	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
0	C1=CC=CC=C1	b3lyp/6-311+G(d,p)	First excited	0.2572752	6.598216937
1	C1=CC=C2C=CC=CC2=C1	b3lyp/6-311+G(d,p)	First excited	0.5595376	4.747842672
2	C1CCC2=CC=CC=C2C1	b3lyp/6-311+G(d,p)	First excited	5.741634	6.192767282
3	C1CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	First excited	37.2958892	4.958730916
4	C1CC2=C(C=C1)C3=CC=CC=C3C=C2	b3lyp/6-311+G(d,p)	First excited	37.533064	4.098578996
5	C1CCC2=C(C1)C=CC3=CC=CC=C23	b3lyp/6-311+G(d,p)	First excited	111.2251852	4.646616315
6	C1C=CCC2=CC=CC=C21	b3lyp/6-311+G(d,p)	First excited	27.9542996	5.944327325
7	C1CC2=CC3=CC=CC=C3C=C2C=C1	b3lyp/6-311+G(d,p)	First excited	4.5231728	4.405523433
8	C1CCC2=CC3=CC=CC=C3C=C2C1	b3lyp/6-311+G(d,p)	First excited	73.11939	4.702943885
9	C1=CC=C2C=C3C=CC=CC3=CC2=C1	b3lyp/6-311+G(d,p)	First excited	0.4320904	3.551630133
10	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	b3lyp/6-311+G(d,p)	First excited	0.2606232	4.68144689
11	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	b3lyp/6-311+G(d,p)	First excited	0.3859996	4.219125437
12	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	b3lyp/6-311+G(d,p)	First excited	0.4032356	3.723878208
13	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	b3lyp/6-311+G(d,p)	First excited	0.3034404	3.849322698
14	C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	First excited	0.343666	2.752159605
15	C1=CC=C2C=C3C4=CC=CC=C4C5=CC=CC=C5C3=CC2=C1	b3lyp/6-311+G(d,p)	First excited	0.3816596	3.849594812
16	C1=CC=C2C(=C1)C=CC3=C2C4=CC=CC=C4C5=CC=CC=C35	b3lyp/6-311+G(d,p)	First excited	0.5098136	4.051503298
17	C1=CC=C2C(=C1)C=CC3=C2C4=CC=CC=C4C=C3	b3lyp/6-311+G(d,p)	First excited	0.2646532	4.171505512
18	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3C5=CC=CC=C5C=C4	b3lyp/6-311+G(d,p)	First excited	0.2517448	4.209057225
19	C1=CC=C2C(=C1)C=CC3=CC4=C(C=C32)C5=CC=CC=C5C=C4	b3lyp/6-311+G(d,p)	First excited	0.2118664	3.887418639
20	C1CC2=CC=CC=C2C3=CC=CC=C31	b3lyp/6-311+G(d,p)	First excited	37.2856592	4.88226692
21	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC5=CC=CC=C5C=C43	b3lyp/6-311+G(d,p)	First excited	0.3758192	3.477615162
22	C1C2=CC=CC=C2CC3=CC4=CC=CC=C4C=C31	b3lyp/6-311+G(d,p)	First excited	0.926714	4.666480627
23	C1CCC2=CC3=C(CCCC3)C=C2C1	b3lyp/6-311+G(d,p)	First excited	74.2574372	5.681465334
24	C1C2=CC=CC=C2CC3=CC=CC=C31	b3lyp/6-311+G(d,p)	First excited	27.8148988	5.945415781
25	C1=CC=C2C=C3C(=CC2=C1)C=CC4=C3C=CC5=CC6=CC=CC=C6C=C54	b3lyp/6-311+G(d,p)	First excited	0.313906	3.126316166
26	C1CCC2=C(C1)C=CC3=C2CCCC3	b3lyp/6-311+G(d,p)	First excited	116.747984	5.938612934
27	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3C=CC5=CC=CC=C54	b3lyp/6-311+G(d,p)	First excited	0.2253328	4.206880314
28	C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	First excited	0.2881016	2.190244479
29	C1CC2=C(C3=CC=CC=C3C=C2)C4=C1C=CC5=CC=CC=C54	b3lyp/6-311+G(d,p)	First excited	37.3873764	3.923881897
30	C1CC2=C(C=CC3=CC=CC=C23)C4=CC=CC=C41	b3lyp/6-311+G(d,p)	First excited	32.9120676	4.247425279
31	C1=CC=C2C=C3C(=CC2=C1)C=CC4=CC5=CC=CC=C5C=C43	b3lyp/6-311+G(d,p)	First excited	0.2543612	3.748640569
32	C1CCC2=C(C1)C=CC3=C2C=CC4=CC=CC=C43	b3lyp/6-311+G(d,p)	First excited	5.3047076	4.562261018
33	C1CCC2=C(C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C23	b3lyp/6-311+G(d,p)	First excited	41.6004004	3.710272515
34	C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	First excited	0.2518316	1.77962466
35	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	First excited	0.2822488	3.810138302
36	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	b3lyp/6-311+G(d,p)	First excited	0.3203416	3.348361078
37	C1=CC=C2C(=C1)C3=CC=CC4=C3C5=C(C=CC=C25)C=C4	b3lyp/6-311+G(d,p)	First excited	0.2163552	3.958984585
38	C1=CC=C2C(=C1)C=C3C=CC4=C5C3=C2C6=CC=CC=C6C5=CC=C4	b3lyp/6-311+G(d,p)	First excited	0.382788	3.381286855
39	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	b3lyp/6-311+G(d,p)	First excited	0.3386068	3.481968984
40	C1=CC=C2C3=C4C(=CC2=C1)C5=CC=CC=C5C6=CC=CC(=C64)C=C3	b3lyp/6-311+G(d,p)	First excited	0.3151832	3.51271785
41	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC6=CC=CC=C56)C=C3	b3lyp/6-311+G(d,p)	First excited	0.2733084	2.877604096
42	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=CC6=CC=CC=C6C(=C54)C=C3	b3lyp/6-311+G(d,p)	First excited	0.2797068	3.224821384
43	C1=CC2=C3C(=C1)C4=CC=CC5=C4C(=CC=C5)C3=CC=C2	b3lyp/6-311+G(d,p)	First excited	0.3224372	2.985089071
44	C1=CC=C2C(=C1)C3=CC=CC=C3C4=CC=CC=C24	b3lyp/6-311+G(d,p)	First excited	0.2690924	4.838728702
45	C1=CC2=C3C(=C1)C=C4C=CC5=C6C4=C3C(=CC6=CC=C5)C=C2	b3lyp/6-311+G(d,p)	First excited	0.2358356	2.867535883

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
46	C1=CC2=C3C4=C1C=CC5=C4C6=C(C=C5)C=CC7=C6C3=C(C=C2)C=C7	b3lyp/6-311+G(d,p)	First excited	0.1260088	4.00089012
47	C1=CC=C2C(=C1)C=C3C4=CC=CC=C4C5=C3C2=CC6=CC=CC=C65	b3lyp/6-311+G(d,p)	First excited	0.6044752	3.241964557
48	C1=CC2=C3C4=C1C=CC5=CC6=C7C8=C(C=CC9=C8C1=C(C=C9)C=C(C3=C1C7=C54)C=C2)C=C6	b3lyp/6-311+G(d,p)	First excited	0.2047364	2.916244264
49	C1=CC=C2C(=C1)C=CC3=C2C=C4C=CC=C5C4=C3C=C5	b3lyp/6-311+G(d,p)	First excited	0.921692	3.238154963
50	C1=CC=C2C=C3C4=C5C(=CC3=CC2=C1)C=CC6=C5C(=CC=C6)C=C4	b3lyp/6-311+G(d,p)	First excited	0.2987532	2.843045635
51	C1=CC=C2C3=C4C(=CC=CC4=CC2=C1)C=C3	b3lyp/6-311+G(d,p)	First excited	0.9005748	3.079512581
52	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C6=CC=CC(=C64)C2=C1	b3lyp/6-311+G(d,p)	First excited	0.2169256	4.104837615
53	C1=CC=C2C(=C1)C3=CC=CC=C3C4=C2C5=CC=CC6=C5C4=CC=C6	b3lyp/6-311+G(d,p)	First excited	0.6884604	3.252304884
54	C1=CC=C2C(=C1)C=C3C=C4C=CC=CC4=C5C3=C2C6=CC=CC=C65	b3lyp/6-311+G(d,p)	First excited	0.2828688	2.460997772
55	C1=CC=C2C(=C1)C=C3C=CC=C4C3=C2C5=CC=CC6=C5C4=CC=C6	b3lyp/6-311+G(d,p)	First excited	0.3040356	2.539094451
56	C1=CC=C2C(=C1)C3=CC=CC=C3C4=C2C5=CC=CC=C5C6=CC=CC=C64	b3lyp/6-311+G(d,p)	First excited	0.3879588	3.975583531
57	C1CC2=CC=CC3=C2C4=C(C=CC=C41)C=C3	b3lyp/6-311+G(d,p)	First excited	36.0939448	4.611785741
58	C1=CC=C2C=C3C4=CC=CC5=C4C6=C(C=CC=C6C3=CC2=C1)C=C5	b3lyp/6-311+G(d,p)	First excited	0.2402128	3.86211205
59	C1=CC=C2C3=C4C(=CC2=C1)C5=CC=CC=C5C6=CC7=CC=CC=C7C(=C64)C=C3	b3lyp/6-311+G(d,p)	First excited	0.2897012	3.406865558
60	C1=CC2=C3C4=C1C=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	b3lyp/6-311+G(d,p)	First excited	0.6490036	4.161437299
61	C1CC2=C3C(=CC=C4C3=C(CCC4)C=C2)C1	b3lyp/6-311+G(d,p)	First excited	79.3815016	4.446068399
62	CC1=CC2=C3C(=C1)C=CC4=CC(=CC(=C43)C=C2)C	b3lyp/6-311+G(d,p)	First excited	0.3751248	3.789457649
63	CC1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	First excited	0.385578	3.800070089
64	CC1=C2C=CC3=CC=CC4=C3C2=C(C=C1)C=C4	b3lyp/6-311+G(d,p)	First excited	2.0037904	3.724966663
65	CC1=CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	First excited	0.7756076	4.756278202
66	CC1=CC=CC2=CC=CC=C12	b3lyp/6-311+G(d,p)	First excited	16.6651288	4.655596073
67	C1=CC2=C3C(=C1)C=CC3=CC=C2	b3lyp/6-311+G(d,p)	First excited	1.0726	3.886602298
68	CC1=C2C=CC3=CC=CC=C3C2=C(C4=CC=CC=C14)C	b3lyp/6-311+G(d,p)	First excited	5.5073112	3.535575415
69	CC1=CC2=CC=CC=C2C3=C1C4=CC=CC=C4C=C3	b3lyp/6-311+G(d,p)	First excited	16.8443336	4.099939566
70	CC1=CC2=C(C=C1)C=C(C=C2)C	b3lyp/6-311+G(d,p)	First excited	16.6800708	4.746754217
71	CC1=CC2=CC=CC(=C2C=C1)C	b3lyp/6-311+G(d,p)	First excited	16.9045604	4.665664286
72	CC(C)C1=CC2=C(C=C1)C=C(C=C2)C(C)C	b3lyp/6-311+G(d,p)	First excited	70.5567936	4.662671033
73	CC1=C2C=CC3=CC=CC=C3C2=CC4=CC=CC=C14	b3lyp/6-311+G(d,p)	First excited	1.2319648	3.629726811
74	CC1=C2C(=CC3=CC=CC=C13)C=CC4=CC=CC=C42	b3lyp/6-311+G(d,p)	First excited	17.2317592	3.627277787
75	CC1=C2C=C3C=CC4=CC=CC=C4C3=CC2=CC=C1	b3lyp/6-311+G(d,p)	First excited	0.403496	3.696938935
76	CC(C)C1=CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	First excited	22.9467208	4.671378677
77	CC1=CC=C(C2=CC=CC=C12)C	b3lyp/6-311+G(d,p)	First excited	18.2250612	4.555186058
78	CC1=CC=C(C=C1)S(=O)(=O)O	b3lyp/6-311+G(d,p)	First excited	15.9317184	5.972082939
159	C1=CC=C2C(=C1)C3=C4C2=CC5=CC=CC6=C5C4=C(C=C6)C=C3	b3lyp/6-311+G(d,p)	First excited	0.6843808	3.31189782
241	C1=CSC2=CC3=CC4=C(C=C3C=C21)C=C5C(=C4)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2588624	2.73773757
242	C1=CC2=C(C=CC3=C2C=CC4=C3SC=C4)C5=C1C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2206456	4.358447735
243	C1=CC=C2C(=C1)C3=CC4=C(C=C3S2)SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	First excited	0.224874	4.273276096
244	C1=CC=C2C(=C1)C3=CC4=C(C=C3S2)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	First excited	0.2078984	4.002250689
245	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	First excited	0.2501948	4.273003982
246	C1=CSC(=C1)C#CC2=CC=C(C=C2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	First excited	1.199762	4.406067661
247	C1=CC=C2C=C3C(=CC2=C1)C4=C(C5=C3SC=C5)SC=C4	b3lyp/6-311+G(d,p)	First excited	0.3795392	3.515983217
248	C1=CC=C(C(=C1)C#CC2=CC=CS2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	First excited	29.1408804	3.606052905
249	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	First excited	0.2084936	4.39681579
250	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	First excited	0.3844992	4.103204932
251	C1=CC=C2C(=C1)C3=C(C4=C(C=C3)SC=C4)C5=C2SC=C5	b3lyp/6-311+G(d,p)	First excited	0.5476584	4.23762918
252	C1=CSC2=CC3=CC4=C(C=C5C=CSC5=C4)C=C3C=C21	b3lyp/6-311+G(d,p)	First excited	0.2634876	2.748077897

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
253	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	First excited	0.2856464	4.022659229
254	C1=CC2=C3C=CSC4=CC=CC(=C34)C5=C2C(=C1)SC=C5	b3lyp/6-311+G(d,p)	First excited	0.301382	2.354601252
255	C1=CC=C2C(=C1)C=C3C=C4C=CC=CC4=C5C3=C2SS5	b3lyp/6-311+G(d,p)	First excited	0.2653352	2.338002306
256	C1=CC2=C(C=CS2)C3=CC4=C(C=C31)C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	First excited	0.39184	3.535303301
257	C1=CC2=C(C=C3C=CSC3=C2)C4=C1C=C5C(=C4)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2155244	3.8846975
258	C1=CC=C2C(=C1)C=CC3=C2SC4=C3SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	First excited	0.3477456	4.081707937
259	C1=CC=C2C=C3C(=CC2=C1)C4=C(S3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	First excited	0.3264424	3.62891047
260	C1=CC2=CC3=C(C=CC4=C3SC=C4)C=C2C5=C1C=CS5	b3lyp/6-311+G(d,p)	First excited	0.355508	3.502921751
261	C1=CC=C2C(=C1)C=CC3=C2C4=C(S3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	First excited	0.3962172	3.921432872
262	C1=CC2=C(C=CC3=C2C=CS3)C4=C1C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	First excited	0.44206	4.153545997
263	C#CC1=CC(=C(C=C1C2=CC=CS2)C#C)C3=CC=CS3	b3lyp/6-311+G(d,p)	First excited	0.5060688	3.863472619
264	C1=CC=C2C(=C1)C3=C(S2)C=C4C=C5C(=CC4=C3)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2540636	3.467819063
265	C1=CC2=C(C=CC3=C2C=CC4=C3C=CS4)C5=C1C=CS5	b3lyp/6-311+G(d,p)	First excited	0.4085056	4.245792596
266	C1=CC=C2C(=C1)C=C(S2)C#CC3=CC4=CC=CC=C4S3	b3lyp/6-311+G(d,p)	First excited	0.4005324	3.588909732
267	C1=CC2=CC3=C(C=C2C4=C1C=CS4)C5=C(C=C3)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.35898	3.506187118
268	C1=CC=C2C(=C1)SC3=C(S2)C4=CC=CC5=C4C3=CC=C5	b3lyp/6-311+G(d,p)	First excited	1.4241896	3.034885908
269	C#CC1=CC(=C(C=C1C2=CSC=C2)C#C)C3=CSC=C3	b3lyp/6-311+G(d,p)	First excited	4.307264	4.195451531
270	[2H]C1=CC2=C(C=CS2)C3=CC4=C(C=C13)C5=C(C=C4[2H])SC=C5	b3lyp/6-311+G(d,p)	First excited	0.3918276	3.535303301
271	[2H]C#CC1=CC(=C(C=C1C2=CSC=C2)C#C[2H])C3=CSC=C3	b3lyp/6-311+G(d,p)	First excited	2.901972	4.236812839
272	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CC5=C4SC=C5	b3lyp/6-311+G(d,p)	First excited	0.3231688	4.101844363
273	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	First excited	0.5110908	4.092592491
274	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=C(C=C4)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2139248	4.209601452
275	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	First excited	0.4110972	4.240078205
276	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=C(C=C4)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.6709888	4.058850372
277	C1=CC=C2C(=C1)C3=C(S2)C=C4C(=C3)C=CC5=C4SC=C5	b3lyp/6-311+G(d,p)	First excited	0.257548	3.852043837
278	C1=CC=C2C(=C1)C3=C(S2)C=C4C(=C3)C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2943512	3.906738723
279	C1=CC=C2C(=C1)C3=C4C(=CC=C3)SC5=CC=CC(=C54)S2	b3lyp/6-311+G(d,p)	First excited	1.2734428	4.237357066
280	[2H]C1=C2C(=CC=C1)C3=C4C(=CC=C3)SC5=CC=CC(=C54)S2	b3lyp/6-311+G(d,p)	First excited	1.271496	4.236812839
281	C1=CC=C2C=C3C(=CC2=C1)C4=C(C=CS4)C5=C3SC=C5	b3lyp/6-311+G(d,p)	First excited	0.3602696	3.492037197
282	C1=CC2=C(C3=CSC=C3C=C2)C4=C1C=CC5=CSC=C54	b3lyp/6-311+G(d,p)	First excited	0.2969552	3.737211787
283	C1=CC2=C(C3=C(C=C2)SC=C3)C4=C1C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2566552	4.239533977
284	C1=CC2=C3C=CC=C4C3=C(C=CS4)C5=C2C(=C1)SC=C5	b3lyp/6-311+G(d,p)	First excited	0.3761168	3.111622017
285	C1=CC(=CC(=C1)C#CC2=CC=CS2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	First excited	2.9436236	3.906194496
286	C1=CC2=CC3=C(C=C2C4=CC5=C(C=CS5)C=C41)SC=C3	b3lyp/6-311+G(d,p)	First excited	0.233678	3.974222961
287	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3SC5=C4SC=C5	b3lyp/6-311+G(d,p)	First excited	0.2380924	4.255316581
288	C1=CC=C2C3=C4C(=CC=C3)SSC5=CC=CC(=C54)C2=C1	b3lyp/6-311+G(d,p)	First excited	2.3272816	3.91354157
289	C#CC1=C(C=CS1)C2=CC=C(C=C2)C3=C(SC=C3)C#C	b3lyp/6-311+G(d,p)	First excited	5.5001812	4.085789645
290	C1=CC(=CC=C1C#CC2=CSC=C2)C#CC3=CSC=C3	b3lyp/6-311+G(d,p)	First excited	5.5536004	3.712993653
291	C1=CC=C2C(=C1)C=CC3=C2C4=C(C=CS4)C5=C3SC=C5	b3lyp/6-311+G(d,p)	First excited	0.2971536	4.096402085
292	C1=CC=C2C=C3C=C4C(=CC3=CC2=C1)C5=C(S4)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.2867252	3.038151274
293	C1=CC=C(C=C1)C#CC2=CC3=C(S2)C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	First excited	1.9651148	4.143477784
294	C1=CC2=C(C=C3C=CSC3=C2)C4=CC5=C(C=CS5)C=C41	b3lyp/6-311+G(d,p)	First excited	0.2294992	4.041707199
295	C1=CC2=C(C=CS2)C3=CC4=C(C=C31)C=C5C=CSC5=C4	b3lyp/6-311+G(d,p)	First excited	0.3143772	3.136112265
296	C#CC1=CC(=C(C=C1C2=CSC=C2)C3=CSC=C3)C#C	b3lyp/6-311+G(d,p)	First excited	4.2123172	4.253411784
297	C1=CC2=C(C=CS2)C3=CC4=C(C=CC5=C4C=CS5)C=C31	b3lyp/6-311+G(d,p)	First excited	0.3933156	3.569861762
298	C1=CC2=CSC=C2C3=CC4=C(C=CC5=CSC=C54)C=C31	b3lyp/6-311+G(d,p)	First excited	0.2357116	3.740749267

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
299	C1=CC2=CC3=CSC=C3C=C2C4=CC5=CSC=C5C=C41	b3lyp/6-311+G(d,p)	First excited	0.2930988	3.207133983
300	C1=CC2=CSC=C2C3=CC4=C(C=C31)C5=CSC=C5C=C4	b3lyp/6-311+G(d,p)	First excited	0.3172168	3.672992915
301	C1=CC2=C(C=CC3=C2C=CC4=CSC=C43)C5=CSC=C51	b3lyp/6-311+G(d,p)	First excited	0.2618012	3.861567822
302	C1=CC=C(C=C1)C#CC2=CC3=C(S2)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	First excited	2.8269768	3.569589648
303	C1=CC=C2C=C3C(=CC2=C1)C=CC4=C3C5=C(S4)C=CS5	b3lyp/6-311+G(d,p)	First excited	0.3882564	3.38727336
304	C1=CC2=C3C4C1C5=CSC=C5C4=CC=C3C6=CSC=C26	b3lyp/6-311+G(d,p)	First excited	0.551986	2.724403991
305	C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC5=C4C(=CC=C5)S3	b3lyp/6-311+G(d,p)	First excited	0.4743744	3.28087684
422	C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC=C4S3	b3lyp/6-311+G(d,p)	First excited	0.4053932	4.234363814
423	C1=CC2=C(C=CC3=C2SC=C3)C4=C1C=CS4	b3lyp/6-311+G(d,p)	First excited	0.2478636	4.420489696
424	C1=CSC2=CC3=C(C=C21)C=C4C(=C3)C=CS4	b3lyp/6-311+G(d,p)	First excited	0.2754412	3.438430766
425	C1=CC=C2C3=C(C4=C(C2=C1)C=CS4)SC=C3	b3lyp/6-311+G(d,p)	First excited	0.2330828	4.229737878
426	C1=CC2=C3C(=CC=C4C3=C1C=CS4)C=CS2	b3lyp/6-311+G(d,p)	First excited	0.6904072	3.062913636
427	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)SC=C4	b3lyp/6-311+G(d,p)	First excited	0.2710392	4.569608092
428	C1=CC=C2C(=C1)C3=C(C4=C2SC=C4)SC=C3	b3lyp/6-311+G(d,p)	First excited	0.4482848	4.345658383
429	C1=CC=C2C(=C1)C(=S)C3=CC=CC=C3C2=S	b3lyp/6-311+G(d,p)	First excited	0.1986232	2.456916064
430	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3SC=C4	b3lyp/6-311+G(d,p)	First excited	0.3138316	4.492871983
431	C1=CC=C2C(=C1)C=C(S2)C#CC3=CSC=C3	b3lyp/6-311+G(d,p)	First excited	1.6256648	3.961161496
432	C1=CC=C2C(=C1)C3=C(S2)SC4=CC=CC=C43	b3lyp/6-311+G(d,p)	First excited	0.3846852	4.666752741
433	C1=CC=C2C(=C1)C=C(S2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	First excited	2.7037456	3.720612841
434	C1=CC2=C(C=CS2)C3=C1C4=C(C=C3)SC=C4	b3lyp/6-311+G(d,p)	First excited	0.460412	4.274092438
435	C1=CSC2=CC3=C(C=C21)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	First excited	0.2845304	3.478703618
436	C1=CC2=C3C(=CC=C4C3=C1C=CS4)SC=C2	b3lyp/6-311+G(d,p)	First excited	0.6218724	2.889032878
437	C1=CC2=C(C3=C1C=CC4=C3SC=C4)SC=C2	b3lyp/6-311+G(d,p)	First excited	0.215822	4.584302241
438	C1=CC=C2C(=C1)C=CC3=C2C4=C(S3)SC=C4	b3lyp/6-311+G(d,p)	First excited	0.4627556	4.35735928
439	C1=C/C(=C\2/C=CC3=C2SC=C3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	First excited	1.088906	2.861549378
440	C1=CSC(=C1)C#C/C=C\C#CC2=CC=CS2	b3lyp/6-311+G(d,p)	First excited	5.5621688	3.231624231
441	C1=CC=C2C(=C1)C3=C(S2)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	First excited	0.2171116	4.159804615
442	C#CC1=C(SC2=CC=CC=C21)C3=CC=CS3	b3lyp/6-311+G(d,p)	First excited	5.9720384	3.870003352
443	C1=CC=C2C(=C1)C(=C3C=CC=CC3=C2[S-])[S-]	b3lyp/6-311+G(d,p)	First excited	0.2025912	2.456371836
444	C1=CC2=C3C(=C1)C4=C(C3=CC=C2)SC=CS4	b3lyp/6-311+G(d,p)	First excited	1.3719856	2.887944422
445	C1=C/C(=C/2\C=CC3=C2SC=C3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	First excited	0.8028752	2.942367195
446	C1=CC=C2C=C3C(=CC2=C1)C4=C(S3)C=CS4	b3lyp/6-311+G(d,p)	First excited	0.313472	3.797076837
447	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C=CS4	b3lyp/6-311+G(d,p)	First excited	0.2622724	4.427564656
448	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	First excited	0.2567668	4.378856275
449	C1=CC2=C(C=CS2)C3=C1C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	First excited	0.3214328	4.41232628
450	C#CC1=C2C(=CC=C1)SC3=CC=CC=C3S2	b3lyp/6-311+G(d,p)	First excited	2.4114404	4.507566132
451	C\1=CC2=C(/C1=C/3\C=CC4=C3C=CS4)C=CS2	b3lyp/6-311+G(d,p)	First excited	0.8097448	2.871073363
452	C1=CC=C2C(=C1)C3=CSC=C3C4=CSC=C24	b3lyp/6-311+G(d,p)	First excited	0.3108804	4.489334503
453	C1=CC2=C(C3=C1C=CC4=C3C=CS4)SC=C2	b3lyp/6-311+G(d,p)	First excited	0.2185128	4.305113418
454	C1=C/C(=C\2/C=CC3=C2C=CS3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	First excited	1.0225784	2.856923442
455	C1=CC=C2C(=C1)C3=CC=CC=C3C2=C([S-])[S-]	b3lyp/6-311+G(d,p)	First excited	0.2403616	2.186706999
456	C\1=CC2=C(/C1=C\3/C=CC4=C3C=CS4)C=CS2	b3lyp/6-311+G(d,p)	First excited	1.2501432	2.890121333
457	C1=C/C(=C/2\C=CC3=C2C=CS3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	First excited	1.054806	2.858011897
458	C1=CC=C2C(=C1)C3=C(S2)C=CC4=CSC=C43	b3lyp/6-311+G(d,p)	First excited	0.4315944	3.70782349
459	C1=CC=C2C(=C1)C3=C(C=CS3)C4=C2SC=C4	b3lyp/6-311+G(d,p)	First excited	0.2668728	4.421850265
460	C1=CC=C2C(=C1)C3=C(S2)C4=CSC=CC4=C3	b3lyp/6-311+G(d,p)	First excited	0.8989132	3.187269671

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
461	C1=CC=C2C(=C1)C3=CC4=CC=CSC4=C3S2	b3lyp/6-311+G(d,p)	First excited	0.7959808	2.63487853
462	C#CC1=CC2=C(C=C1)SC3=CC=CC=C3S2	b3lyp/6-311+G(d,p)	First excited	2.4903292	4.458041409
463	C1=CC2=C(C=CC3=CSC=C32)C4=CSC=C41	b3lyp/6-311+G(d,p)	First excited	0.370884	3.412307835
464	C1=CC2=CSC=C2C3=C1C=CC4=CSC=C43	b3lyp/6-311+G(d,p)	First excited	0.33604	3.367681162
465	C1=CC2=C(C=C3C=CSC3=C2)C4=C1C=CS4	b3lyp/6-311+G(d,p)	First excited	0.3290712	3.924154011
563	C1=CSC2=CC3=C(C=C21)SC=C3	b3lyp/6-311+G(d,p)	First excited	0.2801036	4.296405774
564	C1=CSC2=CC3=C(C=CS3)C=C21	b3lyp/6-311+G(d,p)	First excited	0.330832	4.48280377
565	C1=CC2=CSC=C2C3=CSC=C31	b3lyp/6-311+G(d,p)	First excited	0.3617204	4.38348221
566	C1=CC=C2C(=C1)C3=C(S2)SC=C3	b3lyp/6-311+G(d,p)	First excited	0.5541932	4.963084737
567	C1=CC2=C(C3=C1C=CS3)SC=C2	b3lyp/6-311+G(d,p)	First excited	0.2497236	4.718182261
568	C1=CC=C2C(=C1)C3=C(S2)C=CS3	b3lyp/6-311+G(d,p)	First excited	0.4020204	4.623758751
569	C1=CC2=C(C=CS2)C3=C1C=CS3	b3lyp/6-311+G(d,p)	First excited	0.2899492	4.879545782
570	C1=CC2=C(C=CS2)C3=C1SC=C3	b3lyp/6-311+G(d,p)	First excited	0.456816	4.601717528
571	C1=CC(=S)C=C2C1=CC(=S)C=C2	b3lyp/6-311+G(d,p)	First excited	0.1983876	1.993506156
572	C1=CC=C2C(=S)C=CC(=S)C2=C1	b3lyp/6-311+G(d,p)	First excited	0.2466484	2.342900356
573	C=C1C2=C(C3=C1C=CS3)SC=C2	b3lyp/6-311+G(d,p)	First excited	20.8524228	3.518976469
574	C1=CSC2=CC3=CSC=C3C=C21	b3lyp/6-311+G(d,p)	First excited	0.3349116	3.294482533
575	C1=CC2=C(C=CS2)C3=CSC=C31	b3lyp/6-311+G(d,p)	First excited	0.4920072	3.918983847
609	C1=CSC2=C1SC=C2	b3lyp/6-311+G(d,p)	First excited	0.623596	5.059957272
610	C1=CSC2=C1C=CS2	b3lyp/6-311+G(d,p)	First excited	0.3141044	5.489625061
611	C1=CC(=S)C=CC1=S	b3lyp/6-311+G(d,p)	First excited	0.2129452	2.16357732
612	[2H]C1=C(SC2=C1C(=C(S2)[2H])[2H])[2H]	b3lyp/6-311+G(d,p)	First excited	0.3141168	5.489352947
613	[2H]C1=C(SC2=C1SC(=C2[2H])[2H])[2H]	b3lyp/6-311+G(d,p)	First excited	0.6236208	5.059957272
614	C1=C2C=S=CC2=CS1	b3lyp/6-311+G(d,p)	First excited	0.4233112	2.993252487
79	C1=CC=CC=C1	b3lyp/6-311+G(d,p)	Cationic	0.2944628	6.598216937
80	C1=CC=C2C=CC=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.1813996	4.747842672
81	C1CCC2=CC=CC=C2C1	b3lyp/6-311+G(d,p)	Cationic	36.96502	6.088003445
82	C1CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	Cationic	35.3355732	4.958730916
83	C1CC2=C(C=C1)C3=CC=CC=C3C=C2	b3lyp/6-311+G(d,p)	Cationic	0.231942	4.098578996
84	C1CCC2=C(C1)C=CC3=CC=CC=C23	b3lyp/6-311+G(d,p)	Cationic	6.2023312	4.646616315
85	C1C=CCC2=CC=CC=C21	b3lyp/6-311+G(d,p)	Cationic	0.2573992	5.944327325
86	C1CC2=CC3=CC=CC=C3C=C2C=C1	b3lyp/6-311+G(d,p)	Cationic	31.5613852	4.405523433
87	C1CCC2=CC3=CC=CC=C3C=C2C1	b3lyp/6-311+G(d,p)	Cationic	78.3852236	4.593826226
88	C1=CC=C2C=C3C=CC=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.1396364	3.551630133
89	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	b3lyp/6-311+G(d,p)	Cationic	0.2199388	4.68144689
90	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	b3lyp/6-311+G(d,p)	Cationic	0.1686524	4.219125437
91	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	b3lyp/6-311+G(d,p)	Cationic	0.1432324	3.723878208
92	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	b3lyp/6-311+G(d,p)	Cationic	0.1692848	3.849322698
93	C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.1144892	2.751887491
94	C1=CC=C2C=C3C4=CC=CC=C4C5=CC=CC=C5C3=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.1272364	3.849594812
95	C1=CC=C2C(=C1)C=CC3=C2C4=CC=CC=C4C5=CC=CC=C35	b3lyp/6-311+G(d,p)	Cationic	0.1880832	4.051503298
96	C1=CC=C2C(=C1)C=CC3=C2C4=CC=CC=C4C=C3	b3lyp/6-311+G(d,p)	Cationic	0.1616092	4.171505512
97	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3C5=CC=CC=C5C=C4	b3lyp/6-311+G(d,p)	Cationic	0.2183144	4.208785111
98	C1=CC=C2C(=C1)C=CC3=CC4=C(C=C32)C5=CC=CC=C5C=C4	b3lyp/6-311+G(d,p)	Cationic	0.1326552	3.887418639
99	C1CC2=CC=CC=C2C3=CC=CC=C31	b3lyp/6-311+G(d,p)	Cationic	31.9738588	4.88226692
100	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC5=CC=CC=C5C=C43	b3lyp/6-311+G(d,p)	Cationic	0.12431	3.477615162

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
101	C1C2=CC=CC=C2CC3=CC4=CC=CC=C4C=C31	b3lyp/6-311+G(d,p)	Cationic	29.5613644	4.666480627
102	C1CCC2=CC3=C(CCCC3)C=C2C1	b3lyp/6-311+G(d,p)	Cationic	134.0260448	5.761194696
103	C1C2=CC=CC=C2CC3=CC=CC=C31	b3lyp/6-311+G(d,p)	Cationic	0.477648	5.945687895
104	C1=CC=C2C=C3C(=CC2=C1)C=CC4=C3C=CC5=CC6=CC=CC=C6C=C54	b3lyp/6-311+G(d,p)	Cationic	0.0974392	3.126316166
105	C1CCC2=C(C1)C=CC3=C2CCCC3	b3lyp/6-311+G(d,p)	Cationic	94.177814	5.899972766
106	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3C=CC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Cationic	0.187426	4.206880314
107	C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.0973648	2.190516593
108	C1CC2=C(C3=CC=CC=C3C=C2)C4=C1C=CC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Cationic	0.2271308	3.923337669
109	C1CC2=C(C=CC3=CC=CC=C23)C4=CC=CC=C41	b3lyp/6-311+G(d,p)	Cationic	0.191766	4.247425279
110	C1=CC=C2C=C3C(=CC2=C1)C=CC4=CC5=CC=CC=C5C=C43	b3lyp/6-311+G(d,p)	Cationic	0.1804572	3.748640569
111	C1CCC2=C(C1)C=CC3=C2C=CC4=CC=CC=C43	b3lyp/6-311+G(d,p)	Cationic	76.3040944	4.562261018
112	C1CCC2=C(C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C23	b3lyp/6-311+G(d,p)	Cationic	4.8524424	3.656938198
113	C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.0842952	1.77962466
114	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.1531772	3.810410416
115	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.146072	3.348088964
116	C1=CC=C2C(=C1)C3=CC=CC4=C3C5=C(C=CC=C25)C=C4	b3lyp/6-311+G(d,p)	Cationic	0.1472376	3.958984585
117	C1=CC=C2C(=C1)C=C3C=CC4=C5C3=C2C6=CC=CC=C6C5=CC=C4	b3lyp/6-311+G(d,p)	Cationic	0.15469	3.381286855
118	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.138012	3.481968984
119	C1=CC=C2C3=C4C(=CC2=C1)C5=CC=CC=C5C6=CC=CC(=C64)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.1386816	3.51271785
120	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC6=CC=CC=C56)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.128216	2.877876209
121	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=CC6=CC=CC=C6C(=C54)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.1634692	3.224821384
122	C1=CC2=C3C(=C1)C4=CC=CC5=C4C(=CC=C5)C3=CC=C2	b3lyp/6-311+G(d,p)	Cationic	0.1469276	2.985089071
123	C1=CC=C2C(=C1)C3=CC=CC=C3C4=CC=CC=C24	b3lyp/6-311+G(d,p)	Cationic	0.1850204	4.838728702
124	C1=CC2=C3C(=C1)C=C4C=CC5=C6C4=C3C(=CC6=CC=C5)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.1159772	2.867807996
125	C1=CC=C2C(=C1)C=C3C4=CC=CC=C4C5=C3C2=CC6=CC=CC=C65	b3lyp/6-311+G(d,p)	Cationic	0.1511932	3.241964557
126	C1=CC2=C3C4=C1C=CC5=CC6=C7C8=C(C=CC9=C8C1=C(C=C9)C=C(C3=C1C7=C54)C=C2)C=C6	b3lyp/6-311+G(d,p)	Cationic	0.0955296	2.91597215
127	C1=CC=C2C(=C1)C=CC3=C2C=C4C=CC=C5C4=C3C=C5	b3lyp/6-311+G(d,p)	Cationic	0.2145572	3.238154963
128	C1=CC=C2C=C3C4=C5C(=CC3=CC2=C1)C=CC6=C5C(=CC=C6)C=C4	b3lyp/6-311+G(d,p)	Cationic	0.1239008	2.843317749
129	C1=CC=C2C3=C4C(=CC=CC4=CC2=C1)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.2170868	3.079784695
130	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C6=CC=CC(=C64)C2=C1	b3lyp/6-311+G(d,p)	Cationic	0.1369332	4.105109729
131	C1=CC=C2C(=C1)C3=CC=CC=C3C4=C2C5=CC=CC6=C5C4=CC=C6	b3lyp/6-311+G(d,p)	Cationic	0.2124616	3.252304884
132	C1=CC=C2C(=C1)C=C3C=C4C=CC=CC4=C5C3=C2C6=CC=CC=C65	b3lyp/6-311+G(d,p)	Cationic	0.1005516	2.460997772
133	C1=CC=C2C(=C1)C=C3C=CC=C4C3=C2C5=CC=CC6=C5C4=CC=C6	b3lyp/6-311+G(d,p)	Cationic	0.1473988	2.538822337
134	C1=CC=C2C(=C1)C3=CC=CC=C3C4=C2C5=CC=CC=C5C6=CC=CC=C64	b3lyp/6-311+G(d,p)	Cationic	10.9663988	3.976127758
135	C1CC2=CC=CC3=C2C4=C(C=CC=C41)C=C3	b3lyp/6-311+G(d,p)	Cationic	36.040662	4.611785741
136	C1=CC=C2C=C3C4=CC=CC5=C4C6=C(C=CC=C6C3=CC2=C1)C=C5	b3lyp/6-311+G(d,p)	Cationic	0.1250912	3.86211205
137	C1=CC=C2C3=C4C(=CC2=C1)C5=CC=CC=C5C6=CC7=CC=CC=C7C(=C64)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.15128	3.406865558
138	C1=CC2=C3C4=C1C=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.1904764	4.161437299
139	C1CC2=C3C(=CC=C4C3=C(CCC4)C=C2)C1	b3lyp/6-311+G(d,p)	Cationic	71.727428	4.446068399
140	CC1=CC2=C3C(=C1)C=CC4=CC(=CC(=C43)C=C2)C	b3lyp/6-311+G(d,p)	Cationic	0.2394316	3.789457649
141	CC1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.18321	3.800070089
142	CC1=C2C=CC3=CC=CC4=C3C2=C(C=C1)C=C4	b3lyp/6-311+G(d,p)	Cationic	16.1239432	3.724694549
143	CC1=CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	Cationic	16.7850492	4.756278202
144	CC1=CC=CC2=CC=CC=C12	b3lyp/6-311+G(d,p)	Cationic	1.3446436	4.655323959
145	C1=CC2=C3C(=C1)C=CC3=CC=C2	b3lyp/6-311+G(d,p)	Cationic	0.4145196	3.886602298
146	CC1=C2C=CC3=CC=CC=C3C2=C(C4=CC=CC=C14)C	b3lyp/6-311+G(d,p)	Cationic	18.0141248	3.535575415

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
147	CC1=CC2=CC=CC=C2C3=C1C4=CC=CC=C4C=C3	b3lyp/6-311+G(d,p)	Cationic	0.1957588	4.099939566
148	CC1=CC2=C(C=C1)C=C(C=C2)C	b3lyp/6-311+G(d,p)	Cationic	15.9425808	4.746754217
149	CC1=CC2=CC=CC(=C2C=C1)C	b3lyp/6-311+G(d,p)	Cationic	33.1261164	4.665664286
150	CC(C)C1=CC2=C(C=C1)C=C(C=C2)C(C)C	b3lyp/6-311+G(d,p)	Cationic	24.9330148	4.662126806
151	CC1=C2C=CC3=CC=CC=C3C2=CC4=CC=CC=C14	b3lyp/6-311+G(d,p)	Cationic	16.3096456	3.629454697
152	CC1=C2C(=CC3=CC=CC=C13)C=CC4=CC=CC=C42	b3lyp/6-311+G(d,p)	Cationic	5.3257504	3.6275499
153	CC1=C2C=C3C=CC4=CC=CC=C4C3=CC2=CC=C1	b3lyp/6-311+G(d,p)	Cationic	1.4968164	3.696938935
154	CC(C)C1=CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	Cationic	22.8050012	4.747842672
155	CC1=CC=C(C2=CC=CC=C12)C	b3lyp/6-311+G(d,p)	Cationic	17.3522376	4.555458171
156	CC1=CC=C(C=C1)S(=O)(=O)O	b3lyp/6-311+G(d,p)	Cationic	0.7946416	5.974531964
157	CC1=CC=C(C=C1)S(=O)(=O)Cl	b3lyp/6-311+G(d,p)	Cationic	62.5300504	5.124720372
158	C1=CC2=CC3=C4C5=C(C=C3)C=C6C=CC7=C8C6=C5C9=C3C4=C2C2=C1C=CC1=CC4=C(C3=C12)C1=C(C=C4)C=C(C8=C19)C=C7	b3lyp/6-311+G(d,p)	Cationic	0.068014	2.520862822
160	C1=CC=C2C(=C1)C3=C4C2=CC5=CC=CC6=C5C4=C(C=C6)C=C3	b3lyp/6-311+G(d,p)	Cationic	0.16213	3.31189782
306	C1=CSC2=CC3=CC4=C(C=C3C=C21)C=C5C(=C4)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.0945004	2.73773757
307	C1=CC2=C(C=CC3=C2C=CC4=C3SC=C4)C5=C1C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.1961184	4.358447735
308	C1=CC=C2C(=C1)C3=CC4=C(C=C3S2)SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Cationic	0.0839604	4.273276096
309	C1=CC=C2C(=C1)C3=CC4=C(C=C3S2)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Cationic	0.1198088	4.002250689
310	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Cationic	0.136958	4.272731868
311	C1=CC=C2C=C3C(=CC2=C1)C4=C(C5=C3SC=C5)SC=C4	b3lyp/6-311+G(d,p)	Cationic	0.1440012	3.515983217
312	C1=CC=C(C(=C1)C#CC2=CC=CS2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	Cationic	2.7106896	3.604420222
313	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Cationic	0.1503872	4.397632131
314	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.2009296	4.103204932
315	C1=CC=C2C(=C1)C3=C(C4=C(C=C3)SC=C4)C5=C2SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.2041908	4.228649423
316	C1=CSC2=CC3=CC4=C(C=C5C=CSC5=C4)C=C3C=C21	b3lyp/6-311+G(d,p)	Cationic	0.0941532	2.748077897
317	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Cationic	0.1780268	4.022659229
318	C1=CC2=C3C=CSC4=CC=CC(=C34)C5=C2C(=C1)SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.1854792	2.354329138
319	C1=CC2=CC3=CC4=CC5=CSSC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.2573496	1.373630778
320	C1=CC=C2C(=C1)C=C3C=C4C=CC=CC4=C5C3=C2SS5	b3lyp/6-311+G(d,p)	Cationic	0.1422156	2.338002306
321	C1=CC2=C(C=CS2)C3=CC4=C(C=C31)C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.1578272	3.535575415
322	C1=CC2=C(C=C3C=CSC3=C2)C4=C1C=C5C(=C4)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.20522	3.8846975
323	C1=CC=C2C=C3C(=CC2=C1)C4=C(S3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Cationic	0.1546156	3.62891047
324	C1=CC2=CC3=C(C=CC4=C3SC=C4)C=C2C5=C1C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.1356436	3.502921751
325	C1=CC=C2C(=C1)C=CC3=C2C4=C(S3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Cationic	0.2102916	3.921432872
326	C1=CC2=C(C=CC3=C2C=CS3)C4=C1C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.210924	4.153001769
327	C#CC1=CC(=C(C=C1C2=CC=CS2)C#C)C3=CC=CS3	b3lyp/6-311+G(d,p)	Cationic	0.3881448	3.864288961
328	C1=CC=C2C(=C1)C3=C(S2)C=C4C=C5C(=CC4=C3)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.093186	3.467819063
329	C1=CC2=C(C=CC3=C2C=CC4=C3C=CS4)C5=C1C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.2012892	4.245248368
330	C1=CC=C2C(=C1)C=C(S2)C#CC3=CC4=CC=CC=C4S3	b3lyp/6-311+G(d,p)	Cationic	0.2513728	3.589181846
331	C1=CC2=CC3=C(C=C2C4=C1C=CS4)C5=C(C=C3)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.136648	3.506187118
332	C1=CC=C2C(=C1)SC3=C(S2)C4=CC=CC5=C4C3=CC=C5	b3lyp/6-311+G(d,p)	Cationic	1.0813048	3.034885908
333	C#CC1=CC(=C(C=C1C2=CSC=C2)C#C)C3=CSC=C3	b3lyp/6-311+G(d,p)	Cationic	4.141166	4.155722907
334	[2H]C1=CC2=C(C=CS2)C3=CC4=C(C=C13)C5=C(C=C4[2H])SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.1578644	3.535575415
335	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CC5=C4SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.19344	4.101844363
336	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=C(C=C4)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.1632088	4.209601452
337	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.180544	4.240078205
338	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=C(C=C4)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.1807176	4.058850372

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
339	C1=CC=C2C(=C1)C3=C(S2)C=C4C(=C3)C=CC5=C4SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.1131128	3.852043837
340	C1=CC=C2C(=C1)C3=C(S2)C=C4C(=C3)C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.1368588	3.906738723
341	C1=CC=C2C(=C1)C3=C4C(=CC=C3)SC5=CC=CC(=C54)S2	b3lyp/6-311+G(d,p)	Cationic	0.6864516	4.237357066
342	[2H]C1=C2C(=CC=C1)C3=C4C(=CC=C3)SC5=CC=CC(=C54)S2	b3lyp/6-311+G(d,p)	Cationic	0.68727	4.237357066
343	C1=CC=C2C=C3C(=CC2=C1)C4=C(C=CS4)C5=C3SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.1355692	3.492037197
344	C1=CC2=C(C3=CSC=C3C=C2)C4=C1C=CC5=CSC=C54	b3lyp/6-311+G(d,p)	Cationic	0.1836564	3.737483901
345	C1=CC2=C(C3=C(C=C2)SC=C3)C4=C1C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.2449372	4.239261863
346	C1=CC2=C3C=CC=C4C3=C(C=CS4)C5=C2C(=C1)SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.2395184	3.111894131
347	C1=CC(=CC(=C1)C#CC2=CC=CS2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	Cationic	3.1869488	3.905378154
348	C1=CC2=CC3=C(C=C2C4=CC5=C(C=CS5)C=C41)SC=C3	b3lyp/6-311+G(d,p)	Cationic	0.18352	3.974222961
349	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3SC5=C4SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.2312228	4.255316581
350	C1=CC=C2C3=C4C(=CC=C3)SSC5=CC=CC(=C54)C2=C1	b3lyp/6-311+G(d,p)	Cationic	0.8475524	3.913813684
351	C#CC1=C(C=CS1)C2=CC=C(C=C2)C3=C(SC=C3)C#C	b3lyp/6-311+G(d,p)	Cationic	4.186674	4.092048264
352	C1=CC=C2C(=C1)C=CC3=C2C4=C(C=CS4)C5=C3SC=C5	b3lyp/6-311+G(d,p)	Cationic	0.173786	4.096402085
353	C1=CC=C2C=C3C=C4C(=CC3=CC2=C1)C5=C(S4)C=CS5	b3lyp/6-311+G(d,p)	Cationic	0.1124184	3.038423388
354	C1=CC=C(C=C1)C#CC2=CC3=C(S2)C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	Cationic	2.923114	3.683333242
355	C#CC1=CC(=C(C=C1C2=CSC=C2)C3=CSC=C3)C#C	b3lyp/6-311+G(d,p)	Cationic	0.247256	4.286881789
356	C1=CC2=CSC=C2C3=CC4=C(C=CC5=CSC=C54)C=C31	b3lyp/6-311+G(d,p)	Cationic	0.100254	3.740749267
357	C1=CC2=CC3=CSC=C3C=C2C4=CC5=CSC=C5C=C41	b3lyp/6-311+G(d,p)	Cationic	0.1939112	3.207133983
358	C1=CC2=CSC=C2C3=CC4=C(C=C31)C5=CSC=C5C=C4	b3lyp/6-311+G(d,p)	Cationic	0.1596252	3.672992915
359	C1=CC2=C(C=CC3=C2C=CC4=CSC=C43)C5=CSC=C51	b3lyp/6-311+G(d,p)	Cationic	0.1988092	3.861567822
360	C1=CC2=C3C4C1C5=CSC=C5C4=CC=C3C6=CSC=C26	b3lyp/6-311+G(d,p)	Cationic	69.5200668	2.724403991
361	C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC5=C4C(=CC=C5)S3	b3lyp/6-311+G(d,p)	Cationic	0.175088	3.28087684
466	C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC=C4S3	b3lyp/6-311+G(d,p)	Cationic	0.2284204	4.234363814
467	C1=CC2=C(C=CC3=C2SC=C3)C4=C1C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.2761604	4.420489696
468	C1=CC2=C3C(=C1)SSC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.7743924	3.888234981
469	C1=CC=C2C3=C4C(=CC=C3)SSC4=CC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.1512924	3.379109944
470	C1=CSC2=CC3=C(C=C21)C=C4C(=C3)C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.1002788	3.438430766
471	C1=CC=C2C3=C(C4=C(C2=C1)C=CS4)SC=C3	b3lyp/6-311+G(d,p)	Cationic	0.1762164	4.229737878
472	C1=CC2=C3C(=CC=C4C3=C1C=CS4)C=CS2	b3lyp/6-311+G(d,p)	Cationic	0.214458	3.062913636
473	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)SC=C4	b3lyp/6-311+G(d,p)	Cationic	0.17112	4.569608092
474	C1=CC2=CC3=C4C(=CC=CS4)SC3=C2C=C1	b3lyp/6-311+G(d,p)	Cationic	0.3695076	1.617716912
475	C1=CC2=C3C(=C1)C=CC4=C3C(=CSS4)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.6092492	2.626715114
476	C1=CC=C2C(=C1)C3=C(C4=C2SC=C4)SC=C3	b3lyp/6-311+G(d,p)	Cationic	0.2313716	4.345658383
477	C1=CC=C2C(=C1)C(=S)C3=CC=CC=C3C2=S	b3lyp/6-311+G(d,p)	Cationic	0.0263004	2.455827609
478	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3SC=C4	b3lyp/6-311+G(d,p)	Cationic	0.213714	4.492871983
479	C1=CC=C2C(=C1)C=C(S2)C#CC3=CSC=C3	b3lyp/6-311+G(d,p)	Cationic	0.2726512	3.961161496
480	C1=CC=C2C(=C1)C3=C(S2)SC4=CC=CC=C43	b3lyp/6-311+G(d,p)	Cationic	0.1278564	4.666752741
481	C1=CC=C2C(=C1)C=C(S2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	Cationic	0.450988	3.720884955
482	C1=CC2=C(C=CS2)C3=C1C4=C(C=C3)SC=C4	b3lyp/6-311+G(d,p)	Cationic	0.2472064	4.274092438
483	C1=CSC2=CC3=C(C=C21)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	Cationic	0.096968	3.478703618
484	C1=CC2=C3C(=CC=C4C3=C1C=CS4)SC=C2	b3lyp/6-311+G(d,p)	Cationic	0.214334	2.889032878
485	C1=CC2=C(C3=C1C=CC4=C3SC=C4)SC=C2	b3lyp/6-311+G(d,p)	Cationic	0.158782	4.584302241
486	C1=CC=C2C(=C1)C=CC3=C2C4=C(S3)SC=C4	b3lyp/6-311+G(d,p)	Cationic	0.237522	4.35735928
487	C1=C/C(=C\2/C=CC3=C2SC=C3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.2830176	2.861549378
488	C1=CC=C2C(=C1)C3=CSC(=C23)C4=CC=CS4	b3lyp/6-311+G(d,p)	Cationic	0.6806608	3.845513104

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
489	C1=CSC(=C1)C#C/C=C\C#CC2=CC=CS2	b3lyp/6-311+G(d,p)	Cationic	4.3437696	3.232440572
490	C1=CC=C2C(=C1)C3=C(S2)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	Cationic	0.0976004	4.159804615
491	C#CC1=C(SC2=CC=CC=C21)C3=CC=CS3	b3lyp/6-311+G(d,p)	Cationic	1.6564912	3.750273252
492	C1=CC=C2C(=C1)C(=C3C=CC=CC3=C2[S-])[S-]	b3lyp/6-311+G(d,p)	Cationic	0.0265236	2.456371836
493	C1=CC2=C3C(=C1)C4=C(C3=CC=C2)SC=CS4	b3lyp/6-311+G(d,p)	Cationic	0.8726252	2.887944422
494	C1=C/C(=C/2\C=CC3=C2SC=C3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.2726016	2.942367195
495	C1=CC=C2C=C3C(=CC2=C1)C4=C(S3)C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.1434432	3.797348951
496	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.1861984	4.427292542
497	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.1531524	4.378856275
498	C#CC1=C2C(=CC=C1)SC3=CC=CC=C3S2	b3lyp/6-311+G(d,p)	Cationic	1.3996624	4.507566132
499	C\1=CC2=C(/C1=C/3\C=CC4=C3C=CS4)C=CS2	b3lyp/6-311+G(d,p)	Cationic	0.286998	2.871073363
500	C1=CC=C2C(=C1)C3=CSC=C3C4=CSC=C24	b3lyp/6-311+G(d,p)	Cationic	0.3566364	4.489334503
501	C1=CC2=C(C3=C1C=CC4=C3C=CS4)SC=C2	b3lyp/6-311+G(d,p)	Cationic	0.2310368	4.305113418
502	C1=C/C(=C\2/C=CC3=C2C=CS3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.5224492	2.856923442
503	C1=CC=C2C(=C1)C3=CC=CC=C3C2=C([S-])[S-]	b3lyp/6-311+G(d,p)	Cationic	0.1622292	2.187251226
504	C\1=CC2=C(/C1=C\3/C=CC4=C3C=CS4)C=CS2	b3lyp/6-311+G(d,p)	Cationic	0.4494752	2.88848865
505	C1=C/C(=C/2\C=CC3=C2C=CS3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.4985544	2.858011897
506	C1=CC=C2C(=C1)C3=C(S2)C=CC4=CSC=C43	b3lyp/6-311+G(d,p)	Cationic	0.1636428	3.70782349
507	C1=CC=C2C(=C1)C3=C(C=CS3)C4=C2SC=C4	b3lyp/6-311+G(d,p)	Cationic	0.220348	4.421850265
508	C1=CC=C2C(=C1)C3=C(S2)C4=CSC=CC4=C3	b3lyp/6-311+G(d,p)	Cationic	0.3142036	3.187269671
509	C1=CC=C2C(=C1)C3=CC4=CC=CSC4=C3S2	b3lyp/6-311+G(d,p)	Cationic	0.2507652	2.63487853
510	C#CC1=CC2=C(C=C1)SC3=CC=CC=C3S2	b3lyp/6-311+G(d,p)	Cationic	1.3449164	4.458041409
511	C1=CC2=C(C=CC3=CSC=C32)C4=CSC=C41	b3lyp/6-311+G(d,p)	Cationic	0.125736	3.412307835
512	C1=CC2=CSC=C2C3=C1C=CC4=CSC=C43	b3lyp/6-311+G(d,p)	Cationic	0.1198212	3.367409048
513	C1=CC2=CC3=C4C(=CSS4)C=CC3=C2C=C1	b3lyp/6-311+G(d,p)	Cationic	0.2238944	1.640846591
514	C1=CC2=C(C=C3C=CSC3=C2)C4=C1C=CS4	b3lyp/6-311+G(d,p)	Cationic	0.1290964	3.924154011
576	C1=CSC2=CC3=C(C=C21)SC=C3	b3lyp/6-311+G(d,p)	Cationic	0.1581	4.296405774
577	C1=CC2=C3C(=C1)SSC3=CC=C2	b3lyp/6-311+G(d,p)	Cationic	0.1405292	3.351898558
578	C1=CSC2=CC3=C(C=CS3)C=C21	b3lyp/6-311+G(d,p)	Cationic	0.1030936	4.482531656
579	C1=CC2=CSC=C2C3=CSC=C31	b3lyp/6-311+G(d,p)	Cationic	0.2985796	4.38348221
580	C1=CC=C2C(=C1)C3=C(S2)SC=C3	b3lyp/6-311+G(d,p)	Cationic	0.2392952	4.963084737
581	C1=CC2=C(C3=C1C=CS3)SC=C2	b3lyp/6-311+G(d,p)	Cationic	0.2017356	4.718182261
582	C1=CC=C2C(=C1)C3=C(S2)C=CS3	b3lyp/6-311+G(d,p)	Cationic	0.2550184	4.623758751
583	C1=CC2=C(C=CS2)C3=C1C=CS3	b3lyp/6-311+G(d,p)	Cationic	0.2419488	4.879817895
584	C1=CC2=C(C=CS2)C3=C1SC=C3	b3lyp/6-311+G(d,p)	Cationic	0.2885108	4.601717528
585	C1=CC(=S)C=C2C1=CC(=S)C=C2	b3lyp/6-311+G(d,p)	Cationic	0.03906	1.993506156
586	C1=CC=C2C(=C1)C=CC(=S)C2=S	b3lyp/6-311+G(d,p)	Cationic	0.9801828	2.148338944
587	C1=CC=C2C(=S)C=CC(=S)C2=C1	b3lyp/6-311+G(d,p)	Cationic	0.0795584	2.342900356
588	C=C1C2=C(C3=C1C=CS3)SC=C2	b3lyp/6-311+G(d,p)	Cationic	42.8313112	3.518976469
589	C1=CSC2=CC3=CSC=C3C=C21	b3lyp/6-311+G(d,p)	Cationic	0.1049908	3.294482533
590	C1=CC2=C(C=CS2)C3=CSC=C31	b3lyp/6-311+G(d,p)	Cationic	0.1967136	3.918983847
591	C1=CC2=C3C=CC=C3SSC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.6642184	2.329566777
592	C1=CC=C2C(=C1)C=CC3=C2SS3	b3lyp/6-311+G(d,p)	Cationic	0.2196412	3.431083692
615	C1=CSC2=C1SC=C2	b3lyp/6-311+G(d,p)	Cationic	0.4038928	5.059957272
616	C1=CSC2=C1C=CS2	b3lyp/6-311+G(d,p)	Cationic	0.132494	5.489625061
617	C1=CC(=S)C=CC1=S	b3lyp/6-311+G(d,p)	Cationic	0.0560232	2.16357732

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
618	C1=CC(=S)C(=S)C=C1	b3lyp/6-311+G(d,p)	Cationic	0.7926204	1.789692873
619	[2H]C1=C(SC2=C1C(=C(S2)[2H])[2H])[2H]	b3lyp/6-311+G(d,p)	Cationic	0.1325064	5.489625061
620	[2H]C1=C(SC2=C1SC(=C2[2H])[2H])[2H]	b3lyp/6-311+G(d,p)	Cationic	0.4038308	5.059957272
621	C1=CC2=C(S2)C=C1S	b3lyp/6-311+G(d,p)	Cationic	0.5741696	4.576138825
622	C1=C2C=S=CC2=CS1	b3lyp/6-311+G(d,p)	Cationic	0.060326	2.994068829
623	C1=CC2=CSSC2=C1	b3lyp/6-311+G(d,p)	Cationic	0.4316936	3.39081084
161	C1CCC2=CC3=C(CCCC3)C=C2C1	b3lyp/6-311+G(d,p)	Anionic	184.8776884	5.76146681
162	C1CCC2=C(C1)C=CC3=C2CCCC3	b3lyp/6-311+G(d,p)	Anionic	207.4216572	5.93834082
163	C1CCC2=CC3=CC=CC=C3C=C2C1	b3lyp/6-311+G(d,p)	Anionic	0.2377204	4.593826226
164	C1CCC2=C(C1)C=CC3=C2C=CC4=CC=CC=C43	b3lyp/6-311+G(d,p)	Anionic	41.600326	4.583758013
165	C1CCC2=CC=CC=C2C1	b3lyp/6-311+G(d,p)	Anionic	75.01411	6.088003445
166	C1CCC2=C(C1)C=CC3=CC=CC=C23	b3lyp/6-311+G(d,p)	Anionic	106.4849008	4.646616315
167	C1CC2=C3C(=CC=C4C3=C(CCC4)C=C2)C1	b3lyp/6-311+G(d,p)	Anionic	52.9133668	4.449061651
168	C1CC2=CC3=CC=CC=C3C=C2C=C1	b3lyp/6-311+G(d,p)	Anionic	37.0171992	4.405523433
169	C1CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	Anionic	33.02244	4.958730916
170	C1CC2=C(C=C1)C3=CC=CC=C3C=C2	b3lyp/6-311+G(d,p)	Anionic	37.3657756	4.098578996
171	C1C=CCC2=CC=CC=C21	b3lyp/6-311+G(d,p)	Anionic	30.8223204	5.944327325
172	CC1=CC=C(C2=CC=CC=C12)C	b3lyp/6-311+G(d,p)	Anionic	18.6709652	4.555186058
173	CC1=CC2=CC=CC(=C2C=C1)C	b3lyp/6-311+G(d,p)	Anionic	0.3947044	4.665664286
174	CC1=C2C(=CC3=CC=CC=C13)C=CC4=CC=CC=C42	b3lyp/6-311+G(d,p)	Anionic	18.429314	3.6275499
175	CC1=CC=CC2=CC=CC=C12	b3lyp/6-311+G(d,p)	Anionic	0.2305904	4.655323959
176	CC1=C2C=CC3=CC=CC4=C3C2=C(C=C1)C=C4	b3lyp/6-311+G(d,p)	Anionic	0.2053936	3.724694549
177	CC(C)C1=CC2=C(C=C1)C=C(C=C2)C(C)C	b3lyp/6-311+G(d,p)	Anionic	90.2407768	4.662671033
178	CC1=CC2=C(C=C1)C=C(C=C2)C	b3lyp/6-311+G(d,p)	Anionic	33.4431348	4.746754217
179	CC1=CC2=C3C(=C1)C=CC4=CC(=CC(=C43)C=C2)C	b3lyp/6-311+G(d,p)	Anionic	16.5499328	3.789457649
180	CC1=CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	Anionic	0.4182768	4.756278202
181	CC1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.3536232	3.800070089
182	CC(C)C1=CC2=CC=CC=C2C=C1	b3lyp/6-311+G(d,p)	Anionic	44.6110708	4.747842672
183	C1CC2=CC=CC3=C2C4=C(C=CC=C41)C=C3	b3lyp/6-311+G(d,p)	Anionic	31.7317984	4.611785741
184	C1C2=CC=CC=C2CC3=CC4=CC=CC=C4C=C31	b3lyp/6-311+G(d,p)	Anionic	30.8957532	4.666208513
185	C1CC2=C(C=CC3=CC=CC=C23)C4=CC=CC=C41	b3lyp/6-311+G(d,p)	Anionic	36.7601596	4.247425279
186	CC1=CC2=CC=CC=C2C3=C1C4=CC=CC=C4C=C3	b3lyp/6-311+G(d,p)	Anionic	16.8097872	4.099939566
187	CC1=C2C=CC3=CC=CC=C3C2=C(C4=CC=CC=C14)C	b3lyp/6-311+G(d,p)	Anionic	35.9539488	3.535575415
188	CC1=C2C=CC3=CC=CC=C3C2=CC4=CC=CC=C14	b3lyp/6-311+G(d,p)	Anionic	0.2187608	3.629454697
189	C1CCC2=C(C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C23	b3lyp/6-311+G(d,p)	Anionic	36.6384536	3.710272515
190	CC1=C2C=C3C=CC4=CC=CC=C4C3=CC2=CC=C1	b3lyp/6-311+G(d,p)	Anionic	0.1854668	3.696938935
191	C1C2=CC=CC=C2CC3=CC=CC=C31	b3lyp/6-311+G(d,p)	Anionic	30.7856536	5.945687895
192	C1CC2=CC=CC=C2C3=CC=CC=C31	b3lyp/6-311+G(d,p)	Anionic	37.0302812	4.88226692
193	C1=CC=C2C3=C4C(=CC=CC4=CC2=C1)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.2321032	3.079784695
194	C1=CC2=C3C(=C1)C=CC3=CC=C2	b3lyp/6-311+G(d,p)	Anionic	0.2856712	3.886874411
195	C1=CC=C2C=C3C=CC=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.1962672	3.551630133
196	C1=CC=CC=C1	b3lyp/6-311+G(d,p)	Anionic	0.0022816	6.598216937
197	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	b3lyp/6-311+G(d,p)	Anionic	0.1847848	3.723878208
198	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.2005452	3.348088964
199	C1=CC=C2C=C3C4=CC=CC=C4C5=CC=CC=C5C3=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.163804	3.849594812
200	C1=CC=C2C(=C1)C=CC3=C2C4=CC=CC=C4C=C3	b3lyp/6-311+G(d,p)	Anionic	0.174902	4.171233398

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
201	C1=CC=C2C(=C1)C3=CC=CC4=C3C5=C(C=CC=C25)C=C4	b3lyp/6-311+G(d,p)	Anionic	0.1972468	3.958984585
202	C1=CC=C2C(=C1)C=CC3=C2C=C4C=CC=C5C4=C3C=C5	b3lyp/6-311+G(d,p)	Anionic	0.2263868	3.238154963
203	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	b3lyp/6-311+G(d,p)	Anionic	0.2145572	4.219125437
204	C1=CC2=C3C4=C1C=CC5=C4C6=C(C=C5)C=CC7=C6C3=C(C=C2)C=C7	b3lyp/6-311+G(d,p)	Anionic	0.16957	4.001162234
205	C1=CC=C2C3=C4C(=CC2=C1)C5=CC=CC=C5C6=CC7=CC=CC=C7C(=C64)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.200818	3.406865558
206	C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.1147248	1.77962466
207	C1=CC=C2C=C3C4=CC=CC5=C4C6=C(C=CC=C6C3=CC2=C1)C=C5	b3lyp/6-311+G(d,p)	Anionic	0.162812	3.86211205
208	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C6=CC=CC(=C64)C2=C1	b3lyp/6-311+G(d,p)	Anionic	0.1752988	4.105109729
209	C1=CC=C2C3=C4C(=CC2=C1)C5=CC=CC=C5C6=CC=CC(=C64)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.1818088	3.51271785
210	C1=CC=C2C(=C1)C=C3C=CC4=C5C3=C2C6=CC=CC=C6C5=CC=C4	b3lyp/6-311+G(d,p)	Anionic	0.2059268	3.381286855
211	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC6=CC=CC=C56)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.1660732	2.877876209
212	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=CC6=CC=CC=C6C(=C54)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.225494	3.225093498
213	C1=CC2=C3C4=C1C=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.2176448	4.161437299
214	C1=CC2=C3C(=C1)C=C4C=CC5=C6C4=C3C(=CC6=CC=C5)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.1576288	2.867807996
215	C1=CC=C2C(=C1)C=C3C=CC=C4C3=C2C5=CC=CC6=C5C4=CC=C6	b3lyp/6-311+G(d,p)	Anionic	0.1600592	2.539094451
216	C1=CC=C2C=C3C(=CC2=C1)C=CC4=C3C=CC5=CC6=CC=CC=C6C=C54	b3lyp/6-311+G(d,p)	Anionic	0.1355816	3.126044052
217	C1=CC=C2C(=C1)C3=CC=CC=C3C4=C2C5=CC=CC=C5C6=CC=CC=C64	b3lyp/6-311+G(d,p)	Anionic	0.2570272	3.823199768
218	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.175274	3.481968984
219	C1=CC=C2C=C3C4=C5C(=CC3=CC2=C1)C=CC6=C5C(=CC=C6)C=C4	b3lyp/6-311+G(d,p)	Anionic	0.165044	2.843045635
220	C1=CC=C2C(=C1)C3=CC=CC=C3C4=C2C5=CC=CC6=C5C4=CC=C6	b3lyp/6-311+G(d,p)	Anionic	0.2232744	3.252304884
221	C1=CC=C2C(=C1)C=C3C4=CC=CC=C4C5=C3C2=CC6=CC=CC=C65	b3lyp/6-311+G(d,p)	Anionic	0.2053688	3.241964557
222	C1=CC=C2C(=C1)C=C3C=C4C=CC=CC4=C5C3=C2C6=CC=CC=C65	b3lyp/6-311+G(d,p)	Anionic	0.1808292	2.460997772
223	C1=CC=C2C(=C1)C3=C4C2=CC5=CC=CC6=C5C4=C(C=C6)C=C3	b3lyp/6-311+G(d,p)	Anionic	0.2246136	3.31189782
224	C1=CC=C2C=CC=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.2423952	4.747842672
225	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	b3lyp/6-311+G(d,p)	Anionic	0.1906872	3.849322698
226	C1=CC2=C3C4=C1C=CC5=CC6=C7C8=C(C=CC9=C8C1=C(C=C9)C=C(C3=C1C7=C54)C=C2)C=C6	b3lyp/6-311+G(d,p)	Anionic	0.1215572	2.91597215
227	C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.1355568	2.190516593
228	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3C5=CC=CC=C5C=C4	b3lyp/6-311+G(d,p)	Anionic	0.30752	4.209057225
229	C1CC2=C(C3=CC=CC=C3C=C2)C4=C1C=CC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Anionic	37.411792	3.923881897
230	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC5=CC=CC=C5C=C43	b3lyp/6-311+G(d,p)	Anionic	0.1695948	3.477615162
231	C1=CC=C2C(=C1)C=CC3=C2C4=CC=CC=C4C5=CC=CC=C35	b3lyp/6-311+G(d,p)	Anionic	0.2394192	4.051503298
232	C1=CC=C2C(=C1)C=CC3=CC4=C(C=C32)C5=CC=CC=C5C=C4	b3lyp/6-311+G(d,p)	Anionic	0.1694212	3.887418639
233	C1=CC=C2C=C3C(=CC2=C1)C=CC4=CC5=CC=CC=C5C=C43	b3lyp/6-311+G(d,p)	Anionic	0.2502568	3.748640569
234	C1=CC2=C3C(=C1)C4=CC=CC5=C4C(=CC=C5)C3=CC=C2	b3lyp/6-311+G(d,p)	Anionic	0.1690244	2.985361185
235	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	b3lyp/6-311+G(d,p)	Anionic	0.3118476	4.68144689
236	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3C=CC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Anionic	0.2766688	4.206880314
237	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.213962	3.810138302
238	C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.1621176	2.751887491
239	C1=CC2=CC3=C4C5=C(C=C3)C=C6C=CC7=C8C6=C5C9=C3C4=C2C2=C1C=CC1=CC4=C(C3=C12)C1=C(C=C4)C=C(C8=C19)C=C7	b3lyp/6-311+G(d,p)	Anionic	0.1439392	2.520318594
240	C1=CC=C2C(=C1)C3=CC=CC=C3C4=CC=CC=C24	b3lyp/6-311+G(d,p)	Anionic	0.2497732	4.839000816
362	C1=CC2=C(C=CC3=C2C=CC4=C3SC=C4)C5=C1C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2895152	4.358447735
363	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Anionic	0.2516456	4.273003982
364	C1=CC=C2C=C3C(=CC2=C1)C4=C(C5=C3SC=C5)SC=C4	b3lyp/6-311+G(d,p)	Anionic	0.1844252	3.515983217
365	C1=CC=C(C(=C1)C#CC2=CC=CS2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	Anionic	1.96416	3.627277787
366	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Anionic	0.2094236	4.397632131
367	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.2613176	4.103204932

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
368	C1=CSC2=CC3=CC4=C(C=C5C=CSC5=C4)C=C3C=C21	b3lyp/6-311+G(d,p)	Anionic	0.1624524	2.748077897
369	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Anionic	0.2608092	4.022659229
370	C1=CC2=C3C=CSC4=CC=CC(=C34)C5=C2C(=C1)SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.1811888	2.354601252
371	C1=CC2=CC3=CC4=CC5=CSSC5=CC4=CC3=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.2593832	1.373358664
372	C1=CC=C2C(=C1)C=C3C=C4C=CC=CC4=C5C3=C2SS5	b3lyp/6-311+G(d,p)	Anionic	0.1471756	2.338002306
373	C1=CC2=C(C=CS2)C3=CC4=C(C=C31)C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.220224	3.535303301
374	C1=CC2=C(C=C3C=CSC3=C2)C4=C1C=C5C(=C4)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2634628	3.8846975
375	C1=CC=C2C(=C1)C=CC3=C2SC4=C3SC5=CC=CC=C54	b3lyp/6-311+G(d,p)	Anionic	0.2340252	4.081707937
376	C1=CC=C2C=C3C(=CC2=C1)C4=C(S3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Anionic	0.2249732	3.62891047
377	C1=CC2=CC3=C(C=CC4=C3SC=C4)C=C2C5=C1C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.1605552	3.502921751
378	C1=CC=C2C(=C1)C=CC3=C2C4=C(S3)C5=CC=CC=C5S4	b3lyp/6-311+G(d,p)	Anionic	0.2499096	3.921432872
379	C1=CC2=C(C=CC3=C2C=CS3)C4=C1C5=C(C=C4)SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.2883248	4.153001769
380	C#CC1=CC(=C(C=C1C2=CC=CS2)C#C)C3=CC=CS3	b3lyp/6-311+G(d,p)	Anionic	1.0342716	3.863744733
381	C1=CC=C2C(=C1)C3=C(S2)C=C4C=C5C(=CC4=C3)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.1813996	3.467819063
382	C1=CC2=C(C=CC3=C2C=CC4=C3C=CS4)C5=C1C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2894532	4.245792596
383	C1=CC=C2C(=C1)C=C(S2)C#CC3=CC4=CC=CC=C4S3	b3lyp/6-311+G(d,p)	Anionic	10.0116236	3.589181846
384	C1=CC2=CC3=C(C=C2C4=C1C=CS4)C5=C(C=C3)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.1576412	3.506187118
385	C1=CC=C2C(=C1)SC3=C(S2)C4=CC=CC5=C4C3=CC=C5	b3lyp/6-311+G(d,p)	Anionic	0.2880644	3.034885908
386	C#CC1=CC(=C(C=C1C2=CSC=C2)C#C)C3=CSC=C3	b3lyp/6-311+G(d,p)	Anionic	6.0705316	4.195179418
387	[2H]C1=CC2=C(C=CS2)C3=CC4=C(C=C13)C5=C(C=C4[2H])SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.220224	3.535303301
388	[2H]C#CC1=CC(=C(C=C1C2=CSC=C2)C#C[2H])C3=CSC=C3	b3lyp/6-311+G(d,p)	Anionic	5.5174792	4.195179418
389	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CC5=C4SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.2292636	4.101844363
390	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2461896	4.092592491
391	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C5=C(C=C4)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2365052	4.209601452
392	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C5=C(C=C4)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2594824	4.058850372
393	C1=CC=C2C(=C1)C3=C(S2)C=C4C(=C3)C=CC5=C4SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.1945808	3.851771723
394	C1=CC=C2C(=C1)C3=C(S2)C=C4C(=C3)C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2008676	3.906738723
395	C1=CC=C2C(=C1)C3=C4C(=CC=C3)SC5=CC=CC(=C54)S2	b3lyp/6-311+G(d,p)	Anionic	0.3219536	4.237084952
396	[2H]C1=C2C(=CC=C1)C3=C4C(=CC=C3)SC5=CC=CC(=C54)S2	b3lyp/6-311+G(d,p)	Anionic	0.3220156	4.237084952
397	C1=CC=C2C=C3C(=CC2=C1)C4=C(C=CS4)C5=C3SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.1580504	3.492037197
398	C1=CC2=C(C3=CSC=C3C=C2)C4=C1C=CC5=CSC=C54	b3lyp/6-311+G(d,p)	Anionic	0.2428788	3.737756015
399	C1=CC2=C(C3=C(C=C2)SC=C3)C4=C1C=CC5=C4C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2768548	4.239533977
400	C1=CC2=C3C=CC=C4C3=C(C=CS4)C5=C2C(=C1)SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.592224	3.111894131
401	C1=CC(=CC(=C1)C#CC2=CC=CS2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	Anionic	5.83668	3.905378154
402	C1=CC2=CC3=C(C=C2C4=CC5=C(C=CS5)C=C41)SC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2287428	3.974222961
403	C1=CC=C2C(=C1)C=CC3=C2C=CC4=C3SC5=C4SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.2181532	4.255044467
404	C#CC1=C(C=CS1)C2=CC=C(C=C2)C3=C(SC=C3)C#C	b3lyp/6-311+G(d,p)	Anionic	10.7060608	4.084156962
405	C1=CC(=CC(=C1)C#CC2=CSC=C2)C#CC3=CSC=C3	b3lyp/6-311+G(d,p)	Anionic	13.6600012	4.190825596
406	C1=CC(=CC=C1C#CC2=CSC=C2)C#CC3=CSC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2336656	3.712993653
407	C1=CC=C2C(=C1)C=CC3=C2C4=C(C=CS4)C5=C3SC=C5	b3lyp/6-311+G(d,p)	Anionic	0.1995904	4.096402085
408	C1=CC=C2C=C3C=C4C(=CC3=CC2=C1)C5=C(S4)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.1639404	3.038423388
409	C1=CC=C(C=C1)C#CC2=CC3=C(S2)C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	Anionic	2.548262	3.683605356
410	C1=CC2=C(C=C3C=CSC3=C2)C4=CC5=C(C=CS5)C=C41	b3lyp/6-311+G(d,p)	Anionic	0.2631652	4.041707199
411	C1=CC2=C(C=CS2)C3=CC4=C(C=C31)C=C5C=CSC5=C4	b3lyp/6-311+G(d,p)	Anionic	0.1840656	3.136384379
412	C#CC1=CC(=C(C=C1C2=CSC=C2)C3=CSC=C3)C#C	b3lyp/6-311+G(d,p)	Anionic	0.3195356	4.286609675
413	C1=CC2=C(C=CS2)C3=CC4=C(C=CC5=C4C=CS5)C=C31	b3lyp/6-311+G(d,p)	Anionic	0.2083572	3.569861762

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
414	C1=CC2=CSC=C2C3=CC4=C(C=CC5=CSC=C54)C=C31	b3lyp/6-311+G(d,p)	Anionic	0.1496556	3.740749267
415	C1=CC2=CC3=CSC=C3C=C2C4=CC5=CSC=C5C=C41	b3lyp/6-311+G(d,p)	Anionic	0.182962	3.207133983
416	C1=CC2=CSC=C2C3=CC4=C(C=C31)C5=CSC=C5C=C4	b3lyp/6-311+G(d,p)	Anionic	0.1811516	3.672992915
417	C1=CC2=C(C=CC3=C2C=CC4=CSC=C43)C5=CSC=C51	b3lyp/6-311+G(d,p)	Anionic	0.2625204	3.861567822
418	C1=CC=C(C=C1)C#CC2=CC3=C(S2)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	Anionic	0.2927888	3.569589648
419	C1=CC=C2C=C3C(=CC2=C1)C=CC4=C3C5=C(S4)C=CS5	b3lyp/6-311+G(d,p)	Anionic	0.2006692	3.38727336
420	C1=CC2=C3C4C1C5=CSC=C5C4=CC=C3C6=CSC=C26	b3lyp/6-311+G(d,p)	Anionic	71.1481124	2.724403991
421	C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC5=C4C(=CC=C5)S3	b3lyp/6-311+G(d,p)	Anionic	0.269018	3.28087684
515	C1=CC=C2C(=C1)C3=C(S2)C4=CC=CC=C4S3	b3lyp/6-311+G(d,p)	Anionic	0.2881264	4.234363814
516	C1=CC2=C(C=CC3=C2SC=C3)C4=C1C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2149168	4.420217582
517	C1=CC2=C3C(=C1)SSC4=CC=CC(=C43)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.3128644	3.888234981
518	C1=CC=C2C3=C4C(=CC=C3)SSC4=CC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.2900608	3.379382058
519	C1=CSC2=CC3=C(C=C21)C=C4C(=C3)C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2112836	3.438430766
520	C1=CC=C2C3=C(C4=C(C2=C1)C=CS4)SC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2485952	4.230009992
521	C1=CC2=C3C(=CC=C4C3=C1C=CS4)C=CS2	b3lyp/6-311+G(d,p)	Anionic	0.2691544	3.062913636
522	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)SC=C4	b3lyp/6-311+G(d,p)	Anionic	0.216008	4.569608092
523	C1=CC2=CC3=C4C(=CC=CS4)SC3=C2C=C1	b3lyp/6-311+G(d,p)	Anionic	0.3686148	1.619349595
524	C1=CC=C2C(=C1)C3=C(C4=C2SC=C4)SC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2411428	4.345658383
525	C1=CC=C2C(=C1)C(=S)C3=CC=CC=C3C2=S	b3lyp/6-311+G(d,p)	Anionic	0.2611936	2.456099723
526	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3SC=C4	b3lyp/6-311+G(d,p)	Anionic	0.273668	4.492871983
527	C1=CC=C2C(=C1)C=C(S2)C#CC3=CSC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2887464	3.961161496
528	C1=CC=C2C(=C1)C3=C(S2)SC4=CC=CC=C43	b3lyp/6-311+G(d,p)	Anionic	0.2128708	4.666752741
529	C1=CC=C2C(=C1)C=C(S2)C#CC3=CC=CS3	b3lyp/6-311+G(d,p)	Anionic	0.2880892	3.721157069
530	C1=CC2=C(C=CS2)C3=C1C4=C(C=C3)SC=C4	b3lyp/6-311+G(d,p)	Anionic	0.283526	4.274092438
531	C1=CSC2=CC3=C(C=C21)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	Anionic	0.1984124	3.478703618
532	C1=CC2=C3C(=CC=C4C3=C1C=CS4)SC=C2	b3lyp/6-311+G(d,p)	Anionic	0.273358	2.889032878
533	C1=CC2=C(C3=C1C=CC4=C3SC=C4)SC=C2	b3lyp/6-311+G(d,p)	Anionic	0.2114076	4.584302241
534	C1=CC=C2C(=C1)C=CC3=C2C4=C(S3)SC=C4	b3lyp/6-311+G(d,p)	Anionic	0.2485456	4.35735928
535	C1=C/C(=C\2/C=CC3=C2SC=C3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.3368708	2.861549378
536	C1=CC=C2C(=C1)C3=CSC(=C23)C4=CC=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2708656	3.845513104
537	C1=CSC(=C1)C#C/C=C\C#CC2=CC=CS2	b3lyp/6-311+G(d,p)	Anionic	3.1184636	3.231624231
538	C1=CC=C2C(=C1)C3=C(S2)C=C4C=CSC4=C3	b3lyp/6-311+G(d,p)	Anionic	0.2504924	4.159804615
539	C#CC1=C(SC2=CC=CC=C21)C3=CC=CS3	b3lyp/6-311+G(d,p)	Anionic	4.0064276	3.751633822
540	C1=CC=C2C(=C1)C(=C3C=CC=CC3=C2[S-])[S-]	b3lyp/6-311+G(d,p)	Anionic	0.2614044	2.456371836
541	C1=CC2=C3C(=C1)C4=C(C3=CC=C2)SC=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2793224	2.88848865
542	C1=C/C(=C/2\C=CC3=C2SC=C3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.3430584	2.942367195
543	C1=CC=C2C=C3C(=CC2=C1)C4=C(S3)C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2100064	3.797348951
544	C1=CC=C2C(=C1)C3=C(S2)C4=C(C=C3)C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2705184	4.427564656
545	C1=CC=C2C(=C1)C3=C(S2)C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2579944	4.378584161
546	C1=CC2=C(C=CS2)C3=C1C=CC4=C3C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.2483472	4.41232628
547	C\1=CC2=C(/C1=C/3\C=CC4=C3C=CS4)C=CS2	b3lyp/6-311+G(d,p)	Anionic	0.414408	2.871073363
548	C1=CC=C2C(=C1)C3=CSC=C3C4=CSC=C24	b3lyp/6-311+G(d,p)	Anionic	0.1420048	4.489334503
549	C1=CC2=C(C3=C1C=CC4=C3C=CS4)SC=C2	b3lyp/6-311+G(d,p)	Anionic	0.245644	4.305113418
550	C1=C/C(=C\2/C=CC3=C2C=CS3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.3724836	2.856923442
551	C1=CC=C2C(=C1)C3=CC=CC=C3C2=C([S-])[S-]	b3lyp/6-311+G(d,p)	Anionic	0.174034	2.188067568
552	C\1=CC2=C(/C1=C\3/C=CC4=C3C=CS4)C=CS2	b3lyp/6-311+G(d,p)	Anionic	0.5758188	2.889849219

	SMILES	Functional/Basis Set	Transition	Reorganisation Energy/eV	HOMO-LUMO gap
553	C1=C/C(=C/2\C=CC3=C2C=CS3)/C4=C1C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.3787332	2.858011897
554	C1=CC(=C2C=CC(=C3C=CC#S3)C=C2)S#C1	b3lyp/6-311+G(d,p)	Anionic	0.4013012	1.545062511
555	C1=CC=C2C(=C1)C3=C(S2)C=CC4=CSC=C43	b3lyp/6-311+G(d,p)	Anionic	0.25327	3.70782349
556	C1=CC=C2C(=C1)C3=C(C=CS3)C4=C2SC=C4	b3lyp/6-311+G(d,p)	Anionic	0.1731908	4.421850265
557	C1=CC=C2C(=C1)C3=C(S2)C4=CSC=CC4=C3	b3lyp/6-311+G(d,p)	Anionic	0.3328408	3.187269671
558	C1=CC=C2C(=C1)C3=CC4=CC=CSC4=C3S2	b3lyp/6-311+G(d,p)	Anionic	0.2778096	2.63487853
559	C1=CC2=C(C=CC3=CSC=C32)C4=CSC=C41	b3lyp/6-311+G(d,p)	Anionic	0.1983628	3.412035721
560	C1=CC2=CSC=C2C3=C1C=CC4=CSC=C43	b3lyp/6-311+G(d,p)	Anionic	0.1637792	3.367681162
561	C1=CC2=CC3=C4C(=CSS4)C=CC3=C2C=C1	b3lyp/6-311+G(d,p)	Anionic	0.2637108	1.640846591
562	C1=CC2=C(C=C3C=CSC3=C2)C4=C1C=CS4	b3lyp/6-311+G(d,p)	Anionic	0.1977552	3.924154011
593	C1=CSC2=CC3=C(C=C21)SC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2929748	4.296405774
594	C1=CC2=C3C(=C1)SSC3=CC=C2	b3lyp/6-311+G(d,p)	Anionic	0.2134412	3.351898558
595	C1=CSC2=CC3=C(C=CS3)C=C21	b3lyp/6-311+G(d,p)	Anionic	0.251658	4.482531656
596	C1=CC2=CSC=C2C3=CSC=C31	b3lyp/6-311+G(d,p)	Anionic	0.3487624	4.38348221
597	C1=CC=C2C(=C1)C3=C(S2)SC=C3	b3lyp/6-311+G(d,p)	Anionic	0.2564692	4.963084737
598	C1=CC2=C(C3=C1C=CS3)SC=C2	b3lyp/6-311+G(d,p)	Anionic	0.2930368	4.715733236
599	C1=CC=C2C(=C1)C3=C(S2)C=CS3	b3lyp/6-311+G(d,p)	Anionic	0.2995344	4.623758751
600	C1=CC2=C(C=CS2)C3=C1C=CS3	b3lyp/6-311+G(d,p)	Anionic	0.3261324	4.879817895
601	C1=CC2=C(C=CS2)C3=C1SC=C3	b3lyp/6-311+G(d,p)	Anionic	0.3090824	4.601717528
602	C1=CC(=S)C=C2C1=CC(=S)C=C2	b3lyp/6-311+G(d,p)	Anionic	0.2937808	1.993506156
603	C1=CC=C2C(=C1)C=CC(=S)C2=S	b3lyp/6-311+G(d,p)	Anionic	0.4457304	2.148338944
604	C1=CC=C2C(=S)C=CC(=S)C2=C1	b3lyp/6-311+G(d,p)	Anionic	0.3226356	2.342900356
605	C=C1C2=C(C3=C1C=CS3)SC=C2	b3lyp/6-311+G(d,p)	Anionic	0.4044756	3.518976469
606	C1=CSC2=CC3=CSC=C3C=C21	b3lyp/6-311+G(d,p)	Anionic	0.2290404	3.294482533
607	C1=CC2=C(C=CS2)C3=CSC=C31	b3lyp/6-311+G(d,p)	Anionic	0.2742508	3.918983847
608	C1=CC2=C3C=CC=C3SSC2=C1	b3lyp/6-311+G(d,p)	Anionic	0.4723904	2.329294663
624	C1=CSC2=C1SC=C2	b3lyp/6-311+G(d,p)	Anionic	0.3677964	5.059957272
625	C1=CC(=S)C=CC1=S	b3lyp/6-311+G(d,p)	Anionic	0.3362508	2.16357732
626	C1=CC(=S)C(=S)C=C1	b3lyp/6-311+G(d,p)	Anionic	0.2937932	1.786971735
627	[2H]C1=C(SC2=C1SC(=C2[2H])[2H])[2H]	b3lyp/6-311+G(d,p)	Anionic	0.3682676	5.059957272
628	C1=C2C=S=CC2=CS1	b3lyp/6-311+G(d,p)	Anionic	0.2594824	2.993252487