Supporting Information

DMABI Tripod Structures with Sensing Capabilities: Synthesis, Characterization and Fluorescence Analysis

Rafael Contreras-Cáceres,[a] Manolo Doña,[a] Maria Rosa López-Ramírez,[b] Manuel Algarra,[c] Jesus Hierrezuelo,[a] Miguel Angel Casado-Rodríguez,[a] Maria Sánchez-Molina,[a] Amelia Díaz,[a] Bruno B. Campos,[d] Joaquim C. G. Esteves da Silva,[d] and Juan Manuel López-Romero[a,*,†]

[a]*Dep. Química Orgánica, Facultad de Ciencias, Universidad de Málaga, Campus de Teatinos s/n, 29071 Málaga, Spain.*

[b]*Dep. Química Física, Facultad de Ciencias, Universidad de Málaga, Campus de Teatinos s/n, 29071 Málaga, Spain.*

[c]*Dep. Química Inorgánica, Facultad de Ciencias, Universidad de Málaga, Campus de Teatinos s/n, 29071 Málaga, Spain.*

[d]*Centro de Investigação em Química, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, Porto, Portugal.*

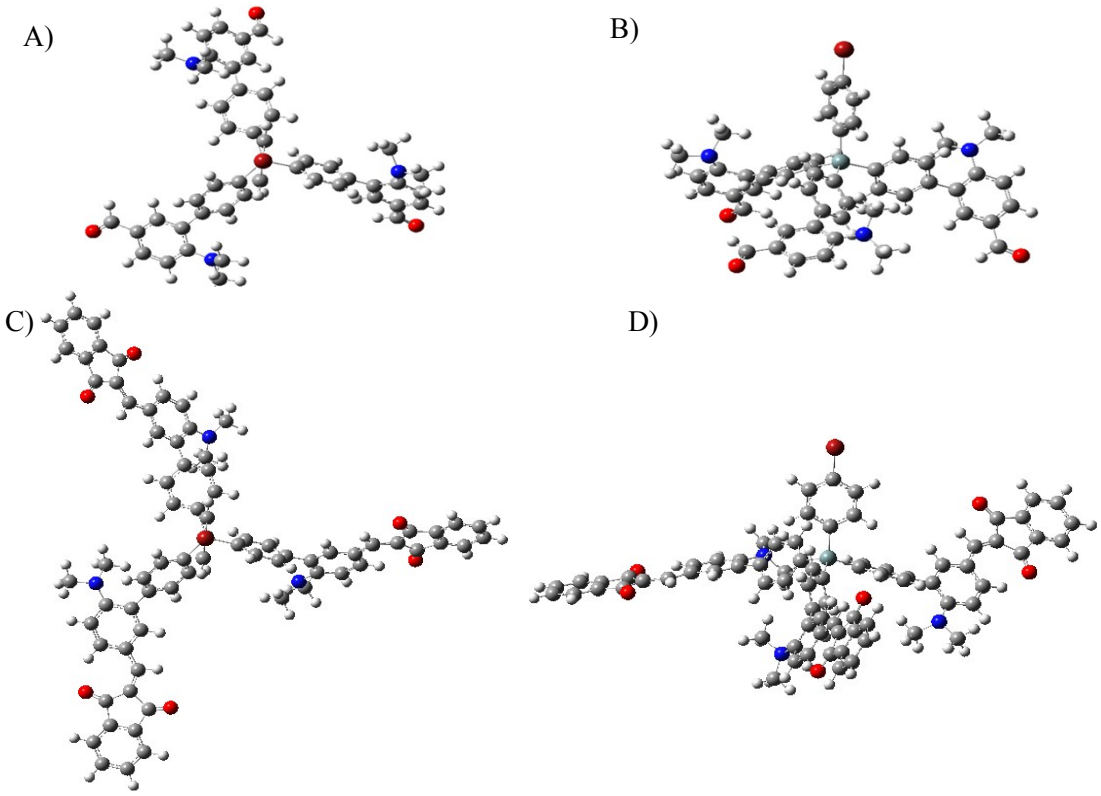
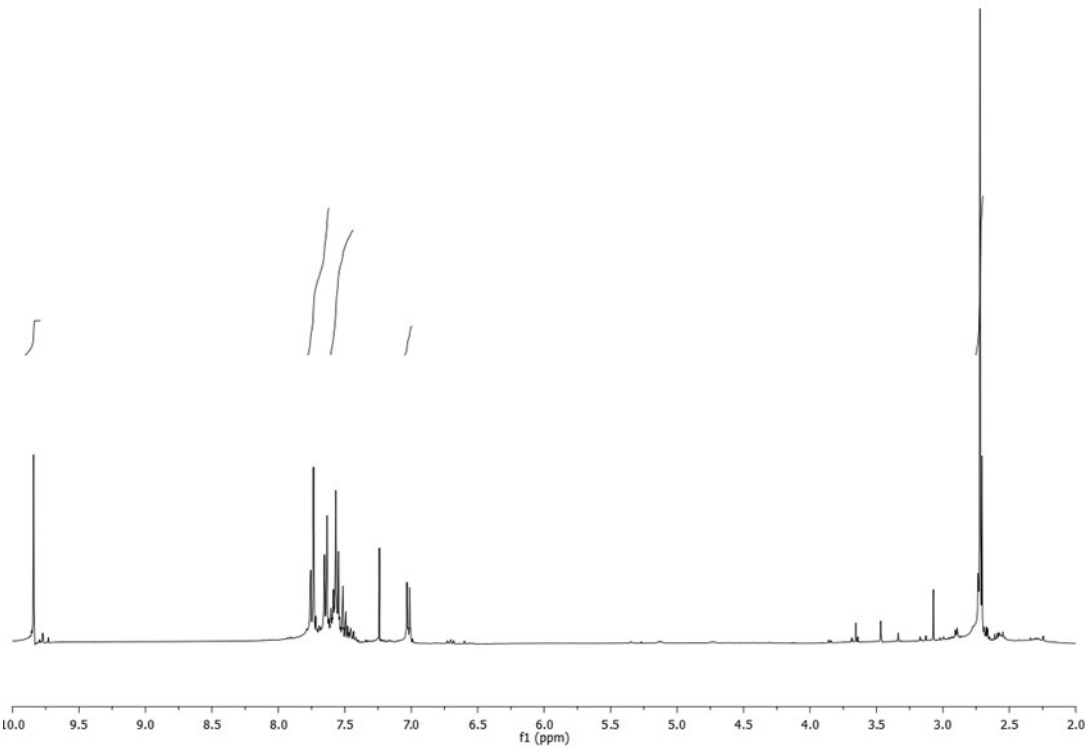
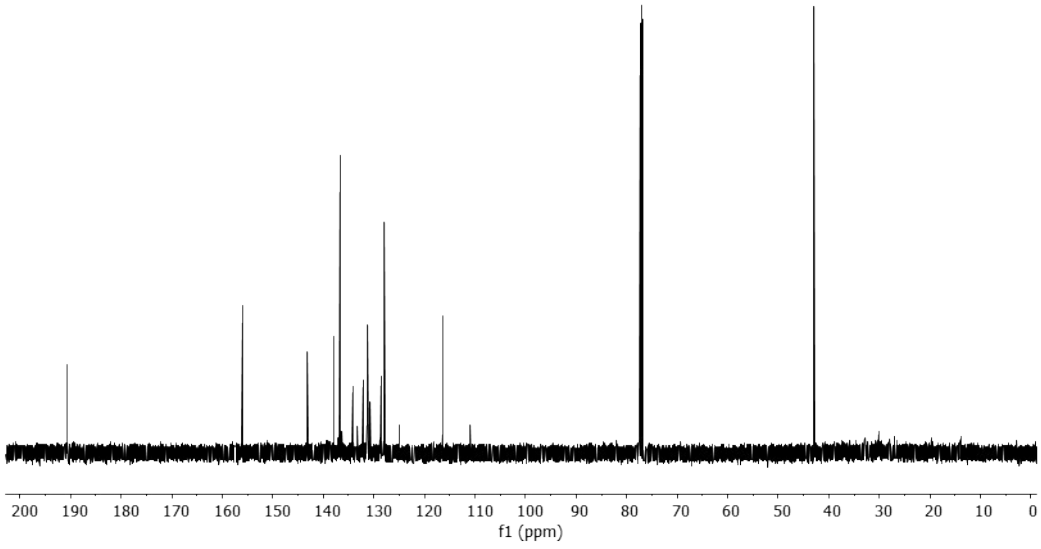


Figure S1. Top view (A) and side view (B) of optimized geometries obtained for **4** and top view (C) and side view (D) of optimized geometries obtained for **1.**

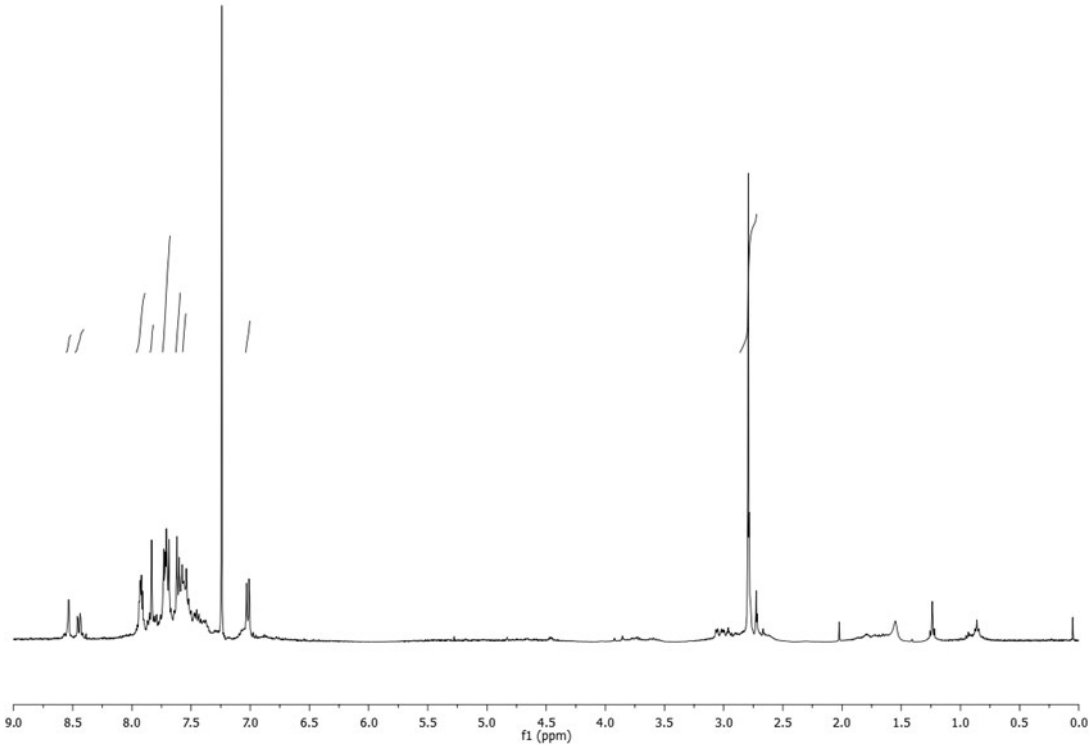


^{1}H NMR spectrum of compound **4**

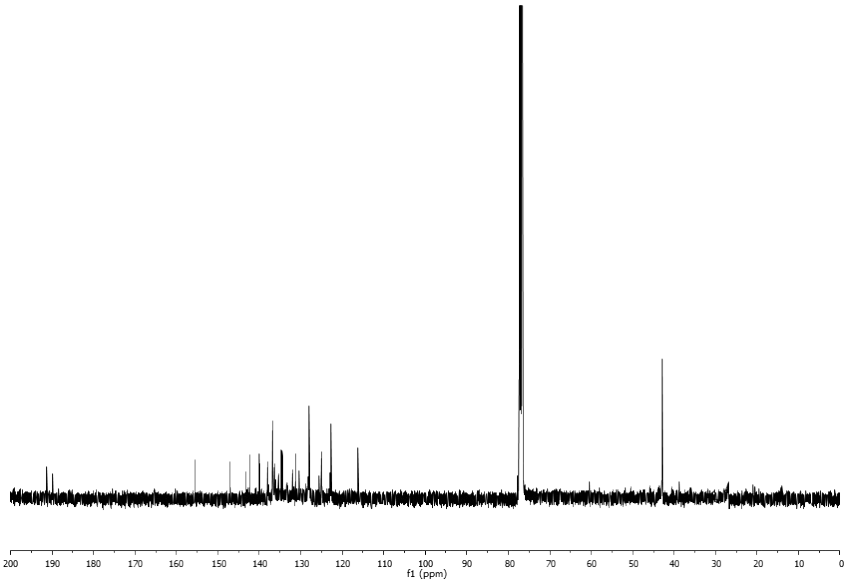


^{13}C NMR spectrum of compound **4**

Figure S2. ^{1}H and ^{13}C NMR spectra for compund **4**



^{1}H NMR spectrum of compound **1**



^{13}C NMR spectrum of compound **1**

Figure S3. ^{1}H and ^{13}C NMR spectra for compund **4**

Figure S2. Optimized molecular structure of compound 4 (top view) with the corresponding atom labels calculated at the B3LYP/6-31G* level of theory.

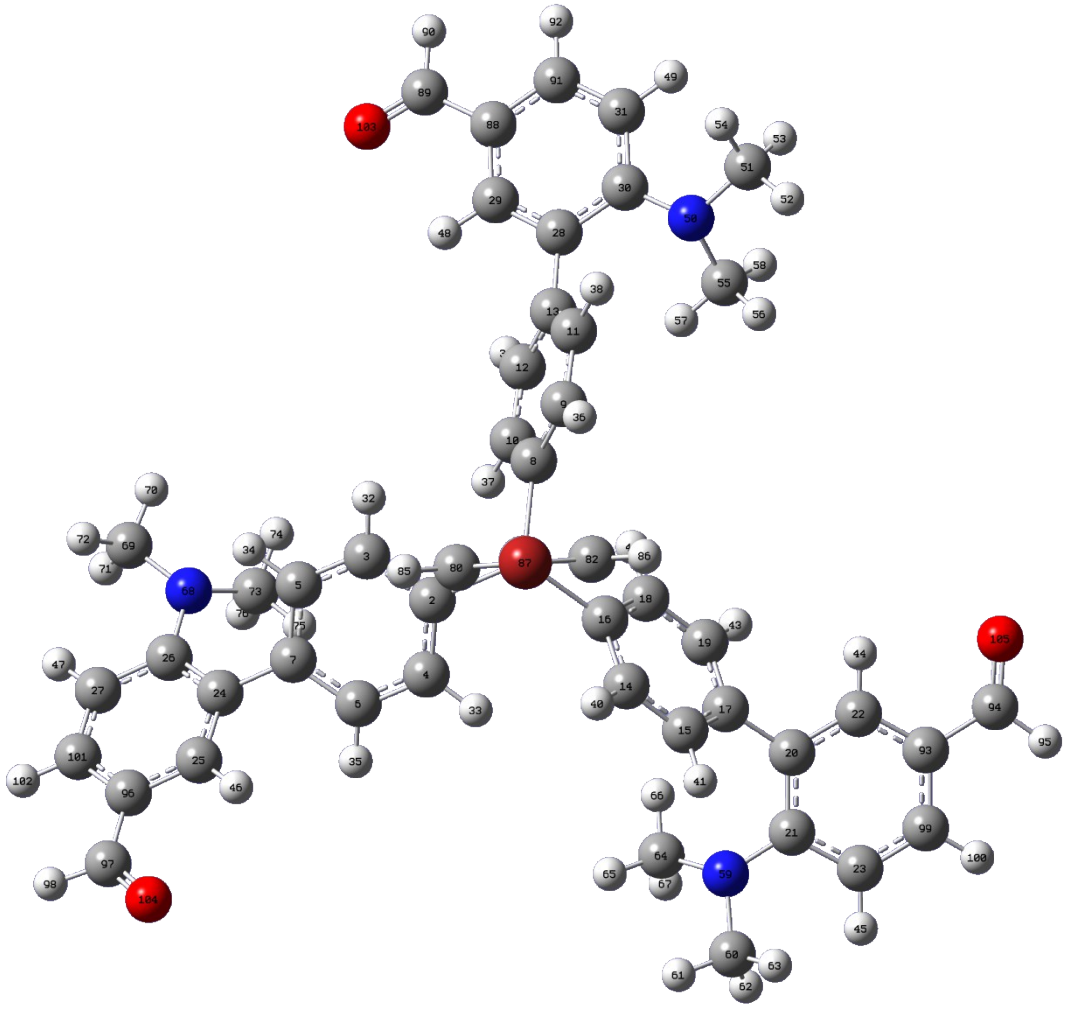


Table S1. Cartesian coordinates (x,y,z) in the optimized molecular structure of compound 4calculated at the B3LYP/6-31G* level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.020522	0.063924	0.770610
2	6	0	1.785462	-0.162188	0.128844
3	6	0	2.431750	-1.412989	0.197074
4	6	0	2.521810	0.909861	-0.403101
5	6	0	3.745008	-1.583396	-0.234375
6	6	0	3.837517	0.745824	-0.836568
7	6	0	4.474421	-0.502704	-0.759289
8	6	0	-0.999308	-1.454293	0.285550
9	6	0	-1.960237	-2.012936	1.149195
10	6	0	-0.851504	-2.052284	-0.979436
11	6	0	-2.742283	-3.101020	0.768994
12	6	0	-1.631665	-3.141854	-1.366421
13	6	0	-2.593857	-3.684953	-0.500113
14	6	0	-0.505306	2.897840	0.576714
15	6	0	-1.042014	4.054531	0.016216
16	6	0	-0.749681	1.623838	0.025533
17	6	0	-1.858430	3.987471	-1.125593
18	6	0	-1.567106	1.568739	-1.116435
19	6	0	-2.110037	2.722963	-1.680757
20	6	0	-2.517736	5.203101	-1.685897
21	6	0	-1.828400	6.430527	-1.945119
22	6	0	-3.894143	5.155073	-1.896809
23	6	0	-2.580720	7.555400	-2.339072
24	6	0	5.906609	-0.645371	-1.152240
25	6	0	6.818653	0.263508	-0.619951
26	6	0	6.398787	-1.703356	-1.981014
27	6	0	7.790828	-1.820483	-2.167843
28	6	0	-3.366612	-4.898088	-0.896098
29	6	0	-2.653798	-5.992997	-1.379320
30	6	0	-4.784168	-5.019469	-0.737177
31	6	0	-5.387943	-6.263052	-1.012584
32	1	0	1.898884	-2.275937	0.590426
33	1	0	2.061473	1.891067	-0.488510
34	1	0	4.213509	-2.559902	-0.168062
35	1	0	4.377594	1.593379	-1.250848
36	1	0	-2.094185	-1.599100	2.145529
37	1	0	-0.109164	-1.669875	-1.676602
38	1	0	-3.472218	-3.509271	1.460346
39	1	0	-1.498658	-3.576665	-2.353834
40	1	0	0.101934	2.990767	1.474354
41	1	0	-0.836567	5.019577	0.467756
42	1	0	-1.792965	0.608892	-1.574234
43	1	0	-2.736053	2.645727	-2.566093
44	1	0	-4.439054	4.238973	-1.689658
45	1	0	-2.074968	8.492022	-2.542372
46	1	0	6.467869	1.063853	0.024713
47	1	0	8.180918	-2.614647	-2.793573
48	1	0	-1.575731	-5.926676	-1.491053
49	1	0	-6.460171	-6.373158	-0.900282
50	7	0	-5.552633	-3.933042	-0.285246
51	6	0	-6.879907	-4.204252	0.245274

52	1	0	-7.223116	-3.316402	0.786465
53	1	0	-7.629070	-4.430526	-0.533924
54	1	0	-6.842994	-5.040114	0.948953
55	6	0	-5.516410	-2.690708	-1.060563
56	1	0	-5.790581	-1.848875	-0.415762
57	1	0	-4.518452	-2.505993	-1.453959
58	1	0	-6.224779	-2.726407	-1.905366
59	7	0	-0.435110	6.521621	-1.778902
60	6	0	0.155255	7.845332	-1.652222
61	1	0	1.174288	7.733839	-1.267195
62	1	0	0.217621	8.393648	-2.608884
63	1	0	-0.415116	8.447430	-0.940061
64	6	0	0.411946	5.617718	-2.559947
65	1	0	1.377913	5.496635	-2.057701
66	1	0	-0.048580	4.635827	-2.653104
67	1	0	0.594552	6.016126	-3.572364
68	7	0	5.515097	-2.624954	-2.569914
69	6	0	6.058115	-3.888925	-3.044142
70	1	0	5.225784	-4.578464	-3.219055
71	1	0	6.622592	-3.799344	-3.989186
72	1	0	6.711907	-4.327971	-2.286005
73	6	0	4.475714	-2.107011	-3.462223
74	1	0	3.648641	-2.823304	-3.514327
75	1	0	4.083187	-1.160314	-3.094968
76	1	0	4.865610	-1.951990	-4.482611
77	6	0	0.040959	0.249054	2.656383
78	6	0	1.123497	-0.204658	3.430992
79	6	0	-1.048675	0.820980	3.340728
80	6	0	1.124481	-0.104514	4.823184
81	1	0	1.992304	-0.640722	2.944875
82	6	0	-1.068862	0.929191	4.731865
83	1	0	-1.900055	1.204297	2.783200
84	6	0	0.022891	0.461480	5.460125
85	1	0	1.969903	-0.457232	5.404329
86	1	0	-1.916305	1.373920	5.242650
87	35	0	0.010383	0.607328	7.367413
88	6	0	-3.268603	-7.218858	-1.676327
89	6	0	-2.476391	-8.355337	-2.173232
90	1	0	-3.065897	-9.282705	-2.355290
91	6	0	-4.644942	-7.344701	-1.468879
92	1	0	-5.141696	-8.288525	-1.685394
93	6	0	-4.630516	6.274098	-2.314197
94	6	0	-6.086643	6.184047	-2.510732
95	1	0	-6.568719	7.138051	-2.823938
96	6	0	8.201000	0.153806	-0.834209
97	6	0	9.132478	1.128687	-0.243259
98	1	0	10.206476	0.930025	-0.461883
99	6	0	-3.956840	7.481659	-2.515895
100	1	0	-4.509134	8.364369	-2.832439
101	6	0	8.677159	-0.912717	-1.601364
102	1	0	9.746202	-1.021750	-1.773617
103	8	0	-1.276251	-8.333747	-2.385543
104	8	0	8.806129	2.088735	0.432811
105	8	0	-6.753221	5.175132	-2.358095

Figure S3. Optimized molecular structure (top view) of compound 1 with the corresponding atom labels calculated at the B3LYP/6-31G* level of theory.

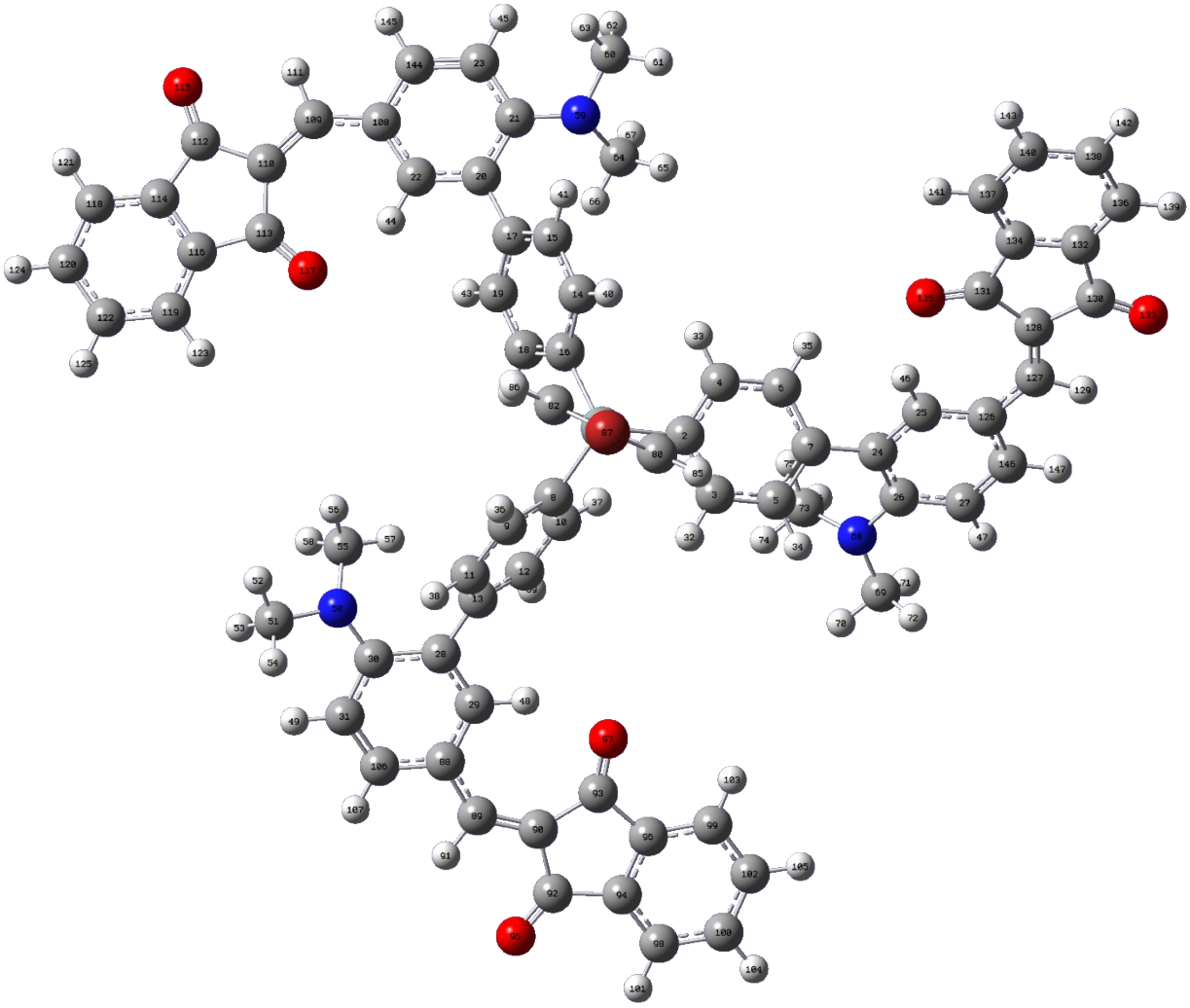


Table S2. Cartesian coordinates (x,y,z) in the optimized molecular structure of compound 1calculated at the B3LYP/6-31G* level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.061038	0.369744	1.114465
2	6	0	1.703622	0.031326	0.239409
3	6	0	2.339431	-1.222718	0.335877
4	6	0	2.362671	1.026440	-0.502524
5	6	0	3.565761	-1.470062	-0.276441
6	6	0	3.592106	0.786114	-1.115774
7	6	0	4.214705	-0.468204	-1.018370
8	6	0	-1.014973	-1.183221	1.014218
9	6	0	-1.864765	-1.565526	2.069263
10	6	0	-1.026024	-1.988761	-0.139263
11	6	0	-2.693082	-2.680953	1.974368
12	6	0	-1.849353	-3.110279	-0.238921
13	6	0	-2.702759	-3.473597	0.814386
14	6	0	-0.482403	3.157984	0.592014
15	6	0	-1.103614	4.233018	-0.038894
16	6	0	-0.829021	1.824433	0.295469
17	6	0	-2.112004	4.021801	-0.994957
18	6	0	-1.842794	1.625270	-0.657336
19	6	0	-2.473305	2.697658	-1.288309
20	6	0	-2.842986	5.164533	-1.618597
21	6	0	-2.187225	6.313299	-2.166525
22	6	0	-4.234896	5.129692	-1.584499
23	6	0	-2.985616	7.406712	-2.567260
24	6	0	5.558432	-0.696914	-1.627183
25	6	0	6.550168	0.244533	-1.362576
26	6	0	5.888078	-1.861158	-2.392439
27	6	0	7.235790	-2.049138	-2.769215
28	6	0	-3.529281	-4.713704	0.727494
29	6	0	-2.880924	-5.890925	0.362723
30	6	0	-4.916896	-4.759040	1.076683
31	6	0	-5.550743	-6.020269	1.116746
32	1	0	1.866281	-2.027866	0.893397
33	1	0	1.907908	2.007754	-0.612906
34	1	0	4.026244	-2.448578	-0.184105
35	1	0	4.075860	1.577868	-1.681394
36	1	0	-1.872813	-0.988770	2.990824
37	1	0	-0.373431	-1.747831	-0.975194
38	1	0	-3.334496	-2.948943	2.808049
39	1	0	-1.830688	-3.714842	-1.141720
40	1	0	0.276662	3.365815	1.343004
41	1	0	-0.813915	5.247876	0.214583
42	1	0	-2.154902	0.615127	-0.910434
43	1	0	-3.258879	2.508463	-2.014867
44	1	0	-4.728440	4.261164	-1.163614
45	1	0	-2.515659	8.291248	-2.980701
46	1	0	6.298389	1.122787	-0.779124
47	1	0	7.515315	-2.923660	-3.344796
48	1	0	-1.827993	-5.853143	0.106859
49	1	0	-6.599924	-6.085223	1.379336
50	7	0	-5.625253	-3.598811	1.403551
51	6	0	-6.891076	-3.727590	2.108334

52	1	0	-7.153962	-2.749946	2.525373
53	1	0	-7.723100	-4.049406	1.458051
54	1	0	-6.796355	-4.436626	2.934666
55	6	0	-5.622872	-2.466583	0.474378
56	1	0	-5.726061	-1.528253	1.030079
57	1	0	-4.695118	-2.426523	-0.091776
58	1	0	-6.461747	-2.544232	-0.236902
59	7	0	-0.794202	6.375415	-2.275067
60	6	0	-0.164464	7.672603	-2.466545
61	1	0	0.903367	7.573358	-2.245760
62	1	0	-0.259304	8.057444	-3.496794
63	1	0	-0.588547	8.406661	-1.776710
64	6	0	-0.080438	5.305698	-2.975063
65	1	0	0.924358	5.191441	-2.553550
66	1	0	-0.602753	4.356890	-2.874603
67	1	0	0.017241	5.538567	-4.048306
68	7	0	4.917917	-2.808647	-2.733883
69	6	0	5.349719	-4.130347	-3.159861
70	1	0	4.490036	-4.806621	-3.109196
71	1	0	5.733656	-4.152892	-4.194659
72	1	0	6.124067	-4.511818	-2.489386
73	6	0	3.699332	-2.376913	-3.421400
74	1	0	2.864737	-3.031195	-3.146294
75	1	0	3.437592	-1.356825	-3.149146
76	1	0	3.832168	-2.422696	-4.514996
77	6	0	0.384168	0.814157	2.928435
78	6	0	1.580606	0.451017	3.572182
79	6	0	-0.581255	1.494821	3.694791
80	6	0	1.808606	0.740570	4.918376
81	1	0	2.360545	-0.062810	3.016263
82	6	0	-0.374570	1.792320	5.042651
83	1	0	-1.513730	1.814246	3.235216
84	6	0	0.823328	1.408298	5.641215
85	1	0	2.739124	0.455424	5.397469
86	1	0	-1.129098	2.318120	5.618109
87	35	0	1.123422	1.813302	7.487432
88	6	0	-3.526127	-7.148806	0.365838
89	6	0	-2.912204	-8.404478	0.012575
90	6	0	-1.673782	-8.780460	-0.425735
91	1	0	-3.580790	-9.262839	0.114245
92	6	0	-1.421402	-10.232738	-0.682629
93	6	0	-0.423608	-8.044555	-0.741561
94	6	0	-0.006579	-10.350859	-1.143360
95	8	0	-2.213167	-11.153442	-0.544389
96	6	0	0.570942	-9.076850	-1.177229
97	8	0	-0.180687	-6.843278	-0.685877
98	6	0	0.718589	-11.482915	-1.501611
99	6	0	1.893609	-8.897313	-1.570596
100	6	0	2.047669	-11.308436	-1.897211
101	1	0	0.255972	-12.464867	-1.469753
102	6	0	2.628198	-10.030346	-1.930864
103	1	0	2.329805	-7.902980	-1.590176
104	1	0	2.643419	-12.171301	-2.182545
105	1	0	3.664434	-9.925358	-2.241185
106	6	0	-4.875940	-7.178514	0.775257
107	1	0	-5.404251	-8.128523	0.800428
108	6	0	-5.035926	6.207138	-2.026744
109	6	0	-6.477455	6.235702	-2.016049

110	6	0	-7.453949	5.339486	-1.684294
111	1	0	-6.899875	7.184404	-2.356124
112	6	0	-8.883114	5.759848	-1.825901
113	6	0	-7.444596	3.934554	-1.203773
114	6	0	-9.719523	4.590111	-1.425948
115	8	0	-9.296906	6.847729	-2.198591
116	6	0	-8.880358	3.529196	-1.067938
117	8	0	-6.499292	3.194746	-0.950182
118	6	0	-11.104350	4.462845	-1.381019
119	6	0	-9.402130	2.307350	-0.654105
120	6	0	-11.633883	3.237799	-0.966023
121	1	0	-11.742500	5.295333	-1.662097
122	6	0	-10.792376	2.172585	-0.606985
123	1	0	-8.738844	1.492710	-0.379019
124	1	0	-12.711273	3.103881	-0.919384
125	1	0	-11.232742	1.231589	-0.288097
126	6	0	7.890793	0.077652	-1.778049
127	6	0	8.963118	1.010904	-1.534923
128	6	0	9.049170	2.244839	-0.955251
129	1	0	9.934586	0.667380	-1.898798
130	6	0	10.386314	2.914824	-0.901990
131	6	0	8.060814	3.165542	-0.337681
132	6	0	10.180591	4.238417	-0.243934
133	8	0	11.447720	2.472869	-1.316599
134	6	0	8.827244	4.382027	0.081855
135	8	0	6.852752	3.029036	-0.174254
136	6	0	11.103352	5.238678	0.045754
137	6	0	8.355796	5.531508	0.708866
138	6	0	10.635453	6.395532	0.675139
139	1	0	12.150314	5.112655	-0.213619
140	6	0	9.277646	6.539916	1.002947
141	1	0	7.303252	5.628776	0.957755
142	1	0	11.329147	7.196449	0.916437
143	1	0	8.942845	7.450095	1.493321
144	6	0	-4.366249	7.356994	-2.495442
145	1	0	-4.947262	8.212010	-2.832505
146	6	0	8.207335	-1.111446	-2.467770
147	1	0	9.230631	-1.282718	-2.792988
