	7.369094	2.164831	1.052210
15	1	0	10.145465	5.386065	2.093280
16	1	0	6.424932	1.654806	0.920469
17	1	0	8.925936	0.741911	0.366718
18	1	0	10.627584	2.741051	1.033768
19	1	0	9.037482	7.891048	3.018109
20	6	0	6.397802	9.121714	3.621796
21	1	0	6.770227	9.894404	2.931154
22	1	0	5.320993	9.260072	3.742684
23	1	0	6.883566	9.327536	4.588440
24	6	0	4.425993	6.579294	2.901102
25	1	0	4.002747	6.358188	1.916016
26	1	0	4.136830	5.756716	3.563790
27	1	0	3.980338	7.504399	3.276383

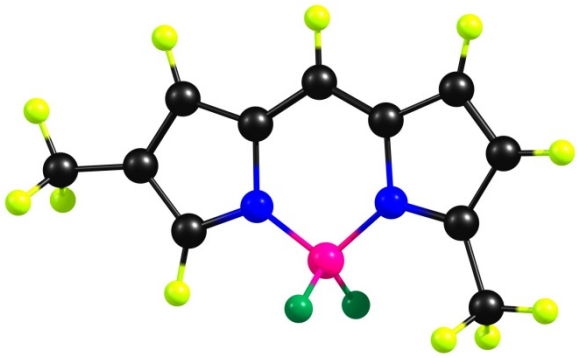

Figure S-15: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.10**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.130079	4.269819	1.867167
2	9	0	5.335006	4.482455	0.752272
3	9	0	5.418745	3.650694	2.882566
4	7	0	6.704731	5.638952	2.379148
5	7	0	7.380985	3.400556	1.478597
6	6	0	5.991744	6.686403	2.816147
7	6	0	6.841826	7.754041	3.199592
8	6	0	8.137737	7.302215	2.972243
9	6	0	8.051954	5.982322	2.460265
10	6	0	9.031575	5.073782	2.067027
11	6	0	8.711503	3.809809	1.586094
12	6	0	9.538347	2.746863	1.138574
13	6	0	8.697573	1.711010	0.767174
14	6	0	7.364817	2.145280	0.989114
15	1	0	10.076668	5.360208	2.137786

16	1	0	8.975808	0.740929	0.377474
17	1	0	10.619946	2.768638	1.104566
18	1	0	9.057335	7.846407	3.148577
19	6	0	6.405221	9.086068	3.736835
20	1	0	5.767712	9.622998	3.023467
21	1	0	5.832208	8.981450	4.666521
22	1	0	7.269831	9.721794	3.951122
23	1	0	4.910241	6.641899	2.841279
24	6	0	6.094122	1.399295	0.747789
25	1	0	5.522672	1.306522	1.677799
26	1	0	5.458388	1.945157	0.042129
27	1	0	6.300209	0.402407	0.350462

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.136676	4.278643	1.871057
2	9	0	5.324735	4.490885	0.754066
3	9	0	5.410179	3.656782	2.889613
4	7	0	6.704962	5.643748	2.381504
5	7	0	7.375332	3.402078	1.479129
6	6	0	5.992052	6.691206	2.819145
7	6	0	6.844765	7.754643	3.200397
8	6	0	8.139140	7.302156	2.971885
9	6	0	8.051117	5.983211	2.460244
10	6	0	9.027935	5.075060	2.066461
11	6	0	8.704789	3.813727	1.586729
12	6	0	9.530773	2.752589	1.139221
13	6	0	8.691957	1.716517	0.768103
14	6	0	7.359331	2.146747	0.989455
15	1	0	10.071607	5.358453	2.135400
16	1	0	8.971952	0.749568	0.379225
17	1	0	10.609761	2.775156	1.104871
18	1	0	9.058201	7.842749	3.146272
19	6	0	6.410129	9.085820	3.737697
20	1	0	5.774681	9.619533	3.024369
21	1	0	5.839777	8.978418	4.665403
22	1	0	7.273703	9.718750	3.950708
23	1	0	4.912574	6.649529	2.846052
24	6	0	6.099656	1.388901	0.743848
25	1	0	5.526326	1.283255	1.668685
26	1	0	5.460929	1.921629	0.034326
27	1	0	6.323947	0.398218	0.347917

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142899	4.279251	1.870608
2	9	0	5.336674	4.491083	0.757864
3	9	0	5.421173	3.660326	2.885096
4	7	0	6.709816	5.638883	2.379095
5	7	0	7.377893	3.408313	1.481439
6	6	0	5.997871	6.679974	2.814063
7	6	0	6.845055	7.742351	3.195452
8	6	0	8.136277	7.292406	2.968437
9	6	0	8.047859	5.977988	2.458452
10	6	0	9.023643	5.073432	2.066534
11	6	0	8.699803	3.815859	1.588243
12	6	0	9.523977	2.758458	1.142661
13	6	0	8.686506	1.726248	0.772737
14	6	0	7.359142	2.159073	0.994333
15	1	0	10.066748	5.356682	2.135821
16	1	0	8.964068	0.758951	0.384000

17	1	0	10.602626	2.780957	1.108706
18	1	0	9.054775	7.833115	3.143203
19	6	0	6.409440	9.066489	3.729889
20	1	0	5.775570	9.598479	3.015619
21	1	0	5.837878	8.957194	4.655272
22	1	0	7.270828	9.699811	3.944836
23	1	0	4.918706	6.635398	2.839510
24	6	0	6.101634	1.410342	0.751773
25	1	0	5.530744	1.309749	1.677519
26	1	0	5.465843	1.947717	0.044645
27	1	0	6.319537	0.419439	0.355975

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142455	4.270698	1.892163
2	9	0	5.311992	4.471898	0.790646
3	9	0	5.443129	3.649160	2.927092
4	7	0	6.709361	5.636419	2.385650
5	7	0	7.378037	3.405712	1.483417
6	6	0	5.996601	6.676295	2.827301
7	6	0	6.843519	7.742410	3.201484
8	6	0	8.137079	7.297934	2.964436
9	6	0	8.050203	5.982266	2.454838
10	6	0	9.027938	5.077973	2.055494
11	6	0	8.704568	3.817972	1.579058
12	6	0	9.527754	2.760969	1.124052
13	6	0	8.687959	1.726170	0.760300
14	6	0	7.359729	2.157756	0.994627
15	1	0	10.072626	5.365857	2.116843
16	1	0	8.964085	0.757800	0.367766
17	1	0	10.608130	2.784610	1.080260
18	1	0	9.055130	7.845322	3.134278
19	6	0	6.406076	9.073513	3.733883
20	1	0	5.876379	9.654763	2.972095
21	1	0	5.733875	8.960241	4.589900
22	1	0	7.268874	9.659068	4.060607
23	1	0	4.916167	6.626892	2.863807
24	6	0	6.096176	1.407599	0.748733
25	1	0	5.461688	1.417844	1.638592
26	1	0	5.527964	1.875716	-0.060630
27	1	0	6.319491	0.375115	0.475091

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.172072	4.249366	1.918823
2	9	0	5.308064	4.472470	0.854060
3	9	0	5.501224	3.659368	2.982757
4	7	0	6.729633	5.642827	2.400037
5	7	0	7.405032	3.425636	1.492344
6	6	0	5.941409	6.670596	2.852565
7	6	0	6.743617	7.732625	3.192212
8	6	0	8.149706	7.282508	2.909003
9	6	0	8.082308	6.014679	2.432978
10	6	0	9.116532	5.081609	1.992945
11	6	0	8.755262	3.837555	1.541994
12	6	0	9.551145	2.748460	1.055672
13	6	0	8.680973	1.721821	0.728779
14	6	0	7.362463	2.156923	1.004747
15	1	0	10.154108	5.386043	2.026870
16	1	0	8.935000	0.747691	0.330801
17	1	0	10.629343	2.760786	0.972109
18	1	0	9.040842	7.877388	3.063226
19	6	0	6.362602	9.059557	3.727095
20	1	0	6.711652	9.867245	3.065171

21	1	0	5.280674	9.155167	3.849282
22	1	0	6.841349	9.245078	4.701117
23	1	0	4.868493	6.561928	2.896887
24	6	0	6.080745	1.417374	0.824454
25	1	0	5.545942	1.327105	1.778089
26	1	0	5.410857	1.958464	0.144849
27	1	0	6.265935	0.417700	0.422919

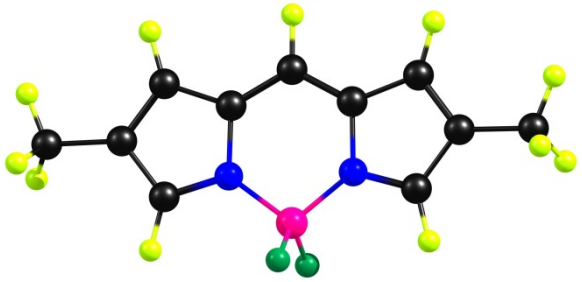

Figure S-16: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.11**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.142551	4.219685	1.993371
2	9	0	5.232416	4.365455	0.965199
3	9	0	5.582122	3.589773	3.088690
4	7	0	6.705503	5.626160	2.419337
5	7	0	7.394144	3.406238	1.495020
6	6	0	5.990059	6.680699	2.830340
7	6	0	6.836964	7.758688	3.196066
8	6	0	8.133906	7.304509	2.985601
9	6	0	8.052870	5.973690	2.498675
10	6	0	9.036115	5.073105	2.099509
11	6	0	8.723233	3.812690	1.598891
12	6	0	9.541399	2.767292	1.096407
13	6	0	8.705834	1.734173	0.687595
14	6	0	7.386112	2.180362	0.956506
15	1	0	10.078971	5.368856	2.166160
16	1	0	10.622784	2.790601	1.041175
17	1	0	9.051514	7.855770	3.150205
18	6	0	6.393880	9.102055	3.698165
19	1	0	5.767790	9.623847	2.963752
20	1	0	5.806396	9.017131	4.620740
21	1	0	7.255744	9.741474	3.912187
22	1	0	4.908414	6.635004	2.851584
23	1	0	6.450429	1.664145	0.781830
24	6	0	9.088552	0.415468	0.081292
25	1	0	8.736698	-0.427886	0.688292
26	1	0	8.662590	0.290855	-0.922025
27	1	0	10.175763	0.328567	-0.007550

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.145321	4.260723	1.896996
2	9	0	5.308161	4.457779	0.800085
3	9	0	5.463183	3.619236	2.929497
4	7	0	6.706004	5.636114	2.397792

5	7	0	7.394971	3.414902	1.472941
6	6	0	5.992238	6.671702	2.857577
7	6	0	6.840288	7.747195	3.219331
8	6	0	8.133230	7.313959	2.954564
9	6	0	8.050269	5.994206	2.440904
10	6	0	9.031596	5.105053	2.019299
11	6	0	8.719242	3.837451	1.542889
12	6	0	9.539006	2.781776	1.067480
13	6	0	8.707583	1.727086	0.712712
14	6	0	7.388948	2.168748	0.982664
15	1	0	10.070896	5.409084	2.063332
16	1	0	10.617014	2.811933	1.000849
17	1	0	9.049034	7.867061	3.105672
18	6	0	6.400044	9.069896	3.772263
19	1	0	5.737214	9.595158	3.077875
20	1	0	5.856471	8.950704	4.714463
21	1	0	7.259100	9.715548	3.963908
22	1	0	4.914427	6.615384	2.913893
23	1	0	6.458431	1.637559	0.841258
24	6	0	9.092868	0.388302	0.157464
25	1	0	8.765117	-0.426745	0.809918
26	1	0	8.645893	0.217704	-0.826674
27	1	0	10.176201	0.310889	0.048062

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.152597	4.263390	1.895991
2	9	0	5.321911	4.460815	0.802830
3	9	0	5.474243	3.625089	2.923825
4	7	0	6.712459	5.632648	2.395315
5	7	0	7.398269	3.421632	1.474819
6	6	0	5.999968	6.662084	2.852483
7	6	0	6.842872	7.736030	3.214901
8	6	0	8.132534	7.304812	2.951833
9	6	0	8.048634	5.989682	2.439568
10	6	0	9.028508	5.103858	2.019889
11	6	0	8.715384	3.840106	1.544655
12	6	0	9.533415	2.788496	1.071403
13	6	0	8.703459	1.737689	0.717347
14	6	0	7.389802	2.181383	0.986866
15	1	0	10.067317	5.407474	2.064558
16	1	0	10.611117	2.818331	1.005431
17	1	0	9.048044	7.857536	3.103560
18	6	0	6.402049	9.051645	3.765327
19	1	0	5.739359	9.574683	3.070938
20	1	0	5.858866	8.930566	4.706181
21	1	0	7.258947	9.698161	3.957366
22	1	0	4.922453	6.603180	2.907035
23	1	0	6.457920	1.652977	0.845918
24	6	0	9.084292	0.404369	0.164751
25	1	0	8.755742	-0.408550	0.817540
26	1	0	8.636298	0.235133	-0.817880
27	1	0	10.166292	0.325187	0.054566

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.152429	4.262302	1.898400
2	9	0	5.317891	4.459774	0.802422
3	9	0	5.473894	3.621968	2.930731
4	7	0	6.712765	5.633082	2.396213
5	7	0	7.398968	3.420986	1.475126

6	6	0	6.000380	6.657995	2.866729
7	6	0	6.842550	7.737631	3.219718
8	6	0	8.133062	7.316343	2.936763
9	6	0	8.050968	6.000256	2.421985
10	6	0	9.031468	5.116377	1.992100
11	6	0	8.718987	3.846779	1.525305
12	6	0	9.536503	2.792101	1.052927
13	6	0	8.705056	1.733513	0.719679
14	6	0	7.391145	2.174618	0.999908
15	1	0	10.071413	5.425932	2.023421
16	1	0	10.615582	2.823673	0.975340
17	1	0	9.048209	7.876378	3.079220
18	6	0	6.397009	9.055025	3.778032
19	1	0	5.808377	9.620281	3.048205
20	1	0	5.776788	8.920059	4.669524
21	1	0	7.257246	9.667232	4.059501
22	1	0	4.922583	6.589867	2.938229
23	1	0	6.457983	1.640232	0.877265
24	6	0	9.084417	0.391690	0.170728
25	1	0	8.673677	-0.418503	0.781078
26	1	0	8.712711	0.257568	-0.850299
27	1	0	10.170690	0.275245	0.148767

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.260496	4.100718	2.387697
2	9	0	5.125114	4.044654	1.601351
3	9	0	6.062630	3.491971	3.617681
4	7	0	6.768256	5.550465	2.535496
5	7	0	7.439604	3.353764	1.657804
6	6	0	6.010116	6.629859	2.820755
7	6	0	6.823836	7.751420	3.108244
8	6	0	8.143653	7.321395	2.991409
9	6	0	8.124496	5.943050	2.611750
10	6	0	9.130415	5.067702	2.276806
11	6	0	8.779280	3.768958	1.705860
12	6	0	9.524132	2.828378	1.071267
13	6	0	8.586252	1.760124	0.591371
14	6	0	7.331598	2.169003	0.977521
15	1	0	10.171294	5.357038	2.335810
16	1	0	10.595493	2.836982	0.915860
17	1	0	9.039140	7.915762	3.119021
18	6	0	6.329009	9.127180	3.443022
19	1	0	6.282525	9.768395	2.552301
20	1	0	5.322523	9.096063	3.873844
21	1	0	6.988614	9.621988	4.164185
22	1	0	4.930877	6.555759	2.832293
23	1	0	6.369158	1.698648	0.844951
24	6	0	8.987075	0.529924	-0.129854
25	1	0	8.125274	-0.092707	-0.383567
26	1	0	9.526790	0.774100	-1.057887
27	1	0	9.685098	-0.072187	0.472025

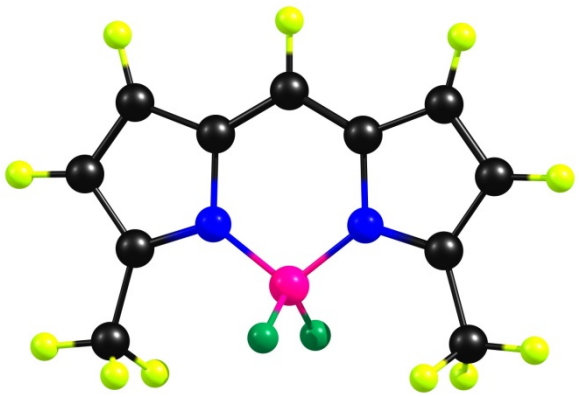

Figure S-17: DFT B3LYP/6-31G(d) optimised ground-state structure of **2.12**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.128107	4.267794	1.868031
2	9	0	5.334564	4.487945	0.748398
3	9	0	5.407901	3.626729	2.869072
4	7	0	6.686885	5.633022	2.403132
5	7	0	7.378937	3.405750	1.474691
6	6	0	5.960543	6.676943	2.852184
7	6	0	6.835668	7.720822	3.245839
8	6	0	8.131406	7.282635	3.023084
9	6	0	8.037735	5.970616	2.493513
10	6	0	9.021858	5.072438	2.094722
11	6	0	8.708036	3.813350	1.594253
12	6	0	9.537299	2.757967	1.136973
13	6	0	8.698303	1.726193	0.746981
14	6	0	7.365259	2.156061	0.967661
15	1	0	10.065079	5.362518	2.176445
16	1	0	10.619050	2.780512	1.108716
17	1	0	9.053994	7.817421	3.208360
18	1	0	8.979369	0.761696	0.345571
19	1	0	6.520323	8.675792	3.644554
20	6	0	6.096870	1.411295	0.709071
21	1	0	5.520255	1.303310	1.634170
22	1	0	5.463977	1.964299	0.006513
23	1	0	6.308181	0.420453	0.299385
24	6	0	4.467881	6.653968	2.894473
25	1	0	4.058451	6.487755	1.892127
26	1	0	4.114735	5.826797	3.519797
27	1	0	4.078808	7.595388	3.290216

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134065	4.269292	1.868856
2	9	0	5.325936	4.486207	0.746097
3	9	0	5.400408	3.623379	2.871481
4	7	0	6.682136	5.633732	2.403564
5	7	0	7.375367	3.402742	1.473574
6	6	0	5.957421	6.678790	2.853208
7	6	0	6.836131	7.718523	3.244501
8	6	0	8.129644	7.277776	3.020247
9	6	0	8.033515	5.967595	2.491740
10	6	0	9.016409	5.071303	2.093433

11	6	0	8.702631	3.814213	1.594099
12	6	0	9.532885	2.761801	1.137761
13	6	0	8.697354	1.728650	0.747621
14	6	0	7.363772	2.152810	0.966552
15	1	0	10.057405	5.360960	2.174539
16	1	0	10.612011	2.786504	1.109972
17	1	0	9.051147	7.809748	3.203915
18	1	0	8.981738	0.767564	0.347489
19	1	0	6.525510	8.672311	3.642582
20	6	0	6.107290	1.394941	0.702913
21	1	0	5.528570	1.274263	1.622416
22	1	0	5.471611	1.934489	-0.004030
23	1	0	6.337750	0.410407	0.295187
24	6	0	4.467417	6.672454	2.902848
25	1	0	4.048156	6.515499	1.905575
26	1	0	4.105147	5.855197	3.531989
27	1	0	4.098050	7.618317	3.299798

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138111	4.270471	1.869028
2	9	0	5.335861	4.487473	0.750550
3	9	0	5.409103	3.627620	2.867596
4	7	0	6.685950	5.628554	2.401642
5	7	0	7.375689	3.408902	1.476276
6	6	0	5.962194	6.667039	2.848279
7	6	0	6.834884	7.706281	3.239515
8	6	0	8.125235	7.268183	3.016650
9	6	0	8.028775	5.962095	2.490064
10	6	0	9.010493	5.069520	2.093301
11	6	0	8.695613	3.816163	1.595491
12	6	0	9.523718	2.767449	1.140635
13	6	0	8.689262	1.738281	0.751910
14	6	0	7.361044	2.165147	0.971682
15	1	0	10.050939	5.359028	2.174483
16	1	0	10.602498	2.791989	1.112903
17	1	0	9.046400	7.800021	3.200337
18	1	0	8.970905	0.776842	0.351667
19	1	0	6.521746	8.659032	3.637124
20	6	0	6.106628	1.416410	0.711440
21	1	0	5.530013	1.301312	1.631813
22	1	0	5.474060	1.960035	0.006331
23	1	0	6.330673	0.431337	0.304475
24	6	0	4.479106	6.654197	2.894888
25	1	0	4.064807	6.495062	1.896952
26	1	0	4.121606	5.834262	3.521565
27	1	0	4.104163	7.596765	3.291333

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.137301	4.269879	1.869874
2	9	0	5.331687	4.486928	0.748626
3	9	0	5.409227	3.625063	2.874097
4	7	0	6.685830	5.629974	2.401654
5	7	0	7.376263	3.407942	1.475445
6	6	0	5.962886	6.668507	2.849449
7	6	0	6.834836	7.710529	3.241796
8	6	0	8.127928	7.273278	3.017900
9	6	0	8.032782	5.965983	2.490116
10	6	0	9.015357	5.071429	2.092325
11	6	0	8.700884	3.815819	1.593862

12	6	0	9.528738	2.765044	1.138712
13	6	0	8.691774	1.734341	0.750710
14	6	0	7.362590	2.163829	0.971745
15	1	0	10.058066	5.361683	2.173261
16	1	0	10.609577	2.789016	1.110408
17	1	0	9.050424	7.806845	3.202011
18	1	0	8.971959	0.770272	0.350393
19	1	0	6.519164	8.664107	3.640827
20	6	0	6.100249	1.415323	0.711552
21	1	0	5.515374	1.321018	1.630494
22	1	0	5.480938	1.950818	-0.013371
23	1	0	6.324395	0.419755	0.324981
24	6	0	4.473196	6.651679	2.894242
25	1	0	4.062172	6.516827	1.889907
26	1	0	4.118483	5.816655	3.504438
27	1	0	4.097395	7.586926	3.312477

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139876	4.271409	1.868173
2	9	0	5.332601	4.486972	0.749313
3	9	0	5.404002	3.627230	2.864921
4	7	0	6.699203	5.620414	2.397488
5	7	0	7.382046	3.422712	1.481383
6	6	0	5.953925	6.655850	2.843472
7	6	0	6.825019	7.707804	3.241916
8	6	0	8.141761	7.284669	3.026071
9	6	0	8.068123	5.979270	2.497655
10	6	0	9.081905	5.088312	2.101436
11	6	0	8.738873	3.820525	1.597574
12	6	0	9.547608	2.760045	1.139515
13	6	0	8.681972	1.731002	0.750436
14	6	0	7.347453	2.170617	0.973886
15	1	0	10.122347	5.377259	2.183808
16	1	0	10.628529	2.765469	1.105576
17	1	0	9.054148	7.832505	3.218428
18	1	0	8.954020	0.763419	0.348046
19	1	0	6.500328	8.660782	3.640102
20	6	0	6.072895	1.444768	0.721511
21	1	0	5.492394	1.348528	1.648505
22	1	0	5.438456	2.007832	0.024367
23	1	0	6.266637	0.450325	0.311395
24	6	0	4.466550	6.614985	2.876479
25	1	0	4.061908	6.438405	1.871172
26	1	0	4.116188	5.778091	3.494888
27	1	0	4.060710	7.550269	3.270415

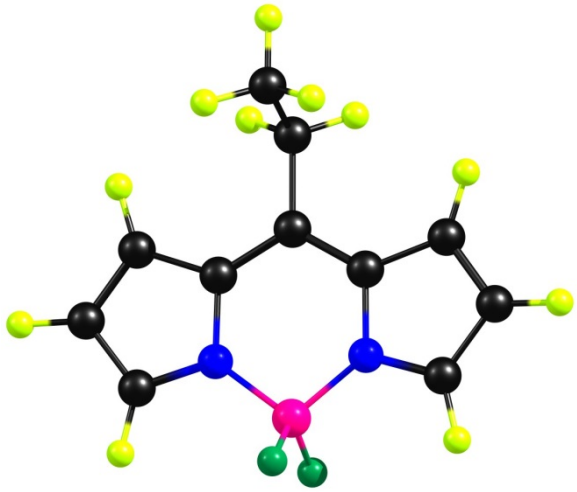

Figure S-18: DFT B3LYP/6-31G(d) optimised ground-state structure of **3.01**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.117317	4.235157	2.007791
2	9	0	5.240993	4.421116	0.956096
3	9	0	5.510448	3.589716	3.069371
4	7	0	6.693625	5.615323	2.480948
5	7	0	7.368124	3.417614	1.530328
6	6	0	5.972036	6.663243	2.900835
7	6	0	6.821766	7.713096	3.306048
8	1	0	6.503996	8.674283	3.685871
9	6	0	8.122684	7.265310	3.119155
10	1	0	9.033566	7.811397	3.323506
11	6	0	8.043483	5.946433	2.596468
12	6	0	9.049149	5.052265	2.198984
13	6	0	8.702073	3.800556	1.668268
14	6	0	9.509765	2.745805	1.164242
15	1	0	10.590675	2.737887	1.128959
16	6	0	8.653364	1.745224	0.724642
17	1	0	8.921491	0.797393	0.278719
18	6	0	7.341656	2.200628	0.970529
19	1	0	6.398575	1.708801	0.772615
20	1	0	4.890987	6.620951	2.897368
21	6	0	10.500242	5.464705	2.275077
22	1	0	10.643499	6.130813	3.131538
23	1	0	11.119018	4.581434	2.461354
24	6	0	10.982108	6.168571	0.989731
25	1	0	10.400161	7.075334	0.796829
26	1	0	12.036110	6.450185	1.086529
27	1	0	10.880147	5.511402	0.120349

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.127958	4.273286	1.928173
2	9	0	5.356068	4.529128	0.795306
3	9	0	5.372896	3.619104	2.900054
4	7	0	6.700618	5.609733	2.500101
5	7	0	7.374521	3.412785	1.545066
6	6	0	5.979324	6.634687	2.972090

7	6	0	6.830350	7.675794	3.390027
8	1	0	6.515319	8.616469	3.813311
9	6	0	8.129145	7.247933	3.154779
10	1	0	9.036706	7.793285	3.361139
11	6	0	8.049797	5.947432	2.592704
12	6	0	9.054171	5.065480	2.170948
13	6	0	8.706497	3.806551	1.662147
14	6	0	9.513023	2.736678	1.194840
15	1	0	10.591129	2.726245	1.159672
16	6	0	8.658332	1.716959	0.801177
17	1	0	8.927382	0.753661	0.397476
18	6	0	7.347371	2.175026	1.034376
19	1	0	6.408282	1.671724	0.859634
20	1	0	4.901008	6.585141	2.994605
21	6	0	10.501505	5.488057	2.219913
22	1	0	10.653840	6.156997	3.069149
23	1	0	11.127606	4.611713	2.398658
24	6	0	10.957367	6.190077	0.924529
25	1	0	10.369943	7.091430	0.737388
26	1	0	12.008652	6.477674	1.004657
27	1	0	10.848246	5.531596	0.060231

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139174	4.279817	1.921321
2	9	0	5.381739	4.540624	0.788178
3	9	0	5.380482	3.628840	2.882559
4	7	0	6.711069	5.607987	2.497963
5	7	0	7.382018	3.420482	1.546520
6	6	0	5.991967	6.627986	2.966770
7	6	0	6.838990	7.666342	3.386283
8	1	0	6.523181	8.606314	3.809500
9	6	0	8.134116	7.238560	3.153862
10	1	0	9.042660	7.781515	3.361634
11	6	0	8.051875	5.943208	2.593103
12	6	0	9.053958	5.063955	2.174341
13	6	0	8.706210	3.809843	1.665259
14	6	0	9.512403	2.745038	1.201178
15	1	0	10.590491	2.735422	1.168763
16	6	0	8.660135	1.729070	0.806380
17	1	0	8.928089	0.765790	0.402999
18	6	0	7.353622	2.188666	1.037437
19	1	0	6.413517	1.688288	0.861097
20	1	0	4.913847	6.577457	2.985995
21	6	0	10.493172	5.484679	2.221696
22	1	0	10.645565	6.153973	3.070017
23	1	0	11.119207	4.608782	2.399835
24	6	0	10.934356	6.180887	0.928843
25	1	0	10.341547	7.078314	0.744344
26	1	0	11.984185	6.472786	0.998178
27	1	0	10.819482	5.520020	0.068095

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139609	4.254641	1.981325
2	9	0	5.309497	4.476266	0.886609
3	9	0	5.452622	3.601275	3.000295
4	7	0	6.710187	5.607772	2.503052
5	7	0	7.381252	3.416985	1.550803
6	6	0	5.990144	6.642570	2.941017
7	6	0	6.837958	7.690183	3.343695

8	1	0	6.521165	8.644401	3.738073
9	6	0	8.136294	7.250956	3.135186
10	1	0	9.047148	7.798004	3.334445
11	6	0	8.054351	5.941730	2.604831
12	6	0	9.056691	5.055164	2.195494
13	6	0	8.709361	3.803349	1.675287
14	6	0	9.514771	2.750973	1.179445
15	1	0	10.594994	2.745131	1.138378
16	6	0	8.659509	1.743859	0.759520
17	1	0	8.926741	0.791647	0.325574
18	6	0	7.351769	2.197629	1.009122
19	1	0	6.408035	1.703598	0.823824
20	1	0	4.910066	6.593608	2.949202
21	6	0	10.499927	5.475295	2.245987
22	1	0	10.654251	6.147700	3.093678
23	1	0	11.128728	4.598619	2.420759
24	6	0	10.930728	6.172310	0.945218
25	1	0	10.330421	7.068496	0.766159
26	1	0	11.981691	6.466964	1.007963
27	1	0	10.809146	5.505519	0.087207

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.209973	4.074201	2.326134
2	9	0	5.088755	3.957836	1.528669
3	9	0	6.033722	3.466702	3.559517
4	7	0	6.668925	5.535343	2.451029
5	7	0	7.424246	3.356018	1.620968
6	6	0	5.862330	6.593792	2.693864
7	6	0	6.636543	7.731354	2.982553
8	1	0	6.246740	8.714721	3.209822
9	6	0	7.974581	7.353959	2.914658
10	1	0	8.840241	7.986522	3.052905
11	6	0	8.010359	5.967751	2.561745
12	6	0	9.071760	5.128326	2.273531
13	6	0	8.754251	3.808182	1.696898
14	6	0	9.533129	2.875205	1.095777
15	1	0	10.606162	2.899181	0.965775
16	6	0	8.626859	1.783600	0.613089
17	1	0	8.938984	0.878467	0.110460
18	6	0	7.356949	2.154190	0.954507
19	1	0	6.406446	1.665382	0.809032
20	1	0	4.787683	6.479723	2.669489
21	6	0	10.504894	5.565875	2.377015
22	1	0	10.598653	6.304405	3.181662
23	1	0	11.126840	4.712006	2.678775
24	6	0	11.076708	6.171305	1.075215
25	1	0	11.026455	5.458509	0.245125
26	1	0	10.509683	7.061042	0.782308
27	1	0	12.125186	6.461045	1.211627

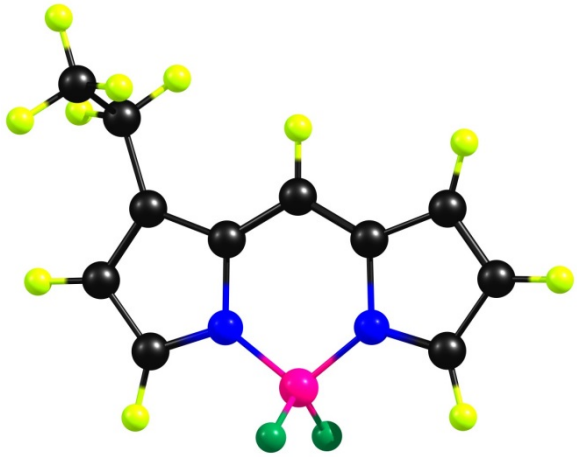

Figure S-19: DFT B3LYP/6-31G(d) optimised ground-state structure of **3.02**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134419	4.162158	2.005186
2	9	0	5.246070	4.387886	0.971540
3	9	0	5.533494	3.502522	3.059823
4	7	0	6.735322	5.529676	2.502733
5	7	0	7.365824	3.332894	1.484368
6	6	0	6.050922	6.551951	3.029802
7	6	0	6.920956	7.613235	3.355009
8	1	0	6.626780	8.558937	3.791118
9	6	0	8.209085	7.216967	3.006792
10	6	0	8.081267	5.898235	2.468338
11	6	0	9.031465	5.024326	1.955950
12	6	0	8.691599	3.762245	1.471523
13	6	0	9.487926	2.727456	0.917127
14	1	0	10.560469	2.769837	0.778419
15	6	0	8.631314	1.681019	0.600663
16	1	0	8.888440	0.727540	0.160309
17	6	0	7.332908	2.096563	0.966185
18	1	0	6.395783	1.563322	0.876473
19	1	0	4.977212	6.490373	3.149717
20	1	0	10.073175	5.330013	1.928691
21	6	0	9.487409	7.981567	3.198919
22	1	0	10.196215	7.735990	2.397868
23	1	0	9.278657	9.053925	3.103653
24	6	0	10.151893	7.715520	4.564509
25	1	0	10.401960	6.655556	4.682673
26	1	0	11.074551	8.298095	4.664808
27	1	0	9.481741	7.991964	5.385264

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.149359	4.158061	2.018381
2	9	0	5.226611	4.376209	0.997167
3	9	0	5.553530	3.490570	3.087092
4	7	0	6.744004	5.524161	2.505793
5	7	0	7.364736	3.329384	1.478290
6	6	0	6.062632	6.547721	3.032082
7	6	0	6.936705	7.604083	3.355123
8	1	0	6.644813	8.548825	3.788429

9	6	0	8.222521	7.203150	3.006970
10	6	0	8.091334	5.886226	2.468923
11	6	0	9.036215	5.013395	1.951970
12	6	0	8.689778	3.756130	1.464105
13	6	0	9.479097	2.724083	0.898963
14	1	0	10.548466	2.763324	0.755421
15	6	0	8.618127	1.683444	0.577845
16	1	0	8.870345	0.735386	0.129622
17	6	0	7.323700	2.097451	0.950851
18	1	0	6.387645	1.566927	0.860288
19	1	0	4.990882	6.492534	3.153769
20	1	0	10.076766	5.314357	1.921841
21	6	0	9.499408	7.967042	3.197449
22	1	0	10.220864	7.687017	2.423364
23	1	0	9.297228	9.032809	3.054482
24	6	0	10.133005	7.754030	4.586130
25	1	0	10.377871	6.701790	4.751518
26	1	0	11.052656	8.337485	4.682321
27	1	0	9.448558	8.064179	5.379267

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.158699	4.164613	2.020571
2	9	0	5.242546	4.379994	1.001991
3	9	0	5.567247	3.500729	3.085176
4	7	0	6.749750	5.526323	2.504777
5	7	0	7.371994	3.341365	1.485133
6	6	0	6.068744	6.543967	3.027655
7	6	0	6.936911	7.600259	3.350022
8	1	0	6.643175	8.544207	3.782806
9	6	0	8.219215	7.201614	3.002888
10	6	0	8.088290	5.888842	2.468524
11	6	0	9.033959	5.020906	1.955232
12	6	0	8.689231	3.765896	1.470712
13	6	0	9.478615	2.738114	0.909863
14	1	0	10.547675	2.778790	0.767012
15	6	0	8.620924	1.699433	0.591168
16	1	0	8.872806	0.750833	0.144833
17	6	0	7.330744	2.114161	0.962482
18	1	0	6.394141	1.584827	0.873284
19	1	0	4.997301	6.485194	3.148544
20	1	0	10.073468	5.324171	1.926069
21	6	0	9.491995	7.959130	3.193051
22	1	0	10.207800	7.686052	2.412226
23	1	0	9.290160	9.025502	3.061335
24	6	0	10.123143	7.727597	4.569744
25	1	0	10.363178	6.673084	4.721474
26	1	0	11.044383	8.305232	4.674054
27	1	0	9.440762	8.028940	5.366833

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.149869	4.184858	1.994678
2	9	0	5.269166	4.395354	0.938259
3	9	0	5.517371	3.528134	3.045540
4	7	0	6.724328	5.551720	2.490311
5	7	0	7.381728	3.356966	1.508043
6	6	0	6.030302	6.566277	3.002716
7	6	0	6.889312	7.633555	3.331064
8	1	0	6.588086	8.578283	3.761636
9	6	0	8.177752	7.243002	2.996761

10	6	0	8.064600	5.926431	2.465881
11	6	0	9.026319	5.060174	1.977388
12	6	0	8.699944	3.791435	1.505644
13	6	0	9.505601	2.758030	0.977699
14	1	0	10.578511	2.802700	0.849651
15	6	0	8.658373	1.704535	0.665571
16	1	0	8.925154	0.747310	0.242619
17	6	0	7.357919	2.117917	1.008409
18	1	0	6.424263	1.580840	0.914263
19	1	0	4.956831	6.497395	3.115335
20	1	0	10.065767	5.373556	1.960582
21	6	0	9.451927	8.003156	3.202768
22	1	0	10.115211	7.858419	2.342272
23	1	0	9.223167	9.072689	3.241261
24	6	0	10.179722	7.586592	4.489699
25	1	0	10.442019	6.524486	4.466692
26	1	0	11.099672	8.164266	4.618559
27	1	0	9.543941	7.751696	5.364157

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.230686	4.081275	2.279229
2	9	0	5.093368	4.070631	1.496467
3	9	0	6.037592	3.422611	3.483297
4	7	0	6.772702	5.508436	2.471636
5	7	0	7.391533	3.326536	1.516481
6	6	0	6.040368	6.603285	2.778479
7	6	0	6.890708	7.676803	3.097972
8	1	0	6.566791	8.672245	3.374587
9	6	0	8.208805	7.236746	2.985512
10	6	0	8.137860	5.858660	2.568341
11	6	0	9.123581	4.972019	2.206899
12	6	0	8.745854	3.702429	1.582550
13	6	0	9.462951	2.765374	0.918358
14	1	0	10.533720	2.746712	0.765528
15	6	0	8.489234	1.747599	0.402953
16	1	0	8.741807	0.855259	-0.153234
17	6	0	7.247407	2.165038	0.792003
18	1	0	6.269994	1.733582	0.643783
19	1	0	4.960219	6.559967	2.770564
20	1	0	10.170966	5.234166	2.272454
21	6	0	9.470211	8.008803	3.230701
22	1	0	10.192397	7.805712	2.426933
23	1	0	9.249661	9.081930	3.179564
24	6	0	10.130379	7.691497	4.588017
25	1	0	10.377829	6.627297	4.667654
26	1	0	11.054150	8.267855	4.715452
27	1	0	9.456083	7.937308	5.415280

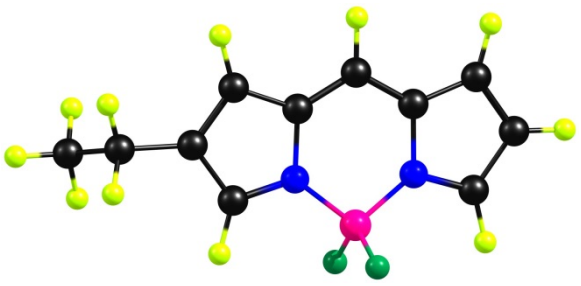

Figure S-20: DFT B3LYP/6-31G(d) optimised ground-state structure of **3.03**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.136008	4.167561	2.067401
2	9	0	5.200344	4.273520	1.057858
3	9	0	5.608837	3.567256	3.194774
4	7	0	6.691243	5.594686	2.437410
5	7	0	7.385614	3.355469	1.563538
6	6	0	5.973901	6.647738	2.844949
7	6	0	6.814169	7.750665	3.153004
8	6	0	8.110381	7.312243	2.908996
9	6	0	8.035244	5.966705	2.460468
10	6	0	9.018866	5.070026	2.060098
11	6	0	8.710078	3.787289	1.611126
12	6	0	9.535006	2.742256	1.121102
13	1	0	10.612808	2.785720	1.032866
14	6	0	8.696706	1.688783	0.779849
15	1	0	8.976815	0.728792	0.368666
16	6	0	7.380630	2.109166	1.068993
17	1	0	6.449807	1.572234	0.942965
18	1	0	4.894916	6.583681	2.911318
19	1	0	10.058645	5.382611	2.084227
20	1	0	9.024731	7.879945	3.030671
21	6	0	6.358595	9.110356	3.607522
22	1	0	5.567982	9.000771	4.361504
23	1	0	7.191513	9.617793	4.109069
24	6	0	5.840017	9.995089	2.458787
25	1	0	4.986347	9.528330	1.954745
26	1	0	5.517694	10.972489	2.835457
27	1	0	6.620308	10.158114	1.707336

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139415	4.191759	1.997967
2	9	0	5.262603	4.327710	0.923752
3	9	0	5.504454	3.589451	3.082022
4	7	0	6.692199	5.599361	2.417423
5	7	0	7.389463	3.349596	1.569833
6	6	0	5.976511	6.641715	2.853695
7	6	0	6.816558	7.746751	3.145497
8	6	0	8.107917	7.322636	2.862039
9	6	0	8.032257	5.980094	2.406667
10	6	0	9.014620	5.088806	2.000177
11	6	0	8.708504	3.795264	1.586813
12	6	0	9.536500	2.737907	1.135251
13	1	0	10.610871	2.784089	1.039201
14	6	0	8.704872	1.663376	0.850156
15	1	0	8.989951	0.689695	0.484134
16	6	0	7.389205	2.082331	1.131762
17	1	0	6.465407	1.531295	1.037779
18	1	0	4.902351	6.569674	2.949996
19	1	0	10.050253	5.408087	2.003376
20	1	0	9.019604	7.893115	2.967089
21	6	0	6.364161	9.096237	3.627658
22	1	0	5.582839	8.968691	4.384543
23	1	0	7.199522	9.592021	4.131138
24	6	0	5.835050	10.002371	2.501493
25	1	0	4.978753	9.546548	1.997380
26	1	0	5.516531	10.969750	2.899590
27	1	0	6.606835	10.180960	1.748269

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.144879	4.201283	2.003188
2	9	0	5.267249	4.337634	0.938548
3	9	0	5.521183	3.601161	3.086467
4	7	0	6.698344	5.602890	2.418632
5	7	0	7.388849	3.364286	1.570170
6	6	0	5.984826	6.641243	2.848695
7	6	0	6.821670	7.742266	3.145000
8	6	0	8.109783	7.316620	2.869756
9	6	0	8.031434	5.978745	2.415425
10	6	0	9.011242	5.089183	2.011993
11	6	0	8.701907	3.801884	1.593728
12	6	0	9.526463	2.749095	1.140176
13	1	0	10.600909	2.793113	1.047650
14	6	0	8.694246	1.682588	0.846675
15	1	0	8.975788	0.710400	0.475085
16	6	0	7.383938	2.105511	1.126561
17	1	0	6.457448	1.560419	1.027122
18	1	0	4.910264	6.569731	2.938175
19	1	0	10.047260	5.405198	2.020152
20	1	0	9.022150	7.884579	2.978805
21	6	0	6.369526	9.086825	3.620492
22	1	0	5.594665	8.960465	4.382993
23	1	0	7.205863	9.587226	4.115785
24	6	0	5.834345	9.974561	2.494893
25	1	0	4.978504	9.510582	1.999398
26	1	0	5.513652	10.944202	2.882784
27	1	0	6.600818	10.147604	1.736351

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.143294	4.194803	2.018420
2	9	0	5.251892	4.329329	0.959380
3	9	0	5.530900	3.590654	3.111536
4	7	0	6.695894	5.599638	2.429762
5	7	0	7.387115	3.362374	1.572652
6	6	0	5.980741	6.637525	2.860668
7	6	0	6.816814	7.740887	3.157887
8	6	0	8.107369	7.319428	2.881637
9	6	0	8.032317	5.979540	2.426069
10	6	0	9.012889	5.090969	2.016620
11	6	0	8.703653	3.802040	1.592802
12	6	0	9.527611	2.752660	1.127997
13	1	0	10.603489	2.799501	1.029193
14	6	0	8.693626	1.684831	0.830710
15	1	0	8.975959	0.714947	0.448562
16	6	0	7.382134	2.105234	1.120080
17	1	0	6.452856	1.561299	1.021186
18	1	0	4.904467	6.563726	2.949944
19	1	0	10.050607	5.409239	2.022857
20	1	0	9.018759	7.893055	2.990907
21	6	0	6.358586	9.091371	3.625383
22	1	0	5.565521	8.970111	4.371884
23	1	0	7.188108	9.593230	4.134628
24	6	0	5.849980	9.974233	2.478150
25	1	0	5.007129	9.501059	1.964809
26	1	0	5.517294	10.946733	2.853200
27	1	0	6.638203	10.140880	1.737775

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.238776	3.991162	2.455781
2	9	0	5.040665	3.907067	1.772823
3	9	0	6.143752	3.452533	3.729291
4	7	0	6.645769	5.508680	2.605991
5	7	0	7.392937	3.363538	1.646022
6	6	0	5.789799	6.531730	2.930128
7	6	0	6.516099	7.684776	3.097936
8	6	0	7.945136	7.302971	2.816537
9	6	0	7.962757	5.977872	2.525111
10	6	0	9.038982	5.089276	2.086063
11	6	0	8.721174	3.841939	1.603411
12	6	0	9.508885	2.849028	0.935610
13	1	0	10.567757	2.933227	0.732215
14	6	0	8.650463	1.819852	0.570523
15	1	0	8.904788	0.914607	0.035346
16	6	0	7.360650	2.165754	1.021078
17	1	0	6.434581	1.613563	0.942225
18	1	0	4.732052	6.346273	3.038610
19	1	0	10.054978	5.460278	2.060216
20	1	0	8.791368	7.977635	2.839485
21	6	0	6.047044	9.040781	3.478624
22	1	0	4.981592	9.005850	3.729837
23	1	0	6.578686	9.363629	4.388485
24	6	0	6.292969	10.100498	2.378319
25	1	0	5.746264	9.844782	1.465558
26	1	0	5.953439	11.082605	2.723507
27	1	0	7.355843	10.179383	2.125965

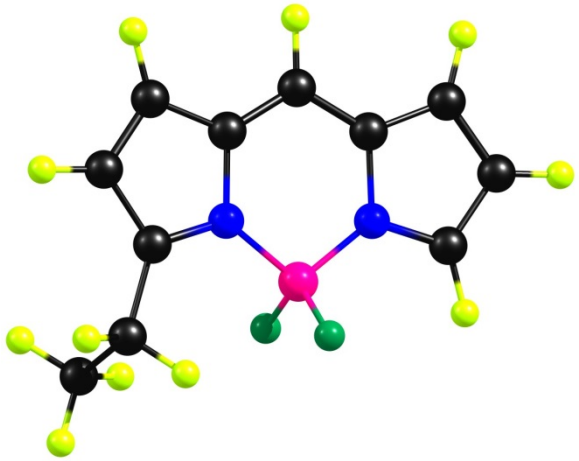

Figure S-21: DFT B3LYP/6-31G(d) optimised ground-state structure of **3.04**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.169565	4.135870	1.852639
2	9	0	5.445575	4.277054	0.676631
3	9	0	5.407993	3.539075	2.844286
4	7	0	6.687800	5.545344	2.332858
5	7	0	7.451029	3.274446	1.580233
6	6	0	5.945581	6.588726	2.754039
7	6	0	6.802228	7.686365	3.045557
8	6	0	8.098320	7.282894	2.787132
9	6	0	8.030699	5.935790	2.340856
10	6	0	9.037010	5.050354	1.983837
11	6	0	8.765031	3.733619	1.612412

12	6	0	9.619210	2.660503	1.256831
13	1	0	10.698623	2.712915	1.198324
14	6	0	8.807310	1.557806	1.015446
15	1	0	9.115521	0.562718	0.725618
16	6	0	7.478706	1.979610	1.225795
17	1	0	6.560606	1.414168	1.137960
18	1	0	10.068200	5.390043	2.007162
19	1	0	9.009184	7.855675	2.904742
20	1	0	6.469915	8.649445	3.409877
21	6	0	4.450339	6.555872	2.841410
22	1	0	4.132955	5.550418	3.130994
23	1	0	4.138736	7.244813	3.635512
24	6	0	3.767154	6.951638	1.514840
25	1	0	4.039613	6.245701	0.727132
26	1	0	2.678636	6.936753	1.636748
27	1	0	4.061719	7.959421	1.201729

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.187290	4.088897	1.943277
2	9	0	5.350194	4.164332	0.827199
3	9	0	5.515534	3.499644	3.016451
4	7	0	6.685418	5.525815	2.340486
5	7	0	7.462443	3.256247	1.593841
6	6	0	5.934271	6.573754	2.728332
7	6	0	6.784140	7.680267	3.002018
8	6	0	8.082930	7.275948	2.768163
9	6	0	8.026658	5.919833	2.352247
10	6	0	9.037378	5.039562	2.006113
11	6	0	8.771535	3.724297	1.630332
12	6	0	9.629466	2.666684	1.246170
13	1	0	10.705282	2.727909	1.179370
14	6	0	8.823638	1.565460	0.981291
15	1	0	9.136277	0.583327	0.663370
16	6	0	7.494920	1.970481	1.207847
17	1	0	6.583513	1.400105	1.110118
18	1	0	10.064535	5.384151	2.029357
19	1	0	8.987433	7.855272	2.878886
20	1	0	6.446848	8.649412	3.336729
21	6	0	4.441068	6.544146	2.805903
22	1	0	4.109787	5.531131	3.038506
23	1	0	4.133909	7.188169	3.635629
24	6	0	3.766221	7.027416	1.505042
25	1	0	4.027016	6.371521	0.673548
26	1	0	2.680009	7.015794	1.625107
27	1	0	4.069548	8.047464	1.255266

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.190008	4.082606	1.972547
2	9	0	5.331804	4.142621	0.880724
3	9	0	5.552340	3.501840	3.062614
4	7	0	6.686905	5.519223	2.344216
5	7	0	7.459146	3.260212	1.603646
6	6	0	5.935572	6.562613	2.718977
7	6	0	6.777440	7.672767	2.981934
8	6	0	8.073595	7.270551	2.753588
9	6	0	8.018914	5.914535	2.351973
10	6	0	9.027919	5.038055	2.006686
11	6	0	8.760773	3.725761	1.634133
12	6	0	9.615956	2.675099	1.242601

13	1	0	10.690864	2.738608	1.169243
14	6	0	8.811647	1.577465	0.979187
15	1	0	9.121922	0.596942	0.655369
16	6	0	7.488711	1.981724	1.214913
17	1	0	6.576012	1.413080	1.121497
18	1	0	10.054228	5.383786	2.024639
19	1	0	8.976839	7.852463	2.857533
20	1	0	6.436209	8.643799	3.305877
21	6	0	4.449146	6.524055	2.791253
22	1	0	4.123343	5.502701	2.989694
23	1	0	4.136177	7.138452	3.640187
24	6	0	3.788735	7.044145	1.508668
25	1	0	4.058813	6.416132	0.659552
26	1	0	2.702298	7.026703	1.616127
27	1	0	4.091942	8.071100	1.293222

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.186442	4.078592	1.993347
2	9	0	5.309155	4.132731	0.910627
3	9	0	5.566477	3.495745	3.098012
4	7	0	6.682296	5.519697	2.357889
5	7	0	7.454552	3.262329	1.605843
6	6	0	5.933234	6.562135	2.736823
7	6	0	6.774809	7.674211	3.005610
8	6	0	8.072951	7.273001	2.776889
9	6	0	8.019365	5.916151	2.368862
10	6	0	9.027913	5.041515	2.015172
11	6	0	8.759981	3.727741	1.633142
12	6	0	9.612841	2.680494	1.226360
13	1	0	10.689330	2.745211	1.146479
14	6	0	8.804720	1.582938	0.955927
15	1	0	9.113375	0.604501	0.618504
16	6	0	7.481768	1.986152	1.203665
17	1	0	6.565157	1.420299	1.112462
18	1	0	10.056330	5.388102	2.031168
19	1	0	8.977662	7.856490	2.879981
20	1	0	6.429689	8.645265	3.331832
21	6	0	4.440591	6.531252	2.792899
22	1	0	4.101150	5.515934	3.009119
23	1	0	4.119763	7.171357	3.621366
24	6	0	3.810399	7.025771	1.480818
25	1	0	4.092791	6.370255	0.654136
26	1	0	2.720301	7.024373	1.566306
27	1	0	4.134215	8.044796	1.247364

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.198305	4.218693	1.718781
2	9	0	5.625902	4.385053	0.461723
3	9	0	5.326948	3.568031	2.581087
4	7	0	6.717868	5.548422	2.302695
5	7	0	7.469557	3.301069	1.543951
6	6	0	5.954055	6.571792	2.782313
7	6	0	6.798022	7.660403	3.110322
8	6	0	8.103793	7.302950	2.818763
9	6	0	8.071299	5.963599	2.314346
10	6	0	9.096052	5.133222	1.930836
11	6	0	8.805174	3.747121	1.580087
12	6	0	9.601119	2.685260	1.309754
13	1	0	10.681579	2.672927	1.261433

14	6	0	8.702907	1.505594	1.099098
15	1	0	9.021752	0.502180	0.852245
16	6	0	7.421059	1.955383	1.269110
17	1	0	6.473528	1.443777	1.206740
18	1	0	10.123188	5.472393	1.944475
19	1	0	9.003039	7.886837	2.960700
20	1	0	6.451991	8.601440	3.518885
21	6	0	4.460029	6.524096	2.861613
22	1	0	4.145441	5.518499	3.156494
23	1	0	4.137268	7.215667	3.649149
24	6	0	3.768388	6.902918	1.532624
25	1	0	4.062299	6.212666	0.738305
26	1	0	2.679609	6.857241	1.649204
27	1	0	4.037087	7.919804	1.225871

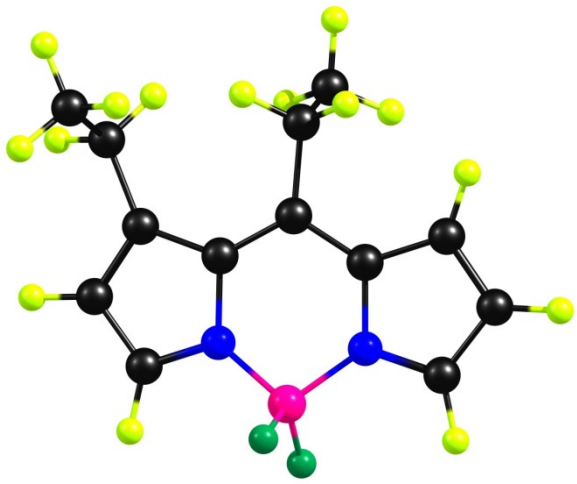

Figure S-22: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.01**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.181271	4.172295	2.134819
2	9	0	5.160886	4.316282	1.213540
3	9	0	5.739400	3.547339	3.288686
4	7	0	6.784248	5.574316	2.490605
5	7	0	7.370585	3.375374	1.516905
6	6	0	6.061225	6.622337	2.893240
7	6	0	6.906944	7.687347	3.245787
8	6	0	8.220777	7.269055	3.051612
9	6	0	8.141763	5.917093	2.560810
10	6	0	9.106467	4.996296	2.116171
11	6	0	8.709218	3.748883	1.594023
12	6	0	9.479748	2.701893	1.020056
13	1	0	10.556227	2.686496	0.919429
14	6	0	8.593198	1.717762	0.599261
15	1	0	8.831425	0.782663	0.111381
16	6	0	7.301840	2.172855	0.927747
17	1	0	6.344474	1.693784	0.772177
18	1	0	6.589993	8.660717	3.596982
19	1	0	4.980801	6.567449	2.911254
20	6	0	10.582492	5.325768	2.097212
21	1	0	10.832933	5.976715	2.935919
22	1	0	11.152939	4.404530	2.247512
23	6	0	9.416401	8.127893	3.372723
24	1	0	10.213782	8.000470	2.634063
25	1	0	9.104550	9.176542	3.296731
26	6	0	11.024927	5.982991	0.773355
27	1	0	12.096927	6.206393	0.801437

28	1	0	10.834171	5.317319	-0.074183
29	1	0	10.484073	6.917215	0.591107
30	6	0	9.973895	7.888337	4.790370
31	1	0	10.821634	8.553865	4.988878
32	1	0	9.203250	8.080505	5.544030
33	1	0	10.312994	6.855349	4.925317

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.173787	4.269589	1.902555
2	9	0	5.439322	4.557899	0.749556
3	9	0	5.360881	3.657172	2.856555
4	7	0	6.787828	5.581465	2.483369
5	7	0	7.385817	3.362232	1.554012
6	6	0	6.069773	6.594862	2.972228
7	6	0	6.917313	7.645678	3.353821
8	6	0	8.225690	7.256636	3.083705
9	6	0	8.143891	5.934018	2.524547
10	6	0	9.109630	5.024152	2.066608
11	6	0	8.720368	3.751083	1.608349
12	6	0	9.500748	2.657113	1.152354
13	1	0	10.576387	2.630053	1.079871
14	6	0	8.624874	1.628312	0.830125
15	1	0	8.874110	0.647434	0.457123
16	6	0	7.328538	2.105229	1.091277
17	1	0	6.378683	1.607001	0.968580
18	1	0	6.603610	8.586750	3.779998
19	1	0	4.993032	6.531433	3.024135
20	6	0	10.574905	5.381765	1.995974
21	1	0	10.845392	6.020184	2.834566
22	1	0	11.169256	4.473260	2.101645
23	6	0	9.422125	8.107332	3.415238
24	1	0	10.196586	8.019962	2.651158
25	1	0	9.099766	9.152674	3.393718
26	6	0	10.945097	6.074956	0.668932
27	1	0	12.011077	6.316270	0.654943
28	1	0	10.730424	5.425770	-0.182542
29	1	0	10.382707	7.001084	0.531594
30	6	0	10.019050	7.810104	4.804935
31	1	0	10.867080	8.469945	5.007871
32	1	0	9.271487	7.965896	5.586228
33	1	0	10.366222	6.776817	4.885924

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.186117	4.280497	1.893881
2	9	0	5.473320	4.572981	0.736839
3	9	0	5.364490	3.673174	2.833264
4	7	0	6.797583	5.583744	2.481795
5	7	0	7.395774	3.372756	1.560580
6	6	0	6.081330	6.591445	2.969311
7	6	0	6.925045	7.640527	3.351229
8	6	0	8.229163	7.252004	3.080147
9	6	0	8.144419	5.935511	2.523078
10	6	0	9.109278	5.029704	2.069739
11	6	0	8.722265	3.759630	1.614912
12	6	0	9.504083	2.670221	1.166736
13	1	0	10.579942	2.645210	1.097017
14	6	0	8.632094	1.642200	0.848094
15	1	0	8.881760	0.660022	0.479930
16	6	0	7.339400	2.119685	1.104843

17	1	0	6.389337	1.622186	0.982717
18	1	0	6.611385	8.580523	3.778900
19	1	0	5.004887	6.525622	3.020031
20	6	0	10.564909	5.389946	1.998341
21	1	0	10.832897	6.029362	2.837058
22	1	0	11.162188	4.483608	2.102420
23	6	0	9.424415	8.092424	3.409830
24	1	0	10.193713	8.007125	2.640476
25	1	0	9.106102	9.138356	3.396446
26	6	0	10.917629	6.080782	0.675895
27	1	0	11.980059	6.332304	0.651789
28	1	0	10.701138	5.428754	-0.172009
29	1	0	10.344529	7.000100	0.541701
30	6	0	10.017845	7.779386	4.787497
31	1	0	10.871710	8.427957	4.996749
32	1	0	9.272824	7.934006	5.570261
33	1	0	10.353825	6.742377	4.859454

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.188763	4.217357	2.043786
2	9	0	5.268236	4.414872	1.017161
3	9	0	5.582888	3.592664	3.132812
4	7	0	6.793697	5.581717	2.487906
5	7	0	7.389659	3.376914	1.541204
6	6	0	6.074240	6.615149	2.914877
7	6	0	6.918683	7.676603	3.272273
8	6	0	8.226519	7.265217	3.053392
9	6	0	8.146074	5.926249	2.549756
10	6	0	9.111099	5.012249	2.111778
11	6	0	8.720868	3.755280	1.615083
12	6	0	9.497340	2.698680	1.085611
13	1	0	10.574433	2.681460	0.997484
14	6	0	8.618527	1.696778	0.696262
15	1	0	8.863567	0.744797	0.248966
16	6	0	7.327417	2.157168	0.998443
17	1	0	6.372641	1.671202	0.853402
18	1	0	6.603179	8.640237	3.647683
19	1	0	4.994827	6.556745	2.943914
20	6	0	10.576039	5.357732	2.072419
21	1	0	10.835527	6.000978	2.912610
22	1	0	11.162462	4.444441	2.194178
23	6	0	9.425999	8.109216	3.378528
24	1	0	10.206864	8.002681	2.621092
25	1	0	9.114390	9.158181	3.343898
26	6	0	10.958171	6.036590	0.747527
27	1	0	12.022651	6.286522	0.744130
28	1	0	10.755252	5.373711	-0.097847
29	1	0	10.386226	6.956285	0.594440
30	6	0	9.994834	7.810128	4.773758
31	1	0	10.856188	8.450434	4.985467
32	1	0	9.235818	7.989088	5.540362
33	1	0	10.312379	6.766806	4.866598

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.255384	4.089529	2.377392
2	9	0	5.055215	4.065450	1.692828
3	9	0	6.166273	3.441849	3.600770
4	7	0	6.796280	5.520644	2.508820
5	7	0	7.357684	3.361805	1.532082

6	6	0	6.036622	6.593659	2.814576
7	6	0	6.859964	7.682633	3.128577
8	6	0	8.192523	7.279391	3.016075
9	6	0	8.164333	5.895562	2.591044
10	6	0	9.151016	5.004608	2.194495
11	6	0	8.713439	3.745679	1.550999
12	6	0	9.401957	2.824251	0.832012
13	1	0	10.463816	2.803839	0.632053
14	6	0	8.412764	1.821623	0.332418
15	1	0	8.643174	0.940495	-0.250745
16	6	0	7.184389	2.226997	0.784214
17	1	0	6.202940	1.794663	0.667169
18	1	0	6.517929	8.671156	3.408811
19	1	0	4.958477	6.517097	2.816468
20	6	0	10.630801	5.271998	2.235255
21	1	0	10.868109	5.946313	3.062054
22	1	0	11.153093	4.332109	2.461239
23	6	0	9.371791	8.163781	3.312151
24	1	0	10.187567	7.989110	2.601967
25	1	0	9.062903	9.206101	3.162677
26	6	0	11.211763	5.856143	0.926967
27	1	0	12.294951	6.000179	1.017116
28	1	0	11.026446	5.193963	0.075057
29	1	0	10.756197	6.823854	0.692790
30	6	0	9.905165	8.016988	4.752156
31	1	0	10.749387	8.695003	4.924906
32	1	0	9.121013	8.253297	5.479286
33	1	0	10.242093	6.994362	4.955273

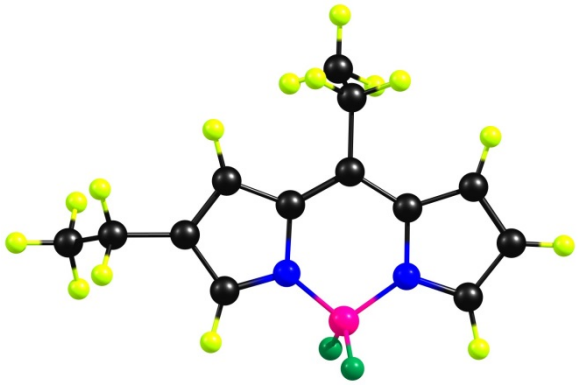

Figure S-23: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.02**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.570929	-1.435475	-0.160103
2	9	0	2.018725	-1.818825	-1.411681
3	9	0	2.035239	-2.282476	0.827811
4	7	0	0.002562	-1.398875	-0.145593
5	7	0	2.011072	0.038926	0.137458
6	6	0	-0.808006	-2.457380	-0.260581
7	6	0	-2.167140	-2.056666	-0.279681
8	6	0	-2.148894	-0.670290	-0.168614
9	6	0	-0.792314	-0.254657	-0.083875
10	6	0	-0.222863	1.016284	0.072376
11	6	0	1.170728	1.149902	0.193424
12	6	0	1.981083	2.294974	0.412886
13	1	0	1.626880	3.311990	0.512354
14	6	0	3.298736	1.859770	0.486579
15	1	0	4.182274	2.460556	0.652680
16	6	0	3.271529	0.462069	0.311763
17	1	0	4.091726	-0.243332	0.305221

18	1	0	-0.397070	-3.457531	-0.317824
19	6	0	-1.101710	2.244514	0.065774
20	1	0	-2.073406	1.999999	0.506011
21	1	0	-0.656664	3.015051	0.702826
22	6	0	-1.308506	2.808486	-1.354984
23	1	0	-1.949341	3.696090	-1.319402
24	1	0	-0.352959	3.091899	-1.807415
25	1	0	-1.783107	2.067122	-2.005604
26	1	0	-3.013213	-0.019538	-0.136379
27	6	0	-3.358632	-2.963946	-0.421962
28	1	0	-4.244597	-2.459901	-0.016717
29	1	0	-3.211474	-3.863426	0.190254
30	6	0	-3.633788	-3.384777	-1.877340
31	1	0	-4.506995	-4.044795	-1.933729
32	1	0	-3.825022	-2.509756	-2.508285
33	1	0	-2.777110	-3.919279	-2.302943

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.564730	-1.441570	-0.077649
2	9	0	2.071897	-1.932447	-1.281366
3	9	0	1.987952	-2.231511	0.990629
4	7	0	0.003497	-1.403889	-0.131638
5	7	0	2.013416	0.038611	0.131542
6	6	0	-0.804146	-2.462161	-0.263183
7	6	0	-2.160754	-2.059859	-0.287882
8	6	0	-2.144522	-0.676087	-0.162968
9	6	0	-0.789953	-0.260246	-0.065736
10	6	0	-0.223589	1.010282	0.084285
11	6	0	1.169752	1.145556	0.191578
12	6	0	1.980220	2.294077	0.374476
13	1	0	1.627307	3.309443	0.465318
14	6	0	3.300613	1.864980	0.419839
15	1	0	4.183442	2.470489	0.551581
16	6	0	3.276777	0.466991	0.266306
17	1	0	4.099699	-0.231677	0.249697
18	1	0	-0.395038	-3.460488	-0.325974
19	6	0	-1.103230	2.235929	0.085123
20	1	0	-2.067370	1.988570	0.533906
21	1	0	-0.653566	3.003045	0.718670
22	6	0	-1.326731	2.805262	-1.330541
23	1	0	-1.966560	3.690037	-1.282295
24	1	0	-0.380379	3.092932	-1.793357
25	1	0	-1.808566	2.070098	-1.978680
26	1	0	-3.006897	-0.027038	-0.132677
27	6	0	-3.349917	-2.964778	-0.447496
28	1	0	-4.231601	-2.471937	-0.026412
29	1	0	-3.196446	-3.873878	0.143810
30	6	0	-3.631779	-3.354025	-1.909579
31	1	0	-4.501702	-4.013536	-1.974912
32	1	0	-3.829336	-2.468213	-2.519065
33	1	0	-2.778551	-3.876260	-2.350646

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.548493	-1.435059	-0.089893
2	9	0	2.044280	-1.916381	-1.294256
3	9	0	1.973115	-2.226529	0.967668
4	7	0	-0.007406	-1.393475	-0.134795
5	7	0	1.997914	0.038245	0.123796
6	6	0	-0.812542	-2.445464	-0.268838

7	6	0	-2.165316	-2.043385	-0.288232
8	6	0	-2.146245	-0.664390	-0.157040
9	6	0	-0.794453	-0.256033	-0.061868
10	6	0	-0.227736	1.009211	0.090616
11	6	0	1.162364	1.140179	0.191358
12	6	0	1.970220	2.284453	0.372987
13	1	0	1.617848	3.299501	0.468400
14	6	0	3.286463	1.854346	0.409927
15	1	0	4.171266	2.456941	0.538589
16	6	0	3.257388	0.460962	0.252551
17	1	0	4.077508	-0.240452	0.228769
18	1	0	-0.403478	-3.443136	-0.338191
19	6	0	-1.099745	2.230055	0.095233
20	1	0	-2.062443	1.984284	0.546831
21	1	0	-0.645891	2.995317	0.727193
22	6	0	-1.319028	2.788955	-1.315357
23	1	0	-1.955238	3.675498	-1.274842
24	1	0	-0.371420	3.069311	-1.778292
25	1	0	-1.801326	2.051170	-1.958861
26	1	0	-3.006384	-0.012775	-0.122462
27	6	0	-3.349826	-2.942940	-0.450445
28	1	0	-4.237028	-2.435392	-0.062156
29	1	0	-3.214665	-3.836074	0.167653
30	6	0	-3.593476	-3.362571	-1.901493
31	1	0	-4.463422	-4.019307	-1.976610
32	1	0	-3.769188	-2.490807	-2.535686
33	1	0	-2.731934	-3.897556	-2.307549

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.569758	-1.445804	0.019381
2	9	0	2.107677	-2.006457	-1.136274
3	9	0	1.961112	-2.164853	1.145560
4	7	0	0.014917	-1.412467	-0.079215
5	7	0	2.011454	0.041378	0.150574
6	6	0	-0.782958	-2.470019	-0.228995
7	6	0	-2.138159	-2.075889	-0.271428
8	6	0	-2.131872	-0.695020	-0.138222
9	6	0	-0.783450	-0.278181	-0.018864
10	6	0	-0.225295	0.994284	0.119420
11	6	0	1.166457	1.141175	0.204083
12	6	0	1.968477	2.298393	0.328544
13	1	0	1.608482	3.315483	0.396040
14	6	0	3.291668	1.879751	0.346172
15	1	0	4.175397	2.494981	0.429376
16	6	0	3.270854	0.479320	0.235370
17	1	0	4.095701	-0.219288	0.214044
18	1	0	-0.365913	-3.466548	-0.295560
19	6	0	-1.110249	2.210353	0.100780
20	1	0	-2.064597	1.974525	0.578735
21	1	0	-0.650761	3.006177	0.691940
22	6	0	-1.355559	2.705204	-1.333820
23	1	0	-1.988929	3.596336	-1.320763
24	1	0	-0.412112	2.958940	-1.824767
25	1	0	-1.852115	1.936273	-1.931689
26	1	0	-2.998553	-0.047210	-0.124764
27	6	0	-3.316586	-2.982903	-0.474157
28	1	0	-4.188586	-2.559057	0.035600
29	1	0	-3.118580	-3.948788	0.003749
30	6	0	-3.645919	-3.204820	-1.956292
31	1	0	-4.503126	-3.875650	-2.068888
32	1	0	-3.885114	-2.256456	-2.447187
33	1	0	-2.794850	-3.646460	-2.483778

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.677773	-1.336637	-0.359187
2	9	0	2.027771	-1.409156	-1.699247
3	9	0	2.238545	-2.365557	0.373894
4	7	0	0.110343	-1.418680	-0.261600
5	7	0	2.010271	0.036241	0.254291
6	6	0	-0.630206	-2.569226	-0.263631
7	6	0	-1.965804	-2.241544	-0.281683
8	6	0	-2.009041	-0.739331	-0.259089
9	6	0	-0.727034	-0.293022	-0.241621
10	6	0	-0.172598	1.067748	-0.089880
11	6	0	1.169530	1.173380	0.224125
12	6	0	1.963407	2.289392	0.647498
13	1	0	1.611057	3.305610	0.754092
14	6	0	3.231012	1.806209	0.950025
15	1	0	4.075343	2.375077	1.316459
16	6	0	3.227327	0.421866	0.696960
17	1	0	4.029689	-0.296975	0.786822
18	1	0	-0.143949	-3.532900	-0.275706
19	6	0	-1.083394	2.251949	-0.231601
20	1	0	-2.027471	2.062583	0.300331
21	1	0	-0.631989	3.120051	0.260328
22	6	0	-1.402191	2.615455	-1.698045
23	1	0	-2.086424	3.470913	-1.744285
24	1	0	-0.486707	2.876935	-2.238522
25	1	0	-1.870371	1.775844	-2.222824
26	1	0	-2.911790	-0.143665	-0.234912
27	6	0	-3.148457	-3.136645	-0.340609
28	1	0	-3.811078	-2.912252	0.511345
29	1	0	-2.828850	-4.178259	-0.229260
30	6	0	-3.970697	-2.977140	-1.641379
31	1	0	-4.843841	-3.637195	-1.615511
32	1	0	-4.326370	-1.949024	-1.767467
33	1	0	-3.365133	-3.235343	-2.515408

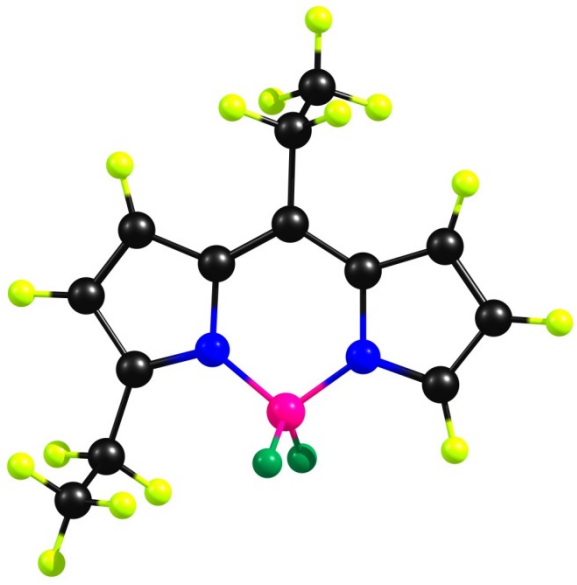

Figure S-24: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.03**

DFT B3LYP/6-31G(d) optimised ground state structure:

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

1	5	0	6.148657	4.164231	1.806822
2	9	0	5.322923	4.370964	0.711912
3	9	0	5.489532	3.456410	2.804269
4	7	0	6.663785	5.535362	2.373226
5	7	0	7.426853	3.382205	1.364756
6	6	0	5.905559	6.561580	2.808686
7	6	0	6.751742	7.598065	3.282496
8	6	0	8.057843	7.172258	3.127063
9	6	0	8.010243	5.873590	2.550452
10	6	0	9.045462	5.017853	2.161015
11	6	0	8.745650	3.777857	1.569592
12	6	0	9.589146	2.754824	1.066634
13	1	0	10.670620	2.763167	1.076836
14	6	0	8.766018	1.754691	0.559225
15	1	0	9.068334	0.825855	0.095440
16	6	0	7.440678	2.181032	0.764402
17	1	0	6.513944	1.682941	0.512997
18	6	0	10.485925	5.448796	2.311692
19	1	0	10.584205	6.095808	3.188735
20	1	0	11.107204	4.568671	2.505316
21	1	0	8.956311	7.718123	3.381085
22	1	0	6.409331	8.542533	3.684372
23	6	0	4.406981	6.540513	2.812553
24	1	0	4.054900	5.971602	1.947933
25	1	0	4.051336	7.571560	2.697809
26	6	0	11.016323	6.187737	1.065983
27	1	0	10.433623	7.093452	0.869938
28	1	0	12.062263	6.477037	1.214775
29	1	0	10.958484	5.551116	0.177530
30	6	0	3.821396	5.933322	4.105143
31	1	0	4.134626	4.891784	4.206457
32	1	0	4.152823	6.488286	4.989892
33	1	0	2.726894	5.967301	4.071619

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.157400	4.203548	1.697571
2	9	0	5.433297	4.487868	0.535566
3	9	0	5.361915	3.488832	2.599142
4	7	0	6.664349	5.529294	2.357196
5	7	0	7.429027	3.378945	1.343135
6	6	0	5.903722	6.537986	2.822702
7	6	0	6.748423	7.560922	3.325339
8	6	0	8.053925	7.144445	3.153388
9	6	0	8.010701	5.863930	2.540794
10	6	0	9.045563	5.015199	2.144000
11	6	0	8.745591	3.774019	1.557066
12	6	0	9.588407	2.736990	1.089454
13	1	0	10.666816	2.736202	1.117979
14	6	0	8.767245	1.728911	0.595948
15	1	0	9.070706	0.788622	0.163255
16	6	0	7.442888	2.164031	0.771362
17	1	0	6.520530	1.663944	0.517356
18	6	0	10.484172	5.444359	2.299384
19	1	0	10.578971	6.088284	3.175798
20	1	0	11.101897	4.565091	2.493592
21	1	0	8.948056	7.682858	3.426423
22	1	0	6.407011	8.488911	3.758276
23	6	0	4.407637	6.520176	2.828052
24	1	0	4.047617	5.911056	1.997974
25	1	0	4.058167	7.543370	2.658429
26	6	0	11.021711	6.185026	1.058227
27	1	0	10.444352	7.090753	0.860331
28	1	0	12.064649	6.472086	1.214772
29	1	0	10.971106	5.553061	0.169127
30	6	0	3.822237	5.991780	4.154008
31	1	0	4.123044	4.956123	4.317242
32	1	0	4.158020	6.592239	5.003540

33	1	0	2.730464	6.031664	4.120228

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.162120	4.218040	1.679105
2	9	0	5.463344	4.518416	0.513723
3	9	0	5.352278	3.506726	2.559125
4	7	0	6.670515	5.528077	2.353982
5	7	0	7.428715	3.389869	1.337824
6	6	0	5.912350	6.528194	2.821942
7	6	0	6.751756	7.545098	3.334528
8	6	0	8.053674	7.129583	3.163533
9	6	0	8.007907	5.858003	2.543423
10	6	0	9.039456	5.011626	2.148391
11	6	0	8.737859	3.777629	1.556721
12	6	0	9.579215	2.744777	1.092798
13	1	0	10.657376	2.742484	1.127058
14	6	0	8.759850	1.742936	0.594628
15	1	0	9.061460	0.802794	0.161284
16	6	0	7.440457	2.181906	0.765658
17	1	0	6.516934	1.686948	0.506797
18	6	0	10.470644	5.434980	2.306514
19	1	0	10.564300	6.078979	3.182384
20	1	0	11.085059	4.554326	2.502384
21	1	0	8.948545	7.663486	3.442611
22	1	0	6.409020	8.469251	3.773642
23	6	0	4.423150	6.504855	2.821411
24	1	0	4.070977	5.870726	2.007624
25	1	0	4.069941	7.520332	2.620858
26	6	0	10.999861	6.168112	1.068592
27	1	0	10.420057	7.071311	0.870521
28	1	0	12.042262	6.457132	1.218008
29	1	0	10.944794	5.533638	0.182483
30	6	0	3.846373	6.013334	4.154256
31	1	0	4.155549	4.985810	4.346360
32	1	0	4.178584	6.638584	4.985931
33	1	0	2.755233	6.042560	4.122558

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.163382	4.205687	1.695458
2	9	0	5.452881	4.493961	0.529017
3	9	0	5.363332	3.490991	2.588371
4	7	0	6.665066	5.527094	2.358936
5	7	0	7.434942	3.386177	1.349716
6	6	0	5.905029	6.533798	2.808111
7	6	0	6.740090	7.562922	3.309182
8	6	0	8.045311	7.147537	3.151006
9	6	0	8.005291	5.864160	2.550053
10	6	0	9.040023	5.016443	2.166312
11	6	0	8.745572	3.777684	1.571824
12	6	0	9.591939	2.752466	1.099991
13	1	0	10.672588	2.755601	1.130706
14	6	0	8.774930	1.748269	0.593120
15	1	0	9.081466	0.811941	0.150763
16	6	0	7.452266	2.180528	0.768135
17	1	0	6.528530	1.683889	0.506328
18	6	0	10.473624	5.445918	2.322694
19	1	0	10.567819	6.106151	3.188422
20	1	0	11.093261	4.569258	2.528522
21	1	0	8.939464	7.690276	3.423748

22	1	0	6.391105	8.493932	3.733321
23	6	0	4.410556	6.506857	2.813206
24	1	0	4.050253	5.883483	1.992282
25	1	0	4.054149	7.526854	2.635333
26	6	0	10.989827	6.163972	1.065617
27	1	0	10.401054	7.062390	0.860987
28	1	0	12.034172	6.457978	1.201417
29	1	0	10.925825	5.511344	0.190680
30	6	0	3.853585	5.988130	4.148429
31	1	0	4.175069	4.958153	4.317863
32	1	0	4.196829	6.605429	4.984472
33	1	0	2.760384	6.011251	4.132632

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.134205	4.117661	1.957974
2	9	0	5.155394	4.207016	0.973812
3	9	0	5.648550	3.427343	3.067691
4	7	0	6.656037	5.522464	2.372022
5	7	0	7.377608	3.395320	1.372215
6	6	0	5.903267	6.597377	2.705734
7	6	0	6.767369	7.643518	3.134939
8	6	0	8.081115	7.180958	3.062230
9	6	0	8.024193	5.851941	2.578459
10	6	0	9.073986	4.961441	2.266103
11	6	0	8.735434	3.748852	1.597109
12	6	0	9.538824	2.773931	0.993635
13	1	0	10.619430	2.762186	0.975260
14	6	0	8.670076	1.837247	0.389594
15	1	0	8.951247	0.950166	-0.162669
16	6	0	7.350287	2.267316	0.644408
17	1	0	6.410107	1.818877	0.355476
18	6	0	10.511031	5.336107	2.497690
19	1	0	10.584958	5.953094	3.401579
20	1	0	11.092649	4.428319	2.701026
21	1	0	8.983019	7.728089	3.297365
22	1	0	6.434963	8.619937	3.464482
23	6	0	4.408553	6.610540	2.686455
24	1	0	4.055196	6.053523	1.813471
25	1	0	4.075256	7.649980	2.580818
26	6	0	11.151290	6.093187	1.313329
27	1	0	10.616007	7.027190	1.112101
28	1	0	12.197477	6.336497	1.531562
29	1	0	11.122478	5.488574	0.400686
30	6	0	3.781711	5.996228	3.961078
31	1	0	4.092353	4.954666	4.072435
32	1	0	4.087119	6.549795	4.855836
33	1	0	2.688424	6.031185	3.892751

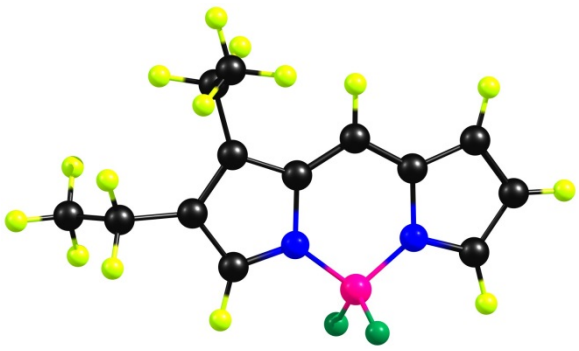

Figure S-25: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.04**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.176484	4.280491	1.905403
2	9	0	5.305232	4.506281	0.857430
3	9	0	5.542740	3.675669	2.975026
4	7	0	6.820030	5.640100	2.369465
5	7	0	7.382810	3.394303	1.425916
6	6	0	6.165593	6.726528	2.790668
7	6	0	7.065466	7.746454	3.187722
8	6	0	8.349767	7.235055	2.986710
9	6	0	8.185073	5.910990	2.471150
10	6	0	9.113354	4.962979	2.064221
11	6	0	8.730714	3.726076	1.543194
12	6	0	9.498731	2.646628	1.038506
13	1	0	10.579690	2.614953	0.994068
14	6	0	8.602231	1.671129	0.618348
15	1	0	8.830922	0.711387	0.175858
16	6	0	7.309342	2.172912	0.875208
17	1	0	6.348606	1.711589	0.688892
18	1	0	5.082688	6.744767	2.801525
19	1	0	10.172562	5.191254	2.137205
20	6	0	9.662626	7.900657	3.290467
21	1	0	10.424665	7.564492	2.575979
22	1	0	9.566258	8.982462	3.139995
23	6	0	6.669463	9.114349	3.676070
24	1	0	7.451603	9.512715	4.333500
25	1	0	5.767736	9.031394	4.296455
26	6	0	10.160917	7.632118	4.724781
27	1	0	10.300645	6.559660	4.898421
28	1	0	11.117794	8.135754	4.902762
29	1	0	9.440676	7.995833	5.465442
30	6	0	6.405007	10.116551	2.536564
31	1	0	6.113909	11.094624	2.936549
32	1	0	7.298374	10.253669	1.917021
33	1	0	5.600248	9.764058	1.881980

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.186394	4.319727	1.822309
2	9	0	5.393649	4.582678	0.705644
3	9	0	5.430518	3.725048	2.831917
4	7	0	6.826215	5.651060	2.347702
5	7	0	7.385025	3.393783	1.427846
6	6	0	6.173136	6.728940	2.789625
7	6	0	7.075713	7.744013	3.188594
8	6	0	8.357368	7.238761	2.968955
9	6	0	8.191604	5.921297	2.438162
10	6	0	9.116572	4.974315	2.032607
11	6	0	8.730952	3.729954	1.534730
12	6	0	9.497141	2.633109	1.072461
13	1	0	10.575533	2.596627	1.033767
14	6	0	8.600485	1.642314	0.690645
15	1	0	8.829163	0.667162	0.290450
16	6	0	7.309176	2.151571	0.925316
17	1	0	6.351481	1.682950	0.755174
18	1	0	5.092422	6.746097	2.812375
19	1	0	10.174153	5.200809	2.099689
20	6	0	9.669058	7.903229	3.271616
21	1	0	10.425684	7.572419	2.553088
22	1	0	9.568426	8.982597	3.125197
23	6	0	6.680870	9.101303	3.702130
24	1	0	7.477189	9.498579	4.338270
25	1	0	5.802518	8.999766	4.348295

26	6	0	10.174268	7.631226	4.702268
27	1	0	10.322667	6.561665	4.870658
28	1	0	11.126223	8.139681	4.878089
29	1	0	9.456899	7.986019	5.446272
30	6	0	6.369950	10.112772	2.583602
31	1	0	6.082895	11.080925	3.003505
32	1	0	7.239341	10.266235	1.938676
33	1	0	5.549270	9.761251	1.952866

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.195447	4.330987	1.820568
2	9	0	5.413096	4.594702	0.705166
3	9	0	5.439870	3.739531	2.822910
4	7	0	6.833231	5.655733	2.346845
5	7	0	7.391122	3.408639	1.432603
6	6	0	6.181379	6.727209	2.788169
7	6	0	7.079592	7.740476	3.187362
8	6	0	8.356989	7.237858	2.966097
9	6	0	8.190393	5.925642	2.436840
10	6	0	9.115056	4.982910	2.034269
11	6	0	8.729597	3.741445	1.539084
12	6	0	9.494534	2.648066	1.081261
13	1	0	10.572621	2.611572	1.044114
14	6	0	8.599949	1.660292	0.701502
15	1	0	8.827031	0.684497	0.303052
16	6	0	7.313645	2.171448	0.934493
17	1	0	6.354835	1.705324	0.765194
18	1	0	5.100831	6.741893	2.810345
19	1	0	10.171930	5.210594	2.102561
20	6	0	9.662083	7.898977	3.269458
21	1	0	10.418278	7.571774	2.549879
22	1	0	9.559460	8.978026	3.126187
23	6	0	6.689764	9.092004	3.699483
24	1	0	7.492660	9.489610	4.326171
25	1	0	5.819450	8.991407	4.355227
26	6	0	10.156797	7.619748	4.692477
27	1	0	10.301285	6.549655	4.855323
28	1	0	11.107654	8.124551	4.878247
29	1	0	9.435609	7.970205	5.433630
30	6	0	6.370766	10.090113	2.583755
31	1	0	6.088091	11.061185	2.997215
32	1	0	7.233516	10.237284	1.930028
33	1	0	5.545397	9.734527	1.962987

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.191762	4.315765	1.824000
2	9	0	5.403012	4.576366	0.706626
3	9	0	5.439667	3.719009	2.832116
4	7	0	6.824155	5.644649	2.349224
5	7	0	7.392307	3.399300	1.432727
6	6	0	6.170244	6.710006	2.805048
7	6	0	7.067763	7.729068	3.197199
8	6	0	8.345233	7.239932	2.951466
9	6	0	8.184497	5.926579	2.422152
10	6	0	9.114501	4.987774	2.019283
11	6	0	8.734024	3.737457	1.531809
12	6	0	9.500860	2.645007	1.073317
13	1	0	10.581021	2.610782	1.031906
14	6	0	8.605839	1.651037	0.698966

15	1	0	8.835187	0.674371	0.299048
16	6	0	7.317242	2.159472	0.936704
17	1	0	6.356474	1.691748	0.772380
18	1	0	5.088135	6.716737	2.841518
19	1	0	10.172501	5.223171	2.082617
20	6	0	9.650754	7.913316	3.245443
21	1	0	10.413116	7.572830	2.536267
22	1	0	9.545294	8.991762	3.086572
23	6	0	6.683151	9.082302	3.720882
24	1	0	7.475405	9.457650	4.378005
25	1	0	5.787767	8.988734	4.345566
26	6	0	10.129326	7.650804	4.681054
27	1	0	10.254890	6.578525	4.858572
28	1	0	11.086780	8.145643	4.868272
29	1	0	9.401291	8.024412	5.407162
30	6	0	6.421714	10.098867	2.601470
31	1	0	6.149218	11.074405	3.015444
32	1	0	7.311552	10.227518	1.977186
33	1	0	5.607274	9.762884	1.952499

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.252417	4.148831	2.155820
2	9	0	5.141310	4.308605	1.349713
3	9	0	5.927603	3.550440	3.363660
4	7	0	6.850740	5.577143	2.491271
5	7	0	7.384762	3.407014	1.422933
6	6	0	6.103804	6.666129	2.867591
7	6	0	6.951004	7.688651	3.206376
8	6	0	8.356378	7.149306	2.995413
9	6	0	8.214235	5.865896	2.554312
10	6	0	9.190491	4.869407	2.119321
11	6	0	8.757113	3.704985	1.523705
12	6	0	9.469535	2.652175	0.867590
13	1	0	10.544941	2.604275	0.761988
14	6	0	8.524063	1.759203	0.372798
15	1	0	8.710498	0.854694	-0.190779
16	6	0	7.256140	2.249581	0.730689
17	1	0	6.277700	1.831587	0.539548
18	1	0	5.025635	6.613988	2.870407
19	1	0	10.247062	5.089042	2.195567
20	6	0	9.617490	7.890226	3.286863
21	1	0	10.435738	7.470448	2.691436
22	1	0	9.511837	8.940290	2.983185
23	6	0	6.596869	9.071532	3.625442
24	1	0	7.272441	9.408150	4.423767
25	1	0	5.582281	9.076487	4.039487
26	6	0	10.008350	7.843658	4.783840
27	1	0	10.165899	6.810846	5.109034
28	1	0	10.933970	8.405746	4.948262
29	1	0	9.228411	8.279829	5.416924
30	6	0	6.665563	10.092144	2.460429
31	1	0	6.398358	11.090165	2.823906
32	1	0	7.670126	10.143899	2.028101
33	1	0	5.969195	9.813509	1.663901

Figure S-26: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.05**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.179032	4.106548	1.806407
2	9	0	5.449258	4.309511	0.641944
3	9	0	5.410185	3.483609	2.777250
4	7	0	6.725470	5.484469	2.341223
5	7	0	7.441043	3.234468	1.490817
6	6	0	6.004825	6.522781	2.806559
7	6	0	6.880053	7.592500	3.131358
8	6	0	8.177689	7.192904	2.853301
9	6	0	8.075263	5.855698	2.353487
10	6	0	9.058954	4.970576	1.945471
11	6	0	8.761140	3.672252	1.523960
12	6	0	9.594185	2.603021	1.115201
13	1	0	10.673550	2.641468	1.045190
14	6	0	8.762186	1.521712	0.840440
15	1	0	9.052340	0.534748	0.507306
16	6	0	7.443894	1.953627	1.083933
17	1	0	6.515622	1.407300	0.983717
18	1	0	10.097108	5.288518	1.963370
19	1	0	6.564973	8.548298	3.531290
20	6	0	9.446824	7.961901	3.084632
21	1	0	10.188389	7.702659	2.318388
22	1	0	9.241413	9.032038	2.961655
23	6	0	4.509970	6.512991	2.903936
24	1	0	4.176617	5.503378	3.159061
25	1	0	4.216366	7.178134	3.724775
26	6	0	10.053311	7.720794	4.481441
27	1	0	10.296789	6.663070	4.629040
28	1	0	10.971655	8.304703	4.609615
29	1	0	9.349455	8.012540	5.267940
30	6	0	3.824924	6.968957	1.597719
31	1	0	4.078288	6.286551	0.783395
32	1	0	2.737224	6.970555	1.727672
33	1	0	4.136666	7.981633	1.318741

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	5	0	6.198733	4.045017	1.918423
2	9	0	5.332274	4.176461	0.828756
3	9	0	5.541546	3.426268	2.985720
4	7	0	6.730002	5.456126	2.358391
5	7	0	7.448818	3.207432	1.504887
6	6	0	6.004032	6.503259	2.787900
7	6	0	6.875868	7.579943	3.097168
8	6	0	8.175059	7.173304	2.846476
9	6	0	8.080425	5.826126	2.375413
10	6	0	9.063231	4.945113	1.968453
11	6	0	8.765195	3.651409	1.535812
12	6	0	9.596364	2.601512	1.082949
13	1	0	10.671473	2.648383	0.995521
14	6	0	8.765816	1.526185	0.782135
15	1	0	9.055713	0.556061	0.410289
16	6	0	7.450479	1.940420	1.055584
17	1	0	6.527045	1.391537	0.948971
18	1	0	10.098733	5.263942	1.981553
19	1	0	6.556853	8.544278	3.465439
20	6	0	9.437528	7.951610	3.072095
21	1	0	10.187772	7.670259	2.326271
22	1	0	9.229758	9.013548	2.910757
23	6	0	4.510761	6.502587	2.868089
24	1	0	4.158073	5.487718	3.056773
25	1	0	4.217871	7.117148	3.724886
26	6	0	10.024781	7.759112	4.483962
27	1	0	10.272334	6.710960	4.669558
28	1	0	10.935893	8.351286	4.605059
29	1	0	9.310715	8.072189	5.249375
30	6	0	3.846359	7.055205	1.589568
31	1	0	4.091449	6.428080	0.731636
32	1	0	2.760196	7.064053	1.710642
33	1	0	4.173512	8.077385	1.381723

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.204186	4.045739	1.931690
2	9	0	5.335261	4.172622	0.852358
3	9	0	5.561094	3.430165	3.000717
4	7	0	6.733473	5.452671	2.362481
5	7	0	7.451066	3.215750	1.514332
6	6	0	6.007184	6.493454	2.785254
7	6	0	6.870984	7.572953	3.089654
8	6	0	8.167192	7.169564	2.840330
9	6	0	8.074278	5.824567	2.377227
10	6	0	9.057165	4.949007	1.972369
11	6	0	8.759864	3.657670	1.543076
12	6	0	9.590028	2.613128	1.091063
13	1	0	10.664603	2.661655	1.002701
14	6	0	8.762140	1.540562	0.791735
15	1	0	9.051077	0.570845	0.419305
16	6	0	7.451586	1.954741	1.066845
17	1	0	6.527412	1.407124	0.962269
18	1	0	10.091436	5.270601	1.984009
19	1	0	6.548463	8.537338	3.453599
20	6	0	9.424761	7.944088	3.060956
21	1	0	10.171020	7.662809	2.312119
22	1	0	9.216924	9.005284	2.900608
23	6	0	4.520475	6.483685	2.859255
24	1	0	4.173076	5.461640	3.012187
25	1	0	4.220854	7.067401	3.734223
26	6	0	10.007539	7.746130	4.463939
27	1	0	10.250448	6.697165	4.645987
28	1	0	10.919747	8.333833	4.589378
29	1	0	9.294071	8.057714	5.229247
30	6	0	3.872491	7.072847	1.600208
31	1	0	4.128345	6.474023	0.726045

32	1	0	2.785870	7.076841	1.707394
33	1	0	4.200548	8.100296	1.427673

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.202452	4.051593	1.951922
2	9	0	5.309269	4.160237	0.885025
3	9	0	5.584287	3.439957	3.043455
4	7	0	6.727252	5.468708	2.363034
5	7	0	7.449216	3.229999	1.517397
6	6	0	6.003995	6.509994	2.786567
7	6	0	6.868299	7.594287	3.087547
8	6	0	8.164111	7.190043	2.838086
9	6	0	8.073366	5.841847	2.378485
10	6	0	9.058518	4.965318	1.982942
11	6	0	8.762695	3.668310	1.553172
12	6	0	9.591345	2.625957	1.094488
13	1	0	10.668395	2.671384	1.008356
14	6	0	8.759078	1.555400	0.782154
15	1	0	9.047929	0.587802	0.398889
16	6	0	7.447867	1.970908	1.057875
17	1	0	6.520003	1.427845	0.945522
18	1	0	10.095133	5.287418	2.001050
19	1	0	6.545078	8.560527	3.451914
20	6	0	9.429864	7.956671	3.067603
21	1	0	10.170000	7.693365	2.303748
22	1	0	9.225259	9.025244	2.947680
23	6	0	4.512220	6.503709	2.863006
24	1	0	4.160824	5.489242	3.064026
25	1	0	4.213510	7.133858	3.707001
26	6	0	10.017479	7.699347	4.463425
27	1	0	10.246245	6.638416	4.601995
28	1	0	10.938534	8.271656	4.606911
29	1	0	9.305587	7.991222	5.240611
30	6	0	3.872061	7.031994	1.568994
31	1	0	4.131576	6.384920	0.728713
32	1	0	2.783457	7.047457	1.670561
33	1	0	4.209757	8.049278	1.348079

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.199934	4.195340	1.685129
2	9	0	5.624908	4.414171	0.436398
3	9	0	5.319388	3.527753	2.526240
4	7	0	6.737535	5.496947	2.313724
5	7	0	7.458853	3.270475	1.478593
6	6	0	5.988409	6.515905	2.822546
7	6	0	6.845635	7.583807	3.176330
8	6	0	8.155120	7.233249	2.876607
9	6	0	8.095158	5.898740	2.333309
10	6	0	9.109144	5.072127	1.917884
11	6	0	8.802361	3.701835	1.523002
12	6	0	9.587664	2.641100	1.218493
13	1	0	10.667760	2.620081	1.167891
14	6	0	8.678884	1.480519	0.976411
15	1	0	8.984826	0.481540	0.697110
16	6	0	7.398460	1.938570	1.165205
17	1	0	6.447076	1.435673	1.089764
18	1	0	10.139790	5.400112	1.928016
19	1	0	6.511423	8.520147	3.607371
20	6	0	9.408834	8.018310	3.120504

21	1	0	10.093430	7.901343	2.268704
22	1	0	9.158696	9.085376	3.166823
23	6	0	4.494389	6.485707	2.903091
24	1	0	4.166403	5.474166	3.160578
25	1	0	4.181920	7.152095	3.716198
26	6	0	10.145368	7.616552	4.415087
27	1	0	10.424422	6.557442	4.397052
28	1	0	11.058774	8.209050	4.543554
29	1	0	9.507263	7.776744	5.290751
30	6	0	3.806464	6.923559	1.589978
31	1	0	4.089010	6.258631	0.770293
32	1	0	2.717265	6.889882	1.706922
33	1	0	4.090095	7.946964	1.320679

Figure S-27: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.06**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.087739	4.357934	1.859609
2	9	0	5.297618	4.549027	0.736680
3	9	0	5.347768	3.830913	2.910187
4	7	0	6.722122	5.722448	2.297195
5	7	0	7.296215	3.404796	1.525293
6	6	0	6.055502	6.845157	2.604595
7	6	0	6.952199	7.851434	3.009708
8	6	0	8.238051	7.314388	2.947083
9	6	0	8.079086	5.970578	2.494804
10	6	0	9.011824	4.971579	2.228854
11	6	0	8.638675	3.721675	1.750565
12	6	0	9.427365	2.601259	1.380073
13	1	0	10.507317	2.552883	1.435315
14	6	0	8.555094	1.625278	0.933264
15	1	0	8.800772	0.639122	0.561971
16	6	0	7.238088	2.149079	1.035606
17	1	0	10.066805	5.173592	2.388353
18	1	0	6.680933	8.854138	3.313295
19	6	0	9.537276	8.011372	3.234760
20	1	0	10.272084	7.292562	3.619214
21	1	0	9.379259	8.743705	4.035824
22	1	0	4.976881	6.881914	2.527963
23	6	0	5.953557	1.450900	0.707597
24	1	0	5.237599	2.184512	0.326978

25	1	0	6.150919	0.731179	-0.095832
26	6	0	5.344988	0.716916	1.921592
27	1	0	6.038572	-0.031102	2.321636
28	1	0	5.106194	1.431866	2.712173
29	1	0	4.423955	0.203396	1.624658
30	6	0	10.125376	8.729210	2.003794
31	1	0	11.065999	9.229530	2.260472
32	1	0	10.324590	8.021002	1.192154
33	1	0	9.429506	9.483923	1.622396

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.094814	4.402660	1.786552
2	9	0	5.377829	4.629719	0.608524
3	9	0	5.251312	3.882920	2.773674
4	7	0	6.732768	5.737718	2.284233
5	7	0	7.282383	3.411716	1.516493
6	6	0	6.075157	6.857119	2.619871
7	6	0	6.982370	7.849710	3.028408
8	6	0	8.264066	7.307977	2.937650
9	6	0	8.093365	5.973861	2.467579
10	6	0	9.015248	4.969111	2.196148
11	6	0	8.627529	3.720877	1.732038
12	6	0	9.401246	2.584004	1.386162
13	1	0	10.477916	2.523346	1.442830
14	6	0	8.518343	1.607508	0.966119
15	1	0	8.753723	0.612077	0.621460
16	6	0	7.207809	2.146483	1.057733
17	1	0	10.070852	5.160412	2.348578
18	1	0	6.719116	8.844549	3.354810
19	6	0	9.566421	7.996136	3.223366
20	1	0	10.312159	7.263829	3.548637
21	1	0	9.426386	8.681966	4.064597
22	1	0	4.997998	6.903058	2.560125
23	6	0	5.921502	1.449224	0.746665
24	1	0	5.183002	2.181315	0.416515
25	1	0	6.101949	0.766009	-0.088939
26	6	0	5.366043	0.655403	1.947516
27	1	0	6.081022	-0.096773	2.291099
28	1	0	5.140008	1.327353	2.776310
29	1	0	4.445211	0.142014	1.659099
30	6	0	10.116530	8.781632	2.017190
31	1	0	11.058691	9.273167	2.274995
32	1	0	10.298262	8.120460	1.166033
33	1	0	9.408896	9.549604	1.695759

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.097704	4.417926	1.763545
2	9	0	5.411524	4.654226	0.576780
3	9	0	5.236923	3.900590	2.726384
4	7	0	6.732618	5.741676	2.277327
5	7	0	7.281076	3.427618	1.513810
6	6	0	6.076463	6.853680	2.615883
7	6	0	6.978791	7.843156	3.029452
8	6	0	8.256519	7.303061	2.937331
9	6	0	8.084885	5.976522	2.461835
10	6	0	9.006633	4.976613	2.191041
11	6	0	8.618733	3.732283	1.727886
12	6	0	9.388909	2.595431	1.392078
13	1	0	10.464953	2.532672	1.451593

14	6	0	8.506056	1.621145	0.979903
15	1	0	8.737395	0.622221	0.643847
16	6	0	7.202054	2.166066	1.066801
17	1	0	10.061413	5.168452	2.345762
18	1	0	6.714591	8.835755	3.360570
19	6	0	9.555186	7.983393	3.223279
20	1	0	10.292157	7.250445	3.564501
21	1	0	9.412995	8.680230	4.053842
22	1	0	4.999526	6.897731	2.554410
23	6	0	5.916104	1.477817	0.766770
24	1	0	5.167565	2.218172	0.483279
25	1	0	6.075261	0.825966	-0.096900
26	6	0	5.407328	0.647307	1.951142
27	1	0	6.137355	-0.108384	2.249399
28	1	0	5.203046	1.290704	2.807107
29	1	0	4.481957	0.135896	1.678058
30	6	0	10.110887	8.741783	2.013925
31	1	0	11.053851	9.232937	2.265166
32	1	0	10.291142	8.066468	1.174782
33	1	0	9.408327	9.506607	1.677239

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.081317	4.428487	1.774162
2	9	0	5.387073	4.675230	0.589272
3	9	0	5.227386	3.887495	2.736192
4	7	0	6.705504	5.752868	2.302529
5	7	0	7.275338	3.452297	1.506697
6	6	0	6.042019	6.857815	2.654109
7	6	0	6.940805	7.853225	3.072264
8	6	0	8.222675	7.321856	2.969217
9	6	0	8.060191	5.998778	2.482875
10	6	0	8.993170	5.011420	2.192404
11	6	0	8.616510	3.767468	1.714737
12	6	0	9.394846	2.639677	1.359876
13	1	0	10.473774	2.585092	1.412458
14	6	0	8.515652	1.661032	0.942593
15	1	0	8.750266	0.664569	0.595452
16	6	0	7.206695	2.195510	1.046071
17	1	0	10.048765	5.215281	2.344193
18	1	0	6.674176	8.844563	3.411300
19	6	0	9.527306	8.005543	3.243822
20	1	0	10.229536	7.298535	3.700470
21	1	0	9.364435	8.798515	3.980808
22	1	0	4.962790	6.891758	2.595667
23	6	0	5.919848	1.491773	0.759476
24	1	0	5.153083	2.222955	0.495234
25	1	0	6.073111	0.843727	-0.109834
26	6	0	5.451204	0.650774	1.957339
27	1	0	6.200666	-0.098298	2.230779
28	1	0	5.265533	1.293033	2.821063
29	1	0	4.522068	0.130550	1.708377
30	6	0	10.153701	8.605302	1.976245
31	1	0	11.100756	9.101014	2.209204
32	1	0	10.347394	7.828368	1.230139
33	1	0	9.482336	9.339952	1.522642

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.182462	4.297485	1.889707
2	9	0	5.334553	4.518141	0.813830

3	9	0	5.471851	3.888594	3.013323
4	7	0	6.844578	5.691760	2.257004
5	7	0	7.340520	3.346518	1.544618
6	6	0	6.118497	6.848034	2.466904
7	6	0	6.988923	7.828427	2.833744
8	6	0	8.370985	7.215304	2.838514
9	6	0	8.208806	5.914103	2.474029
10	6	0	9.151264	4.818718	2.258360
11	6	0	8.705226	3.606265	1.785661
12	6	0	9.434709	2.432738	1.416687
13	1	0	10.509926	2.330672	1.475246
14	6	0	8.511854	1.503919	0.957379
15	1	0	8.714468	0.507344	0.586209
16	6	0	7.225997	2.078053	1.044961
17	1	0	10.206531	4.982845	2.430650
18	1	0	6.758086	8.854924	3.086199
19	6	0	9.617544	7.960211	3.166266
20	1	0	10.459659	7.264825	3.240992
21	1	0	9.504716	8.426841	4.157123
22	1	0	5.047491	6.848907	2.340296
23	6	0	5.913499	1.437744	0.713121
24	1	0	5.244338	2.187667	0.280065
25	1	0	6.091010	0.675244	-0.054991
26	6	0	5.225134	0.784189	1.931710
27	1	0	5.859284	0.005442	2.369783
28	1	0	5.016462	1.533024	2.699508
29	1	0	4.278266	0.323153	1.627927
30	6	0	9.944210	9.066924	2.138629
31	1	0	10.850563	9.603514	2.438226
32	1	0	10.107709	8.637962	1.145116
33	1	0	9.130806	9.796672	2.061031

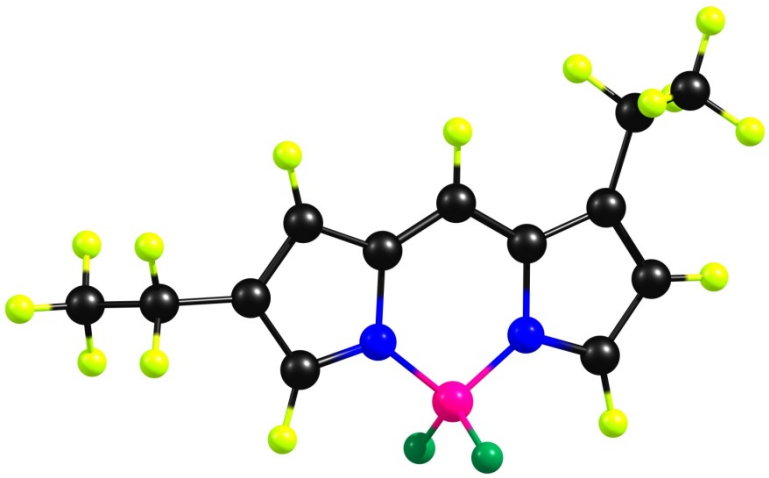

Figure S-28: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.07**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.088828	4.336940	1.667368
2	9	0	5.431620	4.680289	0.500589
3	9	0	5.242434	3.716761	2.565695
4	7	0	6.723125	5.619170	2.320732
5	7	0	7.305544	3.395939	1.335571
6	6	0	6.058070	6.665672	2.827365
7	6	0	6.959509	7.649943	3.279609
8	6	0	8.247502	7.178540	3.035494
9	6	0	8.086703	5.893658	2.431215
10	6	0	9.024414	4.955829	2.011867

11	6	0	8.652337	3.724893	1.478216
12	6	0	9.423827	2.624897	1.021878
13	1	0	10.506122	2.583709	1.007414
14	6	0	8.542032	1.632234	0.606013
15	6	0	7.243405	2.160690	0.822065
16	1	0	10.081685	5.181477	2.115124
17	1	0	6.687775	8.591849	3.737945
18	6	0	9.547528	7.882395	3.301223
19	1	0	10.327720	7.150944	3.547955
20	1	0	9.434396	8.518577	4.187282
21	1	0	4.976223	6.669599	2.850335
22	1	0	6.285373	1.698013	0.620369
23	6	0	8.863514	0.261360	0.076332
24	1	0	8.176053	0.012732	-0.742785
25	1	0	9.869322	0.272154	-0.361093
26	6	0	8.787532	-0.840063	1.149796
27	1	0	7.783786	-0.898402	1.585504
28	1	0	9.028307	-1.819600	0.721016
29	1	0	9.491728	-0.640994	1.965120
30	6	0	10.019617	8.746911	2.115143
31	1	0	10.965145	9.246877	2.353598
32	1	0	10.171358	8.136703	1.218191
33	1	0	9.277822	9.514996	1.872441

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.087816	4.329609	1.700925
2	9	0	5.368280	4.638711	0.546812
3	9	0	5.264347	3.714526	2.642889
4	7	0	6.719592	5.629682	2.303409
5	7	0	7.291656	3.391877	1.344498
6	6	0	6.058730	6.698876	2.764727
7	6	0	6.964850	7.676741	3.215404
8	6	0	8.249829	7.177674	3.017888
9	6	0	8.084230	5.882398	2.442246
10	6	0	9.016132	4.928642	2.054856
11	6	0	8.637148	3.704178	1.516277
12	6	0	9.403372	2.602533	1.058196
13	1	0	10.482876	2.552433	1.058932
14	6	0	8.517921	1.628051	0.611182
15	6	0	7.223073	2.165627	0.810000
16	1	0	10.072047	5.139249	2.177043
17	1	0	6.696401	8.632500	3.639600
18	6	0	9.550673	7.869316	3.301323
19	1	0	10.323540	7.129989	3.534428
20	1	0	9.435599	8.483307	4.199712
21	1	0	4.979070	6.724058	2.759629
22	1	0	6.266386	1.716909	0.583089
23	6	0	8.834266	0.265286	0.062056
24	1	0	8.105265	0.009081	-0.713838
25	1	0	9.809463	0.297401	-0.433646
26	6	0	8.843124	-0.839548	1.133736
27	1	0	7.870510	-0.918008	1.626757
28	1	0	9.076163	-1.810862	0.688468
29	1	0	9.589573	-0.630359	1.904558
30	6	0	10.031231	8.759334	2.138600
31	1	0	10.974294	9.250060	2.394311
32	1	0	10.187540	8.171510	1.230522
33	1	0	9.295361	9.533910	1.909997

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

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

1	5	0	6.101408	4.328946	1.697957
2	9	0	5.391387	4.639989	0.546622
3	9	0	5.280082	3.713130	2.631291
4	7	0	6.728554	5.622133	2.303981
5	7	0	7.303625	3.397809	1.345327
6	6	0	6.067143	6.682875	2.766508
7	6	0	6.966704	7.660858	3.217832
8	6	0	8.248710	7.166605	3.018032
9	6	0	8.084293	5.877452	2.441232
10	6	0	9.017709	4.931193	2.052872
11	6	0	8.641233	3.710070	1.514581
12	6	0	9.408152	2.614158	1.058421
13	1	0	10.487385	2.565861	1.059472
14	6	0	8.526284	1.641168	0.614097
15	6	0	7.235404	2.176980	0.814125
16	1	0	10.072530	5.145458	2.174771
17	1	0	6.695692	8.614339	3.644500
18	6	0	9.544433	7.855454	3.295902
19	1	0	10.315729	7.116533	3.532221
20	1	0	9.430754	8.473091	4.190898
21	1	0	4.987596	6.703194	2.761579
22	1	0	6.278441	1.728331	0.589295
23	6	0	8.840743	0.283248	0.070019
24	1	0	8.121856	0.033002	-0.716035
25	1	0	9.821879	0.310856	-0.412031
26	6	0	8.826589	-0.811768	1.138791
27	1	0	7.847484	-0.881331	1.618154
28	1	0	9.058768	-1.786096	0.702245
29	1	0	9.562019	-0.604728	1.919388
30	6	0	10.015455	8.731414	2.130643
31	1	0	10.958947	9.224855	2.374966
32	1	0	10.165409	8.137002	1.226849
33	1	0	9.277961	9.502610	1.900082

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.118411	4.287111	1.791869
2	9	0	5.338394	4.560443	0.672009
3	9	0	5.370130	3.638464	2.770333
4	7	0	6.717112	5.610751	2.363183
5	7	0	7.343323	3.405019	1.386916
6	6	0	6.034686	6.662462	2.818154
7	6	0	6.917248	7.668748	3.251962
8	6	0	8.208856	7.199114	3.049520
9	6	0	8.071386	5.899612	2.489475
10	6	0	9.027394	4.977654	2.091110
11	6	0	8.678670	3.747994	1.547739
12	6	0	9.467157	2.674058	1.071648
13	1	0	10.549203	2.646166	1.063344
14	6	0	8.602987	1.686341	0.622254
15	6	0	7.299547	2.188193	0.841589
16	1	0	10.079393	5.220638	2.206068
17	1	0	6.631945	8.625109	3.667455
18	6	0	9.499617	7.919233	3.293679
19	1	0	10.245954	7.220705	3.689203
20	1	0	9.343125	8.677086	4.067669
21	1	0	4.953201	6.657370	2.817735
22	1	0	6.348937	1.718556	0.624408
23	6	0	8.944261	0.338802	0.055951
24	1	0	8.360054	0.165067	-0.855166
25	1	0	9.996560	0.336718	-0.247296
26	6	0	8.693035	-0.804678	1.047456
27	1	0	7.641899	-0.835311	1.350774
28	1	0	8.945015	-1.771060	0.600442
29	1	0	9.295809	-0.674124	1.951193
30	6	0	10.044850	8.587968	2.022787
31	1	0	10.988550	9.101000	2.229892
32	1	0	10.221906	7.848375	1.235944

33	1	0	9.331743	9.321108	1.635291

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.022488	4.278459	2.136601
2	9	0	4.986122	4.369519	1.226785
3	9	0	5.614250	3.683843	3.321119
4	7	0	6.684588	5.650531	2.374885
5	7	0	7.175006	3.390396	1.526713
6	6	0	6.036602	6.812058	2.613944
7	6	0	6.952186	7.802621	3.014888
8	6	0	8.225181	7.237387	3.027832
9	6	0	8.060812	5.868192	2.603573
10	6	0	8.982727	4.880082	2.358804
11	6	0	8.540626	3.634469	1.728875
12	6	0	9.229153	2.611098	1.164990
13	1	0	10.304158	2.490186	1.126009
14	6	0	8.222626	1.667883	0.562823
15	6	0	6.995069	2.230811	0.817786
16	1	0	10.037709	5.032553	2.543481
17	1	0	6.698890	8.824655	3.267598
18	6	0	9.534114	7.904778	3.327534
19	1	0	10.175587	7.224235	3.904701
20	1	0	9.353044	8.773739	3.972158
21	1	0	4.962141	6.871285	2.509401
22	1	0	6.001605	1.889238	0.569900
23	6	0	8.543244	0.393946	-0.128089
24	1	0	7.632226	-0.028525	-0.565202
25	1	0	9.232603	0.601776	-0.962903
26	6	0	9.212972	-0.649761	0.797097
27	1	0	8.545234	-0.920799	1.620480
28	1	0	9.450973	-1.555107	0.229170
29	1	0	10.143522	-0.265557	1.228347
30	6	0	10.295431	8.362999	2.066561
31	1	0	11.248105	8.833905	2.335979
32	1	0	10.507652	7.515806	1.405304
33	1	0	9.703709	9.087992	1.497446

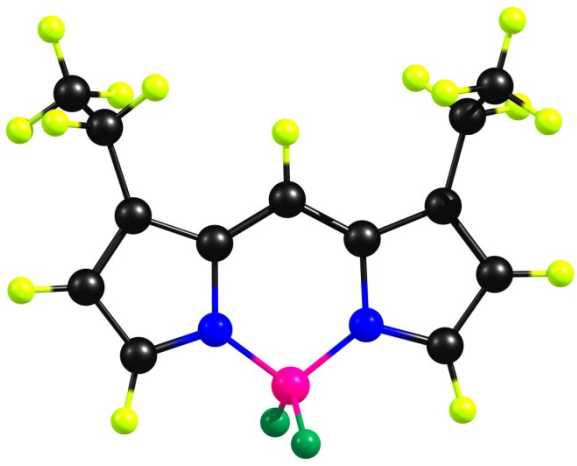

Figure S-29: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.08**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.174291	4.207037	2.050197
2	9	0	5.263754	4.306832	1.016184
3	9	0	5.610970	3.624572	3.171056
4	7	0	6.736785	5.629355	2.414425
5	7	0	7.426012	3.373675	1.590210
6	6	0	6.020442	6.704169	2.769236
7	6	0	6.872623	7.779704	3.089595
8	6	0	8.183003	7.337181	2.920674
9	6	0	8.085280	5.977573	2.493196
10	6	0	9.067951	5.053254	2.152331
11	6	0	8.757755	3.773053	1.704260
12	6	0	9.595738	2.706009	1.256474
13	6	0	8.735267	1.678951	0.874661
14	6	0	7.418182	2.128880	1.095849
15	1	0	10.111164	5.346423	2.222323
16	1	0	6.554462	8.764329	3.406522
17	6	0	9.447470	8.131142	3.086213
18	1	0	10.267403	7.471848	3.398519
19	1	0	9.311052	8.853905	3.899851
20	1	0	4.939238	6.662786	2.784260
21	1	0	6.482776	1.614387	0.919092
22	1	0	9.013466	0.713164	0.473413
23	6	0	11.097856	2.694319	1.249735
24	1	0	11.481147	3.704826	1.058477
25	1	0	11.446746	2.072988	0.416066
26	6	0	9.860749	8.884190	1.806177
27	1	0	10.781774	9.454157	1.972912
28	1	0	10.033609	8.188485	0.977769
29	1	0	9.077535	9.583193	1.494474
30	6	0	11.703273	2.162752	2.564173
31	1	0	12.797976	2.163105	2.513617
32	1	0	11.399381	2.780311	3.416396
33	1	0	11.369998	1.138421	2.761080

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.183169	4.241781	1.961613
2	9	0	5.367472	4.397560	0.840907
3	9	0	5.471890	3.653120	3.007163
4	7	0	6.748787	5.631083	2.411154
5	7	0	7.430637	3.366461	1.601310
6	6	0	6.037543	6.692713	2.810958
7	6	0	6.893957	7.763322	3.128256
8	6	0	8.199964	7.332096	2.909377
9	6	0	8.097467	5.982433	2.457997
10	6	0	9.075431	5.061691	2.103980
11	6	0	8.761319	3.774667	1.686360
12	6	0	9.595892	2.690654	1.281089
13	6	0	8.735290	1.645235	0.955545
14	6	0	7.420392	2.100308	1.165972
15	1	0	10.116616	5.356852	2.155232
16	1	0	6.580132	8.734508	3.480168
17	6	0	9.461809	8.129230	3.063571
18	1	0	10.297894	7.463028	3.298795
19	1	0	9.354515	8.798028	3.923091
20	1	0	4.959511	6.648430	2.857912
21	1	0	6.488287	1.574751	1.020065
22	1	0	9.009982	0.662961	0.601691
23	6	0	11.096199	2.676547	1.262860
24	1	0	11.476986	3.687708	1.087507
25	1	0	11.433657	2.072971	0.414689
26	6	0	9.810329	8.962500	1.814993
27	1	0	10.728786	9.533252	1.977260
28	1	0	9.956341	8.321730	0.941637
29	1	0	9.008995	9.666867	1.579601
30	6	0	11.714219	2.117314	2.559033

31	1	0	12.805842	2.116386	2.495711
32	1	0	11.422978	2.716940	3.425223
33	1	0	11.382837	1.091847	2.738699

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.194831	4.245037	1.961611
2	9	0	5.384164	4.404134	0.846190
3	9	0	5.488937	3.656237	3.001651
4	7	0	6.759738	5.627361	2.412700
5	7	0	7.438247	3.375046	1.600336
6	6	0	6.050618	6.682839	2.812297
7	6	0	6.902664	7.751450	3.130733
8	6	0	8.204585	7.321166	2.911769
9	6	0	8.100164	5.977443	2.459767
10	6	0	9.076814	5.061912	2.103859
11	6	0	8.761286	3.780047	1.684408
12	6	0	9.594472	2.702062	1.278718
13	6	0	8.736880	1.659544	0.953537
14	6	0	7.426594	2.115188	1.165420
15	1	0	10.117797	5.357027	2.155086
16	1	0	6.588260	8.721550	3.483907
17	6	0	9.462960	8.111797	3.062095
18	1	0	10.295348	7.444588	3.304338
19	1	0	9.356147	8.786322	3.916072
20	1	0	4.972880	6.636199	2.858698
21	1	0	6.493468	1.591752	1.020030
22	1	0	9.010670	0.677865	0.598545
23	6	0	11.088085	2.691558	1.264074
24	1	0	11.465892	3.701590	1.080151
25	1	0	11.428546	2.082149	0.422429
26	6	0	9.808214	8.926538	1.811599
27	1	0	10.726662	9.498130	1.963905
28	1	0	9.950452	8.276725	0.945428
29	1	0	9.007298	9.627979	1.570200
30	6	0	11.693271	2.147952	2.562151
31	1	0	12.784428	2.145949	2.508918
32	1	0	11.394657	2.754554	3.419824
33	1	0	11.360098	1.125282	2.748972

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.170241	4.236628	1.961101
2	9	0	5.350112	4.419287	0.851076
3	9	0	5.470962	3.622388	2.996403
4	7	0	6.736219	5.611688	2.438854
5	7	0	7.413982	3.375612	1.572348
6	6	0	6.028372	6.658585	2.865016
7	6	0	6.883972	7.723068	3.203101
8	6	0	8.185431	7.296318	2.969436
9	6	0	8.080616	5.963068	2.487924
10	6	0	9.057429	5.056728	2.103077
11	6	0	8.740837	3.782998	1.654630
12	6	0	9.572592	2.715780	1.219170
13	6	0	8.715895	1.676009	0.879383
14	6	0	7.402557	2.124407	1.110816
15	1	0	10.101223	5.353216	2.154402
16	1	0	6.574136	8.688295	3.578780
17	6	0	9.452582	8.080387	3.126514
18	1	0	10.234171	7.444844	3.559048
19	1	0	9.280693	8.889094	3.843723

20	1	0	4.949267	6.607550	2.914780
21	1	0	6.466793	1.603122	0.961976
22	1	0	8.993986	0.701765	0.502143
23	6	0	11.070811	2.717211	1.198072
24	1	0	11.438390	3.679173	0.822045
25	1	0	11.414595	1.957330	0.489315
26	6	0	9.948387	8.671620	1.798390
27	1	0	10.863184	9.251870	1.950942
28	1	0	10.160267	7.881535	1.071469
29	1	0	9.191379	9.328961	1.361524
30	6	0	11.680050	2.439864	2.580533
31	1	0	12.772669	2.429817	2.526690
32	1	0	11.379006	3.204623	3.303070
33	1	0	11.344320	1.472133	2.963667

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.243242	4.216165	2.242475
2	9	0	5.231153	4.096692	1.310411
3	9	0	5.895259	3.645991	3.457271
4	7	0	6.723470	5.667243	2.386172
5	7	0	7.510574	3.415811	1.716910
6	6	0	5.930522	6.750366	2.581110
7	6	0	6.716418	7.869980	2.889462
8	6	0	8.055050	7.472731	2.889710
9	6	0	8.059864	6.071577	2.558648
10	6	0	9.102690	5.193912	2.363772
11	6	0	8.834782	3.845014	1.861675
12	6	0	9.649616	2.855453	1.403070
13	6	0	8.739156	1.739984	0.942693
14	6	0	7.460244	2.157844	1.150034
15	1	0	10.126712	5.509072	2.512082
16	1	0	6.340728	8.865867	3.087860
17	6	0	9.271843	8.322449	3.104104
18	1	0	10.014395	7.768449	3.695363
19	1	0	8.996125	9.198144	3.704649
20	1	0	4.855667	6.663190	2.505458
21	1	0	6.509575	1.682480	0.966708
22	1	0	9.066619	0.796486	0.526433
23	6	0	11.135774	2.804629	1.335347
24	1	0	11.555009	3.787195	1.574342
25	1	0	11.436524	2.575316	0.301214
26	6	0	9.929659	8.798145	1.792293
27	1	0	10.821195	9.402220	1.998315
28	1	0	10.228905	7.946243	1.171961
29	1	0	9.232190	9.405923	1.205928
30	6	0	11.745466	1.735872	2.270110
31	1	0	12.834953	1.718323	2.161676
32	1	0	11.504475	1.951537	3.315637
33	1	0	11.367273	0.734673	2.036525

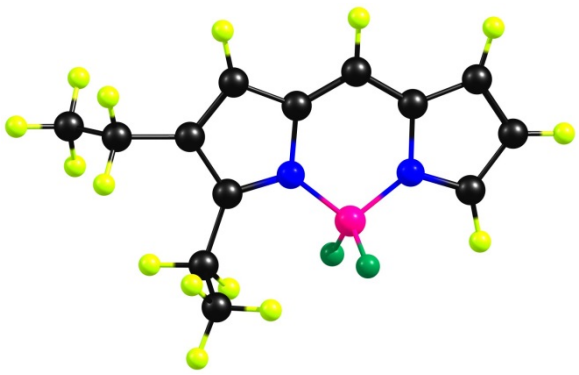

Figure S-30: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.09**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.152957	4.097094	1.850546
2	9	0	5.279750	4.218815	0.781120
3	9	0	5.556802	3.431891	2.914012
4	7	0	6.644452	5.519950	2.321683
5	7	0	7.436900	3.322468	1.399102
6	6	0	5.884874	6.556038	2.725997
7	6	0	6.724068	7.644639	3.129582
8	6	0	8.029093	7.218484	2.950726
9	6	0	7.986379	5.892760	2.443929
10	6	0	9.005751	5.031170	2.071857
11	6	0	8.748574	3.762488	1.547651
12	6	0	9.613819	2.749437	1.068501
13	6	0	8.809656	1.701552	0.630355
14	6	0	7.475682	2.095314	0.852375
15	1	0	10.035625	5.358529	2.179199
16	1	0	6.560496	1.556752	0.645862
17	1	0	9.127707	0.762740	0.198256
18	1	0	10.694476	2.805968	1.050545
19	1	0	8.934018	7.779769	3.149722
20	6	0	6.256267	8.993324	3.606509
21	1	0	5.348848	8.880970	4.213217
22	1	0	7.016361	9.418007	4.273694
23	6	0	4.387670	6.497216	2.773470
24	1	0	4.032318	5.877622	1.945816
25	1	0	3.992226	7.507917	2.620320
26	6	0	3.854037	5.930515	4.107228
27	1	0	4.200865	4.903828	4.243447
28	1	0	4.190536	6.530782	4.960121
29	1	0	2.758577	5.931980	4.101529
30	6	0	5.980526	9.986562	2.461745
31	1	0	5.205438	9.609744	1.785064
32	1	0	5.644931	10.952298	2.856694
33	1	0	6.884426	10.156335	1.866492

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.159509	4.118336	1.757383
2	9	0	5.359458	4.290391	0.624679
3	9	0	5.449912	3.441164	2.753717
4	7	0	6.640789	5.515165	2.295309
5	7	0	7.444822	3.315802	1.384050
6	6	0	5.875926	6.537769	2.720119
7	6	0	6.710409	7.629178	3.122238
8	6	0	8.015553	7.217726	2.924417
9	6	0	7.980151	5.896880	2.406040
10	6	0	9.002401	5.043182	2.034994
11	6	0	8.751291	3.767473	1.528065
12	6	0	9.623100	2.745874	1.086624
13	6	0	8.827095	1.680449	0.677404
14	6	0	7.491433	2.071720	0.876808
15	1	0	10.028480	5.375876	2.139214
16	1	0	6.583737	1.521310	0.680467
17	1	0	9.152483	0.731322	0.281570
18	1	0	10.701088	2.804833	1.077547
19	1	0	8.916447	7.781478	3.121208
20	6	0	6.237952	8.968465	3.616277
21	1	0	5.322777	8.844979	4.203571
22	1	0	6.985865	9.375834	4.303560

23	6	0	4.382656	6.470279	2.788621
24	1	0	4.016242	5.808590	2.002579
25	1	0	3.981798	7.467570	2.585729
26	6	0	3.868105	5.979755	4.159071
27	1	0	4.211869	4.963119	4.352393
28	1	0	4.213468	6.625171	4.970905
29	1	0	2.775166	5.981263	4.166335
30	6	0	5.983589	9.984057	2.487059
31	1	0	5.224035	9.621594	1.789387
32	1	0	5.639845	10.939032	2.894293
33	1	0	6.896653	10.167321	1.914735

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.158208	4.133550	1.746837
2	9	0	5.375314	4.316234	0.611904
3	9	0	5.439541	3.459857	2.729221
4	7	0	6.642892	5.518159	2.292322
5	7	0	7.438405	3.329379	1.383622
6	6	0	5.881241	6.533533	2.717534
7	6	0	6.710156	7.621133	3.124144
8	6	0	8.011946	7.212133	2.927088
9	6	0	7.974337	5.896916	2.405721
10	6	0	8.993478	5.045024	2.036432
11	6	0	8.738694	3.773782	1.529442
12	6	0	9.606910	2.753642	1.092761
13	6	0	8.810607	1.693886	0.683228
14	6	0	7.480490	2.090742	0.879320
15	1	0	10.019720	5.374704	2.142778
16	1	0	6.570380	1.545197	0.681742
17	1	0	9.132573	0.743487	0.288693
18	1	0	10.684737	2.809746	1.087107
19	1	0	8.912984	7.774111	3.126215
20	6	0	6.230584	8.950704	3.616339
21	1	0	5.310944	8.819396	4.193889
22	1	0	6.968901	9.358748	4.312159
23	6	0	4.395255	6.464090	2.787232
24	1	0	4.030776	5.790846	2.010751
25	1	0	3.993341	7.457647	2.570912
26	6	0	3.895284	5.993725	4.159572
27	1	0	4.243418	4.981218	4.362699
28	1	0	4.246342	6.648975	4.959875
29	1	0	2.803494	5.991979	4.177518
30	6	0	5.984420	9.957269	2.489480
31	1	0	5.235846	9.588835	1.784392
32	1	0	5.631180	10.910952	2.888785
33	1	0	6.901705	10.143360	1.926652

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.160627	4.149127	1.712986
2	9	0	5.407807	4.355445	0.556692
3	9	0	5.403817	3.478618	2.674930
4	7	0	6.651383	5.524969	2.281130
5	7	0	7.438661	3.330101	1.377845
6	6	0	5.895366	6.542049	2.705839
7	6	0	6.727165	7.622652	3.131500
8	6	0	8.028659	7.211260	2.940742
9	6	0	7.989557	5.896620	2.407477
10	6	0	9.005181	5.038440	2.044654
11	6	0	8.744975	3.764031	1.533630

12	6	0	9.608162	2.734119	1.110988
13	6	0	8.804191	1.675842	0.699049
14	6	0	7.474791	2.086174	0.880349
15	1	0	10.035299	5.360501	2.158897
16	1	0	6.559089	1.548113	0.679072
17	1	0	9.122295	0.719107	0.311888
18	1	0	10.688621	2.779506	1.114765
19	1	0	8.931047	7.770860	3.151409
20	6	0	6.237662	8.951167	3.629068
21	1	0	5.342399	8.807536	4.244790
22	1	0	6.996127	9.387861	4.287228
23	6	0	4.403954	6.486558	2.776755
24	1	0	4.022649	5.821037	1.999513
25	1	0	4.011897	7.488606	2.574105
26	6	0	3.920739	6.011261	4.157068
27	1	0	4.262147	4.991130	4.344015
28	1	0	4.299675	6.658701	4.954159
29	1	0	2.828116	6.024519	4.196369
30	6	0	5.921723	9.931226	2.490900
31	1	0	5.152915	9.527817	1.824288
32	1	0	5.563046	10.886171	2.886565
33	1	0	6.814360	10.121833	1.887701

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.180618	4.019792	2.046705
2	9	0	5.153768	4.013778	1.112302
3	9	0	5.785299	3.394565	3.226092
4	7	0	6.596080	5.505127	2.391279
5	7	0	7.440410	3.359566	1.449712
6	6	0	5.741159	6.532584	2.741832
7	6	0	6.512875	7.647441	3.031135
8	6	0	7.934941	7.243494	2.822685
9	6	0	7.936151	5.941637	2.441668
10	6	0	9.036747	5.071279	2.061812
11	6	0	8.768622	3.826022	1.544755
12	6	0	9.616224	2.823867	0.975953
13	6	0	8.794610	1.792972	0.536691
14	6	0	7.466510	2.153489	0.840651
15	1	0	10.050398	5.442917	2.136800
16	1	0	6.550044	1.608328	0.662841
17	1	0	9.098072	0.877531	0.046207
18	1	0	10.691937	2.897403	0.891406
19	1	0	8.799068	7.882444	2.952443
20	6	0	6.079728	8.999789	3.466136
21	1	0	5.004199	9.006938	3.668401
22	1	0	6.582284	9.248201	4.415213
23	6	0	4.250317	6.365510	2.835799
24	1	0	3.917059	5.716295	2.022214
25	1	0	3.783300	7.344371	2.673432
26	6	0	3.774861	5.784489	4.182459
27	1	0	4.209892	4.795542	4.344915
28	1	0	4.064594	6.432023	5.018470
29	1	0	2.683003	5.688862	4.189914
30	6	0	6.424912	10.106855	2.440266
31	1	0	5.907908	9.930456	1.492024
32	1	0	6.118152	11.084293	2.827270
33	1	0	7.500362	10.145099	2.236885

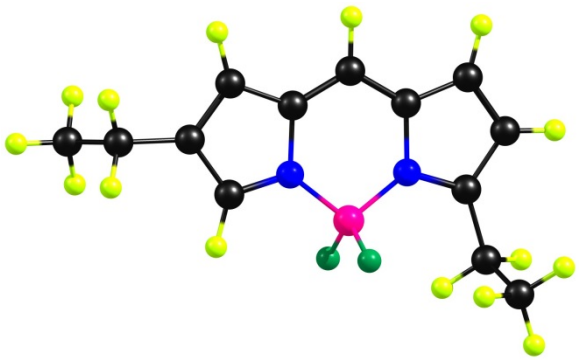

Figure S-31: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.10**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.045899	4.316831	1.878872
2	9	0	5.244371	4.493134	0.761993
3	9	0	5.340794	3.718354	2.914590
4	7	0	6.599193	5.704420	2.356205
5	7	0	7.308381	3.447612	1.515441
6	6	0	5.869247	6.772234	2.711282
7	6	0	6.700838	7.835468	3.140300
8	6	0	8.005639	7.359855	3.029094
9	6	0	7.939884	6.031811	2.538863
10	6	0	8.932404	5.104713	2.228153
11	6	0	8.632056	3.845996	1.724030
12	6	0	9.483969	2.787589	1.312518
13	6	0	8.668012	1.767318	0.858954
14	6	0	7.322111	2.202463	0.996699
15	1	0	9.973685	5.376357	2.373911
16	1	0	8.969367	0.807502	0.460689
17	1	0	10.565618	2.808157	1.347913
18	1	0	8.917208	7.893244	3.269407
19	6	0	6.240921	9.199873	3.576760
20	1	0	5.306891	9.107858	4.146072
21	1	0	6.979516	9.625395	4.267258
22	1	0	4.788406	6.741573	2.655428
23	6	0	6.079374	1.429940	0.675007
24	1	0	5.309242	2.123480	0.326252
25	1	0	6.306668	0.744311	-0.150045
26	6	0	5.545610	0.628604	1.881580
27	1	0	6.295344	-0.080543	2.249695
28	1	0	5.276256	1.307680	2.693628
29	1	0	4.654693	0.062058	1.589316
30	6	0	6.022877	10.173485	2.403638
31	1	0	5.264762	9.792139	1.710492
32	1	0	5.689912	11.152880	2.766045
33	1	0	6.949193	10.315696	1.836195

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.028777	4.367854	1.822829
2	9	0	5.261965	4.581583	0.674339
3	9	0	5.249620	3.780608	2.823814
4	7	0	6.607811	5.726567	2.332463
5	7	0	7.260360	3.453431	1.487454
6	6	0	5.902218	6.792447	2.739912

7	6	0	6.761991	7.844837	3.130351
8	6	0	8.055691	7.366694	2.940001
9	6	0	7.956680	6.044766	2.441778
10	6	0	8.926518	5.111341	2.089071
11	6	0	8.593673	3.848545	1.623379
12	6	0	9.416295	2.769539	1.210702
13	6	0	8.574222	1.741665	0.831812
14	6	0	7.239713	2.191851	1.013687
15	1	0	9.973231	5.376572	2.180879
16	1	0	8.851812	0.767755	0.458342
17	1	0	10.496037	2.779674	1.199226
18	1	0	8.980267	7.890209	3.137091
19	6	0	6.334929	9.203436	3.610932
20	1	0	5.423257	9.106347	4.209683
21	1	0	7.100920	9.602356	4.283179
22	1	0	4.821908	6.767938	2.745443
23	6	0	5.984382	1.415070	0.773064
24	1	0	5.177753	2.100565	0.509153
25	1	0	6.152433	0.760459	-0.087639
26	6	0	5.566444	0.564215	1.990497
27	1	0	6.353171	-0.141122	2.270622
28	1	0	5.349901	1.204460	2.846556
29	1	0	4.666243	-0.007924	1.751932
30	6	0	6.086962	10.205920	2.469357
31	1	0	5.302009	9.850035	1.796759
32	1	0	5.778902	11.177765	2.865300
33	1	0	6.992251	10.352024	1.874265

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.032984	4.385288	1.799862
2	9	0	5.296705	4.610679	0.641664
3	9	0	5.233324	3.804980	2.778545
4	7	0	6.614977	5.730872	2.323272
5	7	0	7.257602	3.465863	1.486854
6	6	0	5.914003	6.791885	2.730365
7	6	0	6.772130	7.837930	3.126820
8	6	0	8.060859	7.357835	2.938721
9	6	0	7.956911	6.042560	2.437053
10	6	0	8.922636	5.108517	2.088759
11	6	0	8.584859	3.850335	1.625215
12	6	0	9.401005	2.767315	1.225328
13	6	0	8.555892	1.745251	0.851851
14	6	0	7.228754	2.207693	1.024792
15	1	0	9.969665	5.368609	2.185013
16	1	0	8.826931	0.766464	0.487469
17	1	0	10.480490	2.770450	1.219822
18	1	0	8.986630	7.876732	3.140338
19	6	0	6.348426	9.190003	3.608124
20	1	0	5.452199	9.089722	4.227853
21	1	0	7.126169	9.596338	4.260623
22	1	0	4.833839	6.769395	2.731183
23	6	0	5.970946	1.446167	0.790323
24	1	0	5.162289	2.143021	0.568553
25	1	0	6.114862	0.819541	-0.094376
26	6	0	5.589048	0.566820	1.987082
27	1	0	6.381448	-0.146057	2.225561
28	1	0	5.398969	1.182274	2.866580
29	1	0	4.681818	0.002722	1.761083
30	6	0	6.070806	10.174261	2.469647
31	1	0	5.275058	9.806991	1.817632
32	1	0	5.764988	11.147610	2.860801
33	1	0	6.961119	10.319419	1.853820

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.063195	4.415111	1.784085
2	9	0	5.352661	4.661204	0.608969
3	9	0	5.231873	3.843583	2.747655
4	7	0	6.660320	5.748078	2.323877
5	7	0	7.277594	3.472749	1.492082
6	6	0	5.970554	6.826628	2.706835
7	6	0	6.841260	7.855893	3.125620
8	6	0	8.125523	7.348105	2.976498
9	6	0	8.008493	6.031868	2.476352
10	6	0	8.965171	5.075737	2.151717
11	6	0	8.613761	3.825724	1.671480
12	6	0	9.415382	2.723482	1.287478
13	6	0	8.555229	1.723656	0.882004
14	6	0	7.234105	2.219216	1.020547
15	1	0	10.016356	5.312948	2.280923
16	1	0	8.810396	0.738391	0.517961
17	1	0	10.496271	2.697821	1.315233
18	1	0	9.056120	7.852824	3.201711
19	6	0	6.429703	9.221493	3.594584
20	1	0	5.670187	9.126342	4.379638
21	1	0	7.292584	9.711556	4.057638
22	1	0	4.888925	6.828268	2.671244
23	6	0	5.961901	1.482689	0.752494
24	1	0	5.165363	2.195641	0.530391
25	1	0	6.108167	0.863235	-0.138622
26	6	0	5.554731	0.596208	1.939977
27	1	0	6.329172	-0.144337	2.163021
28	1	0	5.388139	1.206390	2.830504
29	1	0	4.628015	0.063857	1.708720
30	6	0	5.883323	10.101450	2.463090
31	1	0	5.001030	9.646569	2.002160
32	1	0	5.597724	11.088012	2.840612
33	1	0	6.635116	10.237088	1.679754

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.041319	4.204684	2.127506
2	9	0	4.987823	4.302403	1.227368
3	9	0	5.619021	3.634658	3.325564
4	7	0	6.550554	5.661904	2.437058
5	7	0	7.251711	3.453788	1.527252
6	6	0	5.736527	6.710518	2.772583
7	6	0	6.514777	7.809547	3.057675
8	6	0	7.933730	7.361767	2.848087
9	6	0	7.896222	6.058446	2.474070
10	6	0	8.944202	5.121445	2.083536
11	6	0	8.597464	3.886930	1.593485
12	6	0	9.410825	2.846903	1.037036
13	6	0	8.557911	1.831931	0.640793
14	6	0	7.230889	2.217524	0.953688
15	1	0	9.979351	5.432821	2.128989
16	1	0	8.827465	0.895149	0.169535
17	1	0	10.486574	2.893364	0.934743
18	1	0	8.813760	7.979183	2.973441
19	6	0	6.092015	9.166590	3.484385
20	1	0	5.010653	9.179717	3.657612
21	1	0	6.572733	9.406896	4.446847
22	1	0	4.664367	6.588106	2.797468
23	6	0	5.983883	1.410769	0.767215
24	1	0	5.160809	2.076689	0.491054
25	1	0	6.145648	0.719817	-0.069077
26	6	0	5.585768	0.607047	2.025571
27	1	0	6.377504	-0.094815	2.310271
28	1	0	5.401233	1.280919	2.865523
29	1	0	4.672827	0.032348	1.831588

30	6	0	6.475172	10.270745	2.470119
31	1	0	5.983498	10.099470	1.507661
32	1	0	6.165785	11.250155	2.849627
33	1	0	7.556323	10.300064	2.297960

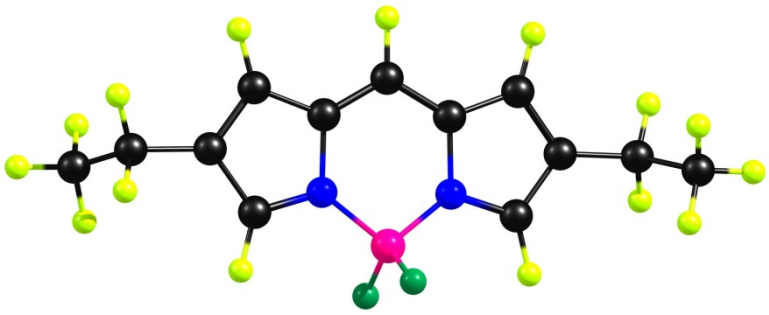

Figure S-32: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.11**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.046371	4.248683	1.863810
2	9	0	5.184629	4.447318	0.803077
3	9	0	5.420698	3.613129	2.919785
4	7	0	6.635625	5.626116	2.345399
5	7	0	7.290640	3.406127	1.396600
6	6	0	5.938167	6.687064	2.770776
7	6	0	6.802693	7.734630	3.181311
8	6	0	8.092963	7.254067	2.982916
9	6	0	7.989293	5.938767	2.460037
10	6	0	8.959048	5.020991	2.067032
11	6	0	8.626853	3.776695	1.539094
12	6	0	9.431054	2.719010	1.040423
13	6	0	8.579934	1.712736	0.595066
14	6	0	7.265865	2.188823	0.839160
15	1	0	10.007071	5.288972	2.163505
16	1	0	10.513730	2.718463	1.009120
17	1	0	9.020919	7.775316	3.183842
18	6	0	6.377774	9.087542	3.683612
19	1	0	5.552001	8.972790	4.398220
20	1	0	7.206221	9.538234	4.243434
21	1	0	4.855514	6.665416	2.775544
22	1	0	6.322109	1.701418	0.628537
23	6	0	8.942289	0.376407	0.006760
24	1	0	8.279226	0.154630	-0.839869
25	1	0	9.957357	0.428881	-0.405357
26	6	0	8.864182	-0.777730	1.023230
27	1	0	7.852567	-0.875348	1.432773
28	1	0	9.132655	-1.730411	0.552527
29	1	0	9.546479	-0.606352	1.863023
30	6	0	5.941280	10.045464	2.559755
31	1	0	5.094042	9.635704	1.998551
32	1	0	5.638174	11.015447	2.970230
33	1	0	6.758516	10.214245	1.849971

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.052192	4.284849	1.760220
2	9	0	5.255487	4.528531	0.642530
3	9	0	5.319418	3.642922	2.757381
4	7	0	6.636215	5.632495	2.306886
5	7	0	7.289390	3.411409	1.357080
6	6	0	5.939107	6.677869	2.770298
7	6	0	6.805532	7.721195	3.179538
8	6	0	8.093698	7.256419	2.941307
9	6	0	7.988414	5.951262	2.396292
10	6	0	8.956586	5.041088	1.989111
11	6	0	8.622916	3.791944	1.479333
12	6	0	9.426507	2.723438	1.005944
13	6	0	8.576187	1.701848	0.599183
14	6	0	7.263232	2.177715	0.836667
15	1	0	10.002341	5.313380	2.071526
16	1	0	10.506527	2.725386	0.970655
17	1	0	9.020642	7.777038	3.134761
18	6	0	6.383619	9.057099	3.723591
19	1	0	5.566126	8.916954	4.439039
20	1	0	7.214379	9.488911	4.289781
21	1	0	4.859150	6.648422	2.800516
22	1	0	6.322265	1.680959	0.647185
23	6	0	8.940006	0.350818	0.050553
24	1	0	8.272216	0.104223	-0.781943
25	1	0	9.948737	0.397970	-0.370675
26	6	0	8.876084	-0.773223	1.100152
27	1	0	7.870369	-0.865044	1.518792
28	1	0	9.145873	-1.735344	0.655772
29	1	0	9.562562	-0.574961	1.927435
30	6	0	5.937517	10.048341	2.633801
31	1	0	5.087318	9.656925	2.068906
32	1	0	5.638406	11.002827	3.075873
33	1	0	6.746923	10.239578	1.924402

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.063977	4.288215	1.759548
2	9	0	5.273391	4.532765	0.646132
3	9	0	5.335445	3.648403	2.751731
4	7	0	6.646656	5.629581	2.305428
5	7	0	7.297312	3.419364	1.358633
6	6	0	5.950487	6.668748	2.766083
7	6	0	6.811686	7.710237	3.176753
8	6	0	8.096614	7.247805	2.940683
9	6	0	7.990658	5.947481	2.396433
10	6	0	8.957576	5.041069	1.990661
11	6	0	8.623479	3.796178	1.480957
12	6	0	9.425758	2.732106	1.009393
13	6	0	8.577214	1.714595	0.602859
14	6	0	7.269145	2.191709	0.840170
15	1	0	10.002767	5.312977	2.074160
16	1	0	10.505456	2.733759	0.975315
17	1	0	9.023110	7.768122	3.135071
18	6	0	6.388283	9.039750	3.716973
19	1	0	5.578207	8.897238	4.439090
20	1	0	7.220342	9.477248	4.275130
21	1	0	4.870748	6.636935	2.793750
22	1	0	6.327045	1.697491	0.650942
23	6	0	8.936671	0.368400	0.057634
24	1	0	8.276688	0.128373	-0.781886
25	1	0	9.948938	0.410703	-0.353210
26	6	0	8.853613	-0.746122	1.102821
27	1	0	7.843654	-0.829412	1.510591
28	1	0	9.121069	-1.711213	0.666047
29	1	0	9.530838	-0.550025	1.936964
30	6	0	5.932143	10.014077	2.628811

31	1	0	5.081782	9.613388	2.072421
32	1	0	5.630178	10.970150	3.062913
33	1	0	6.735010	10.203148	1.912890

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.057500	4.287467	1.753957
2	9	0	5.267707	4.538682	0.636199
3	9	0	5.324832	3.641130	2.744770
4	7	0	6.640061	5.627001	2.307954
5	7	0	7.292673	3.419693	1.351526
6	6	0	5.942510	6.665353	2.771460
7	6	0	6.803585	7.705021	3.191461
8	6	0	8.091268	7.244922	2.957371
9	6	0	7.987536	5.945839	2.405626
10	6	0	8.956267	5.039794	1.995643
11	6	0	8.622951	3.795822	1.477104
12	6	0	9.425642	2.731987	1.000933
13	6	0	8.574732	1.716847	0.588548
14	6	0	7.265257	2.193183	0.827582
15	1	0	10.003556	5.311601	2.082957
16	1	0	10.507540	2.731198	0.967226
17	1	0	9.017885	7.766988	3.158537
18	6	0	6.374520	9.039903	3.727021
19	1	0	5.543018	8.902871	4.427654
20	1	0	7.196903	9.474577	4.305075
21	1	0	4.860811	6.633517	2.794553
22	1	0	6.321400	1.699317	0.635618
23	6	0	8.933117	0.363618	0.047101
24	1	0	8.259180	0.109934	-0.779042
25	1	0	9.941472	0.404082	-0.378320
26	6	0	8.868806	-0.736922	1.114277
27	1	0	7.862864	-0.811452	1.538926
28	1	0	9.130905	-1.709952	0.687757
29	1	0	9.560147	-0.522449	1.934804
30	6	0	5.952998	10.014359	2.619345
31	1	0	5.116117	9.610615	2.041054
32	1	0	5.642501	10.974825	3.041838
33	1	0	6.779680	10.193872	1.925380

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	5.983708	4.154244	2.306367
2	9	0	4.898707	4.207871	1.451412
3	9	0	5.662630	3.532209	3.503412
4	7	0	6.589189	5.556553	2.529399
5	7	0	7.146739	3.339547	1.627124
6	6	0	5.898327	6.685697	2.790341
7	6	0	6.775157	7.733792	3.163071
8	6	0	8.062745	7.202861	3.122643
9	6	0	7.963652	5.839109	2.705890
10	6	0	8.919662	4.894846	2.411904
11	6	0	8.509761	3.644637	1.778175
12	6	0	9.221732	2.667036	1.161250
13	6	0	8.240109	1.694508	0.579174
14	6	0	6.995858	2.192067	0.897014
15	1	0	9.973290	5.100207	2.547597
16	1	0	10.298799	2.600444	1.076222
17	1	0	8.990258	7.721919	3.327433
18	6	0	6.368417	9.143866	3.486792
19	1	0	5.407185	9.136668	4.017097

20	1	0	7.099435	9.581796	4.177551
21	1	0	4.818177	6.694331	2.729065
22	1	0	6.011535	1.804630	0.681551
23	6	0	8.587416	0.449865	-0.152037
24	1	0	7.679049	-0.000995	-0.565868
25	1	0	9.236508	0.703780	-1.006076
26	6	0	9.332661	-0.584932	0.724202
27	1	0	8.706831	-0.902334	1.563817
28	1	0	9.587827	-1.466671	0.127228
29	1	0	10.260911	-0.170474	1.131529
30	6	0	6.247576	10.041450	2.239952
31	1	0	5.500091	9.647123	1.542742
32	1	0	5.949556	11.058546	2.519861
33	1	0	7.202442	10.099047	1.706059

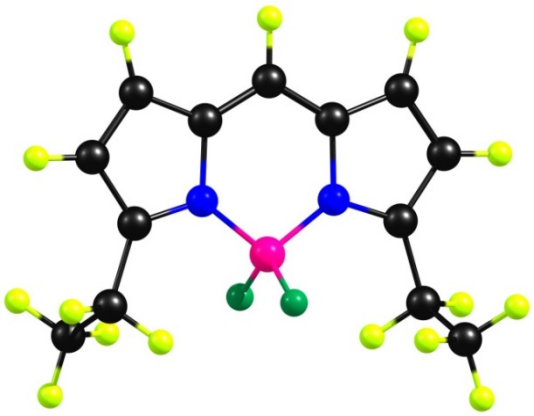

Figure S-33: DFT B3LYP/6-31G(d) optimised ground-state structure of **4.12**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.088762	4.268504	1.829825
2	9	0	5.332146	4.435701	0.673110
3	9	0	5.322715	3.697694	2.842625
4	7	0	6.648540	5.653884	2.314054
5	7	0	7.331749	3.360980	1.515989
6	6	0	5.932866	6.729090	2.710800
7	6	0	6.823206	7.770172	3.081183
8	6	0	8.113213	7.299736	2.903283
9	6	0	8.004075	5.969964	2.424332
10	6	0	8.981600	5.035300	2.103261
11	6	0	8.662923	3.757057	1.659667
12	6	0	9.493167	2.676282	1.269513
13	6	0	8.654746	1.641669	0.890430
14	6	0	7.318786	2.092634	1.050374
15	1	0	10.026906	5.312378	2.202068
16	1	0	10.575493	2.688873	1.269822
17	1	0	9.042929	7.820470	3.093157
18	1	0	8.936895	0.661661	0.528843
19	1	0	6.519194	8.744384	3.440707
20	6	0	6.061936	1.317727	0.793704
21	1	0	5.289086	1.999825	0.428065
22	1	0	6.266135	0.594823	-0.005253
23	6	0	4.434860	6.773777	2.707083
24	1	0	4.046460	5.783867	2.962960
25	1	0	4.114030	7.465760	3.495020
26	6	0	3.849432	7.227336	1.353415
27	1	0	4.125047	6.519137	0.569001
28	1	0	2.756489	7.273111	1.414413
29	1	0	4.217265	8.221330	1.075599

30	6	0	5.548120	0.572798	2.043478
31	1	0	6.301589	-0.123972	2.427278
32	1	0	5.297992	1.287758	2.830296
33	1	0	4.648756	-0.001077	1.794175

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.082426	4.266228	1.830075
2	9	0	5.308964	4.437444	0.674653
3	9	0	5.309447	3.682927	2.842411
4	7	0	6.633555	5.650898	2.311866
5	7	0	7.318463	3.357786	1.513645
6	6	0	5.916834	6.729125	2.694981
7	6	0	6.807341	7.769118	3.063352
8	6	0	8.096354	7.296029	2.893321
9	6	0	7.988762	5.965174	2.421764
10	6	0	8.966043	5.034625	2.096899
11	6	0	8.647887	3.758881	1.652162
12	6	0	9.477444	2.677744	1.267331
13	6	0	8.641133	1.638319	0.900646
14	6	0	7.305343	2.085077	1.063005
15	1	0	10.008998	5.312542	2.193407
16	1	0	10.557174	2.691723	1.264311
17	1	0	9.023307	7.816771	3.082019
18	1	0	8.925851	0.658774	0.547729
19	1	0	6.506032	8.744238	3.414747
20	6	0	6.055566	1.297425	0.825668
21	1	0	5.249027	1.973270	0.537910
22	1	0	6.236237	0.626488	-0.019859
23	6	0	4.421766	6.785359	2.678330
24	1	0	4.018427	5.787116	2.854130
25	1	0	4.099646	7.418601	3.510770
26	6	0	3.857954	7.349717	1.357826
27	1	0	4.132494	6.706803	0.520596
28	1	0	2.767274	7.400219	1.410368
29	1	0	4.235692	8.357022	1.163981
30	6	0	5.627095	0.468656	2.054357
31	1	0	6.413174	-0.228546	2.355874
32	1	0	5.400291	1.124282	2.896008
33	1	0	4.731108	-0.111202	1.817995

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.078622	4.264947	1.830461
2	9	0	5.308855	4.436106	0.680926
3	9	0	5.312376	3.683946	2.839661
4	7	0	6.629914	5.643904	2.307142
5	7	0	7.311050	3.361990	1.516711
6	6	0	5.913655	6.716475	2.681606
7	6	0	6.797068	7.758367	3.046148
8	6	0	8.083291	7.287557	2.880801
9	6	0	7.976455	5.958819	2.416224
10	6	0	8.952613	5.031642	2.093768
11	6	0	8.633258	3.758917	1.652491
12	6	0	9.459909	2.679294	1.273224
13	6	0	8.624032	1.642512	0.912985
14	6	0	7.294028	2.093873	1.074804
15	1	0	9.995044	5.309669	2.189357
16	1	0	10.539303	2.692377	1.269948
17	1	0	9.009490	7.809454	3.068022
18	1	0	8.905605	0.660927	0.564341

19	1	0	6.492810	8.734014	3.392392
20	6	0	6.044485	1.315340	0.848526
21	1	0	5.231172	1.999527	0.605588
22	1	0	6.200909	0.672366	-0.022274
23	6	0	4.425121	6.764694	2.656715
24	1	0	4.028421	5.757791	2.788544
25	1	0	4.092789	7.360709	3.511400
26	6	0	3.879025	7.376099	1.360987
27	1	0	4.166530	6.768595	0.502758
28	1	0	2.788561	7.421198	1.399550
29	1	0	4.255398	8.390373	1.211067
30	6	0	5.660654	0.456043	2.058955
31	1	0	6.457396	-0.245056	2.316942
32	1	0	5.459250	1.086720	2.924971
33	1	0	4.760019	-0.120555	1.837536

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.073025	4.262555	1.831258
2	9	0	5.296646	4.435152	0.681386
3	9	0	5.310939	3.675863	2.846040
4	7	0	6.623862	5.642888	2.309156
5	7	0	7.307727	3.362815	1.510150
6	6	0	5.908048	6.712484	2.691866
7	6	0	6.789429	7.757990	3.057104
8	6	0	8.078872	7.291575	2.884425
9	6	0	7.974125	5.962906	2.414797
10	6	0	8.952092	5.037487	2.084055
11	6	0	8.634252	3.763286	1.639537
12	6	0	9.461977	2.685602	1.251783
13	6	0	8.624432	1.646684	0.892350
14	6	0	7.293432	2.096703	1.063332
15	1	0	9.996454	5.318591	2.175754
16	1	0	10.543347	2.701445	1.242299
17	1	0	9.006102	7.816369	3.070269
18	1	0	8.903762	0.663880	0.539242
19	1	0	6.480090	8.732716	3.407578
20	6	0	6.041291	1.308470	0.849747
21	1	0	5.218801	1.983868	0.605251
22	1	0	6.197460	0.653971	-0.014227
23	6	0	4.414188	6.761596	2.664341
24	1	0	4.010628	5.756187	2.801182
25	1	0	4.080528	7.368318	3.512732
26	6	0	3.883069	7.365487	1.354902
27	1	0	4.179343	6.747853	0.504148
28	1	0	2.790878	7.416250	1.381783
29	1	0	4.269285	8.378158	1.203294
30	6	0	5.677083	0.463589	2.080573
31	1	0	6.486019	-0.227393	2.337116
32	1	0	5.483261	1.108799	2.940324
33	1	0	4.776661	-0.123507	1.878732

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.103968	4.272376	1.831461
2	9	0	5.335159	4.428226	0.673779
3	9	0	5.321538	3.705029	2.842078
4	7	0	6.664294	5.644481	2.307649
5	7	0	7.340026	3.376892	1.525381
6	6	0	5.931696	6.712176	2.706554
7	6	0	6.821251	7.760629	3.083079

8	6	0	8.128445	7.304989	2.908618
9	6	0	8.035650	5.979655	2.428462
10	6	0	9.043006	5.051874	2.110662
11	6	0	8.695686	3.764846	1.663970
12	6	0	9.510674	2.680315	1.270012
13	6	0	8.650340	1.649930	0.889242
14	6	0	7.310071	2.107069	1.053757
15	1	0	10.085456	5.328263	2.209913
16	1	0	10.592206	2.681006	1.263905
17	1	0	9.050184	7.835616	3.105035
18	1	0	8.924471	0.668490	0.523045
19	1	0	6.508299	8.731862	3.445362
20	6	0	6.053830	1.342069	0.794222
21	1	0	5.288554	2.027701	0.415714
22	1	0	6.258568	0.606451	0.006456
23	6	0	4.438561	6.748050	2.704533
24	1	0	4.056026	5.758085	2.974051
25	1	0	4.112821	7.451767	3.480598
26	6	0	3.835861	7.175483	1.344763
27	1	0	4.122461	6.463043	0.568607
28	1	0	2.742196	7.198761	1.413922
29	1	0	4.181991	8.173878	1.055675
30	6	0	5.510165	0.610418	2.044804
31	1	0	6.245091	-0.101158	2.436794
32	1	0	5.267480	1.334484	2.825180
33	1	0	4.601085	0.055880	1.784992

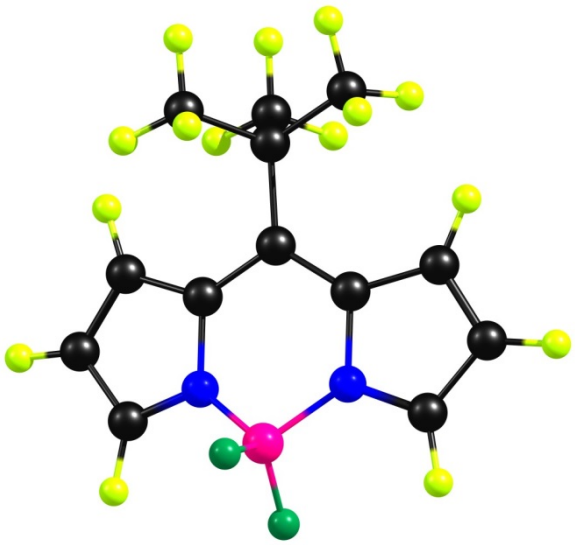

Figure S-34: DFT B3LYP/6-31G(d) optimised ground-state structure of **5.01**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.157956	4.170384	2.288274
2	9	0	5.039725	4.103177	1.477940
3	9	0	5.897188	3.696273	3.563610
4	7	0	6.699237	5.623563	2.355906
5	7	0	7.334735	3.376765	1.651632
6	6	0	5.951605	6.715767	2.553213
7	6	0	6.777649	7.836151	2.748881
8	1	0	6.448043	8.852698	2.912987
9	6	0	8.085533	7.378612	2.676479
10	6	0	8.050699	5.973858	2.419624
11	6	0	9.074672	5.018218	2.162843
12	6	0	8.691080	3.730533	1.709511

13	6	0	9.408099	2.628362	1.140730
14	1	0	10.469831	2.552998	0.994402
15	6	0	8.487757	1.667741	0.754970
16	1	0	8.694284	0.721142	0.275122
17	6	0	7.218294	2.167547	1.097263
18	1	0	6.241936	1.717978	0.975443
19	1	0	4.872359	6.643572	2.551780
20	1	0	8.964442	7.995785	2.769645
21	6	0	10.550726	5.446100	2.375414
22	6	0	11.600378	4.321342	2.236000
23	1	0	11.357926	3.444754	2.843152
24	1	0	11.745334	4.012535	1.197705
25	1	0	12.562898	4.710090	2.584860
26	6	0	10.716836	5.971902	3.830070
27	1	0	10.048620	6.794681	4.078748
28	1	0	10.525497	5.165505	4.547094
29	1	0	11.748408	6.312030	3.974940
30	6	0	10.944235	6.528034	1.333702
31	1	0	10.337380	7.431360	1.393799
32	1	0	11.992551	6.811340	1.483318
33	1	0	10.845388	6.130418	0.317432

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138828	4.200965	2.182616
2	9	0	5.082005	4.178108	1.273345
3	9	0	5.729668	3.702839	3.423554
4	7	0	6.698919	5.633405	2.338791
5	7	0	7.334637	3.374278	1.644999
6	6	0	5.957930	6.722909	2.570025
7	6	0	6.791486	7.828341	2.801326
8	1	0	6.468903	8.837733	3.001909
9	6	0	8.094812	7.365157	2.714839
10	6	0	8.052863	5.971338	2.416387
11	6	0	9.074973	5.017641	2.157638
12	6	0	8.690609	3.726362	1.721409
13	6	0	9.413289	2.600088	1.215133
14	1	0	10.475040	2.510932	1.103583
15	6	0	8.499255	1.627247	0.850742
16	1	0	8.712364	0.660426	0.422966
17	6	0	7.225764	2.142853	1.140952
18	1	0	6.254320	1.689063	1.014200
19	1	0	4.880086	6.662928	2.564759
20	1	0	8.973650	7.972302	2.834352
21	6	0	10.550684	5.452623	2.359277
22	6	0	11.610942	4.347001	2.172714
23	1	0	11.425142	3.477605	2.805019
24	1	0	11.701594	4.029836	1.133624
25	1	0	12.579883	4.761224	2.461599
26	6	0	10.735715	5.945118	3.822344
27	1	0	10.086124	6.772793	4.092127
28	1	0	10.536147	5.129378	4.522587
29	1	0	11.772181	6.262573	3.964899
30	6	0	10.917204	6.560808	1.335419
31	1	0	10.301020	7.452309	1.418069
32	1	0	11.961032	6.852963	1.480304
33	1	0	10.814233	6.182069	0.314985

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.152160	4.197056	2.190903

2	9	0	5.096829	4.166410	1.290803
3	9	0	5.757095	3.706589	3.431091
4	7	0	6.707790	5.627079	2.334851
5	7	0	7.344731	3.376493	1.651400
6	6	0	5.967469	6.711508	2.557293
7	6	0	6.795668	7.817006	2.783962
8	1	0	6.471352	8.826723	2.977864
9	6	0	8.095967	7.355259	2.703187
10	1	0	8.975235	7.962904	2.821260
11	6	0	8.052538	5.965132	2.413232
12	6	0	9.072823	5.015166	2.159367
13	6	0	8.691803	3.726882	1.727712
14	6	0	9.416273	2.607355	1.223987
15	1	0	10.478803	2.521335	1.113051
16	6	0	8.506276	1.636137	0.859618
17	1	0	8.719855	0.670107	0.431312
18	6	0	7.236342	2.150624	1.149665
19	1	0	6.264438	1.698082	1.023476
20	1	0	4.890030	6.648041	2.549746
21	6	0	10.536012	5.450480	2.358451
22	6	0	11.591161	4.351955	2.179234
23	1	0	11.401543	3.482753	2.810176
24	1	0	11.689532	4.037229	1.140294
25	1	0	12.557066	4.767437	2.474875
26	6	0	10.714956	5.945617	3.810947
27	1	0	10.053501	6.763463	4.081045
28	1	0	10.528000	5.128415	4.511901
29	1	0	11.746870	6.277027	3.950647
30	6	0	10.897284	6.546957	1.334859
31	1	0	10.275824	7.435193	1.408351
32	1	0	11.938787	6.844349	1.481491
33	1	0	10.799475	6.160178	0.317697

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.159545	4.195247	2.217634
2	9	0	5.078499	4.153787	1.342071
3	9	0	5.801412	3.704864	3.473812
4	7	0	6.709416	5.630353	2.341998
5	7	0	7.344942	3.380519	1.649417
6	6	0	5.966933	6.714652	2.567658
7	6	0	6.794871	7.824878	2.783927
8	1	0	6.470403	8.837098	2.974373
9	6	0	8.098041	7.365081	2.696264
10	6	0	8.056988	5.972530	2.412360
11	6	0	9.078096	5.019624	2.153907
12	6	0	8.696627	3.731560	1.714995
13	6	0	9.415091	2.617405	1.185754
14	1	0	10.477042	2.531067	1.051830
15	6	0	8.499657	1.648919	0.820185
16	1	0	8.708964	0.688244	0.373871
17	6	0	7.231175	2.159302	1.135105
18	1	0	6.256837	1.705298	1.018170
19	1	0	4.888029	6.645985	2.569368
20	1	0	8.976441	7.979893	2.803869
21	6	0	10.545929	5.450575	2.363572
22	6	0	11.597920	4.340223	2.196925
23	1	0	11.385388	3.467891	2.819686
24	1	0	11.713380	4.032524	1.155638
25	1	0	12.563813	4.744283	2.513513
26	6	0	10.712963	5.950092	3.820511
27	1	0	10.059585	6.780268	4.078960
28	1	0	10.502999	5.136404	4.521948
29	1	0	11.748509	6.269619	3.973675
30	6	0	10.918107	6.544246	1.335269
31	1	0	10.317711	7.447966	1.422089
32	1	0	11.969031	6.819122	1.471252
33	1	0	10.796953	6.161698	0.316886

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.433366	3.961574	2.778035
2	9	0	5.113893	3.722624	2.451580
3	9	0	6.794212	3.430458	4.000621
4	7	0	6.723840	5.497857	2.761795
5	7	0	7.373632	3.480620	1.644554
6	6	0	5.833005	6.513279	2.758686
7	6	0	6.517393	7.697568	2.531037
8	1	0	6.109774	8.699479	2.556343
9	6	0	7.928558	7.338873	2.324710
10	6	0	8.035234	5.996118	2.503236
11	6	0	9.151755	5.046056	2.208154
12	6	0	8.726607	3.905571	1.526652
13	6	0	9.337627	3.036879	0.566521
14	1	0	10.348591	3.120505	0.196453
15	6	0	8.358944	2.163341	0.106128
16	1	0	8.478828	1.386905	-0.638223
17	6	0	7.164538	2.460721	0.794598
18	1	0	6.202403	1.969740	0.754348
19	1	0	4.782127	6.324600	2.917896
20	1	0	8.718053	8.029698	2.068452
21	6	0	10.606950	5.395042	2.514448
22	6	0	11.427422	4.120565	2.828442
23	1	0	10.990097	3.577078	3.672659
24	1	0	11.483943	3.432036	1.983468
25	1	0	12.452594	4.401243	3.096349
26	6	0	10.702628	6.298171	3.768091
27	1	0	10.242598	7.277894	3.622448
28	1	0	10.218721	5.826373	4.630340
29	1	0	11.757343	6.459368	4.018296
30	6	0	11.255497	6.130715	1.309999
31	1	0	10.728229	7.061354	1.073613
32	1	0	12.299025	6.383608	1.535751
33	1	0	11.243873	5.505305	0.411013

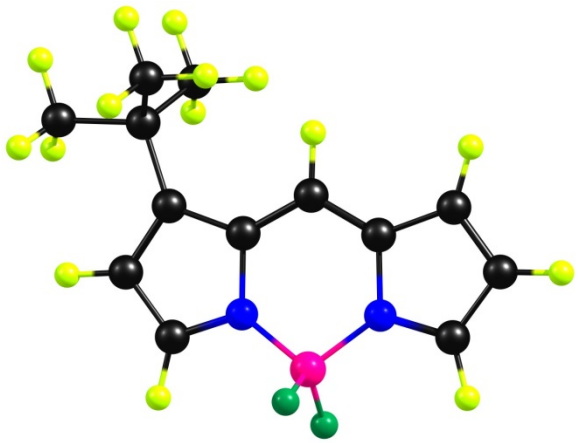

Figure S-35: DFT B3LYP/6-31G(d) optimised ground-state structure of **5.02**

DFT B3LYP/6-31G(d) optimised ground state structure:

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

1	5	0	6.141108	4.145950	2.066256
2	9	0	5.182326	4.273019	1.080866
3	9	0	5.634710	3.533740	3.197890
4	7	0	6.710159	5.565377	2.444667
5	7	0	7.373605	3.338980	1.528549
6	6	0	5.981792	6.616217	2.827660
7	6	0	6.820435	7.692798	3.180939
8	1	0	6.477108	8.658969	3.520811
9	6	0	8.139843	7.282123	3.005475
10	6	0	8.059257	5.924883	2.532286
11	6	0	9.025226	5.006191	2.135178
12	6	0	8.700730	3.745475	1.633076
13	6	0	9.522843	2.710524	1.118267
14	1	0	10.603195	2.740312	1.059622
15	6	0	8.677720	1.688515	0.703496
16	1	0	8.954587	0.745243	0.253226
17	6	0	7.361309	2.116994	0.975731
18	1	0	6.425386	1.603538	0.799915
19	1	0	4.901033	6.562211	2.837652
20	1	0	10.074022	5.273041	2.191539
21	6	0	9.393300	8.110071	3.255234
22	6	0	9.012962	9.510283	3.777546
23	1	0	8.454281	9.450227	4.718140
24	1	0	9.919268	10.096888	3.964190
25	1	0	8.403884	10.059438	3.050972
26	6	0	10.190044	8.290275	1.939176
27	1	0	10.539623	7.337602	1.529671
28	1	0	9.573478	8.774225	1.173871
29	1	0	11.070229	8.920087	2.115798
30	6	0	10.284975	7.426672	4.320875
31	1	0	9.741290	7.304489	5.264001
32	1	0	10.625966	6.436199	4.004688
33	1	0	11.173454	8.038879	4.516678

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.138084	4.194651	1.948128
2	9	0	5.305737	4.396986	0.848277
3	9	0	5.442446	3.572527	2.983725
4	7	0	6.710487	5.569662	2.442310
5	7	0	7.377205	3.336087	1.537298
6	6	0	5.985939	6.597691	2.885983
7	6	0	6.826431	7.669037	3.245074
8	1	0	6.484748	8.614902	3.632277
9	6	0	8.141335	7.278889	3.009409
10	6	0	8.058895	5.937773	2.497127
11	6	0	9.022754	5.029045	2.084056
12	6	0	8.699916	3.757513	1.614320
13	6	0	9.525674	2.702464	1.154037
14	1	0	10.603424	2.732614	1.096026
15	6	0	8.686564	1.652618	0.803391
16	1	0	8.968498	0.687509	0.412963
17	6	0	7.369689	2.084352	1.055061
18	1	0	6.440302	1.554156	0.910666
19	1	0	4.908608	6.535955	2.931870
20	1	0	10.068384	5.301738	2.121642
21	6	0	9.393532	8.110471	3.249372
22	6	0	9.015653	9.496088	3.808643
23	1	0	8.489068	9.414606	4.763078
24	1	0	9.920736	10.085273	3.977445
25	1	0	8.382189	10.051744	3.112334
26	6	0	10.159813	8.322736	1.921061
27	1	0	10.507027	7.383030	1.487611
28	1	0	9.524721	8.815518	1.180514
29	1	0	11.036313	8.954832	2.092104
30	6	0	10.312509	7.411884	4.280926
31	1	0	9.786457	7.254017	5.225878
32	1	0	10.665226	6.439901	3.931179
33	1	0	11.190783	8.033168	4.480157

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.148908	4.204063	1.951209
2	9	0	5.321827	4.406116	0.855948
3	9	0	5.458451	3.585035	2.982984
4	7	0	6.720326	5.573239	2.442978
5	7	0	7.384318	3.349851	1.542126
6	6	0	5.997521	6.595950	2.884338
7	6	0	6.833825	7.665798	3.243131
8	1	0	6.493181	8.612013	3.630303
9	6	0	8.144094	7.275535	3.007869
10	6	0	8.060369	5.939887	2.497855
11	6	0	9.023287	5.035433	2.086573
12	6	0	8.699926	3.767505	1.618219
13	6	0	9.523939	2.716753	1.159792
14	1	0	10.601354	2.747284	1.101996
15	6	0	8.686536	1.670517	0.810371
16	1	0	8.966674	0.705278	0.420031
17	6	0	7.374698	2.103896	1.062199
18	1	0	6.444019	1.576158	0.918755
19	1	0	4.920511	6.531674	2.929125
20	1	0	10.068583	5.309010	2.124608
21	6	0	9.390275	8.101044	3.245919
22	6	0	9.012664	9.477815	3.801622
23	1	0	8.486037	9.394761	4.755256
24	1	0	9.916482	10.067669	3.970845
25	1	0	8.379375	10.031739	3.104654
26	6	0	10.149633	8.310514	1.924410
27	1	0	10.494503	7.370881	1.490386
28	1	0	9.513861	8.803495	1.185654
29	1	0	11.026591	8.941201	2.094153
30	6	0	10.301295	7.404712	4.271613
31	1	0	9.774241	7.248357	5.215414
32	1	0	10.651697	6.432208	3.922786
33	1	0	11.180148	8.024044	4.470820

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.146274	4.202042	1.949104
2	9	0	5.317331	4.405628	0.849907
3	9	0	5.453078	3.581920	2.984392
4	7	0	6.717014	5.572873	2.441917
5	7	0	7.382920	3.348307	1.540877
6	6	0	5.993417	6.595538	2.883353
7	6	0	6.830210	7.668475	3.243884
8	1	0	6.488098	8.616256	3.631765
9	6	0	8.141741	7.278473	3.009052
10	6	0	8.060995	5.942155	2.498211
11	6	0	9.025243	5.037117	2.087295
12	6	0	8.702528	3.765612	1.617426
13	6	0	9.526293	2.713981	1.158885
14	1	0	10.605904	2.744273	1.101503
15	6	0	8.686364	1.665825	0.808041
16	1	0	8.966766	0.698934	0.416920
17	6	0	7.373068	2.100970	1.060055
18	1	0	6.438788	1.575949	0.917217
19	1	0	4.914776	6.527818	2.926531
20	1	0	10.073366	5.310001	2.125574
21	6	0	9.392539	8.104169	3.247639
22	6	0	9.014358	9.485022	3.805101

23	1	0	8.485545	9.399794	4.759812
24	1	0	9.920330	10.075039	3.975331
25	1	0	8.380157	10.038819	3.105485
26	6	0	10.152559	8.311490	1.921931
27	1	0	10.506889	7.369652	1.494956
28	1	0	9.511264	8.794674	1.178480
29	1	0	11.026161	8.950743	2.089411
30	6	0	10.303386	7.402638	4.275433
31	1	0	9.769984	7.235361	5.216150
32	1	0	10.662235	6.433652	3.918740
33	1	0	11.179566	8.026238	4.483564

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.223142	4.084834	2.289109
2	9	0	5.091598	4.050918	1.498556
3	9	0	6.022009	3.462958	3.511375
4	7	0	6.757015	5.520422	2.445085
5	7	0	7.392137	3.319073	1.559859
6	6	0	5.999864	6.607708	2.701937
7	6	0	6.821903	7.695471	3.039504
8	1	0	6.461885	8.683097	3.291104
9	6	0	8.154002	7.279780	2.993196
10	6	0	8.116822	5.887367	2.590016
11	6	0	9.104311	4.980485	2.278297
12	6	0	8.742290	3.703124	1.659021
13	6	0	9.481999	2.765417	1.021121
14	1	0	10.556311	2.751993	0.895440
15	6	0	8.527927	1.739322	0.488813
16	1	0	8.799154	0.842815	-0.051699
17	6	0	7.272383	2.153945	0.841302
18	1	0	6.301733	1.715563	0.670276
19	1	0	4.921383	6.548708	2.656918
20	1	0	10.152480	5.216734	2.383823
21	6	0	9.389165	8.120841	3.269735
22	6	0	8.982291	9.541110	3.710611
23	1	0	8.369571	9.519196	4.618945
24	1	0	9.876762	10.137165	3.924402
25	1	0	8.416249	10.058920	2.927991
26	6	0	10.255065	8.247433	1.991023
27	1	0	10.591684	7.274057	1.621975
28	1	0	9.687756	8.728089	1.186185
29	1	0	11.143678	8.858107	2.193159
30	6	0	10.225149	7.487355	4.409272
31	1	0	9.638952	7.430581	5.333150
32	1	0	10.555226	6.472963	4.166345
33	1	0	11.117252	8.093885	4.608097

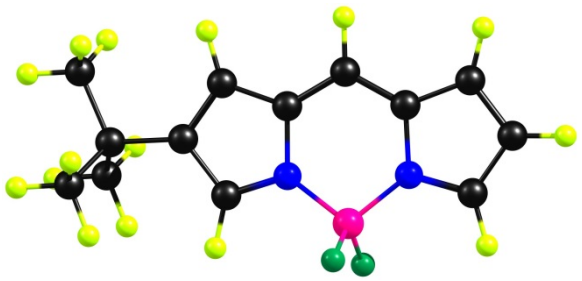

Figure S-36: DFT B3LYP/6-31G(d) optimised ground-state structure of **5.03**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.124634	4.259821	1.885525
2	9	0	5.307451	4.445222	0.788258
3	9	0	5.449175	3.662643	2.932926
4	7	0	6.712606	5.643953	2.356627
5	7	0	7.375139	3.392440	1.490641
6	6	0	6.013801	6.726073	2.713426
7	6	0	6.873200	7.776352	3.143103
8	6	0	8.161882	7.266976	3.027822
9	6	0	8.063459	5.937790	2.535503
10	6	0	9.034939	4.998842	2.212241
11	6	0	8.707852	3.747224	1.691850
12	6	0	9.523527	2.671230	1.258010
13	1	0	10.605286	2.656149	1.285540
14	6	0	8.671497	1.675714	0.796115
15	1	0	8.942871	0.712809	0.386025
16	6	0	7.356732	2.161540	0.957887
17	1	0	6.417433	1.681687	0.716982
18	1	0	4.933247	6.717541	2.652481
19	1	0	10.081377	5.251761	2.355270
20	1	0	9.090930	7.771582	3.256712
21	6	0	6.420042	9.147965	3.615759
22	6	0	5.499953	8.991492	4.849088
23	1	0	5.159214	9.973397	5.199509
24	1	0	4.611291	8.394356	4.615154
25	1	0	6.026922	8.498470	5.673534
26	6	0	5.637764	9.852976	2.483108
27	1	0	5.297197	10.842609	2.811302
28	1	0	6.265338	9.985120	1.594703
29	1	0	4.753404	9.278028	2.185780
30	6	0	7.631989	10.015199	4.001902
31	1	0	8.208792	9.559217	4.815052
32	1	0	8.304216	10.167557	3.149402
33	1	0	7.297520	11.001485	4.342758

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.135611	4.299209	1.792600
2	9	0	5.409473	4.519689	0.623972
3	9	0	5.334166	3.711576	2.769284
4	7	0	6.714373	5.658195	2.324833
5	7	0	7.376567	3.391651	1.494288
6	6	0	6.013535	6.730691	2.704212
7	6	0	6.874114	7.779498	3.129550
8	6	0	8.162602	7.281325	2.987179
9	6	0	8.065057	5.956414	2.484661
10	6	0	9.035878	5.019472	2.165845
11	6	0	8.707372	3.756575	1.678559
12	6	0	9.521281	2.662788	1.295168
13	1	0	10.600349	2.646557	1.327004
14	6	0	8.669204	1.646552	0.882396
15	1	0	8.940040	0.666446	0.522718
16	6	0	7.355974	2.136651	1.020822
17	1	0	6.419899	1.644777	0.802602
18	1	0	4.934290	6.716803	2.661025
19	1	0	10.080454	5.275656	2.299070
20	1	0	9.091088	7.784538	3.209352
21	6	0	6.420449	9.141584	3.626775
22	6	0	5.528130	8.964274	4.876795
23	1	0	5.192056	9.938184	5.245582
24	1	0	4.639326	8.367668	4.654800
25	1	0	6.074767	8.464643	5.680947
26	6	0	5.610110	9.852501	2.518541
27	1	0	5.274902	10.835412	2.863458
28	1	0	6.215937	9.994284	1.619670
29	1	0	4.723318	9.278083	2.237765

30	6	0	7.632645	10.013962	3.997472
31	1	0	8.227034	9.556872	4.793786
32	1	0	8.284652	10.181473	3.135402
33	1	0	7.296025	10.991216	4.353863

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139483	4.310569	1.797806
2	9	0	5.417349	4.530917	0.634713
3	9	0	5.344020	3.726269	2.771768
4	7	0	6.718049	5.663590	2.327140
5	7	0	7.375880	3.407315	1.500150
6	6	0	6.018806	6.730127	2.704546
7	6	0	6.875115	7.776890	3.128747
8	6	0	8.160060	7.281671	2.987012
9	6	0	8.060922	5.961113	2.486080
10	6	0	9.029676	5.027361	2.168101
11	6	0	8.699535	3.768301	1.682243
12	6	0	9.511216	2.678690	1.299903
13	1	0	10.589949	2.662464	1.331298
14	6	0	8.660356	1.666320	0.888813
15	1	0	8.928938	0.686148	0.528800
16	6	0	7.352435	2.158240	1.028661
17	1	0	6.414779	1.669267	0.811782
18	1	0	4.939637	6.714336	2.660926
19	1	0	10.073892	5.282939	2.300758
20	1	0	9.087904	7.785885	3.209277
21	6	0	6.422494	9.131306	3.623129
22	6	0	5.534722	8.952039	4.864364
23	1	0	5.197477	9.924522	5.233830
24	1	0	4.647327	8.355320	4.640175
25	1	0	6.080812	8.451722	5.667421
26	6	0	5.617973	9.835662	2.519685
27	1	0	5.281496	10.817928	2.863057
28	1	0	6.224535	9.976446	1.622082
29	1	0	4.732693	9.260065	2.239018
30	6	0	7.628622	9.996728	3.992090
31	1	0	8.221257	9.538195	4.788008
32	1	0	8.279962	10.163206	3.130120
33	1	0	7.293307	10.973669	4.348494

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.139267	4.311730	1.796388
2	9	0	5.415849	4.537000	0.629774
3	9	0	5.339252	3.728663	2.773603
4	7	0	6.721651	5.664448	2.327191
5	7	0	7.374195	3.405488	1.498772
6	6	0	6.023620	6.731966	2.704706
7	6	0	6.881431	7.779337	3.130059
8	6	0	8.167504	7.284884	2.989533
9	6	0	8.068851	5.962205	2.487383
10	6	0	9.036091	5.025219	2.168436
11	6	0	8.702645	3.763701	1.680966
12	6	0	9.511781	2.671726	1.298076
13	1	0	10.592586	2.653146	1.329479
14	6	0	8.656734	1.659129	0.885952
15	1	0	8.924857	0.677064	0.525234
16	6	0	7.348184	2.155046	1.026461
17	1	0	6.406667	1.669385	0.809939
18	1	0	4.942348	6.717814	2.660794

19	1	0	10.082971	5.279311	2.301436
20	1	0	9.096084	7.792135	3.213827
21	6	0	6.422617	9.135506	3.624989
22	6	0	5.531591	8.948955	4.867344
23	1	0	5.183476	9.920124	5.235924
24	1	0	4.649866	8.341589	4.639147
25	1	0	6.082839	8.452455	5.672093
26	6	0	5.614092	9.834952	2.516314
27	1	0	5.267047	10.815956	2.858941
28	1	0	6.224948	9.979460	1.619665
29	1	0	4.734175	9.248576	2.232911
30	6	0	7.628209	10.007933	3.996052
31	1	0	8.221875	9.549418	4.794335
32	1	0	8.280283	10.175705	3.132003
33	1	0	7.287092	10.985192	4.352271

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.427508	4.024848	2.760465
2	9	0	5.111989	3.898785	2.356466
3	9	0	6.615587	3.553295	4.050564
4	7	0	6.831345	5.550736	2.745177
5	7	0	7.391466	3.361548	1.754549
6	6	0	6.047996	6.581538	3.203202
7	6	0	6.769077	7.750277	3.153821
8	6	0	8.110215	7.362061	2.581396
9	6	0	8.087732	6.025230	2.353091
10	6	0	9.057115	5.124153	1.729721
11	6	0	8.667162	3.848656	1.395573
12	6	0	9.311079	2.826092	0.626440
13	1	0	10.297801	2.908097	0.191265
14	6	0	8.416711	1.768674	0.516600
15	1	0	8.567872	0.835970	-0.010467
16	6	0	7.249821	2.128218	1.219552
17	1	0	6.341321	1.563799	1.376915
18	1	0	5.045002	6.384253	3.546388
19	1	0	10.034460	5.501844	1.460043
20	1	0	8.929995	8.038922	2.379921
21	6	0	6.380215	9.135242	3.569242
22	6	0	4.942425	9.171283	4.116125
23	1	0	4.674893	10.192383	4.408981
24	1	0	4.221211	8.838386	3.361617
25	1	0	4.836593	8.529828	4.997801
26	6	0	6.487960	10.078696	2.339044
27	1	0	6.233555	11.102120	2.639158
28	1	0	7.500907	10.093102	1.922610
29	1	0	5.798172	9.769581	1.547071
30	6	0	7.362715	9.631076	4.665272
31	1	0	7.308479	8.996209	5.555492
32	1	0	8.399555	9.634250	4.312014
33	1	0	7.102740	10.656067	4.954885

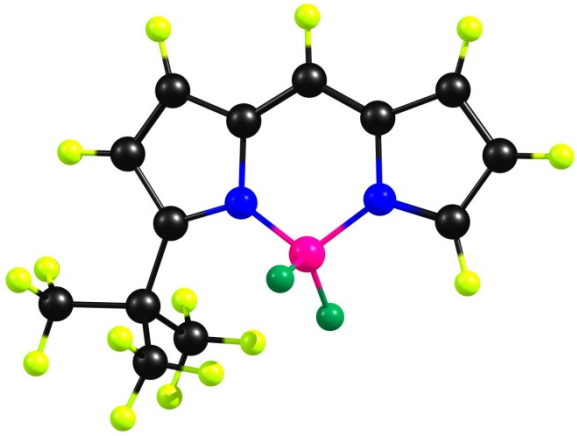

Figure S-37: DFT B3LYP/6-31G(d) optimised ground-state structure of **5.04**

DFT B3LYP/6-31G(d) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.217224	4.018783	2.185431
2	9	0	5.161415	3.903494	1.292163
3	9	0	5.914322	3.446067	3.409347
4	7	0	6.648100	5.529962	2.412084
5	7	0	7.456189	3.283690	1.567789
6	6	0	5.920598	6.622430	2.770283
7	6	0	6.816283	7.689509	3.070163
8	6	0	8.104556	7.230837	2.893698
9	6	0	8.005797	5.881375	2.478732
10	6	0	9.024317	5.009900	2.116629
11	6	0	8.770859	3.726312	1.641226
12	6	0	9.612194	2.716783	1.110989
13	1	0	10.689028	2.778937	1.023207
14	6	0	8.785932	1.670336	0.716192
15	1	0	9.079690	0.735717	0.258586
16	6	0	7.463825	2.060152	1.016826
17	1	0	6.538948	1.520341	0.864850
18	1	0	10.049725	5.362075	2.178163
19	1	0	9.029605	7.777494	3.024374
20	1	0	6.521853	8.681830	3.374995
21	6	0	4.398887	6.733686	2.786163
22	6	0	3.989464	8.074351	3.436616
23	1	0	4.356619	8.937124	2.870153
24	1	0	2.896888	8.141351	3.462263
25	1	0	4.353568	8.155522	4.467155
26	6	0	3.874113	6.728566	1.326336
27	1	0	4.306929	7.556241	0.752233
28	1	0	4.113520	5.790147	0.825776
29	1	0	2.784585	6.854422	1.331359
30	6	0	3.727812	5.596282	3.591771
31	1	0	3.853682	4.625244	3.117252
32	1	0	4.133201	5.536776	4.607457
33	1	0	2.653586	5.803375	3.665388

DFT B3LYP/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.224825	4.014815	2.176784
2	9	0	5.156763	3.898463	1.288069
3	9	0	5.918917	3.424013	3.405179

4	7	0	6.645081	5.523303	2.414086
5	7	0	7.459442	3.278889	1.562608
6	6	0	5.916884	6.616304	2.769678
7	6	0	6.812665	7.682842	3.063318
8	6	0	8.099370	7.225474	2.883558
9	6	0	8.002322	5.876534	2.472359
10	6	0	9.021014	5.012552	2.103287
11	6	0	8.769848	3.729445	1.630801
12	6	0	9.614309	2.722147	1.106150
13	1	0	10.688068	2.788460	1.016247
14	6	0	8.793471	1.668186	0.722509
15	1	0	9.091057	0.733329	0.274292
16	6	0	7.471418	2.049647	1.024447
17	1	0	6.553338	1.500041	0.882347
18	1	0	10.043145	5.367991	2.160233
19	1	0	9.021711	7.772778	3.009323
20	1	0	6.520785	8.673705	3.365923
21	6	0	4.396970	6.735605	2.789634
22	6	0	3.994285	8.073581	3.448914
23	1	0	4.359115	8.937060	2.887180
24	1	0	2.904309	8.140240	3.477911
25	1	0	4.359774	8.146666	4.476798
26	6	0	3.871623	6.745256	1.330362
27	1	0	4.315866	7.568092	0.762742
28	1	0	4.091373	5.809191	0.820600
29	1	0	2.786957	6.889318	1.339690
30	6	0	3.723573	5.599051	3.591201
31	1	0	3.868731	4.624380	3.134865
32	1	0	4.108082	5.557961	4.613447
33	1	0	2.648224	5.793793	3.641106

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.223457	4.021876	2.187363
2	9	0	5.156983	3.900151	1.307163
3	9	0	5.930169	3.435557	3.413214
4	7	0	6.641925	5.523977	2.417520
5	7	0	7.451899	3.292090	1.568109
6	6	0	5.916931	6.611323	2.768041
7	6	0	6.806175	7.676866	3.062356
8	6	0	8.089890	7.219866	2.888123
9	6	0	7.990859	5.874596	2.479677
10	6	0	9.008512	5.013814	2.114025
11	6	0	8.756210	3.735524	1.639345
12	6	0	9.597049	2.733854	1.110778
13	1	0	10.670635	2.798727	1.021692
14	6	0	8.775752	1.687771	0.721436
15	1	0	9.069819	0.755048	0.267354
16	6	0	7.459197	2.071919	1.025141
17	1	0	6.538521	1.527832	0.880070
18	1	0	10.030006	5.368962	2.173897
19	1	0	9.012706	7.765214	3.015795
20	1	0	6.510614	8.667237	3.363207
21	6	0	4.405839	6.727503	2.784451
22	6	0	4.004561	8.057187	3.438941
23	1	0	4.367431	8.919809	2.875532
24	1	0	2.915009	8.121932	3.467937
25	1	0	4.370070	8.131247	4.466116
26	6	0	3.889951	6.737113	1.332129
27	1	0	4.336105	7.559641	0.767042
28	1	0	4.111999	5.801063	0.824045
29	1	0	2.805839	6.880656	1.337715
30	6	0	3.738413	5.595740	3.578976
31	1	0	3.889343	4.622029	3.122772
32	1	0	4.118719	5.556678	4.602032
33	1	0	2.662731	5.786308	3.623656

DFT mpw1pw91/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.222882	4.026224	2.189621
2	9	0	5.146563	3.897812	1.315711
3	9	0	5.941889	3.445247	3.426025
4	7	0	6.642048	5.531385	2.412938
5	7	0	7.447118	3.295927	1.562747
6	6	0	5.920721	6.618134	2.768594
7	6	0	6.811949	7.684039	3.068157
8	6	0	8.096736	7.225482	2.892529
9	6	0	7.996547	5.879871	2.478469
10	6	0	9.012311	5.016641	2.109091
11	6	0	8.756722	3.734853	1.633815
12	6	0	9.593816	2.729796	1.104011
13	1	0	10.669678	2.789390	1.013603
14	6	0	8.766380	1.684334	0.714395
15	1	0	9.057450	0.749030	0.259629
16	6	0	7.450004	2.073694	1.020105
17	1	0	6.525291	1.532588	0.876642
18	1	0	10.037529	5.367658	2.170436
19	1	0	9.021412	7.770932	3.023758
20	1	0	6.519542	8.676079	3.373738
21	6	0	4.403718	6.728792	2.784110
22	6	0	3.995156	8.064499	3.431324
23	1	0	4.357399	8.926211	2.861919
24	1	0	2.903423	8.126586	3.456853
25	1	0	4.358627	8.145301	4.461024
26	6	0	3.888231	6.722892	1.328844
27	1	0	4.320476	7.553980	0.761332
28	1	0	4.132276	5.787251	0.826045
29	1	0	2.799331	6.842420	1.332325
30	6	0	3.747003	5.594406	3.592169
31	1	0	3.879829	4.621311	3.124241
32	1	0	4.158988	5.545878	4.604453
33	1	0	2.672270	5.790468	3.666995

DFT wb97xd/6-31++G(d,p) optimised ground state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.222882	4.026224	2.189621
2	9	0	5.146563	3.897812	1.315711
3	9	0	5.941889	3.445247	3.426025
4	7	0	6.642048	5.531385	2.412938
5	7	0	7.447118	3.295927	1.562747
6	6	0	5.920721	6.618134	2.768594
7	6	0	6.811949	7.684039	3.068157
8	6	0	8.096736	7.225482	2.892529
9	6	0	7.996547	5.879871	2.478469
10	6	0	9.012311	5.016641	2.109091
11	6	0	8.756722	3.734853	1.633815
12	6	0	9.593816	2.729796	1.104011
13	1	0	10.669678	2.789390	1.013603
14	6	0	8.766380	1.684334	0.714395
15	1	0	9.057450	0.749030	0.259629
16	6	0	7.450004	2.073694	1.020105
17	1	0	6.525291	1.532588	0.876642
18	1	0	10.037529	5.367658	2.170436
19	1	0	9.021412	7.770932	3.023758
20	1	0	6.519542	8.676079	3.373738
21	6	0	4.403718	6.728792	2.784110
22	6	0	3.995156	8.064499	3.431324
23	1	0	4.357399	8.926211	2.861919
24	1	0	2.903423	8.126586	3.456853
25	1	0	4.358627	8.145301	4.461024
26	6	0	3.888231	6.722892	1.328844
27	1	0	4.320476	7.553980	0.761332

28	1	0	4.132276	5.787251	0.826045
29	1	0	2.799331	6.842420	1.332325
30	6	0	3.747003	5.594406	3.592169
31	1	0	3.879829	4.621311	3.124241
32	1	0	4.158988	5.545878	4.604453
33	1	0	2.672270	5.790468	3.666995

DFT B3LYP/6-31G(d) optimised 1st excited-state structure:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	6.249766	3.986832	2.338487
2	9	0	5.114396	3.811210	1.553172
3	9	0	6.082784	3.410569	3.590173
4	7	0	6.666481	5.489940	2.498003
5	7	0	7.438360	3.315777	1.593505
6	6	0	5.922770	6.603877	2.770031
7	6	0	6.819110	7.668768	3.076425
8	6	0	8.128934	7.194747	2.994118
9	6	0	8.048737	5.842437	2.619994
10	6	0	9.091947	4.958990	2.309876
11	6	0	8.795129	3.713824	1.707204
12	6	0	9.581700	2.768340	1.052779
13	1	0	10.657437	2.799600	0.947967
14	6	0	8.693755	1.797742	0.514529
15	1	0	8.962662	0.915881	-0.051923
16	6	0	7.385866	2.184352	0.867347
17	1	0	6.441414	1.701063	0.663070
18	1	0	10.118842	5.280870	2.428660
19	1	0	9.045069	7.748354	3.148551
20	1	0	6.521071	8.671134	3.346046
21	6	0	4.404855	6.715893	2.750995
22	6	0	3.987170	8.104777	3.285289
23	1	0	4.371571	8.919033	2.660705
24	1	0	2.894528	8.176977	3.281299
25	1	0	4.327671	8.265195	4.314661
26	6	0	3.882825	6.593990	1.293994
27	1	0	4.312440	7.379513	0.661323
28	1	0	4.129860	5.622424	0.866854
29	1	0	2.792066	6.711768	1.286336
30	6	0	3.731526	5.648410	3.648920
31	1	0	3.886775	4.638072	3.274347
32	1	0	4.114106	5.700519	4.674172
33	1	0	2.651691	5.838234	3.678739