

Supplementary Information

A computational study on boron dipyrromethene ancillary acceptor-based dyes for dye-sensitized solar cells

Ganapathi Rao Kandregula¹, Sudip Mandal^{1,2}, Gollapalli Prince³, Satyesh Kumar Yadav³,
Kothandaraman Ramanujam^{1,4*}

¹*Department of Chemistry, Indian Institute of Technology Madras, Chennai, India, 600 036*

²*Division of Chemistry, Department of Sciences and Humanities, Vignan's Foundation for Science, Technology and Research, Vadlamudi, Guntur, Andhra Pradesh, India, 522 213*

³*Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India, 600 036*

⁴*DST-IITM Solar Energy Harnessing Centre, Indian Institute of Technology Madras, Chennai, India, 600 036.*

**Corresponding author's e-mail: rkraman@iitm.ac.in*

Table of Contents:

Fig S1. The frontier orbital diagram of D1 showing the transition corresponds to π - π^* transition.

Fig S2. The frontier orbital diagram of D2 showing the transition corresponds to π - π^* transition.

Fig S3. The frontier orbital diagram of D3 showing the transition corresponds to π - π^* transition.

Fig S4. The frontier orbital diagram of D4 showing the transition corresponds to π - π^* transition.

Fig. S5. Ground state optimized geometries of dyes@TiO₂ with an expanded view of the interface between dyes and TiO₂ surface displaying the a) monodentate b) chelating of dye onto TiO₂

Table S1. Comparison of the electrical performance of BODIPY-based dyes known for OPV and DSSC applications.

Table S2. The calculated HOMO, LUMO, bandgap energy and driving force for dye regeneration (in eV) of four dyes obtained using five different functionals (**B3LYP**, **CAM-B3LYP**, **M06-2XWB97XD**, and **PBE1PBE**) along with experimentally measured values (shown within parenthesis)

Table S3 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D1 obtained using M06-2X/6-31G(d,p) method.

Table S4 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D2 obtained using M06-2X/6-31G(d,p) method.

Table S5 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D3 obtained using M06-2X/6-31G(d,p) method.

Table S6 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D4 obtained using M06-2X/6-31G(d,p) method.

Table S7 The list of frequencies for optimized ground and excited state geometries of four dyes obtained using M06-2X/6-31G(d,p) method.

Table S8 Computed absorption wavelength (λ_c), and oscillator strength (f) for the singlet-singlet transitions for metal-free organic dyes in DCM solvent medium (IEF-PCM simulation) using 6-31G(d,p) and 6-31+G(d,p) basis sets with various functionals (B3LYP, CAM-B3LYP, M06-2X, WB97XD, PBE1PBE, and sTPSSH).

Table S9 Calculated adsorption energy (E_{ads} in eV) and bond lengths (in Å) of the optimized dye structures.

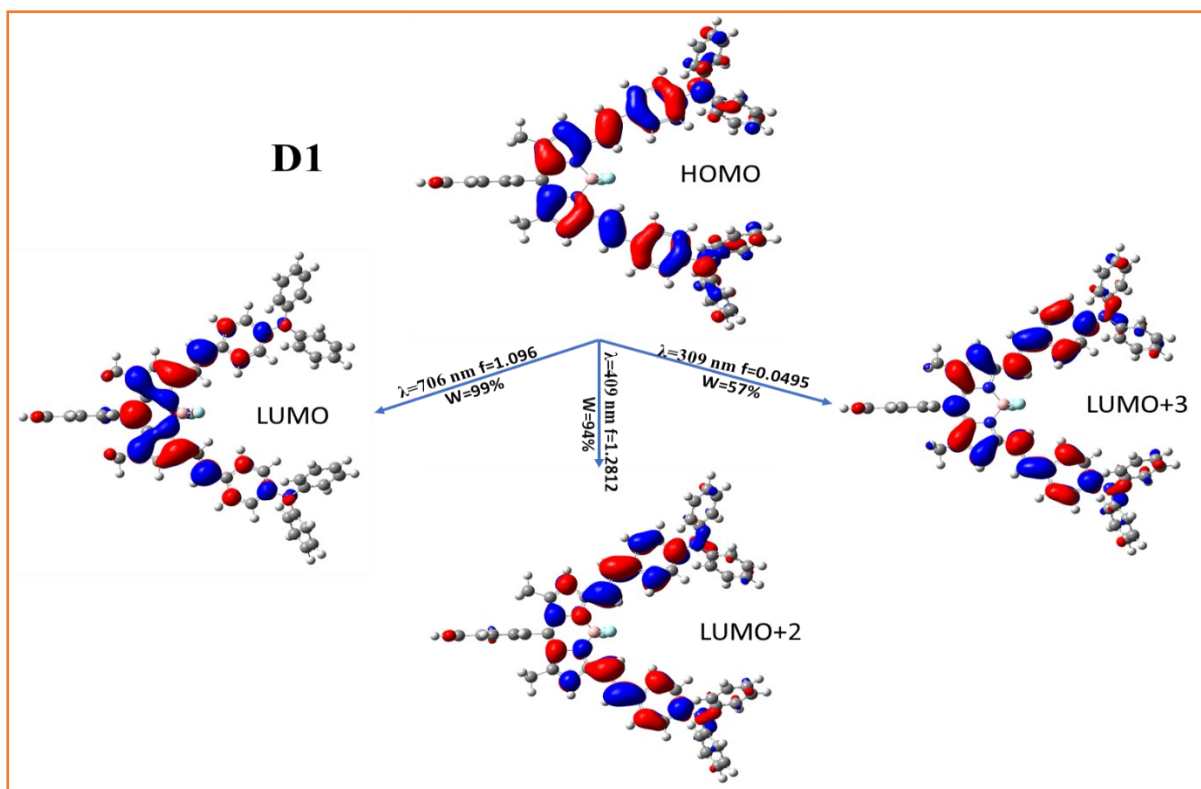


Fig S1. The frontier orbital diagram of D1 showing the transition corresponds to $\pi-\pi^*$ transition.

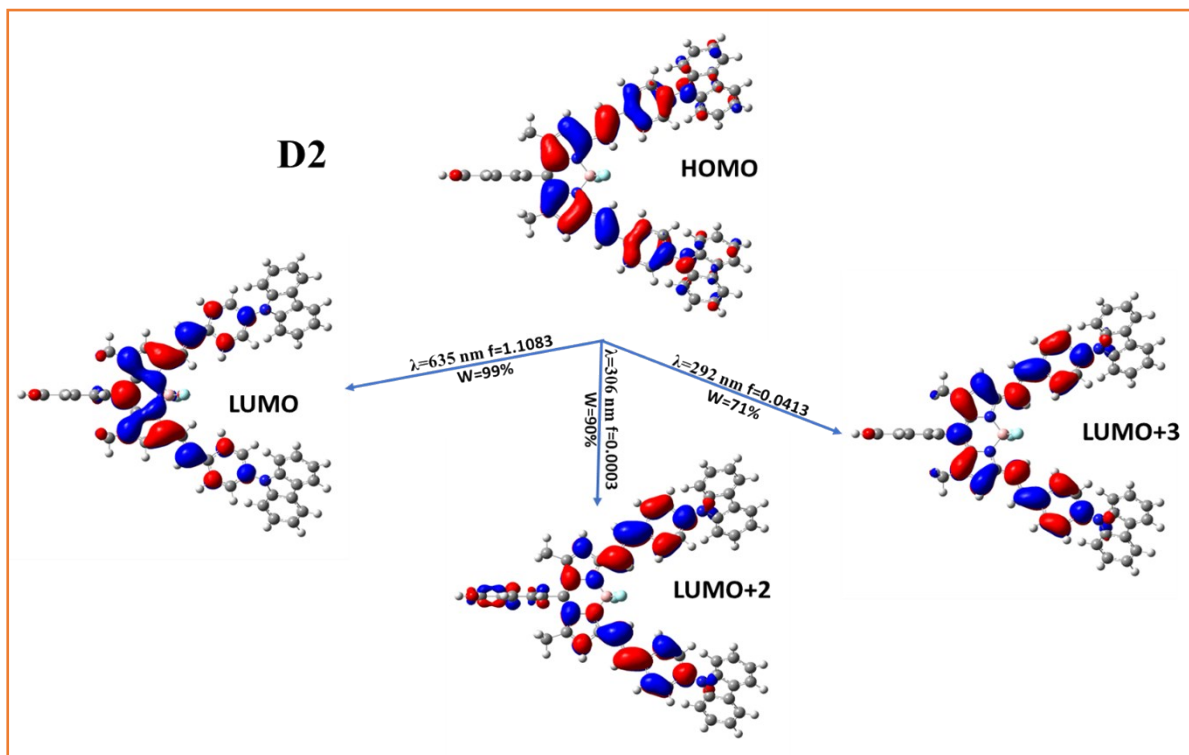


Fig S2. The frontier orbital diagram of D2 showing the transition corresponds to $\pi-\pi^*$ transition.

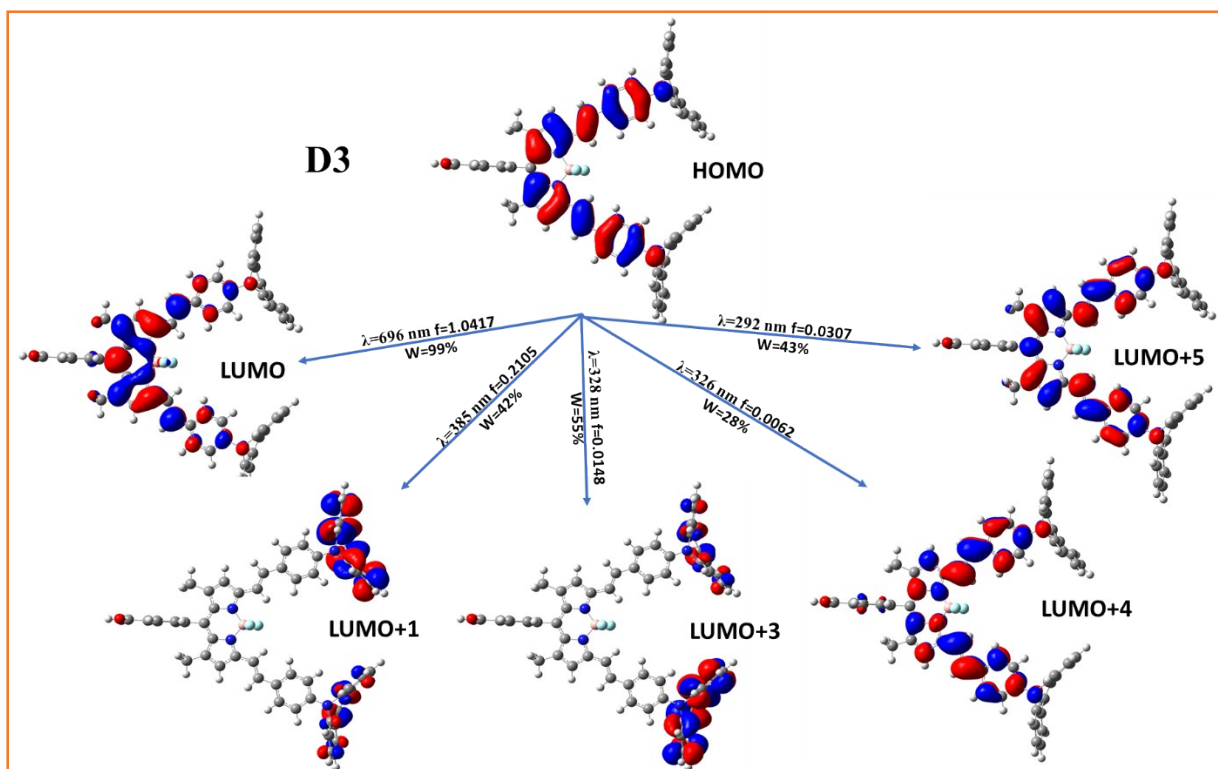


Fig S3. The frontier orbital diagram of D3 showing the transition corresponds to π - π^* transition.

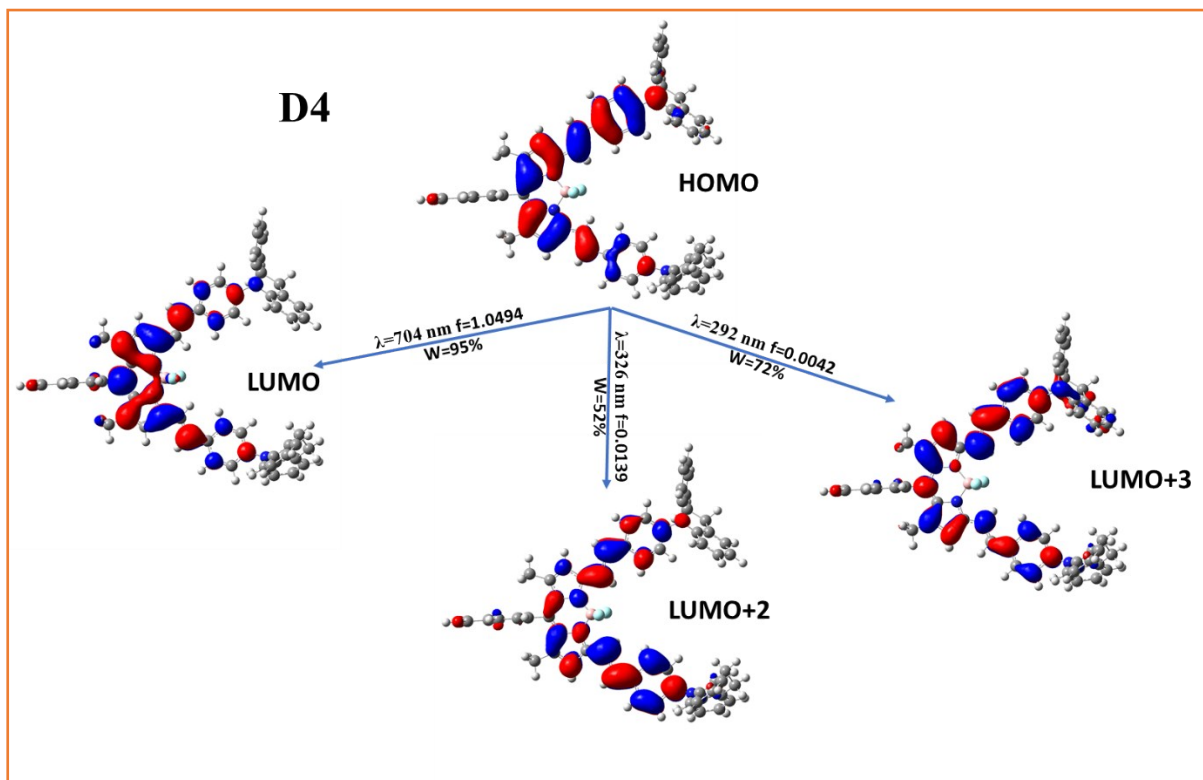


Fig S4. The frontier orbital diagram of D4 showing the transition corresponds to π - π^* transition.

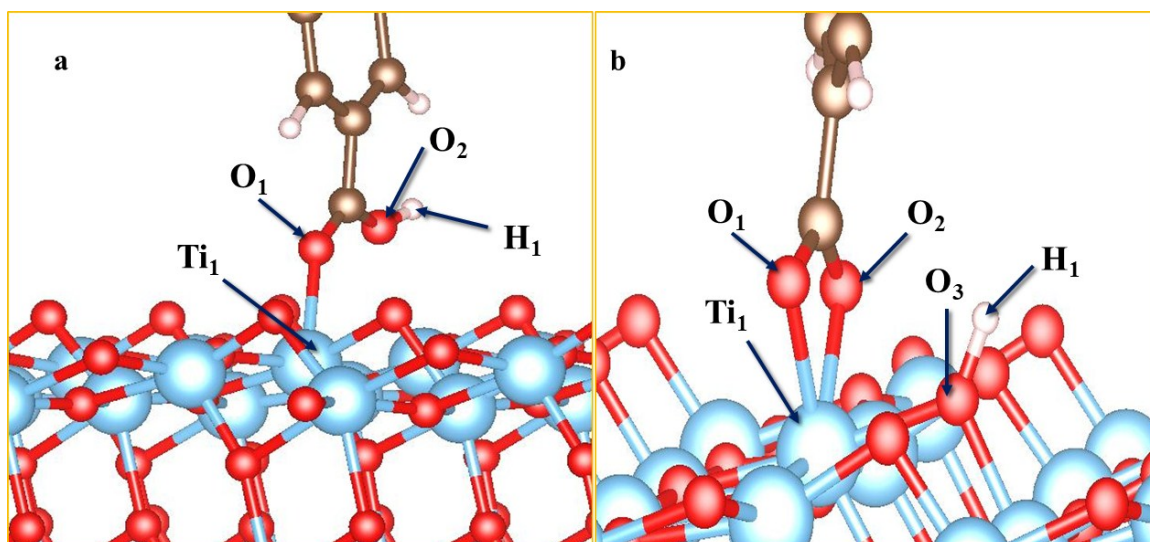
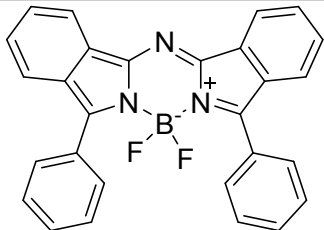
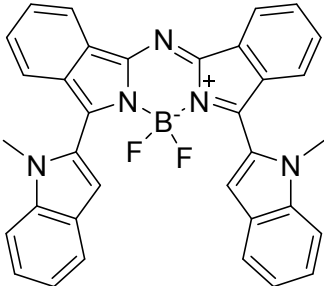
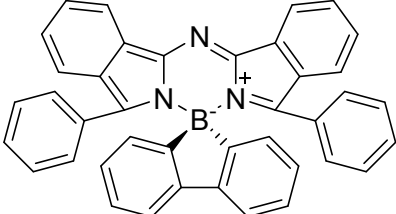
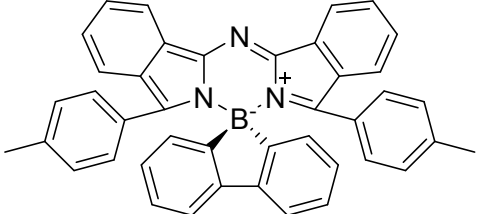
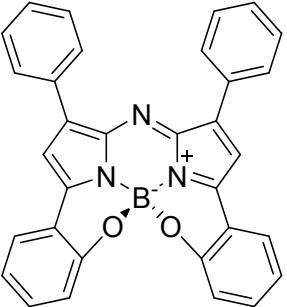
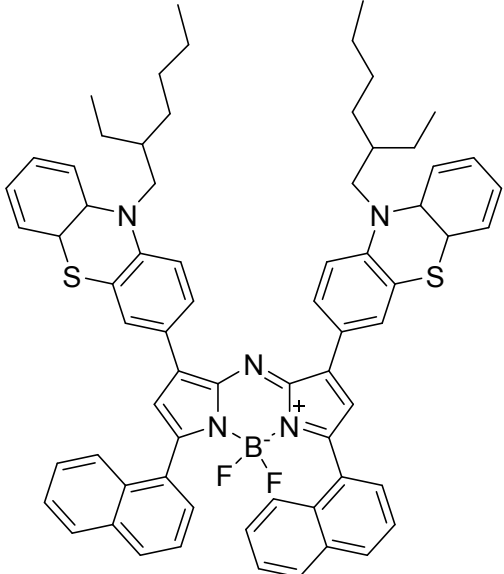
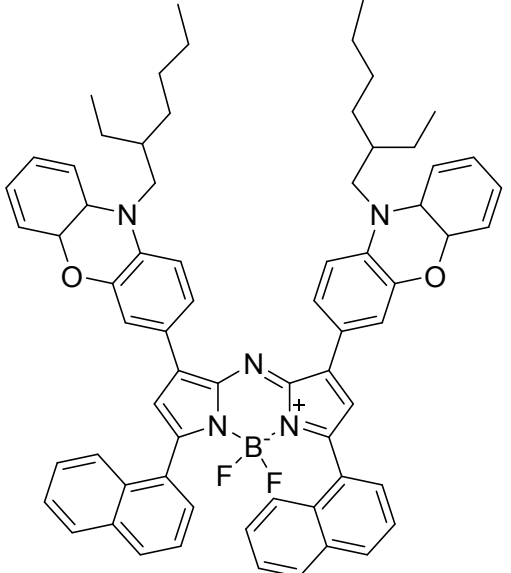
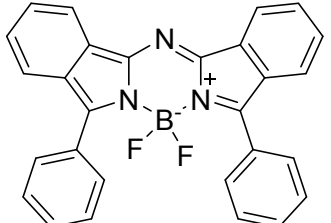
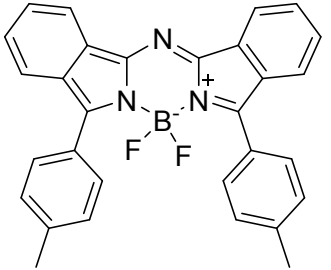
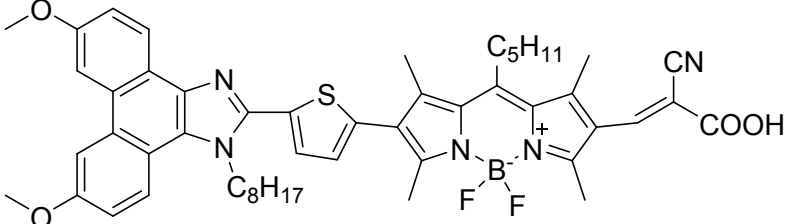


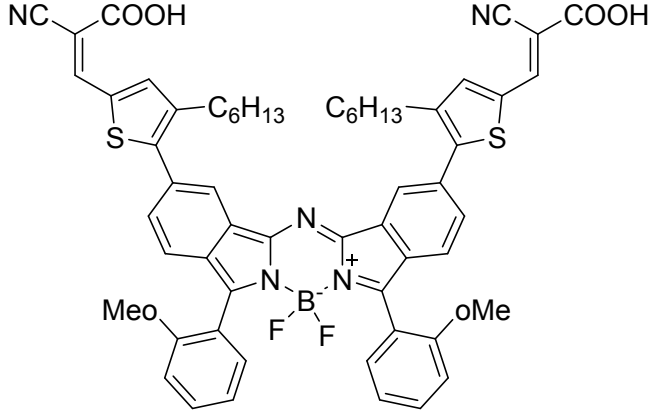
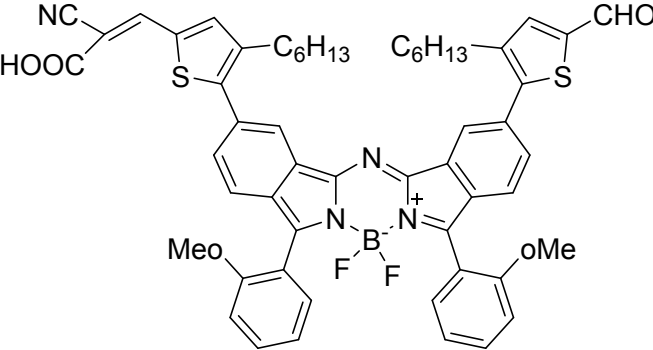
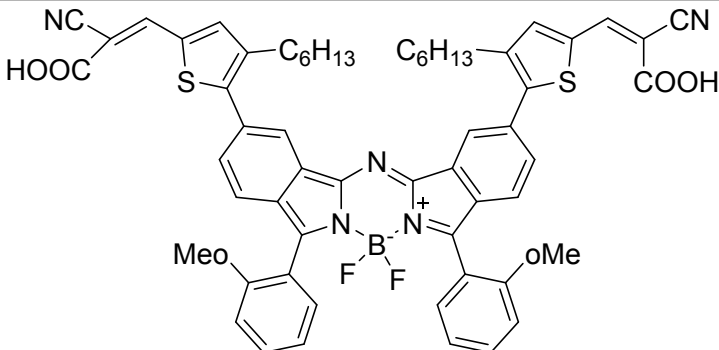
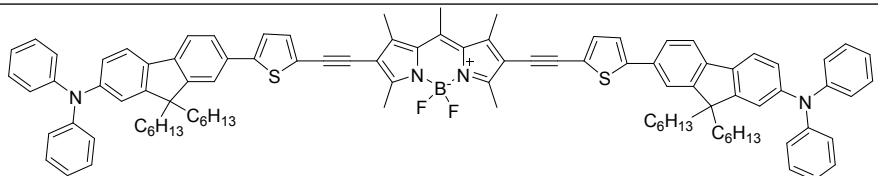
Fig. S5. Ground state optimized geometries of dyes@TiO₂ with an expanded view of the interface between dyes and TiO₂ surface displaying the a) monodentate b) chelating of dye onto TiO₂

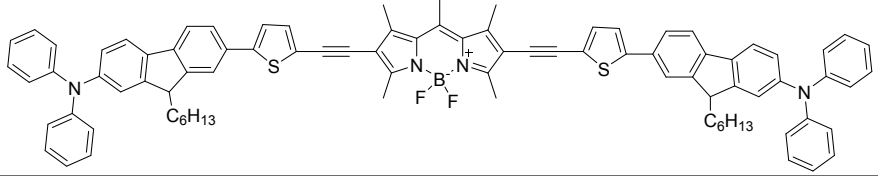
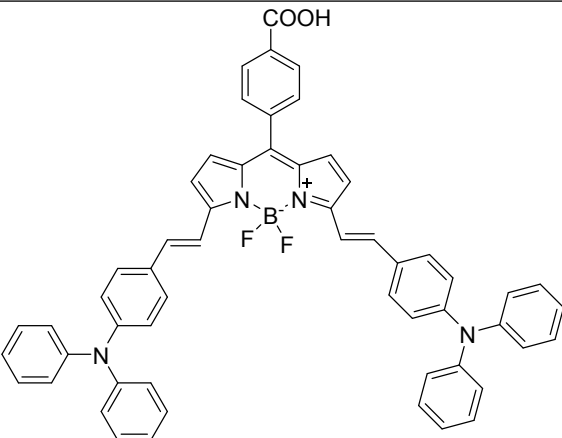
Table S1. Comparison of the electrical performance of BODIPY-based dyes known for OPV and DSSC applications.

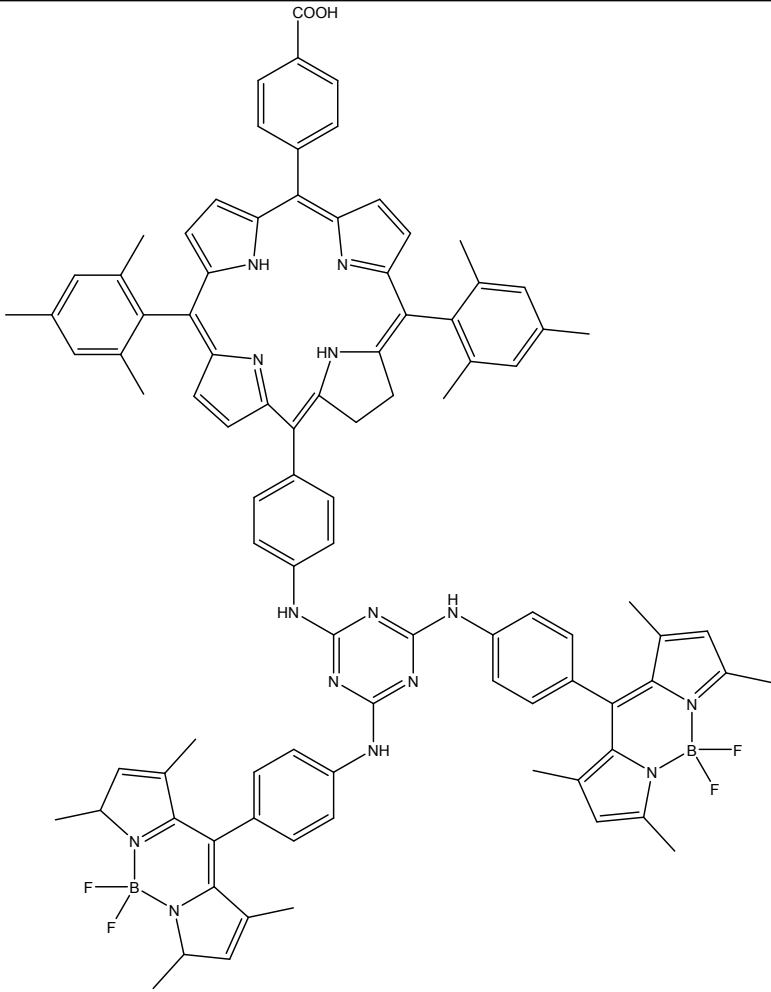
S. No.	Structure	V _{oc} / (V)	J _{sc} / (mA cm ⁻²)	FF	PCE / %	Type of cell	Intensity of irradiation (mW cm ⁻²)	Ref.
1		0.92	3.15	48	1.2	OPV (Organic Photovoltaics)	122 mW cm ⁻² with AM1.5G irradiation	¹
2		0.56	4.7	63	1.6	OPV	104 mW cm ⁻² with AM1.5G irradiation	²
3		0.77	10.4	57.3	4.5	OPV	103 mW cm ⁻²	³
4		0.74	8.6	57.3	3.7	OPV	98 mW cm ⁻²	³

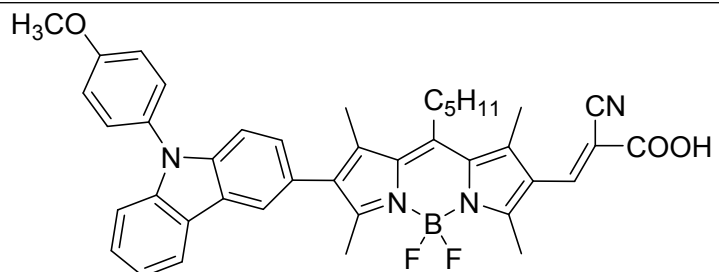
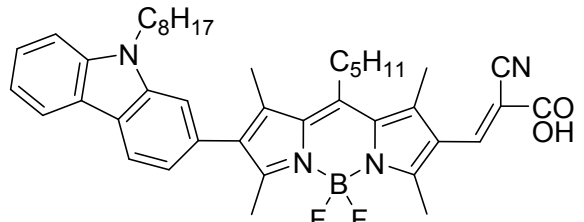
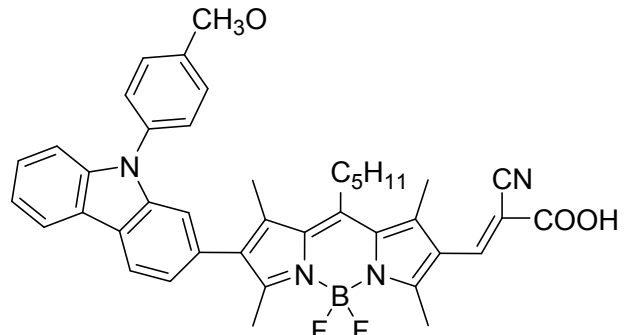
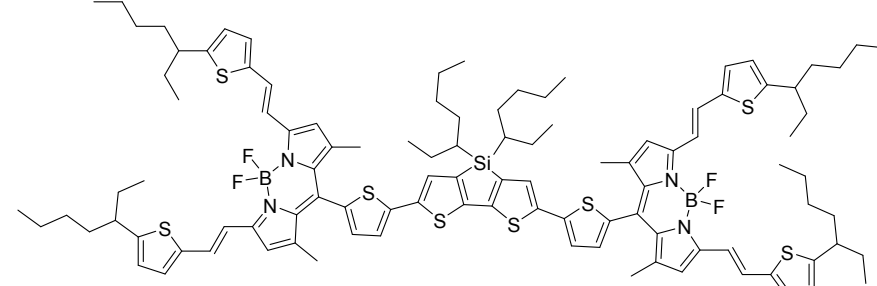
5		0.796	5.88	56.2	2.63	OPV	1 sun with AM 1.5G filter	⁴
6		0.79	16.28	64	8.23	OPV	NA	⁵

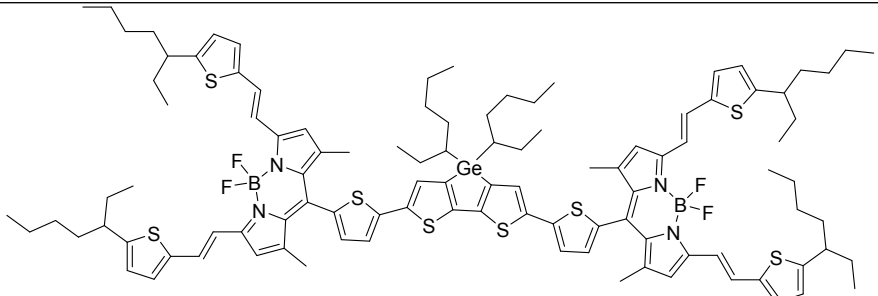
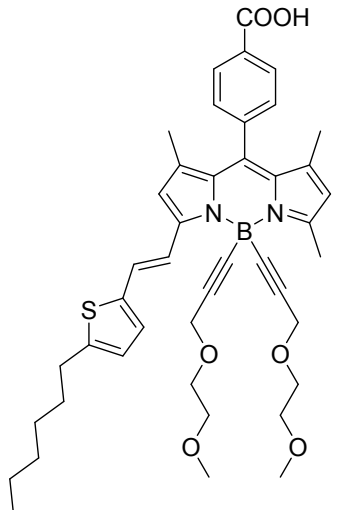
7		0.93	13.43	58	7.24	OPV	NA	⁵
8		0.81	8	59	3.8	OPV	1 sun with AM 1.5G filter	⁶
9		0.71	7	55	2.7	OPV	1 sun with AM 1.5G filter	⁶
10		0.61	5.1	72	2.26	DSSC	100 mW cm ⁻² with AM 1.5G filter	⁷

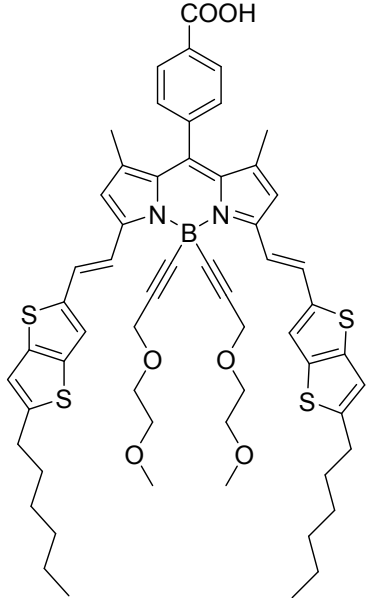
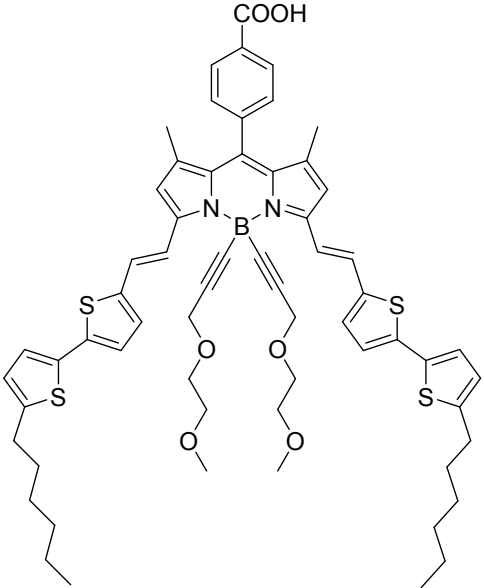
11		0.54	19.02	59	6.06	DSSC	100 mW cm ⁻² with AM 1.5G filter	8
12		0.55	17.2	57.9	5.48	DSSC	100 mW cm ⁻² with AM 1.5G filter	8
13		0.53	19.24	51.4	5.24	DSSC	100 mW cm ⁻² with AM 1.5G filter	8
14		0.988	8.25	39.5	3.22	OPV	NA	9

15		0.928	7.51	36.7	2.56	OPV	NA	⁹
16		0.43	9.17	62	2.46	DSSC	NA	¹⁰

17	 This molecule is adsorbed on TiO₂	0.68	10.86	70	5.17	DSSC	100 mW cm ⁻² with AM 1.5G filter	11
----	--	------	-------	----	------	------	---	----

20		0.56	9.18	73	3.74	DSSC	100 mW cm ⁻² with AM 1.5G filter	¹²
21		0.54	6.84	73	2.68	DSSC	100 mW cm ⁻² with AM 1.5G filter	¹²
22		0.600	10.2	70	4.28	DSSC	100 mW cm ⁻² with AM 1.5G filter	¹²
23		0.769	10.58	56.4	4.58	OPV	1000 W m ⁻² ; Model-SS 150, class-AAA at 1 sun	¹³

24		0.774	9.41	56.6	4.12	OPV	1000 W m ⁻² ; Model-SS 150, class-AAA at 1 sun	¹³
25		0.526	11.40	71	4.26	DSSC	100 mW cm ⁻² with AM 1.5G filter	¹⁴

26		0.536	16.10	70.2	6.06	DSSC	100 mW cm ⁻² with AM 1.5G filter	14
27		0.457	12.0	62.8	3.44	DSSC	100 mW cm ⁻² with AM 1.5G filter	14

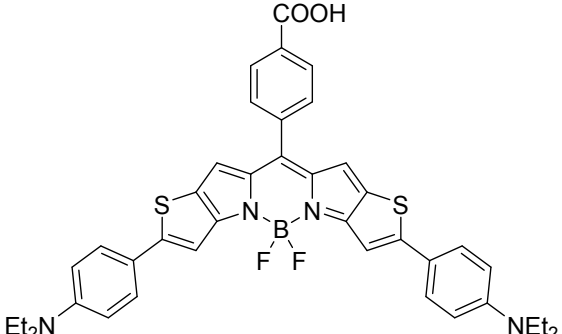
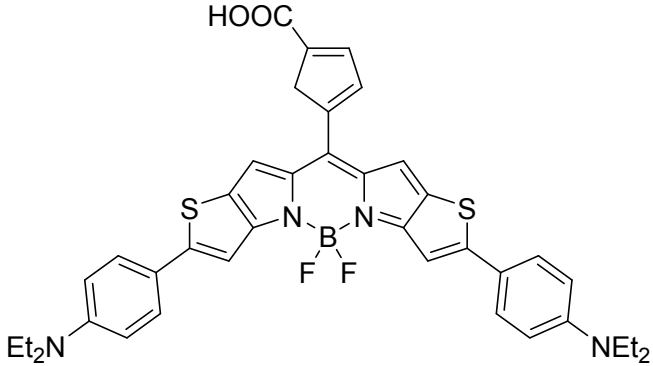
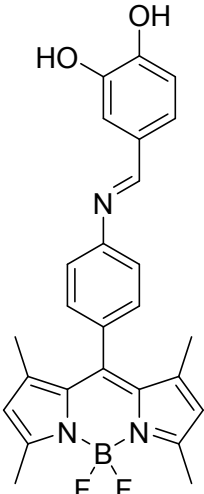
28		0.431	4.98	65	1.4	DSSC	100 mW cm ⁻² with AM 1.5G filter	15
29		0.435	3.96	65	1.12	DSSC	100 mW cm ⁻² with AM 1.5G filter	15
30		0.49	1.66	52	0.42	DSSC	100 mW cm ⁻² with AM 1.5G filter	16

Table S2 The calculated HOMO, LUMO, bandgap energy and driving force for dye regeneration (in eV) of four dyes obtained using five different functionals (**B3LYP**, **CAM-B3LYP**, **M06-2XWB97XD**, and **PBE1PBE**) along with experimentally measured values (shown within parenthesis)

	B3LYP			CAM-B3LYP			M06-2X			WB97XD			PBE1PBE		
	E_{HOMO} (eV)	E_{LUMO} (eV)	Driving force for dye regenerati on (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	Driving force for dye regenerati on (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	Driving force for dye regenerati on (eV)	E_{HOM} o (eV)	E_{LUMO} (eV)	Driving force for dye regeneratio n (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	Driving force for dye regenerat ion (eV)
D1	-4.68	-2.73	-0.12	-5.85	-1.83	1.05	-4.99 (-5.06)	-2.65 (-3.41)	0.19	-6.44	-1.37	1.64	-4.92	-2.72	0.12
D2	-5.05	-2.91	0.25	-6.20	-1.96	1.40	-5.33 (-5.30)	-2.81 (-3.52)	0.53	-6.79	-1.49	1.99	-5.29	-2.89	0.49
D3	-4.82	-2.75	0.02	-5.79	-1.73	0.99	-4.97 (-4.98)	-2.54 (-3.3)	0.17	-6.40	-1.27	1.60	-4.85	-2.59	0.05
D4	-4.81	-2.75	0.01	-5.96	-1.83	1.16	-5.12 (-4.96)	-2.67 (-3.31)	0.32	-6.56	-1.36	1.76	-5.05	-2.74	0.25

Table S3 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D1 obtained using M06-2X/6-31G(d,p) method.

D1					Ground state parameters						Excited state parameters					
Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z	Bond	Angle	Dihedral	X	Y	Z
1	C							-9.01258	-0.22598	1.231708				-9.09047	-0.35653	1.17797
2	C	1			1.387548			-7.62549	-0.19098	1.225509	1.389499			-7.70099	-0.35015	1.175184
3	C	2	1		1.395912	120.232		-6.92808	-0.18047	0.016343	1.39973	120.6005		-6.99212	-0.0637	0.002711
4	C	3	2	1	1.396567	119.8208	-0.0056	-7.63024	-0.20542	-1.19061	1.400211	119.2359	-0.00093	-7.69934	0.217583	-1.17258
5	C	4	3	2	1.386452	120.0135	-0.0358	-9.01622	-0.24126	-1.18602	1.388319	120.3996	-0.12415	-9.08763	0.210003	-1.17597
6	C	5	4	3	1.396187	120.1309	0.063526	-9.71305	-0.25117	0.023804	1.396411	119.9256	0.148341	-9.78559	-0.0765	-0.00092
7	H	1	2	3	1.085731	120.2562	-179.991	-9.55542	-0.23401	2.17196	1.084026	120.4766	-179.72	-9.63745	-0.57421	2.088212
8	H	2	1	6	1.088407	120.3917	-179.979	-7.07098	-0.1715	2.161869	1.085888	120.2001	179.8046	-7.15195	-0.5635	2.087426
9	H	4	3	2	1.088173	119.4216	179.9563	-7.08005	-0.19631	-2.1294	1.085815	119.2517	-179.907	-7.1497	0.438323	-2.08261
10	H	5	4	3	1.086613	121.0813	-179.962	-9.57993	-0.26167	-2.11475	1.084714	121.1224	-179.705	-9.64724	0.421537	-2.08079
11	C	3	2	1	4.707752	114.1307	-144.089	-2.88983	-2.59874	0.102593	4.743492	107.5936	-147.642	-2.96288	-2.56432	0.11616
12	C	11	3	2	1.413832	68.6247	70.81704	-4.00853	-3.46204	0.14884	1.424746	68.4864	62.24018	-4.10574	-3.41503	0.108447
13	C	12	11	3	1.380232	108.5079	0.217381	-5.15553	-2.69501	0.115704	1.374763	108.8086	0.2457	-5.23787	-2.63608	0.069791
14	C	13	12	11	1.429796	106.1864	-0.02878	-4.72298	-1.33387	0.048424	1.446432	106.2302	-0.26457	-4.78361	-1.26287	0.059476
15	N	11	3	2	1.356145	40.02166	-109.227	-3.33244	-1.31811	0.04601	1.372289	39.31954	-117.904	-3.40603	-1.26591	0.085439
16	H	12	11	3	1.083947	125.8504	-178.683	-3.97366	-4.5432	0.218299	1.081873	125.5058	-179.515	-4.08427	-4.49641	0.133254
17	C	14	13	12	2.434917	160.6467	-176.11	-4.79512	1.09917	-0.01413	2.43406	161.1319	176.6058	-4.80494	1.169631	-0.02492
18	C	17	14	13	1.430581	160.6419	0.442834	-5.30773	2.434756	-0.0125	1.446472	160.8302	14.50219	-5.28476	2.533762	0.0097
19	C	18	17	14	1.380404	106.1555	176.0036	-4.2076	3.268428	-0.02676	1.37455	106.2259	171.4271	-4.16783	3.334531	-0.01507
20	C	19	18	17	1.413445	108.5151	0.031027	-3.04046	2.471252	-0.03772	1.425111	108.8135	-0.5008	-3.00899	2.505889	-0.05226
21	N	20	19	18	1.356058	108.6627	-0.30252	-3.40658	1.16563	-0.02364	1.372126	107.7585	-0.03632	-3.42841	1.199441	-0.0491
22	H	19	18	17	1.083885	125.6031	-178.788	-4.23661	4.351809	-0.01096	1.081841	125.6784	-178.878	-4.16587	4.415887	0.017259
23	C	14	13	12	1.397799	131.2303	-178.898	-5.44599	-0.1381	0.013347	1.410403	130.7857	179.0804	-5.50728	-0.05343	0.006721
24	C	20	19	18	1.434866	128.991	-179.781	-1.66599	2.88301	-0.04971	1.415565	129.5399	-179.181	-1.64113	2.869813	-0.07127
25	H	24	20	19	1.087322	116.0978	172.5099	-0.92887	2.092773	0.070463	1.085012	116.2299	175.2431	-0.9272	2.054442	-0.0191
26	C	24	20	19	1.351787	123.5486	-7.16772	-1.27239	4.16827	-0.19293	1.370301	123.6962	-4.5534	-1.20002	4.165015	-0.14608
27	H	26	24	20	1.092368	118.487	-1.12989	-2.03814	4.936074	-0.32473	1.088806	118.3906	-1.00019	-1.94007	4.961059	-0.21045
28	C	11	3	2	1.435144	162.3998	-107.022	-1.49343	-2.92916	0.125661	1.415672	161.895	-116.629	-1.5881	-2.89983	0.155436
29	H	28	11	3	1.087894	116.1012	4.951106	-0.80459	-2.09116	0.208	1.085144	116.1436	3.283655	-0.89502	-2.06838	0.232153

30	C	28	11	3	1.351825	123.2703	-176.008	-1.03059	-4.19807	0.070099	1.370014	123.6735	-177.242	-1.11859	-4.18617	0.112677
31	H	30	28	11	1.092206	118.3963	0.668035	-1.75464	-5.01216	-0.00681	1.088711	118.3537	0.73088	-1.84009	-4.99752	0.032483
32	C	26	24	20	4.27838	128.0258	179.676	2.717362	5.712015	-0.25027	4.275374	127.7107	179.912	2.844046	5.5505	-0.21511
33	C	32	26	24	1.401795	58.60143	176.8026	1.608847	6.545303	-0.45486	1.408817	58.51632	177.7572	1.758732	6.442837	-0.31803
34	C	32	26	24	1.405317	59.85242	-3.32488	2.493191	4.343865	-0.02043	1.411718	59.84743	-2.6885	2.568741	4.172734	-0.07757
35	C	33	32	26	1.383025	120.3323	0.408204	0.328116	6.024254	-0.42335	1.379634	120.3443	0.284109	0.462803	5.970595	-0.28726
36	H	33	32	26	1.087043	119.5777	-179.404	1.76157	7.605189	-0.64188	1.084191	119.5996	-178.992	1.947227	7.504234	-0.43368
37	C	34	32	26	1.380409	120.7064	0.147008	1.210944	3.832936	-0.00248	1.377697	120.8087	-0.03258	1.270764	3.711536	-0.05303
38	H	34	32	26	1.087118	119.3989	-179.204	3.340913	3.686299	0.155068	1.084305	119.3571	-179.272	3.391535	3.473581	0.021995
39	C	35	33	32	1.403944	121.8054	-0.71087	0.090261	4.658198	-0.20341	1.412973	122.0212	-0.30167	0.169787	4.594229	-0.15978
40	H	35	33	32	1.089066	119.2512	-179.662	-0.52013	6.686634	-0.59006	1.086515	119.1219	-179.239	-0.35906	6.675087	-0.38075
41	H	37	34	32	1.087845	118.6012	-179.293	1.076237	2.770794	0.190173	1.084897	118.444	-179.086	1.102961	2.646706	0.06937
42	C	32	26	24	2.453389	150.895	28.58803	5.111658	5.4476	-0.71562	2.449512	150.3895	27.48144	5.208537	5.194003	-0.74633
43	C	42	32	26	1.39771	98.50033	38.29257	5.012099	4.698932	-1.89171	1.398583	98.11889	36.8882	5.037965	4.474213	-1.93328
44	C	42	32	26	1.397463	137.3858	-115.484	6.304866	5.429943	0.011597	1.398198	137.766	-117.654	6.424371	5.121764	-0.05968
45	C	43	42	32	1.389226	120.0315	-159.281	6.089285	3.934885	-2.32281	1.390639	119.8991	-159.815	6.071405	3.678849	-2.41626
46	H	43	42	32	1.087732	119.4232	20.64738	4.086081	4.720295	-2.46197	1.0854	119.4522	20.21188	4.096557	4.543755	-2.46901
47	C	44	42	32	1.38905	120.1152	150.1116	7.382975	4.677284	-0.43634	1.390619	119.9126	150.6788	7.457396	4.336283	-0.55938
48	H	44	42	32	1.087867	119.2153	-29.921	6.376719	6.011459	0.928183	1.085329	119.3693	-29.3872	6.550188	5.683357	0.860491
49	C	47	44	42	1.392084	120.4217	-0.76813	7.280328	3.92298	-1.60184	1.393746	120.4396	-0.64341	7.285424	3.608052	-1.73524
50	H	45	43	42	1.087353	119.4102	179.9653	6.000596	3.355883	-3.23891	1.085048	119.3987	179.9582	5.930044	3.123356	-3.33755
51	H	47	44	42	1.087384	119.4251	-179.98	8.305982	4.671391	0.138491	1.085074	119.4214	-179.961	8.397373	4.285507	-0.01971
52	H	49	47	44	1.086885	120.2583	-179.579	8.123329	3.329627	-1.94622	1.08464	120.2317	-179.645	8.091464	2.991966	-2.11888
53	C	30	28	11	4.277496	128.3379	-178.763	3.0258	-5.55036	0.188266	4.274534	127.8023	-179.777	2.948758	-5.49585	0.226834
54	C	53	30	28	1.405511	59.88318	-3.09373	2.740794	-4.17406	0.193512	1.411334	59.88003	0.300463	2.646195	-4.11868	0.287819
55	C	53	30	28	1.401641	58.5636	177.521	1.955494	-6.45355	0.130926	1.40853	58.52966	-179.729	1.883611	-6.41231	0.129194
56	C	54	53	30	1.38025	120.7462	0.088397	1.436696	-3.72337	0.157522	1.377885	120.7807	0.112746	1.339913	-3.68156	0.254387
57	H	54	53	30	1.087018	119.369	-179.469	3.560055	-3.46008	0.219033	1.084394	119.3516	-179.097	3.455019	-3.39896	0.348803
58	C	55	53	30	1.383051	120.3044	0.485939	0.653197	-5.99031	0.083457	1.379658	120.3413	0.034286	0.579382	-5.96379	0.09341
59	H	55	53	30	1.086934	119.686	-178.908	2.152434	-7.52249	0.133848	1.084296	119.5576	-179.348	2.094274	-7.4753	0.092334
60	C	58	55	53	1.403698	121.8335	-0.62435	0.353956	-4.61902	0.103612	1.412971	121.982	-0.17501	0.258751	-4.58909	0.155722
61	H	56	54	53	1.08781	118.7095	-179.392	1.254388	-2.65096	0.152716	1.084898	118.4605	-179.142	1.150969	-2.61381	0.289344

62	H	58	55	53	1.089149	119.2248	-179.496	-0.16545	-6.70778	0.047582	1.086607	119.1641	-179.349	-0.22805	-6.68807	0.028618
63	C	53	30	28	2.449735	149.6302	-151.769	4.717173	-7.21542	-0.41839	2.44915	149.4767	-150.128	4.655062	-7.13719	-0.39997
64	C	63	53	30	1.396825	136.2034	-110.723	5.478272	-8.17194	0.257569	1.398297	137.9836	-116.522	5.509181	-8.04269	0.237036
65	C	63	53	30	1.397287	99.19652	42.23243	4.337049	-7.44758	-1.74278	1.398754	97.93158	37.95474	4.195358	-7.40944	-1.69267
66	C	64	63	53	1.389118	120.0735	149.3403	5.859991	-9.3411	-0.3882	1.390729	119.9221	150.6173	5.897859	-9.20712	-0.41655
67	H	64	63	53	1.087848	119.201	-30.901	5.768892	-7.98659	1.289362	1.085299	119.3916	-29.4613	5.863071	-7.82593	1.239857
68	C	65	63	53	1.389201	120.0248	-158.402	4.708908	-8.62672	-2.3762	1.390518	119.9199	-159.867	4.576642	-8.5843	-2.3313
69	H	65	63	53	1.087868	119.2686	21.68462	3.750974	-6.6961	-2.26743	1.085366	119.4361	20.16975	3.542711	-6.69739	-2.1877
70	C	66	64	63	1.3923	120.401	-0.77361	5.475032	-9.57639	-1.70537	1.393652	120.4566	-0.66149	5.430921	-9.48654	-1.69957
71	H	66	64	63	1.08733	119.4798	179.9567	6.452998	-10.0788	0.146942	1.08508	119.4071	-179.987	6.56075	-9.90408	0.085674
72	H	68	65	63	1.087354	119.4577	-179.901	4.409469	-8.79714	-3.40753	1.085077	119.3894	179.9855	4.214775	-8.78693	-3.33399
73	H	70	66	64	1.086917	120.2601	-179.707	5.770996	-10.4941	-2.2069	1.084633	120.2423	-179.646	5.73174	-10.3985	-2.20383
74	N	32	26	24	1.402948	179.306	-162.329	4.019578	6.233791	-0.26596	1.395324	179.4213	149.585	4.159892	6.013704	-0.24544
75	C	74	32	26	1.419553	120.5183	11.94969	4.273343	7.552559	0.194021	1.421927	120.8776	56.38257	4.483999	7.321063	0.210238
76	C	75	74	32	1.397403	120.522	46.0596	3.719932	8.004046	1.395117	1.398656	120.3777	45.28318	3.95433	7.802881	1.411712
77	C	75	74	32	1.397116	119.9877	-134.903	5.098299	8.403511	-0.54575	1.398185	119.8769	-135.71	5.353365	8.122975	-0.53546
78	C	76	75	74	1.38928	120.0653	179.6954	3.979677	9.294454	1.839504	1.390571	119.8969	179.7096	4.282764	9.080735	1.850924
79	H	76	75	74	1.087742	119.4246	-0.2475	3.087191	7.336775	1.976126	1.085399	119.4411	-0.22454	3.289815	7.17153	1.993009
80	C	77	75	74	1.389306	120.0847	-178.832	5.367545	9.686302	-0.08518	1.39058	119.9294	-178.945	5.688341	9.393324	-0.0797
81	H	77	75	74	1.087887	119.19	1.049178	5.525317	8.047664	-1.48091	1.085297	119.3736	0.95841	5.761273	7.743017	-1.46665
82	C	80	77	75	1.392088	120.4346	-0.7813	4.806896	10.14023	1.105421	1.393668	120.436	-0.64966	5.152368	9.88026	1.111073
83	H	78	76	75	1.087398	119.4441	-179.98	3.544075	9.635204	2.77576	1.085074	119.3973	-179.999	3.867243	9.446351	2.784226
84	H	80	77	75	1.087385	119.417	179.9985	6.011087	10.3395	-0.66964	1.085059	119.4185	-179.981	6.363519	10.00874	-0.66515
85	H	82	80	77	1.086903	120.2627	-179.612	5.014392	11.14652	1.459933	1.084627	120.2403	-179.672	5.41167	10.87364	1.460892
86	N	53	30	28	1.40285	179.3228	151.5085	4.351083	-6.00812	0.23382	1.396212	179.395	-163.981	4.273087	-5.93689	0.259207
87	C	86	53	30	1.41816	120.9847	-120.923	5.345148	-5.29606	0.952149	1.421531	120.7359	-165.734	5.268255	-5.19755	0.954744
88	C	87	86	53	1.397677	119.9102	-138.08	6.619032	-5.13075	0.401339	1.398323	119.9545	-136.511	6.522761	-4.99482	0.371286
89	C	87	86	53	1.398154	120.7024	42.97603	5.072953	-4.77333	2.220019	1.398781	120.3191	44.34736	5.005546	-4.68572	2.229734
90	C	88	87	86	1.388802	120.1445	-178.678	7.604343	-4.45807	1.112274	1.390621	119.9195	-179.091	7.502061	-4.28765	1.06028
91	H	88	87	86	1.087846	119.2623	1.190445	6.828022	-5.53611	-0.58629	1.085297	119.3794	0.852304	6.720609	-5.39439	-0.6182
92	C	89	87	86	1.389155	120.0762	179.5756	6.05911	-4.08558	2.915892	1.390566	119.919	179.8746	5.986	-3.9659	2.90371
93	H	89	87	86	1.087704	119.4311	-0.35253	4.085311	-4.9114	2.654302	1.085391	119.4406	-0.09113	4.034448	-4.85648	2.68348

94	C	92	89	87	1.392109	120.5142	-0.99652	7.329957	-3.92776	2.369991	1.393779	120.4467	-0.91994	7.238346	-3.76595	2.32555
95	H	90	88	87	1.087477	119.3951	179.9696	8.591422	-4.33688	0.67228	1.085082	119.406	-179.968	8.472449	-4.13479	0.599431
96	H	92	89	87	1.087411	119.3763	179.9828	5.834947	-3.68353	3.901069	1.085067	119.3964	179.961	5.772881	-3.57216	3.892101
97	H	94	92	89	1.086845	120.313	-179.483	8.101508	-3.39632	2.920907	1.084632	120.2294	-179.562	8.002857	-3.20999	2.857394
98	B	15	11	3	1.555002	126.1073	-172.68	-2.45474	-0.05429	-0.17854	1.544236	125.2183	177.2756	-2.50294	-0.03322	-0.14245
99	F	98	15	11	1.385327	110.3966	65.70574	-1.89655	-0.07314	-1.44629	1.394458	110.846	-67.0549	-1.88778	-0.09838	-1.39219
100	F	98	15	11	1.391394	110.0474	-55.5147	-1.44524	0.001337	0.777391	1.399849	110.2151	53.29834	-1.51059	0.031236	0.842779
101	C	6	5	4	1.480772	117.9735	-179.931	-11.1924	-0.29138	-0.02702	1.487625	117.9972	179.9479	-11.2723	-0.07176	-0.05295
102	O	101	6	5	1.212891	124.5492	0.214842	-11.845	-0.32018	-1.04897	1.211048	124.398	-0.10566	-11.9213	0.166096	-1.04734
103	O	101	6	5	1.341448	112.9003	-179.806	-11.7567	-0.29348	1.18998	1.341574	113.0366	179.877	-11.8398	-0.36164	1.127597
104	H	103	101	6	0.97021	106.8301	-179.966	-12.7169	-0.32123	1.05434	0.970064	107.3974	179.9659	-12.8013	-0.33552	1.001397
105	C	18	17	14	1.490398	129.3131	-3.11022	-6.72223	2.903232	0.019189	1.498092	128.5265	-7.02916	-6.69786	3.024035	0.093732
106	H	105	18	17	1.096048	112.3026	-59.9683	-7.2985	2.544789	-0.84149	1.094145	112.0045	-71.7474	-7.24395	2.862854	-0.84059
107	H	105	18	17	1.096132	112.1442	60.07061	-7.25128	2.559678	0.915619	1.093552	111.8868	48.27189	-7.25961	2.515405	0.88214
108	H	105	18	17	1.094139	109.7207	179.9938	-6.74918	3.997006	0.010734	1.092122	109.36	168.4646	-6.69737	4.095422	0.305535
109	C	13	12	11	1.490474	124.6167	-179.317	-6.54135	-3.2417	0.162136	1.498096	125.1837	178.8941	-6.64223	-3.15588	0.02662
110	H	109	13	12	1.096303	112.1342	116.8626	-7.08489	-2.91411	1.056075	1.094156	112.0696	108.8854	-7.17203	-2.98762	0.969056
111	H	109	13	12	1.09613	112.2854	-123.209	-7.14102	-2.92812	-0.70017	1.093564	111.8615	-131.045	-7.23059	-2.67458	-0.75956
112	H	109	13	12	1.094117	109.7452	-3.05074	-6.5072	-4.33525	0.171054	1.092151	109.3279	-10.891	-6.624	-4.23108	-0.16416

Table S4 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D2 obtained using M06-2X/6-31G(d,p) method.

D2					Ground state parameters						Excited state parameters					
Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z	Bond	Angle	Dihedral	X	Y	Z
1	C							-9.09142	0.01072	1.209362				-9.15235	-0.27365	1.186085
2	C	1			1.387572			-7.70386	0.006562	1.205118	1.389741			-7.76261	-0.27084	1.183003
3	C	2	1		1.395772	120.182		-7.00583	0.007495	-0.00357	1.399174	120.4958		-7.05563	-0.05537	-0.00504
4	C	3	2	1	1.39652	119.9047	0.010196	-7.70594	0.012843	-1.21191	1.399652	119.4103	-0.06374	-7.76052	0.156856	-1.19547
5	C	4	3	2	1.38643	119.9521	-0.09522	-9.09237	0.015217	-1.20861	1.388561	120.2925	-0.09855	-9.14907	0.151558	-1.19773
6	C	5	4	3	1.396111	120.1377	0.099125	-9.79046	0.014361	0.000438	1.39615	119.9153	0.178809	-9.84648	-0.06259	-0.00736
7	H	1	2	3	1.0857	120.2541	-179.958	-9.63557	0.010688	2.148856	1.083967	120.4702	-179.699	-9.69965	-0.43579	2.107583
8	H	2	1	6	1.088373	120.4221	-179.873	-7.14989	0.001616	2.141946	1.085859	120.2109	179.8349	-7.21385	-0.43134	2.106145

9	H	4	3	2	1.088145	119.4735	179.9444	-7.15468	0.014457	-2.15008	1.085761	119.3484	-179.915	-7.21088	0.322583	-2.11705
10	H	5	4	3	1.086569	121.0717	-179.908	-9.65537	0.017873	-2.13794	1.084651	121.1147	-179.736	-9.70868	0.310343	-2.1132
11	C	3	2	1	4.704158	113.0212	-144.22	-3.05183	-2.53618	0.153552	4.740897	108.7749	-147.016	-3.03158	-2.55786	0.138703
12	C	11	3	2	1.41267	68.70088	68.71077	-4.19604	-3.36099	0.231743	1.42694	68.51381	63.65913	-4.17706	-3.40855	0.15781
13	C	12	11	3	1.380424	108.4491	-0.02367	-5.31771	-2.55796	0.181261	1.372899	108.7562	0.0788	-5.30646	-2.62928	0.112724
14	C	13	12	11	1.430369	106.1324	-0.05703	-4.83989	-1.21426	0.071153	1.449091	106.1524	-0.18228	-4.84697	-1.25567	0.068705
15	N	11	3	2	1.355124	40.093	-110.856	-3.45041	-1.24422	0.062299	1.369375	39.44859	-116.21	-3.46923	-1.26139	0.08572
16	H	12	11	3	1.083725	125.9749	-179.29	-4.19732	-4.44042	0.328176	1.081633	125.5018	-179.665	-4.15638	-4.48897	0.2047
17	C	14	13	12	2.435292	160.6075	-176.454	-4.83263	1.21701	-0.06858	2.432561	161.0625	177.9028	-4.86509	1.173921	-0.05009
18	C	17	14	13	1.430345	160.5363	2.196925	-5.30246	2.567731	-0.09498	1.449118	160.7957	11.4898	-5.34649	2.540731	-0.04496
19	C	18	17	14	1.380333	106.1287	173.5718	-4.17599	3.365267	-0.11278	1.372735	106.1493	172.2504	-4.23004	3.338871	-0.07531
20	C	19	18	17	1.412652	108.4622	0.06358	-3.03652	2.530395	-0.09929	1.427144	108.7625	-0.42452	-3.0709	2.506436	-0.08908
21	N	20	19	18	1.354925	108.7909	-0.21347	-3.44263	1.238123	-0.06881	1.369264	107.9311	-0.00486	-3.48807	1.202454	-0.06689
22	H	19	18	17	1.083745	125.5874	-178.773	-4.1705	4.448994	-0.11568	1.081623	125.7288	-178.855	-4.22629	4.420416	-0.06287
23	C	17	14	13	1.398146	29.43873	-4.46723	-5.52341	0.0031	-0.00486	1.410169	130.6564	179.1818	-5.56979	-0.04689	-0.00163
24	C	20	19	18	1.43704	128.9459	-179.385	-1.64731	2.898044	-0.09742	1.417495	129.4426	-178.976	-1.70096	2.87032	-0.10018
25	H	24	20	19	1.087617	116.062	173.0966	-0.93774	2.08392	0.031522	1.084987	116.2577	174.817	-0.98752	2.056634	-0.02191
26	C	24	20	19	1.349399	123.3198	-6.0654	-1.21707	4.170316	-0.22818	1.36707	123.4395	-4.868	-1.26552	4.162641	-0.196
27	H	26	24	20	1.091732	118.6263	-0.92791	-1.95748	4.962227	-0.3568	1.088438	118.5742	-1.1866	-2.00525	4.955813	-0.28749
28	C	11	3	2	1.436948	162.2835	-111.44	-1.66447	-2.91022	0.166449	1.417442	161.9638	-115.942	-1.65565	-2.89682	0.171067
29	H	28	11	3	1.087461	116.098	5.818701	-0.94861	-2.09196	0.190074	1.085082	116.2088	3.836121	-0.95862	-2.06667	0.220091
30	C	28	11	3	1.349399	123.4721	-175.125	-1.23889	-4.19074	0.169377	1.366975	123.4053	-176.674	-1.19715	-4.18449	0.153761
31	H	30	28	11	1.091741	118.7603	-0.4038	-1.98144	-4.99107	0.168337	1.08829	118.5262	0.438073	-1.92294	-4.994	0.105741
32	C	26	24	20	4.262166	128.0814	179.3345	2.797755	5.601131	-0.2253	4.259564	127.6142	179.5035	2.76021	5.55425	-0.22457
33	C	32	26	24	1.395288	59.12195	179.2556	1.725089	6.478246	-0.38927	1.399942	59.10561	177.4977	1.69058	6.445312	-0.372
34	C	32	26	24	1.398748	60.48812	-0.83476	2.553328	4.234143	-0.05768	1.402758	60.49906	-2.73493	2.503822	4.184942	-0.06028
35	C	33	32	26	1.38542	119.7923	0.439889	0.428623	5.989957	-0.37748	1.38368	119.8348	0.436069	0.391097	5.970497	-0.35042
36	H	33	32	26	1.087261	119.682	-178.556	1.914587	7.537954	-0.54173	1.084846	119.6049	-178.287	1.889439	7.501005	-0.52319
37	C	34	32	26	1.383154	120.2171	0.363013	1.256577	3.752982	-0.06376	1.381855	120.2821	0.25126	1.204267	3.715221	-0.05374
38	H	34	32	26	1.087334	119.4545	-178.598	3.38969	3.556127	0.094272	1.084967	119.3803	-178.375	3.33404	3.501508	0.083973
39	C	35	33	32	1.402932	121.4447	-0.85255	0.16346	4.621228	-0.22099	1.410673	121.5465	-0.76728	0.10977	4.59657	-0.19818
40	H	35	33	32	1.0885	119.4785	-179.892	-0.4043	6.678531	-0.50763	1.086041	119.4117	-179.596	-0.4333	6.666969	-0.47203

41	H	37	34	32	1.087313	118.9115	-179.831	1.090828	2.686877	0.071133	1.084507	118.7123	-179.321	1.034825	2.653219	0.086252
42	C	32	26	24	2.499983	153.5381	52.46073	5.16922	5.615285	-1.01641	2.496367	153.3357	46.35462	5.137714	5.489386	-0.98293
43	C	42	32	26	1.393315	102.1449	0.171225	5.162766	4.608991	-1.98008	1.396747	102.2029	1.035854	5.127504	4.432821	-1.89642
44	C	42	32	26	1.411747	136.1867	178.1521	6.331401	6.367	-0.7384	1.411483	136.1991	178.8776	6.308311	6.23653	-0.73042
45	C	43	42	32	1.388853	117.5733	179.3291	6.352059	4.352842	-2.65007	1.389083	117.491	179.7575	6.324308	4.119934	-2.52834
46	H	43	42	32	1.087128	121.4101	-0.32317	4.260204	4.046702	-2.20605	1.084003	121.5534	0.332155	4.220656	3.880595	-2.11491
47	C	44	42	32	1.39522	119.6693	-178.704	7.513922	6.089715	-1.42499	1.396713	119.8353	-179.057	7.499349	5.902378	-1.37894
48	C	47	44	42	1.387332	119.0036	0.321297	7.518585	5.079596	-2.37595	1.38817	118.9067	0.430601	7.501949	4.83925	-2.27156
49	H	45	43	42	1.087327	119.0633	179.8753	6.374922	3.571202	-3.40558	1.085061	118.9776	179.8205	6.344488	3.301455	-3.24041
50	H	47	44	42	1.08835	120.2952	-179.958	8.41602	6.662416	-1.21826	1.085739	120.3415	-179.954	8.404802	6.471048	-1.19026
51	H	48	47	44	1.08702	119.8883	-179.916	8.43231	4.850543	-2.9184	1.084587	119.8962	-179.875	8.418377	4.564616	-2.7825
52	C	30	28	11	4.262557	127.8034	-179.701	2.780798	-5.60796	0.224032	4.258907	127.7306	179.9192	2.848824	-5.51173	0.236274
53	C	52	30	28	1.398806	60.45569	-6.77844	2.534124	-4.2386	0.080271	1.402711	60.5204	-0.33717	2.57297	-4.13652	0.25357
54	C	52	30	28	1.395412	59.12876	173.4983	1.708055	-6.49255	0.341887	1.399923	59.10912	179.555	1.792194	-6.4291	0.194435
55	C	53	52	30	1.383198	120.2116	0.347886	1.235372	-3.76286	0.067962	1.381861	120.2693	0.372533	1.266068	-3.68796	0.235035
56	H	53	52	30	1.087286	119.4925	-178.319	3.369906	-3.55424	-0.0435	1.085011	119.366	-178.272	3.395455	-3.42889	0.259252
57	C	54	52	30	1.38542	119.8205	0.679348	0.409947	-6.00974	0.307267	1.383638	119.8264	0.239586	0.486094	-5.97348	0.163213
58	H	54	52	30	1.087198	119.6912	-178.413	1.898051	-7.55469	0.475152	1.084908	119.5904	-178.556	2.005424	-7.49277	0.206619
59	C	57	54	52	1.402788	121.4251	-1.26049	0.14277	-4.63839	0.181507	1.410773	121.5311	-0.65386	0.18466	-4.59548	0.186148
60	H	55	53	52	1.087372	118.9507	-179.225	1.066779	-2.69601	-0.05773	1.084514	118.7172	-179.389	1.081847	-2.61921	0.238925
61	H	57	54	52	1.088503	119.4932	179.9435	-0.42288	-6.70463	0.398751	1.086162	119.4449	-179.65	-0.32912	-6.69075	0.136584
62	C	52	30	28	2.499156	152.6084	-136.272	4.60865	-7.1273	-0.54819	2.496366	152.3837	-132.499	4.731025	-6.92369	-0.59771
63	C	62	52	30	1.411737	136.2436	-178.361	5.970614	-7.32571	-0.23404	1.411568	136.1929	-179.748	6.092308	-7.10342	-0.27041
64	C	62	52	30	1.393162	102.1386	3.144155	3.972868	-7.86935	-1.54119	1.396653	102.1918	2.612635	4.139447	-7.60354	-1.66471
65	C	63	62	52	1.395256	119.6819	-179.539	6.700271	-8.30392	-0.91039	1.396699	119.8217	-178.792	6.87008	-8.00257	-1.00347
66	C	64	62	52	1.388851	117.6138	179.9402	4.720903	-8.83565	-2.2012	1.389038	117.492	179.5369	4.933797	-8.49175	-2.3785
67	H	64	62	52	1.087002	121.3865	0.316533	2.930643	-7.69669	-1.79717	1.084009	121.5153	0.137369	3.102637	-7.44018	-1.93566
68	C	65	63	62	1.387402	119.0082	0.440019	6.068848	-9.05793	-1.889	1.388127	118.9108	0.440287	6.283299	-8.6978	-2.05192
69	H	65	63	62	1.088353	120.3339	-179.867	7.750266	-8.46734	-0.6752	1.085767	120.3472	-179.977	7.917916	-8.14776	-0.75883
70	H	66	64	62	1.087346	119.0412	179.8955	4.247293	-9.42953	-2.97922	1.085067	118.9888	179.8686	4.49829	-9.03461	-3.21098
71	H	68	65	63	1.087015	119.8812	-179.867	6.623243	-9.82526	-2.42327	1.084569	119.8897	-179.91	6.872144	-9.40101	-2.63076
72	N	42	32	26	1.395498	27.22563	178.8467	4.121927	6.09049	-0.22599	1.396765	27.24568	178.8849	4.086209	6.027953	-0.23779

73	C	72	42	32	1.395694	108.3181	-179.633	4.605207	7.138756	0.558575	1.396706	108.4469	179.9721	4.57295	7.114873	0.491919
74	C	73	72	42	1.393175	129.3749	-177.795	3.947354	7.894025	1.526942	1.396697	129.4371	-177.336	3.913058	7.932971	1.411713
75	C	73	72	42	1.411755	108.9691	-0.02261	5.97273	7.336159	0.268808	1.411588	108.9481	-0.06619	5.947752	7.27452	0.214406
76	C	74	73	72	1.388852	117.5971	178.6287	4.679855	8.871645	2.187707	1.38906	117.5029	178.4327	4.653345	8.935557	2.025134
77	H	74	73	72	1.087028	121.358	-0.98795	2.900343	7.722319	1.763407	1.083977	121.5228	-0.9737	2.865191	7.788797	1.648765
78	C	75	73	72	1.395175	119.6812	-179.191	6.686384	8.325935	0.945236	1.396666	119.8305	-179.018	6.670352	8.290132	0.844531
79	C	78	75	73	1.387421	118.9978	0.43455	6.033503	9.092352	1.89985	1.388137	118.9149	0.417095	6.015909	9.120905	1.743667
80	H	76	74	73	1.087349	119.0528	179.9162	4.189472	9.475969	2.947079	1.08507	118.9874	179.8459	4.164041	9.586821	2.741942
81	H	78	75	73	1.08836	120.3349	-179.888	7.740577	8.488477	0.728938	1.085742	120.3397	-179.962	7.727983	8.420775	0.636723
82	H	79	78	75	1.087029	119.879	-179.885	6.575255	9.868672	2.434138	1.084575	119.8928	-179.893	6.561293	9.915783	2.240687
83	N	62	52	30	1.395893	27.26871	-178.939	4.106444	-6.0926	0.242825	1.396622	27.2451	-179.337	4.18183	-5.96528	0.256921
84	C	83	62	52	1.395604	108.3046	179.5615	5.136473	-5.62714	1.061421	1.396479	108.4563	-179.727	5.179643	-5.52861	1.130901
85	C	84	83	62	1.411787	108.9692	-0.12589	6.30633	-6.37112	0.794827	1.411551	108.9513	-0.07756	6.37855	-6.21306	0.836581
86	C	84	83	62	1.393323	129.3683	-177.93	5.107942	-4.63649	2.040781	1.396711	129.4133	-177.403	5.097053	-4.6192	2.187758
87	C	85	84	83	1.395245	119.6732	-179.079	7.474355	-6.10096	1.508579	1.39666	119.8222	-179.049	7.52536	-5.96205	1.593205
88	C	86	84	83	1.388848	117.5851	178.5782	6.28306	-4.38719	2.737807	1.389062	117.4845	178.4913	6.251107	-4.38662	2.925023
89	H	86	84	83	1.087102	121.4163	-1.08496	4.199368	-4.0806	2.258179	1.084074	121.5314	-0.94915	4.167569	-4.11819	2.433255
90	C	87	85	84	1.387361	119.0063	0.345301	7.457163	-5.10585	2.475133	1.388159	118.9101	0.405318	7.456481	-5.04337	2.631597
91	H	87	85	84	1.088355	120.2992	-179.929	8.382304	-6.66747	1.31055	1.08574	120.338	-179.953	8.452192	-6.4832	1.373612
92	H	88	86	84	1.087331	119.0529	179.8692	6.288255	-3.61758	3.505896	1.085068	118.9849	179.8227	6.215176	-3.68244	3.749774
93	H	90	87	85	1.087016	119.894	-179.892	8.35946	-4.8822	3.038554	1.084574	119.8947	-179.883	8.337884	-4.83483	3.228206
94	B	21	20	19	1.555676	126.2379	173.1723	-2.53036	-0.01573	-0.19423	1.546112	125.2308	176.3602	-2.56117	-0.03208	-0.15199
95	F	94	21	20	1.384071	110.4108	-66.6735	-1.97599	-0.08461	-1.46055	1.391851	110.8073	-66.7172	-1.95083	-0.10697	-1.40064
96	F	94	21	20	1.390349	110.1293	54.71515	-1.51993	0.030363	0.759706	1.39751	110.2298	53.9721	-1.57239	0.037191	0.833187
97	C	6	5	4	1.481113	117.9472	179.9729	-11.2706	0.017611	-0.05265	1.488551	117.9604	179.8609	-11.3341	-0.05625	-0.05922
98	O	97	6	5	1.212759	124.5135	-0.01825	-11.9215	0.021294	-1.07594	1.210728	124.332	0.083063	-11.9815	0.121113	-1.06684
99	O	97	6	5	1.341174	112.8863	179.98	-11.8362	0.016029	1.16345	1.341033	113.0016	-179.894	-11.9011	-0.26892	1.137319
100	H	99	97	6	0.970248	106.8539	179.9992	-12.7968	0.018384	1.026966	0.970128	107.4588	179.9136	-12.8628	-0.24712	1.011708
101	C	18	17	14	1.490059	129.315	-5.67466	-6.7013	3.08103	-0.08792	1.497217	128.4016	-6.49225	-6.76091	3.028378	0.012282
102	H	101	18	17	1.096044	112.1481	-62.1349	-7.26511	2.756181	-0.96991	1.094031	111.8529	-69.9283	-7.30132	2.82017	-0.91589
103	H	101	18	17	1.096016	112.2291	57.85217	-7.26436	2.738191	0.787676	1.093514	111.8491	50.00963	-7.32266	2.55355	0.821448
104	H	101	18	17	1.093996	109.7234	177.9397	-6.69312	4.174948	-0.07771	1.091864	109.3666	170.2676	-6.76535	4.108206	0.173895

105	C	13	12	11	1.490269	124.5649	-179.23	-6.71965	-3.05824	0.253349	1.497229	125.414	179.2512	-6.71353	-3.1408	0.099158
106	H	105	13	12	1.096362	111.933	113.7976	-7.22592	-2.72761	1.167889	1.094049	111.9101	110.2373	-7.23611	-2.92309	1.035354
107	H	105	13	12	1.095923	112.4516	-126.244	-7.33188	-2.71033	-0.5864	1.09355	111.8233	-129.782	-7.30153	-2.69188	-0.70619
108	H	105	13	12	1.094028	109.7278	-5.89105	-6.72221	-4.15223	0.245589	1.091909	109.3456	-9.56179	-6.70341	-4.22366	-0.04076

Table S5 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D3 obtained using M06-2X/6-31G(d,p) method.

D3					Ground state parameters						Excited state parameters					
Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z	Bond	Angle	Dihedral	X	Y	Z
1	C							-9.17743	0.325976	-1.3459				-9.22627	0.37351	1.362864
2	C	1			1.387707			-7.79165	0.261566	-1.31149	1.389323			-7.83955	0.376698	1.277944
3	C	2	1		1.395784	120.2096		-7.11909	0.253959	-0.08845	1.400111	120.6332		-7.19715	0.029075	0.083461
4	C	3	2	1	1.396755	119.7886	0.06447	-7.84546	0.310074	1.103252	1.400529	119.174	0.04269	-7.9702	-0.32261	-1.03018
5	C	4	3	2	1.386195	120.0853	-0.0372	-9.22981	0.373886	1.070907	1.388142	120.4356	0.093273	-9.35613	-0.32479	-0.95177
6	C	1	2	3	1.396416	119.907	-0.03736	-9.90163	0.382582	-0.1533	1.39655	119.9324	-0.15547	-9.98694	0.022353	0.244861
7	H	1	2	3	1.08571	120.2254	179.9035	-9.70077	0.333486	-2.29713	1.084078	120.4787	179.6585	-9.72096	0.63777	2.290588
8	H	2	1	6	1.088441	120.4128	179.9871	-7.219	0.216944	-2.23604	1.085896	120.1974	-179.742	-7.23999	0.644192	2.142896
9	H	4	3	2	1.088138	119.3678	179.9231	-7.31422	0.302478	2.052869	1.085854	119.2226	179.8585	-7.47285	-0.59011	-1.95763
10	H	5	4	3	1.086651	121.1337	179.9709	-9.81179	0.417658	1.987523	1.084726	121.1268	179.6797	-9.96582	-0.59027	-1.80875
11	C	3	2	1	4.709072	116.4787	-143.11	-3.03894	2.59913	0.078591	4.741196	123.6662	-141.377	-3.20362	-2.51926	-0.10792
12	C	11	3	2	1.414596	68.56811	71.43537	-4.14035	3.483185	-0.0015	1.424666	68.379	82.28346	-4.35133	-3.35169	0.031675
13	C	12	11	3	1.380167	108.5484	0.097212	-5.30034	2.736583	-0.04492	1.375136	108.8357	-0.44274	-5.4718	-2.5567	0.091151
14	C	13	12	11	1.42932	106.2001	-0.10992	-4.89518	1.366887	0.00738	1.446085	106.2256	0.537571	-5.00627	-1.19276	-0.02759
15	N	11	3	2	1.356487	39.99876	-108.289	-3.50632	1.325706	0.078437	1.372384	39.36247	-97.0509	-3.63287	-1.21597	-0.13283
16	H	12	11	3	1.084022	125.8209	-178.503	-4.08375	4.564797	-0.04639	1.08186	125.4909	-178.765	-4.33905	-4.43078	0.108069
17	C	14	13	12	2.434617	160.562	-173.625	-5.01075	-1.06464	-0.03336	2.434886	160.8154	-170.716	-4.99817	1.242109	-0.03364
18	C	17	14	13	1.43002	160.6213	-0.2651	-5.54312	-2.38846	-0.12845	1.44609	161.1707	-15.3643	-5.46021	2.612325	-0.04776
19	C	18	17	14	1.380297	106.1784	175.2233	-4.46016	-3.2429	-0.08	1.375278	106.2326	-176.641	-4.33255	3.397756	-0.10125
20	C	19	18	17	1.414506	108.5304	0.216742	-3.28268	-2.46949	0.047343	1.424307	108.8359	0.373417	-3.18539	2.554023	-0.12947
21	N	20	19	18	1.356313	108.5681	-0.49414	-3.62743	-1.15786	0.066384	1.372771	107.7741	-0.19774	-3.62107	1.252873	-0.08838
22	H	19	18	17	1.083935	125.5631	-179.567	-4.50752	-4.32443	-0.13453	1.081869	125.6276	-179.663	-4.31819	4.479374	-0.11959
23	C	14	13	12	1.397661	131.2008	-178.002	-5.63868	0.184389	-0.04115	1.411092	30.3867	-11.5677	-5.71532	0.027318	0.000275
24	C	20	19	18	1.434433	129.0244	179.0903	-1.92111	-2.90808	0.1539	1.41633	129.6023	179.9816	-1.81264	2.898202	-0.18518
25	H	24	20	19	1.087371	116.238	178.6023	-1.16807	-2.12648	0.220209	1.08521	116.2249	176.5595	-1.10915	2.073192	-0.13903
26	C	24	20	19	1.352595	123.5567	-0.6416	-1.55312	-4.20965	0.159255	1.370031	123.5883	-2.68127	-1.35753	4.187226	-0.27612
27	H	26	24	20	1.092635	118.4374	1.299088	-2.33049	-4.97057	0.056512	1.089012	118.241	-0.43959	-2.09109	4.991187	-0.31466
28	C	11	3	2	1.434999	162.5805	-106.564	-1.63871	2.908488	0.132322	1.416553	162.1344	-96.3844	-1.83571	-2.87776	-0.19113

29	H	28	11	3	1.087976	116.1897	5.448874	-0.95714	2.063684	0.058483	1.08507	116.3141	3.248699	-1.12432	-2.05874	-0.21362
30	C	28	11	3	1.352624	123.0585	-175.265	-1.16588	4.170063	0.252514	1.369976	123.5339	-177.265	-1.39419	-4.17399	-0.23211
31	H	30	28	11	1.092533	118.1305	1.332078	-1.8885	4.985491	0.333268	1.089017	118.2357	0.827062	-2.1354	-4.9716	-0.21277
32	C	26	24	20	4.285229	128.1146	-179.273	2.394479	-5.84084	0.50401	4.279438	128.0729	179.5859	2.696102	5.549437	-0.43755
33	C	32	26	24	1.404944	58.46235	-173.666	1.281687	-6.65822	0.244309	1.411234	58.44027	-179.363	1.611892	6.452467	-0.46221
34	C	32	26	24	1.408332	59.67906	6.248303	2.182228	-4.45613	0.648661	1.414086	59.81947	0.410309	2.413742	4.16644	-0.35251
35	C	33	32	26	1.382586	120.3643	-0.29506	0.01777	-6.10689	0.143879	1.3796	120.2641	-0.08575	0.31536	5.983813	-0.4106
36	H	33	32	26	1.086479	119.9114	179.9115	1.412893	-7.73011	0.124793	1.083489	119.9026	179.824	1.79786	7.518288	-0.52043
37	C	34	32	26	1.380513	120.7168	-0.04348	0.914111	-3.92179	0.538297	1.378075	120.7164	0.014405	1.112557	3.715583	-0.30022
38	H	34	32	26	1.086618	119.78	179.8626	3.023936	-3.79933	0.850868	1.083602	119.6826	-179.836	3.228901	3.453004	-0.32572
39	C	35	33	32	1.403738	122.1068	0.622739	-0.20788	-4.72822	0.281109	1.412185	122.2498	0.185636	0.014662	4.606469	-0.32831
40	H	35	33	32	1.089412	119.0328	-179.846	-0.83014	-6.76119	-0.05553	1.086808	118.9681	179.9407	-0.50364	6.697966	-0.42992
41	H	37	34	32	1.088148	118.434	179.6522	0.791869	-2.84767	0.662353	1.085192	118.315	-179.919	0.940631	2.646141	-0.23405
42	C	32	26	24	2.440357	150.3658	-3.04994	4.808867	-5.53289	0.680764	2.443441	150.5068	-9.23606	5.09419	5.115745	-0.26009
43	C	42	32	26	1.391842	115.8197	73.44331	5.272764	-5.07107	1.909076	1.393579	114.8189	71.676	5.633242	4.371946	-1.30807
44	C	42	32	26	1.40599	113.0917	-72.2422	5.399531	-5.1042	-0.52096	1.404518	114.8318	-75.4877	5.571594	4.96952	1.052682
45	C	43	42	32	1.388803	120.2647	-141.493	6.313899	-4.15358	1.964054	1.390183	120.0232	-143.674	6.642099	3.448556	-1.05873
46	H	43	42	32	1.087843	118.3813	36.78373	4.781842	-5.42441	2.813263	1.085348	118.6291	34.98047	5.233646	4.515369	-2.30693
47	C	44	42	32	1.403271	117.8556	141.3923	6.434704	-4.16005	-0.44248	1.403616	117.946	142.8436	6.577766	4.018756	1.284635
48	C	47	44	42	1.386493	121.2206	1.841967	6.88928	-3.69201	0.780907	1.388212	121.0986	1.611941	7.109744	3.269352	0.24419
49	H	45	43	42	1.086835	120.0675	179.2842	6.665868	-3.78629	2.924482	1.084633	119.9609	179.3841	7.053977	2.86303	-1.87356
50	H	47	44	42	1.088818	118.666	-178.872	6.8889	-3.80495	-1.36613	1.086197	118.8404	-179.074	6.9469	3.882902	2.297111
51	H	48	47	44	1.087007	119.8284	179.7023	7.695881	-2.96414	0.815501	1.084818	119.8107	179.6806	7.890471	2.543813	0.446398
52	C	30	28	11	4.283982	128.8302	-179.145	2.899774	5.512413	0.397692	4.279596	128.0659	-179.269	2.642078	-5.58141	-0.43875
53	C	52	30	28	1.408663	59.76329	1.839375	2.610073	4.144198	0.229189	1.41405	59.81955	0.529555	2.374593	-4.19364	-0.39292
54	C	52	30	28	1.404866	58.39985	-178.699	1.824049	6.409767	0.503618	1.411149	58.44065	-179.66	1.549272	-6.47377	-0.41043
55	C	53	52	30	1.380306	120.7678	-0.03312	1.304205	3.699578	0.181576	1.378104	120.7183	-0.05461	1.079121	-3.72821	-0.32739
56	H	53	52	30	1.086625	119.7553	179.8548	3.422328	3.428763	0.133538	1.083612	119.6787	179.7412	3.196868	-3.48802	-0.40612
57	C	54	52	30	1.382733	120.283	-0.00536	0.52215	5.946662	0.453184	1.379678	120.2625	0.069679	0.258601	-5.99065	-0.34509
58	H	54	52	30	1.086472	120.0141	-179.942	2.012994	7.472807	0.624722	1.083497	119.9021	-179.778	1.723979	-7.54274	-0.4376
59	C	57	54	52	1.403481	122.1752	-0.09303	0.218676	4.585547	0.294983	1.412133	122.2517	-0.09052	-0.02738	-4.60844	-0.30226
60	H	55	53	52	1.088172	118.4732	179.8699	1.123217	2.634909	0.048006	1.085186	118.3097	179.7804	0.918918	-2.65556	-0.29023
61	H	57	54	52	1.089443	118.9582	-179.948	-0.29563	6.661617	0.536613	1.086798	118.9656	-179.875	-0.56719	-6.69681	-0.32227
62	C	52	30	28	2.440157	149.2337	171.7838	4.501187	7.353565	0.398361	2.441637	149.2074	170.6423	4.223423	-7.439	-0.33726
63	C	62	52	30	1.405843	113.2289	-73.2525	4.646435	7.962553	-0.86038	1.404587	114.6498	-75.4927	4.482903	-7.91735	0.957625
64	C	62	52	30	1.39168	115.8168	72.63309	4.557839	8.107116	1.567003	1.393544	114.9117	71.54752	4.183294	-8.30435	-1.42882
65	C	63	62	52	1.403423	117.8479	141.6182	4.799199	9.357067	-0.90027	1.403689	117.9369	142.6914	4.65532	-9.30025	1.125549
66	C	64	62	52	1.389034	120.2703	-141.735	4.731677	9.483819	1.504682	1.390252	120.022	-143.443	4.375165	-9.66861	-1.24236

67	H	64	62	52	1.087855	118.4098	36.57627	4.435066	7.595537	2.51918	1.085369	118.6273	35.21122	3.978643	-7.89227	-2.41185
68	C	65	63	62	1.386289	121.2417	1.797542	4.844053	10.10903	0.263494	1.388256	121.1001	1.628566	4.605504	-10.166	0.041431
69	H	65	63	62	1.088885	118.6335	-179.078	4.89744	9.84372	-1.86938	1.086206	118.8556	-179.089	4.841809	-9.68798	2.122912
70	H	66	64	62	1.086786	120.047	179.2626	4.763398	10.07025	2.419122	1.084634	119.9714	179.41	4.334249	-10.3426	-2.09122
71	H	68	65	63	1.086975	119.8082	179.7091	4.967857	11.18738	0.205602	1.084821	119.8144	179.6882	4.74659	-11.2306	0.194452
72	N	32	26	24	1.39504	178.6432	126.1522	3.669327	-6.39035	0.641621	1.386102	178.8628	123.6591	4.003509	6.003525	-0.5135
73	C	72	32	26	1.427353	119.6225	76.04609	3.919779	-7.71666	0.177375	1.429044	120.3125	68.59978	4.294352	7.39391	-0.35728
74	C	73	72	32	1.391736	119.582	-91.9734	3.774176	-8.78961	1.051737	1.393582	119.5852	-88.5899	4.280261	8.229342	-1.47259
75	C	73	72	32	1.405874	119.4597	84.86037	4.244996	-7.92625	-1.17421	1.404592	119.3092	88.93066	4.53847	7.905126	0.928001
76	C	74	73	72	1.389167	120.2272	175.2103	3.917203	-10.0921	0.590398	1.390245	120.0217	176.162	4.482988	9.596277	-1.32037
77	H	74	73	72	1.087886	118.3975	-3.13201	3.520675	-8.58109	2.088923	1.085376	118.6293	-2.48371	4.086866	7.792494	-2.44717
78	C	75	73	72	1.403181	117.8743	-174.157	4.361656	-9.25054	-1.62316	1.403645	117.941	-175.345	4.722501	9.290299	1.060848
79	C	78	75	73	1.386423	121.2031	-1.98389	4.203268	-10.3199	-0.75503	1.388286	121.1003	-1.61821	4.698384	10.12643	-0.04714
80	H	76	74	73	1.086763	120	-179.261	3.790874	-10.9276	1.273824	1.084639	119.9688	-179.397	4.462111	10.24703	-2.18785
81	H	78	75	73	1.088836	118.6883	178.9113	4.595384	-9.42833	-2.67165	1.086211	118.8496	179.0978	4.897486	9.703272	2.050135
82	H	79	78	75	1.087029	119.797	-179.659	4.304017	-11.3365	-1.12628	1.084819	119.8181	-179.692	4.847972	11.19347	0.078943
83	N	52	30	28	1.394414	178.5769	-109.52	4.21891	5.957105	0.478435	1.386264	178.9148	-123.801	3.943483	-6.05066	-0.52747
84	C	83	52	30	1.426966	119.7864	125.6035	5.283135	5.096153	0.075424	1.429043	120.4071	135.9397	5.046822	-5.16753	-0.31562
85	C	84	83	52	1.405853	119.5354	85.31725	5.656334	5.042793	-1.27894	1.404566	119.3251	88.71868	5.54545	-4.98944	0.985329
86	C	84	83	52	1.391696	119.4979	-91.4263	5.891116	4.271161	1.017	1.393525	119.5716	-88.8403	5.577151	-4.45903	-1.39204
87	C	85	84	83	1.403465	117.8877	-174.254	6.62149	4.096662	-1.65713	1.403637	117.9411	-175.386	6.563666	-4.04219	1.175473
88	C	86	84	83	1.389126	120.2142	175.2297	6.859872	3.356668	0.623445	1.390207	120.0231	176.2229	6.598318	-3.53895	-1.18385
89	H	86	84	83	1.087785	118.4283	-2.99582	5.567937	4.342102	2.053243	1.085352	118.6264	-2.41539	5.161139	-4.62652	-2.38041
90	C	87	85	84	1.386266	121.1845	-1.83508	7.217957	3.266181	-0.72104	1.388202	121.0978	-1.63925	7.086877	-3.32756	0.10652
91	H	87	85	84	1.088776	118.671	178.9895	6.907806	4.032976	-2.70565	1.086205	118.8455	179.0493	6.94921	-3.88136	2.178136
92	H	88	86	84	1.086781	120.0278	-179.163	7.322922	2.70446	1.359177	1.084626	119.9659	-179.378	7.003491	-2.98067	-2.02085
93	H	90	87	85	1.08701	119.7985	-179.734	7.966142	2.544259	-1.03827	1.084829	119.8113	-179.68	7.877178	-2.60413	0.27659
94	B	15	11	3	1.555009	126.2412	-171.703	-2.66915	0.039146	0.327358	1.543878	125.2145	-177.109	-2.72343	0.017434	-0.32042
95	F	94	15	11	1.386044	110.3191	66.54406	-2.20715	0.01082	1.633829	1.395083	110.8476	67.23668	-2.17656	0.040504	-1.60364
96	F	94	15	11	1.390363	110.2265	-54.7997	-1.59357	-0.01213	-0.55219	1.400007	110.2398	-53.0577	-1.67803	-0.00555	0.610512
97	C	6	1	2	1.480544	122.144	179.7579	-11.3801	0.457699	-0.13232	1.487227	118.0015	-179.905	-11.4736	0.003518	0.281528
98	O	97	6	1	1.21297	124.5517	-179.316	-12.0515	0.520497	0.875941	1.21119	124.4186	-0.06657	-12.1779	-0.29205	-0.65846
99	O	97	6	1	1.34162	112.9268	0.630394	-11.9212	0.450878	-1.35995	1.34178	113.056	179.9265	-11.9742	0.351233	1.476878
100	H	99	97	6	0.970176	106.8205	-179.9	-12.8829	0.504219	-1.24317	0.970028	107.3588	-179.943	-12.941	0.310485	1.408717
101	C	18	17	14	1.490729	129.1867	-3.55195	-6.96037	-2.8251	-0.28019	1.498123	128.6342	2.271502	-6.86785	3.124936	-0.03501
102	H	101	18	17	1.096188	112.5952	-55.0939	-7.6115	-2.42217	0.504228	1.093604	111.8635	-47.4335	-7.49619	2.607875	-0.76562
103	H	101	18	17	1.09662	111.8402	64.81242	-7.38705	-2.50054	-1.23683	1.094233	112.1439	72.66343	-7.34454	2.997051	0.941596
104	H	101	18	17	1.094238	109.7773	-175.538	-7.01756	-3.91714	-0.24106	1.092234	109.3162	-167.556	-6.86636	4.190832	-0.27342

105	C	63	62	52	1.45636	122.7017	-39.5363	4.668268	7.204204	-2.10353	1.465773	122.5276	-38.2129	4.59691	-7.02895	2.117901
106	H	105	63	62	1.09034	115.1149	157.1996	4.398104	7.769994	-2.99557	1.087484	115.2343	154.8667	4.373451	-7.48885	3.077681
107	C	105	63	62	1.348855	127.3689	-29.7608	5.10388	5.940454	-2.28405	1.346255	127.1023	-31.5208	5.056429	-5.7636	2.129842
108	H	107	105	63	1.090302	117.146	-172.904	5.155331	5.573715	-3.30953	1.087472	117.3889	-173.496	5.174363	-5.28332	3.098352
109	C	44	42	32	1.456167	122.6815	-39.4903	4.992072	-5.61356	-1.82287	1.465702	122.5349	-38.0047	5.072476	5.77932	2.167755
110	H	109	44	42	1.090298	115.1122	157.2744	5.221564	-4.96264	-2.6669	1.087468	115.2146	154.7621	5.170481	5.324671	3.150748
111	C	109	44	42	1.348875	127.4049	-29.6122	4.490166	-6.83337	-2.105	1.346208	127.1086	-31.5669	4.625442	7.047995	2.113906
112	H	111	109	44	1.090324	117.1431	-172.99	4.349486	-7.08218	-3.15719	1.08748	117.3821	-173.555	4.391136	7.536185	3.056978
113	C	13	12	11	1.490735	124.6563	-179.033	-6.67288	3.308269	-0.15253	1.498152	125.1885	-177.856	-6.87266	-3.05205	0.282695
114	H	113	13	12	1.096231	112.1513	119.5557	-7.19151	2.970612	-1.05737	1.09361	111.8997	130.436	-7.39293	-2.50771	1.075779
115	H	113	13	12	1.096335	112.2576	-120.561	-7.30826	3.025148	0.694867	1.094283	112.0569	-109.538	-7.4746	-2.94346	-0.62468
116	H	113	13	12	1.094167	109.7666	-0.47177	-6.61743	4.400611	-0.18279	1.09218	109.3581	10.24273	-6.84899	-4.11117	0.548332

Table S6 The optimized ground and excited state parameters (bond length, bond angle, and dihedral angle) of D4 obtained using M06-2X/6-31G(d,p) method.

D4					Ground state parameters						Excited state parameters					
Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z	Bond	Angle	Dihedral	X	Y	Z
1	C							9.338525	-0.07636	1.264594				-9.38568	-0.52138	-1.24567
2	C	1			1.387592			7.951002	-0.08197	1.251997	1.389465			-7.99678	-0.50117	-1.21164
3	C	2	1		1.395895	120.2144		7.259491	-0.07728	0.039432	1.399752	120.5781		-7.31784	-0.20282	-0.02449
4	C	3	2	1	1.396612	119.8354	0.053444	7.967671	-0.06804	-1.16428	1.400226	119.2687	0.024928	-8.05391	0.07578	1.133626
5	C	4	3	2	1.386361	120.011	0.047826	9.353983	-0.06455	-1.15318	1.388297	120.3752	0.112461	-9.44175	0.054084	1.105539
6	C	5	4	3	1.396236	120.1257	-0.09398	10.04507	-0.06827	0.060026	1.396409	119.9284	-0.15714	-10.1099	-0.24377	-0.0839
7	H	1	2	3	1.085705	120.2377	179.9038	9.876748	-0.07843	2.207497	1.08402	120.4692	179.7031	-9.90971	-0.74796	-2.16716
8	H	2	1	6	1.088387	120.4174	179.8639	7.391488	-0.09051	2.185516	1.085878	120.2096	-179.791	-7.42509	-0.71231	-2.11038
9	H	4	3	2	1.088169	119.4248	-179.968	7.421843	-0.06391	-2.10564	1.08581	119.2822	179.8814	-7.52745	0.30534	2.055111
10	H	5	4	3	1.086591	121.0932	179.9329	9.922554	-0.05847	-2.07912	1.084703	121.1187	179.6968	-10.0238	0.263217	1.996624
11	C	3	2	1	4.705285	116.7732	-143.085	3.281577	2.430656	-0.12232	4.743062	122.9424	-141.492	-3.36353	2.413501	0.097666
12	C	11	3	2	1.417275	68.57926	73.77022	4.423282	3.270405	-0.12276	1.426251	68.29249	81.84665	-4.53307	3.227609	0.037733
13	C	12	11	3	1.377075	108.5528	0.27602	5.549379	2.4789	-0.08082	1.373876	108.8591	-0.35216	-5.63913	2.413664	-0.0032
14	C	13	12	11	1.433659	106.2271	-0.06352	5.085078	1.122801	-0.05256	1.447512	106.209	0.561732	-5.14284	1.054776	0.045947
15	N	11	3	2	1.354498	40.05699	-106.291	3.692878	1.140962	-0.07556	1.374317	108.2623	-0.8726	-3.77008	1.099114	0.094092
16	H	12	11	3	1.083798	125.8311	-178.611	4.413784	4.354101	-0.13422	1.081808	125.4774	-178.685	-4.5443	4.308729	0.000834
17	C	14	13	12	2.435078	160.7508	-173.926	5.094121	-1.30758	0.098399	2.434553	160.6215	-171.202	-5.09809	-1.37811	-0.0321
18	C	17	14	13	1.426965	160.5303	-3.11873	5.573757	-2.6467	0.212076	1.446436	161.3177	-14.2333	-5.53547	-2.75671	-0.05122
19	C	18	17	14	1.38353	106.1169	177.5926	4.451452	-3.45505	0.246029	1.375504	106.1921	-176.96	-4.39236	-3.5216	-0.06685

20	C	19	18	17	1.409568	108.4352	0.023296	3.308572	-2.63504	0.155022	1.423117	108.7206	0.335854	-3.26311	-2.65571	-0.05004
21	N	20	19	18	1.357433	108.7399	-0.29383	3.706546	-1.33988	0.072519	1.367081	108.0703	-0.20684	-3.71755	-1.36654	-0.02893
22	H	19	18	17	1.083968	125.6268	-178.948	4.453562	-4.53454	0.34445	1.08174	125.7347	-179.589	-4.35572	-4.60249	-0.08951
23	C	14	13	12	1.392656	131.2486	-178.159	5.777044	-0.0832	0.026353	1.408181	30.43897	-10.9575	-5.8337	-0.17789	0.00428
24	C	20	19	18	1.437997	129.1888	-179.971	1.920048	-3.00895	0.149742	1.424195	129.5551	179.9335	-1.87519	-2.97504	-0.05563
25	H	24	20	19	1.087646	115.8646	171.9037	1.20767	-2.1891	0.207578	1.085209	115.9775	175.7116	-1.19377	-2.13235	-0.11237
26	C	24	20	19	1.348709	123.7502	-7.71039	1.487899	-4.28497	0.086266	1.361319	123.6774	-3.72895	-1.39308	-4.24716	-0.0059
27	H	26	24	20	1.091875	118.764	-0.60167	2.226019	-5.08728	0.02563	1.088543	118.7059	-0.51171	-2.10053	-5.07261	0.049451
28	C	11	3	2	1.432255	162.5247	-104.266	1.896898	2.795794	-0.14861	1.410656	162.0885	-95.9956	-2.00505	2.79212	0.131079
29	H	28	11	3	1.087414	116.2327	3.71887	1.183223	1.982616	-0.03962	1.084936	116.3979	2.204409	-1.27884	1.98688	0.094983
30	C	28	11	3	1.353814	123.185	-177.071	1.469901	4.073401	-0.28355	1.376161	123.5886	-178.255	-1.58046	4.099535	0.19599
31	H	30	28	11	1.092489	118.2477	0.790925	2.219819	4.860702	-0.3899	1.088809	118.2223	1.200434	-2.33414	4.883916	0.243126
32	C	26	24	20	4.26981	127.7397	-179.69	-2.54798	-5.67797	0.036282	4.270517	127.635	179.7342	2.69253	-5.49006	-0.02457
33	C	32	26	24	1.394976	58.94125	179.6667	-1.47771	-6.57073	-0.02253	1.398521	58.89833	179.5304	1.65374	-6.42363	0.047656
34	C	32	26	24	1.397151	60.15061	-0.46414	-2.28616	-4.30785	0.115364	1.398038	60.27173	-0.19114	2.381857	-4.12835	-0.08568
35	C	33	32	26	1.387355	120.1305	0.243845	-0.17384	-6.09726	0.000075	1.386465	120.1643	0.110853	0.334024	-5.99863	0.050094
36	H	33	32	26	1.088569	119.4292	179.9578	-1.67538	-7.63958	-0.08141	1.086311	119.3836	179.8274	1.891223	-7.48252	0.096997
37	C	34	32	26	1.384041	120.7502	-0.13377	-0.98519	-3.83601	0.13561	1.38555	120.7406	0.00741	1.06362	-3.70176	-0.08076
38	H	34	32	26	1.088683	118.6579	179.4132	-3.12672	-3.61701	0.153286	1.085854	118.6563	179.8731	3.195019	-3.41042	-0.13491
39	C	35	33	32	1.402723	121.2984	-0.2056	0.101527	-4.72401	0.077408	1.408779	121.3197	-0.23374	0.005233	-4.63027	-0.01438
40	H	35	33	32	1.088767	119.6664	-179.962	0.655812	-6.80075	-0.04683	1.086276	119.6195	-179.922	-0.46586	-6.73133	0.107764
41	H	37	34	32	1.087425	119.1887	179.7466	-0.81062	-2.76424	0.193439	1.08478	118.9869	-179.942	0.855014	-2.63837	-0.13011
42	C	32	26	24	2.404928	145.4865	83.08782	-4.4819	-6.1	-1.32956	2.404021	145.5308	83.89312	4.655848	-5.86623	1.310789
43	C	42	32	26	1.39831	97.27417	47.11111	-3.8248	-6.77439	-2.36333	1.400754	94.36246	39.74383	3.948939	-6.41954	2.386073
44	C	42	32	26	1.400613	133.5454	-96.5201	-5.64152	-5.36743	-1.61299	1.401273	137.9421	-105.086	5.887849	-5.24224	1.548224
45	C	43	42	32	1.38839	120.8331	-150.944	-4.31358	-6.73501	-3.66224	1.389915	120.7811	-154.384	4.461928	-6.36731	3.6768
46	H	43	42	32	1.08712	119.2378	29.04521	-2.92016	-7.33476	-2.14097	1.084007	119.5222	25.28715	2.988107	-6.88901	2.208666
47	C	44	42	32	1.394685	118.9799	139.1844	-6.13288	-5.35829	-2.91822	1.395781	119.1688	140.4602	6.398715	-5.21737	2.846916
48	C	47	44	42	1.389341	121.4651	-1.8451	-5.4772	-6.02673	-3.94465	1.390711	121.4388	-1.7119	5.695618	-5.7668	3.91362
49	H	45	43	42	1.087321	119.6651	-179.94	-3.78796	-7.26722	-4.45138	1.085088	119.5021	-179.946	3.897185	-6.80336	4.49432
50	H	47	44	42	1.089498	118.5155	179.2877	-7.04197	-4.79558	-3.12782	1.086803	118.5432	179.27	7.360693	-4.7413	3.017507
51	H	48	47	44	1.087137	120.1955	-179.041	-5.87015	-5.99302	-4.95772	1.084882	120.2672	-179.094	6.104013	-5.72395	4.917785
52	C	30	28	11	4.284767	128.4963	-179.56	-2.55311	5.544995	-0.37874	4.276724	127.8045	-179.304	2.442564	5.548779	0.268864
53	C	52	30	28	1.410359	59.63941	0.786883	-2.3018	4.167158	-0.21284	1.418973	59.69609	2.162404	2.184425	4.158253	0.153595
54	C	52	30	28	1.406948	58.32664	179.8405	-1.44783	6.408364	-0.49034	1.416143	58.32153	-179.062	1.334137	6.427913	0.331908
55	C	53	52	30	1.379533	120.8098	-0.0907	-1.01034	3.683073	-0.18271	1.37483	120.8036	-0.07907	0.895287	3.681012	0.130784

56	H	53	52	30	1.086012	119.7098	179.3746	-3.13355	3.478271	-0.0986	1.082877	119.6904	179.1561	3.011514	3.464294	0.070127
57	C	54	52	30	1.381592	120.4354	0.07	-0.16123	5.905966	-0.45791	1.376479	120.3987	0.02589	0.050066	5.932696	0.307063
58	H	54	52	30	1.086116	119.8661	179.8406	-1.60557	7.476665	-0.60653	1.082989	119.803	179.9328	1.497706	7.496207	0.401604
59	C	57	54	52	1.404156	122.1375	-0.30212	0.101667	4.534771	-0.30836	1.415585	122.2875	-0.24679	-0.22433	4.547094	0.213833
60	H	55	53	52	1.0881	118.381	179.7474	-0.86189	2.613525	-0.04858	1.08497	118.2535	179.4885	0.745436	2.610914	0.032832
61	H	57	54	52	1.089347	118.9837	179.7377	0.677128	6.595339	-0.55067	1.086607	118.9816	179.7949	-0.78342	6.62782	0.360081
62	C	52	30	28	2.444112	148.5638	163.8596	-4.08416	7.442399	-0.20723	2.44512	148.7568	171.2587	3.983816	7.444413	0.170248
63	C	62	52	30	1.397989	114.1148	-75.9994	-4.30073	7.885139	1.10099	1.39778	117.1238	-81.5795	4.308171	7.936757	-1.0971
64	C	62	52	30	1.390087	116.5376	73.39697	-4.10318	8.324194	-1.28167	1.39123	113.7904	68.98147	3.92232	8.276228	1.283721
65	C	63	62	52	1.393041	118.4099	148.0297	-4.54414	9.240703	1.310186	1.394513	118.2932	148.3416	4.57883	9.298492	-1.22783
66	C	64	62	52	1.391521	119.5642	-146.78	-4.33689	9.677161	-1.05543	1.392867	119.2743	-148.706	4.183057	9.636167	1.133186
67	H	64	62	52	1.088161	119.0454	32.97812	-3.93014	7.938849	-2.2845	1.08566	119.3428	31.12604	3.669568	7.852696	2.250879
68	C	66	64	62	1.391729	119.753	-0.38025	-4.55689	10.13269	0.241107	1.393486	119.8323	-0.52604	4.511687	10.1442	-0.12209
69	H	65	63	62	1.08914	119.2446	179.5172	-4.72252	9.59916	2.32306	1.086365	119.3127	179.5804	4.839438	9.697643	-2.20402
70	H	66	64	62	1.086904	119.971	179.8371	-4.35056	10.37287	-1.89039	1.084656	119.8939	179.8255	4.135146	10.29432	1.994013
71	H	68	66	64	1.08734	119.9598	-179.841	-4.74242	11.1888	0.421445	1.085027	119.9186	-179.766	4.718778	11.20271	-0.24023
72	N	42	32	26	1.42562	32.81489	-177.956	-3.91243	-6.11162	-0.02267	1.428532	32.96235	-178.153	4.073179	-5.87741	0.006536
73	C	72	42	32	1.417352	126.0932	179.0919	-4.57431	-6.48664	1.173228	1.419272	125.8155	-171.218	4.678724	-6.39239	-1.16924
74	C	73	72	42	1.407301	117.375	151.4803	-3.78582	-7.02211	2.20863	1.409807	117.8981	152.8352	3.833439	-6.86249	-2.19494
75	C	73	72	42	1.41319	124.5832	-29.2039	-5.96226	-6.347	1.399514	1.415828	124.3378	-28.8743	6.075724	-6.43392	-1.39559
76	C	74	73	72	1.384655	122.2533	-179.079	-4.32988	-7.43877	3.411821	1.386605	122.27	-178.841	4.327877	-7.40532	-3.37117
77	H	74	73	72	1.085247	119.0873	0.54435	-2.71512	-7.11885	2.060315	1.08124	119.4979	1.056799	2.761064	-6.80395	-2.06978
78	C	75	73	72	1.399698	118.1822	178.352	-6.48138	-6.79452	2.61992	1.400341	118.342	178.2048	6.539439	-7.0051	-2.58709
79	C	78	75	73	1.38546	123.3112	1.341798	-5.69963	-7.34133	3.624594	1.386772	123.3941	1.693629	5.69989	-7.50189	-3.57273
80	H	76	74	73	1.087606	119.2602	179.8108	-3.67529	-7.84833	4.177755	1.085402	119.0888	179.7129	3.629895	-7.75579	-4.12489
81	H	78	75	73	1.090039	117.4067	179.9162	-7.55318	-6.67942	2.78168	1.087374	117.3587	-179.879	7.615197	-7.03046	-2.74356
82	H	79	78	75	1.086849	120.6019	179.4902	-6.14833	-7.66739	4.559257	1.08444	120.6813	179.5783	6.106872	-7.92932	-4.4825
83	N	52	30	28	1.389584	178.9872	172.1396	-3.84917	6.045233	-0.40894	1.377123	178.9788	166.5906	3.729691	6.038079	0.287751
84	C	83	52	30	1.429933	121.5138	-172.285	-4.98538	5.184556	-0.29503	1.431959	122.2854	-166.613	4.874993	5.179728	0.242764
85	C	84	83	52	1.402484	122.09	108.4012	-5.7844	5.154004	0.857184	1.402321	121.6585	114.8913	5.761461	5.191623	-0.84376
86	C	84	83	52	1.398768	117.4172	-72.9901	-5.29845	4.381918	-1.39699	1.400326	117.5386	-66.8172	5.103395	4.346628	1.344894
87	C	85	84	83	1.400813	117.3169	178.3114	-6.89432	4.299452	0.847313	1.402023	117.1945	178.2946	6.872152	4.338892	-0.77389
88	C	86	84	83	1.385126	121.0316	-179.301	-6.39131	3.531224	-1.37325	1.386273	120.7776	-179.307	6.200026	3.499262	1.378401
89	H	86	84	83	1.088255	118.0631	0.768359	-4.65745	4.444078	-2.27423	1.085942	118.3121	0.77865	4.399236	4.38061	2.170893
90	C	87	85	84	1.386027	122.2858	0.861311	-7.1992	3.494394	-0.23897	1.38754	122.2734	0.788515	7.094329	3.498779	0.307834
91	H	87	85	84	1.089961	118.0952	-179.606	-7.52781	4.270584	1.733806	1.087194	118.1763	-179.794	7.571679	4.337795	-1.60614

92	H	88	86	84	1.086871	120.1567	-179.87	-6.62027	2.912246	-2.23681	1.084606	120.0588	-179.711	6.363148	2.855504	2.235919
93	H	90	87	85	1.087167	119.96	179.6094	-8.06688	2.840335	-0.20345	1.084876	119.9505	179.4865	7.962285	2.848021	0.318907
94	B	15	11	3	1.554669	126.1458	-173.616	2.786038	-0.1158	-0.19882	1.542755	125.7846	177.6208	-2.83156	-0.12004	0.207854
95	F	94	15	11	1.384974	110.4704	66.39257	2.238957	-0.19568	-1.46865	1.393607	110.9726	-109.059	-2.23682	-0.17591	1.466941
96	F	94	15	11	1.391262	110.0946	-54.8885	1.767593	-0.06505	0.747653	1.399082	110.2799	130.3554	-1.82578	-0.04993	-0.76216
97	C	6	5	4	1.480797	117.945	-179.923	11.52519	-0.06253	0.015542	1.487752	117.9899	-179.928	-11.5975	-0.25346	-0.0655
98	O	97	6	5	1.21288	124.5381	0.038774	12.18249	-0.05412	-1.00376	1.210991	124.3826	0.118393	-12.2709	-0.01796	0.913084
99	O	97	6	5	1.341405	112.9072	-179.971	12.08422	-0.06741	1.234896	1.341468	113.0327	-179.869	-12.1352	-0.55354	-1.25729
100	H	99	97	6	0.970215	106.8302	-179.991	13.04545	-0.06296	1.10325	0.97008	107.3997	-179.969	-13.0996	-0.53647	-1.15305
101	C	18	17	14	1.491071	129.382	-1.34586	6.97612	-3.14458	0.305817	1.497605	128.565	2.115708	-6.93372	-3.29287	-0.03531
102	H	101	18	17	1.096042	112.5505	-54.716	7.603226	-2.7928	-0.52141	1.093608	111.843	-47.5993	-7.54419	-2.81447	0.735683
103	H	101	18	17	1.0965	111.9871	65.31822	7.466657	-2.81825	1.230584	1.094249	112.0504	72.43908	-7.44508	-3.13505	-0.98977
104	H	101	18	17	1.094196	109.7153	-175.035	6.981011	-4.23869	0.292971	1.092104	109.3408	-167.792	-6.90704	-4.36689	0.160805
105	C	63	62	52	1.49859	118.2233	-35.1879	-4.33182	6.865076	2.198385	1.504578	118.0488	-34.375	4.406581	6.9555	-2.23342
106	H	105	63	62	1.099478	110.2304	53.00878	-3.42491	6.244331	2.166267	1.095822	109.8399	51.85562	3.498184	6.344127	-2.27659
107	H	105	63	62	1.096445	109.8189	170.3125	-4.33581	7.367492	3.172938	1.093171	109.8586	169.6334	4.481819	7.492708	-3.18251
108	C	85	84	83	1.513185	126.025	-0.58352	-5.57364	5.978367	2.108476	1.52046	126.1265	-1.24769	5.638409	6.05145	-2.0917
109	H	108	85	84	1.101116	107.5653	118.2222	-6.45982	6.61905	2.237518	1.097077	107.4579	119.7411	6.533855	6.68297	-2.14588
110	H	108	85	84	1.098713	107.8369	-128.679	-5.58339	5.294004	2.967966	1.095507	107.6412	-126.494	5.686108	5.385153	-2.95998
111	C	44	42	32	1.492806	119.7116	-44.4758	-6.37251	-4.68187	-0.50658	1.497535	119.4429	-43.4964	6.670561	-4.69552	0.394499
112	H	111	44	42	1.099915	110.8396	55.65558	-5.7037	-4.00294	0.042565	1.096628	110.6166	54.13446	6.055908	-4.00657	-0.19723
113	H	111	44	42	1.096306	109.6103	173.649	-7.18107	-4.07004	-0.92345	1.093189	109.7067	172.8783	7.533639	-4.13697	0.766226
114	C	75	73	72	1.50883	125.9686	-3.74206	-6.95438	-5.71183	0.456738	1.516364	126.1109	-5.11604	7.145015	-5.84929	-0.49327
115	H	114	75	73	1.09771	107.4105	-147.819	-7.73409	-5.2406	1.069078	1.094424	107.142	-146.559	7.957878	-5.50277	-1.13898
116	H	114	75	73	1.101068	110.4303	97.47809	-7.46923	-6.48347	-0.13644	1.097106	110.5972	98.01515	7.574028	-6.62695	0.150806
117	C	13	12	11	1.489872	124.6328	-179.273	6.946642	2.995201	-0.05241	1.498077	125.2154	-177.965	-7.0562	2.886741	-0.11421
118	H	117	13	12	1.096027	112.1734	121.8229	7.497249	2.650191	0.830247	1.093486	111.8853	129.6957	-7.59674	2.370962	-0.91265
119	H	117	13	12	1.096121	112.1297	-118.274	7.523728	2.673086	-0.92687	1.09405	111.9994	-110.255	-7.61755	2.719893	0.809906
120	H	117	13	12	1.094033	109.7541	1.687959	6.936446	4.089111	-0.03958	1.092062	109.3322	9.528395	-7.06414	3.957805	-0.32719

NA: The atom that the actual atom has a distance (RN) with. • NB: The actual atom has an angle (AN) with atoms NA and NB. • NC: The actual atom has a dihedral angle (DN) with atoms NA, NB, and NC. It is the angle between the actual atom and atom NC when looking down the NA-NB axis.

Table S7 The list of frequencies for optimized ground and excited state geometries of four dyes obtained using M06-2X/6-31G(d,p) method.

D1	Ground State		Excited State		D2	Ground State		Excited State		D3	Ground State		Excited State		D4	Ground State		Excited State	
Mod e	Frequenc y	Infrare d	Frequenc y	Infrare d	Mod e	Frequenc y	Infrare d	Frequenc y	Infrare d	Mod e	Frequenc y	Infrare d	Frequenc y	Infrare d	Mod e	Frequenc y	Infrare d	Frequenc y	Infrare d
1	6.46	0.0602	7	0.0602	1	5.99	0.0126	5.6	0.1108	1	7.07	0.0331	6.63	0.0791	1	7.45	0.0127	6.55	0.0651
2	7.44	0.0061	8.56	0.2295	2	8.16	0.0177	6.8	0.0021	2	7.79	0.0089	7.35	0.0607	2	8.23	0.0387	8.93	0.0441
3	8.04	0.021	10.37	0.1627	3	9.18	0.0129	7.77	0.0798	3	9.48	0.0251	9.75	0.0038	3	10.46	0.0804	9.61	0.0938
4	11.64	0.137	11.71	0.3893	4	10.18	0.0458	10.65	0.1527	4	11.54	0.5898	11.41	0.6565	4	10.81	0.0635	11.31	0.2386
5	13.77	0.2612	12.51	0.2648	5	12.48	0.0529	11.03	0.0642	5	12.53	0.0598	13.87	0.0578	5	13.41	0.3723	12.09	0.1527
6	17.96	0.4779	17.85	0.255	6	17.99	0.0738	17.86	0.0243	6	18.54	0.3081	17.82	0.0818	6	18.48	0.144	17.04	0.375
7	25.01	1.9654	24.88	1.8232	7	24.43	0.6002	20.66	1.6654	7	22.06	1.6617	20.3	1.2684	7	20.94	0.2097	19.98	0.1738
8	26.26	0.6524	26.22	0.6727	8	26.05	0.7746	25.96	0.1371	8	23.81	0.5498	21.65	3.6819	8	22.8	0.802	23.16	0.7371
9	27.42	1.5318	28.26	0.7083	9	27.82	0.4655	27.16	0.2073	9	26.68	0.9047	28.09	0.1679	9	24.99	0.8199	24.59	1.0472
10	30.91	0.6911	32.89	0.895	10	34.2	2.5372	34.63	3.7493	10	29.01	1.3873	32.35	3.1909	10	27.34	0.5166	27.26	0.1835
11	34.97	1.7916	34.87	3.518	11	35.12	1.0937	38.78	0.6953	11	30.42	2.3634	34.22	2.0152	11	30.78	0.5736	33.46	3.2496
12	35.21	1.7499	38.55	1.3948	12	43.07	0.2395	44.91	0.1961	12	45.11	0.1552	43.3	0.8329	12	34.66	3.1777	36.28	1.8036
13	36.03	2.5774	42.23	6.605	13	55.61	0.9789	56.25	0.4161	13	46.58	0.0411	45.17	0.0684	13	40.15	0.1708	41.82	0.1253
14	38.67	10.7162	43.39	8.8969	14	64.58	1.1313	62.36	1.8385	14	50.65	0.0302	53.84	0.6933	14	45.63	0.7016	46.88	1.1063
15	41.46	4.8838	44.28	15.1132	15	66.2	5.3323	68.68	0.4488	15	53.55	0.4821	55.32	2.2493	15	46.93	0.6582	49.86	1.3633
16	50.12	0.1798	54.69	0.1848	16	67.55	3.9701	71.71	16.0022	16	53.77	0.1689	55.84	2.4065	16	52.08	0.0061	54.18	1.2949
17	56.39	0.8413	59.85	0.9084	17	70.22	0.3668	73.28	20.6231	17	55.33	0.0342	57.61	0.1654	17	53.7	0.2061	57.14	0.5968
18	64.91	0.9242	64.67	2.0739	18	77.3	0.4016	81	0.1643	18	55.91	1.4163	58.42	0.2442	18	62.07	1.587	65.25	0.6973
19	69.94	1.0129	68.27	0.2383	19	86.5	0.7643	88.33	2.9407	19	62.76	0.5628	62.56	0.1006	19	64.66	0.5383	68.62	3.2451
20	70.51	1.4898	69.17	1.8263	20	92.51	0.2065	99.08	6.813	20	64.14	1.9007	74.49	4.1654	20	76.97	0.4439	80.51	0.9166
21	71.68	2.7362	71.23	1.8853	21	98.57	12.1124	101.45	0.5466	21	78.99	0.794	81.54	1.3358	21	85.19	0.4231	87.94	1.9536
22	77.49	0.9239	82.91	3.3433	22	101.33	0.6995	109.1	0.2739	22	88.02	0.2819	99.14	0.2554	22	91.42	0.4858	95.52	2.1663
23	86.52	0.2961	87.26	0.547	23	105.35	2.2906	113.21	2.002	23	98.55	0.1445	100.87	0.6696	23	94.09	3.2937	99.21	1.1601
24	88.2	0.3217	92.91	0.9431	24	112.61	0.8215	113.58	2.1321	24	100.77	0.327	101.98	1.6265	24	98.2	2.2854	100.25	0.6031
25	91.25	1.4411	95.23	5.3673	25	113.23	1.6426	116.42	1.5353	25	102.09	0.0615	103.37	0.0806	25	100.48	2.4196	103.54	0.7655
26	96.06	0.8032	109.28	0.6511	26	135.01	1.2058	137.1	1.0624	26	110.31	19.8895	112.39	14.0554	26	105.89	4.4574	109.12	0.4252
27	105.48	0.1366	111.4	7.1391	27	147.28	7.3959	147.95	2.2741	27	115.12	0.5212	114.87	2.2241	27	109.22	4.0654	114.42	4.0022
28	112.67	16.3086	116.53	0.0082	28	155.13	4.2273	156.14	10.9708	28	138.67	2.1741	140.04	2.0913	28	123.7	2.1118	125.18	1.2377
29	114.96	0.1793	118.25	10.538	29	157.05	4.388	157.14	11.703	29	148.67	1.8261	153.43	1.1456	29	143.88	3.697	146.65	11.9809
30	140.57	2.7341	142.95	1.1677	30	164.48	1.4387	168.11	3.9046	30	149.83	1.1881	153.71	9.9701	30	146.21	0.8065	148.59	0.2378
31	156.34	34.1134	159.28	33.1664	31	170.48	1.5545	173.78	1.1007	31	154.04	27.9379	157.51	8.3802	31	149.8	9.0848	152.69	0.2833
32	161.34	1.7377	164.58	6.1982	32	174.94	2.0129	180.68	1.1733	32	159.84	1.6295	162.89	19.0532	32	163.18	1.423	164.26	1.1555
33	169.66	1.9964	173.08	1.4762	33	180.88	0.8714	184.03	2.2299	33	167.94	0.7119	170.71	5.4771	33	163.96	5.743	166.1	8.3272
34	175.96	0.2092	180.54	1.4654	34	181.53	0.6559	203.16	1.7787	34	172.32	14.4683	175.91	9.5873	34	166.67	10.0016	170.06	3.1605
35	178.44	2.8261	183.86	1.8093	35	185.81	4.2776	205.14	0.4768	35	173.9	7.0985	181.51	1.1183	35	171.17	5.9591	178.58	3.4044
36	181.52	1.873	201.95	1.0848	36	202.12	0.5207	215.98	0.8712	36	178.08	5.5456	198.34	3.6984	36	177	2.0792	187.75	1.9279
37	182.82	3.7345	206.65	0.7566	37	205.57	0.662	216.9	0.8027	37	181.14	3.4861	200.02	4.1149	37	182.65	3.3115	192.67	1.2136
38	196.07	1.6858	211.67	0.6418	38	213.85	15.0365	218.52	0.015	38	183.73	5.6598	205.66	1.6938	38	185.76	0.2767	198.15	0.2607
39	198.68	1.5061	216.63	0.761	39	217.68	1.1957	219.14	0.3125	39	196.78	5.1867	210.67	2.1055	39	188.12	7.1521	199.58	1.5116
40	223.65	0.7701	224.84	0.4784	40	230.3	2.0123	229.2	1.7667	40	220.87	1.8925	229.74	0.7836	40	194.91	3.0704	214.29	0.4211
41	227	0.3672	230	0.6307	41	234.3	2.4553	230.82	0.3961	41	227.81	2.8352	237.74	0.3504	41	207.94	0.2503	221.96	0.6315
42	231.18	1.8373	233.13	1.4686	42	235.98	0.6048	235.95	1.916	42	232.4	0.5902	243.26	27.9885	42	225.14	0.6392	228.8	0.5382
43	239.8	0.5805	241.98	4.5867	43	252.63	1.2203	250.46	1.3339	43	243.96	0.1751	246.21	10.1051	43	229.75	3.241	232.73	0.6034

44	242.79	2.7325	244.31	2.4262	44	264.01	4.1442	265.48	9.1907	44	246.63	0.9323	247.1	4.7637	44	241.04	3.7277	240.57	2.662
45	250.98	1.9459	251.83	11.4212	45	266.85	0.6752	268.82	1.3342	45	249.03	0.3604	249.36	11.9455	45	244.57	0.329	246.47	3.5647
46	251.62	10.6074	253.59	9.9613	46	291.82	13.5837	292.11	36.5805	46	249.14	0.2737	251.89	3.4966	46	253.07	2.0461	251.69	3.0883
47	252.65	2.9778	254.83	8.573	47	296.84	4.5939	296.72	9.4428	47	254.63	4.7207	253.85	2.942	47	259.22	1.9644	259.05	22.0374
48	276.32	3.2348	277.01	83.8543	48	297.12	1.7318	296.92	22.3482	48	283.49	35.3715	284.93	20.0411	48	269.16	2.7325	268.49	6.417
49	294.69	31.3811	293.51	9.0875	49	303.8	23.2352	301.67	0.1222	49	304.1	6.1919	304.47	13.3008	49	280.31	10.4747	281.09	2.8668
50	297.33	12.4066	296.29	76.3911	50	316.67	7.7671	317.24	48.4886	50	306.97	2.0128	307.55	1.4971	50	290.21	6.0496	287.91	22.5986
51	311.79	3.8585	312.18	5.9291	51	318.38	14.252	320.67	1.0041	51	315.11	3.2577	317.82	60.9071	51	291.41	32.569	291.36	9.7211
52	316.35	0.2669	318.98	6.7773	52	320.63	0.493	325.6	13.7143	52	317.18	23.8696	321.3	0.4372	52	309.23	4.8033	308.6	16.0975
53	318.38	0.3471	322.31	2.1681	53	331.2	4.7453	334.01	16.3641	53	319.19	0.767	326.75	1.7576	53	313.28	1.8188	313.69	1.7334
54	324.13	1.9977	327.66	4.6266	54	357.51	1.4494	352.97	2.537	54	331.08	8.1423	331.66	0.1681	54	316.99	1.272	317.87	6.412
55	329.86	1.1525	329.63	1.5769	55	358.47	3.0953	356.73	0.7637	55	333.11	1.0099	332.41	0.1616	55	318.16	0.7072	320.75	1.8048
56	341.37	20.1661	341.49	1.2146	56	364.05	12.2059	364.71	15.4728	56	334.86	2.8151	334.73	4.9164	56	319.15	4.551	327.15	2.3388
57	349.05	0.9327	348.33	9.1197	57	391.8	1.3741	379.54	6.8373	57	335.85	7.451	335.07	5.8705	57	329.35	1.8478	329.46	0.7057
58	355.98	4.5964	351.46	3.9997	58	393.94	13.378	391.2	1.3576	58	344.1	2.2131	340.52	7.7921	58	340.91	0.569	339.08	10.7035
59	356.93	2.3262	354.12	0.7004	59	411.09	27.9628	405.88	9.1996	59	344.94	12.4043	343.53	1.4359	59	341.28	1.5333	341.11	1.7088
60	360.25	17.9803	360.84	7.5916	60	413.23	0.4259	408.57	12.0817	60	347.75	7.3097	349.36	0.3005	60	346.87	6.9337	346.75	0.3069
61	398.42	11.2701	381.75	12.8325	61	415.67	0.5434	417.21	32.1476	61	361.29	6.1367	359.59	6.7694	61	350.56	2.6852	347.93	6.173
62	401.65	8.5105	400.96	5.9389	62	419.66	19.811	417.87	30.0328	62	365.77	3.334	365.57	0.1844	62	369.17	13.3741	368.44	14.0466
63	413.71	0.6927	408.76	3.17	63	423.82	0.1313	420.22	64.1337	63	397.18	19.2913	381.48	5.9415	63	376.55	0.2859	372.97	5.9282
64	416.7	17.2515	418.25	60.4475	64	435.41	1.1288	426.54	22.0655	64	402.25	0.5727	400.45	9.1013	64	378.67	19.3051	379.26	9.833
65	418.84	22.981	419.17	0.7826	65	437.01	6.1759	437.3	14.9637	65	403.26	1.1799	402.05	2.8433	65	402.32	8.2543	388.13	2.9549
66	419.59	4.6977	419.77	4.4651	66	440.14	1.2686	438.45	0.1222	66	405.57	7.6722	403.58	12.0781	66	408.2	8.0972	407.59	1.4274
67	420.12	1.8898	419.93	13.2244	67	440.89	2.3433	439.82	2.7416	67	413.19	0.5367	407.01	0.4423	67	413.66	0.3497	409.44	3.7283
68	424.41	2.9075	420.52	14.0593	68	442.12	4.7161	440.08	5.1393	68	417.82	0.013	419.95	2.2103	68	418.75	1.6982	419.49	2.6049
69	426.56	3.7191	425.57	53.1025	69	451.07	19.6213	453.04	1.4228	69	422.72	0.4013	421.37	0.3073	69	426.3	3.0262	422.03	3.253
70	428.02	8.4756	426.83	37.6054	70	459.76	13.3014	458.68	12.5435	70	430.92	4.5081	422.33	2.5234	70	431.01	18.4535	428.86	5.3316
71	431.84	16.2026	436.57	13.324	71	461.63	13.1846	462.13	40.8823	71	439.75	27.8886	440.92	82.1944	71	437.17	1.181	432.29	3.7891
72	446.82	1.3887	446.94	1.8824	72	462.55	13.2504	462.82	45.3788	72	450.58	0.3647	450.37	13.1423	72	442.06	6.5075	443.49	10.9307
73	453.73	4.5509	457.83	17.5955	73	488.44	5.2206	480.67	1.7252	73	470.29	21.8655	466.88	59.4271	73	451.06	9.6879	450.94	8.5052
74	460.53	3.8097	461.32	5.6287	74	490.44	0.2282	482.8	3.418	74	472.83	4.5945	467.1	142.802 ₂	74	454.32	7.6815	454.46	36.2331
75	484.34	9.9028	479.67	6.1505	75	506.52	3.7407	500.57	12.4106	75	474.45	49.074	472.82	47.3974	75	456.12	8.5787	455.87	3.0943
76	491.76	4.5542	482.65	0.0569	76	510.27	2.2451	510.73	45.3687	76	481.21	48.7341	477.58	125.321 ₄	76	464.71	23.9341	464.81	36.5738
77	506.23	4.6334	500.77	35.3526	77	527.18	0.0509	522.86	0.5658	77	486.97	2.019	479.95	1.3921	77	475.56	9.8365	474.06	21.4351
78	509.54	9.6513	509.57	186.186 ₁	78	529.27	3.5514	524.7	6.4124	78	487.23	2.6954	486.33	5.1866	78	479.07	2.894	478.38	14.2103
79	513.87	9.5188	513.41	30.0931	79	538.7	7.4937	537.58	1.8436	79	488.4	24.368	486.73	7.4922	79	484.33	5.8379	479.31	18.8474
80	518.4	101.265 ₉	517.25	156.610 ₇	80	541.03	25.4938	538.04	23.708	80	496.8	46.7498	488.42	95.4894	80	488.7	6.8559	485.97	3.5763
81	522.71	3.3226	519.68	0.2012	81	543.18	26.9299	545.3	21.2998	81	506.03	3.3195	500.28	18.6212	81	494.56	23.1413	490.68	48.0719
82	523.5	27.5581	521.29	33.7285	82	551.51	2.6081	548.64	15.5684	82	509.26	0.8182	511.13	58.8006	82	498.8	3.6016	495.85	4.9767
83	535.59	5.3209	536.51	3.5593	83	584	3.1562	560.53	9.3974	83	520.45	0.1423	516.53	36.4835	83	506.3	3.5444	501.03	18.0274
84	538.44	25.3568	537.24	19.9388	84	584.2	3.2832	585.05	2.3735	84	526.69	15.9799	520.56	27.9366	84	510.53	1.9613	511.8	39.5146
85	544.13	58.5687	547.55	9.7242	85	588.64	0.9	585.08	3.9819	85	535.15	28.2044	532.63	3.7119	85	523.63	6.2904	517.69	27.4014
86	552.12	3.1015	550.48	26.185	86	588.82	0.8582	587.88	2.0601	86	540.49	1.5482	537.2	0.5937	86	532.43	5.2781	533.18	4.6433
87	595.38	140.838 ₇	562.4	18.3292	87	595.51	132.48	587.98	2.1513	87	547.75	12.3266	547.78	7.1131	87	536.92	13.2803	537.17	15.9
88	606.13	1.4322	593.43	67.2606	88	607.27	6.7628	592.58	62.0878	88	548.46	0.4839	548.3	1.5171	88	543.28	14.7041	544.42	9.9214

89	606.52	9.9458	605.59	2.2628	89	610.75	0.5673	605.79	2.6043	89	550.88	15.3025	550.48	13.7108	89	547.03	19.6993	546.41	5.5652
90	610.77	2.1723	605.77	6.9727	90	612.22	3.5632	609.89	6.8286	90	554.46	1.4691	554.1	4.1292	90	551.37	3.5389	549.32	20.7458
91	612.01	4.3938	609.93	1.0758	91	616.58	0.8217	614.5	0.6057	91	590.5	146.467 8	561.46	18.2694	91	558.22	0.5744	556.82	9.9929
92	626.04	0.908	625.3	1.0113	92	621.96	1.1461	621.51	1.2903	92	598.86	0.0888	587.48	57.5793	92	571.32	3.2233	561.51	15.6218
93	626.43	0.6359	625.76	0.7819	93	622.16	2.4086	621.74	2.1476	93	599.08	0.1684	598.35	1.4227	93	573.89	9.6096	570.41	14.5292
94	627.11	3.4704	626.77	3.0047	94	633.38	10.2784	630.98	10.7792	94	603.94	94.765	598.54	1.8442	94	587.84	25.1196	573.03	5.2292
95	627.33	4.5464	626.94	3.5008	95	633.88	16.8582	631.54	11.156	95	604.81	106.583 3	599.11	346.868 1	95	595.92	133.916 6	589.88	63.3814
96	632.06	1.9684	631.66	4.4508	96	646.07	34.9797	644.3	46.9785	96	607.21	22.4103	601.59	203.220 7	96	601.2	7.5653	595.39	67.0456
97	632.14	19.5456	631.77	6.0691	97	651.73	5.215	646.63	2.6485	97	610.84	3.3501	606.3	3.081	97	606.59	0.6705	601.24	11.1688
98	644.64	33.1583	643.07	46.2589	98	655.9	8.1362	654.21	9.4925	98	611.28	0.1225	610.97	1.5225	98	608.09	14.5802	605.59	25.9784
99	651.46	4.634	646.63	2.1464	99	656.62	1.2473	654.97	1.9057	99	614.95	2.1509	613.82	3.6763	99	611.4	4.8826	607.33	12.3749
100	652.44	13.8324	649.5	26.2673	100	676.04	1.0209	671.5	0.9882	100	634.94	7.9971	633.47	5.4633	100	613.95	13.1172	613.31	5.8969
101	653.69	1.602	650.82	2.4747	101	681.75	0.2015	678.63	7.4345	101	635.06	4.2274	633.59	1.0115	101	619.04	23.2385	620.35	21.5498
102	674.14	3.5808	670.11	3.2465	102	692.92	61.4134	679.48	2.2441	102	644.41	33.6906	642.63	48.457	102	632.11	16.7237	631.04	15.8693
103	676.7	0.5569	674.66	16.6225	103	703.97	6.2562	692.18	53.7827	103	651.09	4.3479	646.52	2.0969	103	637.49	7.7351	634.61	3.8352
104	688.53	51.966	677.6	5.5388	104	710.83	3.1687	697.71	6.7837	104	652.86	6.23	649.98	15.7084	104	644.94	29.4758	643.44	43.4234
105	702.51	4.8578	688.93	44.3286	105	713.97	0.2628	717.63	93.7637	105	654.23	1.6826	651.18	1.7846	105	651.48	5.8988	646.51	2.2857
106	709.2	5.8521	697.17	10.083	106	730.21	1.1095	729.29	7.2061	106	672.08	11.1624	668.98	4.418	106	653.75	2.409	650.22	10.4753
107	712.33	8.4186	714.46	63.8096	107	732.95	0.236	731.05	5.361	107	674.97	0.1566	671.8	14.54	107	655.21	5.5023	653.1	1.9831
108	715.07	59.5162	714.53	9.1576	108	747.03	22.9627	741.74	4.9046	108	686.06	39.5969	676.38	4.2264	108	673.45	0.2038	668.74	1.4221
109	715.33	23.7588	715.56	1.4135	109	747.76	4.2984	744.06	0.3939	109	700.95	2.2542	686.25	37.2534	109	675.88	2.5314	673.5	4.4965
110	716.87	117.996 2	716.39	159.865 5	110	748.57	39.2663	746.1	15.3081	110	707.27	11.206	696.29	12.5759	110	683.78	58.1513	678.71	6.9609
111	717.27	48.4774	717.35	240.213 4	111	750.65	39.3826	747.38	23.6337	111	709.06	1.9193	709.56	134.907 2	111	701.26	6.6662	684.02	60.5486
112	726.97	3.4005	725.85	57.7382	112	756.31	267.405 8	747.44	21.8607	112	714.72	2.1077	713.38	8.0925	112	703.18	3.3657	697.88	13.6723
113	729.9	14.2584	726.77	142.426 5	113	764.73	14.1599	763.29	30.2695	113	715.96	0.6214	715.75	0.233	113	708.78	7.1741	701.39	58.0493
114	741.39	40.6464	735.53	33.7514	114	766.18	5.4574	766.04	25.7752	114	716.15	0.5671	715.8	0.258	114	710.77	8.7183	707.97	55.7472
115	744.24	20.7218	736.61	6.8115	115	767.1	5.5098	766.92	24.9397	115	718.68	17.4447	720.69	6.9651	115	718.03	7.1793	720.7	39.8996
116	755.51	336.198 4	743.55	3.3702	116	772.25	1.5974	772.58	0.5216	116	734.98	19.834	730.85	17.7713	116	732.5	0.552	731.35	1.5602
117	762.16	56.2548	763.82	115.878 3	117	774.08	7.4478	773.85	10.5769	117	736.84	1.1223	731.48	7.5207	117	735.1	12.0286	732.59	1.2629
118	780.59	91.3196	782.03	85.6851	118	776.33	216.962 6	776.83	149.065 6	118	739.36	17.1494	737.7	16.9253	118	737.77	1.4388	733.45	27.5096
119	781.28	77.1547	782.6	65.8115	119	776.42	45.7721	777.27	109.394 1	119	741.3	15.0987	738.09	0.9354	119	751.44	61.6088	742.87	4.1609
120	782.25	9.7992	783.51	28.9298	120	790.16	40.8206	789.72	63.4512	120	754.52	369.921 3	741.78	6.4211	120	755.89	282.363 8	750.55	10.8653
121	783.67	2.4823	784.67	29.4403	121	796.29	2.9823	795.96	11.2916	121	760.12	41.5053	764.39	63.8463	121	762.17	16.6963	763.59	34.0175
122	789.71	43.8897	789.88	58.1201	122	796.32	3.7585	796.07	10.4083	122	770.25	0.8214	768.22	0.6287	122	765.66	4.4406	765.67	7.4554
123	802.3	3.4411	804.43	1.6586	123	802.27	0.5018	804.04	23.8214	123	770.57	0.8593	768.53	0.6047	123	767.39	7.4345	766.5	7.0908
124	836.95	8.342	834.88	110.788	124	839.1	10.7834	842.22	44.7487	124	778.75	2.4483	780.34	1.2665	124	772.28	30.6179	773.01	30.5962
125	839.92	9.2476	836.42	63.7979	125	842.2	14.1261	843.91	28.6569	125	784.52	10.2514	785.16	4.5702	125	775.01	30.694	775.42	38.4166
126	841.75	7.0177	841.71	62.7399	126	843.38	9.8072	848.45	26.7708	126	792.15	34.6112	791.37	47.2793	126	777.85	83.2752	777.67	99.7432
127	847.79	11.4953	845.07	26.285	127	854.92	1.6233	850.03	23.8462	127	792.27	18.7652	791.75	30.5384	127	784.36	67.3233	784.29	49.6112

128	850.03	10.5124	846.02	17.4293	128	855.31	90.0356	850.38	27.731	128	792.87	86.7304	792.23	98.0276	128	789.3	14.8555	788.9	25.98
129	850.45	56.2403	848.59	63.3862	129	859.33	13.5958	851.08	48.1711	129	802	5.5573	804.49	2.619	129	793.45	27.8002	792.82	53.0772
130	851.96	66.4828	849.93	31.9762	130	859.88	12.3817	854.2	52.0223	130	806.64	6.2618	805.09	22.559	130	795.75	13.4794	795.36	15.827
131	864.19	1.87	864.66	5.5771	131	868.69	5.3897	863.49	7.2106	131	806.87	22.3424	805.4	22.0384	131	799.09	43.9806	798.48	47.8549
132	864.73	2.4103	865.27	5.7633	132	877.38	18.1606	875.44	8.6936	132	829.91	73.9733	829.04	2.7222	132	801.94	0.6574	802.76	13.8019
133	865.22	0.3193	865.79	2.1968	133	881.21	27.9835	878.18	1.6059	133	830.99	77.7358	829.88	57.6013	133	802.97	7.8694	804.53	23.3764
134	866.7	0.3298	866.67	18.1759	134	883.81	4.706	884	4.2125	134	834.78	0.9017	830.12	88.4709	134	836.93	3.2531	826.97	7.9164
135	868.18	6.2857	866.93	45.7353	135	885.64	0.06	886.21	0.4371	135	837.03	0.1194	830.55	5.9275	135	838.71	17.8623	841.34	37.4855
136	877.36	16.1684	873.87	100.535 2	136	885.69	1.0102	886.31	1.5391	136	840.07	3.6454	839.9	40.6706	136	839.66	2.5913	842.71	54.5992
137	881.33	22.1129	878.31	10.2178	137	889.45	0.2077	890.28	3.9663	137	840.75	0.6495	841.05	58.912	137	842.41	9.5526	845.73	1.8951
138	882.84	2.5422	882.82	6.9373	138	890.18	0.1934	890.63	0.4385	138	842.2	11.3814	841.85	40.0704	138	845.12	84.5182	848.72	31.9935
139	895.81	41.8516	886.09	3.8414	139	899.25	177.071 2	896.74	3.3154	139	844.05	55.6013	846.43	51.8256	139	851.87	23.6831	851.19	26.8653
140	899.4	13.0929	893.7	15.0817	140	904.72	24.0427	899.35	8.6721	140	845.13	129.591 1	848.31	20.575	140	864.18	11.2136	854.28	11.6597
141	901.85	151.039 1	910.5	198.107 9	141	906.51	6.5159	908.13	101.201 8	141	866.73	9.8902	864.73	40.3468	141	867.78	14.3075	864.61	58.9683
142	928.21	0.528	926.3	32.5978	142	931.71	49.4923	925.92	21.4069	142	872.53	4.6	873.31	78.362	142	877.29	16.9391	873.85	49.1147
143	928.74	1.0283	928.7	0.1421	143	937.83	10.6892	935.33	1.9694	143	873.06	9.3737	874.59	0.268	143	880.02	0.221	879.21	14.9206
144	931.74	52.6569	929.27	19.3594	144	938.02	14.5137	935.51	11.7906	144	877	13.123	875.17	0.5315	144	881.5	20.2641	880.09	14.0134
145	932.17	13.8771	934.3	0.2662	145	961.35	24.0953	957.55	47.1755	145	880.23	18.6737	879.62	8.5945	145	882.26	2.1698	882.31	5.3039
146	932.77	12.3598	934.48	8.1168	146	961.64	8.1073	958.33	7.6529	146	881.64	0.5544	881.56	3.4423	146	887.59	16.5443	883.33	7.2933
147	951.54	3.559	952.51	6.4836	147	967.76	3.0902	966.86	29.9048	147	891.2	19.7719	882.38	10.9842	147	891.32	1.3928	891.74	4.7094
148	951.94	4.4838	952.6	3.5726	148	967.87	2.8915	967.59	15.3988	148	892.27	26.0472	887.48	2.432	148	893.91	0.1261	894.14	3.2122
149	958.69	17.6408	957.63	150.136 8	149	968.26	0.1752	969.08	0.8622	149	900.65	117.010 8	903.61	32.8771	149	900.7	151.793 2	898.07	3.6947
150	958.94	5.3612	958.65	7.5486	150	969.48	0.0743	969.78	0.8773	150	903.89	28.2167	904.45	5.7339	150	903.45	22.4163	902.24	13.2135
151	978.79	5.5988	962.47	42.578	151	987.47	14.7745	971.21	37.6769	151	905.04	32.4659	911.34	141.164 7	151	906.45	6.5921	910.47	67.7897
152	979.66	7.8456	964.36	24.5504	152	988.66	5.1639	971.75	5.326	152	912.3	2.3039	913.25	6.5391	152	920.33	4.1896	920.22	7.5805
153	989.03	0.4581	986.75	44.87	153	989.32	2.6378	987.71	23.5743	153	913.4	2.8432	913.36	3.1318	153	928.73	2.4216	926.77	7.3867
154	990.65	3.547	988.06	9.604	154	999.02	1.2156	995.46	3.4878	154	931.62	72.1894	927.9	8.6348	154	931.5	58.9996	927.3	8.0172
155	992.51	1.5111	989.12	4.153	155	999.74	0.5785	996.22	2.4908	155	947.22	0.1146	947.5	47.7945	155	942.49	16.4855	940.16	14.3033
156	998.25	0.9549	992.26	3.714	156	1005.34	1.915	998.52	0.9027	156	947.54	0.0797	947.64	1.485	156	946.95	0.6194	945.5	53.8479
157	998.57	0.5597	992.4	6.242	157	1007.01	13.415	999.82	1.0622	157	951.04	27.8857	948.57	106.222 6	157	949.56	14.7544	945.62	61.7157
158	998.93	2.9154	1000.26	5.1814	158	1007.27	3.631	1004.9	0.852	158	951.31	11.0513	949.38	32.1425	158	951.72	15.3549	950.51	12.5334
159	1000.01	3.6474	1000.76	2.5388	159	1007.93	6.2482	1008.51	0.6401	159	972.01	5.2852	958.32	34.5785	159	962.29	1.2067	954.56	34.4377
160	1005.39	3.3223	1000.89	17.9654	160	1008	2.3774	1009.35	0.4198	160	972.96	3.8378	962.64	21.8048	160	972.88	5.8028	962.53	1.1136
161	1008.12	442.771 5	1001.16	15.6819	161	1010.13	468.205	1009.77	0.5817	161	983.59	0.411	982.14	4.6426	161	973.69	2.8695	973.76	8.1704
162	1009.34	584.191 2	1004.67	1.7097	162	1011.58	471.059 4	1009.83	0.4524	162	984.32	0.1303	983.5	4.3445	162	978.74	4.4401	976.41	31.7765
163	1010.86	555.832 4	1011.27	5.2845	163	1012.01	24.9868	1011.48	2.0662	163	985.34	0.6198	986.41	15.3697	163	984.29	1.2375	979.3	15.2412
164	1011.95	6.7585	1015.65	90.1077	164	1013.52	240.710 5	1021.82	176.581	164	986.31	0.4003	986.58	8.8454	164	985.21	0.2459	984.27	1.1001
165	1015.72	0.7539	1015.9	71.4719	165	1023.64	2.2726	1022.71	19.1135	165	988.56	2.4871	986.84	0.8324	165	986.52	1.6818	985.32	1.8301
166	1015.84	0.7389	1016.85	1.0174	166	1023.71	1.9701	1024.11	1.5743	166	988.7	0.7121	987.23	5.7634	166	987.86	9.0965	986.86	54.0565
167	1016.33	0.0613	1017.09	0.7558	167	1026.65	1.6777	1024.12	1.1025	167	989.86	3.5449	988.09	5.247	167	988.93	12.1409	987.64	4.5516

168	1016.42	0.0761	1020.46	245.977 9	168	1035.53	16.772	1029.03	3.9378	168	1005.21	18.5131	989.73	4.63	168	993.98	7.0583	990.87	3.1251
169	1018.9	0.2041	1021.7	0.0849	169	1036.35	13.5972	1029.62	3.5537	169	1007.01	1175.62 6	989.88	3.9958	169	1002.12	0.2384	992.68	5.6853
170	1019.55	0.1621	1021.83	1.3498	170	1041.17	73.1842	1039.02	19.2283	170	1008.97	75.2198	1005.63	0.9667	170	1005.71	3.7554	995.23	17.0303
171	1019.74	0.3277	1021.98	5.3441	171	1055.29	4.6058	1056	7.1756	171	1009.58	392.316 8	1012.67	4.1403	171	1007.11	57.415	1002.52	0.7136
172	1020.21	0.2523	1022.04	0.2616	172	1055.42	13.7221	1056.24	14.3512	172	1010.8	12.8104	1018.74	2.812	172	1007.8	233.067 5	1005.52	0.7785
173	1025.99	0.4297	1022.29	1.6224	173	1057.96	4.4531	1058.09	4.5314	173	1018.15	1.9409	1018.76	0.7883	173	1010.19	934.598 6	1007.9	0.5867
174	1031.95	0.9022	1023.71	1.1729	174	1058.82	5.0835	1059.52	3.6941	174	1018.95	1.5535	1019.53	134.687 2	174	1010.59	103.969 9	1010.52	0.6468
175	1032.65	2.0891	1024.13	8.4348	175	1060.47	15.9018	1061.45	14.6663	175	1022.56	0.2127	1020.91	0.9102	175	1012.03	4.7729	1012.57	6.7594
176	1041.04	74.9128	1038.51	15.5423	176	1061.57	15.8835	1061.93	15.4045	176	1022.75	0.2983	1022.25	36.2745	176	1014.13	69.9238	1016.52	75.9148
177	1054.96	7.9611	1056.08	20.2346	177	1065.12	77.6899	1064.59	3.0109	177	1024.88	16.6241	1023	2.8576	177	1017.88	0.0664	1019.27	1.7111
178	1055.21	11.1954	1056.56	15.3724	178	1123.33	126.534 9	1111.35	26.8203	178	1025.62	0.6385	1023.16	12.7042	178	1019.91	0.0044	1020.89	200.043 5
179	1064.32	43.3683	1064.12	0.6359	179	1133.07	92.2443	1129.1	548.720 7	179	1026.09	0.6605	1023.35	16.3043	179	1025.59	0.28	1021.47	0.0661
180	1065.02	3.8167	1064.28	0.1148	180	1134.16	3.0295	1131.87	196.587 4	180	1028.98	0.2812	1026.19	0.7101	180	1027.6	0.5667	1022.74	58.945
181	1065.28	1.5167	1065.12	24.074	181	1134.66	6.8129	1133.81	19.0711	181	1029.36	2.4893	1026.34	0.6582	181	1035.05	21.1552	1030.83	9.9147
182	1066.74	9.5275	1066.03	13.9896	182	1136.31	1426.64 5	1134.89	38.2952	182	1040.81	73.1018	1038.77	21.6679	182	1041.1	73.1826	1038.7	20.5065
183	1067.24	10.7526	1066.05	3.9352	183	1142.4	39.0462	1144.99	41.2645	183	1054.07	5.3244	1055.28	17.4445	183	1052.5	2.2734	1051.11	5.4755
184	1115.56	11.8498	1112.49	18.3572	184	1143.77	473.923	1146.89	45.8982	184	1055.22	11.1226	1057.12	13.8992	184	1054.88	2.6096	1054.95	22.3619
185	1116.53	12.6942	1116.03	13.5475	185	1152.42	5.1573	1152.57	3.2324	185	1064.21	33.7117	1065.22	2.4026	185	1055.02	18.3321	1056.86	12.6981
186	1117.58	1.9893	1116.57	11.6361	186	1153.12	5.4664	1153.25	99.5673	186	1073.15	4.765	1073.65	5.034	186	1064.44	60.0764	1065.22	31.2503
187	1118.33	0.6504	1117.59	38.445	187	1153.98	85.9695	1153.61	9.1811	187	1073.34	5.1337	1073.78	6.0755	187	1068.68	3.1524	1068.83	4.0083
188	1122.55	82.4558	1118.06	25.3537	188	1170.07	15.9734	1160.65	310.136 6	188	1075.08	5.4573	1075.76	5.2477	188	1072.15	6.8049	1072.64	6.7923
189	1132.81	125.122 8	1125.54	3349.73 8	189	1170.88	15.663	1170.55	51.1681	189	1075.29	4.9067	1075.91	4.221	189	1085	3.3938	1085.86	5.5805
190	1136.12	2253.59 3	1130.73	309.217 6	190	1178.47	0.2126	1171.73	55.5645	190	1121.9	75.7282	1112.02	19.9942	190	1088.73	10.2799	1089.3	11.7389
191	1153.32	29.4886	1150.72	337.860 6	191	1178.99	38.9329	1178.77	0.8465	191	1124	5.4135	1124.97	33.1649	191	1105.07	13.9683	1105.89	15.709
192	1153.81	91.3444	1152.74	94.973	192	1179.18	271.442 7	1179.4	0.772	192	1124.25	10.2115	1125.27	17.9143	192	1121.88	209.608 1	1112.4	67.6801
193	1154.23	98.0828	1156.63	288.052 3	193	1194.1	1106.68 3	1181.44	759.064 7	193	1132.56	111.564 2	1129.21	776.501 4	193	1123.04	19.7011	1124.32	11.5361
194	1173.68	0.3783	1158.46	128.170 7	194	1194.69	131.918	1192.73	124.026 1	194	1135.63	2483.62 8	1132.54	969.375 5	194	1132.75	195.963 7	1129.72	262.010 1
195	1174.93	1.8429	1166.85	4472.39 2	195	1197.16	108.539 3	1193.01	299.387 9	195	1143.73	1.5971	1144.45	2.2401	195	1133.32	43.0322	1132.44	135.340 4
196	1175.66	2.51	1174.65	7.8813	196	1199.35	476.556	1207.51	430.723 6	196	1144.03	1.0192	1144.47	2.2397	196	1135.1	570.152 1	1134.18	79.5242
197	1176.49	8.0407	1175.91	2.2655	197	1216.23	47.2862	1211.21	78.2921	197	1153.4	97.0311	1148.92	335.38	197	1138.49	1398.78 5	1137.12	215.447 7
198	1176.69	303.824 2	1176.38	26.92	198	1218.58	12.5541	1217.36	26.8313	198	1163.31	23.3253	1152.61	93.649	198	1139.88	30.3784	1139.95	4.2735
199	1194.21	2044.35 5	1177.45	32.1498	199	1219.29	13.5173	1219.19	6.7847	199	1163.95	50.3151	1165.54	80.8595	199	1142.71	31.8508	1142.86	34.9163

200	1194.48	141.936	1191.84	207.389 7	200	1222.02	55.6529	1222.27	232.813 4	200	1173.41	9.7974	1166.52	77.1149	200	1153.71	93.6319	1152.97	111.552 2
201	1196.15	83.1429	1194.63	207.177 7	201	1225.44	232.403 9	1223.22	151.844 4	201	1173.84	9.8338	1173.5	1510.73 6	201	1164.16	20.9686	1154.16	311.705 4
202	1196.94	81.8185	1196.53	58.1455	202	1239.93	1894.46	1250.65	150.664 6	202	1175.12	294.999 3	1175.02	25.4161	202	1175.89	1.9357	1168.69	11.7144
203	1198	0.5169	1197.1	0.4888	203	1251	27.3516	1256.61	24.8432	203	1177.27	0.834	1178.31	908.212 4	203	1177.18	289.583 4	1177.24	4.5972
204	1199.13	16.0124	1197.87	15.9526	204	1254.19	461.087 7	1265.11	123.830 8	204	1178.09	1.6875	1178.56	0.2571	204	1177.71	14.9132	1178.66	4.3351
205	1204.63	236.896 3	1200.42	665.683 6	205	1267.41	134.272 8	1265.47	106.685 9	205	1190.77	113.250 2	1178.96	2433.44 1	205	1178.5	0.5519	1179.89	2.2222
206	1206.16	20.3182	1208.62	431.999 9	206	1268.28	135.137 6	1274.02	779.84	206	1191.12	59.7721	1191.33	41.3464	206	1186.4	2.6635	1186.54	169.070 8
207	1216.54	71.3952	1213.08	11.5903	207	1281.27	14.027	1280.36	10.5344	207	1193.84	2455.47 9	1191.83	43.8022	207	1188.62	11.1971	1187.65	480.451 8
208	1221.67	40.6951	1222.01	148.291 9	208	1282.06	14.0318	1281.42	35.9142	208	1195.45	121.508 5	1191.97	206.684 2	208	1190.93	11.4908	1189.67	314.802 3
209	1225.07	250.768 3	1223.2	283.571	209	1304.25	3.6975	1287.48	262.932 6	209	1208.56	205.78	1204.95	1367.07 7	209	1193.58	1266.30 2	1192.81	211.109 1
210	1230.45	348.549 1	1230.63	246.095 2	210	1308.22	26.1647	1310.96	5.3451	210	1209.34	372.148 4	1209.49	17.1436	210	1194.96	118.002 7	1193.04	3.9845
211	1231.21	47.5157	1231.93	79.154	211	1321.91	26.3024	1318.33	33.532	211	1215.5	26.5115	1214.29	2.0563	211	1196.1	954.803 7	1197.94	2216.76 3
212	1238.38	2255.98 8	1257.51	211.394 2	212	1323.2	24.8993	1321.36	50.3661	212	1221.95	21.1081	1222.38	248.974 5	212	1207.16	28.1341	1207.59	6.3248
213	1255.83	8.4257	1261.81	10.7891	213	1324.31	14.0203	1321.89	45.8073	213	1225.26	273.650 8	1223	95.952	213	1207.88	205.422 3	1209.38	160.295 7
214	1258.46	311.383 2	1270.49	2841.61 9	214	1325.45	5.6539	1323.86	70.3416	214	1232.45	394.835 4	1234.79	121.021 4	214	1212.9	13.7703	1211.65	5.8006
215	1302.6	66.1668	1287.16	117.192 3	215	1341.06	13.0861	1325.58	41.881	215	1233.19	14.4824	1235.71	34.2343	215	1215.61	276.193 6	1212.47	33.4035
216	1305.05	46.2936	1310.15	38.934	216	1343.22	119.725 9	1334.71	33.4614	216	1237.85	1124.82 7	1237.88	2.5432	216	1216.65	17.8856	1215.54	363.051 6
217	1311.31	1.5283	1312.78	67.4254	217	1349.28	1.5346	1338.08	5.4073	217	1237.95	709.281 9	1238.54	2.4757	217	1219.26	4.0234	1219.19	10.3912
218	1315.54	21.4705	1314.86	20.8344	218	1349.98	1.6037	1348.6	17.1555	218	1238.17	303.392 7	1256.1	33.0574	218	1221.93	28.45	1222.14	31.207
219	1320.46	44.1671	1316.2	341.722 3	219	1350.25	2.3647	1349.66	18.5966	219	1255.65	7.7972	1256.8	23.0168	219	1225.39	271.089 6	1224.07	309.695 3
220	1321.02	86.1275	1317.3	19.3546	220	1353.43	624.834 6	1350.82	69.5749	220	1255.77	3.4344	1262.57	10.322	220	1238.86	1441.36 9	1243.57	7.615
221	1322.52	49.5847	1318.7	6.133	221	1355.89	102.272 6	1353.45	11.6647	221	1260.23	18.1452	1265.62	7.6691	221	1243.67	16.2882	1244.18	22.6786
222	1326.61	321.787 2	1324.72	39.295	222	1356.59	21.6765	1359.13	101.550 1	222	1262.51	178.504	1275.16	2410.52 5	222	1244.38	9.3667	1245.11	7.4299
223	1327.16	240.478 1	1326.29	149.092 7	223	1364.84	41.0151	1361.27	12.3337	223	1279.25	4.3709	1279.76	16.3654	223	1245.63	750.321 6	1248.94	1.706
224	1328.98	390.830 3	1331.04	229.275 5	224	1371.53	135.889 1	1363.82	109.005 5	224	1279.49	4.304	1280.22	14.9698	224	1250.11	96.0434	1257.92	2.2401
225	1339.7	526.599	1331.67	236.818 5	225	1371.8	212.376 2	1370.89	309.100 2	225	1298.31	18.5378	1288.97	376.111	225	1255.84	14.9555	1266.44	77.3256
226	1341.22	7.9	1336.43	472.204	226	1386.95	636.787 6	1371.51	688.699 3	226	1298.51	22.3852	1299.79	36.5607	226	1263.14	108.750 5	1281.29	611.991 3
227	1347.57	11.747	1338.06	4.6858	227	1392.25	0.6506	1390.73	1.9658	227	1305.47	60.1107	1300.28	20.1653	227	1287.81	11.346	1288.26	26.4989

228	1351.24	541.300 2	1350.47	40.3588	228	1392.82	0.6561	1390.95	1.8294	228	1312.73	61.4539	1314.3	36.4665	228	1294.44	108.887 6	1288.61	534.178 5
229	1353.68	119.239 1	1352.63	0.7841	229	1412.43	442.556 4	1408.45	369.659 1	229	1320.76	51.1376	1319.31	35.5174	229	1297.55	54.7861	1293.57	123.055 4
230	1353.8	18.6608	1354.82	71.3235	230	1416.4	364.952 8	1416.09	328.117 7	230	1322.76	1.2991	1321.3	136.197 4	230	1302.51	21.9644	1298.32	62.0294
231	1354	26.1308	1355.09	58.5836	231	1418.99	8.4145	1417.74	579.139 1	231	1323.62	32.6503	1321.8	39.5223	231	1306.73	192.057 2	1309.7	190.571 2
232	1355.46	188.505 3	1355.91	11.0984	232	1421.59	162.934 6	1420.91	570.930 5	232	1330.63	104.171 3	1326.55	0.8457	232	1310.35	14.9957	1311.28	23.6636
233	1366.22	168.905	1359.16	17.717	233	1422.26	210.162 7	1421.61	4.5954	233	1337.17	988.324 5	1328.3	101.680 1	233	1317.73	52.7457	1316.34	80.8738
234	1367.52	230.228 7	1369.27	1289.91 1	234	1438.21	1044.82 2	1427.44	13.5426	234	1341.33	2.7121	1336.95	217.264	234	1320.98	24.1661	1318.33	46.1273
235	1368.23	21.2655	1373.68	47.3899	235	1450.14	8.3564	1446.79	194.819 6	235	1341.66	4.9601	1339.27	7.0947	235	1322.72	22.646	1319.85	5.6938
236	1371.95	413.890 8	1374.36	4.0908	236	1453.2	111.833 3	1450.82	71.2045	236	1341.95	27.2368	1342.64	1.1632	236	1328	97.9282	1320.82	17.9802
237	1373.03	1168.07 2	1376.83	835.851 9	237	1470.15	44.1905	1458.56	45.5141	237	1346.2	161.617 2	1342.91	0.718	237	1332.71	12.6208	1329.73	15.4087
238	1386.85	566.534 5	1380.18	2596.32 7	238	1470.75	66.1988	1469.95	585.890 5	238	1346.74	178.474 2	1347.75	130.858 1	238	1334.96	66.3223	1332.94	61.0526
239	1412.86	389.631 2	1411.56	622.033 3	239	1482.58	37.6677	1477.92	84.8885	239	1348.13	37.6035	1348.3	144.314 4	239	1338.73	230.218 3	1334.05	157.593 8
240	1416.26	326.936 2	1416.32	78.1334	240	1487.61	14.6134	1478.47	76.7646	240	1353.3	718.739 6	1356.06	139.010 7	240	1341.28	15.2568	1336.02	68.713
241	1418.84	2.3692	1421.83	0.562	241	1488.43	39.7917	1484.8	2.2638	241	1364.43	1158.83 4	1361.71	19.8116	241	1344.12	90.8301	1338.49	14.3066
242	1439.01	1098.76 9	1429.31	49.6679	242	1489.86	61.8852	1485.04	36.0115	242	1365.61	36.9376	1369.81	831.482 3	242	1345.73	641.603 9	1346.21	197.649 5
243	1450.58	9.26	1447.86	54.4231	243	1493.88	652.772 4	1491.47	25.9997	243	1365.96	7.1131	1373.88	1.1417	243	1348.23	106.459 2	1347.88	37.4419
244	1453.23	112.301 8	1451.32	78.7449	244	1502.83	371.164 3	1492.3	465.871 5	244	1366.17	576.337 1	1374.37	1.5557	244	1351.04	110.709 6	1348.71	181.850 5
245	1477.91	104.615	1459.4	54.3574	245	1503.85	193.762 1	1497.43	662.776	245	1368.41	79.3028	1378.57	1406.78	245	1353.54	265.496 3	1352.98	70.2341
246	1478.09	4.7687	1477.04	336.142 2	246	1503.98	360.491 8	1498.63	1428.13 1	246	1386.52	624.464 4	1384.35	3147.79 5	246	1358.1	244.974 2	1357.12	213.091 1
247	1483.28	52.7891	1486.2	13.7061	247	1504.96	132.034 9	1503.57	100.188 5	247	1412.56	330.163 7	1411.7	440.412 3	247	1365.54	258.481 4	1359.89	68.8674
248	1487.61	10.5023	1487.24	39.0535	248	1521.86	17.1083	1503.93	97.8111	248	1416.32	315.137 2	1415.92	85.1656	248	1369.12	49.3072	1370.5	184.472 1
249	1488.51	40.1995	1489.95	256.458 1	249	1524.15	3.3987	1515.26	14.1621	249	1418.14	12.8155	1421.88	0.826	249	1371.42	11.7316	1371.48	20.3469
250	1489.54	168.271 2	1490.64	342.372 3	250	1535.59	105.971 2	1524.11	185.013 3	250	1439.37	1062.31 9	1429.54	25.2086	250	1374.75	1000.60 2	1377.68	22.6824
251	1493.55	413.333 9	1493.99	1.1026	251	1535.74	20.3442	1534.04	150.321 7	251	1445.67	0.5595	1445.81	2.3241	251	1376.16	335.202 1	1378.09	33.2315
252	1502.44	10.0672	1496.92	14.0007	252	1547.99	70.7473	1534.37	20.8591	252	1445.71	0.5448	1447.08	1.9905	252	1387.72	423.877 6	1393.19	38.5066
253	1503.08	6.4834	1503.66	54.9786	253	1548.54	37.8199	1537.77	1.2636	253	1450.69	18.9298	1449.2	133.430 6	253	1393.31	11.1107	1394.02	2299.78 2
254	1509.82	20.9631	1505.14	134.145 8	254	1559.2	11.8648	1548.26	74.654	254	1453.19	97.6698	1452.51	25.6687	254	1393.72	7.7183	1395.6	1472.36 6
255	1510.51	14.9207	1507.24	604.827	255	1564.03	2677.03	1548.87	121.433	255	1480.92	7.7246	1460.88	12.1341	255	1412.57	359.903	1411.06	182.339

				7			7		8								9		7
256	1520.94	133.612 8	1509.97	32.8493	256	1575.57	683.169 5	1571.4	971.830 8	256	1483.26	265.150 2	1476.99	564.185 1	256	1416.55	324.717 1	1416.09	206.310 6
257	1523.61	13.5936	1516.24	322.31	257	1577.07	841.231 1	1573.96	472.743 7	257	1486.27	38.0005	1487.9	11.868	257	1418.86	6.3519	1421.92	4.8087
258	1544.8	418.368 4	1522.9	214.314 6	258	1591.02	46.4484	1575.99	656.624 6	258	1487.02	50.6124	1489.65	330.909 4	258	1438.2	1049.32 8	1428.44	24.0158
259	1545.11	179.339 5	1540.47	21.1358	259	1610.8	458.406 5	1588.81	393.714 4	259	1489.71	48.7684	1489.7	22.2892	259	1450	7.2401	1447.3	134.687
260	1545.69	321.685	1541.74	1674.50 9	260	1612.9	636.178 7	1617.94	55.6485	260	1490.7	315.861 8	1490.23	353.267 2	260	1452.97	122.396 2	1451.15	108.988 5
261	1546.66	477.334 4	1544.02	353.195 1	261	1647.34	18.5848	1618.91	22.5918	261	1491.11	39.7234	1492.7	73.5085	261	1461.91	85.7874	1457.83	30.7044
262	1558.58	2087.99 1	1544.41	241.181 8	262	1648.43	20.3311	1622.59	146.826	262	1491.67	36.8196	1494.19	214.223 8	262	1475.92	4.0051	1468.63	79.1452
263	1559.45	108.705	1544.58	332.393	263	1654.95	14.2492	1633.87	241.207 1	263	1493.98	201.746 1	1497.87	40.4008	263	1481.19	47.2744	1475.42	81.9103
264	1566.32	724.420 5	1559.12	2044.84 6	264	1658.52	0.6421	1643.88	349.806	264	1514.97	5.9358	1501.35	94.6931	264	1484.83	199.412 1	1475.92	84.9656
265	1568.28	1592.55 6	1568.61	868.817 2	265	1658.72	0.6606	1649.97	9.6647	265	1515.08	3.2289	1514.71	52.8221	265	1486.55	13.0198	1486.03	7.0909
266	1591.69	73.511	1575.16	148.588 8	266	1665.12	6.5646	1659.31	0.5068	266	1520.24	208.051 1	1515.2	129.003 1	266	1486.71	10.4935	1486.8	13.2483
267	1610.38	545.769	1580.32	862.980 8	267	1665.49	7.6492	1659.33	0.8815	267	1523.73	24.9153	1517.04	474.557 9	267	1487.51	24.8963	1487	24.1603
268	1615.27	636.535 3	1610.5	132.064 7	268	1682.84	48.3789	1665.03	3.4182	268	1542.02	189.859 4	1523.24	127.363 5	268	1489.33	59.6881	1487.91	54.7946
269	1638.78	54.298	1611	28.7966	269	1682.95	49.8408	1665.11	3.0808	269	1542.87	160.739 4	1540.05	24.3568	269	1490.13	103.117 2	1490.96	147.892 3
270	1639.78	78.0355	1614.48	68.7491	270	1689.27	197.534 7	1681.6	46.1738	270	1550.91	50.4765	1543.38	394.471 1	270	1493.45	21.1936	1492.2	28.9669
271	1654.91	15.8723	1621.42	730.134	271	1689.93	153.859 1	1681.69	45.4695	271	1551.22	41.3736	1544.75	357.953 7	271	1494.06	330.726 7	1493.91	505.955 6
272	1667.06	29.5357	1638.67	1071.94 1	272	1699.69	60.8757	1689.65	54.0789	272	1557.9	2713.11 3	1550.1	349.510 7	272	1497.34	78.2883	1497.28	117.409 5
273	1667.58	30.1816	1648.44	10.8962	273	1709.13	12.5544	1691.45	312.837 1	273	1559.61	15.7877	1550.57	55.5709	273	1502.8	34.8939	1498.78	47.5646
274	1672.56	139.277 8	1667.26	19.1184	274	1709.5	9.6563	1695.09	223.132 7	274	1568.05	782.142	1561.94	2206.53 6	274	1508.3	71.3872	1507.17	17.0881
275	1673.02	190.440 7	1667.3	12.7596	275	1728.74	98.0495	1707.28	12.3964	275	1569.02	1405.19 6	1570.37	1051.08 7	275	1511.61	24.135	1508.38	90.6548
276	1678.18	250.945 2	1673.32	56.0539	276	1729.78	183.172 1	1707.3	7.6641	276	1592.28	89.9079	1575.19	351.295 9	276	1520.07	135.727 8	1511.37	291.552 6
277	1678.36	776.222 5	1673.51	92.2756	277	1860.8	611.706 9	1857.99	708.875 7	277	1610.57	587.271 1	1585.99	1006.30 8	277	1523.93	28.935	1513.88	65.2594
278	1679.94	148.027 9	1678.48	84.4458	278	3083.8	22.4571	3076.85	55.6398	278	1616.64	627.556 3	1611.25	16.8393	278	1543.54	363.642 1	1525.98	121.591 7
279	1680.1	143.810 9	1678.78	71.6	279	3084.46	34.6743	3077.65	60.5649	279	1637.98	66.749	1612.67	29.7458	279	1547.85	96.2394	1539.96	104.326 7
280	1695.3	92.2947	1681.76	326.347 4	280	3153.51	1.6063	3144.12	11.7666	280	1639.09	89.9723	1613.91	171.341 7	280	1549.94	435.474 9	1543.25	346.020 8
281	1695.5	43.6902	1683.39	617.739 2	281	3154.44	16.0897	3145.41	10.7031	281	1646.13	7.7429	1622.39	790.574 5	281	1553.85	488.840 9	1546.39	137.345
282	1699.6	48.8731	1693.05	313.228	282	3172.78	58.2504	3166.89	22.0037	282	1646.46	9.6617	1641.92	1262.11 1	282	1556.42	933.834 4	1548.9	546.953 7

283	1723.03	194.703 3	1695.98	138.888 6	283	3173.07	0.2155	3167.47	11.6216	283	1653.88	5.0574	1647.29	1.9175	283	1561.29	495.317 4	1554.4	70.2503
284	1723.25	231.865 4	1696.4	307.976 2	284	3190.79	20.3201	3197.8	20.9737	284	1654.11	4.8845	1648.05	73.9358	284	1566.95	532.775 6	1565.37	352.086
285	1860.25	616.466 4	1856.19	754.065 1	285	3193.2	20.9801	3199.33	26.2954	285	1655.09	14.5452	1648.59	7.978	285	1568.45	1654.06 1	1569.67	1390.66 2
286	3083.13	25.798	3075.14	68.8461	286	3216.6	16.6206	3218.03	6.044	286	1677.92	328.820 9	1653.84	5.8242	286	1591.83	63.0381	1575.23	290.918 7
287	3083.83	39.4449	3075.71	90.0021	287	3216.76	3.2799	3218.04	8.2824	287	1678.29	957.149 8	1653.87	3.3731	287	1610.73	889.513 6	1591.26	622.959 6
288	3152.55	2.2608	3142.57	12.6648	288	3216.87	0.6807	3218.61	5.07	288	1687.07	3.4108	1681.45	231.415 5	288	1617.49	529.573 4	1602.43	81.7007
289	3153.54	16.3784	3143.14	13.4058	289	3217.09	2.4276	3218.67	15.0007	289	1687.14	3.461	1682.81	475.927 6	289	1633.04	135.658 6	1615.07	83.9286
290	3171.76	58.9832	3163.52	36.625	290	3217.86	6.571	3218.95	3.1641	290	1693.42	304.690 4	1686.9	5.0792	290	1644.49	13.9875	1617.67	592.759 6
291	3172.08	2.1286	3163.73	0.336	291	3218.48	10.3185	3219.6	10.0471	291	1693.58	393.259 8	1687.21	1.4556	291	1655.08	12.9183	1627.93	463.924
292	3184.81	23.3693	3191.48	37.8979	292	3223.62	10.7296	3222.87	3.7069	292	1699.13	21.9004	1691.93	379.976 3	292	1656.23	37.9176	1648.73	12.3442
293	3188.08	26.0988	3192.53	40.7232	293	3223.99	6.7251	3223.96	2.8082	293	1721.07	201.071 1	1696.33	304.964 9	293	1660.8	62.3876	1653.56	104.252 4
294	3210.04	18.6015	3213.09	19.7892	294	3224.17	6.7886	3225.46	4.7063	294	1722.5	170.776 8	1697.68	621.085 2	294	1669.08	147.037 1	1656.97	27.8776
295	3212	16.827	3214.32	21.9264	295	3224.8	9.5396	3225.83	10.4068	295	1725.81	2.921	1725.61	0.1967	295	1670.57	19.5625	1660.7	41.8491
296	3215.91	9.7518	3217.83	6.713	296	3225.41	1.5035	3226.06	7.7997	296	1725.92	5.393	1726.05	0.2148	296	1677.71	929.382 5	1669.96	89.5137
297	3216.26	6.4614	3218.07	6.8152	297	3226.21	1.3641	3226.3	4.9651	297	1860.36	614.856 6	1855.39	750.972 5	297	1684.48	54.908	1670.56	26.3638
298	3217.53	6.4775	3218.17	17.8766	298	3226.91	29.0626	3227.77	25.5424	298	3083.54	23.1012	3074.84	70.2186	298	1686.39	26.4235	1684.24	917.908
299	3217.75	10.2915	3219.42	18.8924	299	3227.4	27.6615	3228.78	26.6125	299	3083.97	44.8919	3075.81	83.7304	299	1689.13	3.5163	1684.6	110.656 9
300	3221.96	5.1647	3222.57	4.7073	300	3237.01	17.459	3237.47	11.1543	300	3152.49	0.2835	3142.11	13.7397	300	1695.82	13.227	1688.75	8.7515
301	3222.18	2.2205	3223.08	3.7617	301	3237.51	22.7526	3238.06	12.9556	301	3153.28	18.9304	3142.38	13.5708	301	1696.55	218.226 3	1688.84	56.6568
302	3222.89	25.6631	3223.64	2.6664	302	3237.61	31.4055	3238.09	55.2659	302	3171.51	45.5786	3163.14	22.6584	302	1699.59	34.4751	1692.99	247.711 3
303	3223.29	4.8182	3223.82	2.1938	303	3237.93	46.569	3238.66	72.841	303	3172.17	17.5435	3164.36	15.9941	303	1719.36	230.745 8	1696.35	53.8366
304	3223.9	6.2973	3224.24	2.9923	304	3239	9.578	3239.47	7.7071	304	3181.62	21.6467	3188.52	37.2276	304	1730.84	62.0722	1697.9	403.555 3
305	3224.04	21.7685	3224.76	2.5396	305	3239.03	1.286	3239.82	19.6732	305	3182.81	23.6569	3189.1	33.5805	305	1860.3	613.383 3	1855.85	729.650 5
306	3225.09	1.667	3225.84	9.4237	306	3239.61	20.3962	3240.55	6.3334	306	3190.85	0.1575	3192.82	0.2211	306	3060.4	39.6584	3061.85	41.9443
307	3225.86	1.4674	3227.1	8.3633	307	3239.79	5.808	3240.64	23.6718	307	3191.17	0.1759	3193.14	0.2129	307	3061.18	34.5744	3064.89	40.7027
308	3229.87	11.8691	3230.65	9.5482	308	3244.67	30.4674	3245.25	15.5658	308	3206.48	19.3143	3209.86	19.2187	308	3075.05	29.3687	3074.81	27.0369
309	3230.36	15.9589	3230.7	9.9437	309	3245.38	14.7977	3246.43	15.2442	309	3207.11	18.8837	3210.07	22.698	309	3080.16	20.3661	3074.85	69.608
310	3231.35	14.4365	3231.49	11.8944	310	3245.7	31.1498	3246.48	1.2904	310	3208.02	21.105	3211.33	34.4701	310	3082.79	33.1096	3076.82	67.3454
311	3231.98	12.3469	3232.49	6.0381	311	3246	12.9988	3247.43	12.378	311	3208.4	21.5839	3211.4	12.8746	311	3084.35	30.5568	3081.12	18.5872
312	3234.42	21.1307	3235.58	17.8704	312	3246.58	11.2429	3248.69	10.0961	312	3212.79	8.2449	3213.39	11.1561	312	3107.33	30.7002	3109.8	24.0373
313	3234.61	19.739	3235.71	18.4276	313	3246.61	7.9395	3248.85	15.2207	313	3213.05	9.3879	3213.68	9.8362	313	3111.82	42.1729	3112.51	41.0736
314	3235.69	21.0375	3236.38	17.689	314	3248.29	0.6083	3249.33	4.2195	314	3214.18	8.9964	3214.76	11.8134	314	3136.08	36.2925	3136.1	37.1245
315	3236.3	19.7969	3236.67	18.52	315	3254.23	0.2567	3252.83	1.0086	315	3214.36	9.3467	3215.97	8.7298	315	3137.16	35.9359	3139.26	50.9639

316	3238.34	23.778	3239.43	1.7993	316	3284.18	8.6824	3278.2	8.721	316	3221.73	20.0848	3221.6	3.9535	316	3151.96	6.8428	3141.69	13.099
317	3238.46	10.6323	3240.71	1.6808	317	3285.66	8.3974	3279.92	8.5898	317	3221.83	18.4661	3221.93	4.7245	317	3154.14	11.696	3144.52	12.2576
318	3239.6	10.5018	3242.25	44.5304	318	3820.8	208.098 2	3822.09	223.633 5	318	3223.98	2.191	3224.37	1.4885	318	3171.1	36.4118	3164.52	38.434
319	3239.61	5.1564	3243.45	17.5872						319	3224.84	0.2119	3224.54	1.6043	319	3172.97	24.9232	3164.74	0.0342
320	3242.19	16.2001	3243.52	23.4651						320	3224.87	5.547	3225	1.1253	320	3183.25	21.4886	3190.85	24.4236
321	3242.4	13.8197	3243.72	33.8805						321	3225.12	3.4003	3225.44	2.2447	321	3189.72	20.3945	3192.37	26.0247
322	3243.44	12.6656	3244.07	44.0371						322	3226.1	1.7143	3226.04	5.3391	322	3196.21	20.2957	3197.65	21.4721
323	3244.12	45.375	3245.27	46.309						323	3226.74	1.5447	3226.18	5.4814	323	3200.3	14.6317	3204.28	16.9583
324	3244.27	16.5191	3245.35	26.6999						324	3232.77	17.7057	3232.34	18.5443	324	3206.96	12.3005	3206.93	12.9311
325	3244.8	42.3498	3245.45	1.2289						325	3233.99	15.4444	3232.71	18.0011	325	3207.6	18.8451	3211.3	21.7824
326	3247.83	0.654	3246.47	39.9648						326	3234.38	14.1446	3233.55	14.6898	326	3209.11	8.6492	3213	9.6701
327	3253.71	0.3271	3252	1.5253						327	3234.39	20.3606	3234.24	14.9691	327	3213.1	18.5352	3214.36	20.6459
328	3283.1	10.2326	3275.09	13.4216						328	3241.43	33.6798	3240.19	4.4528	328	3218.22	1.7966	3219.82	12.5617
329	3285	10.0706	3275.59	13.5488						329	3242.03	29.5873	3240.88	3.9246	329	3220.13	11.8935	3220.88	1.3433
330	3821.03	208.996 7	3822.89	228.900 8						330	3243.33	25.5587	3243.73	32.049	330	3220.54	1.8161	3221.95	21.7926
										331	3243.96	30.5391	3243.82	28.3198	331	3222.18	10.7315	3222.16	9.4188
										332	3244.09	8.2153	3244.7	12.9905	332	3222.24	14.5948	3223.03	3.7531
										333	3244.12	21.3834	3244.71	5.3525	333	3222.77	17.4663	3223.27	4.3132
										334	3245.38	15.1491	3245.1	18.2935	334	3225.03	1.6296	3223.4	1.9181
										335	3246.59	14.5855	3249.08	20.1478	335	3225.72	1.4483	3226.09	40.9849
										336	3246.68	16.9415	3249.53	37.6147	336	3227.89	22.532	3229.94	6.6797
										337	3247.17	17.6654	3249.73	15.4108	337	3228.12	18.6452	3230.05	9.5262
										338	3248.04	0.6938	3250.36	2.6743	338	3228.2	18.6449	3231.8	17.4735
										339	3254.38	0.38	3250.44	40.2471	339	3235.24	11.1768	3233.62	1.8337
										340	3282.68	11.1467	3274.89	12.7103	340	3236.77	29.9471	3236.89	29.8047
										341	3283.77	8.5995	3274.93	9.0735	341	3240.2	29.7277	3240.39	32.0983
										342	3822.67	206.797 4	3823.27	225.719 2	342	3240.52	25.8011	3242.39	9.3243
															343	3240.87	18.1312	3242.65	19.5949
															344	3243.47	26.5973	3243.19	31.7261
															345	3244.52	35.941	3243.36	3.6151
															346	3247.89	0.6106	3246.01	1.3168
															347	3250.94	14.8869	3249.22	7.782
															348	3251.08	7.7661	3251.97	1.4261
															349	3253.53	0.3379	3257.35	17.2218
															350	3253.86	9.6221	3257.99	28.0264
															351	3267.09	4.7035	3271.75	4.5245
															352	3283.62	12.9946	3275.83	7.1392
															353	3284.4	5.6535	3277.95	13.9518
															354	3821.76	208.009	3823.21	224.252 5

Table S8 Computed absorption wavelength (λ_c), and oscillator strength (f) for the singlet-singlet transitions for metal-free organic dyes in DCM solvent medium (IEF-PCM simulation) using 6-31G(d,p) and 6-31+G(d,p) basis sets with various functionals (B3LYP, CAM-B3LYP, M06-2X, WB97XD, PBE1PBE, and TPSSH).

		6-31G(d,p)			6-31+G(d,p)		
Dye	$\lambda_{\text{max}}/\text{nm}$	Method	λ_c/nm	Oscillator strength (f)	Method	λ_c/nm	Oscillator strength (f)
	Exp		Theory			Theory	
D1	693.5, 347.5	B3LYP	723, 575, 413, 365	1.033, 0.6094, 1.1551, 0.8298	B3LYP	734, 579, 427	1.0365, 0.6361, 1.2049
		CAM-B3LYP	611, 407, 334	1.2537, 1.6104, 1.0283	CAM-B3LYP	623, 413, 345	1.241, 1.743, 0.7732
		M06-2X	620, 425, 340, 292	1.2301, 1.3885, 0.3833, 1.1926	M06-2X	631, 430, 352	1.2175, 1.4966, 0.9619
		WB97XD	599, 383, 318	1.2665, 2.1439, 0.5969	WB97XD	608, 389, 325	1.2534, 2.2384, 0.3789
		PBE1PBE	683, 535, 392	1.0876, 0.6944, 1.2847	PBE1PBE	706, 546, 409	1.096, 0.7275, 1.2812
		TPSSH	765, 636, 436, 383	0.8996, 0.5025, 0.9511, 0.8385	TPSSH	788, 648, 514, 453	0.9233, 0.5202, 0.2811, 0.9775
D2	644.5, 347.5	B3LYP	649, 540, 495	1.0247, 0.3402, 0.1502	B3LYP	657, 540, 496	1.0354, 0.3605, 0.1248
		CAM-B3LYP	576, 366, 321	1.2179, 1.5119, 0.9384	CAM-B3LYP	586, 371, 331	1.2028, 1.6928, 0.6927
		M06-2X	579, 381, 326	1.2015, 1.1521, 1.0671	M06-2X	589, 385, 336	1.1866, 1.2759, 0.9307
		WB97XD	569, 346, 309	1.221, 2.2545, 0.3261	WB97XD	578, 352, 313	1.2063, 2.381, 0.2688
		PBE1PBE	617, 494, 352	1.1105, 0.4155, 1.952	PBE1PBE	635, 503, 466	1.1083, 0.4251, 0.0731

		TPSSH	685, 532, 385, 350	0.7913, 0.3817, 1.287, 0.4242	TPSSH	702, 619, 545	0.8125, 0.2834, 0.3475
D3	695, 347.5	B3LYP	660, 566, 477	1.136, 0.0017, 0.4356	B3LYP	670, 481, 417	1.138, 0.4247, 0.25
		CAM-B3LYP	592, 375, 322	1.2408, 1.3258, 0.7681	CAM-B3LYP	602, 379, 335	1.2337, 1.499, 0.8102
		M06-2X	597, 385, 330	1.2283, 1.1455, 0.4889	M06-2X	607, 389, 339	1.2209, 1.2757, 0.9666
		WB97XD	583, 359, 310	1.2435, 1.693, 0.7518	WB97XD	593, 364, 317	1.2362, 1.8714, 0.4862
		PBE1PBE	648, 472, 364	1.1565, 0.6978, 1.4813	PBE1PBE	651, 459, 396	1.1787, 0.5047, 0.0807
		TPSSH	694, 541, 394	1.0598, 0.4814, 1.4233	TPSSH	696, 517, 461	1.0417, 0.2105 , 0.0103
D4	700, 347.5	B3LYP	665,559, 482	1.1373, 0.0057, 0.4562	B3LYP	675, 559, 485	1.1378, 0.006, 0.447
		CAM-B3LYP	594, 378, 323	1.2496, 1.3469, 0.9404	CAM-B3LYP	604, 383, 344	1.2411, 1.5125, 0.0078
		M06-2X	600, 388, 326	1.237, 1.1631, 0.7139	M06-2X	609, 392, 364	1.2287, 1.2893, 0.0039
		WB97XD	586, 362, 310	1.2523, 1.7786, 0.715	WB97XD	595, 367, 330	1.244, 1.9362, 0.1604
		PBE1PBE	634, 453, 351	1.1546, 0.5221, 1.0255	PBE1PBE	657, 516, 464	1.1804, 0.0076, 0.5229
		TPSSH	684, 508, 388	0.85, 0.4151, 0.7006	TPSSH	704, 672, 520	1.0494, 0.0269, 0.3898

Table S9 Calculated adsorption energy (E_{ads} in eV) and bond lengths (in Å) of the optimized dye structures.

Dye	E_{ads} / eV	Distances between the chosen atoms / Å		
D2- bidentate	-0.356	Ti ₁ -O ₁ / 2.004 Å	Ti ₂ -O ₂ / 2.097 Å	O ₃ -H / 0.963 Å
D2-Monodentate	4.955	Ti ₁ -O ₁ / 2.081 Å		O ₂ -H / 0.926 Å
D2-Chelating	0.421	Ti ₁ -O ₁ / 2.153 Å	Ti ₁ -O ₂ / 2.163 Å	O ₃ -H / 0.969 Å

References:

- 1 T. Mueller, R. Gresser, K. Leo and M. Riede, *Sol. Energy Mater. Sol. Cells*, 2012, **99**, 176–181.
- 2 T. Y. Li, T. Meyer, R. Meerheim, M. Höppner, C. Körner, K. Vandewal, O. Zeika and K. Leo, *J. Mater. Chem. A*, 2017, **5**, 10696–10703.
- 3 M. Lorenz-Rothe, K. S. Schellhammer, T. Jägeler-Hoheisel, R. Meerheim, S. Kraner, M. P. Hein, C. Schünemann, M. L. Tietze, M. Hummert, F. Ortmann, G. Cuniberti, C. Körner and K. Leo, *Adv. Electron. Mater.*, 2016, **2**, 1–11.
- 4 S. Y. Leblebici, L. Catane, D. E. Barclay, T. Olson, T. L. Chen and B. Ma, *ACS Appl. Mater. Interfaces*, 2011, **3**, 4469–4474.
- 5 R. S. Rao, B. Yadagiri, G. D. Sharma and S. P. Singh, *Chem. Commun.*, 2019, **55**, 12535–12538.
- 6 S. Kraner, J. Widmer, J. Benduhn, E. Hieckmann, T. Jägeler-Hoheisel, S. Ullbrich, D. Schütze, K. Sebastian Radke, G. Cuniberti, F. Ortmann, M. Lorenz-Rothe, R. Meerheim, D. Spoltore, K. Vandewal, C. Koerner and K. Leo, *Phys. Status Solidi Appl. Mater. Sci.*, 2015, **212**, 2747–2753.
- 7 M. Mao, J. B. Wang, Z. F. Xiao, S. Y. Dai and Q. H. Song, *Dye. Pigment.*, 2012, **94**, 224–232.
- 8 Y. Kubo, D. Eguchi, A. Matsumoto, R. Nishiyabu, H. Yakushiji, K. Shigaki and M. Kaneko, *J. Mater. Chem. A*, 2014, **2**, 5204–5211.
- 9 H. Y. Lin, W. C. Huang, Y. C. Chen, H. H. Chou, C. Y. Hsu, J. T. Lin and H. W. Lin, *Chem. Commun.*, 2012, **48**, 8913–8915.
- 10 S. Kolemen, O. A. Bozdemir, Y. Cakmak, G. Barin, S. Erten-Ela, M. Marszalek, J. H. Yum, S. M. Zakeeruddin, M. K. Nazeeruddin, M. Grätzel and E. U. Akkaya, *Chem. Sci.*, 2011, **2**, 949–954.
- 11 Z. E. Galateia, N. Agapi, N. Vasilis, G. D. Sharma and C. G. Athanassios, *J. Mater. Chem. C*, 2015, **3**, 5652–5664.
- 12 J. Liao, H. Zhao, Y. Xu, W. Zhou, F. Peng, Y. Wang and Y. Fang, *RSC Adv.*, 2017, **7**, 33975–33985.
- 13 G. Thumuganti, V. Gupta and S. P. Singh, *New J. Chem.*, 2019, **43**, 8735–8740.
- 14 M. F. Shah, A. Mirloup, T. H. Chowdhury, S. Alexandra, A. S. Hanbazazah, A. Ahmed, J.-J. Lee, N. Leclerc, M. Abdel-Shakour and A. Islam, *Sustain. Energy Fuels*, , DOI:10.1039/c9se00300b.
- 15 Y. Kubota, K. Kimura, J. Jin, K. Manseki, K. Funabiki and M. Matsui, *New J. Chem.*, 2019, **43**, 1156–1165.
- 16 E. A. Yildiz, G. Sevinc, H. G. Yaglioglu and M. Hayvali, *Opt. Mater. (Amst.)*, 2019, **91**, 50–57.