补充材料

附表 I 多氯联苯化合物各理化性质和生物活性的文献报道值 [a]

Table S1 List of experimental values of physicochemical properties and biological activities under study

No.	logS_W	logK_{OW}	logK_{OA}	logK_{OC}	logY_W	logP_L	*TSA*	*RRT*	ΔH_{subl}	ΔH_{vap}	ΔH_{fus}	pEC_{50}	Biodeg %	–log*k*
1			6.65		4.67	.2800	208.3	.1544	86.3	72.1	14.5			
2	5.39	4.66		4.58	4.94		209.9	.1937		74.3				
3	5.33	4.63	6.99	4.71	4.78	-.0288	209.9	.1975	82.4	71.6	13.3			
4	5.72	4.72	6.86	4.74	5.06	-.4850	224.3	.2245	96.9				85	.553
5	5.35	4.99	7.59			-.8310	223.9	.2785					80	.032
6	5.26	4.84	7.55	4.85	5.59	-.7610		.2790					95	
7	5.56	5.15	7.39	4.76	5.36	-.7330	225.9	.2566		75.4			85	
8	5.46	5.09	7.61	4.76	5.40	-.8010	225.9	.2783					80	.008
9			7.40		5.39	-.7330	225.9	.2570		76.8			85	
10					5.17	-.4750	224.3	.2243			12.6			1.086
11	6.45	5.27	7.90		5.76	-1.0600	227.4	.3238		81.0				.432
12	6.39	5.23	7.80			-1.1100	225.4	.3298						.055
13	6.40	5.15				-1.0800		.3315						
14			7.78			-.9000	227.4	.2973						.016
15	6.37	5.23	7.88	4.79	5.65	-1.1390		.3387	105.1	81.4			20	.298
16	6.10	5.12	7.98	4.78	5.91	-1.2680		.3625					80	
17	6.49	5.39	7.74	4.81		-1.1480		.3398					50	
18	6.17	5.33		4.79	5.84			.3378	99.5	80.2			45	.991
19	5.90	5.04		4.71	5.15	-.9360		.3045					50	
20		5.60	8.49	4.94		-1.5500	241.4	.4170						
21	6.18	5.68				-1.5600	241.4	.4135						.194
22	5.80	5.29	8.58	4.98	5.82	-1.5900		.4267					60	
23						-1.3100		.3770						
24	6.49	5.44			6.05	-1.1800		.3508						
25	6.11	5.54	8.28			-1.4300		.3937					35	
26	6.14	5.65	8.52	4.80	5.98	-1.5800	239.4	.3911					90	.083
27			8.27	4.79	6.82	-1.3900		.3521					70	
28	6.22	5.71		4.98	6.00	-1.3000	241.4	.4031						.095

29					5.77	-1.2300	241.4	.3820	103.6		22.8		80	.188
30			8.40		5.70	-1.4700	241.8	.3165	95.6		16.5		15	.036
31	6.18	5.68	8.05	4.96	5.98	-1.3500	234.4	.4024					20	.216
32	6.16	5.24				-1.0100		.3636						
33	6.21	5.71	8.40		5.94	-1.4600	241.4	.4163						.112
34	6.30	5.71	7.97			-1.2700		.3782					60	
35						-1.8600	241.4	.4738						
36						-1.7500		.4375						
37					6.25	-1.9000	243.2	.4858					0	
38								.4593						
39						-1.7000		.4488						
40	6.83	5.67		5.14	6.08	-2.0100	255.4	.5102					75	.836
41	7.00	5.79				-1.9600		.4990					70	
42	6.96	5.72	8.82		6.25	-1.9300		.4870					40	
43						-1.7800		.4587						
44	6.91	5.73	8.71	5.10	6.28	-1.8900	257.4	.4832					60	
45	6.30	4.84		4.94		-1.6500	256.9	.4334					35	
46	6.30	4.84	8.56	5.00	5.44	-1.7300		.4450					60	
47	7.23	5.94	8.56		6.43	-1.8100	259.4	.4639				3.886	5	
48	6.86	5.69	8.50		6.68	-1.8100		.4651					5	
49	7.12	5.87		5.09			259.4	.4610	108.3	87.4	23.4		30	
50	6.94	5.75			5.46		247.8	.4007						
51	6.65	5.51				-1.6100	257.8	.4242					40	
52	7.00	5.79	8.49	5.10	6.20	-1.7900	259.4	.4557	101.0				20	1.155
53	6.65	5.55	8.18		5.85	-1.5600		.4187	101.0	84.9			25	
54	6.20	5.24			6.33	-1.4100	256.3	.3800						
55	6.77	6.10				-2.2400		.5562						
56					6.16	-2.3700		.5676					40	
57								.5155						
58								.5267						
59								.4860						
60	6.86	6.24		5.38	5.72	-2.2800	259.2	.5676					40	
61			8.93		6.60	-1.9200	255.0	.5331			25.2	3.854		.420

62								.4685						
63	6.77	6.10	9.06		6.26	-2.1700		.5290					20	
64	7.02	5.76	8.63			-1.8800		.4999					70	
65	7.25	5.96				-1.8500	255.4	.4671						
66	6.63	5.98	9.29	5.38	5.90	-2.2100	259.0	.5447					0	
67		6.32				-2.1800		.5214					5	
68	7.13							.5040						
69	7.26	6.03			6.94	-1.7500		.4510						
70	6.69	6.22	9.22	5.26	6.21	-2.2600	259.0	.5407					70	
71	7.02	5.76						.4989						
72			8.84	5.27		-2.0400		.4984						
73						-2.0000		.4554						
74	6.77	6.10			6.02			.5341						
75	7.26	6.03	9.14		6.15	-2.1400	258.5	.4643					0	
76	6.71	5.98			6.06	-1.7400		.5408					5	
77			9.92	5.71	7.19	-2.6600	258.5	.6295				6.149		
78						-2.5000		.6204						
79						-2.4700		.5894						
80					7.28	-2.2600	262.5	.5464						
81						-2.5400		.6149				4.553		
82					6.12			.6453						
83							272.9	.6029						
84	6.78	5.60					272.3	.5744						
85	7.62	6.18					272.3	.6224						
86	7.87	6.38			6.32		270.9	.6105						
87	7.66	6.23		5.82	6.53		273.0	.6175						
88	7.92	6.50			7.06		271.4	.5486						
89	6.78	5.60						.5779						
90	7.82	6.32						.5814						
91	7.17	5.87						.5549						
92	7.82	6.32						.5742					30	
93	7.40	6.06						.5437						
94				5.39				.5331						

95	7.19	5.92		5.62	6.10		273.4	.5464		92.3				
96								.5057		89.6				
97	7.76	6.30		5.91	6.51			.6100					0	
98	7.40	6.04						.5415						
99	7.95	6.41					274.9	.5880						
100	7.66	6.23			6.94		275.4	.5212						
101				5.78	6.91		275.0	.5816	109.8		18.8			
102								.5431						
103	7.47	6.11						.5142		91.6				
104					6.73		273.8	.4757						
105	7.52	6.79		6.07			272.5	.7049				5.367		
106	7.68	6.92						.6680						
107								.6628						
108								.6626						
109								.6016						
110	7.65	6.20		5.80	7.05		273.0	.6314						
111								.6183						
112	7.95	6.45						.5986						
113	7.76	6.41						.5862						
114	7.50	6.71			6.59			.6828						
115	7.96	6.44						.6171				5.387		
116					6.82		269.0	.6132			21.8			
117	7.88	6.39						.6150						
118	7.33	6.57		5.99	6.55		274.5	.6693						
119	7.91	6.40						.5968				5.041		
120		6.30						.6256				4.854		
121	7.92	6.42						.5518						
122					6.48			.6871						
123	7.42	6.64						.6658						
124					6.52		274.5	.6584						
125	7.57							.6142						
126				5.87				.7512				6.886		
127				5.82				.7078						

128	8.33				7.53		286.5	.7761	122.7		29.2			
129	8.42	6.76			7.15		286.5	.7501						
130		7.30						.7284						
131	8.48	6.78						.6853						
132	7.65	6.20						.7035						
133		6.72						.6871						
134	7.65	6.20			7.08		286.9	.6796						
135	7.82	6.32			6.70			.6563						
136					6.91		287.4	.6257			21.1			
137	8.52	6.82			7.12			.7329						
138	8.38	6.73		6.20	7.14		288.5	.7403						
139					7.00			.6707						
140	8.24	6.58						.6707						
141	8.42	6.75			7.09			.7203						
142								.6848						
143	8.13	6.56						.6789						
144	8.01	6.45						.6563						
145								.6149						
146	8.58	6.85		6.18				.6955						
147								.6608						
148				5.95				.6243						
149	7.94	6.41		6.05			289.0	.6672						
150								.5969						
151	7.93	6.42		6.02	6.68			.6499						
152								.6062						
153	8.49	6.80		6.19	7.50		290.5	.7036		103.5		4.102		
154	8.12	6.65						.6349						
155	8.12	6.54			7.88		291.4	.5666	101.5		17.5			
156	8.31	7.44			6.81		288.1	.8105		112.6		5.149		
157							287.8	.8184				5.301		
158	8.48	6.78			6.84			.7429						
159								.7655						
160								.7396						

161								.6968						
162								.7737						
163	8.48	6.78			7.21			.7396						
164	8.27	6.63						.7399						
165		7.00						.6920						
166								.7572						
167	8.21	7.29						.7814				4.796		
168								.7068				4.004		
169	8.85	7.55					289.6	.8625						
170	8.90	7.08			6.97			.8740						
171					7.22		302.5	.8089	122.7	109.1	20.3			
172	9.10	7.21						.8278						
173								.8152						
174	8.59	6.85		6.30	6.84			.7965						
175	8.68	6.92						.7611						
176	8.15	6.55						.7305						
177	8.42	6.73		6.35				.8031						
178	8.59	6.85						.7537						
179	7.94	6.41						.7205						
180	9.10	7.21		6.37	7.15		304.5	.8362						
181	8.97	7.13						.7968						
182	8.68	6.92						.7653						
183	8.85	7.04		6.32	7.33			.7720						
184								.7016						
185	8.75	6.99			7.10		302.5	.7848						
186								.7416						
187					7.16		304.5	.7654						
188	8.49	6.78						.6920						
189	8.72	7.72						.9142						
190	8.90	7.08						.8740						
191	9.10	7.21						.8447						
192	9.10	7.21						.8269						
193	9.10	7.21						.8397						

194	9.70	7.62			8.23		317.6	.9620						
195	9.29	7.35						.9321						
196	9.42	7.43						.8938						
197	9.10	7.21						.8293						
198	9.42	7.43						.8845						
199	9.10	7.21						.8494						
200	9.20	7.30						.8197						
201	9.29	7.35						.8875						
202					8.29		318.5	.8089	114.2		22.8			
203	9.50	7.49						.8938						
204	9.48	7.48						.8217						
205	9.70	7.62						.9678						
206	10.18	7.94			8.21		331.6	1.0103						
207	10.07	7.88					332.0	.9423						
208					9.02		332.0	.9320			22.6			
209		8.20			8.75		345.6	1.0496	119.1		28.7			

[a] 单位：*S*: mol·L^{-1}; P_L: Pa; *TSA*: Å^2; ΔH_{subl}, ΔH_{vap}, ΔH_{fus}: kJ·mol; EC_{50}: mol·L^{-1}; *k*: hr^{-1}.

附表 II　209 个多氯联苯化合物计算的结构参数 [a]

Table S2　List of computational descriptors for 209 PCBs

No.	ε_{HOMO}	ε_{LUMO}	μ	V_{min}	$V_{s,min}$	$V_{s,max}$	$\overline{V_s}$	Π	σ^2_{tot}	ΣV_s^-	ΣV_s^+
1	-.31684	.11773	1.910	-1.0900	-1.0282	.8424	-.0590	.4072	.1122	-26.6001	19.6418
2	-.31044	.10490	2.292	-.7888	-.6867	.8504	.0461	.4086	.0802	-22.8881	21.9741
3	-.30610	.10507	2.378	-.7742	-.6921	.7953	.0183	.4037	.0838	-23.4767	22.8372
4	-.33398	.12177	2.528	-.9988	-.9680	.8630	-.0376	.4187	.1131	-29.7970	22.0705
5	-.32596	.10991	3.174	-.9818	-.9117	.9998	-.0210	.4120	.1243	-27.1420	23.4799
6	-.32760	.10802	3.503	-.8643	-.8338	.9460	-.0012	.4091	.1204	-24.4034	21.8230
7	-.32248	.10594	2.380	-.8946	-.8744	.9792	.0145	.3573	.0938	-20.5025	22.1397
8	-.32189	.10697	3.373	-.8480	-.8127	.9522	.0116	.4003	.1137	-22.9559	24.2975
9	-.32464	.10552	.686	-.8996	-.8810	.9750	.0192	.3640	.1017	-22.0008	19.8230
10	-.33322	.11642	1.210	-1.0125	-.9906	1.0214	-.0718	.4176	.1418	-25.5411	21.0404
11	-.32076	.09420	3.318	-.6956	-.6219	.9536	.0292	.3880	.1058	-20.5119	25.7041
12	-.31429	.09528	3.578	-.9257	-.8602	.9337	.0113	.3897	.1124	-23.0471	27.6049
13	-.31601	.09419	2.072	-.6828	-.6052	.9733	.0570	.3787	.1013	-19.5922	26.9029
14	-.32035	.09364	2.585	-.6011	-.5452	.8918	.0467	.3354	.0839	-17.6539	23.2539
15	-.31190	.09439	0.000	-.6715	-.5940	.9567	.0542	.3986	.1049	-19.6607	27.8504
16	-.33898	.11209	3.746	-.9602	-.8970	1.0224	-.0538	.4227	.1363	-28.6868	27.7917
17	-.34012	.11041	3.272	-.8432	-.8118	.9629	-.0248	.3929	.1251	-22.5282	23.6686
18	-.33646	.11028	2.110	-.8532	-.8137	1.0065	.0350	.3891	.1232	-22.3582	25.6744
19	-.33558	.11438	1.850	-.8940	-.8392	1.0605	-.0584	.4303	.1404	-28.3554	23.0038
20	-.33701	.10200	3.969	-.8803	-.8205	1.1067	-.0045	.4011	.1362	-24.9569	25.0275
21	-.32989	.09988	3.679	-.8114	-.7717	1.0610	-.0348	.3813	.1225	-25.5442	24.1472
22	-.33020	.10032	3.348	-.8585	-.7945	1.0951	.0004	.3812	.1363	-21.9134	26.9417
23	-.33342	.09780	2.220	-.7820	-.7498	1.0032	.0343	.3320	.1134	-19.7902	22.0052
24	-.33795	.10464	1.315	-.8704	-.8468	1.1275	.0057	.3787	.1348	-25.5849	23.7131
25	-.33268	.09730	2.800	-.7226	-.6524	1.0667	.0247	.3541	.1243	-17.9051	24.7120
26	-.33037	.09875	4.578	-.9173	-.8622	1.0146	.0535	.4213	.1410	-23.8268	27.9921
27	-.33386	.09672	1.808	-.7231	-.6426	1.0317	.0634	.3374	.1073	-19.1827	24.3726
28	-.33669	.09729	3.501	-.6688	-.6288	1.0120	.0472	.3568	.1279	-18.9107	24.3243

29	-.33641	.10953	3.094	-.7822	-.7375	1.0951	.0122	.4086	.1461	-23.8961	23.2966
30	-.32716	.09635	1.665	-.6775	-.6104	1.0801	.0621	.3540	.1242	-18.1833	25.6901
31	-.32866	.09554	2.467	-.7482	-.7052	.9343	.0119	.3332	.0952	-20.4030	23.5060
32	-.33949	.10293	.993	-.8321	-.7789	.9300	.0120	.3413	.0920	-19.4927	22.5575
33	-.32913	.09591	1.653	-.6808	-.6249	1.0718	.0643	.3659	.1162	-18.2393	24.8915
34	-.33555	.10933	3.530	-.7574	-.7331	1.1205	-.0122	.3855	.1250	-23.1158	23.8563
35	-.32395	.08529	3.565	-.8328	-.7850	1.0655	.0486	.3721	.1412	-18.5879	27.0361
36	-.33039	.08369	2.157	-.6050	-.5356	1.0444	.0850	.3374	.1320	-15.2342	24.5024
37	-.31950	.08530	1.772	-.8192	-.7754	1.1120	.0678	.3914	.1498	-18.8941	29.5456
38	-.32191	.08583	3.965	-.7675	-.7220	.9966	.0227	.3564	.1354	-21.2963	24.1321
39	-.32511	.08372	.252	-.5916	-.5240	1.0426	.1161	.3600	.1262	-14.8968	27.1168
40	-.34469	.10442	4.235	-.8761	-.8291	1.1024	-.0186	.4225	.1593	-28.1677	28.7541
41	-.34347	.10180	4.381	-.7963	-.7584	1.0743	.0019	.3977	.1420	-25.2530	24.9492
42	-.34602	.10288	3.496	-.8494	-.7853	1.1171	.0326	.3709	.1427	-22.5571	25.8449
43	-.34392	.10019	3.176	-.7676	-.7284	1.0153	.0090	.3590	.1262	-23.5913	25.3762
44	-.34073	.10278	2.951	-.8588	-.8000	1.0932	.0207	.4064	.1540	-23.1183	27.7084
45	-.33988	.10317	2.233	-.8032	-.7360	1.1371	-.0215	.3875	.1482	-27.0538	24.7302
46	-.34164	.10791	3.553	-.9376	-.8797	1.1322	-.0821	.3920	.1555	-27.7408	23.6449
47	-.34756	.10135	2.217	-.6563	-.6296	1.0850	.0494	.3431	.1284	-18.8039	26.3825
48	-.34328	.10017	3.432	-.7376	-.7108	.9865	.0109	.3505	.1129	-22.2177	27.4625
49	-.34181	.10125	1.855	-.6726	-.6569	1.1033	.0779	.3710	.1367	-18.5811	26.0059
50	-.34116	.10154	2.306	-.7549	-.7163	1.0039	.0122	.3584	.1155	-20.5225	21.7635
51	-.34355	.10650	3.267	-.7033	-.6749	1.0765	.0045	.3765	.1355	-22.7657	23.5460
52	-.34136	.10118	.171	-.6789	-.6484	1.0919	.0477	.3550	.1306	-18.5414	25.4541
53	-.33758	.10649	1.847	-.7120	-.6726	1.0577	-.0239	.3762	.1411	-23.0830	22.8136
54	-.34062	.11159	.000	-.7384	-.7169	1.0194	-.0576	.3891	.1403	-29.9991	22.8461
55	-.34043	.09287	3.724	-.7123	-.6563	1.1884	.0351	.3976	.1431	-21.9446	27.6861
56	-.33914	.09367	4.388	-.8423	-.7840	1.1718	.0390	.3973	.1605	-20.9889	29.1549
57	-.34243	.09044	2.417	-.6853	-.6416	1.0928	.0793	.3530	.1227	-18.4562	28.1968
58	-.34570	.09218	3.386	-.7729	-.7121	1.1490	.0489	.3642	.1461	-18.8124	26.5581
59	-.34051	.09843	2.546	-.7125	-.6528	1.2088	.0115	.3756	.1273	-21.7830	23.3249
60	-.33393	.09127	2.556	-.6937	-.6470	1.2054	.0703	.3918	.1351	-19.3057	28.1407
61	-.33572	.08964	3.358	-.6733	-.6492	1.0626	.0071	.3590	.0942	-22.3253	26.9036

62	-.34265	.09360	2.051	-.7322	-.7046	1.0909	.0088	.3357	.0864	-21.9777	22.7537
63	-.33694	.08918	1.198	-.6636	-.6256	1.0852	.0901	.3384	.1038	-16.0201	28.0616
64	-.33980	.09821	2.621	-.6943	-.6466	1.2261	.0232	.3704	.1361	-20.8704	26.8195
65	-.34219	.09374	1.149	-.7357	-.7180	1.0987	.0407	.3373	.0906	-21.5508	23.6453
66	-.33518	.08905	2.900	-.8200	-.7242	1.1598	.0967	.3735	.1430	-18.2690	31.7366
67	-.33790	.08747	2.035	-.6483	-.6085	1.0823	.0840	.3325	.1151	-16.2878	28.3362
68	-.34117	.08772	1.717	-.5384	-.4869	1.1672	.1084	.3178	.1174	-14.0835	27.5083
69	-.34162	.09677	1.821	-.6863	-.6213	1.0919	.0457	.3355	.1038	-16.5909	25.5796
70	-.33665	.08847	2.838	-.8257	-.7619	1.1481	.1029	.3861	.1570	-17.4443	27.8229
71	-.33738	.08940	4.718	-.7596	-.7170	1.0945	.0503	.3674	.1454	-21.0322	25.7604
72	-.34198	.10331	4.583	-.9044	-.8307	1.1668	.0055	.3904	.1569	-22.9486	26.3340
73	-.34191	.08756	1.848	-.5386	-.4919	1.1479	.0939	.3004	.1133	-13.8422	24.6427
74	-.34486	.10227	3.682	-.5984	-.5473	1.1814	.0428	.3649	.1459	-18.9803	23.9213
75	-.33283	.08676	.159	-.6430	-.5984	1.0987	.0842	.3382	.1139	-16.8582	26.4247
76	-.34118	.09656	1.332	-.6664	-.5985	1.0940	.0749	.3309	.1003	-15.4953	26.1563
77	-.32697	.07701	2.801	-.7518	-.7128	1.2302	.0825	.3829	.1808	-17.8390	29.3514
78	-.33136	.07647	3.126	-.6759	-.6384	1.1341	.0707	.3386	.1314	-17.4619	28.8172
79	-.33291	.07547	1.625	-.7410	-.6971	1.2120	.1042	.3224	.1376	-13.7482	26.9940
80	-.34045	.07415	0.000	-.4271	-.3845	1.1421	.1371	.2868	.1056	-11.2758	29.9990
81	-.32655	.07652	1.626	-.6663	-.6255	1.1124	.0533	.3392	.1280	-16.5430	28.6026
82	-.34916	.09563	4.281	-.7902	-.7501	1.1790	.0241	.4159	.1670	-25.5376	28.4209
83	-.34805	.09412	3.337	-.7797	-.7312	1.1495	.0552	.3735	.1553	-21.0723	27.5102
84	-.34538	.09793	3.283	-.8568	-.8022	1.2138	.0470	.4203	.1602	-23.6951	26.6137
85	-.35109	.09425	3.100	-.6868	-.6535	1.1807	.0601	.3579	.1473	-18.9326	26.6071
86	-.34736	.09147	4.201	-.6798	-.6421	1.1067	.0089	.3515	.1324	-21.6122	24.2918
87	-.34484	.09419	3.131	-.6952	-.6586	1.1974	.0466	.3730	.1428	-20.1436	25.5120
88	-.34424	.09240	3.045	-.6997	-.6559	1.1099	-.0044	.3704	.1121	-21.5320	22.6253
89	-.34923	.09995	4.485	-.7728	-.7244	1.2047	.0032	.3856	.1690	-23.3949	22.7362
90	-.34906	.09275	1.929	-.6584	-.5908	1.1431	.0722	.3165	.1247	-16.5674	25.7052
91	-.34780	.09405	3.353	-.7691	-.7306	1.1638	.0507	.3729	.1598	-19.4461	25.0403
92	-.34726	.09667	2.582	-.6790	-.6447	1.2205	.0271	.3516	.1429	-19.6129	24.6363
93	-.34678	.09634	2.942	-.8350	-.7509	1.0843	.0638	.3657	.1353	-20.1073	22.9022
94	-.34554	.09272	1.621	-.6667	-.6117	1.1363	.0838	.3415	.1310	-15.5819	26.8754

95	-.34390	.09255	2.395	-.6968	-.6621	1.1152	.0143	.3551	.1124	-21.5767	23.3492
96	-.34484	.09853	3.221	-.7476	-.7050	1.1737	.0286	.3485	.1549	-20.5698	25.2526
97	-.34157	.09673	1.431	-.6846	-.6457	1.2278	-.0034	.3441	.1405	-20.9410	23.1020
98	-.34292	.10112	1.787	-.7678	-.7159	1.1420	-.0191	.3682	.1469	-24.8027	22.6540
99	-.34864	.09267	1.695	-.6361	-.6042	1.1639	.0683	.3251	.1177	-15.4515	27.0968
100	-.34908	.09510	1.682	-.5723	-.5052	1.1258	.0802	.3032	.1095	-15.0248	23.2562
101	-.34566	.09264	1.754	-.6444	-.6152	1.1608	.0924	.3194	.1198	-16.8654	26.7531
102	-.34488	.09848	3.597	-.7222	-.6843	1.1555	.0696	.3490	.1484	-19.3893	22.7060
103	-.34263	.09516	.342	-.5789	-.5403	1.0972	.0585	.3226	.1251	-17.0704	21.5719
104	-.34689	.09962	2.166	-.6019	-.5746	1.0832	-.0271	.3026	.1161	-18.5643	18.6508
105	-.34251	.08561	3.346	-.7675	-.7173	1.2567	.0649	.3658	.1513	-20.5768	31.9211
106	-.34496	.08289	2.897	-.5997	-.5261	1.1824	.0566	.3420	.1147	-17.3242	24.6689
107	-.34841	.08424	2.490	-.6123	-.5658	1.2726	.1248	.3765	.1411	-15.8657	30.3804
108	-.34449	.08781	2.097	-.6391	-.5709	.9844	.0798	.3491	.0908	-18.4347	25.4055
109	-.34495	.08317	2.446	-.7581	-.7073	1.1965	.1308	.3689	.1362	-16.0004	32.8733
110	-.34592	.08472	4.201	-.7047	-.6524	1.1810	.0814	.3788	.1466	-19.9648	30.9891
111	-.34592	.09313	3.657	-.8340	-.7850	1.2899	.0473	.4039	.1549	-20.3742	29.4914
112	-.35128	.08237	1.266	-.5844	-.5377	1.1639	.1050	.3115	.1005	-13.6545	26.6598
113	-.34429	.08794	1.781	-.6446	-.5836	.9988	.0612	.3507	.0889	-18.6016	24.2339
114	-.34871	.09230	2.761	-.6054	-.5412	1.3042	.0917	.3571	.1387	-16.2612	27.0148
115	-.33919	.08172	4.867	-.5650	-.5031	1.1774	.0686	.3330	.1129	-16.9189	28.4959
116	-.34402	.08758	1.179	-.6210	-.5545	1.2057	.0719	.3548	.0952	-17.0815	27.2883
117	-.34518	.08471	2.409	-.6413	-.6195	.8585	.0076	.3319	.0806	-20.3666	21.8107
118	-.34360	.08771	1.160	-.6247	-.5618	1.1750	.0768	.3543	.1050	-17.7171	29.3927
119	-.34027	.08002	1.595	-.7516	-.7089	1.2209	.0898	.3450	.1342	-14.8369	30.8721
120	-.34174	.08062	2.625	-.6650	-.6114	1.2433	.1149	.3470	.1475	-15.6374	29.5993
121	-.34715	.09151	2.624	-.8136	-.7522	1.0679	.0720	.3391	.1175	-16.1139	26.1172
122	-.34613	.07916	.117	-.5720	-.5319	1.1665	.0964	.3019	.0931	-12.8312	27.3703
123	-.34973	.09068	1.518	-.5064	-.4571	1.1611	.1337	.3204	.0983	-12.3206	26.4074
124	-.34312	.08043	3.186	-.6707	-.6352	1.2253	.1151	.3447	.1351	-16.7180	29.3537
125	-.35175	.09628	5.024	-.7481	-.6998	1.2431	.0107	.3546	.1614	-19.6223	24.9359
126	-.33388	.06875	1.687	-.6809	-.6474	1.2978	.1275	.3450	.1448	-15.1435	31.7407
127	-.34047	.06746	1.342	-.5883	-.5528	1.2600	.1438	.3101	.1166	-13.4107	31.0349

128	-.35718	.08854	3.573	-.6302	-.5989	1.2797	.0683	.3896	.1638	-20.2327	29.8686
129	-.35284	.08620	3.892	-.7191	-.6443	1.1972	.0646	.3820	.1471	-20.6047	29.3509
130	-.35195	.08719	2.837	-.6190	-.5933	1.2713	.1022	.3385	.1366	-17.8436	28.6558
131	-.34963	.08771	3.237	-.7775	-.7194	1.2071	.0373	.3501	.1425	-19.8823	24.9318
132	-.35075	.09200	3.735	-.6962	-.6603	1.2784	.0276	.3542	.1594	-22.3886	26.3096
133	-.35253	.08590	1.581	-.5936	-.5658	1.2007	.0919	.3155	.1127	-15.7744	29.7383
134	-.34916	.08788	2.923	-.7840	-.7296	1.2056	.0438	.3575	.1338	-21.3799	29.2612
135	-.34856	.09087	2.460	-.6683	-.6239	1.2905	.0861	.3193	.1345	-16.5147	25.8009
136	-.34611	.09568	1.819	-.6896	-.6519	1.2057	.0179	.3333	.1565	-21.1750	24.4248
137	-.35384	.08494	2.343	-.5475	-.5167	1.2173	.0696	.3213	.1241	-15.7184	25.4666
138	-.35173	.08704	2.502	-.6148	-.5755	1.3077	.0827	.3303	.1500	-16.4979	27.7548
139	-.35186	.08655	1.834	-.5295	-.5102	1.1792	.0361	.2905	.1032	-15.8410	25.2374
140	-.35560	.09050	2.938	-.6771	-.6363	1.1852	.0489	.3333	.1311	-17.7873	26.6397
141	-.34844	.08494	2.649	-.5541	-.5134	1.2190	.0486	.3239	.1071	-16.9042	25.0461
142	-.34691	.08368	3.391	-.6235	-.5725	1.0534	.0013	.3377	.1072	-22.3921	22.8938
143	-.35021	.09052	4.421	-.6303	-.5774	1.2648	.0196	.3408	.1465	-18.8371	24.9309
144	-.34545	.08651	1.492	-.5367	-.5133	1.2143	.0449	.3160	.1093	-15.9731	22.2309
145	-.34951	.09020	3.099	-.6141	-.5768	1.1886	-.0235	.3108	.1259	-19.0583	19.9662
146	-.35230	.08574	1.234	-.5856	-.5444	1.2345	.1025	.3325	.1243	-14.4734	24.9465
147	-.35119	.08673	1.596	-.5264	-.5040	1.1577	.0479	.3017	.0986	-17.5478	24.7642
148	-.34969	.08940	1.404	-.6479	-.6003	1.1684	.0967	.3033	.1001	-13.2005	24.6534
149	-.34866	.09070	2.684	-.6578	-.6026	1.2617	.0347	.3016	.1372	-17.4935	24.5786
150	-.34813	.09430	1.587	-.6654	-.6278	1.2091	.0222	.3140	.1481	-16.8355	23.5436
151	-.34523	.08657	.499	-.5369	-.4990	1.0992	.0260	.2827	.0931	-16.4422	23.6190
152	-.34713	.09012	2.323	-.6155	-.5820	1.1891	-.0351	.2943	.1290	-20.1760	21.5108
153	-.35172	.08561	.029	-.5744	-.5449	1.2420	.0957	.2861	.0997	-14.8826	29.7331
154	-.34981	.08924	1.434	-.6381	-.6087	1.1863	.0890	.2954	.0973	-11.8326	22.6763
155	-.35885	.09295	0.000	-.4358	-.4176	1.1147	.0647	.2568	.0837	-15.3878	21.4959
156	-.34708	.07635	1.983	-.7051	-.6632	1.2824	.1375	.3695	.1400	-16.0786	30.5033
157	-.34862	.07758	2.788	-.6139	-.5755	1.3356	.1004	.3372	.1201	-17.6746	30.8488
158	-.34978	.08301	2.280	-.7614	-.7127	1.2409	.0840	.3444	.1173	-15.4041	30.2004
159	-.35344	.07564	1.140	-.4698	-.4387	1.1933	.1338	.3253	.1003	-13.3234	28.2101
160	-.34699	.07921	2.064	-.5940	-.5370	1.0690	.0933	.3370	.0890	-16.4986	26.8499

161	-.35245	.08228	1.272	-.4606	-.4289	1.2179	.1296	.3136	.0928	-13.7501	28.7251
162	-.35177	.07578	2.243	-.6072	-.5587	1.1688	.1370	.3303	.1081	-15.1600	32.0430
163	-.34945	.08314	2.474	-.7697	-.6912	1.2522	.0827	.3346	.1169	-16.6214	30.9871
164	-.35415	.08765	3.991	-.6800	-.6343	1.3624	.1163	.3884	.1770	-18.3045	29.0279
165	-.35226	.08243	1.350	-.4676	-.4321	1.3111	.1167	.3253	.1104	-13.3113	27.8657
166	-.34631	.07897	.092	-.5746	-.4942	1.0653	.0947	.3321	.1035	-16.6773	28.6731
167	-.34670	.07271	1.432	-.5994	-.5634	1.2480	.1136	.3281	.1238	-14.6328	31.4539
168	-.35670	.08610	2.860	-.6602	-.6219	1.2262	.0951	.3081	.1099	-13.9721	28.1218
169	-.34085	.06119	.000	-.5343	-.5004	1.3595	.1208	.3521	.1321	-15.5259	33.5199
170	-.35707	.08042	2.763	-.5663	-.5008	1.3556	.0777	.3291	.1384	-16.1176	27.5522
171	-.35814	.08285	2.796	-.6286	-.5745	1.3148	.0872	.3236	.1362	-16.4944	27.4170
172	-.35537	.07930	1.954	-.5352	-.5073	1.3315	.0953	.3059	.1098	-15.2304	29.9741
173	-.35208	.07915	3.306	-.7283	-.6774	1.1804	.0077	.3140	.1222	-20.8304	23.5636
174	-.35338	.08477	3.462	-.5544	-.5274	1.2651	.0331	.2916	.0979	-16.6734	23.9610
175	-.35238	.08192	1.498	-.5923	-.5120	1.2679	.0943	.3036	.0931	-14.3159	26.5729
176	-.35462	.08300	2.820	-.6320	-.5924	1.2586	.0914	.3222	.1347	-17.1552	28.4785
177	-.35079	.08562	2.349	-.6119	-.5702	1.2710	-.0094	.2755	.1225	-18.0891	19.9511
178	-.35207	.08211	1.292	-.5935	-.5632	1.2937	.1038	.3115	.1178	-15.2131	26.0298
179	-.34986	.08556	1.680	-.6163	-.5713	1.2778	.0304	.2990	.1228	-18.1003	22.0593
180	-.35515	.07911	1.197	-.5277	-.4809	1.2529	.0805	.3012	.0984	-13.8553	27.5297
181	-.35418	.07794	1.662	-.4501	-.4213	1.2133	.0820	.2928	.0889	-14.6540	24.5474
182	-.35507	.08347	2.360	-.5314	-.4953	1.2392	.1067	.3008	.1113	-14.6790	26.4272
183	-.35243	.08170	1.222	-.5890	-.5246	1.2929	.0946	.2745	.0974	-12.9469	22.7706
184	-.35642	.08468	1.277	-.5172	-.4907	1.2136	.0618	.2642	.0927	-14.3559	25.2210
185	-.34792	.07777	1.716	-.4555	-.4101	1.1637	.0575	.2849	.0872	-15.7133	24.0784
186	-.35184	.08125	3.558	-.5102	-.4832	1.1980	-.0016	.3119	.1179	-19.8512	21.9276
187	-.35212	.08189	1.259	-.5958	-.5661	1.2922	.0981	.2894	.1057	-14.0425	26.2578
188	.35225	.08459	.173	-.5184	-.4829	1.1668	.0541	.2761	.0954	-13.9101	21.7787
189	.35350	.06968	1.153	-.5560	-.5207	1.3791	.1594	.3405	.1335	-14.8007	34.6932
190	.35197	.07472	1.667	-.7199	-.6577	1.2246	.0868	.3043	.1153	-15.3243	28.4024
191	.35930	.07838	2.330	-.6135	-.5793	1.2654	.0954	.3069	.1147	-14.0584	29.3148
192	.35485	.07407	.125	-.4192	-.3749	1.1977	.1025	.2832	.1016	-12.1541	27.2505
193	.35800	.07853	2.679	-.6156	-.5822	1.3140	.1329	.3137	.1001	-14.9356	27.9033

194	.36003	.07389	1.374	-.4257	-.4093	1.4228	.1221	.3111	.1049	-13.7125	31.8785
195	.36014	.07477	2.470	-.5859	-.5496	1.3322	.0356	.2820	.1027	-16.8651	25.4837
196	.35760	.07749	1.969	-.4844	-.4568	1.3463	.0751	.2703	.0877	-12.7344	25.8858
197	.35828	.08100	1.440	-.4687	-.4433	1.2894	.0618	.2608	.0737	-15.2111	24.6897
198	.35470	.07375	1.204	-.5445	-.5003	1.3314	.0986	.2832	.0887	-12.7149	25.8686
199	.35688	.07765	2.189	-.4887	-.4630	1.3148	.0661	.2677	.0856	-13.4125	27.2708
200	.35309	.07686	2.644	-.5629	-.5179	1.3198	.0411	.2840	.1049	-16.7884	22.3287
201	.35469	.08120	1.171	-.4720	-.4473	1.2765	.0709	.2726	.0853	-13.5865	22.0251
202	.35346	.08144	0.000	-.4713	-.4469	1.2176	.0316	.2558	.0771	-17.8270	23.8346
203	.35469	.07336	.041	-.5471	-.4418	1.3090	.0997	.2507	.0727	-11.1017	26.6239
204	.35822	.07589	1.401	-.4119	-.3890	1.2243	.0840	.2399	.0578	-12.4257	21.7736
205	.36143	.07507	1.459	-.5704	-.5398	1.2931	.1294	.2993	.1080	-13.3746	30.2167
206	.35975	.07059	1.210	-.4435	-.4199	1.3891	.1252	.2734	.0808	-11.6909	29.1546
207	.36005	.07278	1.197	-.4235	-.3965	1.2934	.1005	.2512	.0635	-12.5340	24.3231
208	.35684	.07291	1.218	-.4189	-.3923	1.2431	.0708	.2459	.0658	-11.9031	24.7382
209	.36182	.07013	0.000	-.3224	-.3071	.8060	.0668	.2440	.0425	-12.8796	26.2859

[a] 单位：ε_{HOMO}, ε_{LUMO}: a.u.; μ: Debye; V_{min}, $V_{s,min}$, $V_{s,max}$, $\overline{V_s}$, Π, ΣV_s^+, ΣV_s^-: eV; σ_{tot}^2: eV^2.