Temperature-dependent Changes in the Molecular Orientation and Visible Color of Phthalocyanine Films

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Supporting information

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Additional Experimental and Computational Results

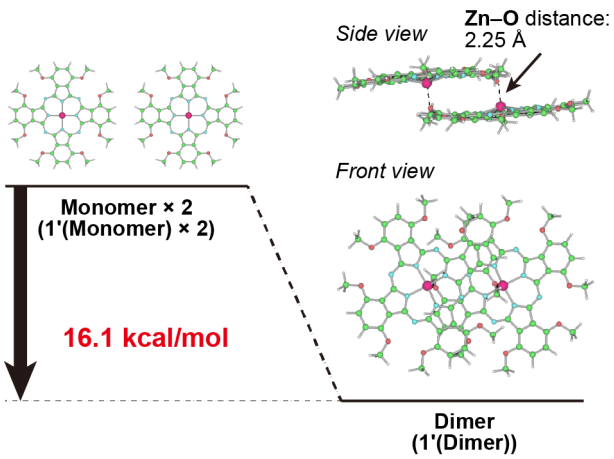
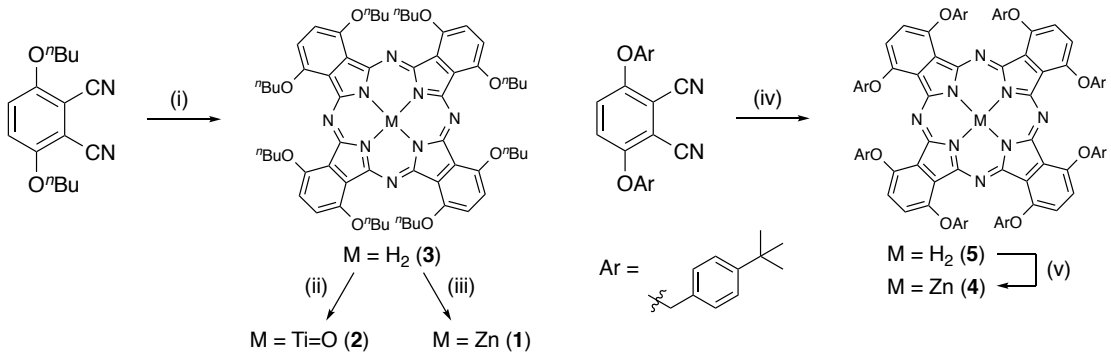


Fig. S1 Zn–O coordination of the Pc model complex (**1′**). Calculations were carried out at the B3LYP/6-31G* level of theory.



Scheme S1 Synthesis of Pcs in this work. *Reagents and conditions*: (i) ^{n}BuOLi, ^{n}BuOH, reflux, 3 h, 61%; (ii) $Ti(OEt)_4$, DMF, 130°C, 1 h, 63%; (iii) $Zn(OAc)_2$•$2H_2O$, DMSO, 100°C, 4 h, 96%; (iv) ^{n}BuOLi, ^{n}BuOH, reflux, 3 h, 33%; (v) $Zn(OAc)_2$•$2H_2O$, DMSO, 100°C, 4 h, 73%.

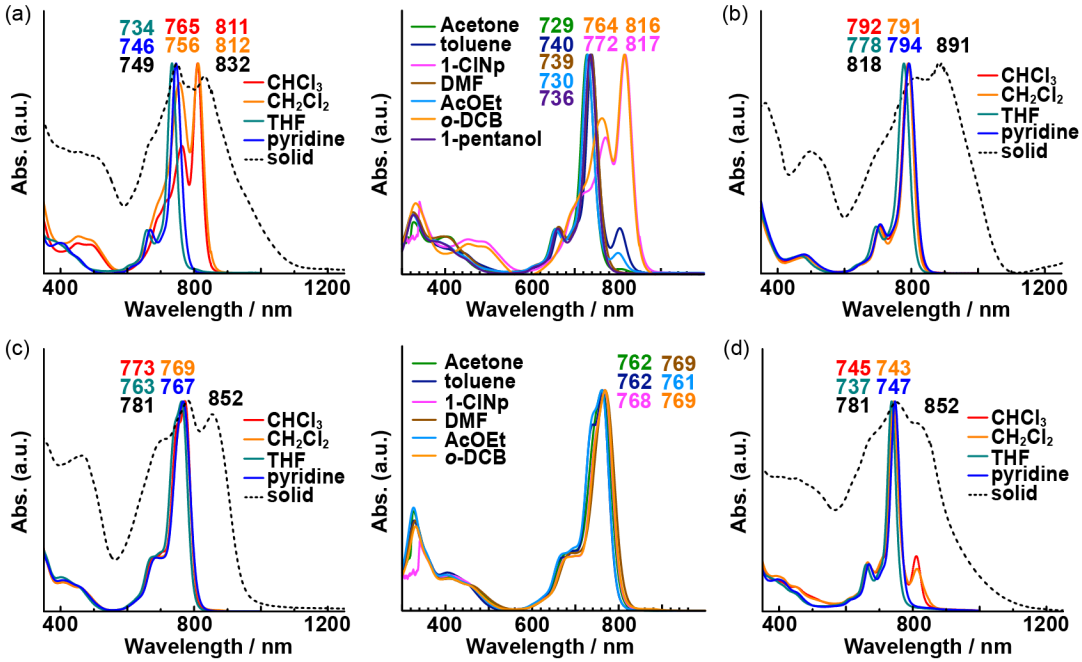


Fig. S2 UV-vis-NIR absorption spectra of **1** (a), **2** (b), **3** (c) and **4** (d) in various solvents and in the powder state.

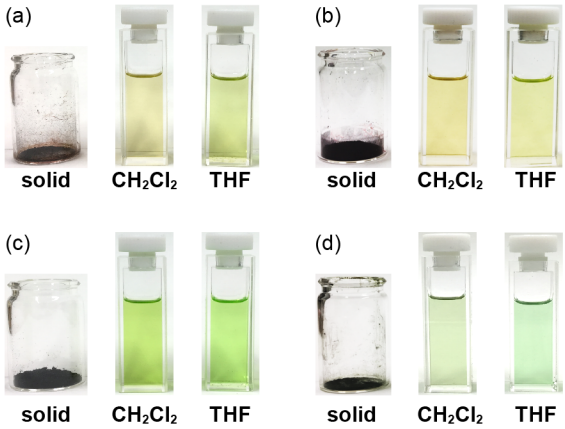


Fig. S3 Photographs of **1** (a), **2** (b), **3** (c), and **4** (d) in various solvents and in the powder state.

Table S1. Fluorescence lifetime parameters of **1** in CH_2Cl_2 at various emission wavelengths.[a]

λ_{em} / nm	τ_1 / ns	a_1 / %	τ_2 / ns	a_2 / %	χ^2
780	1.52	100	-[b]	-	1.12
800	1.13	86	0.30	14	1.16
810	1.01	84	0.40	16	1.13
820	1.20	56	0.57	44	1.08
830	-	-	0.87	100	1.24
850	-	-	0.89	100	1.03

[a] λ_{ex} = 630 nm. [b] Not detected.

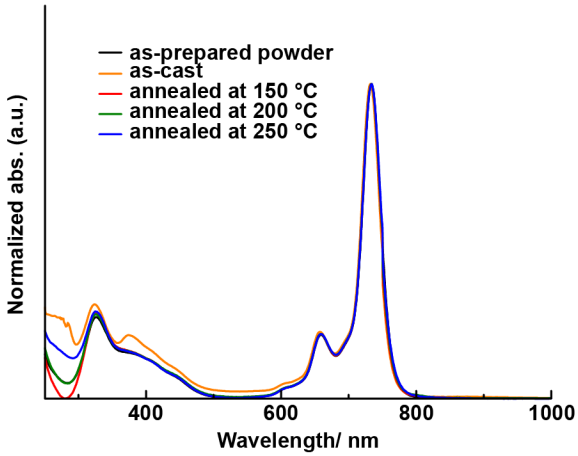


Fig. S4 UV-vis-NIR absorption spectra of the as-prepared powder of **1** (black line) and the partial dissolution of the annealed films of **1** (orange, red, green, and blue lines) in THF.

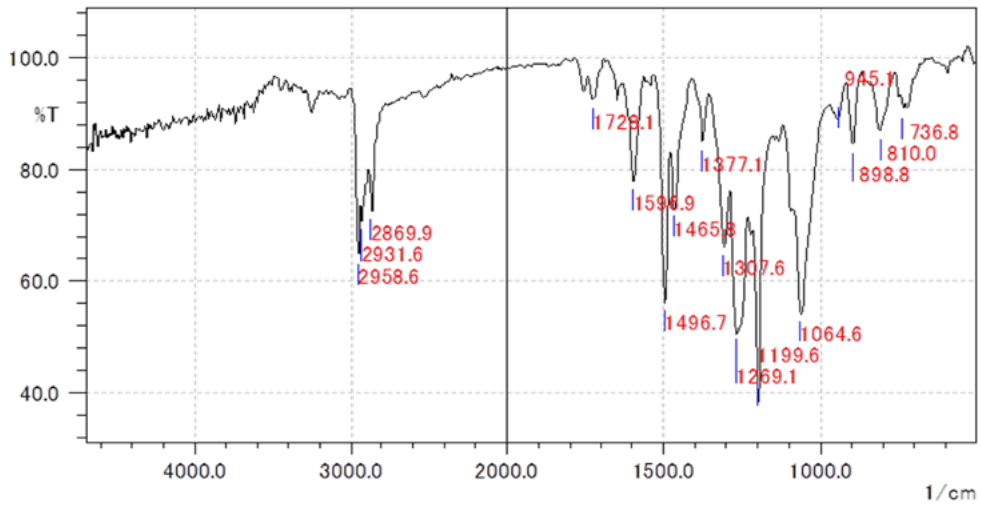


Fig. S5 FT-IR spectrum of **1** dispersed in a KBr pellet.

Table S2. Assignment of vibrational modes from DFT calculations at the B3LYP/6-31G* level of theory.

1			
Assignment	Calculated		Observed
	Frequency (cm^{-1})	IR Intensity	Frequency (cm^{-1})
Out-of-plane	813	144	810
In-plane	1114	954	1065
Unsubstituted ZnPc			
Assignment[1]	Calculated		Observed[1]
	Frequency (cm^{-1})	IR Intensity	Frequency (cm^{-1})
Out-of-plane	739	156	727
In-plane	1149	187	1120

Table S3. IR-RAS orientation parameters.

Temp.	out-of-plane/in-plane (*R*)	*S*	θ/degree
rt	0.93	-0.01	55.34
150°C	1.02	-0.04	56.56
200°C	1.09	-0.06	57.37
250°C	0.61	0.13	49.48

Based on previous reports in the literature,[2] the orientation parameter *S* was calculated as follows:

$$S = \frac{1}{2} < 3cos^2\theta - 1 > = \frac{3}{2 + \frac{R}{R_r}} - \frac{1}{2}$$

where θ is the angle between the long molecular axis and the direction perpendicular to the substrate surface, *R* is the peak intensity ratio, and R_r is the value of *R* in the KBr-dispersed pellet.

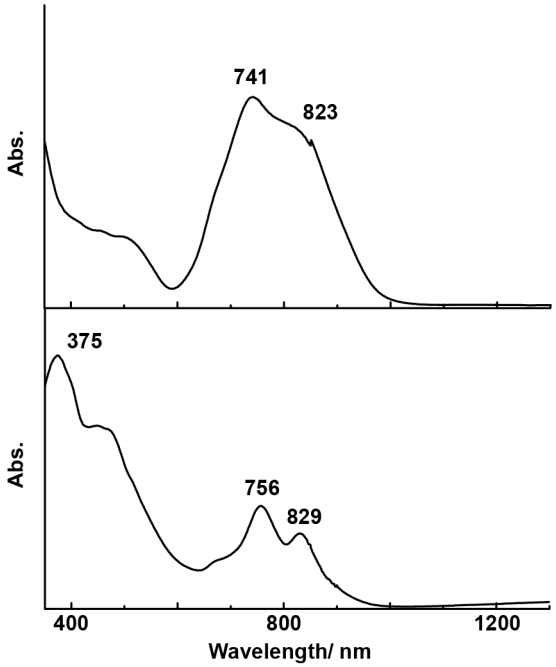


Fig. S6 UV-vis-NIR absorption spectra of the thin films of **1** on a glass (top) and Au (bottom) substrates.

Copies of the NMR Spectra of Studied Compounds

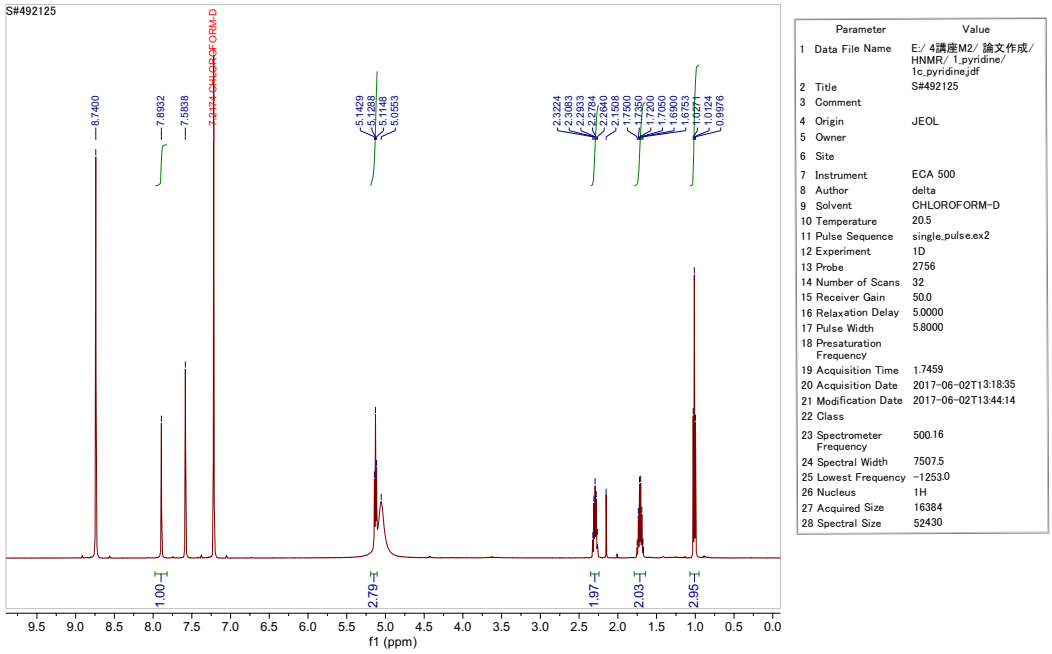


Fig. S7 ^{1}H NMR spectra of **1** in pyridine-d_5.

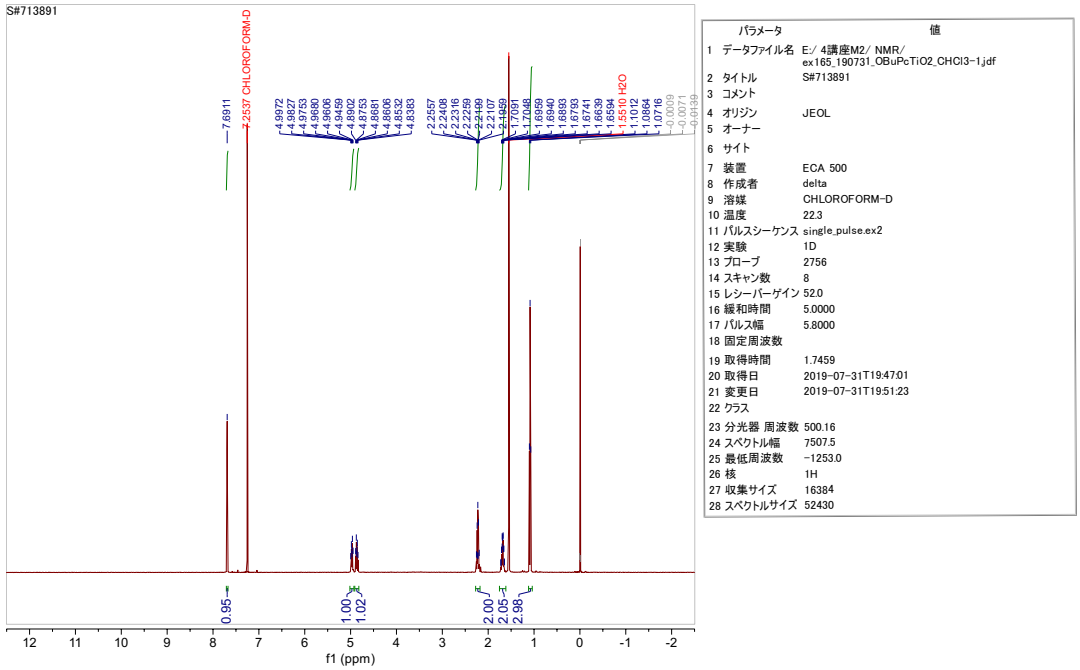
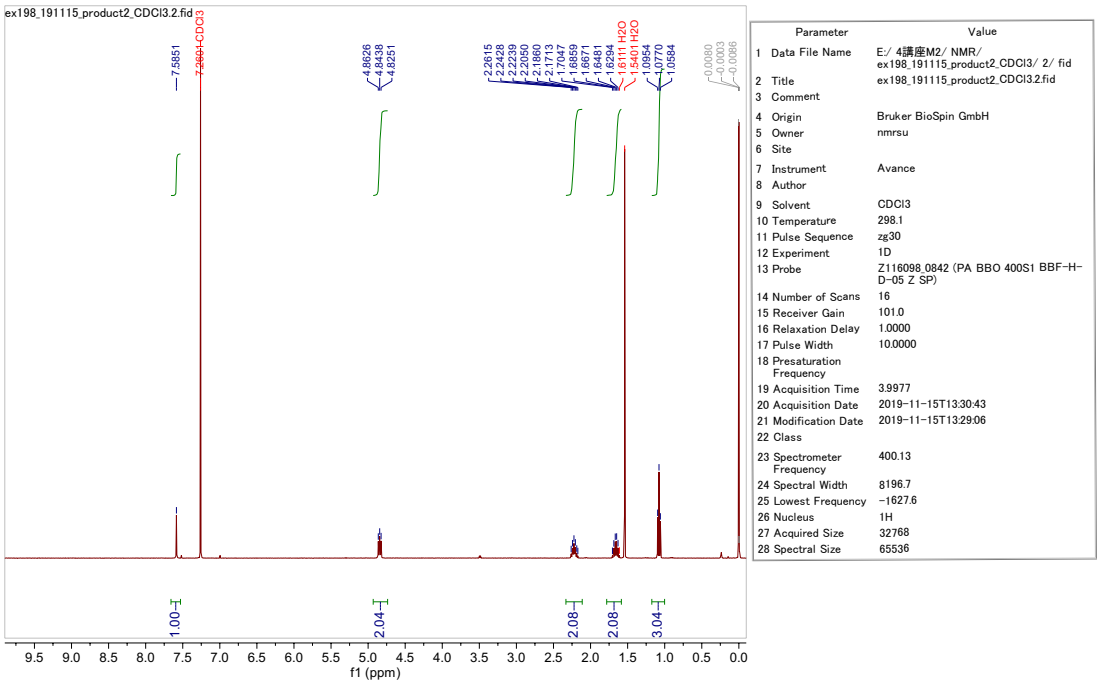


Fig. S8 ^{1}H NMR spectra of **2** in $CDCl_3$.



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4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0842 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	16
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16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-11-15T13:30:43
21 Modification Date	2019-11-15T13:29:06
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24 Spectral Width	8196.7
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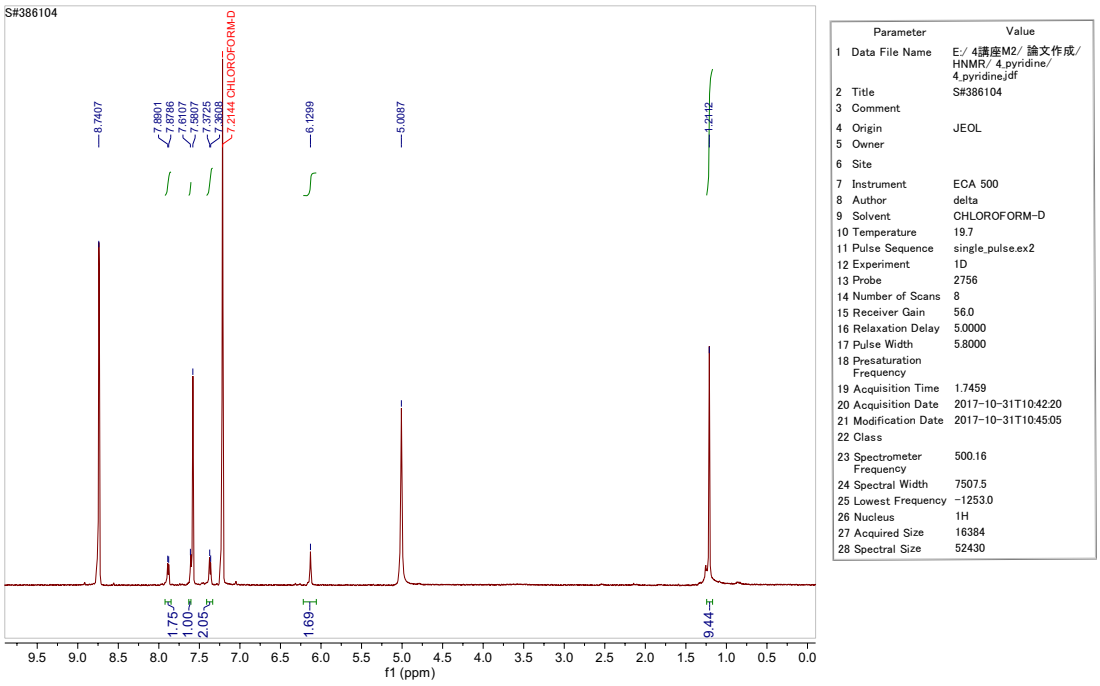
28 Spectral Size	65536

Fig. S9 ^{1}H NMR spectra of **3** in $CDCl_3$.



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3 Comment	
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5 Owner	
6 Site	
7 Instrument	ECA 500
8 Author	delta
9 Solvent	CHLOROFORM-D
10 Temperature	19.7
11 Pulse Sequence	single_pulse.ex2
12 Experiment	1D
13 Probe	2756
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19 Acquisition Time	1.7459
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23 Spectrometer Frequency	500.16
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28 Spectral Size	52430

Fig. S10 ^{1}H NMR spectra of **4** in pyridine-d_5.

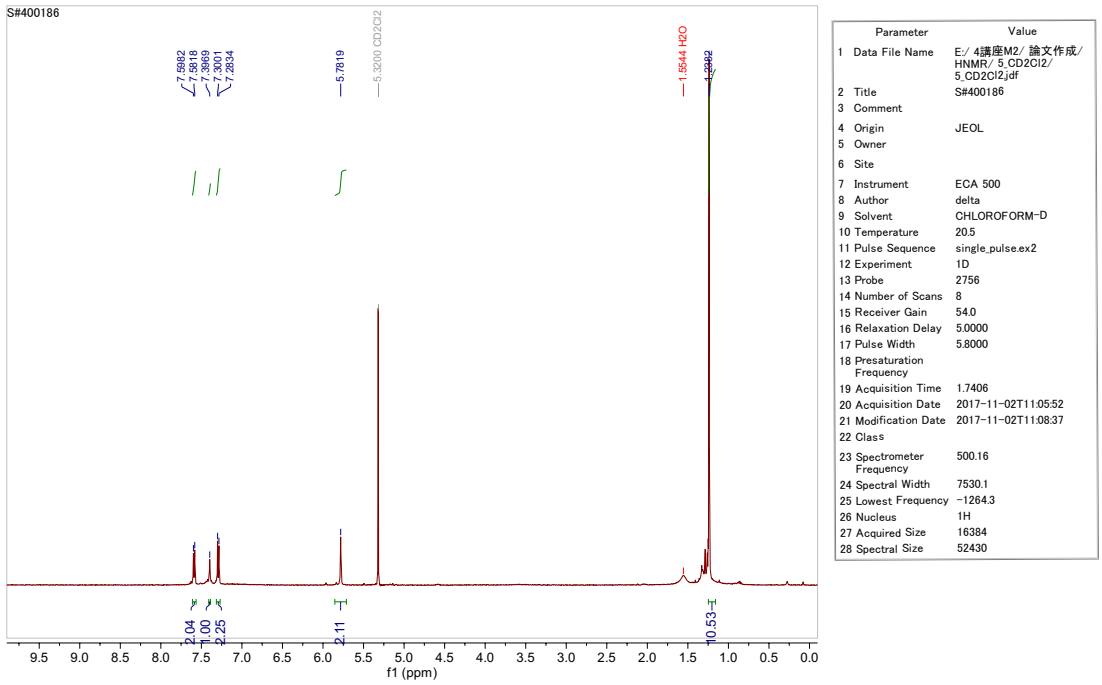

Fig. S11 ^{1}H NMR spectra of **5** in CD_2Cl_2.

Full Computational Details

Computational Details

Geometry optimization for all molecules was performed at the DFT level, by means of the hybrid Becke3LYP[3] (B3LYP) functional as implemented in Gaussian 2009.[4] The 6-31G(d) basis set was used for the all atoms. All stationary points were characterized by normal coordinate analysis at the same level of the theory (the number of imaginary frequency, Nimag, 0).

Cartesian Coordinates and Total Electron Energies

1'(Monomer)

SCF Done: E(RB3LYP) = -4362.44748304 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.995919	0.000000
2	6	0	1.121990	2.787878	0.000000
3	6	0	0.705729	4.189563	0.000000
4	6	0	1.434311	5.395648	0.000000
5	6	0	0.702327	6.585558	0.000000
6	6	0	-0.702327	6.585558	-0.000000
7	6	0	-1.434311	5.395648	-0.000000
8	6	0	-0.705729	4.189563	-0.000000
9	6	0	-1.121990	2.787878	-0.000000
10	7	0	-2.389805	2.389805	0.000000
11	1	0	1.211241	7.542384	0.000000
12	1	0	-1.211241	7.542384	-0.000000
13	7	0	-1.995919	0.000000	0.000000
14	6	0	-2.787878	1.121990	0.000000
15	6	0	-4.189563	0.705729	0.000000
16	6	0	-5.395648	1.434311	0.000000
17	6	0	-6.585558	0.702327	0.000000
18	6	0	-6.585558	-0.702327	-0.000000
19	6	0	-5.395648	-1.434311	-0.000000
20	6	0	-4.189563	-0.705729	-0.000000
21	6	0	-2.787878	-1.121990	-0.000000
22	7	0	-2.389805	-2.389805	-0.000000
23	1	0	-7.542384	1.211241	0.000000
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25	7	0	-0.000000	-1.995919	0.000000
26	6	0	-1.121990	-2.787878	0.000000
27	6	0	-0.705729	-4.189563	0.000000
28	6	0	-1.434311	-5.395648	0.000000
29	6	0	-0.702327	-6.585558	0.000000
30	6	0	0.702327	-6.585558	-0.000000
31	6	0	1.434311	-5.395648	-0.000000
32	6	0	0.705729	-4.189563	-0.000000
33	6	0	1.121990	-2.787878	-0.000000
34	7	0	2.389805	-2.389805	0.000000
35	1	0	-1.211241	-7.542384	0.000000
36	1	0	1.211241	-7.542384	-0.000000
37	7	0	1.995919	-0.000000	0.000000
38	6	0	2.787878	-1.121990	0.000000
39	6	0	4.189563	-0.705729	0.000000
40	6	0	5.395648	-1.434311	0.000000
41	6	0	6.585558	-0.702327	0.000000
42	6	0	6.585558	0.702327	-0.000000

43	6	0	5.395648	1.434311	-0.000000
44	6	0	4.189563	0.705729	-0.000000
45	6	0	2.787878	1.121990	-0.000000
46	7	0	2.389805	2.389805	0.000000
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48	1	0	7.542384	1.211241	-0.000000
49	8	0	-2.791595	5.328380	0.000000
50	8	0	-5.328380	2.791595	-0.000000
51	8	0	-5.328380	-2.791595	0.000000
52	8	0	-2.791595	-5.328380	-0.000000
53	8	0	2.791595	-5.328380	0.000000
54	8	0	5.328380	-2.791595	-0.000000
55	8	0	5.328380	2.791595	0.000000
56	8	0	2.791595	5.328380	0.000000
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59	1	0	-3.302497	7.145247	-0.894817
60	1	0	-4.569810	6.262592	0.000000
61	6	0	3.515235	6.543873	0.000000
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64	1	0	4.569810	6.262592	0.000000
65	6	0	6.543873	3.515235	0.000000
66	1	0	7.145247	3.302497	0.894817
67	1	0	7.145247	3.302497	-0.894817
68	1	0	6.262592	4.569810	0.000000
69	6	0	6.543873	-3.515235	-0.000000
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73	6	0	3.515235	-6.543873	0.000000
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76	1	0	4.569810	-6.262592	0.000000
77	6	0	-3.515235	-6.543873	-0.000000
78	1	0	-3.302497	-7.145247	-0.894817
79	1	0	-3.302497	-7.145247	0.894817
80	1	0	-4.569810	-6.262592	-0.000000
81	6	0	-6.543873	-3.515235	0.000000
82	1	0	-7.145247	-3.302497	0.894817
83	1	0	-7.145247	-3.302497	-0.894817
84	1	0	-6.262592	-4.569810	0.000000
85	6	0	-6.543873	3.515235	-0.000000
86	1	0	-7.145247	3.302497	-0.894817
87	1	0	-7.145247	3.302497	0.894817
88	1	0	-6.262592	4.569810	-0.000000
89	30	0	0.000000	0.000000	0.000000

1'(Dimer)

SCF Done: E(RB3LYP) = -8724.92058429 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.772489	-0.909254	-1.349980
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3	6	0	-0.444321	-1.321708	-1.836473
4	6	0	-1.840629	-1.304686	-1.959367
5	6	0	-2.502858	-2.494450	-2.237887
6	6	0	-1.812588	-3.707624	-2.349454
7	6	0	-0.429787	-3.763371	-2.136120
8	6	0	0.244107	-2.556085	-1.865068
9	6	0	1.628319	-2.263466	-1.494797
10	7	0	2.552348	-3.200541	-1.309904
11	1	0	-3.585367	-2.481020	-2.319207
12	1	0	-2.378716	-4.608733	-2.550022

13	7	0	4.353279	-1.758315	-0.573492
14	6	0	3.794529	-2.967448	-0.899290
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16	6	0	4.774778	-5.410693	-0.938423
17	6	0	5.961888	-6.116404	-0.733238
18	6	0	7.147444	-5.466163	-0.349494
19	6	0	7.190167	-4.084631	-0.150288
20	6	0	5.995636	-3.364361	-0.353285
21	6	0	5.675669	-1.940004	-0.260706
22	7	0	6.573054	-1.006137	0.040108
23	1	0	5.990818	-7.191912	-0.863767
24	1	0	8.036195	-6.069733	-0.206101
25	7	0	5.167842	0.918498	-0.372043
26	6	0	6.339307	0.300232	-0.022235
27	6	0	7.365249	1.318139	0.211591
28	6	0	8.713186	1.234833	0.611861
29	6	0	9.421080	2.433307	0.730228
30	6	0	8.815672	3.673318	0.466507
31	6	0	7.477856	3.766241	0.074833
32	6	0	6.756594	2.562599	-0.052099
33	6	0	5.371299	2.271078	-0.430066
34	7	0	4.496011	3.202110	-0.793238
35	1	0	10.461463	2.429228	1.034033
36	1	0	9.417979	4.567218	0.579310
37	7	0	2.585142	1.757784	-1.167913
38	6	0	3.235126	2.962700	-1.139239
39	6	0	2.296967	4.018696	-1.512537
40	6	0	2.458859	5.410377	-1.653640
41	6	0	1.320111	6.159231	-1.958427
42	6	0	0.067402	5.547452	-2.116008
43	6	0	-0.098512	4.164661	-1.998763
44	6	0	1.045873	3.394321	-1.708835
45	6	0	1.273202	1.956491	-1.510140
46	7	0	0.337384	1.017081	-1.661409
47	1	0	1.382256	7.234892	-2.076841
48	1	0	-0.782919	6.181317	-2.335551
49	8	0	0.297357	-4.905875	-2.168128
50	8	0	3.590081	-5.986821	-1.286525
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52	8	0	9.235103	0.005212	0.866842
53	8	0	6.832565	4.936632	-0.179579
54	8	0	3.702159	5.937936	-1.489933
55	8	0	-1.299899	3.540491	-2.135621
56	8	0	-2.618695	-0.185228	-1.668878
57	6	0	-0.394483	-6.131947	-2.327875
58	1	0	-1.118108	-6.292978	-1.518321
59	1	0	-0.911665	-6.186041	-3.295599
60	1	0	0.370628	-6.909282	-2.289489
61	6	0	-2.799938	0.749572	-2.753566
62	1	0	-1.878850	1.312347	-2.908698
63	1	0	-3.099996	0.204816	-3.655321
64	1	0	-3.607263	1.414569	-2.442859
65	6	0	-2.460311	4.361619	-2.179294
66	1	0	-2.520365	5.003424	-1.293072
67	1	0	-2.486664	4.974903	-3.090551
68	1	0	-3.311020	3.680258	-2.183807
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73	6	0	7.560768	6.139316	-0.028921
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77	6	0	10.579674	-0.067795	1.298390
78	1	0	11.274356	0.319098	0.539622
79	1	0	10.737229	0.479072	2.238678

80	1	0	10.782394	-1.127689	1.463647
81	6	0	9.505806	-4.118715	0.385497
82	1	0	9.430419	-4.866241	1.187860
83	1	0	9.807423	-4.621363	-0.543983
84	1	0	10.262259	-3.379089	0.654122
85	6	0	3.582753	-7.378404	-1.542067
86	1	0	4.267947	-7.644985	-2.358369
87	1	0	3.848544	-7.961008	-0.648503
88	1	0	2.560656	-7.622338	-1.836943
89	30	0	3.346332	0.007661	-0.448847
90	7	0	-5.167683	-0.918547	0.371670
91	6	0	-6.339138	-0.300326	0.021769
92	6	0	-7.364917	-1.318292	-0.212521
93	6	0	-8.712774	-1.235038	-0.613066
94	6	0	-9.420524	-2.433557	-0.731835
95	6	0	-8.815049	-3.673561	-0.468233
96	6	0	-7.477306	-3.766433	-0.076295
97	6	0	-6.756186	-2.562746	0.051030
98	6	0	-5.371000	-2.271156	0.429350
99	7	0	-4.495665	-3.202158	0.792485
100	1	0	-10.460839	-2.429522	-1.035871
101	1	0	-9.417244	-4.567498	-0.581345
102	7	0	-2.584995	-1.757697	1.167721
103	6	0	-3.234865	-2.962672	1.138747
104	6	0	-2.296672	-4.018638	1.512020
105	6	0	-2.458460	-5.410367	1.652761
106	6	0	-1.319706	-6.159181	1.957618
107	6	0	-0.067103	-5.547308	2.115658
108	6	0	0.098697	-4.164473	1.998796
109	6	0	-1.045681	-3.394178	1.708706
110	6	0	-1.273088	-1.956340	1.510137
111	7	0	-0.337330	-1.016883	1.661526
112	1	0	-1.381758	-7.234878	2.075746
113	1	0	0.783231	-6.181144	2.335225
114	7	0	-1.772557	0.909374	1.350266
115	6	0	-0.574954	0.293188	1.582831
116	6	0	0.444280	1.321970	1.836531
117	6	0	1.840609	1.305075	1.959244
118	6	0	2.502790	2.494916	2.237552
119	6	0	1.812459	3.708054	2.349082
120	6	0	0.429623	3.763671	2.135956
121	6	0	-0.244234	2.556306	1.865179
122	6	0	-1.628494	2.263582	1.495195
123	7	0	-2.552699	3.200566	1.310742
124	1	0	3.585309	2.481555	2.318736
125	1	0	2.378543	4.609226	2.549488
126	7	0	-4.353432	1.758302	0.573915
127	6	0	-3.794910	2.967392	0.900249
128	6	0	-4.809135	4.014005	0.752688
129	6	0	-4.775698	5.410384	0.940893
130	6	0	-5.962897	6.115990	0.735848
131	6	0	-7.148226	5.465760	0.351381
132	6	0	-7.190650	4.084337	0.151371
133	6	0	-5.996030	3.364172	0.354216
134	6	0	-5.675820	1.939914	0.261038
135	7	0	-6.573028	1.006032	-0.040244
136	1	0	-5.992087	7.191402	0.867105
137	1	0	-8.037053	6.069251	0.208130
138	8	0	-6.831958	-4.936815	0.178023
139	8	0	-3.701668	-5.938008	1.488628
140	8	0	1.299972	-3.540213	2.136210
141	8	0	2.618769	0.185657	1.668843
142	8	0	-0.297574	4.906146	2.167860
143	8	0	-3.591266	5.986484	1.289907
144	8	0	-8.301087	3.395996	-0.223626
145	8	0	-9.234750	-0.005415	-0.867921
146	6	0	-7.560040	-6.139531	0.027031

147	1	0	-8.410757	-6.192410	0.720857
148	1	0	-7.929261	-6.267735	-1.000335
149	1	0	-6.858544	-6.943599	0.257254
150	6	0	-10.579277	0.067566	-1.299610
151	1	0	-10.736667	-0.479077	-2.240056
152	1	0	-11.274008	-0.319592	-0.541023
153	1	0	-10.782084	1.127481	-1.464624
154	6	0	-9.506183	4.118288	-0.384887
155	1	0	-9.808095	4.620318	0.544832
156	1	0	-9.430773	4.866310	-1.186783
157	1	0	-10.262434	3.378675	-0.654116
158	6	0	-3.584315	7.377885	1.546447
159	1	0	-3.849813	7.961084	0.653184
160	1	0	-4.269922	7.643758	2.362634
161	1	0	-2.562401	7.621797	1.841975
162	6	0	0.394264	6.132294	2.327005
163	1	0	0.911422	6.186876	3.294716
164	1	0	1.117908	6.292911	1.517391
165	1	0	-0.370838	6.909616	2.288191
166	6	0	2.799964	-0.749113	2.753568
167	1	0	3.099733	-0.204295	3.655380
168	1	0	1.878954	-1.312069	2.908505
169	1	0	3.607493	-1.413945	2.443029
170	6	0	2.460429	-4.361240	2.180376
171	1	0	2.486156	-4.974976	3.091346
172	1	0	2.521272	-5.002560	1.293854
173	1	0	3.311057	-3.679781	2.185926
174	6	0	-3.866326	-7.324203	1.710290
175	1	0	-3.295583	-7.926313	0.988415
176	1	0	-3.569096	-7.613378	2.727957
177	1	0	-4.931777	-7.522269	1.579231
178	30	0	-3.346284	-0.007513	0.448925

1

SCF Done: E(RB3LYP) = -5305.98422339 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.000000	0.000000	0.715715
2	7	0	1.411807	1.411807	0.667847
3	6	0	2.765250	1.178319	0.656207
4	6	0	3.462653	2.463684	0.634751
5	6	0	4.831406	2.797760	0.615271
6	6	0	5.150960	4.158302	0.576687
7	6	0	4.158302	5.150960	0.576687
8	6	0	2.797760	4.831406	0.615271
9	6	0	2.463684	3.462653	0.634751
10	6	0	1.178319	2.765250	0.656207
11	7	0	0.000000	3.379519	0.651695
12	1	0	6.185070	4.480356	0.540893
13	1	0	4.480356	6.185070	0.540893
14	8	0	1.783166	5.735763	0.648433
15	8	0	5.735763	1.783166	0.648433
16	6	0	2.072392	7.130440	0.624813
17	1	0	2.917367	7.364056	1.287487
18	1	0	1.183060	7.599216	1.058371
19	6	0	7.130440	2.072392	0.624813
20	1	0	7.364056	2.917367	1.287487
21	1	0	7.599216	1.183060	1.058371
22	6	0	2.305323	7.663839	-0.790080
23	1	0	3.170292	7.159503	-1.239506
24	1	0	1.435705	7.393073	-1.403220
25	6	0	7.663839	2.305323	-0.790080
26	1	0	7.159503	3.170292	-1.239506
27	1	0	7.393073	1.435705	-1.403220

28	6	0	2.517388	9.183565	-0.816390
29	1	0	3.388049	9.444066	-0.197481
30	1	0	1.654357	9.680788	-0.350157
31	6	0	9.183565	2.517388	-0.816390
32	1	0	9.444066	3.388049	-0.197481
33	1	0	9.680788	1.654357	-0.350157
34	6	0	2.716915	9.734443	-2.232424
35	1	0	2.865163	10.820206	-2.220829
36	1	0	3.592808	9.282334	-2.713366
37	1	0	1.846479	9.522123	-2.864999
38	6	0	9.734443	2.716915	-2.232424
39	1	0	9.282334	3.592808	-2.713366
40	1	0	10.820206	2.865163	-2.220829
41	1	0	9.522123	1.846479	-2.864999
42	7	0	-1.411807	1.411807	0.667847
43	6	0	-1.178319	2.765250	0.656207
44	6	0	-2.463684	3.462653	0.634751
45	6	0	-2.797760	4.831406	0.615271
46	6	0	-4.158302	5.150960	0.576687
47	6	0	-5.150960	4.158302	0.576687
48	6	0	-4.831406	2.797760	0.615271
49	6	0	-3.462653	2.463684	0.634751
50	6	0	-2.765250	1.178319	0.656207
51	7	0	-3.379519	0.000000	0.651695
52	1	0	-4.480356	6.185070	0.540893
53	1	0	-6.185070	4.480356	0.540893
54	8	0	-5.735763	1.783166	0.648433
55	8	0	-1.783166	5.735763	0.648433
56	6	0	-7.130440	2.072392	0.624813
57	1	0	-7.364056	2.917367	1.287487
58	1	0	-7.599216	1.183060	1.058371
59	6	0	-2.072392	7.130440	0.624813
60	1	0	-2.917367	7.364056	1.287487
61	1	0	-1.183060	7.599216	1.058371
62	6	0	-7.663839	2.305323	-0.790080
63	1	0	-7.159503	3.170292	-1.239506
64	1	0	-7.393073	1.435705	-1.403220
65	6	0	-2.305323	7.663839	-0.790080
66	1	0	-3.170292	7.159503	-1.239506
67	1	0	-1.435705	7.393073	-1.403220
68	6	0	-9.183565	2.517388	-0.816390
69	1	0	-9.444066	3.388049	-0.197481
70	1	0	-9.680788	1.654357	-0.350157
71	6	0	-2.517388	9.183565	-0.816390
72	1	0	-3.388049	9.444066	-0.197481
73	1	0	-1.654357	9.680788	-0.350157
74	6	0	-9.734443	2.716915	-2.232424
75	1	0	-10.820206	2.865163	-2.220829
76	1	0	-9.282334	3.592808	-2.713366
77	1	0	-9.522123	1.846479	-2.864999
78	6	0	-2.716915	9.734443	-2.232424
79	1	0	-3.592808	9.282334	-2.713366
80	1	0	-2.865163	10.820206	-2.220829
81	1	0	-1.846479	9.522123	-2.864999
82	7	0	-1.411807	-1.411807	0.667847
83	6	0	-2.765250	-1.178319	0.656207
84	6	0	-3.462653	-2.463684	0.634751
85	6	0	-4.831406	-2.797760	0.615271
86	6	0	-5.150960	-4.158302	0.576687
87	6	0	-4.158302	-5.150960	0.576687
88	6	0	-2.797760	-4.831406	0.615271
89	6	0	-2.463684	-3.462653	0.634751
90	6	0	-1.178319	-2.765250	0.656207
91	7	0	-0.000000	-3.379519	0.651695
92	1	0	-6.185070	-4.480356	0.540893
93	1	0	-4.480356	-6.185070	0.540893
94	8	0	-1.783166	-5.735763	0.648433

95	8	0	-5.735763	-1.783166	0.648433
96	6	0	-2.072392	-7.130440	0.624813
97	1	0	-2.917367	-7.364056	1.287487
98	1	0	-1.183060	-7.599216	1.058371
99	6	0	-7.130440	-2.072392	0.624813
100	1	0	-7.364056	-2.917367	1.287487
101	1	0	-7.599216	-1.183060	1.058371
102	6	0	-2.305323	-7.663839	-0.790080
103	1	0	-3.170292	-7.159503	-1.239506
104	1	0	-1.435705	-7.393073	-1.403220
105	6	0	-7.663839	-2.305323	-0.790080
106	1	0	-7.159503	-3.170292	-1.239506
107	1	0	-7.393073	-1.435705	-1.403220
108	6	0	-2.517388	-9.183565	-0.816390
109	1	0	-3.388049	-9.444066	-0.197481
110	1	0	-1.654357	-9.680788	-0.350157
111	6	0	-9.183565	-2.517388	-0.816390
112	1	0	-9.444066	-3.388049	-0.197481
113	1	0	-9.680788	-1.654357	-0.350157
114	6	0	-2.716915	-9.734443	-2.232424
115	1	0	-2.865163	-10.820206	-2.220829
116	1	0	-3.592808	-9.282334	-2.713366
117	1	0	-1.846479	-9.522123	-2.864999
118	6	0	-9.734443	-2.716915	-2.232424
119	1	0	-9.282334	-3.592808	-2.713366
120	1	0	-10.820206	-2.865163	-2.220829
121	1	0	-9.522123	-1.846479	-2.864999
122	7	0	1.411807	-1.411807	0.667847
123	6	0	1.178319	-2.765250	0.656207
124	6	0	2.463684	-3.462653	0.634751
125	6	0	2.797760	-4.831406	0.615271
126	6	0	4.158302	-5.150960	0.576687
127	6	0	5.150960	-4.158302	0.576687
128	6	0	4.831406	-2.797760	0.615271
129	6	0	3.462653	-2.463684	0.634751
130	6	0	2.765250	-1.178319	0.656207
131	7	0	3.379519	-0.000000	0.651695
132	1	0	4.480356	-6.185070	0.540893
133	1	0	6.185070	-4.480356	0.540893
134	8	0	5.735763	-1.783166	0.648433
135	8	0	1.783166	-5.735763	0.648433
136	6	0	7.130440	-2.072392	0.624813
137	1	0	7.364056	-2.917367	1.287487
138	1	0	7.599216	-1.183060	1.058371
139	6	0	2.072392	-7.130440	0.624813
140	1	0	2.917367	-7.364056	1.287487
141	1	0	1.183060	-7.599216	1.058371
142	6	0	7.663839	-2.305323	-0.790080
143	1	0	7.159503	-3.170292	-1.239506
144	1	0	7.393073	-1.435705	-1.403220
145	6	0	2.305323	-7.663839	-0.790080
146	1	0	3.170292	-7.159503	-1.239506
147	1	0	1.435705	-7.393073	-1.403220
148	6	0	9.183565	-2.517388	-0.816390
149	1	0	9.444066	-3.388049	-0.197481
150	1	0	9.680788	-1.654357	-0.350157
151	6	0	2.517388	-9.183565	-0.816390
152	1	0	3.388049	-9.444066	-0.197481
153	1	0	1.654357	-9.680788	-0.350157
154	6	0	9.734443	-2.716915	-2.232424
155	1	0	10.820206	-2.865163	-2.220829
156	1	0	9.282334	-3.592808	-2.713366
157	1	0	9.522123	-1.846479	-2.864999
158	6	0	2.716915	-9.734443	-2.232424
159	1	0	3.592808	-9.282334	-2.713366
160	1	0	2.865163	-10.820206	-2.220829
161	1	0	1.846479	-9.522123	-2.864999

Unsubstituted Pc zinc complex

SCF Done: E(RB3LYP) = -3446.32687847 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.991218	0.000000
2	6	0	1.120915	2.784704	0.000000
3	6	0	0.705099	4.185053	0.000000
4	6	0	1.425693	5.380346	0.000000
5	6	0	0.704407	6.573447	0.000000
6	6	0	-0.704407	6.573447	-0.000000
7	6	0	-1.425693	5.380346	-0.000000
8	6	0	-0.705099	4.185053	-0.000000
9	6	0	-1.120915	2.784704	-0.000000
10	7	0	-2.391659	2.391659	0.000000
11	1	0	1.234585	7.521945	0.000000
12	1	0	-1.234585	7.521945	-0.000000
13	7	0	-1.991218	0.000000	0.000000
14	6	0	-2.784704	1.120915	0.000000
15	6	0	-4.185053	0.705099	0.000000
16	6	0	-5.380346	1.425693	0.000000
17	6	0	-6.573447	0.704407	0.000000
18	6	0	-6.573447	-0.704407	-0.000000
19	6	0	-5.380346	-1.425693	-0.000000
20	6	0	-4.185053	-0.705099	-0.000000
21	6	0	-2.784704	-1.120915	-0.000000
22	7	0	-2.391659	-2.391659	-0.000000
23	1	0	-7.521945	1.234585	0.000000
24	1	0	-7.521945	-1.234585	-0.000000
25	7	0	-0.000000	-1.991218	0.000000
26	6	0	-1.120915	-2.784704	0.000000
27	6	0	-0.705099	-4.185053	0.000000
28	6	0	-1.425693	-5.380346	0.000000
29	6	0	-0.704407	-6.573447	0.000000
30	6	0	0.704407	-6.573447	-0.000000
31	6	0	1.425693	-5.380346	-0.000000
32	6	0	0.705099	-4.185053	-0.000000
33	6	0	1.120915	-2.784704	-0.000000
34	7	0	2.391659	-2.391659	0.000000
35	1	0	-1.234585	-7.521945	0.000000
36	1	0	1.234585	-7.521945	-0.000000
37	7	0	1.991218	-0.000000	0.000000
38	6	0	2.784704	-1.120915	0.000000
39	6	0	4.185053	-0.705099	0.000000
40	6	0	5.380346	-1.425693	0.000000
41	6	0	6.573447	-0.704407	0.000000
42	6	0	6.573447	0.704407	-0.000000
43	6	0	5.380346	1.425693	-0.000000
44	6	0	4.185053	0.705099	-0.000000
45	6	0	2.784704	1.120915	-0.000000
46	7	0	2.391659	2.391659	0.000000
47	1	0	7.521945	-1.234585	0.000000
48	1	0	7.521945	1.234585	-0.000000
49	30	0	0.000000	0.000000	0.000000
50	1	0	-2.511322	5.371882	0.000000
51	1	0	2.511322	5.371882	0.000000
52	1	0	5.371882	2.511322	0.000000
53	1	0	5.371882	-2.511322	-0.000000
54	1	0	2.511322	-5.371882	0.000000
55	1	0	-2.511322	-5.371882	-0.000000
56	1	0	-5.371882	-2.511322	0.000000
57	1	0	-5.371882	2.511322	-0.000000

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