

	SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation	DUSHIN Reorganisation	Difference (4-point & Difference Percentage (4-	
						Energy	Energy	DUSHIN)	point & DUSHIN)
0	C1=CC=CC=C1	B3LYP	6-31G	COS1	6.855908765	0.281382496	0.276931106	0.00445139	1.582
1	C1=CC=CC=C1	B3LYP	6-31G	C1S0	6.855908765	0.300064228	0.299111879	0.00095235	0.317
2	C1=CC=CC=C1	B3LYP	6-31G	C-1S0	6.855908765	0.392677501	0.393439057	-0.000761556	-0.194
3	C1=CC=CC=C1	B3LYP	6-311+G(d,p)	COS1	6.597672709	0.260298053	0.255990174	0.004307878	1.655
4	C1=CC=CC=C1	B3LYP	6-311+G(d,p)	C1S0	6.597672709	0.293965449	0.293854949	0.000110501	0.038
5	C1=CC=CC=C1	B3LYP	6-311+G(d,p)	C-1S0	6.597672709	0.004218309	0.002182122	0.002036187	48.270
6	C1=CC=CC=C1	B3LYP	6-311+G(2d,p)	COS1	6.611006288	0.261824856	0.25987088	0.001953977	0.746
7	C1=CC=CC=C1	B3LYP	6-311+G(2d,p)	C1S0	6.611006288	0.292792638	0.297004147	-0.004211509	-1.438
8	C1=CC=CC=C1	B3LYP	6-311+G(2d,p)	C-1S0	6.611006288	0.004175778	0.002058138	0.00211764	50.712
9	C1=CC=CC=C1	CAM-B3LYP	6-31G	COS1	9.71092741	0.274877396	0.271240231	0.003637166	1.323
10	C1=CC=CC=C1	CAM-B3LYP	6-31G	C1S0	9.71092741	0.32816793	0.327417471	0.000750459	0.229
11	C1=CC=CC=C1	CAM-B3LYP	6-31G	C-1S0	9.71092741	0.411856467	0.41373527	-0.001878803	-0.456
12	C1=CC=CC=C1	CAM-B3LYP	6-311+G(d,p)	COS1	9.332689141	0.257088279	0.252630203	0.004458077	1.734
13	C1=CC=CC=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	9.332689141	0.316271003	0.317052392	-0.000781389	-0.247
14	C1=CC=CC=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	9.332689141	0.355935898	0.359219418	-0.00328352	-0.923
15	C1=CC=CC=C1	CAM-B3LYP	6-311+G(2d,p)	COS1	9.343301581	0.259256755	0.257725953	0.001530801	0.590
16	C1=CC=CC=C1	CAM-B3LYP	6-311+G(2d,p)	C1S0	9.343301581	0.319722768	0.322098549	-0.002375781	-0.743
17	C1=CC=CC=C1	CAM-B3LYP	6-311+G(2d,p)	C-1S0	9.343301581	0.358548083	0.364129192	-0.00558111	-1.557
36	C1=CC=CC=C1	B3LYP	cc-pVDZ	C1S0	6.711960531	0.291691176	0.29117689	0.000514286	0.176
37	C1=CC=CC=C1	B3LYP	cc-pVDZ	COS1	6.711960531	0.268359752	0.263887968	0.004471785	1.666
38	C1=CC=CC=C1	CAM-B3LYP	cc-pVDZ	COS1	9.543033156	0.263384178	0.260094051	0.003290126	1.249
39	C1=CC=CC=C1	CAM-B3LYP	cc-pVDZ	C1S0	9.543033156	0.314131753	0.315180231	-0.001048478	-0.334
40	C1=CC=CC=C1	CAM-B3LYP	cc-pVDZ	C-1S0	9.543033156	0.42543748	0.42809264	-0.002655161	-0.624
41	C1=CC=CC=C1	B3LYP	STO-3G	COS1	7.657828317	0.395435674	0.390004694	0.00543098	1.373
42	C1=CC=CC=C1	CAM-B3LYP	STO-3G	COS1	10.70577569	0.386016562	0.380569497	0.005447065	1.411
43	C1=CC=CC=C1	CAM-B3LYP	STO-3G	C1S0	10.70577569	0.541853695	0.54194733	-9.36349E-05	-0.017
44	C1=CC=CC=C1	CAM-B3LYP	STO-3G	C-1S0	10.70577569	0.501498365	0.501416895	8.14702E-05	0.016
47	C1=CC=CC=C1	B3LYP	cc-pVTZ	COS1	6.700531749	0.268911137	0.264445897	0.00446524	1.660
48	C1=CC=CC=C1	B3LYP	cc-pVTZ	C1S0	6.700531749	0.297823997	0.297698459	0.000125538	0.042
49	C1=CC=CC=C1	B3LYP	cc-pVTZ	C-1S0	6.700531749	0.391486568	0.393029909	-0.001543341	-0.394
50	C1=CC=CC=C1	CAM-B3LYP	cc-pVTZ	C1S0	9.499494938	0.327597525	0.327603447	-5.92216E-06	-0.002
51	C1=CC=CC=C1	CAM-B3LYP	cc-pVTZ	C-1S0	9.499494938	0.421386003	0.423133272	-0.001747269	-0.415
52	C1=CC=CC=C1	CAM-B3LYP	AUG-cc-pVTZ	C1S0	8.812951663	0.326490321	0.327615846	-0.001125525	-0.345
53	C1=CC=CC=C1	CAM-B3LYP	AUG-cc-pVTZ	C-1S0	8.812951663	0.001295235	0.001388623	-9.33882E-05	-7.210
54	C1=CC=CC=C1	B3LYP	STO-4G	COS1	7.565309604	0.378805245	0.373080851	0.005724394	1.511
55	C1=CC=CC=C1	B3LYP	STO-4G	C1S0	7.565309604	0.510019012	0.501912832	0.00810618	1.589
56	C1=CC=CC=C1	B3LYP	STO-4G	C-1S0	7.565309604	0.447936371	0.452467934	-0.004531563	-1.012
57	C1=CC=CC=C1	B3LYP	STO-6G	COS1	7.560139441	0.385156274	0.382392065	0.002764209	0.718
58	C1=CC=CC=C1	B3LYP	STO-6G	C1S0	7.560139441	0.503668446	0.504541297	-0.000872851	-0.173
59	C1=CC=CC=C1	B3LYP	STO-6G	C-1S0	7.560139441	0.451550641	0.457538887	-0.005988246	-1.326
60	C1=CC=CC=C1	CAM-B3LYP	STO-4G	COS1	10.61162429	0.369589756	0.363732443	0.005857313	1.585
61	C1=CC=CC=C1	CAM-B3LYP	STO-4G	C1S0	10.61162429	0.534356822	0.532164976	0.002191845	0.410
62	C1=CC=CC=C1	CAM-B3LYP	STO-4G	C-1S0	10.61162429	0.491579407	0.481083487	0.01049592	2.135
63	C1=CC=CC=C1	CAM-B3LYP	STO-6G	COS1	10.60890316	0.376519761	0.374072725	0.002447036	0.650
64	C1=CC=CC=C1	CAM-B3LYP	STO-6G	C1S0	10.60890316	0.542687669	0.543819491	-0.001131822	-0.209
65	C1=CC=CC=C1	CAM-B3LYP	STO-6G	C-1S0	10.60890316	0.486354113	0.486699971	-0.000345858	-0.071
138	C1=CC=CC=C1	B3LYP	AUG-cc-pVTZ	COS1	6.614815883	0.260134295	0.257998718	0.002135576	0.821
139	C1=CC=CC=C1	B3LYP	cc-pVDZ	C-1S0	6.711960531	0.396208187	0.396427076	-0.001218889	-0.308
140	C1=CC=CC=C1	B3LYP	AUG-cc-pVTZ	C1S0	6.614815883	0.296366745	0.29737361	-0.001009355	-0.341
141	C1=CC=CC=C1	CAM-B3LYP	cc-pVTZ	COS1	9.499494938	0.26369885	0.259040186	0.004658664	1.767

SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation Energy	DUSHIN Reorganisation Energy	Difference (4-point & DUSHIN)	Difference Percentage (4- point & DUSHIN)
142 C1=CC=CC=C1	CAM-B3LYP	AUG-cc-pVTZ	COS1	8.812951663	0.25708466	0.254564356	0.002520304	0.980
18 C1=CC=C2C=CC=CC2=C1	B3LYP	6-31G	COS1	4.86321895	0.546883339	0.551196551	-0.004313212	-0.789
19 C1=CC=C2C=CC=CC2=C1	B3LYP	6-31G	C1S0	4.86321895	0.18573714	0.186373047	-0.000635907	-0.342
20 C1=CC=C2C=CC=CC2=C1	B3LYP	6-31G	C-1S0	4.86321895	0.251026834	0.249580191	0.001446643	0.576
21 C1=CC=C2C=CC=CC2=C1	B3LYP	6-311+G(d,p)	COS1	4.746754217	0.555239819	0.559689468	-0.004449649	-0.801
22 C1=CC=C2C=CC=CC2=C1	B3LYP	6-311+G(d,p)	C1S0	4.746754217	0.185750855	0.187439311	-0.001688457	-0.909
23 C1=CC=C2C=CC=CC2=C1	B3LYP	6-311+G(d,p)	C-1S0	4.746754217	0.243364461	0.243529762	-0.000165301	-0.068
24 C1=CC=C2C=CC=CC2=C1	B3LYP	6-311+G(2d,p)	COS1	4.757366657	0.569287044	0.576501726	-0.007214681	-1.267
25 C1=CC=C2C=CC=CC2=C1	B3LYP	6-311+G(2d,p)	C1S0	4.757366657	0.187509989	0.188418786	-0.000908797	-0.485
26 C1=CC=C2C=CC=CC2=C1	B3LYP	6-311+G(2d,p)	C-1S0	4.757366657	0.24805614	0.251700321	-0.003644181	-1.469
27 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-31G	COS1	7.470886094	0.276803228	0.275666467	0.001136761	0.411
28 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-31G	C1S0	7.470886094	0.243929533	0.246108634	-0.002179101	-0.893
29 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-31G	C-1S0	7.470886094	0.309091742	0.309700129	-0.000608387	-0.197
30 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-311+G(d,p)	COS1	7.301631271	0.274849559	0.273558735	0.001290824	0.470
31 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	7.301631271	0.246068375	0.24653018	-0.000461805	-0.188
32 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	7.301631271	0.302716277	0.302099898	0.000616379	0.204
33 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	COS1	7.313604281	0.27813049	0.281047381	-0.00291689	-1.049
34 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C1S0	7.313604281	0.25004151	0.251997883	-0.001956373	-0.782
35 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C-1S0	7.313604281	0.307691444	0.310865581	-0.003174137	-1.032
45 C1=CC=C2C=CC=CC2=C1	B3LYP	cc-pVDZ	C1S0	4.7758704	0.18254802	0.183571004	-0.001022984	-0.560
46 C1=CC=C2C=CC=CC2=C1	B3LYP	cc-pVDZ	C-1S0	4.7758704	0.256816329	0.255729808	0.001086521	0.423
66 C1=CC=C2C=CC=CC2=C1	B3LYP	cc-pVTZ	C1S0	4.793285687	0.188341487	0.188579966	-0.000238478	-0.127
67 C1=CC=C2C=CC=CC2=C1	B3LYP	cc-pVTZ	C-1S0	4.793285687	0.261778488	0.260726371	0.001052117	0.402
68 C1=CC=C2C=CC=CC2=C1	B3LYP	AUG-cc-pVTZ	C-1S0	4.758455113	0.240533906	0.24143443	-0.000900524	-0.374
69 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	cc-pVDZ	COS1	7.372925103	0.270145881	0.26920689	0.000938991	0.348
70 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	cc-pVDZ	C1S0	7.372925103	0.243011911	0.245265541	-0.002253631	-0.927
71 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	cc-pVDZ	C-1S0	7.372925103	0.317893183	0.318205445	-0.000312262	-0.098
72 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	cc-pVTZ	C1S0	7.375918356	0.250480402	0.251489548	-0.001009146	-0.403
73 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	cc-pVTZ	C-1S0	7.375918356	0.322917711	0.322656478	0.000261233	0.081
74 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-3G	COS1	5.445814729	0.315813988	0.313680022	0.002133966	0.676
75 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-3G	C1S0	5.445814729	0.318955815	0.319321303	-0.000365488	-0.115
76 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-3G	C-1S0	5.445814729	0.311005818	0.310877979	0.000127839	0.041
77 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-4G	COS1	5.378058378	0.304616748	0.302831405	0.001785343	0.586
78 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-4G	C1S0	5.378058378	0.31386998	0.31432474	-0.00045476	-0.145
79 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-4G	C-1S0	5.378058378	0.299951083	0.300463306	-0.000512223	-0.171
80 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-6G	COS1	5.378330492	0.310094753	0.310840784	-0.00074603	-0.241
81 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-6G	C1S0	5.378330492	0.319124934	0.321267855	-0.002142921	-0.671
82 C1=CC=C2C=CC=CC2=C1	B3LYP	STO-6G	C-1S0	5.378330492	0.304051948	0.3060054	-0.001953452	-0.642
83 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-3G	COS1	8.243145235	0.408017294	0.407734435	0.000282859	0.069
84 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-3G	C1S0	8.243145235	0.415753573	0.417839147	-0.002085574	-0.502
85 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-3G	C-1S0	8.243145235	0.411315804	0.413611286	-0.002295482	-0.558
86 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-4G	COS1	8.172939859	0.395941752	0.396538662	-0.00059691	-0.151
87 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-4G	C1S0	8.172939859	0.410313228	0.412978966	-0.002665739	-0.650
88 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-4G	C-1S0	8.172939859	0.398149983	0.400816117	-0.002666134	-0.670
89 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-6G	COS1	8.175660998	0.402306223	0.405167962	-0.002861739	-0.711
90 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-6G	C1S0	8.175660998	0.416456117	0.420579198	-0.004123081	-0.990
91 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	STO-6G	C-1S0	8.175660998	0.403282377	0.407139311	-0.003856934	-0.956
146 C1=CC=C2C=CC=CC2=C1	B3LYP	cc-pVTZ	COS1	4.793285687	0.577827746	0.58258935	-0.004761604	-0.824
147 C1=CC=C2C=CC=CC2=C1	B3LYP	AUG-cc-pVTZ	COS1	4.758455113	0.566389413	0.572720208	-0.006330795	-1.118
148 C1=CC=C2C=CC=CC2=C1	B3LYP	AUG-cc-pVTZ	C1S0	4.758455113	0.187259944	0.188307201	-0.001047257	-0.559

SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation Energy	DUSHIN Reorganisation Energy	Difference (4-point & DUSHIN)	Difference Percentage (4-point & DUSHIN)
149 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	cc-pVTZ	COS1	7.375918356	0.277154309	0.27712948	2.48289E-05	0.009
150 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	AUG-cc-pVTZ	COS1	7.312243712	0.275233512	0.27658395	-0.001350438	-0.491
151 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	AUG-cc-pVTZ	C1S0	7.312243712	0.249436138	0.251191986	-0.001755848	-0.704
152 C1=CC=C2C=CC=CC2=C1	CAM-B3LYP	AUG-cc-pVTZ	C-1S0	7.312243712	0.301971638	0.303538115	-0.001566477	-0.519
92 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-31G	C1S0	3.621019168	0.1364097	0.13684136	-0.00043166	-0.316
93 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-31G	C-1S0	3.621019168	0.190755246	0.189385863	0.001369383	0.718
94 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C1S0	3.549725336	0.138350933	0.138081202	0.000269731	0.195
95 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C-1S0	3.549725336	0.196507624	0.19568426	0.000823364	0.419
96 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C1S0	3.554623385	0.140648308	0.140784057	-0.000135749	-0.097
97 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C-1S0	3.554623385	0.198471361	0.198325124	0.000146238	0.074
98 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-31G	COS1	6.030859534	0.549204878	0.554060586	-0.004855708	-0.884
99 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-31G	C1S0	6.030859534	0.196469474	0.197791992	-0.001322518	-0.673
100 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-31G	C-1S0	6.030859534	0.251621784	0.251563939	5.78453E-05	0.023
101 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	5.935075454	0.202347242	0.202453798	-0.000106555	-0.053
102 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	5.935075454	0.260698822	0.259697302	0.00100152	0.384
103 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C1S0	5.941061959	0.205247105	0.206098933	-0.000851828	-0.415
104 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C-1S0	5.941061959	0.262833773	0.262747313	8.64597E-05	0.033
105 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	cc-pVDZ	C1S0	3.554351271	0.136417183	0.13715132	-0.000734137	-0.538
106 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	cc-pVDZ	C-1S0	3.554351271	0.197881582	0.197283656	0.000597925	0.302
107 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	cc-pVTZ	C1S0	3.573399242	0.141349464	0.141242799	0.000106665	0.075
108 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	cc-pVTZ	C-1S0	3.573399242	0.203066113	0.202057048	0.001009065	0.497
109 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C1S0	5.961470499	0.199103917	0.200656027	-0.001552109	-0.780
110 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C-1S0	5.961470499	0.261641316	0.26151987	0.000121446	0.046
111 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-3G	COS1	4.093953061	0.549882318	0.549882318	-0.003992522	-0.731
112 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-3G	C1S0	4.093953061	0.230882544	0.231453702	-0.000571157	-0.247
113 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-3G	C-1S0	4.093953061	0.224955823	0.224113837	0.000841986	0.374
114 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-4G	COS1	4.042523541	0.526470554	0.532016195	-0.005545641	-1.053
115 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-4G	C1S0	4.042523541	0.227168653	0.227634988	-0.000466336	-0.205
116 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-6G	C-1S0	4.044972565	0.221520412	0.223097167	-0.001576754	-0.712
117 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-3G	C1S0	6.682844348	0.331173646	0.333715868	-0.002542223	-0.768
118 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-3G	C-1S0	6.682844348	0.321281001	0.322904446	-0.001623446	-0.505
119 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-4G	COS1	6.628149462	0.730546073	0.742082623	-0.01153655	-1.579
120 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-4G	C1S0	6.628149462	0.326663141	0.329016867	-0.002353727	-0.721
121 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-4G	C-1S0	6.628149462	0.312645712	0.315638972	-0.00299326	-0.957
122 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-6G	COS1	6.63223117	0.737653388	0.748244637	-0.01059125	-1.436
123 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-6G	C1S0	6.63223117	0.329373993	0.33087663	-0.001502637	-0.456
124 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	STO-6G	C-1S0	6.63223117	0.316196553	0.318701382	-0.002504829	-0.792
130 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C-1S0	5.974804078	0.26750956	0.26654123	0.00096833	0.362
154 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-311+G(d,p)	COS1	3.549725336	0.431201314	0.432022939	-0.000821626	-0.191
155 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	COS1	3.554623385	0.441441013	0.443268306	-0.001827293	-0.414
156 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	COS1	5.935075454	0.58270155	0.586879203	-0.004177653	-0.717
157 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	COS1	5.941061959	0.596500499	0.602464017	-0.005963518	-1.000
159 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	cc-pVTZ	COS1	3.573399242	0.444981105	0.446132341	-0.001151236	-0.259
160 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	COS1	3.555439727	0.440153615	0.442573995	-0.00242038	-0.550
161 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	C1S0	3.555439727	0.140523816	0.141019627	-0.000495811	-0.353
162 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	C-1S0	3.555439727	0.196739819	0.197035688	-0.000295869	-0.150
164 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	COS1	5.974804078	0.599724966	0.60486931	-0.005144344	-0.858
165 C1=CC=C2C=C3C=CC=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C1S0	5.974804078	0.205772203	0.206322105	-0.000549901	-0.267
169 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-4G	C-1S0	4.042523541	0.218153275	0.218720524	-0.000567249	-0.260
170 C1=CC=C2C=C3C=CC=CC3=CC2=C1	B3LYP	STO-6G	COS1	4.044972565	0.533009396	0.539926387	-0.006916992	-1.298

SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation Energy	DUSHIN Reorganisation Energy	Difference (4-point & DUSHIN)	Difference Percentage (4- point & DUSHIN)
171 C1=CC=C2C=C3C=C4C=CC3=CC2=C1	B3LYP	STO-6G	C1S0	4.044972565	0.230213471	0.231366913	-0.001153442	-0.501
125 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-31G	C0S1	2.803589125	0.321969884	0.32413189	-0.002162006	-0.671
126 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-31G	C1S0	2.803589125	0.108929873	0.109180485	-0.000250612	-0.230
127 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-31G	C-1S0	2.803589125	0.152007375	0.150764785	0.00124259	0.817
128 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C1S0	5.063766867	0.171715875	0.172573606	-0.000857731	-0.500
131 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C0S1	5.063766867	0.457759736	0.460626094	-0.002866358	-0.626
132 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C-1S0	5.063766867	0.215951575	0.215943278	8.29653E-06	0.004
133 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C0S1	2.745356758	0.334678527	0.335736811	-0.001058284	-0.316
134 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C1S0	2.745356758	0.110742424	0.111288216	-0.000545793	-0.493
135 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C-1S0	2.745356758	0.158819664	0.158203837	0.000615827	0.388
136 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C1S0	5.008255639	0.176753519	0.177904926	-0.001151408	-0.651
137 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C-1S0	5.008255639	0.226442952	0.227052263	-0.00060931	-0.269
173 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C0S1	2.749438466	0.342700552	0.341539271	0.001161281	0.339
174 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C1S0	2.749438466	0.112430074	0.111523786	0.000906287	0.806
175 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C-1S0	2.749438466	0.160469191	0.159022133	0.001447058	0.902
176 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C0S1	2.751071149	0.35156077	0.351817561	-0.000256791	-0.073
177 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C1S0	2.751071149	0.114666768	0.11440022	0.000266548	0.232
178 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C-1S0	2.751071149	0.162789179	0.162282917	0.000506262	0.311
179 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C0S1	4.999275881	0.494074609	0.494510975	-0.000436366	-0.088
180 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	4.999275881	0.17971839	0.178686027	0.001032363	0.574
181 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	4.999275881	0.229153669	0.228031738	0.001121931	0.490
182 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C0S1	5.003085475	0.506496471	0.509190704	-0.002694233	-0.532
183 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C1S0	5.003085475	0.182851373	0.182926286	-7.49138E-05	-0.041
184 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C-1S0	5.003085475	0.231887646	0.230022832	0.001864814	0.099
185 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C0S1	2.761139362	0.352115039	0.351507601	0.000607438	0.173
186 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C1S0	2.761139362	0.114909031	0.114313431	0.0005956	0.518
187 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C-1S0	2.761139362	0.163431667	0.162121738	0.00130993	0.802
188 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	C0S1	2.750526922	0.350099845	0.350391743	-0.000291898	-0.083
189 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	C1S0	2.750526922	0.114314	0.114090259	0.00022374	0.196
190 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	C-1S0	2.750526922	0.161402433	0.161043075	0.000359357	0.223
192 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C0S1	5.021861332	0.506021551	0.507690496	-0.001668945	-0.330
193 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C1S0	5.021861332	0.182819345	0.18250474	0.000314605	0.172
194 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C-1S0	5.021861332	0.231972632	0.231180936	0.000791696	0.341
196 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	AUG-cc-pVTZ	C1S0	5.001180678	0.182026595	0.182058397	-3.18015E-05	-0.017
197 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	AUG-cc-pVTZ	C-1S0	5.001180678	0.229577051	0.229655931	-7.888E-05	-0.034
198 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-3G	C0S1	3.216930082	0.427881008	0.432853633	-0.004972626	-1.162
199 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-3G	C1S0	3.216930082	0.181878538	0.183434622	-0.001556083	-0.856
200 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-3G	C-1S0	3.216930082	0.178053869	0.179107573	-0.001053704	-0.592
201 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-4G	C0S1	3.175296661	0.411270007	0.416363735	-0.005093728	-1.239
202 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-4G	C1S0	3.175296661	0.177808368	0.179082776	-0.001274408	-0.717
203 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-4G	C-1S0	3.175296661	0.172582993	0.174160603	-0.001577611	-0.914
204 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-6G	C0S1	3.176929344	0.414597144	0.41875663	-0.004159487	-1.003
205 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-6G	C1S0	3.176929344	0.179801058	0.180607782	-0.000806724	-0.449
206 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	B3LYP	STO-6G	C-1S0	3.176929344	0.173578304	0.174396173	-0.00081787	-0.471
207 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C0S1	5.650716468	0.631753775	0.640341189	-0.008587415	-1.359
208 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C1S0	5.650716468	0.287094356	0.290631359	-0.003537003	-1.232
209 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C-1S0	5.650716468	0.277001245	0.280613436	-0.003612191	-1.304
210 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C0S1	5.605001339	0.609649204	0.617478503	-0.0078293	-1.284
211 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C1S0	5.605001339	0.281663862	0.284618126	-0.002954264	-1.049
212 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C-1S0	5.605001339	0.26965428	0.273323165	-0.003668886	-1.361

SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation Energy	DUSHIN Reorganisation Energy	Difference (4-point & DUSHIN)	Difference Percentage (4-point & DUSHIN)
213 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	COS1	5.610443616	0.614913546	0.620664897	-0.005751352	-0.935
214 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	C1S0	5.610443616	0.284109512	0.285609999	-0.001500487	-0.528
215 C1=CC=C2C=C3C=C4C=CC=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	C-1S0	5.610443616	0.271655296	0.273806704	-0.002151408	-0.792
216 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	COS1	2.234871152	0.265502312	0.266826393	-0.001324081	-0.499
217 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	C1S0	2.234871152	0.089994912	0.090223301	-0.00022839	-0.254
218 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	C-1S0	2.234871152	0.124291707	0.123178301	0.001113406	0.896
219 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	COS1	2.187251226	0.286782596	0.285362031	0.001420565	0.495
220 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C1S0	2.187251226	0.094391156	0.093174125	0.001217031	1.289
221 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C-1S0	2.187251226	0.133203981	0.131609227	0.001594754	1.197
223 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C1S0	2.185890657	0.096649048	0.096124949	0.000524099	0.542
224 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C-1S0	2.185890657	0.13543194	0.134808019	0.000623921	0.461
225 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	COS1	4.379128389	0.399999949	0.402217138	-0.002217189	-0.554
226 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C1S0	4.379128389	0.1548797	0.155686958	-0.000807258	-0.521
227 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C-1S0	4.379128389	0.19023959	0.190402533	-0.000162943	-0.086
228 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	COS1	4.327970982	0.435572687	0.433027211	0.002545476	0.584
229 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	4.327970982	0.164272472	0.162431698	0.001840774	1.121
230 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	4.327970982	0.203275749	0.200618831	0.002656918	1.307
231 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	COS1	4.330692121	0.448350582	0.449603899	-0.001253316	-0.280
232 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C1S0	4.330692121	0.168086148	0.167775417	0.000310731	0.185
233 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C-1S0	4.330692121	0.207110405	0.206917229	0.000193176	0.093
234 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	COS1	2.180992608	0.279074889	0.280353069	-0.001278181	-0.458
235 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C1S0	2.180992608	0.092858556	0.093335305	-0.000476748	-0.513
236 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C-1S0	2.180992608	0.130697839	0.130071823	0.000626017	0.479
237 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	COS1	2.191332934	0.293098974	0.293086247	0.000912727	0.310
238 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C1S0	2.191332934	0.096530243	0.095703403	0.00082684	0.857
239 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C-1S0	2.191332934	0.134709342	0.133196224	0.001513117	1.123
242 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	AUG-cc-pVTZ	C-1S0	2.184530088	0.133704942	0.132551507	0.001153436	0.863
244 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C1S0	4.330964235	0.161753596	0.162902838	-0.001149243	-0.710
245 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C-1S0	4.330964235	0.200756383	0.201424729	-0.000668346	-0.333
246 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	COS1	4.341848789	0.446269673	0.446367911	-9.82378E-05	-0.022
247 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C1S0	4.341848789	0.167570601	0.166882731	0.00068787	0.410
248 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C-1S0	4.341848789	0.205812803	0.204685513	0.00112729	0.548
252 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	COS1	2.609027713	0.351655629	0.355028752	-0.003373123	-0.959
253 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C1S0	2.609027713	0.147720167	0.149041405	-0.001321238	-0.894
254 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C-1S0	2.609027713	0.144329084	0.144652364	-0.00032328	-0.224
255 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-4G	COS1	2.576646164	0.338196986	0.342307973	-0.004110987	-1.216
256 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-4G	C1S0	2.576646164	0.144276593	0.145619441	-0.001342848	-0.931
257 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-4G	C-1S0	2.576646164	0.140674132	0.142135485	-0.001461353	-1.039
258 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-6G	COS1	2.579367302	0.340503233	0.342828707	-0.002325474	-0.683
259 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-6G	C1S0	2.579367302	0.145198787	0.145445863	-0.000247076	-0.170
260 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	B3LYP	STO-6G	C-1S0	2.579367302	0.141357628	0.141788329	-0.000430702	-0.305
261 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	COS1	4.924716683	0.55784784	0.565975467	-0.008127627	-1.457
262 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C1S0	4.924716683	0.258327431	0.262486946	-0.004159515	-1.610
263 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C-1S0	4.924716683	0.247252533	0.251030807	-0.003778273	-1.528
264 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	COS1	4.88716497	0.538019012	0.545406489	-0.007387477	-1.373
265 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C1S0	4.88716497	0.252732906	0.256114159	-0.003381252	-1.338
266 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C-1S0	4.88716497	0.241262953	0.245228346	-0.003965393	-1.644
267 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	COS1	4.893695702	0.542517435	0.547154666	-0.004637231	-0.855
268 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	C1S0	4.893695702	0.254699201	0.256238143	-0.001538942	-0.604
269 C1=CC=C2C=C3C=C4C=C5C=CC=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	C-1S0	4.893695702	0.242924617	0.245005174	-0.002080558	-0.856

SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation Energy	DUSHIN Reorganisation Energy	Difference (4-point & DUSHIN)	Difference Percentage (4-point & DUSHIN)
270 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	COS1	1.822346537	0.228538365	0.229197189	-0.000658824	-0.288
271 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	C1S0	1.822346537	0.075474753	0.075729548	-0.000254796	-0.338
272 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	C-1S0	1.822346537	0.103310477	0.102187776	0.001122701	1.087
273 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	COS1	1.77608718	0.249754811	0.247075711	0.0026791	1.073
274 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C1S0	1.77608718	0.080335359	0.078829153	0.001506206	1.875
275 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C-1S0	1.77608718	0.111698931	0.109763211	0.00193572	1.733
276 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	COS1	1.772277586	0.257421347	0.25649851	0.000922837	0.358
277 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C1S0	1.772277586	0.082621932	0.082003149	0.000618783	0.749
278 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(2d,p)	C-1S0	1.772277586	0.114051083	0.11329676	0.000754323	0.661
279 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	COS1	3.874629288	0.36048352	0.362517398	-0.002033878	-0.564
280 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C1S0	3.874629288	0.1414748	0.142606625	-0.001131825	-0.800
281 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C-1S0	3.874629288	0.170155111	0.170428679	-0.000273568	-0.161
282 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	COS1	3.829458386	0.39651379	0.392955518	0.003558271	0.897
283 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	3.829458386	0.152195379	0.149611732	0.002583646	1.698
284 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	3.829458386	0.183198753	0.180285423	0.00291333	1.590
285 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	COS1	3.830546842	0.408870671	0.409061066	-0.000190395	-0.047
286 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C1S0	3.830546842	0.155995421	0.155104232	0.000891189	0.571
287 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(2d,p)	C-1S0	3.830546842	0.186831745	0.185703532	0.001128213	0.604
288 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	COS1	1.769556448	0.242693728	0.243219802	-0.000526074	-0.217
289 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C1S0	1.769556448	0.077966608	0.077688499	0.000278109	0.357
290 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C-1S0	1.769556448	0.109339704	0.108585361	0.000754343	0.690
291 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	COS1	1.775270839	0.255821317	0.253560084	0.002261233	0.884
292 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C1S0	1.775270839	0.082135937	0.081036072	0.001099865	1.339
293 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C-1S0	1.775270839	0.112552008	0.1106311	0.001920908	1.707
297 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	COS1	3.8297305	0.385111484	0.387587003	-0.002475519	-0.643
298 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C1S0	3.8297305	0.149599412	0.150839176	-0.001239763	-0.829
299 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C-1S0	3.8297305	0.180337476	0.180496196	-0.00015872	-0.088
300 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	COS1	3.840342941	0.408675293	0.410350501	-0.001675209	-0.410
301 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C1S0	3.840342941	0.156700224	0.156864808	-0.000164584	-0.105
302 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVTZ	C-1S0	3.840342941	0.186891882	0.186683008	0.000208875	0.112
306 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	COS1	2.170924395	0.299051393	0.299892979	-0.000841586	-0.281
307 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C1S0	2.170924395	0.121536473	0.122074842	-0.000538369	-0.443
308 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C-1S0	2.170924395	0.120149753	0.121008578	-0.000858824	-0.715
309 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-4G	COS1	2.145073578	0.28757959	0.289565095	-0.001985505	-0.690
310 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-4G	C1S0	2.145073578	0.118708149	0.119830728	-0.001122579	-0.946
311 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-4G	C-1S0	2.145073578	0.11708167	0.118752065	-0.001670396	-1.427
312 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-6G	COS1	2.149155286	0.290224128	0.290928922	-0.000704793	-0.243
313 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-6G	C1S0	2.149155286	0.119735324	0.120041501	-0.000306177	-0.256
314 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-6G	C-1S0	2.149155286	0.117496997	0.11793377	-0.000436772	-0.372
315 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	COS1	4.390012943	0.507378365	0.513406167	-0.006027802	-1.188
316 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C1S0	4.390012943	0.233842708	0.23601632	-0.002173612	-0.930
317 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C-1S0	4.390012943	0.222590908	0.224213024	-0.001622116	-0.729
318 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	COS1	4.357631393	0.488039423	0.492502431	-0.004463008	-0.914
319 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C1S0	4.357631393	0.228095282	0.229779915	-0.001684633	-0.739
320 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-4G	C-1S0	4.357631393	0.216560158	0.217567471	-0.001007314	-0.465
321 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	COS1	4.370964973	0.497742487	0.504566094	-0.006823607	-1.371
322 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	C1S0	4.370964973	0.232788729	0.235272415	-0.002483686	-1.067
323 C1=CC=C2C=C3C=C4C=C5C=C6C=CC=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-6G	C-1S0	4.370964973	0.221662401	0.224002251	-0.00233985	-1.056
324 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	COS1	1.513769417	0.203053541	0.202156235	0.000897306	0.442
325 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	C1S0	1.513769417	0.063381305	0.063405519	-2.4214E-05	-0.038

SMILES	Functional	Basis Set	Final Charge and State	HOMO-LUMO Gap	4-Point Reorganisation Energy	DUSHIN Reorganisation Energy	Difference (4-point & DUSHIN)	Difference Percentage (4-point & DUSHIN)
326 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-31G	C-1S0	1.513769417	0.086475336	0.08481759	0.001657746	1.917
327 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C0S1	1.470231199	0.230175402	0.229705524	0.000469877	0.204
328 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C1S0	1.470231199	0.070138709	0.069852697	0.000286011	0.408
329 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	6-311+G(d,p)	C-1S0	1.470231199	0.096592802	0.096410113	0.000182689	0.189
333 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C0S1	3.490404514	0.331030595	0.332302449	-0.001271853	-0.384
334 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C1S0	3.490404514	0.129040475	0.129873448	-0.000832973	-0.646
335 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-31G	C-1S0	3.490404514	0.153232758	0.15331886	-8.61015E-05	-0.056
336 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C0S1	3.453397028	0.373911386	0.374308295	-0.000396909	-0.106
337 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C1S0	3.453397028	0.143767278	0.142891789	0.000875489	0.609
338 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	6-311+G(d,p)	C-1S0	3.453397028	0.169562583	0.168965666	0.000596918	0.352
342 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C0S1	1.4604351	0.219349896	0.218410564	0.000939332	0.428
343 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C1S0	1.4604351	0.067110898	0.067199436	-8.85379E-05	-0.132
344 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVDZ	C-1S0	1.4604351	0.092102923	0.090768832	0.001334092	1.448
345 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C0S1	1.463428352	0.234373302	0.232705942	0.00166736	0.711
346 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C1S0	1.463428352	0.070780353	0.070026275	0.000754078	1.065
347 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	cc-pVTZ	C-1S0	1.463428352	0.096387356	0.095393442	0.000993914	1.031
351 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C0S1	3.44713841	0.357349992	0.359231816	-0.001881824	-0.527
352 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C1S0	3.44713841	0.138341871	0.13919706	-0.000855188	-0.618
353 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	cc-pVDZ	C-1S0	3.44713841	0.164011188	0.164130282	-0.000119094	-0.073
360 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C0S1	1.84438776	0.262710968	0.263565609	-0.000854641	-0.325
361 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C1S0	1.84438776	0.101114246	0.101667043	-0.000552797	-0.547
362 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	B3LYP	STO-3G	C-1S0	1.84438776	0.10019559	0.100365209	-0.000169619	-0.169
369 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C0S1	3.986468085	0.471963807	0.478145061	-0.006181254	-1.310
370 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C1S0	3.986468085	0.214595251	0.217021941	-0.00242669	-1.131
371 C1=CC=C2C=C3C=C4C=C5C=C6C=C7C=CC=CC7=CC6=CC5=CC4=CC3=CC2=C1	CAM-B3LYP	STO-3G	C-1S0	3.986468085	0.204091111	0.205937754	-0.001846642	-0.905