Supplementary information

for

Confusion of Möbius aromaticity: Disruption of annulenic pathway in singly N-confused [28]hexaphyrin and its mono-Pd(II) complex

Sabapathi Gokulnath,[a] Motoki Toganoh,[a] Keisuke Yamaguchi,[a] Shigeki Mori,[b] Hidemitsu Uno,[b] and Hiroyuki Furuta*[a,c]

[a]*Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka 819-0395, Japan.*

[b]Integrated Center for Sciences and Graduate School of Science and Engineering, Ehime University, Matsuyama 790-8577, Japan

[c]*International Research Center for Molecular Systems, Kyushu University*

E-mail: hfuruta@cstf.kyushu-u.ac.jp

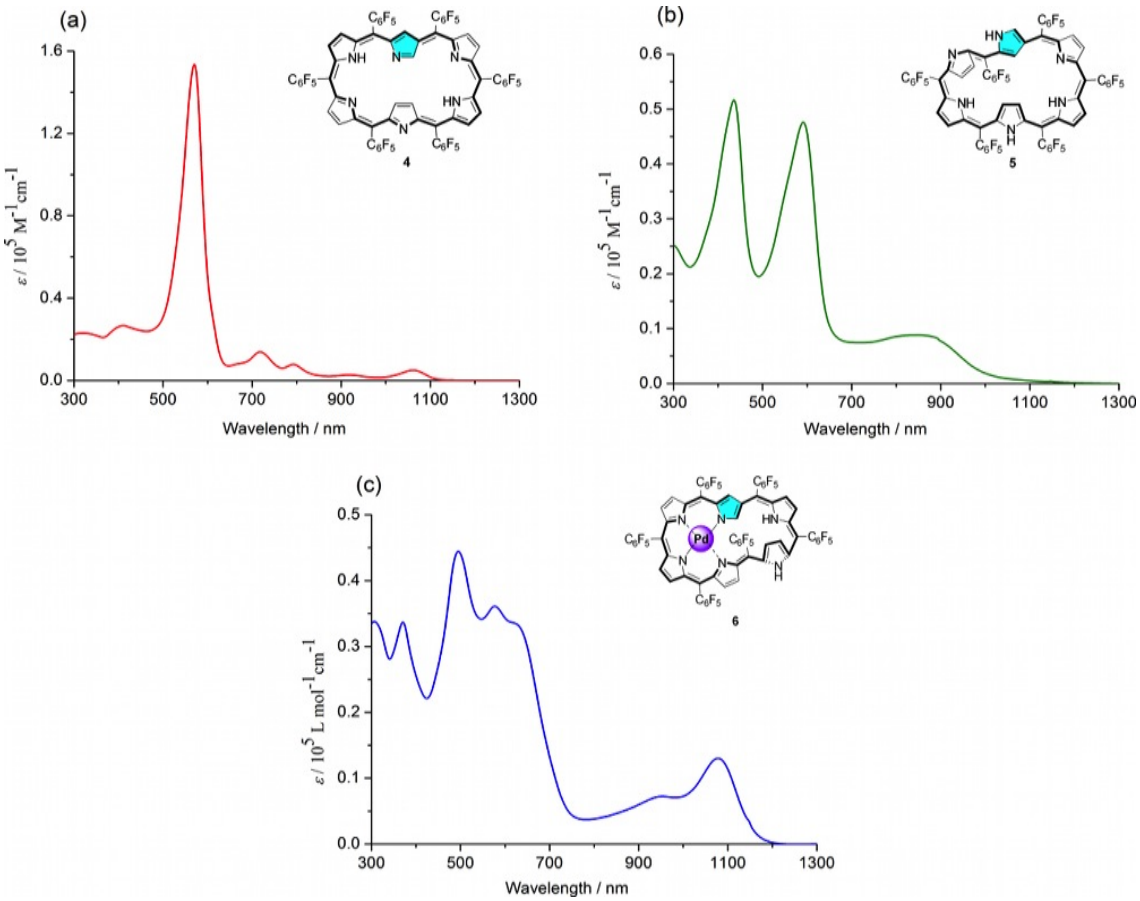


Fig. S1 UV/Vis/NIR absorption spectra of (a) **4**, (b) **5**, and (c) **6** in CH_2Cl_2.

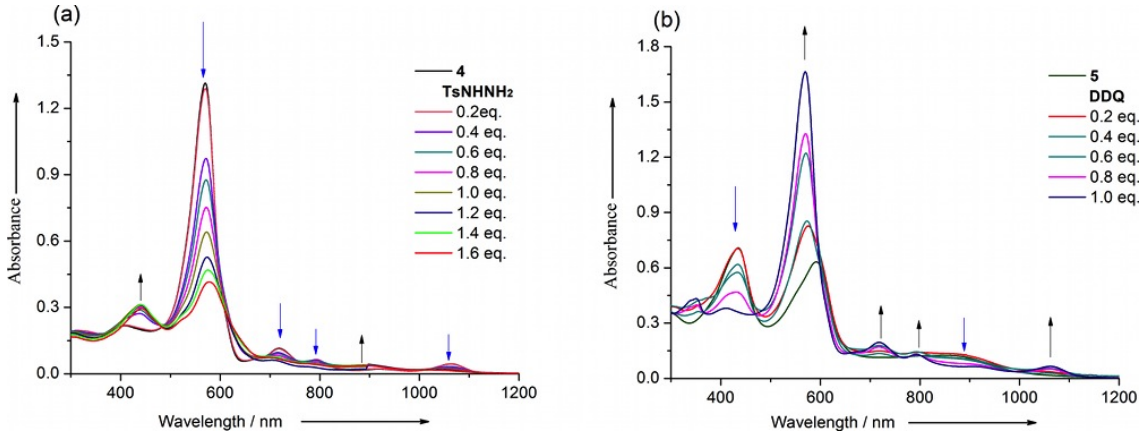


Fig. S2 UV/Vis/NIR absorption spectra for redox reaction between **4** and **5**: (a) reduction of **4** and (b) oxidation of **5** in CH_2Cl_2.

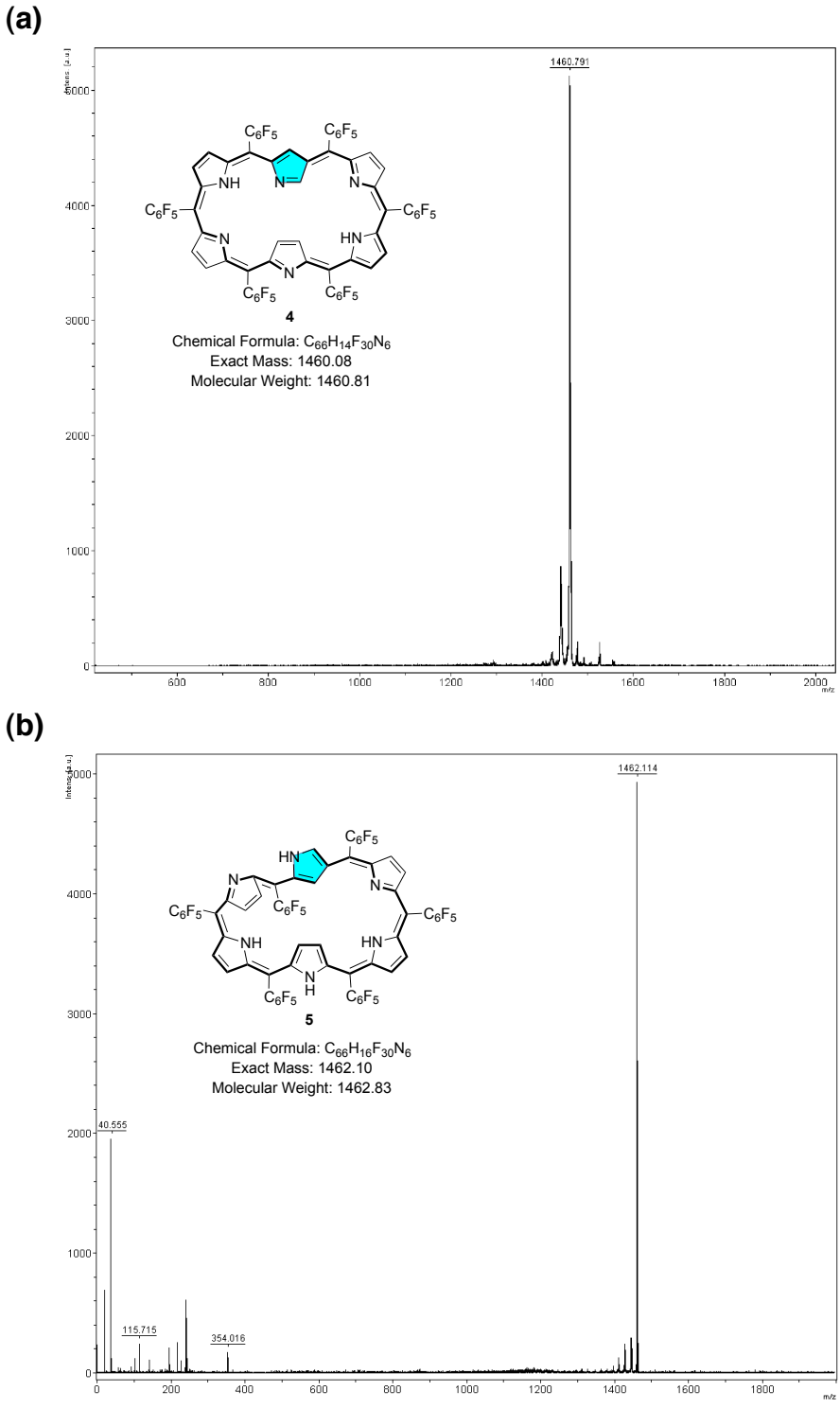


Fig. S3 MALDI-TOF-MS spectra of (a) **4** and (b) **5**.

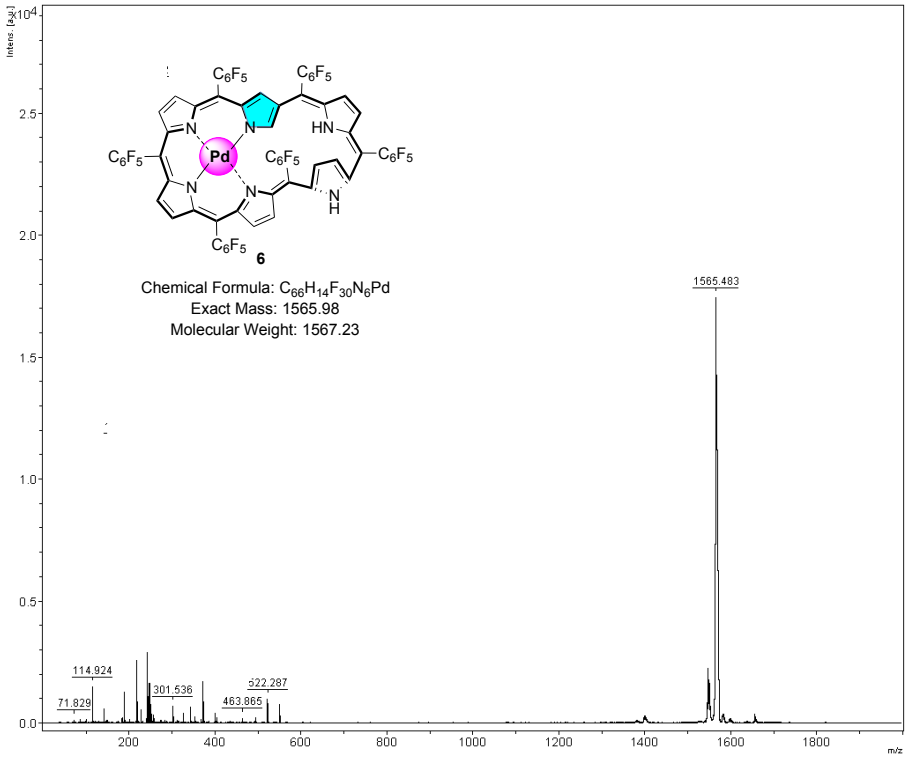


Fig. S4 MALDI-TOF-MS spectrum of **6**.

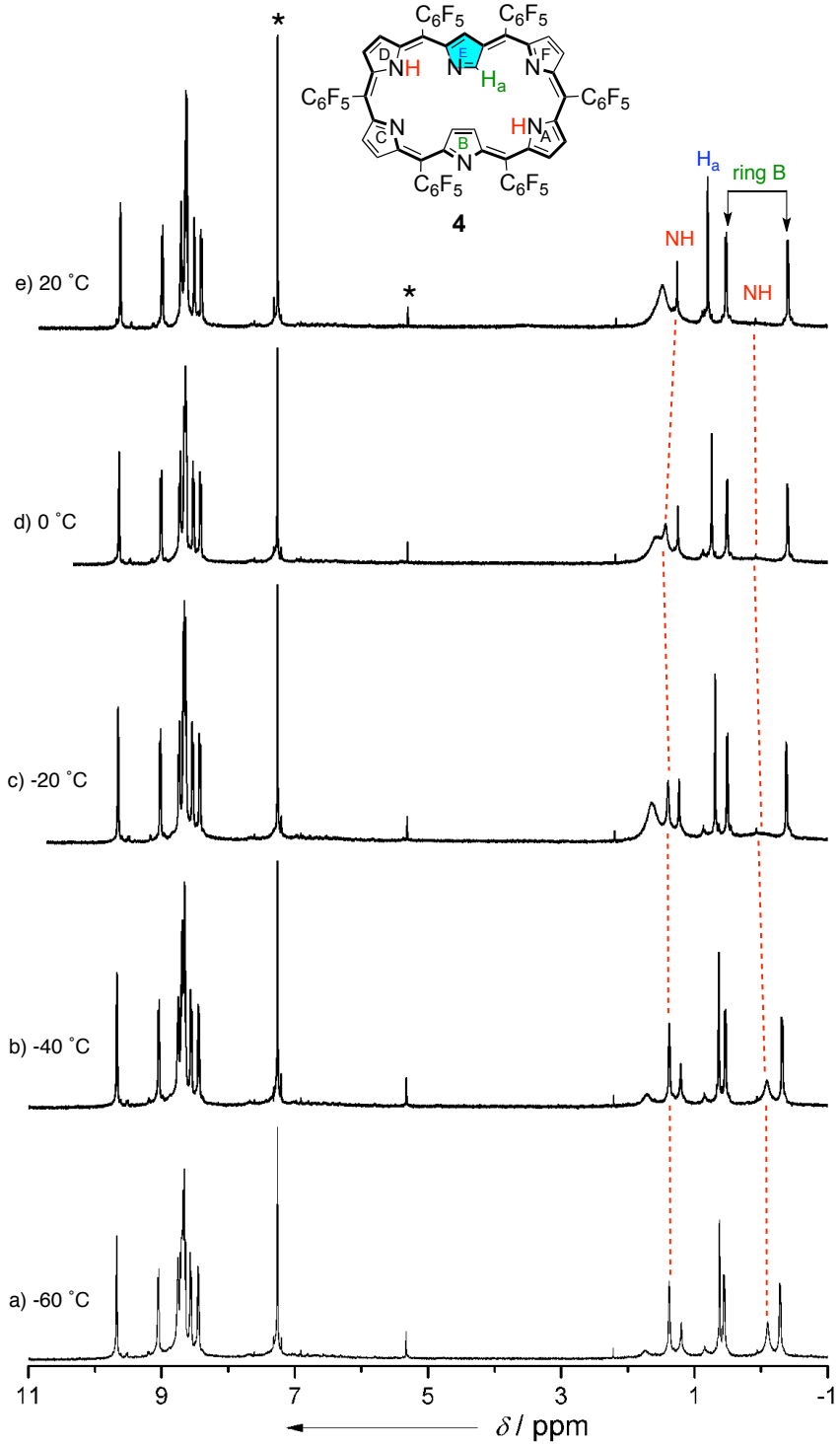


Fig. S5 Variable temperature ^{1}H NMR spectra of **4** in $CDCl_3$. (Peaks marked with * are due to residual solvents.)

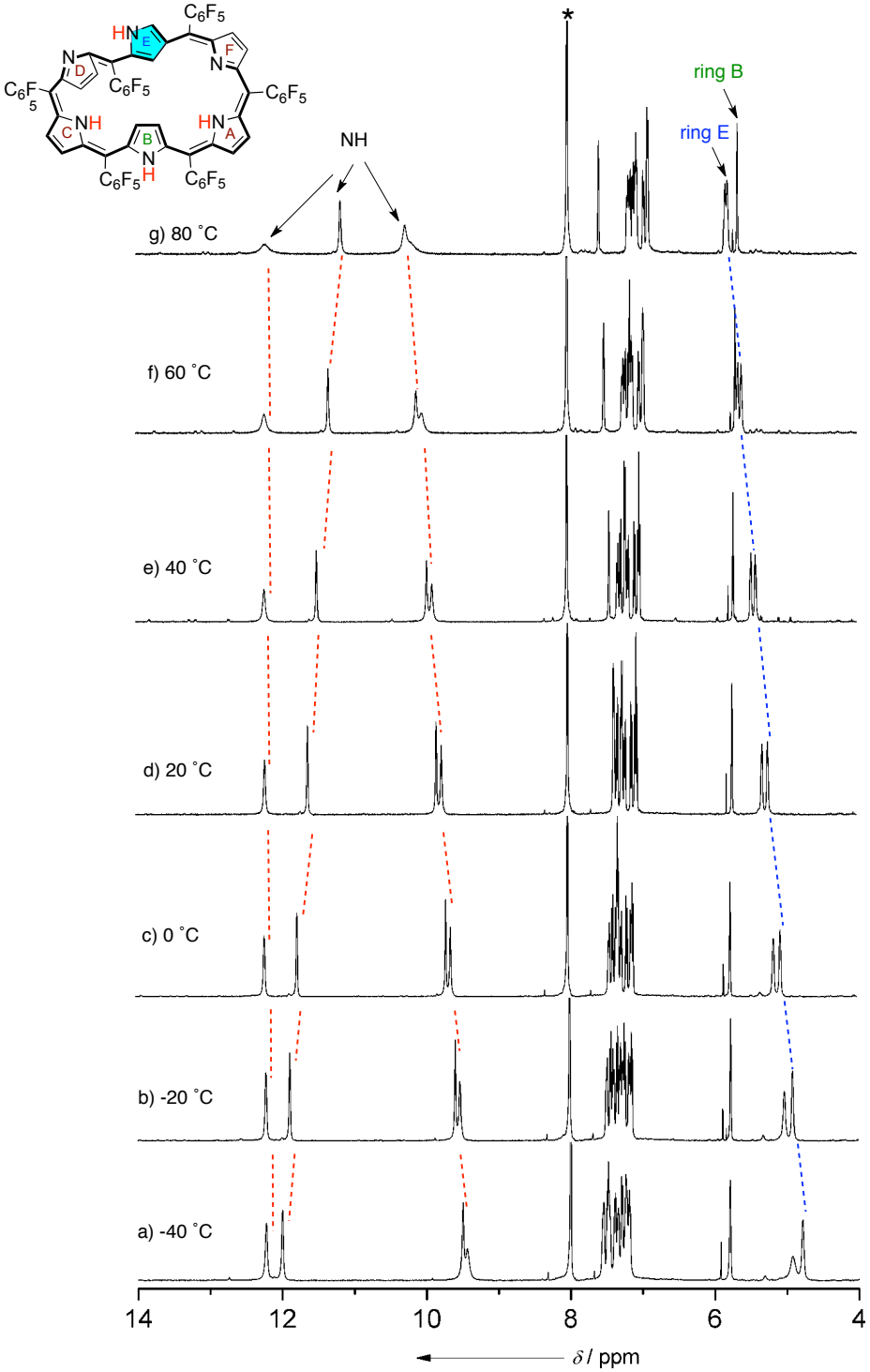


Fig. S6 Variable temperature ^{1}H NMR spectra of **5** in DMF-d_7. (Peaks marked with * is due to residual solvent.)

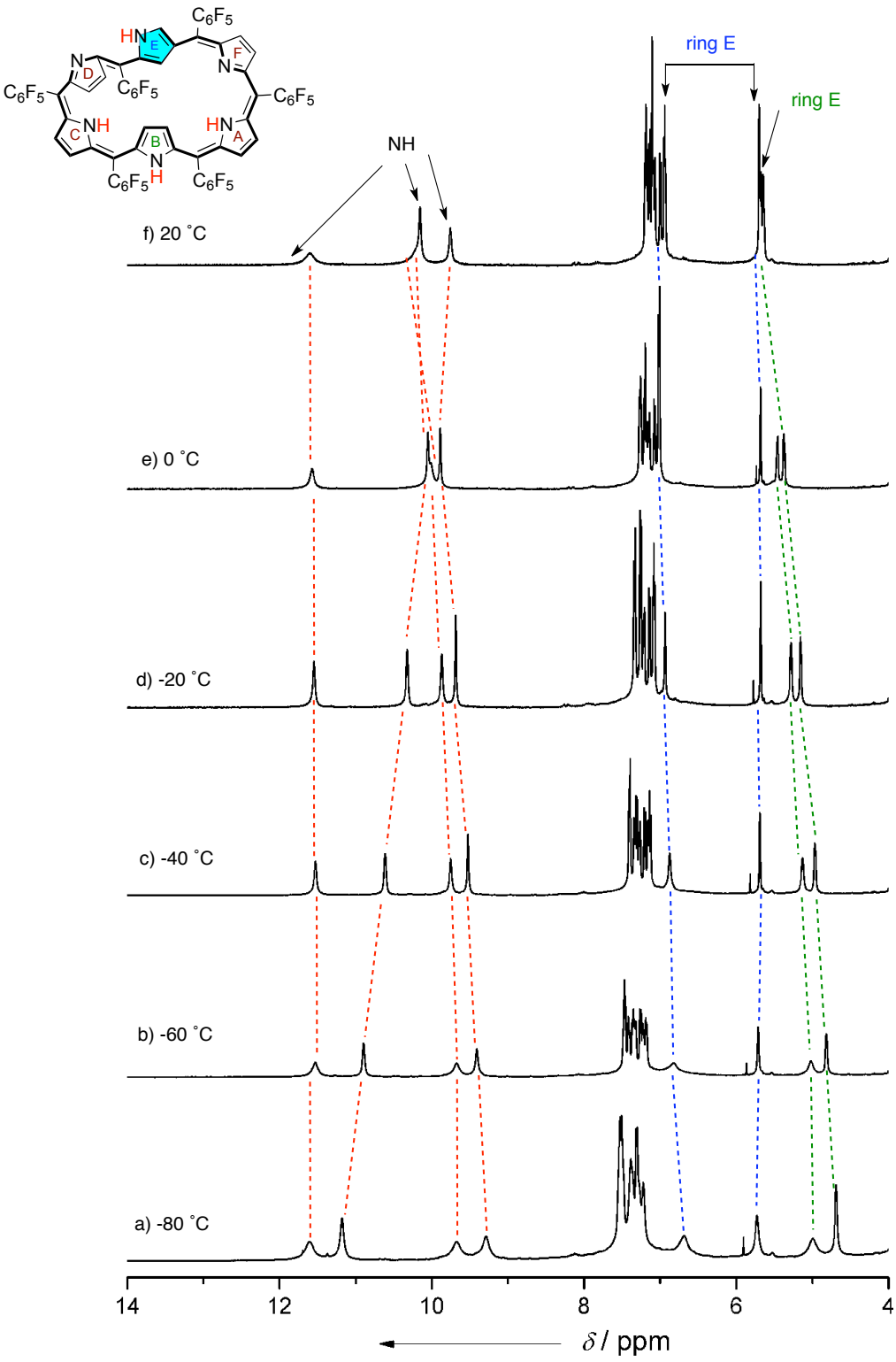


Fig. S7 Variable temperature ^{1}H NMR spectra of **5** in THF-d_8.

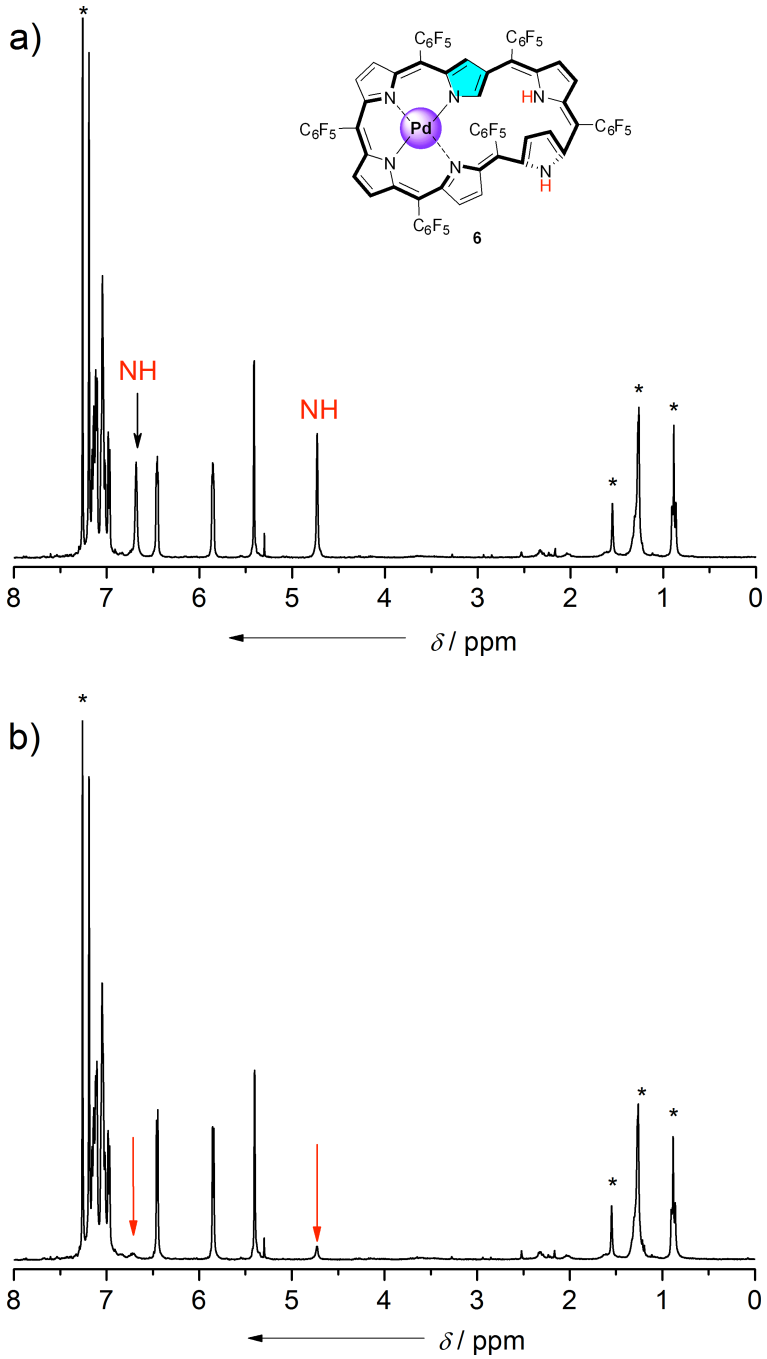


Fig. S8 ^{1}H NMR spectra of **6** in (a) $CDCl_3$ and (b) $CDCl_3$ with D_2O at 25 °C. (Peaks marked with * are due to residual solvents.)

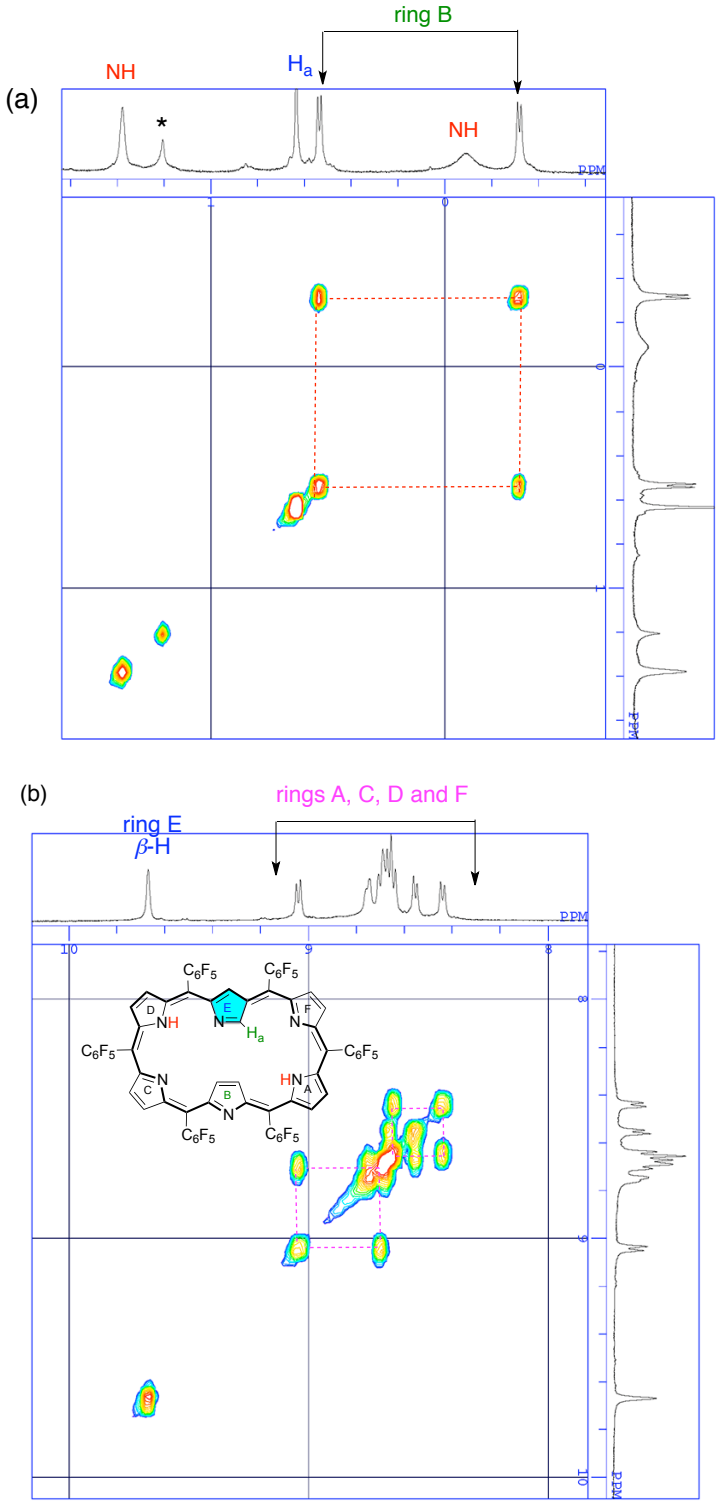


Fig. S9 ^{1}H-^{1}H COSY spectra of **4** in $CDCl_3$ at –60 °C: (a) in the upfield region and (b) in the downfield region.

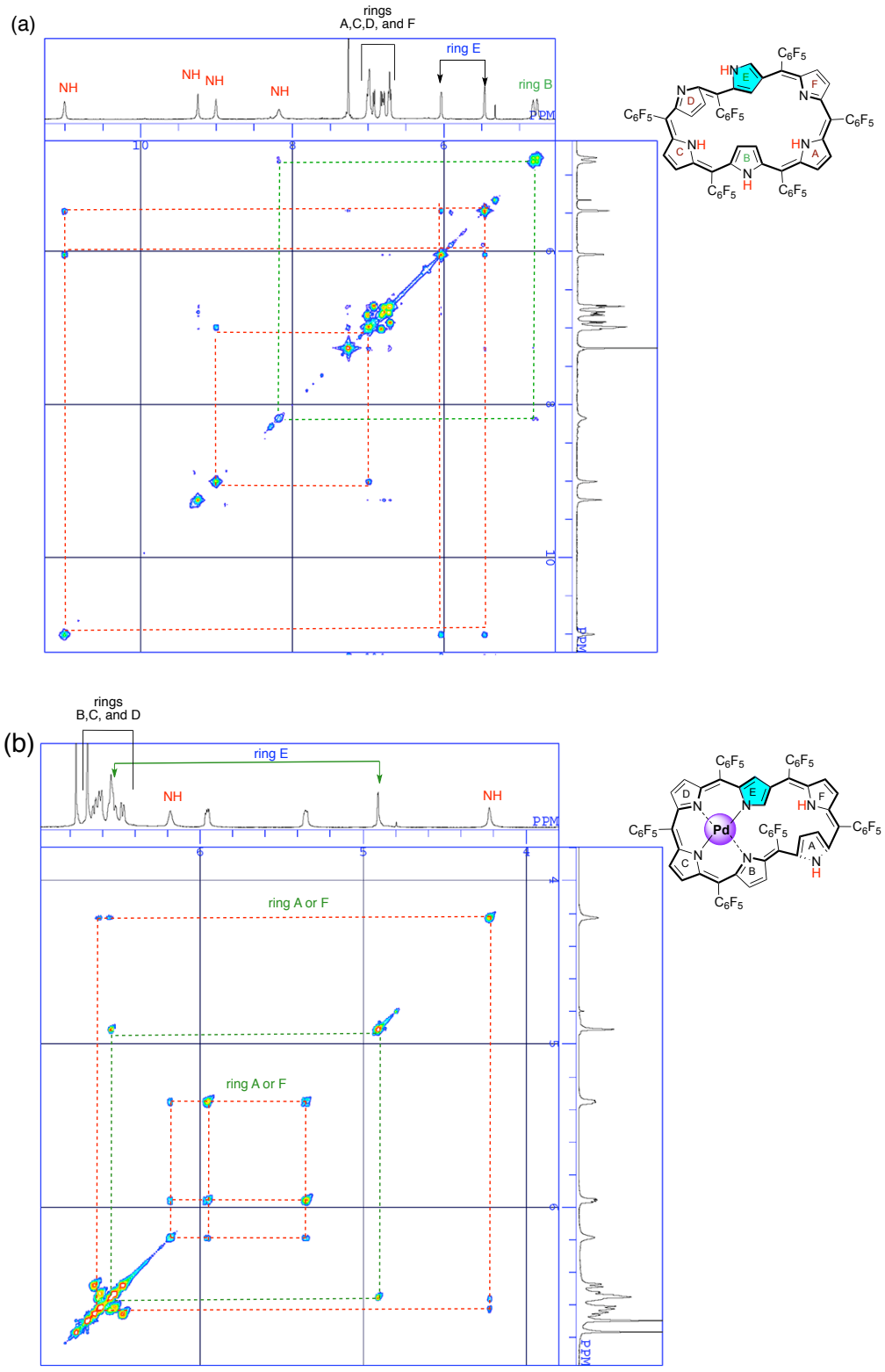


Fig. S10 ^{1}H-^{1}H COSY spectra of (a) **5** at –60 °C and (b) **6** at 25 °C in $CDCl_3$.

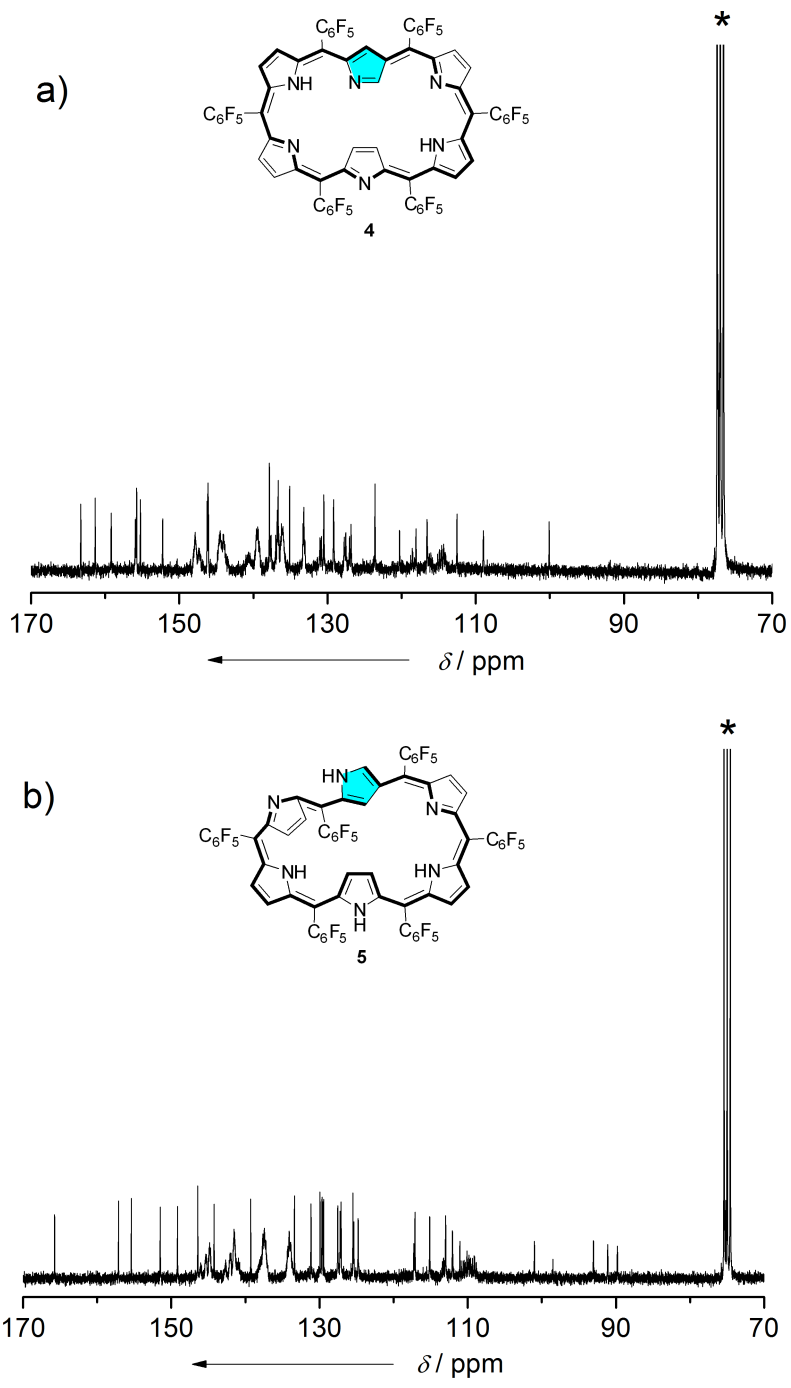


Fig. S11 ^{13}C NMR spectra of (a) **4** and (b) **5** in $CDCl_3$ at 25 °C.

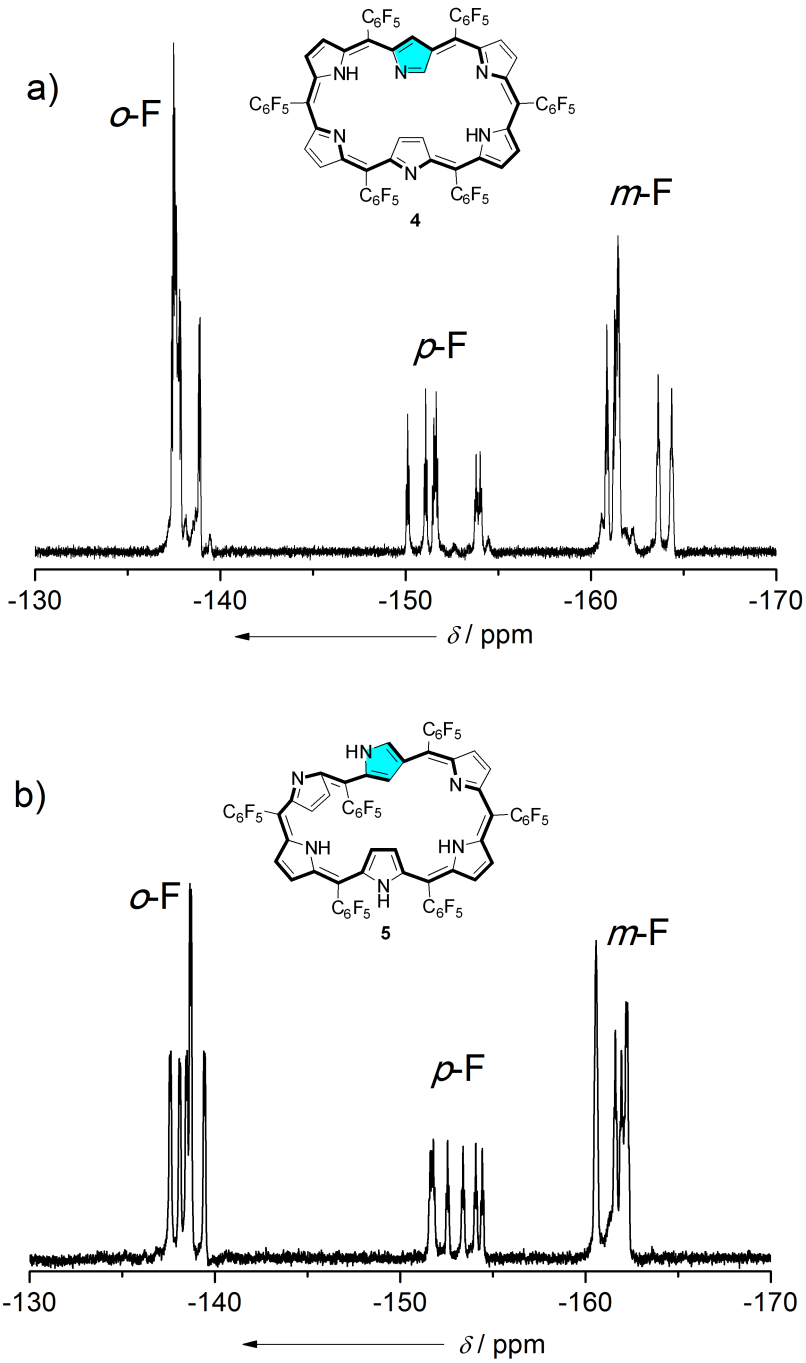


Fig. S12 ^{19}F NMR spectra of (a) **4** and (b) **5** in $CDCl_3$ at 25 °C.

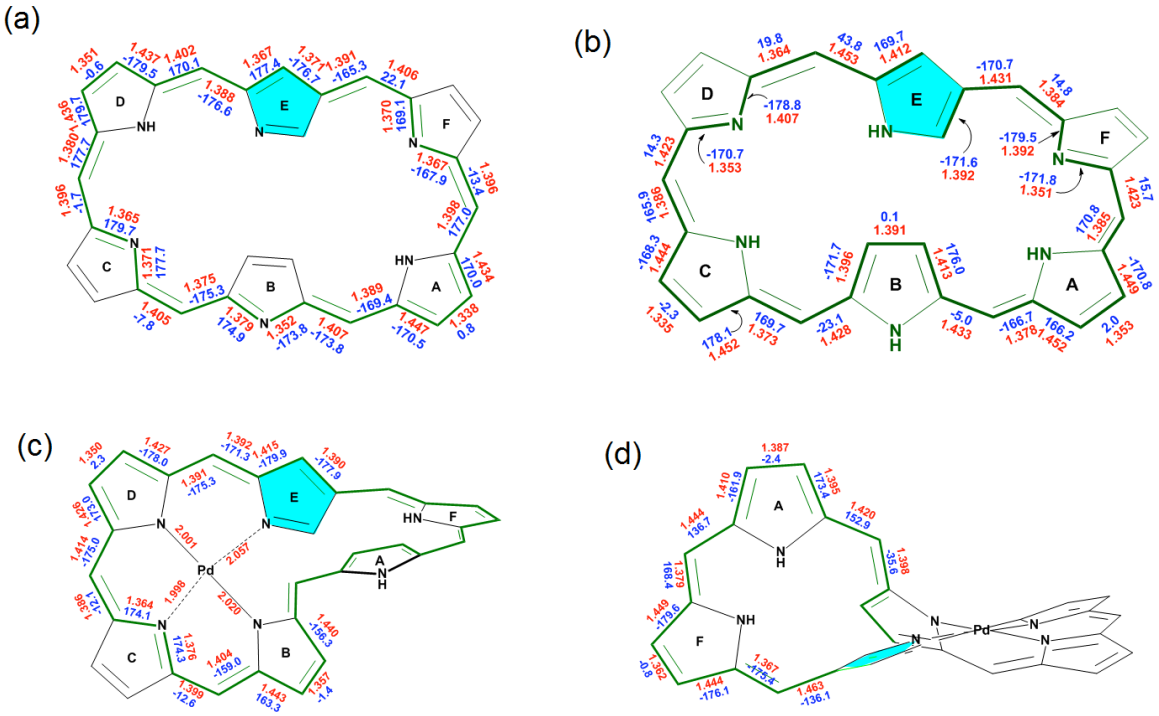
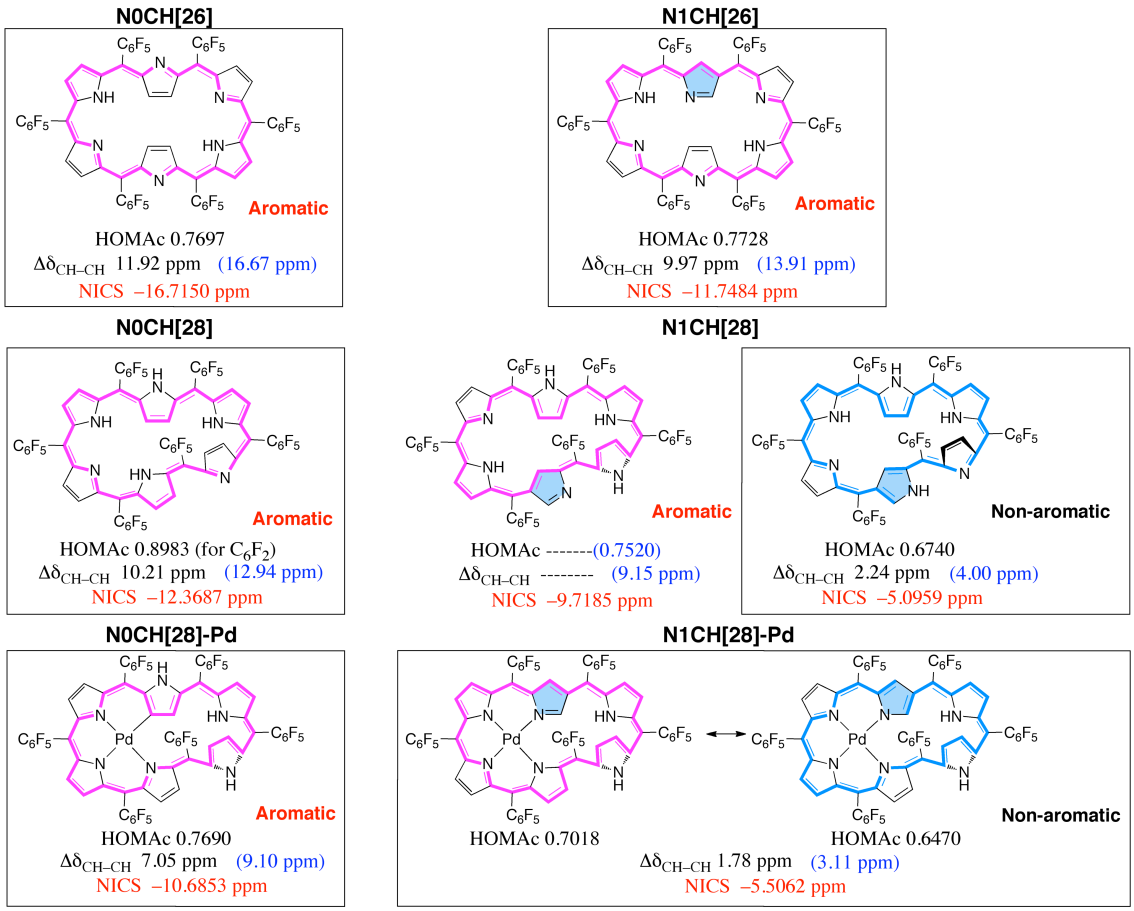


Fig. S13 Detailed structural data for **4** (a), **5** (b), and **6** (c, d). The annulenic circuits are indicated in green along with the bond lengths (Å) indicated in red and dihedral angles (°) indicated in blue.



HOMAc based on X-ray structure
(HOMAc based on optimized structure)

The subscript "c" means the values are calculated for the annulenic circuit indicated by the colored bold lines.

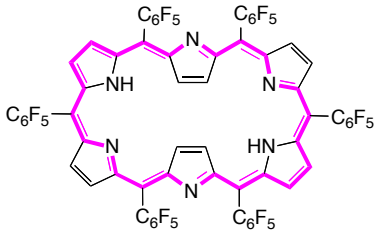
$\Delta\delta_{CH-CH}$ in $CDCl_3$, experimental
($\Delta\delta_{CH-CH}$ for optimized structure, theoretical)

NICS for optimized structure

B3LYP/6-31+G**//B3LYP/6-31G** except for a LANL2DZ basis set for Pd

Fig. S14 Evaluation of aromaticity in regular and singly N-confused [26]- and [28]hexaphyrins and mono-Pd(II) complexes of [28]hexaphyrins.

Energy, Cartesian coordinate and vibrational frequency for the optimized structures



E(RB3LYP) = -5846.75766715 A.U

Stoichiometry	C66H14F30N6			
Framework group	C1[X(C66H14F30N6)]			
Deg. of freedom	342			
Full point group		C1		
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.239627	1.194520	0.154525
2	6	0	5.881598	2.455368	0.367370
3	6	0	4.907524	3.406389	0.491347
4	6	0	3.628425	2.767384	0.373611
5	6	0	2.387841	3.426110	0.404616
6	6	0	1.102760	2.844081	0.483214
7	6	0	0.684055	1.494428	0.882873
8	6	0	–1.066491	2.850481	0.434432
9	6	0	–2.346901	3.423696	0.285125
10	6	0	–3.593362	2.755395	0.318374
11	6	0	–4.857048	3.478863	0.471877
12	6	0	–5.837198	2.549727	0.444869
13	6	0	–5.168652	1.267590	0.242370
14	6	0	–5.852692	0.048354	0.067504
15	6	0	–5.239643	–1.194537	–0.154725
16	6	0	–5.881629	–2.455415	–0.367494
17	6	0	–4.907556	–3.406467	–0.491319
18	6	0	–3.628411	–2.767402	–0.373628
19	6	0	–2.387858	–3.426157	–0.404572
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21	6	0	–0.684056	–1.494536	–0.883027
22	6	0	1.066475	–2.850529	–0.434449
23	6	0	2.346914	–3.423728	–0.285142
24	6	0	3.593361	–2.755397	–0.318528
25	6	0	4.857000	–3.478865	–0.472138
26	6	0	5.837166	–2.549698	–0.445237
27	6	0	5.168636	–1.267593	–0.242677
28	6	0	5.852660	–0.048371	–0.067811
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31	6	0	2.422712	4.917045	0.335952
32	1	0	–1.320742	–0.681745	–1.205308
33	1	0	1.320741	0.681590	1.205093
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35	6	0	–2.375263	4.897283	0.043975
36	6	0	–7.346695	0.059924	0.103713
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38	6	0	2.375307	–4.897254	–0.043809
39	6	0	7.346679	–0.059926	–0.104112
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42	1	0	–4.958699	4.544171	0.616332
43	1	0	–6.900400	2.704363	0.554397
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46	1	0	4.958667	–4.544188	–0.616609
47	1	0	1.350416	–0.713399	–1.146668
48	1	0	–1.350417	0.713274	1.146453
49	1	0	–3.232927	–0.655632	–0.034699
50	1	0	3.232896	0.655599	0.034576
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52	7	0	–0.027033	–3.622163	–0.231004
53	7	0	3.883197	1.422948	0.187377
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55	7	0	–3.883228	–1.422980	–0.187516
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58	6	0	2.903949	6.984183	–0.868928
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60	6	0	1.924228	7.088877	1.332641
61	6	0	1.935363	5.698893	1.390670
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63	9	0	3.369327	7.600652	–1.961335
64	9	0	2.410790	9.066094	0.132156
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66	9	0	1.479719	5.113582	2.502364
67	6	0	–2.915788	5.423651	–1.135606
68	6	0	–2.908415	6.788321	–1.411744
69	6	0	–2.340542	7.669881	–0.496446
70	6	0	–1.795652	7.179188	0.687957
71	6	0	–1.820862	5.812855	0.947067
72	9	0	–3.449559	4.606652	–2.055009
73	9	0	–3.431272	7.252618	–2.552537
74	9	0	–2.322029	8.980290	–0.749879
75	9	0	–1.241344	8.023592	1.566939
76	9	0	–1.302081	5.393359	2.105865
77	6	0	–1.935440	–5.699031	–1.390458
78	6	0	–1.924366	–7.089016	–1.332307
79	6	0	–2.410376	–7.733164	–0.195710
80	6	0	–2.904011	–6.984109	0.869277
81	6	0	–2.904297	–5.593942	0.788924
82	9	0	–1.479811	–5.113843	–2.502213
83	9	0	–1.465948	–7.808056	–2.360703
84	9	0	–2.410943	–9.066126	–0.131638
85	9	0	–3.369420	–7.600501	1.961745
86	9	0	–3.376051	–4.904380	1.838103
87	6	0	1.820876	–5.812994	–0.946717
88	6	0	1.795712	–7.179281	–0.687455
89	6	0	2.340738	–7.669822	0.496947
90	6	0	2.908673	–6.788124	1.412078
91	6	0	2.916016	–5.423471	1.135772
92	9	0	1.301926	–5.393636	–2.105546
93	9	0	1.241343	–8.023807	–1.566300
94	9	0	2.322303	–8.980155	0.750548
95	9	0	3.431667	–7.252253	2.552886
96	9	0	3.449816	–4.606333	2.055022
97	6	0	8.098677	–0.635535	0.926238
98	6	0	9.491026	–0.655314	0.901244
99	6	0	10.167266	–0.082486	–0.173783
100	6	0	9.448396	0.502202	–1.214036
101	6	0	8.056352	0.505929	–1.169221
102	9	0	7.479626	–1.189536	1.976028
103	9	0	10.179561	–1.211133	1.902618
104	9	0	11.500579	–0.093048	–0.206468
105	9	0	10.095324	1.049183	–2.247666
106	9	0	7.394732	1.074291	–2.185914
107	6	0	–8.098617	0.635503	–0.926698
108	6	0	–9.490981	0.655312	–0.901780
109	6	0	–10.167282	0.082560	0.173202
110	6	0	–9.448488	–0.502098	1.213546
111	6	0	–8.056444	–0.505854	1.168792
112	9	0	–7.479505	1.189456	–1.976472
113	9	0	–10.179440	1.211100	–1.903260
114	9	0	–11.500595	0.093138	0.205810
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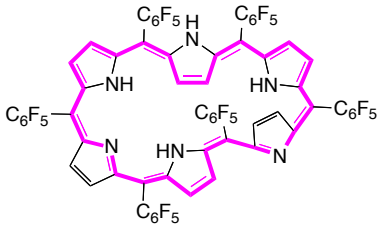
116	9	0	–7.394900	–1.074185	2.185561

Rotational constants (GHZ): 0.0138674 0.0120372 0.0068866

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1 A	2 A	3 A
Frequencies --	3.9526	5.5417	8.0910
Red. masses --	15.0053	14.8872	15.8285
Frc consts --	0.0001	0.0003	0.0006
IR Inten --	0.0992	0.0278	0.0005

E(RB3LYP) = -5848.01558711 A.U.



Stoichiometry	C66H16F30N6
Framework group	C1[X(C66H16F30N6)]
Deg. of freedom	348
Full point group	C1 NOp 1
Largest Abelian subgroup	C1 NOp 1
Largest concise Abelian subgroup	C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.314943	–0.816810	0.315229
2	6	0	6.319267	–0.051595	0.994466
3	6	0	5.723740	1.080983	1.495113
4	6	0	4.331573	1.055667	1.139933
5	6	0	3.342943	2.045163	1.303300
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8	6	0	–0.017803	0.914329	0.374323
9	6	0	–0.095190	2.320011	0.152752
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11	6	0	–2.371005	2.665312	–0.833150
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16	6	0	–4.852774	–0.677851	0.208794
17	6	0	–5.832777	–1.423165	0.980941
18	6	0	–5.129783	–2.142642	1.899042
19	6	0	–3.726947	–1.898907	1.621769
20	6	0	–2.637731	–2.520195	2.274156
21	6	0	–1.365552	–2.650601	1.683667
22	6	0	–0.123726	–3.041078	2.268902
23	6	0	0.825592	–3.090214	1.276063
24	6	0	0.192034	–2.773172	0.031121
25	6	0	0.723384	–2.906529	–1.273024
26	6	0	2.124919	–2.888125	–1.480544
27	6	0	2.864247	–3.604647	–2.509067
28	6	0	4.184890	–3.451292	–2.207189
29	6	0	4.240213	–2.566260	–1.052054
30	6	0	5.398928	–1.973569	–0.483176
31	6	0	3.748454	3.405296	1.740534
32	6	0	3.150660	4.012977	2.857743
33	6	0	3.510301	5.284175	3.295413
34	6	0	4.498966	5.992476	2.615343
35	6	0	5.112018	5.425490	1.500739
36	6	0	4.729818	4.156208	1.072798
37	6	0	–0.764547	4.537015	–0.767723
38	6	0	–1.453887	5.597036	–0.160957
39	6	0	–1.171921	6.928883	–0.455945
40	6	0	–0.170636	7.234155	–1.375290
41	6	0	0.538241	6.207059	–1.994741
42	6	0	0.233995	4.882354	–1.690273
43	6	0	–6.550345	0.482749	–1.205559
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45	6	0	–8.384318	–0.475720	–2.511428
46	6	0	–9.193155	0.615652	–2.203952
47	6	0	–8.696284	1.639724	–1.401516
48	6	0	–7.395731	1.560679	–0.909764
49	6	0	–2.846560	–3.089488	3.629026
50	6	0	–3.336402	–2.300734	4.681885
51	6	0	–3.548612	–2.814251	5.958229
52	6	0	–3.269120	–4.153760	6.217491
53	6	0	–2.781737	–4.967589	5.197607
54	6	0	–2.582249	–4.435385	3.926820
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58	6	0	9.261581	–3.663866	–1.399061
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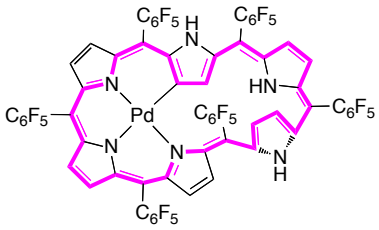
60	6	0	7.745496	–1.792981	–1.416076
61	6	0	–0.180026	–3.138735	–2.423279
62	6	0	–0.066151	–2.389548	–3.607085
63	6	0	–0.894054	–2.605116	–4.704951
64	6	0	–1.875764	–3.591265	–4.646977
65	6	0	–2.020633	–4.354579	–3.490616
66	6	0	–1.179049	–4.127936	–2.405995
67	9	0	2.207530	3.359675	3.548216
68	9	0	5.324705	3.668348	–0.022666
69	9	0	–2.414997	5.345946	0.734526

70	9	0	0.927868	3.920760	–2.314667
71	9	0	–6.334706	–1.589419	–2.344443
72	9	0	–6.968601	2.556201	–0.120482
73	9	0	–3.597002	–1.002253	4.485756
74	9	0	–2.139575	–5.263323	2.971330
75	9	0	6.128641	–4.656875	0.100325
76	9	0	7.526416	–0.516536	–1.761477
77	9	0	–1.334643	–4.906928	–1.327517
78	9	0	0.843094	–1.411782	–3.702201
79	1	0	7.359483	–0.328577	1.081421
80	1	0	6.202604	1.868801	2.057705
81	1	0	1.584238	–0.368011	1.141951
82	1	0	–0.793536	0.194051	0.173908
83	1	0	–3.106877	4.280092	–2.185853
84	1	0	–5.298846	2.776357	–2.412305
85	1	0	–6.906788	–1.358634	0.876299
86	1	0	–5.519817	–2.810338	2.654693
87	1	0	3.285185	–0.513516	0.062899
88	1	0	0.020609	–3.259457	3.316729
89	1	0	1.863268	–3.368665	1.364917
90	1	0	2.434097	–4.199333	–3.303560
91	1	0	5.032768	–3.861351	–2.738712
92	1	0	1.403029	3.788546	0.456157
93	1	0	–2.678397	0.782629	0.203624
94	1	0	–1.839385	–2.145325	–0.292406
95	7	0	4.138185	–0.124863	0.469833
96	7	0	1.123597	2.827344	0.571005
97	7	0	–2.980980	1.487265	–0.464973
98	7	0	–3.585380	–1.008976	0.591501
99	7	0	–1.121197	–2.486310	0.335637
100	7	0	2.981948	–2.255884	–0.635012
101	9	0	1.494346	6.497103	–2.882471
102	9	0	0.110115	8.506120	–1.660741
103	9	0	–1.847041	7.913646	0.143913
104	9	0	8.533701	–5.716891	–0.482212
105	9	0	10.454728	–4.192067	–1.680587
106	9	0	9.931394	–1.586905	–2.306706
107	9	0	–2.525037	–6.257726	5.439890
108	9	0	–3.467105	–4.655713	7.438099
109	9	0	–4.006136	–2.027080	6.938058
110	9	0	–8.855947	–1.457668	–3.287304
111	9	0	–10.439675	0.679909	–2.676794
112	9	0	–9.474851	2.683226	–1.094098
113	9	0	–2.950672	–5.313411	–3.437833
114	9	0	–2.673965	–3.804273	–5.694254
115	9	0	–0.760934	–1.862374	–5.809170
116	9	0	2.923803	5.822775	4.369132
117	9	0	4.853540	7.210103	3.028125
118	9	0	6.047622	6.110067	0.835301

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	7.6238	8.0588	10.6944
Red. masses --	15.1220	15.3773	15.0599
Frc consts --	0.0005	0.0006	0.0010
IR Inten --	0.0012	0.0040	0.0036

E(RB3LYP) = -5973.52314852 A.U.



Stoichiometry	C66H14F30N6Pd
Framework group	C1[X(C66H14F30N6Pd)]
Deg. of freedom	345
Full point group	C1 NOp 1
Largest Abelian subgroup	C1 NOp 1
Largest concise Abelian subgroup	C1 NOp 1

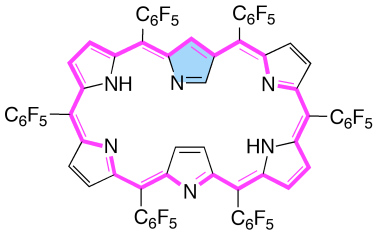
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.368543	–2.600459	–0.710244
2	6	0	0.820605	–3.867959	–0.165088
3	6	0	–0.150283	–4.302585	0.686606
4	6	0	–1.193747	–3.298924	0.697137
5	6	0	–2.480809	–3.466133	1.254939
6	6	0	–3.573754	–2.628341	0.971076
7	6	0	–4.961164	–2.877981	1.318964
8	6	0	–5.689288	–1.843870	0.820441
9	6	0	–4.750443	–0.918260	0.211275
10	6	0	–5.056197	0.356439	–0.291789
11	6	0	–4.112718	1.378986	–0.540212
12	6	0	–4.435442	2.685068	–1.068761
13	6	0	–3.293546	3.427294	–1.044328
14	6	0	–2.255169	2.586680	–0.503563
15	6	0	–0.938188	2.982587	–0.212281
16	6	0	0.022451	2.086198	0.275076
17	6	0	–0.023202	0.653667	0.317752
18	6	0	1.206140	0.262642	0.864762
19	6	0	1.984307	1.409203	1.182800
20	6	0	3.272608	1.541277	1.807085
21	6	0	4.291307	0.625000	1.537503
22	6	0	5.576329	0.395566	2.138785
23	6	0	6.232685	–0.568529	1.414002
24	6	0	5.392730	–0.978320	0.321463
25	6	0	5.610098	–1.837067	–0.762451
26	6	0	4.503828	–2.154013	–1.628412
27	6	0	4.388613	–2.138523	–3.039446
28	6	0	3.033293	–2.076182	–3.362024
29	6	0	2.288082	–2.126166	–2.161369
30	6	0	0.902896	–1.990392	–1.860526
31	6	0	–2.704196	–4.668364	2.109267
32	6	0	–2.129783	–4.758086	3.382922
33	6	0	–2.308320	–5.872314	4.199376
34	6	0	–3.082258	–6.938463	3.746742
35	6	0	–3.666387	–6.882885	2.483296
36	6	0	–3.467781	–5.760778	1.681871
37	6	0	–6.498205	0.669435	–0.511217
38	6	0	–7.241262	–0.004583	–1.488975
39	6	0	–8.591996	0.259465	–1.704393
40	6	0	–9.236189	1.221223	–0.929724
41	6	0	–8.527294	1.908883	0.052948
42	6	0	–7.178477	1.625603	0.253412
43	6	0	–0.557914	4.410678	–0.400248
44	6	0	–1.135025	5.446116	0.346947
45	6	0	–0.779943	6.779777	0.154816
46	6	0	0.181176	7.106377	–0.799616
47	6	0	0.779717	6.100411	–1.555916
48	6	0	0.407478	4.774043	–1.350790
49	6	0	3.532689	2.705124	2.684331
50	6	0	2.655378	3.029804	3.735617
51	6	0	2.872458	4.116588	4.577061
52	6	0	3.997413	4.918659	4.392857
53	6	0	4.888971	4.630217	3.362396
54	6	0	4.648442	3.544973	2.523552
55	6	0	6.958753	–2.314746	–1.117688
56	6	0	7.181062	–3.667567	–1.432497
57	6	0	8.432697	–4.152045	–1.797767
58	6	0	9.519787	–3.282219	–1.854799
59	6	0	9.340102	–1.934707	–1.551123
60	6	0	8.077313	–1.467005	–1.198313
61	6	0	0.063257	–1.174331	–2.762020
62	6	0	–1.161223	–1.644336	–3.261497
63	6	0	–1.983224	–0.854485	–4.058269
64	6	0	–1.589547	0.441453	–4.384586
65	6	0	–0.374234	0.936396	–3.916338
66	6	0	0.434737	0.129592	–3.125208
67	9	0	–1.382948	–3.749236	3.852121
68	9	0	–1.747964	–5.922386	5.412965
69	9	0	–3.262846	–8.011016	4.521057

70	9	0	–4.402443	–7.909570	2.043465
71	9	0	–4.033965	–5.750054	0.467428
72	9	0	–6.653282	–0.928674	–2.258946
73	9	0	–9.270844	–0.397551	–2.651139
74	9	0	–10.530178	1.483357	–1.127359
75	9	0	–9.148156	2.825774	0.803572
76	9	0	–6.535462	2.294495	1.219377
77	9	0	–2.049974	5.170107	1.282893
78	9	0	–1.345445	7.744558	0.886718
79	9	0	0.530626	8.379932	–0.987244
80	9	0	1.699280	6.414519	–2.473683
81	9	0	0.993821	3.832011	–2.100619
82	9	0	1.574802	2.274191	3.961861
83	9	0	2.019494	4.385644	5.569781
84	9	0	4.217290	5.958917	5.197841
85	9	0	5.960022	5.407353	3.171288
86	9	0	5.517787	3.333174	1.525272
87	9	0	6.171357	–4.546245	–1.363677
88	9	0	8.601771	–5.448348	–2.077871
89	9	0	10.725523	–3.737889	–2.198405
90	9	0	10.376339	–1.092402	–1.621175
91	9	0	7.952817	–0.154280	–0.956428
92	9	0	–1.574965	–2.882799	–2.973150
93	9	0	–3.146823	–1.330193	–4.512528
94	9	0	–2.375255	1.208536	–5.143056
95	9	0	–0.006602	2.189585	–4.208290
96	9	0	1.567761	0.667470	–2.646718
97	1	0	1.686950	–4.418208	–0.505243
98	1	0	–0.197931	–5.256893	1.191168
99	1	0	1.542671	3.454043	0.877214
100	1	0	3.532720	–0.138950	–0.252859
101	1	0	2.974546	–2.252351	–0.169591
102	1	0	–5.328855	–3.734809	1.863717
103	1	0	–6.757633	–1.697997	0.891287
104	1	0	–5.411887	2.996108	–1.409406
105	1	0	–3.168737	4.451358	–1.365037
106	1	0	1.494437	–0.746141	1.123035
107	1	0	5.935715	0.888807	3.030421
108	1	0	7.211253	–0.976834	1.621198
109	1	0	5.221140	–2.084857	–3.726638
110	1	0	2.605289	–2.006553	–4.351945
111	7	0	–0.809648	–2.249178	–0.089318
112	7	0	–3.494930	–1.439545	0.293546
113	7	0	–2.773414	1.344713	–0.233002
114	7	0	1.229490	2.497644	0.819453
115	7	0	4.214637	–0.259988	0.481621
116	7	0	3.220067	–2.220657	–1.147178
117	46	0	–1.714116	–0.394289	0.022502

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	8.0297	9.7839	12.3547
Red. masses --	15.4009	15.4632	15.6071
Frc consts --	0.0006	0.0009	0.0014
IR Inten --	0.0049	0.0031	0.0119



E(RB3LYP) = -5846.75450123 A.U.

Stoichiometry	C66H14F30N6		
Framework group	C1[X(C66H14F30N6)]		
Deg. of freedom	342		
Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

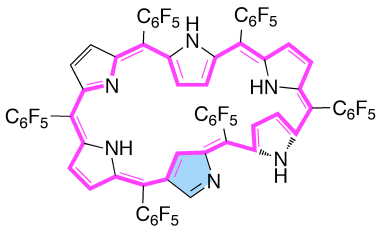
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.020435	1.323291	0.005557
2	6	0	5.710596	2.497879	0.532944
3	6	0	4.743323	3.350889	0.930993
4	6	0	3.465263	2.710199	0.614324
5	6	0	2.250158	3.393315	0.743210
6	6	0	0.927674	2.964924	0.434976
7	6	0	0.350169	1.618803	0.264140
8	6	0	–1.281199	3.014937	–0.040603
9	6	0	–2.555886	3.480261	–0.360332
10	6	0	–3.720116	2.707161	–0.578401
11	6	0	–4.985281	3.220150	–0.990419
12	6	0	–5.874989	2.176396	–1.030604
13	6	0	–5.181856	0.992683	–0.641385
14	6	0	–5.754647	–0.293712	–0.489405
15	6	0	–5.061785	–1.467523	–0.178765
16	6	0	–5.702065	–2.749989	0.111064
17	6	0	–4.697586	–3.611695	0.381972
18	6	0	–3.450980	–2.853900	0.224418
19	6	0	–2.168746	–3.467006	0.332591
20	6	0	–0.953157	–2.920658	–0.091092
21	6	0	1.175643	–2.917046	–0.483744
22	6	0	0.665726	–1.629918	–0.986129
23	6	0	2.479082	–3.469398	–0.614681
24	6	0	3.650701	–2.735755	–0.807614
25	6	0	4.927200	–3.260308	–1.215592
26	6	0	5.828776	–2.238886	–1.232071
27	6	0	5.156418	–1.043329	–0.795372
28	6	0	5.724960	0.194266	–0.504259
29	6	0	2.336644	4.821618	1.201657
30	6	0	2.819005	5.840183	0.374215
31	6	0	2.870364	7.168234	0.792868
32	6	0	2.427466	7.504125	2.070042
33	6	0	1.937513	6.512363	2.917288
34	6	0	1.892656	5.192639	2.475243
35	6	0	–2.727918	4.963116	–0.476895
36	6	0	–3.418551	5.694295	0.495495
37	6	0	–3.576234	7.075036	0.405482
38	6	0	–3.034435	7.758096	–0.681401
39	6	0	–2.341770	7.058217	–1.667038
40	6	0	–2.195718	5.677260	–1.555703
41	6	0	–7.236520	–0.381929	–0.662715
42	6	0	–8.118360	0.215428	0.245931
43	6	0	–9.500390	0.131932	0.098219
44	6	0	–10.034682	–0.568389	–0.981237
45	6	0	–9.185094	–1.175337	–1.903373
46	6	0	–7.805748	–1.075680	–1.737071
47	6	0	–2.110569	–4.842002	0.914638
48	6	0	–2.479511	–5.073651	2.243992
49	6	0	–2.375819	–6.329954	2.835751
50	6	0	–1.881074	–7.398804	2.093470
51	6	0	–1.509043	–7.202186	0.765780
52	6	0	–1.637579	–5.942452	0.190526
53	6	0	2.583629	–4.949033	–0.509261
54	6	0	3.355038	–5.569912	0.480570
55	6	0	3.385753	–6.953452	0.633466
56	6	0	2.627072	–7.755800	–0.214715
57	6	0	1.849367	–7.171204	–1.212828
58	6	0	1.844393	–5.788081	–1.355795
59	6	0	7.200300	0.325521	–0.694840
60	6	0	8.118614	–0.362819	0.106911
61	6	0	9.494688	–0.233980	–0.066585
62	6	0	9.986014	0.609211	–1.060491
63	6	0	9.100006	1.312962	–1.873382
64	6	0	7.728496	1.164502	–1.683972
65	6	0	–0.155875	3.822006	0.252457
66	6	0	–0.671195	–1.642851	–0.756577
67	9	0	3.248520	5.553481	–0.861381
68	9	0	3.336774	8.119195	–0.023261
69	9	0	2.473891	8.772684	2.481968

70	9	0	1.515611	6.831918	4.145013
71	9	0	1.416115	4.263352	3.313075
72	9	0	–3.947882	5.066107	1.552546
73	9	0	–4.237939	7.745841	1.353004
74	9	0	–3.179673	9.080171	–0.778661
75	9	0	–1.826952	7.712479	–2.712258
76	9	0	–1.530146	5.034325	–2.522330
77	9	0	–7.638185	0.889756	1.298612
78	9	0	–10.313949	0.711213	0.986518
79	9	0	–11.356956	–0.656511	–1.131709
80	9	0	–9.696230	–1.842109	–2.942791
81	9	0	–7.019697	–1.665387	–2.645918
82	9	0	–2.937941	–4.062793	2.997486
83	9	0	–2.736084	–6.511393	4.111910
84	9	0	–1.768758	–8.607194	2.650402
85	9	0	–1.024265	–8.224191	0.047307
86	9	0	–1.297219	–5.815523	–1.096599
87	9	0	4.076513	–4.830955	1.336694
88	9	0	4.130411	–7.513145	1.594266
89	9	0	2.651955	–9.082745	–0.077785
90	9	0	1.136242	–7.942374	–2.038043
91	9	0	1.114458	–5.264337	–2.344725
92	9	0	7.682939	–1.174957	1.079507
93	9	0	10.343367	–0.905426	0.718407
94	9	0	11.302049	0.741399	–1.234489
95	9	0	9.570050	2.117687	–2.831578
96	9	0	6.905016	1.851734	–2.484901
97	1	0	6.780181	2.627959	0.607705
98	1	0	4.872093	4.318246	1.392299
99	1	0	3.176384	–0.703465	–0.231047
100	1	0	0.889801	0.687572	0.371869
101	1	0	–5.182856	4.252458	–1.233999
102	1	0	–6.915341	2.218491	–1.313183
103	1	0	–6.764147	–2.946120	0.121189
104	1	0	–4.773573	–4.659886	0.630563
105	1	0	1.231842	–0.874791	–1.515121
106	1	0	5.097449	–4.291029	–1.487692
107	1	0	6.868961	–2.289989	–1.515229
108	1	0	–1.399839	–0.889759	–1.008148
109	1	0	–3.144054	0.701576	–0.117867
110	1	0	–0.141644	4.899305	0.298052
111	7	0	–0.930038	1.643000	0.007347
112	7	0	0.192183	–3.652454	0.047023
113	7	0	3.676228	1.453241	0.083625
114	7	0	–3.877992	1.350729	–0.395074
115	7	0	–3.698240	–1.565972	–0.095172
116	7	0	3.835548	–1.381806	–0.601609

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	3.5825	6.1649	10.4195
Red. masses --	15.0561	14.9485	15.4292
Frc consts --	0.0001	0.0003	0.0010
IR Inten --	0.0258	0.0067	0.0336

E(RB3LYP) = -5848.00462328 A.U.



Stoichiometry	C66H16F30N6		
Framework group	C1[X(C66H16F30N6)]		
Deg. of freedom	348		
Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

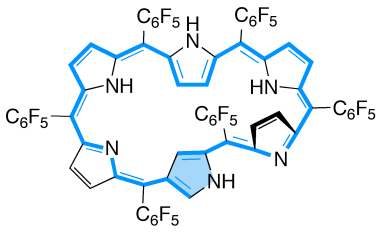
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–4.567169	1.082123	–0.792065
2	6	0	–4.998856	2.228414	–1.590437
3	6	0	–3.923630	3.045170	–1.691731
4	6	0	–2.833035	2.390587	–0.970305
5	6	0	–1.567688	2.958980	–0.772831
6	6	0	–0.459236	2.284734	–0.189287
7	6	0	–0.220902	0.911563	0.032429
8	6	0	1.057213	0.769820	0.554854
9	6	0	1.637501	2.058896	0.677421
10	6	0	2.922479	2.429717	1.196033
11	6	0	4.016876	1.568807	1.112870
12	6	0	5.353460	1.698893	1.630581
13	6	0	6.103924	0.645737	1.180012
14	6	0	5.275820	–0.187236	0.350450
15	6	0	5.605527	–1.294115	–0.437801
16	6	0	4.609540	–2.033729	–1.151893
17	6	0	4.691635	–2.661812	–2.423104
18	6	0	3.417025	–3.072624	–2.782515
19	6	0	2.533594	–2.750750	–1.720380
20	6	0	1.142759	–2.955924	–1.572056
21	6	0	0.464264	–2.771066	–0.353683
22	6	0	0.272309	–2.634279	1.808828
23	6	0	–0.930844	–2.801440	–0.094487
24	6	0	–1.084734	–2.732756	1.292407
25	6	0	–2.288768	–2.822748	2.075514
26	6	0	–3.504807	–2.302808	1.635630
27	6	0	–4.841931	–2.694887	1.993530
28	6	0	–5.721146	–1.959912	1.247194
29	6	0	–4.963544	–1.025577	0.455763
30	6	0	–5.421405	0.044161	–0.326948
31	6	0	3.113212	3.757431	1.850732
32	6	0	2.976204	4.971338	1.169144
33	6	0	3.131908	6.208521	1.786231
34	6	0	3.458691	6.260966	3.138640
35	6	0	3.609151	5.076057	3.854772
36	6	0	3.428475	3.852571	3.214019
37	6	0	7.024373	–1.661874	–0.648917
38	6	0	7.986464	–0.749985	–1.111199
39	6	0	9.314999	–1.111707	–1.317136
40	6	0	9.718019	–2.423554	–1.080509
41	6	0	8.789434	–3.360722	–0.633210
42	6	0	7.469186	–2.974965	–0.422673
43	6	0	0.375506	–3.388675	–2.770532
44	6	0	0.319617	–2.599503	–3.927906
45	6	0	–0.400692	–2.987302	–5.054256
46	6	0	–1.092047	–4.196397	–5.045591
47	6	0	–1.056912	–5.006168	–3.912925
48	6	0	–0.330158	–4.599770	–2.796747
49	6	0	–2.240310	–3.530977	3.373885
50	6	0	–1.608751	–4.780763	3.512632
51	6	0	–1.532239	–5.445471	4.732642
52	6	0	–2.097236	–4.871622	5.869023
53	6	0	–2.731006	–3.635207	5.773814
54	6	0	–2.792810	–2.982900	4.546133
55	6	0	–6.882090	0.117106	–0.601973
56	6	0	–7.530936	–0.875607	–1.349204
57	6	0	–8.896683	–0.833688	–1.616825
58	6	0	–9.658708	0.228252	–1.136435
59	6	0	–9.048883	1.233216	–0.389579
60	6	0	–7.683088	1.164289	–0.126249
61	6	0	–1.359063	4.381789	–1.174497
62	6	0	–0.435310	4.731198	–2.170686
63	6	0	–0.224415	6.051226	–2.559790
64	6	0	–0.949399	7.071174	–1.947404
65	6	0	–1.872888	6.762577	–0.951526
66	6	0	–2.063591	5.435063	–0.574154
67	9	0	2.651282	4.970613	–0.143774
68	9	0	2.982872	7.338046	1.087563
69	9	0	3.621396	7.437645	3.744604

70	9	0	3.913156	5.118901	5.155172
71	9	0	3.573003	2.740918	3.948406
72	9	0	7.640865	0.516124	–1.387090
73	9	0	10.199964	–0.212354	–1.761318
74	9	0	10.988038	–2.780886	–1.280584
75	9	0	9.174427	–4.618967	–0.395385
76	9	0	6.614480	–3.902341	0.027980
77	9	0	0.957278	–1.422077	–3.970920
78	9	0	–0.439297	–2.204017	–6.137277
79	9	0	–1.784029	–4.579056	–6.119921
80	9	0	–1.709460	–6.172960	–3.907960
81	9	0	0.273074	3.775350	–2.787744
82	9	0	–0.304784	–5.418022	–1.738921
83	9	0	–1.078185	–5.391618	2.446201
84	9	0	–0.936224	–6.639674	4.816472
85	9	0	–2.032960	–5.503480	7.042409
86	9	0	–3.260208	–3.072882	6.866176
87	9	0	–3.381092	–1.779341	4.521119
88	9	0	–6.831929	–1.910270	–1.838273
89	9	0	–9.477157	–1.798990	–2.339335
90	9	0	–10.968833	0.282204	–1.389417
91	9	0	–9.780872	2.248106	0.084173
92	9	0	0.657933	6.343725	–3.520498
93	9	0	–7.142476	2.140426	0.614848
94	9	0	–0.758170	8.339803	–2.313029
95	9	0	–2.560815	7.741862	–0.355381
96	9	0	–2.946784	5.185984	0.399182
97	1	0	0.857513	3.925564	0.073864
98	1	0	3.281233	0.138534	–0.254930
99	1	0	–0.917562	0.124967	–0.197418
100	1	0	1.493147	–0.153618	0.901595
101	1	0	5.691335	2.497677	2.273260
102	1	0	7.143841	0.453242	1.398356
103	1	0	5.587578	–2.725566	–3.023457
104	1	0	3.129636	–3.549918	–3.708026
105	1	0	0.548767	–2.538435	2.854100
106	1	0	–1.718727	–2.919994	–0.824153
107	1	0	–5.080236	–3.489277	2.686060
108	1	0	–6.798967	–2.027187	1.257415
109	1	0	–5.983961	2.380005	–2.007872
110	1	0	–3.862008	3.989025	–2.214582
111	7	0	–3.255202	1.183467	–0.469169
112	7	0	0.680874	2.947510	0.238692
113	7	0	4.017279	0.387435	0.389807
114	7	0	3.296841	–2.113479	–0.756606
115	1	0	2.926071	–2.066812	0.197217
116	7	0	1.175529	–2.614198	0.858982
117	7	0	–3.640261	–1.303197	0.684552
118	1	0	–2.939060	–0.617049	0.403048

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	6.8744	8.7787	10.0488
Red. masses --	15.3426	15.2655	15.0522
Frc consts --	0.0004	0.0007	0.0009
IR Inten --	0.0054	0.0032	0.0036

E(RB3LYP) = -5848.00816863 A.U.



Stoichiometry	C66H16F30N6	
Framework group	C1[X(C66H16F30N6)]	
Deg. of freedom	348	
Full point group	C1	NOp 1
Largest Abelian subgroup	C1	NOp 1
Largest concise Abelian subgroup	C1	NOp 1

Standard orientation:

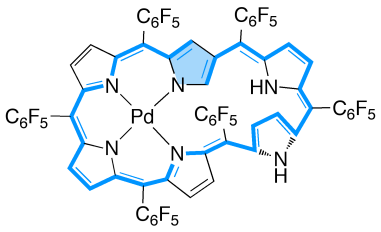
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–4.628697	1.242040	–0.795432
2	6	0	–4.976123	2.388217	–1.603555
3	6	0	–3.882126	3.194659	–1.688551
4	6	0	–2.795915	2.583075	–0.955089
5	6	0	–1.516003	3.087096	–0.765886
6	6	0	–0.441601	2.355118	–0.162543
7	6	0	–0.256228	0.977000	0.059547
8	6	0	1.022580	0.793640	0.586340
9	6	0	1.644042	2.052517	0.705424
10	6	0	2.957624	2.394456	1.187110
11	6	0	4.034321	1.524403	1.071426
12	6	0	5.412409	1.716035	1.471407
13	6	0	6.149195	0.659645	1.022572
14	6	0	5.266218	–0.243134	0.318947
15	6	0	5.544575	–1.385465	–0.432568
16	6	0	4.494744	–2.119517	–1.085029
17	6	0	4.635357	–2.919718	–2.295932
18	6	0	3.375445	–3.259161	–2.683457
19	6	0	2.475733	–2.733351	–1.670463
20	6	0	1.103644	–2.939210	–1.565279
21	6	0	0.385757	–2.722987	–0.339153
22	6	0	0.165949	–2.622720	1.896805
23	6	0	–0.978024	–2.654840	–0.052906
24	6	0	–1.134024	–2.597051	1.357974
25	6	0	–2.363994	–2.626848	2.128352
26	6	0	–3.541586	–2.040952	1.697523
27	6	0	–4.883135	–2.368755	2.173455
28	6	0	–5.745592	–1.658563	1.407419
29	6	0	–4.922268	–0.833331	0.520178
30	6	0	–5.433405	0.205446	–0.329554
31	6	0	3.190606	3.715948	1.842575
32	6	0	3.067841	4.938677	1.174403
33	6	0	3.265861	6.166405	1.798290
34	6	0	3.623362	6.199424	3.143498
35	6	0	3.761493	5.005139	3.846386
36	6	0	3.538991	3.791840	3.199318
37	6	0	6.949248	–1.807404	–0.649712
38	6	0	7.926145	–0.960674	–1.194658
39	6	0	9.239662	–1.374362	–1.400676
40	6	0	9.611401	–2.677432	–1.080229
41	6	0	8.666457	–3.552579	–0.549907
42	6	0	7.362796	–3.112813	–0.340868
43	6	0	0.340237	–3.443115	–2.733075
44	6	0	0.344302	–2.758889	–3.958454
45	6	0	–0.379181	–3.208963	–5.059585
46	6	0	–1.134976	–4.374078	–4.958803
47	6	0	–1.160911	–5.080412	–3.758276
48	6	0	–0.430241	–4.614706	–2.669324
49	6	0	–2.343783	–3.364868	3.415967
50	6	0	–1.867334	–4.684176	3.506069
51	6	0	–1.821798	–5.378033	4.711255
52	6	0	–2.257913	–4.758767	5.880466
53	6	0	–2.734388	–3.451264	5.832360
54	6	0	–2.772112	–2.773555	4.616559
55	6	0	–6.884183	0.211588	–0.647543
56	6	0	–7.479063	–0.870710	–1.312855
57	6	0	–8.838045	–0.907678	–1.611133
58	6	0	–9.651330	0.163262	–1.248128
59	6	0	–9.097685	1.255479	–0.585456
60	6	0	–7.737444	1.263949	–0.286492
61	6	0	–1.237502	4.480555	–1.214618
62	6	0	–0.270103	4.752345	–2.194839
63	6	0	0.017402	6.047266	–2.617272
64	6	0	–0.676830	7.120738	–2.063046
65	6	0	–1.645228	6.889921	–1.089012
66	6	0	–1.909109	5.586720	–0.673421
67	9	0	2.716601	4.958715	–0.131992
68	9	0	3.128790	7.305391	1.112278
69	9	0	3.826880	7.366887	3.755218

70	9	0	4.095041	5.029667	5.140123
71	9	0	3.673236	2.671210	3.921040
72	9	0	7.611405	0.294306	–1.550018
73	9	0	10.139698	–0.534068	–1.924459
74	9	0	10.866938	–3.085411	–1.279717
75	9	0	9.020216	–4.802840	–0.231681
76	9	0	6.489953	–3.982041	0.188004
77	9	0	1.039197	–1.623059	–4.096606
78	9	0	–0.359434	–2.524741	–6.208447
79	9	0	–1.829314	–4.814533	–6.009249
80	9	0	–1.871872	–6.208783	–3.664474
81	9	0	0.406478	3.744195	–2.759998
82	9	0	–0.459236	–5.341299	–1.545731
83	9	0	–1.463986	–5.330863	2.405438
84	9	0	–1.376646	–6.638618	4.751361
85	9	0	–2.219591	–5.415651	7.041185
86	9	0	–3.139243	–2.849014	6.955997
87	9	0	–3.209869	–1.508219	4.631604
88	9	0	–6.728832	–1.915182	–1.690718
89	9	0	–9.364129	–1.956105	–2.254682
90	9	0	–10.955451	0.142603	–1.534704
91	9	0	–9.877537	2.280817	–0.222789
92	9	0	0.940736	6.265027	–3.558456
93	9	0	–7.256138	2.325411	0.377520
94	9	0	–0.414595	8.365367	–2.464327
95	9	0	–2.305093	7.919480	–0.548705
96	9	0	–2.834937	5.413089	0.278136
97	1	0	–2.854930	0.696064	0.129423
98	1	0	0.928312	3.945784	0.100404
99	1	0	3.221861	–0.144376	–0.036486
100	1	0	2.064948	–2.602373	0.918077
101	1	0	–0.950891	0.186016	–0.174009
102	1	0	1.437403	–0.145820	0.910754
103	1	0	5.781341	2.574975	2.011800
104	1	0	7.211963	0.513598	1.143990
105	1	0	5.563426	–3.144487	–2.803311
106	1	0	3.087462	–3.848009	–3.543313
107	1	0	0.485514	–2.582668	2.927975
108	1	0	–1.783888	–2.673094	–0.769900
109	1	0	–5.123003	–3.092508	2.939921
110	1	0	–6.825598	–1.656223	1.457385
111	1	0	–5.943971	2.556427	–2.051007
112	1	0	–3.805327	4.128703	–2.225061
113	7	0	–3.299605	1.391516	–0.467213
114	7	0	0.715437	2.976153	0.271651
115	7	0	4.007689	0.302917	0.427159
116	7	0	3.203478	–2.039344	–0.715196
117	7	0	1.050724	–2.680425	0.885455
118	7	0	–3.616455	–1.089785	0.689560

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	7.3951	8.0127	9.5064
Red. masses --	15.3863	15.1071	15.0701
Frc consts --	0.0005	0.0006	0.0008
IR Inten --	0.0123	0.0060	0.0064

E(RB3LYP) = -5973.53413932 A.U.



Stoichiometry	C66H14F30N6Pd				
Framework group	C1[X(C66H14F30N6Pd)]				
Deg. of freedom	345				
Full point group		C1	NOp	1	
Largest Abelian subgroup		C1	NOp	1	
Largest concise Abelian subgroup		C1	NOp	1	

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	–4.120544	1.324632	–0.510553
2	6	0	–4.468199	2.609331	–1.068724
3	6	0	–3.330385	3.359293	–1.100173
4	6	0	–2.269036	2.552156	–0.554164
5	6	0	–0.962087	2.972219	–0.296249
6	6	0	0.066604	2.166237	0.241470
7	6	0	1.260638	2.611912	0.851004
8	6	0	1.963544	1.483175	1.281662
9	6	0	1.145626	0.368956	0.905478
10	6	0	3.229231	1.453319	2.020369
11	6	0	4.260056	0.628797	1.622080
12	6	0	5.545366	0.308899	2.201803
13	6	0	6.222053	–0.513483	1.346795
14	6	0	5.398000	–0.760618	0.184184
15	6	0	5.628488	–1.486910	–0.982916
16	6	0	4.512411	–1.724959	–1.875013
17	6	0	4.369265	–1.594053	–3.275255
18	6	0	3.004559	–1.593176	–3.572801
19	6	0	2.290142	–1.781813	–2.369072
20	6	0	0.908982	–1.754621	–2.025414
21	6	0	0.458070	–2.445678	–0.885840
22	6	0	0.982170	–3.711777	–0.417830
23	6	0	0.070803	–4.225010	0.460943
24	6	0	–1.005434	–3.268410	0.567548
25	6	0	–2.263927	–3.488027	1.182024
26	6	0	–3.379539	–2.676222	0.943526
27	6	0	–4.749546	–2.973767	1.320604
28	6	0	–5.528658	–1.965600	0.853344
29	6	0	–4.649990	–0.989752	0.233820
30	6	0	–5.030263	0.268909	–0.237399
31	6	0	–0.622333	4.402158	–0.548695
32	6	0	–1.208651	5.447804	0.174532
33	6	0	–0.876170	6.780489	–0.058524
34	6	0	0.067820	7.093747	–1.033792
35	6	0	0.672821	6.075476	–1.767859
36	6	0	0.327552	4.749973	–1.518107
37	6	0	3.405294	2.393603	3.147614
38	6	0	2.437145	2.489229	4.163626
39	6	0	2.556140	3.382941	5.222648
40	6	0	3.668286	4.219570	5.299638
41	6	0	4.647166	4.156019	4.311680
42	6	0	4.506727	3.258981	3.255868
43	6	0	6.975081	–1.935418	–1.376420
44	6	0	8.104653	–1.099575	–1.331624
45	6	0	9.367675	–1.533092	–1.725071
46	6	0	9.537687	–2.830760	–2.201418
47	6	0	8.440052	–3.686154	–2.273059
48	6	0	7.189321	–3.238451	–1.861604
49	6	0	–0.020578	–0.971858	–2.865744
50	6	0	0.246997	0.360134	–3.224025
51	6	0	–0.642381	1.112592	–3.983571
52	6	0	–1.835416	0.538039	–4.417018
53	6	0	–2.128802	–0.784070	–4.090129
54	6	0	–1.228040	–1.520715	–3.328914
55	6	0	–2.415068	–4.713869	2.015086
56	6	0	–1.759943	–4.823227	3.248150
57	6	0	–1.860637	–5.962041	4.043366
58	6	0	–2.636775	–7.035117	3.610817
59	6	0	–3.299641	–6.961474	2.387816
60	6	0	–3.176549	–5.815122	1.605747
61	6	0	–6.485569	0.538017	–0.401840
62	6	0	–7.154109	1.502124	0.364545
63	6	0	–8.515140	1.754535	0.212943
64	6	0	–9.250092	1.026783	–0.720725
65	6	0	–8.618936	0.056598	–1.495674
66	6	0	–7.255224	–0.174825	–1.331192
67	9	0	–2.106766	5.184984	1.131888
68	9	0	–1.449299	7.757047	0.652524
69	9	0	0.392734	8.367037	–1.264718

70	9	0	1.575301	6.377281	–2.706964
71	9	0	0.922294	3.797955	–2.245869
72	9	0	1.365807	1.687462	4.146125
73	9	0	1.620836	3.431398	6.176738
74	9	0	3.794551	5.075137	6.315979
75	9	0	5.709414	4.967131	4.372251
76	9	0	5.461443	3.266312	2.312712
77	9	0	7.990724	0.171982	–0.920190
78	9	0	10.414088	–0.702032	–1.668728
79	9	0	10.743811	–3.253128	–2.585731
80	9	0	8.598832	–4.937379	–2.717753
81	9	0	6.168770	–4.106573	–1.921259
82	9	0	1.355513	0.969415	–2.781333
83	9	0	–0.372749	2.387892	–4.282366
84	9	0	–2.696510	1.254723	–5.141024
85	9	0	–3.271473	–1.335598	–4.509601
86	9	0	–1.544008	–2.788735	–3.045934
87	9	0	–1.008900	–3.808066	3.697281
88	9	0	–1.225126	–6.028993	5.218199
89	9	0	–2.744561	–8.130733	4.365646
90	9	0	–4.037840	–7.994085	1.966411
91	9	0	–3.816260	–5.789066	0.428136
92	9	0	–6.485027	2.207961	1.285448
93	9	0	–9.122923	2.678397	0.965132
94	9	0	–10.556029	1.257961	–0.870573
95	9	0	–9.322458	–0.638716	–2.395684
96	9	0	–6.681716	–1.107785	–2.102070
97	1	0	–5.454958	2.899599	–1.398032
98	1	0	3.561112	0.171441	–0.298225
99	1	0	3.027336	–2.006918	–0.402812
100	1	0	1.561962	3.642710	0.968668
101	1	0	1.315822	–0.676389	1.123900
102	1	0	5.882433	0.650868	3.169673
103	1	0	7.200112	–0.944768	1.504090
104	1	0	5.183407	–1.438680	–3.968786
105	1	0	2.554689	–1.473541	–4.548154
106	1	0	1.850991	–4.211568	–0.823469
107	1	0	0.085721	–5.201983	0.922311
108	1	0	–5.069355	–3.851598	1.861685
109	1	0	–6.599610	–1.862488	0.950724
110	1	0	–3.222762	4.372146	–1.459546
111	7	0	–2.787485	1.311107	–0.225024
112	7	0	0.023744	0.769895	0.295229
113	7	0	4.211366	–0.084569	0.430219
114	7	0	3.248844	–1.902632	–1.380917
115	7	0	–0.706134	–2.177607	–0.188534
116	7	0	–3.368972	–1.471909	0.276675
117	46	0	–1.686767	–0.382467	–0.005512

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	8.6801	9.9565	12.0028
Red. masses --	15.4250	15.5535	15.4293
Frc consts --	0.0007	0.0009	0.0013
IR Inten --	0.0062	0.0081	0.0281