Supporting information for:

Application of an inverse-design method to optimizing porphyrins in dye-sensitized solar cells

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Fig. 1 shows the 41 functional groups that were considered in the PooMa calculations. Moreover, Table 1 lists the 206 dyes that were identified in earlier, experimental studies plus the values for their five descriptors as obtained in the DFTB calculations.

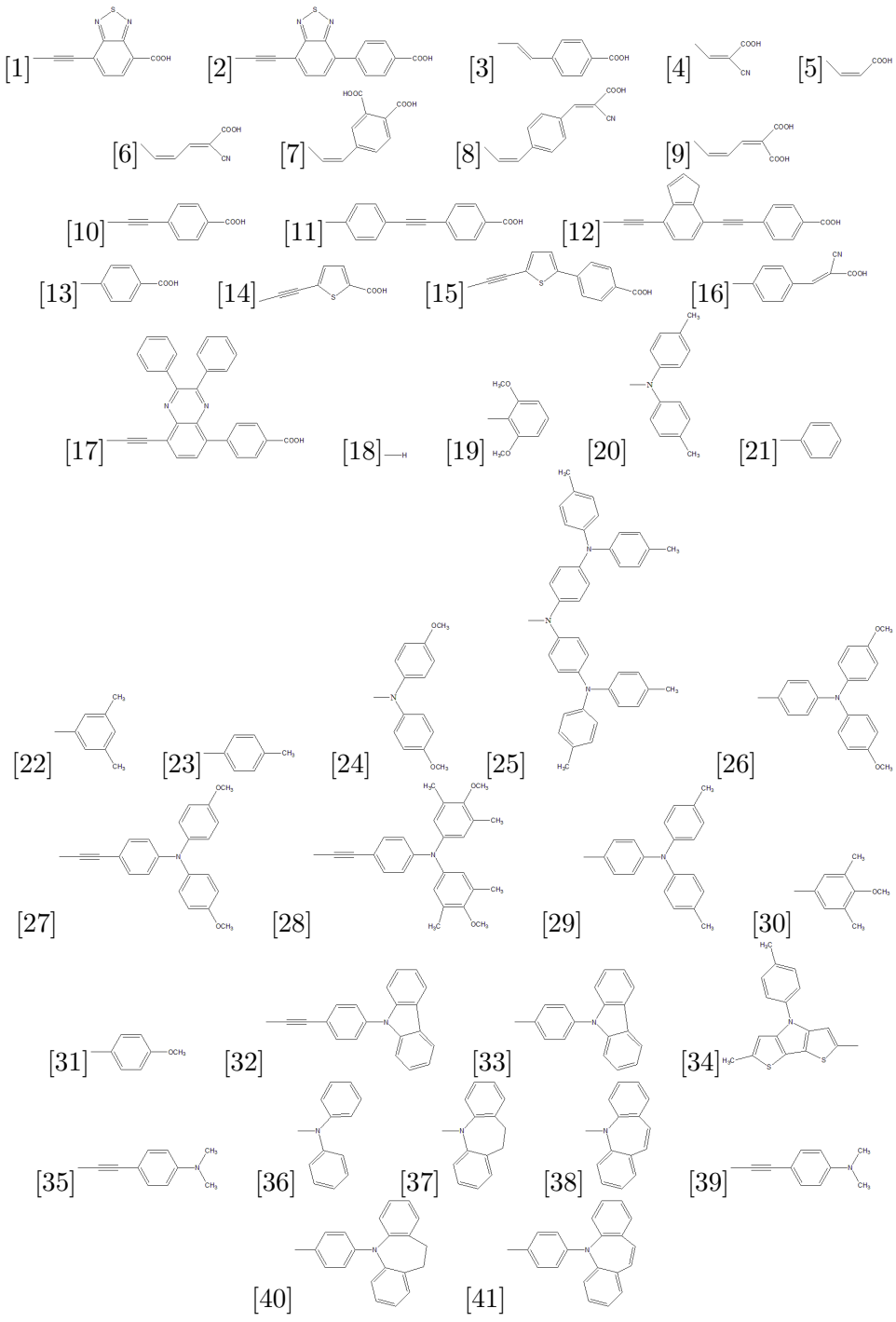

Figure 1: Fourty-one substitutes in the pool.

Table 1: The set of 206 dyes whose PCE was determined experimentally in other studies. Also shown are the calculated values for their electronic properties as calculated using the DFTB method.

Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
1	0.0667663	0.1098637	5.7343099	3.4535395	0.1145571	3.65	Dye-1	[1]
2	0.0663543	0.1096820	6.0609838	3.4544885	0.1138443	2.92	Dye-2	[1]
3	0.0664988	0.1103366	4.8131561	3.4586567	0.1141258	1.85	Dye-3	[1]
4	0.0667569	0.1106514	4.6365321	3.4549942	0.1144396	3.60	Dye-4	[1]
5	0.0585169	0.1340320	10.2152042	4.0362108	0.1120592	3.12	Ia	[2]
6	0.0581445	0.1203809	9.4677291	3.7705729	0.1056630	2.12	Ib	[2]
7	0.0582487	0.1049978	8.3026409	3.2347226	0.0894526	1.56	Ic	[2]
8	0.0585103	0.0972312	7.3989790	3.0272590	0.0844352	1.01	Id	[2]
9	0.0651194	0.1489580	5.0898235	3.8586935	0.1140304	3.55	IIa	[2]
10	0.0646801	0.1383724	4.5471286	3.6183750	0.1074025	4.18	IIb	[2]
11	0.0649658	0.1212406	4.3987205	3.1155014	0.0917486	4.79	IIc	[2]
12	0.0646400	0.1126151	3.8027126	2.9405910	0.0863881	5.08	IId	[2]
13	0.0522444	0.0926442	25.2075402	3.9906128	0.1171719	4.05	4a	[3]
14	0.0538638	0.1097202	20.7111210	3.8794755	0.1079478	5.26	4b	[3]
15	0.0451378	0.1281958	16.3328951	4.1582659	0.1109642	2.62	4c	[3]
16	0.0609398	0.1451275	6.5802371	4.5240353	0.1094510	5.05	LP-1	[4]
17	0.0610683	0.1323146	6.6710082	4.0286502	0.0959868	6.04	LP-2	[4]
18	0.0609842	0.1204137	5.9517260	3.6794902	0.0880607	5.35	LP-3	[4]
19	0.0616440	0.1304654	5.6258422	3.9561696	0.1209219	4.02	LP-4	[5]
20	0.0577100	0.0921068	19.6625025	3.6961125	0.1280541	4.47	LP-5	[5]

Table 1 continued from previous page

Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
21	0.0421651	0.1225426	20.2310204	4.2740513	0.1346527	6.14	LP-6	[5]
22	0.0431682	0.0832682	31.9452022	3.6657477	0.1031059	6.46	LP-11	[6]
23	0.0300687	0.1006932	37.1778862	4.0805418	0.1069056	7.37	LP-12	[6]
24	0.0651594	0.0924354	2.5485089	2.6158141	0.0594725	3.94	N-1	[7]
25	0.0636379	0.0849677	0.9614710	2.4923765	0.0635152	2.93	N-2	[7]
26	0.0614332	0.0902923	3.9628319	2.7286297	0.0559813	4.16	N-3	[7]
27	0.0623167	0.1319958	16.7910857	4.4047664	0.0927662	1.69	cz-4	[8]
28	0.0624102	0.1261617	15.8280472	4.1983894	0.0886179	2.13	cz-6	[8]
29	0.0623065	0.1152013	14.7572428	3.8539791	0.0813854	1.30	cz-10	[8]
30	0.0657199	0.1581280	4.5349031	4.5953904	0.1068553	3.01	ZnP	[9]
31	0.0652765	0.1240605	9.0586813	3.7328133	0.1144729	3.47	CZ-ZnP	[9]
32	0.0540346	0.1245887	8.9207224	3.6745778	0.1086988	3.62	IDB-ZnP	[9]
33	0.0542926	0.1312902	4.9425365	3.6583189	0.1141326	2.55	ISB-ZnP	[9]
34	0.0641569	0.1674612	4.4436781	4.5929910	0.1072287	0.95	4a	[10]
35	0.0643061	0.1241872	3.5871889	3.3790816	0.0777495	1.23	4b	[10]
36	0.0613149	0.1523029	4.0288707	4.2330484	0.1136030	0.55	5a	[10]
37	0.0614268	0.1202159	2.5602694	3.2368591	0.0848363	0.90	5b	[10]
38	0.0305762	0.0850418	7.1037800	2.1842021	0.0630336	4.84	GY21	[11]
39	0.0381284	0.0913519	5.7311743	2.1392080	0.0654496	8.90	GY50	[11]
40	0.0698013	0.1340860	12.2788772	3.9427723	0.1108234	4.11	Zn-1	[12]
41	0.0694326	0.1195924	11.2653050	3.4081137	0.0944323	4.80	Zn-2	[12]
42	0.0714856	0.1359144	5.2975855	3.6566619	0.1040171	0.89	Zn-4	[12]
43	0.0681198	0.1270787	9.9687732	3.8465629	0.1137559	5.20	Zn-3	[13]

Table 1 continued from previous page

Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
44	0.0701037	0.1369030	8.4470794	3.9188586	0.1102227	4.00	Zn-5	[13]
45	0.0606876	0.1390918	17.4673304	4.2028109	0.1092884	4.00	Zn-8	[13]
46	0.0699891	0.1261839	12.3239482	3.7383974	0.1082790	2.40	Zn-11	[13]
47	0.0647567	0.1188279	23.4547244	4.1144920	0.1151459	3.70	Zn-13	[13]
48	0.0574624	0.1354942	16.3196090	4.0872576	0.1061092	5.10	GD-1	[14]
49	0.0576122	0.1242851	15.3547937	3.8095844	0.0999381	7.10	GD-2	[14]
50	0.0578275	0.1148293	14.2016937	3.5310991	0.0931519	5.80	GD-3	[14]
51	0.0579618	0.1003757	12.4794999	3.0905908	0.0813659	6.40	GD-4	[14]
52	0.0580412	0.0798598	10.0239670	2.4717253	0.0653706	5.30	GD-5	[14]
53	0.0574176	0.1220547	14.2477433	3.5191403	0.0919278	6.10	GD-6	[14]
54	0.0633787	0.0996594	11.8911212	2.9677537	0.0637155	2.08	1b-d-Zn	[15]
55	0.0583384	0.0724674	16.5569083	3.2440629	0.0688259	2.37	2b-bd-Zn	[15]
56	0.0518869	0.0723033	17.3013189	3.0943628	0.0677597	3.03	2b-bdta-Zn	[15]
57	0.0711670	0.1112677	2.3188779	2.5824263	0.0704301	4.34	YD-0	[16]
58	0.0571101	0.1044525	3.6465939	2.5374905	0.0726405	6.15	YD-1	[16]
59	0.0707163	0.1077785	2.4395716	2.5352951	0.0589497	6.56	YD-2	[16]
60	0.0477547	0.1072710	4.8059315	2.6988464	0.0774612	5.34	YD-3	[16]
61	0.0529775	0.0992576	3.3021361	2.3825721	0.0687246	5.65	YD-4	[16]
62	0.0395915	0.0795812	4.2701956	2.1760608	0.0820473	2.10	YD-5	[16]
63	0.0458267	0.1040151	5.9300487	2.6847999	0.0822526	5.13	YD-6	[16]
64	0.0434028	0.0969086	14.8000218	2.9669484	0.0867171	4.38	YD-7	[16]
65	0.0513111	0.0706299	14.4246611	2.4099288	0.0734713	4.27	YD-8	[16]
66	0.0711670	0.1112677	2.3188779	2.5824263	0.0704301	5.00	YD0	[17]

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Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
67	0.0707163	0.1077785	2.4395716	2.5352951	0.0589497	7.10	YD2	[17]
68	0.0542112	0.0772139	4.0564086	2.3031583	0.0732740	6.80	YD14	[17]
69	0.0439099	0.0694964	15.4810452	2.6246536	0.0880480	4.20	YD15	[17]
70	0.0519541	0.0689608	8.8103707	2.2925680	0.0848171	5.50	YD16	[17]
71	0.0561651	0.0926398	3.2137225	2.1946879	0.0616570	7.00	YD17	[17]
72	0.0317356	0.0430464	28.3898544	2.2488689	0.1006172	6.69	XY1	[18]
73	0.0307369	0.0464320	27.0144801	2.3217648	0.0995922	6.89	XY2	[18]
74	0.0246106	0.0435574	30.4748570	2.2702888	0.0990199	5.50	XY3	[18]
75	0.0597190	0.0587322	22.1780946	2.3657366	0.0860160	3.64	CCT1A	[19]
76	0.0533135	0.0637261	27.7841165	2.6894384	0.0914474	4.80	CCT2A	[19]
77	0.0489295	0.0682620	35.6102724	2.9571414	0.0925016	5.25	CCT3A	[19]
78	0.0555831	0.0730346	4.2128616	1.9403036	0.0561517	7.60	YD-2-OC8	[20]
79	0.0555831	0.0730346	4.2128616	1.9403036	0.0561517	9.40	YD-2-OC8	[20]
80	0.0741501	0.1123608	1.0770695	2.3705037	0.0688793	4.01	1PEP	[21]
81	0.0740513	0.1280516	3.6765154	2.6671958	0.0797870	2.55	2PEP	[21]
82	0.0740785	0.1327977	10.0882432	2.9577075	0.0915939	0.58	3PEP	[21]
83	0.0612046	0.0808118	17.5427761	2.7310944	0.0796227	2.22	Q1	[22]
84	0.0643443	0.0793069	13.3271717	2.5787145	0.0770773	5.51	Q2	[22]
85	0.0651000	0.0628752	8.7421524	1.8751841	0.0563655	7.13	XW1	[22]
86	0.0633436	0.0679377	9.2710832	1.9548001	0.0590251	6.84	XW2	[22]
87	0.0601367	0.0710189	6.1817574	1.8861611	0.0571289	7.32	XW3	[22]
88	0.0615689	0.0691939	3.7172860	1.7146918	0.0516344	7.94	XW4	[22]
89	0.0552887	0.0758360	32.3656110	2.8962656	0.1117750	9.10	TA-ST-CA	[23]

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Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
90	0.0524638	0.0783148	29.8457557	3.3269538	0.1064191	6.72	DPTP	[24]
91	0.0488015	0.0745953	28.6722651	3.0716907	0.0952905	7.05	OMeDPTP	[24]
92	0.0503438	0.0542790	20.7832498	2.2597189	0.0717968	7.64	OHexDPTP	[24]
93	0.0481101	0.0767060	31.6898283	3.3072438	0.1135833	5.22	M-TP	[24]
94	0.0520232	0.0448104	12.8216249	1.4405117	0.0593717	4.60	PFT1	[25]
95	0.0527270	0.0580806	16.1220258	1.8478817	0.0745614	5.81	PFT2	[25]
96	0.0498505	0.0463602	18.2618960	1.7550009	0.0653839	6.10	PFT4	[25]
97	0.0490678	0.0578566	25.0361823	2.2980821	0.0810550	6.19	PFT5	[25]
98	0.0500541	0.0575150	23.8612992	2.2342677	0.0812448	5.76	PFT6	[25]
99	0.0549575	0.0884838	34.8488172	3.4904077	0.1125149	3.50	DP1	[26]
100	0.0461346	0.0996140	24.9309775	4.0957710	0.1132304	4.70	DP2	[26]
101	0.0493274	0.0817432	37.2108174	3.5345121	0.1058133	1.50	DP3	[26]
102	0.0407387	0.0892162	27.3739533	3.8124314	0.1063739	2.20	DP4	[26]
103	0.0841135	0.2057307	7.1010683	2.7208610	0.0664321	1.32	PR1	[27]
104	0.0517700	0.1100617	28.0466053	3.7487154	0.1069148	2.01	PR2	[27]
105	0.0552221	0.0880710	37.5865174	3.2462465	0.1093803	4.51	1a	[28]
106	0.0515456	0.0737763	38.6887253	3.1875722	0.1159729	4.30	2a	[28]
107	0.0448888	0.0806014	43.4726481	3.4968618	0.1139284	1.87	3a	[28]
108	0.0617975	0.0825254	32.6481218	3.0964956	0.1122582	3.40	4a	[28]
109	0.0508722	0.0699902	37.6127881	3.1095210	0.1164795	4.81	5a	[28]
110	0.0563576	0.0601751	26.4729997	2.2710818	0.0797090	4.01	1b	[28]
111	0.0520953	0.0519731	27.7355773	2.2763563	0.0844611	4.53	2b	[28]
112	0.0453090	0.0571239	30.8566665	2.5021194	0.0831224	3.60	3b	[28]

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Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
113	0.0641378	0.0582832	21.5817121	2.0887966	0.0829236	3.31	4b	[28]
114	0.0519093	0.0478448	25.8112761	2.1736651	0.0837734	4.89	5b	[28]
115	0.0345478	0.1158408	22.4026301	3.6692020	0.1043632	0.95	4a	[29]
116	0.0313985	0.0958721	24.1906637	3.2062762	0.1334664	4.51	4b	[29]
117	0.0500921	0.0891723	37.2959570	3.6383843	0.1148349	3.68	3a	[30]
118	0.0439812	0.0787065	37.1605931	3.4551607	0.1125992	0.35	3b	[30]
119	0.0553125	0.0651710	8.2952616	2.0958641	0.0608170	7.95	JY47	[31]
120	0.0360465	0.0753090	11.4781473	2.3113859	0.0710253	8.44	JY48	[31]
121	0.0361144	0.0742704	12.0550747	2.3025053	0.0739827	7.84	JY49	[31]
122	0.0726905	0.1329466	2.1572703	3.2870702	0.0677228	1.87	PD1	[32]
123	0.0542564	0.0879329	9.4990120	3.2851808	0.1168215	2.74	PD2	[32]
124	0.0411915	0.0919867	23.8557771	3.0991290	0.0867796	1.61	CVHTP	[33]
125	0.0618008	0.0858590	22.5883618	2.9804705	0.0835124	1.12	CVHTC	[33]
126	0.0413066	0.0959144	28.5044492	3.4460743	0.0980040	3.20	CVTC-H-CVTP	[33]
127	0.0394775	0.0372875	12.1225083	1.3838718	0.0763475	6.20	C1	[34]
128	0.0456119	0.0312782	11.7898422	1.3341227	0.0758650	4.74	C2	[34]
129	0.0344904	0.0305524	13.4128932	1.3582548	0.0765701	1.42	C3	[34]
130	0.0291520	0.0716024	10.9348966	1.6340496	0.0940685	6.14	ND	[35]
131	0.0460617	0.0628970	20.4731641	2.6530180	0.0837996	7.42	SC1	[36]
132	0.0455990	0.0645827	19.3184989	2.7756639	0.0840953	6.45	SC2	[36]
133	0.0456559	0.0517875	16.1174775	2.2321817	0.0688872	6.53	SC3	[36]
134	0.0541271	0.0490485	31.4490748	2.5346917	0.0930642	6.90	M81	[37]
135	0.0534775	0.0699740	38.1812534	3.1046537	0.0996195	6.15	M82	[37]

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Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
136	0.0479043	0.0497461	15.8997758	1.9558896	0.0709909	4.43	M83	[37]
137	0.0500849	0.0529846	16.4925284	1.9671548	0.0680051	7.59	M84	[37]
138	0.0582135	0.0878282	14.5325216	2.8137256	0.0696394	5.99	M85	[37]
139	0.0841303	0.1048041	8.8130411	1.8789629	0.0704406	0.72	DEA-Q	[38]
140	0.0506190	0.0810102	19.6715293	2.4798638	0.0966150	0.75	CBZ-Q	[38]
141	0.0427224	0.0587965	19.0172584	2.1543939	0.0815758	3.07	BPA-Q	[38]
142	0.0604350	0.0693764	19.8577933	2.8935371	0.1174360	5.65	FWD1	[39]
143	0.0580204	0.0904394	25.7566080	3.8867700	0.1120075	6.04	FWD2	[39]
144	0.0603457	0.0841191	24.1186544	3.0040282	0.1209318	5.19	FWD3	[39]
145	0.0447695	0.0547394	14.2904317	1.9386081	0.0923815	5.64	ZHG5	[40]
146	0.0451923	0.0616264	15.9976067	2.0818389	0.0926777	5.32	ZHG6	[40]
147	0.0458692	0.0373386	23.6356043	1.8225969	0.0889805	2.74	ZHG7	[40]
148	0.0494562	0.0880206	13.2479744	2.3711061	0.0752384	7.55	TBCPCA-1	[41]
149	0.0492978	0.0832383	12.9728251	2.2690494	0.0724452	7.97	TBCPCA-2	[41]
150	0.0485320	0.0512228	14.9746384	2.0241526	0.0883079	7.11	TBTCPCA-1	[41]
151	0.0483990	0.0496290	14.8755703	1.9700435	0.0861409	6.17	TBTCPCA-2	[41]
152	0.0492426	0.0283154	12.9889047	2.1688351	0.0802441	1.40	FBA1	[42]
153	0.0602150	0.0240906	13.0003237	1.6102805	0.0687187	2.10	FBA2	[42]
154	0.0600001	0.0184357	9.9806662	1.2505838	0.0533310	2.50	FBA3	[42]
155	0.0644035	0.0660986	26.6569484	2.6446677	0.0830919	5.20	CD-1	[43]
156	0.0663843	0.0592458	24.1027450	2.3756802	0.0912346	4.10	CD-2	[43]
157	0.0687606	0.0537808	22.3137242	2.2149987	0.0990528	3.50	CD-3	[43]
158	0.0156502	0.0539460	18.7662736	1.9177332	0.0854602	3.37	SC32	[44]

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Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
159	0.0442793	0.0535942	23.5056563	2.2802517	0.0823760	6.52	SC33	[44]
160	0.0437057	0.0534638	23.9861220	2.2521598	0.0812267	7.07	SC35	[44]
161	0.0430359	0.0390825	20.6383475	1.8277278	0.0692110	7.38	SC36	[44]
162	0.0442080	0.0424417	21.7986307	1.9608395	0.0737957	6.70	SC36N	[44]
163	0.0527280	0.0575476	17.7988149	3.0560310	0.0944754	7.44	D1	[45]
164	0.0522667	0.0940092	22.8766610	3.0570864	0.0904328	6.64	D2	[45]
165	0.0521401	0.0628896	31.3356719	2.8531441	0.0880253	6.72	D3	[45]
166	0.0527717	0.0704874	37.1575169	3.0258481	0.0983773	6.06	D4	[45]
167	0.0659430	0.0741071	21.0042222	2.4773849	0.0765677	7.39	QX11	[46]
168	0.0695141	0.0792216	15.6467279	2.3310899	0.0709776	7.64	QX12	[46]
169	0.0657324	0.0589542	16.9540920	1.9888067	0.0620891	6.95	QX13	[46]
170	0.0692903	0.0572709	13.9197013	1.8434155	0.0581264	6.52	QX14	[46]
171	0.0317029	0.0510672	40.7211582	2.8327700	0.0826220	1.10	DPP1	[47]
172	0.0322922	0.0353959	25.9853729	1.9561253	0.0669555	1.40	DPP2	[47]
173	0.0315614	0.0362411	30.0719430	2.0737607	0.0601351	1.80	DPP3	[47]
174	0.0345150	0.0332382	26.2949546	1.8979877	0.0684235	2.20	DPP4	[47]
175	0.0417351	0.0745864	50.8924433	3.7784633	0.1065326	0.60	PE4T	[47]
176	0.0468692	0.0581254	28.2242522	2.7360594	0.0668775	3.40	MK-2	[47]
177	0.0392516	0.0690701	15.5298974	2.4799794	0.0930063	7.19	QBT-3	[48]
178	0.0388931	0.0701548	13.8409102	2.4168808	0.0868444	6.78	CTY-1	[48]
179	0.0292251	0.0640481	17.4939690	2.5255762	0.0904998	8.27	CTY-2	[48]
180	0.0388931	0.0701548	13.8409102	2.4168808	0.0868444	7.60	CTY-3	[48]
181	0.0292251	0.0640481	17.4939690	2.5255762	0.0904998	8.10	CTY-4	[48]

Table 1 continued from previous page

Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
182	0.0712902	0.0833525	1.2577618	2.0866102	0.0536498	5.03	ZnP3C	[49]
183	0.0504375	0.0716576	26.5928157	2.8331785	0.0632194	1.65	X66	[50]
184	0.0508574	0.0682930	23.8054083	2.6036665	0.0662447	3.67	X67	[50]
185	0.0505090	0.0706008	24.3234921	2.6846997	0.0675389	3.24	X68	[50]
186	0.0509958	0.0609839	22.9207043	2.4686164	0.0739502	4.21	X69	[50]
187	0.0671807	0.0805556	1.0923534	1.8670982	0.0481617	9.01	LD14	[51]
188	0.0669543	0.0880626	1.2356082	1.9481770	0.0490203	9.53	LW4	[51]
189	0.0669449	0.0900709	2.4224591	2.0487544	0.0517304	8.16	LW5	[51]
190	0.0489638	0.1000547	2.5089851	2.1347794	0.0576524	9.21	LW24	[51]
191	0.0525938	0.1101084	17.2953206	3.1584463	0.0835753	4.39	T2-1	[52]
192	0.0225351	0.0843428	22.3894841	2.8046683	0.1199625	5.89	PZ-1	[52]
193	0.0180974	0.0672775	22.0673579	2.4616481	0.1245091	2.62	PZ-2	[52]
194	0.0209844	0.0739312	22.0094535	2.5514273	0.1238206	4.97	PZ-3	[52]
195	0.0208503	0.0634133	21.2871276	2.3910134	0.1047528	6.35	PZ-4	[52]
196	0.0689817	0.0648257	12.9473879	3.2856018	0.0957432	1.37	OF-Car-Car	[53]
197	0.0819577	0.0826697	4.6338681	2.7784854	0.0916952	2.04	OF-Py-Py	[53]
198	0.0705968	0.0729861	32.3979744	3.2201559	0.0995803	0.07	OF-Cat-Cat	[53]
199	0.0749618	0.0810413	27.3428612	2.9627925	0.0992052	1.51	OF-Py-Car	[53]
200	0.0753765	0.0785730	10.4911300	3.1440620	0.0995364	0.06	OF-Py-Cat	[53]
201	0.0632342	0.0887058	20.0629795	2.8690664	0.1030617	1.75	MH	[54]
202	0.0601685	0.0807677	21.7355627	3.0067993	0.1096920	0.99	MT	[54]
203	0.0569366	0.0858796	10.8433973	3.6573353	0.0965582	2.70	DH	[54]
204	0.0551298	0.0692840	11.0962548	3.6412735	0.1094707	1.42	DT	[54]

Table 1 continued from previous page

Molecule	G	O	D	A	LHE	PCE (exp.)	Molecule name in Ref.	Ref.
205	0.0642779	0.0940782	18.5053841	3.0665354	0.1097282	2.31	TPAC1	[54]
206	0.0578251	0.0767625	11.2128556	3.6531465	0.1069505	2.73	TPAC2	[54]

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