Electronic Supplementary Information

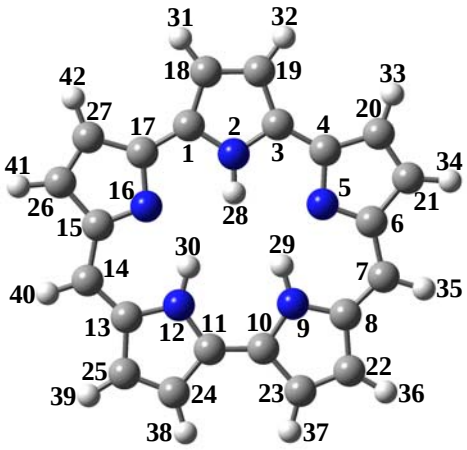
Prediction of the Main Macrocyclic Conjugation Pathway of Porphyrinoids from the Ring Current Distribution

Jun-ichi Aihara and Masakazu Makino

B3LYL/6-31G**-optimized geometries of orangarin (**7**), sapphyrin (**8**), and amethyrin (**9**) are presented numerically in Table S1 and graphically in Figure S1. These geometries were used to evaluate ring and circuit currents induced in the π-systems.

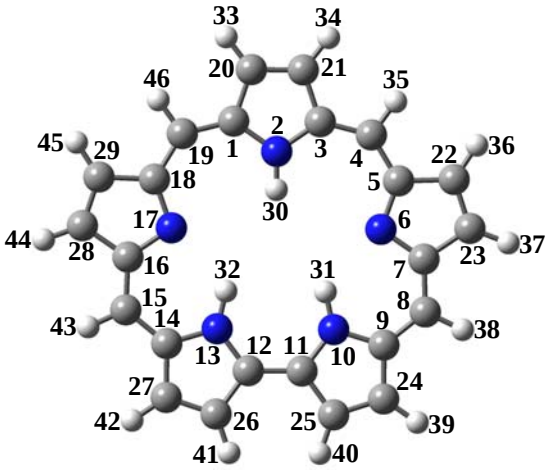
Table S1 B3LYL/6-31G**-optimized geometries of orangarin (**7**), sapphyrin (**8**), and amethyrin (**9**).

A. Orangarin (**7**)



Position Number	Atomic Number	Cartesian Coordinates / Å X	Y	Z
1	6	–1.142780	2.859596	–0.016244
2	7	–0.000001	2.111309	–0.053510
3	6	1.142777	2.859597	–0.016236
4	6	2.351597	2.177004	–0.010895
5	7	2.267391	0.786808	–0.026769
6	6	3.518117	0.317059	–0.007994
7	6	3.806333	–1.093410	–0.003533
8	6	2.813025	–2.054421	–0.000864
9	7	1.466336	–1.761294	–0.003407
10	6	0.689396	–2.910440	0.005439
11	6	–0.689393	–2.910441	0.005439
12	7	–1.466335	–1.761295	–0.003410
13	6	–2.813022	–2.054424	–0.000859
14	6	–3.806332	–1.093412	–0.003526
15	6	–3.518117	0.317054	–0.007998
16	7	–2.267390	0.786805	–0.026781
17	6	–2.351598	2.177000	–0.010907
18	6	–0.684918	4.239294	0.030448
19	6	0.684912	4.239295	0.030454
20	6	3.736142	2.584654	0.015605
21	6	4.471078	1.430926	0.015621
22	6	2.893127	–3.509975	0.007968
23	6	1.626865	–4.014641	0.011835
24	6	–1.626860	–4.014642	0.011842
25	6	–2.893123	–3.509977	0.007982
26	6	–4.471079	1.430921	0.015631
27	6	–3.736145	2.584650	0.015584
28	1	0.000000	1.108452	–0.094584
29	1	1.202032	–0.776616	–0.000817
30	1	–1.202032	–0.776617	–0.000828
31	1	–1.331594	5.104799	0.066697
32	1	1.331586	5.104801	0.066708
33	1	4.105509	3.601642	0.030204
34	1	5.549568	1.339025	0.032770
35	1	4.840137	–1.417844	0.003856
36	1	3.818527	–4.069247	0.010604
37	1	1.342767	–5.057945	0.018142
38	1	–1.342762	–5.057946	0.018152
39	1	–3.818522	–4.069249	0.010627
40	1	–4.840136	–1.417846	0.003877
41	1	–5.549568	1.339019	0.032796
42	1	–4.105513	3.601638	0.030174

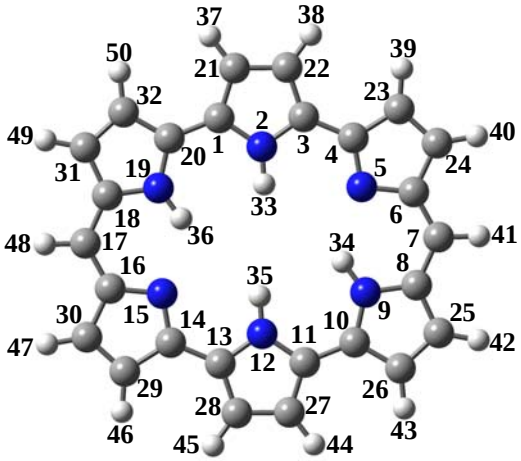
B. Sapphyrin (**8**)



Position Number	Atomic Number	Cartesian Coordinates / Å X	Y	Z
1	6	–1.137116	3.412159	–0.000298
2	7	0.000001	2.622175	0.000003
3	6	1.137119	3.412158	0.000296
4	6	2.483752	3.074422	0.000493
5	6	3.206514	1.868592	0.000102
6	7	2.752403	0.587979	–0.000111
7	6	3.888959	–0.188253	–0.000316
8	6	3.935398	–1.579775	–0.000315
9	6	2.851760	–2.459650	–0.000059
10	7	1.530506	–2.061276	–0.000330
11	6	0.705648	–3.159309	0.000073
12	6	–0.705651	–3.159308	–0.000068
13	7	–1.530508	–2.061275	0.000361
14	6	–2.851762	–2.459648	0.000057
15	6	–3.935400	–1.579772	0.000302
16	6	–3.888959	–0.188250	0.000313
17	7	–2.752403	0.587981	0.000128
18	6	–3.206513	1.868594	–0.000097
19	6	–2.483750	3.074424	–0.000496
20	6	–0.681769	4.773576	–0.000234
21	6	0.681773	4.773576	0.000221
22	6	4.667029	1.915691	–0.000014
23	6	5.091370	0.629772	–0.000295
24	6	2.856044	–3.879436	0.000538
25	6	1.544698	–4.307395	0.000619

26	6	–1.544701	–4.307394	–0.000630
27	6	–2.856047	–3.879434	–0.000549
28	6	–5.091369	0.629776	0.000287
29	6	–4.667027	1.915695	0.000020
30	1	0.000001	1.613850	0.000009
31	1	1.307360	–1.068488	–0.000365
32	1	–1.307361	–1.068487	0.000420
33	1	–1.346332	5.626452	–0.000494
34	1	1.346336	5.626451	0.000473
35	1	3.120529	3.954834	0.000871
36	1	5.259779	2.821566	0.000125
37	1	6.105496	0.251367	–0.000480
38	1	4.918728	–2.039632	–0.000411
39	1	3.746916	–4.491686	0.000878
40	1	1.192600	–5.328323	0.001116
41	1	–1.192604	–5.328323	–0.001137
42	1	–3.746919	–4.491683	–0.000900
43	1	–4.918729	–2.039628	0.000379
44	1	–6.105495	0.251372	0.000463
45	1	–5.259776	2.821570	–0.000117
46	1	–3.120526	3.954837	–0.000881

C. Amethyrin (**9**)



Position Number	Atomic Number	Cartesian Coordinates / Å X	Y	Z
1	6	–1.067461	3.297210	0.000164
2	7	0.055929	2.501688	–0.000080
3	6	1.195219	3.272858	0.000140
4	6	2.509778	2.681214	–0.000035
5	7	2.704894	1.362774	–0.000090
6	6	4.093880	1.193842	–0.000194
7	6	4.728775	–0.030307	–0.000190
8	6	4.111658	–1.301480	–0.000146
9	7	2.737335	–1.462321	–0.000219
10	6	2.414613	–2.789207	0.000053
11	6	1.067459	–3.297157	0.000156
12	7	–0.055958	–2.501693	0.000045
13	6	–1.195211	–3.272897	0.000160
14	6	–2.509796	–2.681272	0.000031
15	7	–2.704877	–1.362828	–0.000218
16	6	–4.093855	–1.193862	–0.000216
17	6	–4.728743	0.030299	–0.000177
18	6	–4.111639	1.301482	–0.000154
19	7	–2.737324	1.462382	–0.000276
20	6	–2.414643	2.789281	0.000038
21	6	–0.622853	4.622099	0.000530
22	6	0.783725	4.606199	0.000516
23	6	3.758099	3.421917	–0.000139
24	6	4.748163	2.484685	–0.000227
25	6	4.672056	–2.591139	–0.000146
26	6	3.622717	–3.512940	0.000105
27	6	0.622904	–4.622070	0.000509
28	6	–0.783672	–4.606224	0.000382
29	6	–3.758139	–3.421949	0.000030
30	6	–4.748183	–2.484687	–0.000287
31	6	–4.672082	2.591122	–0.000136
32	6	–3.622770	3.512964	0.000130
33	1	0.095092	1.495518	–0.000409
34	1	2.148281	–0.630787	–0.000380
35	1	–0.095145	–1.495522	–0.000159
36	1	–2.148200	0.630930	–0.000478
37	1	–1.260972	5.493720	0.000788
38	1	1.439239	5.464850	0.000759
39	1	3.858934	4.498645	–0.000136
40	1	5.818521	2.646118	–0.000310
41	1	5.815187	–0.029355	–0.000210
42	1	5.731031	–2.809023	–0.000187
43	1	3.701020	–4.590142	0.000255
44	1	1.261051	–5.493669	0.000744
45	1	–1.439147	–5.464905	0.000517

46	1	–3.859008	–4.498672	0.000137
47	1	–5.818545	–2.646099	–0.000442
48	1	–5.815153	0.029342	–0.000162
49	1	–5.731065	2.808968	–0.000155
50	1	–3.701124	4.590163	0.000311

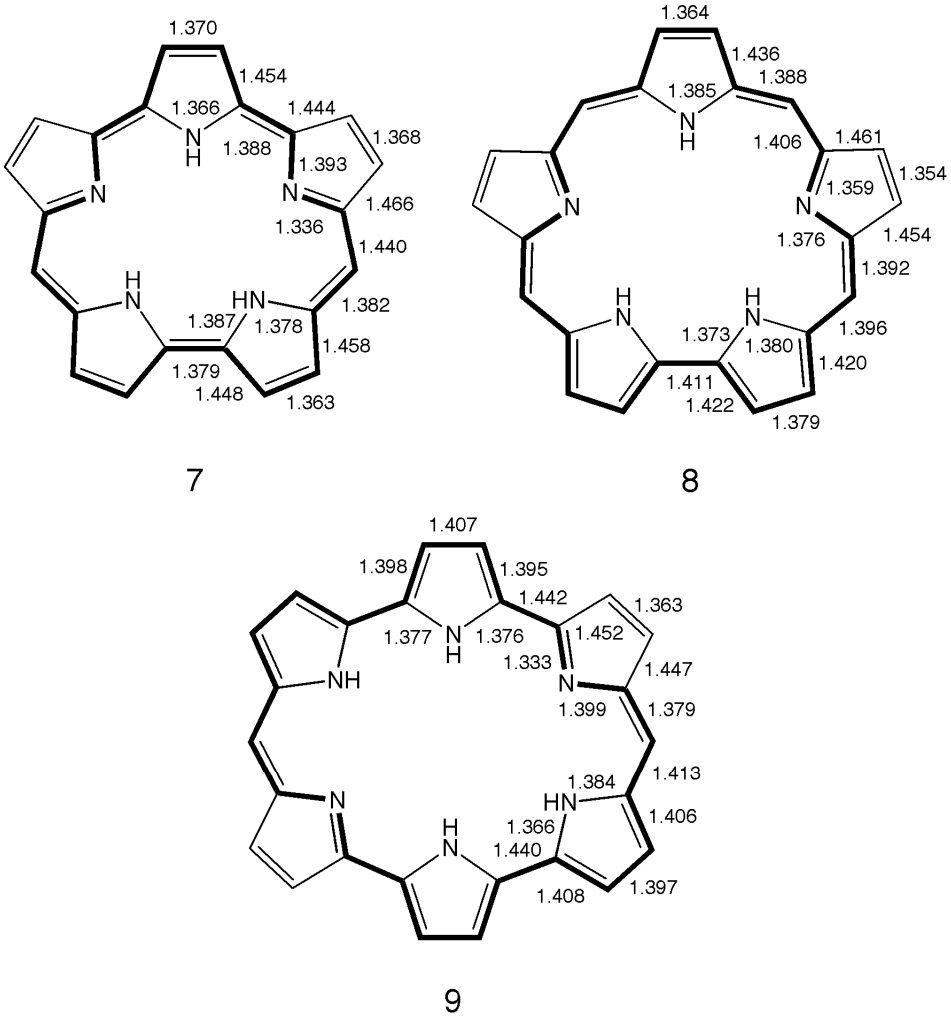


Fig. S1 Calculated bond lengths in units of Å.