Supporting Information

Theoretical Study on the Geometry, Aromaticity and Electronic Properties of Porphyrin Analogues

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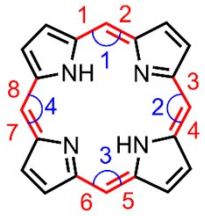
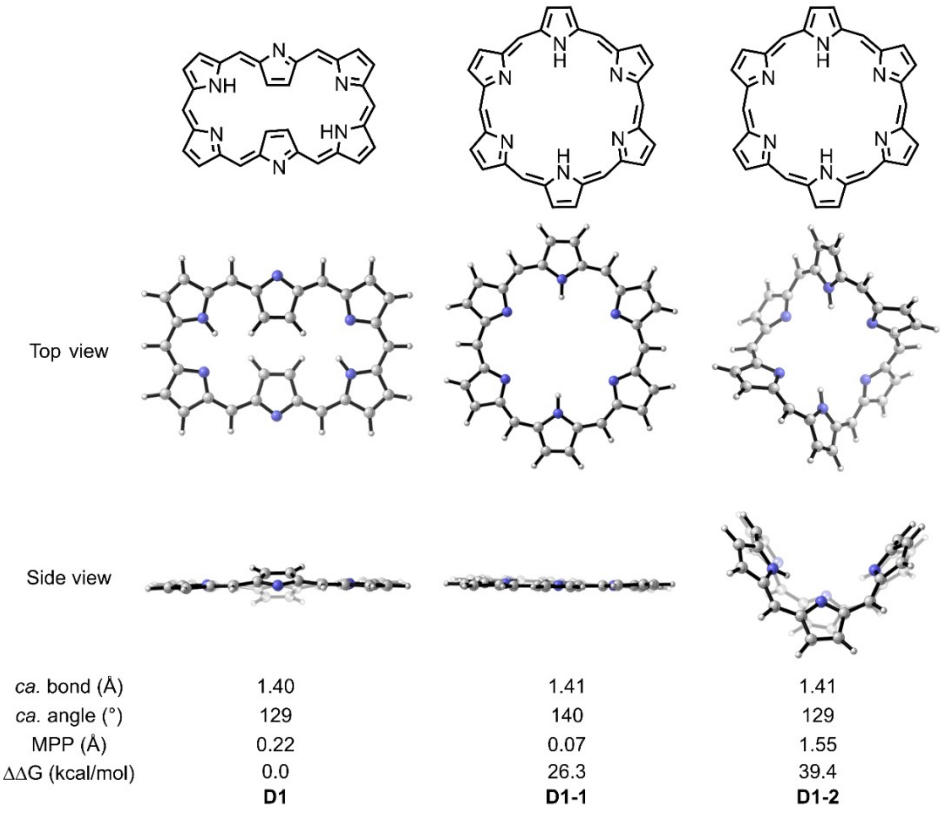


ca. bond = average(1 + 2 + 3 + 4 + 5 + 6 + 7 + 8)

ca. angle = average(1 + 2 + 3 + 4)

Figure S1. Method for calculating average bond lengths and bond angles of porphyrin analogues.



ca. bond (Å)	1.40	1.41	1.41
ca. angle (°)	129	140	129
MPP (Å)	0.22	0.07	1.55
ΔΔG (kcal/mol)	0.0	26.3	39.4
	D1	**D1-1**	**D1-2**

Figure S2. Optimized geometries of **D1**, **D1-1**, and **D1-2**. The structure of **D1-1** was optimized with heavy atoms (*meso* atoms, $N_{pyrrole}$ atoms, and α-$C_{pyrrole}$ atoms) constrained to maintain planarity. **D1-2** represents the most stable conformation among the circular geometries of **D1**.

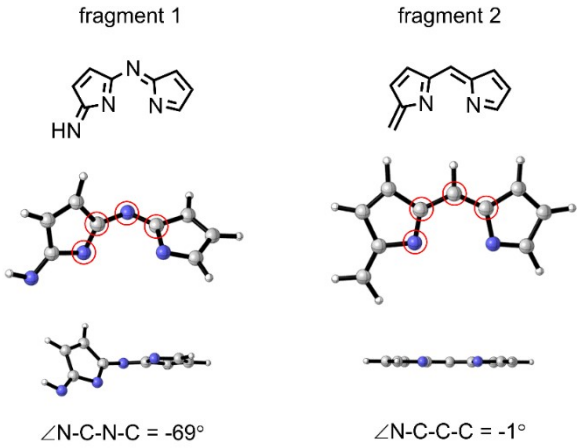


Figure S3. Optimized geometries of fragment 1 and fragment 2.

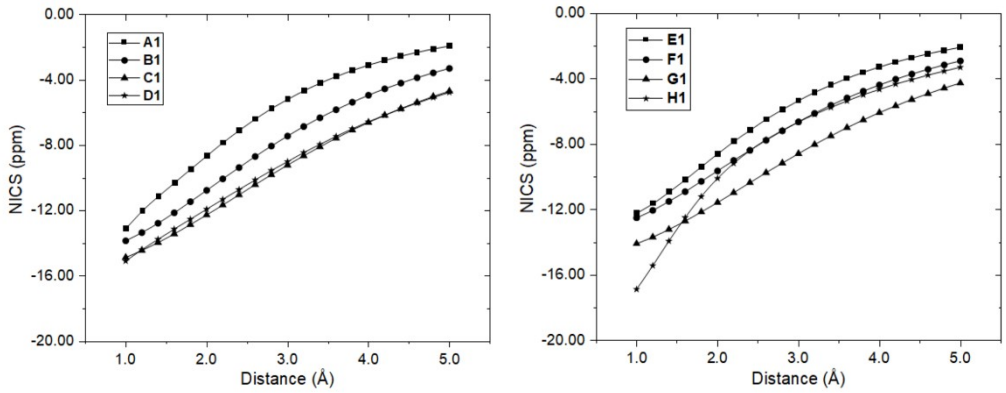


Figure S4. Variation of NICS values for **A1**–**H1** as a function of distance from the ring center.

This scanning procedure was performed by placing the probe (Bq) along the axis perpendicular to the molecular plane above and below the ring center of the molecule, starting at 1.0 Å and extending to 5.0 Å with a step size of 0.2 Å. For example, NICS(1) corresponds to the average of the values calculated at 1 Å above and below the ring center.

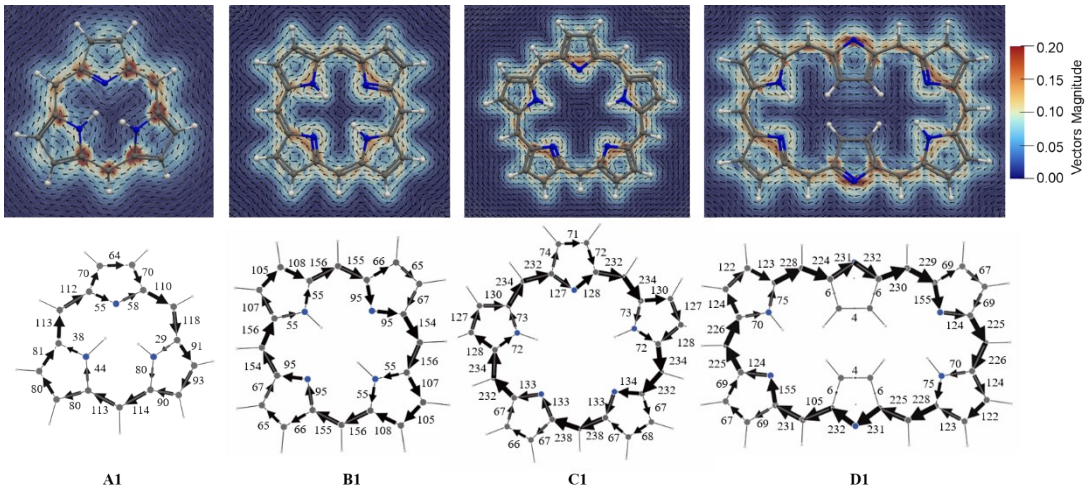


Figure S5. The line integral convolution (LIC) (top panels) and bond current strength (BCS) (bottom panels) for compounds **A1**–**D1**. Values aside each arrow represent the percentage relationship with respect to a reference current strength of 12 nA/T.

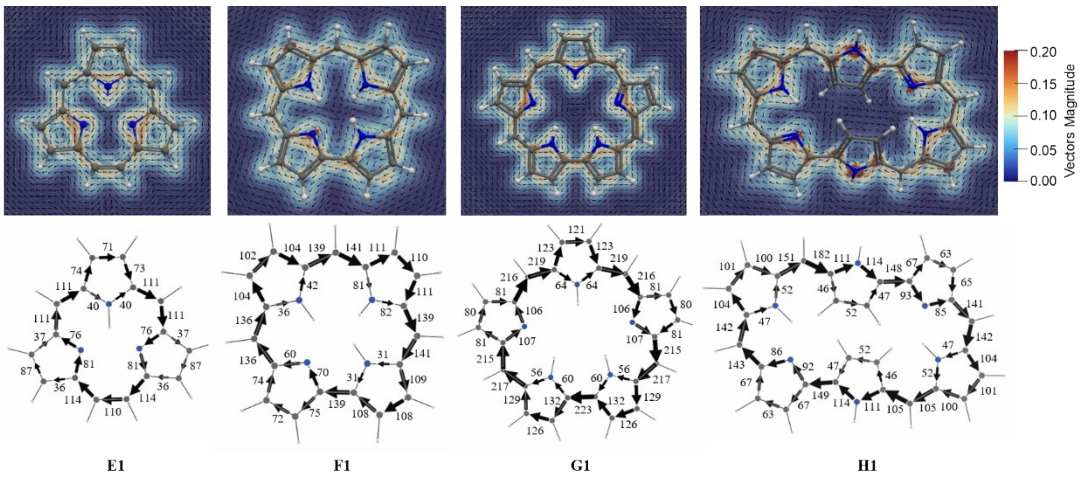


Figure S6. The line integral convolution (LIC) (top panels) and bond current strength (BCS) (bottom panels) for compounds **E1**–**H1**. Values aside each arrow represent the percentage relationship with respect to a reference current strength of 12 nA/T.

The GIMIC calculations were carried out using the GIMIC code. GIMIC employs density matrices obtained from NMR shielding calculations performed with Gaussian 16, which were subsequently transformed into the appropriate format using the Gaussian2gimic.py program written in Python. The line integral convolution (LIC) plots were generated from the corresponding *.pvsm* and *.vti* files using ParaView[1]. In addition, bond current strength (BCS) analyses were performed using the CTOCD-DZ2 method. The BCS is defined as the integral of current density over the plane placed at the midpoint of a bond and perpendicular to it.

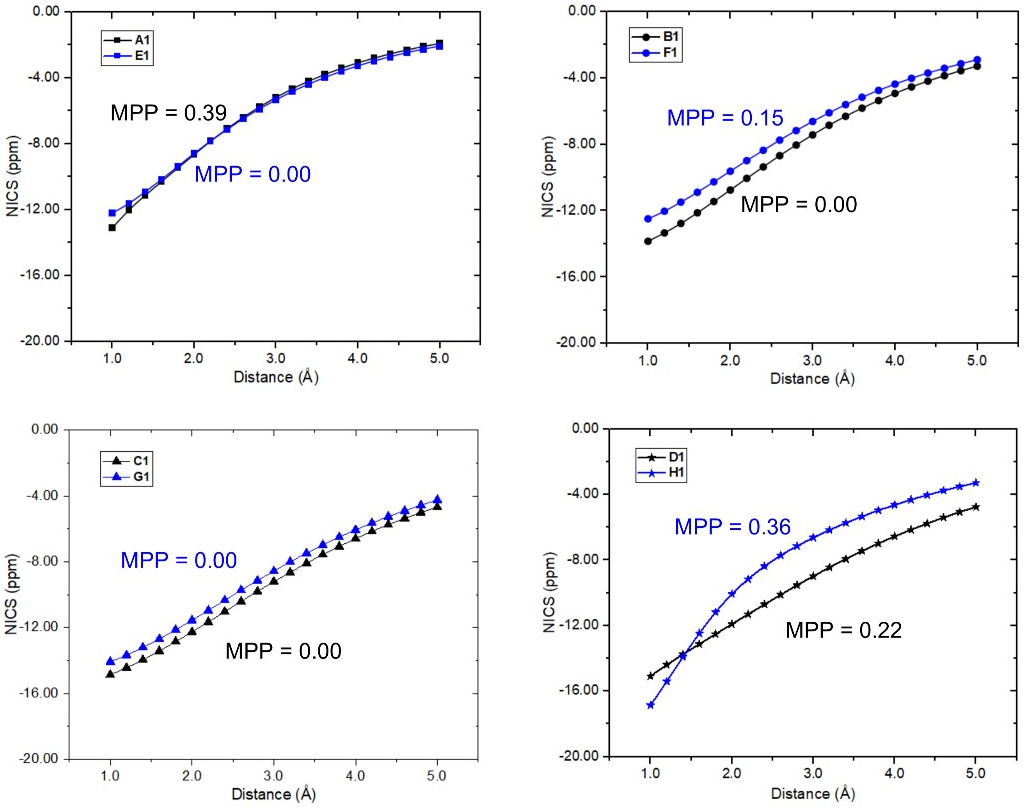


Figure S7. Variation of NICS values within the same series as a function of distance from the ring center.

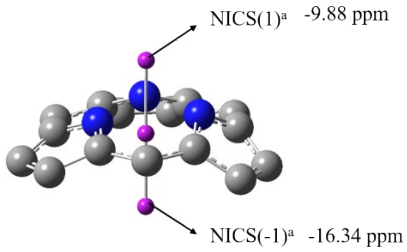
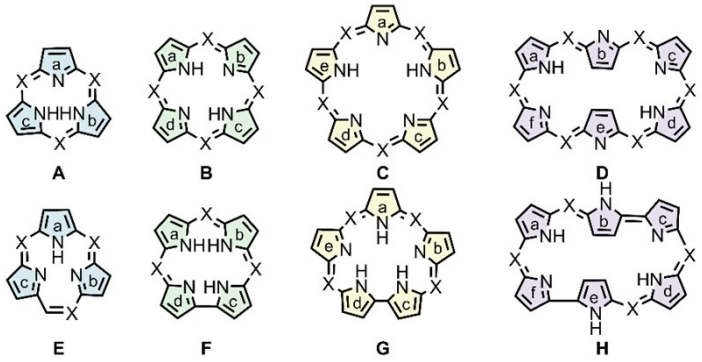


Figure S8. NICS values for **A1**. NICS(1)^a and NICS(−1)^a represent the NICS values evaluated 1 Å from the ring center on the convex and concave faces, respectively.

Table S1. Calculated NICS(1) and NICS(2) values (ppm) for porphyrin analogues.



Molecule	$NICS(1)_a$/ $NICS(2)_a$	$NICS(1)_b$/ $NICS(2)_b$	$NICS(1)_c$/ $NICS(2)_c$	$NICS(1)_d$/ $NICS(2)_d$	$NICS(1)_e$/ $NICS(2)_e$	$NICS(1)_f$/ $NICS(2)_f$	NICS(1)/ NICS(2)
A1	-9.60/-6.49	-13.87/-7.84	-11.77/-6.87	—	—	—	-13.11/-8.66
B1	-11.99/-6.94	-6.00/-5.43	-12.00/-6.94	-6.00/-5.43	—	—	-13.84/-10.75
C1	-4.64/-5.46	-13.33/-7.70	-3.94/-5.27	-3.94/-5.27	-13.34/-7.70	—	-14.86/-12.26
D1	-12.94/-7.47	-21.07/-11.17	-4.46/-5.26	-12.94/-7.48	-21.07/-11.17	-4.46/-5.26	-15.08/-11.91
E1	-8.97/-5.51	-3.92/-4.23	-3.92/-4.23	—	—	—	-12.21/-8.59
F1	-12.21/-6.76	-13.36/-7.03	-13.72/-7.37	-7.76/-5.70	—	—	-12.49/-9.62
G1	-12.90/-7.33	-6.72/-5.88	-13.90/-7.68	-13.90/-7.68	-6.72/-5.88	—	-14.07/-11.55
H1	-11.58/-6.59	-11.07/-7.26	-5.69/-5.10	-11.58/-6.59	-11.07/-7.26	-5.69/-5.11	-16.86/-10.08
A2	-5.67/-4.38	-9.70/-5.07	-9.16/-5.24	—	—	—	-13.45/-6.63
B2	-9.46/-5.86	-3.29/-4.27	-9.46/-5.86	-3.29/-4.27	—	—	-13.80/-10.33
C2	-2.82/-3.64	-7.02/-4.47	0.33/-2.58	-0.15/-2.69	-9.12/-5.17	—	-10.29/-8.42
D2	-9.32/-5.73	-16.56/-9.27	-1.28/-3.61	-9.31/-5.73	-16.56/-9.27	-1.28/-3.61	-13.97/-10.20
E2	-6.85/-4.47	3.40/-3.72	-3.71/-3.73	—	—	—	-10.58/-6.71
F2	-10.46/-6.07	-12.55/-6.65	-13.01/-7.18	-6.26/-5.21	—	—	-13.03/-9.66
G2	-11.08/-6.58	-3.93/-4.77	-12.43/-7.12	-12.43/-7.12	-3.93/-4.77	—	-14.46/-11.61
H2	-9.39/-5.64	-11.23/-7.41	-4.26/-4.56	-9.38/-5.64	-11.23/-7.41	-4.26/-4.56	-16.68/-9.92

Table S2. Calculated NICS(0) values (ppm) for porphyrin analogues.

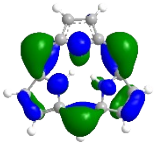
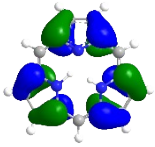
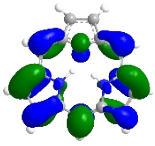
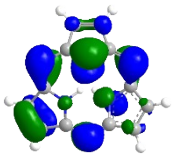
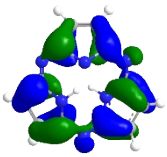
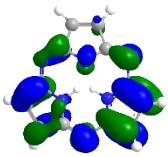
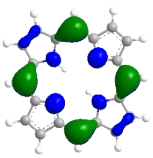
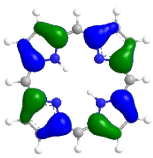
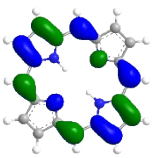
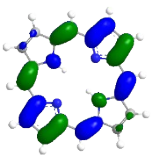
Molecule	$NICS(0)_a$	$NICS(0)_b$	$NICS(0)_c$	$NICS(0)_d$	$NICS(0)_e$	$NICS(0)_f$	NICS(0)
A1	-7.42	-15.31	-11.30	—	—	—	-18.18
B1	-12.48	-2.61	-12.48	-2.61	—	—	-14.92
C1	-0.38	-13.86	0.63	0.63	-13.86	—	-15.87
D1	-13.28	-19.76	-0.31	-13.29	-19.76	-0.31	-17.75
E1	-8.32	-0.27	-0.27	—	—	—	-13.40
F1	-13.31	-14.88	-15.82	-5.67	—	—	-13.27
G1	-13.73	-3.59	-15.42	-15.42	-3.59	—	-15.00
H1	-12.27	-11.88	-3.21	-12.27	-11.88	-3.21	-19.89
A2	-4.04	-12.04	-9.93	—	—	—	-12.78
B2	-8.86	0.94	-8.86	0.95	—	—	-15.19
C2	0.71	-6.71	4.72	3.60	-9.55	—	-11.00
D2	-8.28	-13.90	3.82	-8.28	-13.90	3.82	-16.60
E2	-4.87	1.02	-0.76	—	—	—	-12.12
F2	-10.83	-13.74	-14.84	-3.43	—	—	-14.18
G2	-10.94	0.12	-13.23	-13.23	0.12	—	-15.56
H2	-9.38	-11.74	-1.18	-9.38	-11.74	-1.18	-18.74

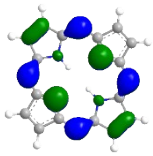
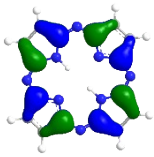
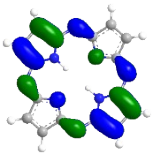
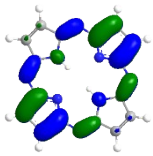
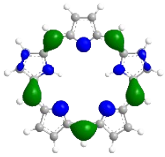
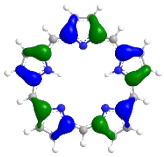
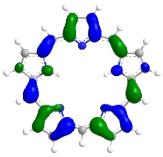
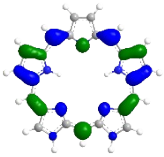
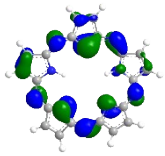
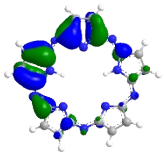
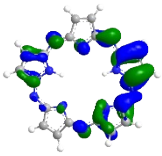
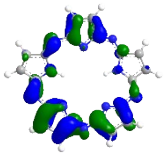
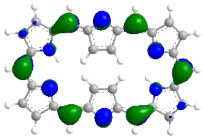
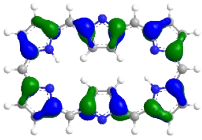
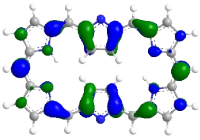
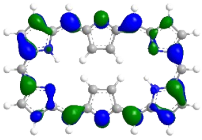
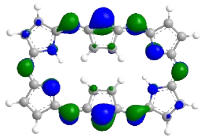
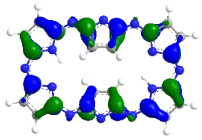
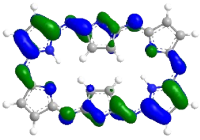
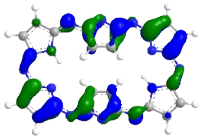
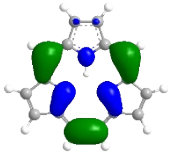
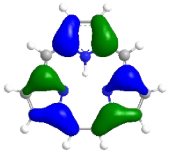
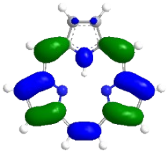
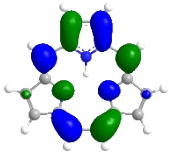
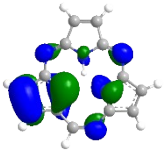
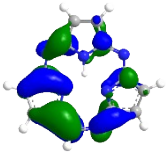
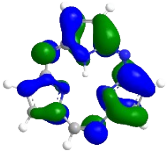
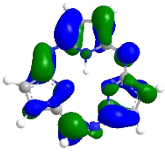
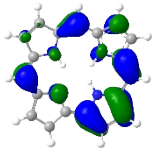
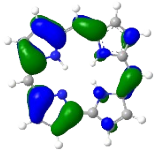
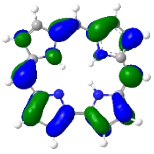
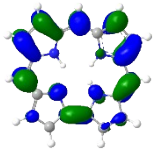
Table S3. Frontier molecular orbital energies and HOMO–LUMO gaps (in eV) for **A1**–**H1** and **A2**–**H2**.

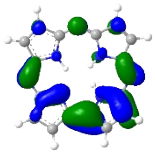
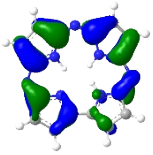
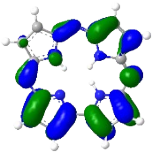
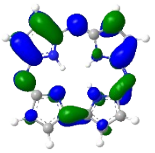
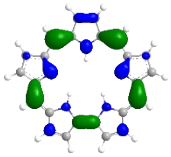
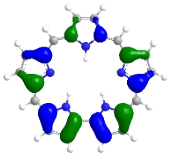
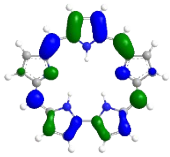
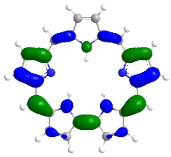
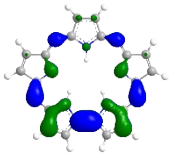
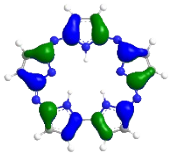
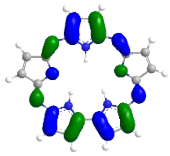
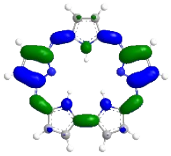
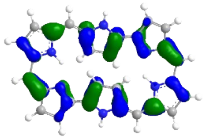
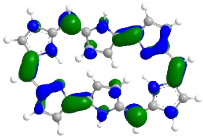
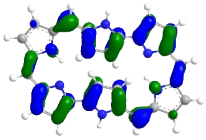
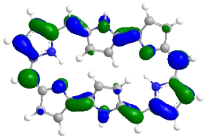
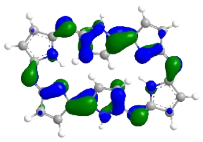
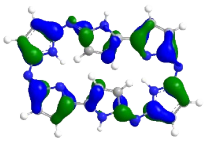
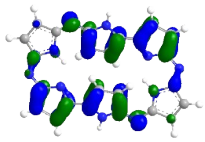
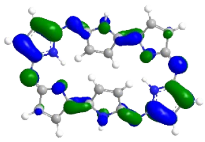
	HOMO			-IP	LUMO			-EA	HOMO-LUMO gap			(-IP)-(-EA)
	HF[a]	DFT1[b]	DFT2[c]	DFT3[d]	HF[a]	DFT1[b]	DFT2[c]	DFT3[d]	HF[a]	DFT1[b]	DFT2[c]	DFT3[d]
A1	-6.55	-6.69	-7.19	-7.14	0.87	-1.19	-0.60	-0.65	7.42	5.50	6.59	6.49
B1	-6.18	-6.52	-6.98	-6.91	0.07	-1.80	-1.27	-1.32	6.25	4.71	5.71	5.59
C1	-5.93	-6.33	-6.75	-6.57	-0.61	-2.38	-1.90	-1.92	5.32	3.95	4.85	4.64
D1	-5.86	-6.20	-6.59	-6.43	-1.27	-2.93	-2.47	-2.47	4.95	3.27	4.12	3.96
E1	-6.86	-6.99	-7.49	-7.42	0.17	-1.88	-1.31	-1.34	7.03	5.11	6.19	6.08
F1	-6.12	-6.10	-6.57	-6.47	0.35	-1.62	-1.08	-1.11	6.47	4.48	5.49	5.36
G1	-5.90	-6.03	-6.46	-6.29	-0.12	-2.03	-1.54	-1.55	5.78	3.99	4.92	4.73
H1	-5.29	-5.41	-5.81	-5.75	-0.54	-2.22	-1.74	-1.71	4.75	3.19	4.07	4.04
A2	-6.48	-6.75	-7.23	-7.29	-0.20	-2.27	-1.66	-1.67	6.28	4.48	5.57	5.62
B2	-6.19	-6.87	-7.31	-7.42	-0.74	-2.68	-2.13	-2.13	5.45	4.19	5.18	5.29
C2	-5.90	-6.42	-6.83	-6.89	-0.85	-2.99	-2.46	-2.55	5.04	3.43	4.37	4.34
D2	-5.52	-6.52	-6.87	-7.04	-1.81	-3.64	-3.15	-3.15	3.72	2.88	3.72	3.89
E2	-7.31	-7.32	-7.81	-7.79	-0.30	-2.56	-1.97	-2.02	7.01	4.75	5.84	5.77
F2	-6.23	-6.59	-7.05	-7.06	-0.36	-2.30	-1.75	-1.73	5.87	4.29	5.30	5.33
G2	-5.68	-6.40	-6.81	-6.87	-0.97	-2.77	-2.28	-2.23	4.72	3.63	4.53	4.64
H2	-5.29	-5.97	-6.38	-6.39	-1.00	-2.80	-2.29	-2.28	4.29	3.18	4.09	4.11

[a]The energies were calculated at the HF/def2-TZVP level, using geometries optimized at the B3LYP-D3/def2-SVP level.
[b]The energies were calculated at the CAM-B3LYP/def2-TZVPD level, using geometries optimized at the B3LYP-D3/def2-SVP level.
[c]The energies were calculated at the *w*B97XD/def2-TZVPD level, using geometries optimized at the B3LYP-D3/def2-SVP level.
[d]The energies were calculated at the B3LYP-D3/def2-TZVP level, using geometries optimized at the B3LYP-D3/def2-SVP level.

Table S4. Frontier molecular orbitals of porphyrin analogues.

Molecule	HOMO-1 (eV)	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)
A1	 -7.19	 -6.55	 0.87	 1.00
A2	 -9.31	 -6.48	 -0.20	 0.23
B1	 -6.75	 -6.18	 0.07	 0.14

B2	 -9.15	 -6.19	 -0.74	 -0.48
C1	 -6.47	 -5.93	 -0.61	 -0.55
C2	 -9.01	 -5.90	 -0.85	 -0.50
D1	 -6.28	 -5.86	 -1.27	 -0.97
D2	 -8.81	 -5.52	 -1.81	 -1.57
E1	 -7.72	 -6.86	 0.17	 0.55
E2	 -9.17	 -7.31	 -0.30	 0.13
F1	 -6.35	 -6.12	 0.35	 0.93

F2	 -7.43	 -6.23	 -0.36	 0.19
G1	 -6.24	 -5.90	 -0.12	 0.24
G2	 -7.70	 -5.68	 -0.97	 -0.39
H1	 -5.50	 -5.29	 -0.54	 0.20
H2	 -6.86	 -5.29	 -1.00	 -0.45

Cartesian coordinates of the structures

A1

C	2.670845	-0.406676	0.101199
C	1.843779	-1.552909	0.204803
N	0.591155	-1.487092	0.770379
N	0.875535	1.119001	0.612432
C	2.151952	0.909498	0.212749
N	-1.419704	0.264676	0.529651
C	-1.895756	1.466358	0.096950
C	-0.970249	2.536830	-0.022282
C	0.428204	2.312173	0.141776
C	-0.296688	-2.375681	0.206477
C	-1.682894	-2.098732	0.091601
C	-2.206846	-0.786935	0.175117
C	1.572935	3.019037	-0.430962

C	2.639860	2.152188	-0.386432
C	1.827420	-2.769321	-0.563791
C	0.531762	-3.268213	-0.561867
C	-3.224753	1.188641	-0.404171
C	-3.416856	-0.183523	-0.349854
H	3.662881	-0.537252	-0.336421
H	0.370569	-0.796543	1.470889
H	-0.367144	0.312021	0.658055
H	-1.311195	3.488126	-0.434536
H	-2.324097	-2.879301	-0.322002
H	1.553912	4.012054	-0.880000
H	3.638586	2.319078	-0.789800
H	2.662495	-3.141209	-1.155351
H	0.158616	-4.102590	-1.153620
H	-3.920072	1.923399	-0.807981
H	-4.289746	-0.730284	-0.704341

A2

C	-1.055327	-1.985132	0.203005
N	0.062903	-1.285682	0.606686
N	-1.224160	0.520161	-0.660413
C	-2.275451	-0.099573	-0.080250
N	1.203763	0.671518	-0.680962
C	1.053596	1.995369	-0.344718
C	-1.251716	1.835990	-0.342742
C	1.237597	-1.880134	0.210887
C	2.291677	0.109400	-0.063721
C	-2.557944	2.126244	0.278647
C	-3.204107	0.924725	0.421623
C	-0.539300	-3.273354	-0.215190
C	0.844348	-3.208384	-0.214825
C	2.310857	2.371930	0.277361
C	3.073505	1.225725	0.430769
H	0.006297	-0.338412	0.944806
H	0.308557	0.209010	-0.969953
H	-2.884342	3.107283	0.621449
H	-4.152457	0.727325	0.918441
H	-1.161008	-4.089568	-0.577089
H	1.540517	-3.962903	-0.575260
H	2.542117	3.371511	0.641108
H	4.026271	1.129435	0.947242
N	2.399191	-1.217559	0.134709
N	-2.270438	-1.436946	0.123927
N	-0.141597	2.604147	-0.283349

B1

C	-0.681594	4.259984	0.000047
C	0.677889	4.260527	-0.000170
C	1.083726	2.854700	-0.000042
N	-0.000912	2.033965	-0.000121
C	-1.086293	2.853824	-0.000007
C	-4.266098	-0.689487	-0.000048
C	-4.266722	0.685691	-0.000010
C	-2.898744	1.127026	0.000065
N	-2.120039	-0.000925	0.000134
C	-2.897721	-1.129582	0.000033
C	-2.426574	2.440655	0.000088
C	0.681676	-4.259935	0.000010
C	-0.677808	-4.260579	-0.000096
C	-1.083733	-2.854773	-0.000038
N	0.000932	-2.033969	-0.000250
C	1.086288	-2.853756	-0.000031
C	-2.424377	-2.442787	0.000067
C	4.266115	0.689503	0.000042
C	4.266738	-0.685704	0.000089
C	2.898818	-1.126954	0.000008
N	2.119840	0.000926	0.000211
C	2.897800	1.129515	0.000016
C	2.424306	2.442703	-0.000067
C	2.426503	-2.440570	-0.000033
H	-1.361108	5.111884	0.000156
H	1.356730	5.112961	-0.000303
H	-5.125425	-1.357731	-0.000127
H	-5.126657	1.353152	-0.000046
H	-1.100985	-0.000433	0.000348
H	-3.188280	3.223301	0.000133
H	1.361261	-5.111776	0.000078
H	-1.356579	-5.113071	-0.000038
H	-3.185387	-3.226110	0.000145
H	5.125364	1.357853	0.000053
H	5.126593	-1.353273	0.000135
H	1.100812	0.000440	0.000405
H	3.185425	3.225940	-0.000187
H	3.188324	-3.223123	-0.000101

B2

C	0.679050	-4.155513	-0.000036
C	-0.675572	-4.156075	-0.000032

C	-1.083581	-2.741318	-0.000001
N	0.000813	-1.920279	-0.000001
C	1.085883	-2.740417	-0.000019
C	4.157328	0.686177	-0.000001
C	4.157906	-0.682705	-0.000010
C	2.778282	-1.129423	-0.000017
N	1.999634	0.000827	-0.000023
C	2.777328	1.131733	-0.000010
C	-0.679051	4.155514	-0.000005
C	0.675571	4.156075	-0.000012
C	1.083578	2.741317	0.000004
N	-0.000812	1.920279	0.000018
C	-1.085886	2.740419	0.000017
C	-4.157327	-0.686178	0.000039
C	-4.157905	0.682706	0.000039
C	-2.778282	1.129422	0.000033
N	-1.999634	-0.000827	-0.000002
C	-2.777328	-1.131731	0.000023
H	1.377120	-4.990475	-0.000053
H	-1.372948	-4.991616	-0.000042
H	5.003148	1.370069	0.000007
H	5.004303	-1.365883	-0.000010
H	0.982702	0.000394	-0.000027
H	-1.377120	4.990476	-0.000012
H	1.372948	4.991615	-0.000028
H	-5.003148	-1.370068	0.000046
H	-5.004303	1.365882	0.000046
H	-0.982702	-0.000394	-0.000030
N	2.371884	-2.385169	-0.000023
N	-2.369874	-2.387138	0.000013
N	-2.371884	2.385169	0.000030
N	2.369876	2.387138	-0.000006

C1

C	1.074412	-3.623311	-0.000250
C	2.443194	-3.326745	0.002612
C	3.212425	-2.163204	0.003750
C	4.648889	-2.215108	0.006059
C	5.121779	-0.931485	0.005472
C	3.992360	-0.048060	0.002895
C	4.110818	1.339021	0.000875
C	3.148445	2.354306	-0.001760
C	3.560272	3.761415	-0.004740
C	2.409732	4.471323	-0.006388

C	1.314827	3.482976	-0.004135
C	0.002613	3.981698	-0.003761
C	-1.310212	3.484610	-0.000773
C	-2.403890	4.474307	0.001085
C	-3.555301	3.765825	0.004399
C	-3.145206	2.358191	0.003916
C	-4.108901	1.344151	0.005306
C	-3.992333	-0.043088	0.003194
C	-5.122999	-0.924940	0.002609
C	-4.651922	-2.209222	-0.001026
C	-3.215387	-2.159326	-0.002231
C	-2.447724	-3.323897	-0.004919
C	-1.079306	-3.622116	-0.004303
C	-0.679003	-5.035772	-0.005611
C	0.672511	-5.036539	-0.002757
N	-0.001977	-2.793678	-0.001325
N	-2.858677	-0.828644	0.000380
N	-1.795784	2.216943	0.000988
N	1.798821	2.214731	-0.001633
N	2.857594	-0.832017	0.002201
H	3.072566	-4.220299	0.003839
H	5.220991	-3.140956	0.007677
H	6.156775	-0.595086	0.006575
H	5.147336	1.685161	0.001206
H	4.588812	4.120900	-0.005387
H	2.278784	5.553165	-0.008643
H	0.003295	5.075798	-0.005582
H	-2.271602	5.555989	0.000110
H	-4.583393	4.126583	0.006651
H	-5.144953	1.691674	0.007523
H	-6.157520	-0.587086	0.004531
H	-5.225322	-3.134268	-0.002507
H	-3.078229	-4.216647	-0.007127
H	-1.362435	-5.884373	-0.008067
H	1.355021	-5.885881	-0.002361
H	-1.909891	-0.457067	-0.000101
H	1.909362	-0.459030	0.000273

C2

C	0.974461	3.385910	-0.159935
C	2.860017	2.045641	-0.755393
C	4.236806	2.006781	-1.233289
C	4.747756	0.781086	-0.954929
C	3.697652	-0.011225	-0.332098

C	2.951608	-2.056077	0.546528
C	3.299971	-3.247343	1.363497
C	2.160789	-3.954547	1.467757
C	1.141196	-3.199541	0.684824
C	-1.094256	-3.288753	-0.184232
C	-1.986129	-4.234507	-0.909302
C	-3.071338	-3.518199	-1.258674
C	-2.843611	-2.162515	-0.708367
C	-3.723139	-0.032583	-0.245790
C	-4.881609	0.767758	0.047728
C	-4.444928	1.955619	0.568481
C	-3.004029	1.954391	0.536807
C	-1.036059	3.314297	0.592515
C	-0.593661	4.706927	0.765406
C	0.650134	4.764276	0.241037
N	-0.041053	2.526306	0.067442
N	-2.606663	0.714727	0.060770
N	-1.617338	-2.053629	-0.113644
N	1.656490	-2.026480	0.201344
N	2.564027	0.773903	-0.280233
H	4.723492	2.877399	-1.667423
H	5.752441	0.395666	-1.112928
H	4.296131	-3.454217	1.750577
H	1.965797	-4.907595	1.956215
H	-1.751554	-5.284245	-1.076053
H	-3.973616	-3.818120	-1.788350
H	-5.896926	0.416959	-0.120715
H	-5.019973	2.814204	0.907384
H	-1.221453	5.492958	1.180451
H	1.330792	5.605632	0.126993
H	-1.647751	0.378417	-0.017830
H	1.652666	0.459484	0.049711
N	-3.807190	-1.266883	-0.724643
N	0.000167	-3.764793	0.401611
N	3.903521	-1.208213	0.155038
N	2.187456	3.153920	-0.682490
N	-2.305106	3.031010	0.825741

D1

C	-5.845231	2.576759	0.107896
C	-4.851218	3.501290	0.160279
C	-3.591025	2.759052	0.052232
N	-3.825447	1.421377	-0.035010
C	-5.177224	1.279859	0.002554

C	-4.902458	-3.446738	-0.129744
C	-5.892809	-2.494472	-0.110501
C	-5.257931	-1.210711	-0.030150
N	-3.902695	-1.431256	0.024652
C	-3.631230	-2.779567	-0.035048
C	-5.855700	0.051114	-0.023505
C	-2.390777	-3.422281	-0.025773
C	-2.349788	3.414166	0.056785
C	1.062277	-2.902784	0.153846
N	-0.023174	-3.682138	-0.066035
C	-1.103869	-2.901514	0.169698
C	-0.694331	-1.562821	0.627533
C	0.664217	-1.566888	0.618343
C	-1.062281	2.902768	-0.154380
N	0.023135	3.682275	0.064818
C	1.103860	2.901489	-0.170495
C	0.694266	1.562499	-0.627381
C	-0.664283	1.566583	-0.618007
C	5.845315	-2.576731	-0.106180
C	4.851305	-3.501259	-0.159131
C	3.591080	-2.758935	-0.051800
N	3.825492	-1.421341	0.035558
C	5.177334	-1.279882	-0.001341
C	2.349763	-3.414038	-0.057366
C	4.902432	3.446800	0.128650
C	5.892777	2.494477	0.110204
C	5.257895	1.210732	0.030368
N	3.902670	1.431277	-0.024813
C	3.631236	2.779598	0.034076
C	2.390750	3.422356	0.024444
C	5.855685	-0.051104	0.024654
H	-6.922809	2.732093	0.149677
H	-4.934491	4.584111	0.247188
H	-5.015764	-4.527730	-0.187761
H	-6.969386	-2.647624	-0.156230
H	-3.262961	-0.632981	0.024307
H	-6.947212	0.073852	-0.032667
H	-2.419701	-4.496100	-0.226748
H	-2.374071	4.486212	0.272224
H	-1.341475	-0.754712	0.962808
H	1.346199	-0.780268	0.925883
H	1.341288	0.754080	-0.962137
H	-1.346296	0.779883	-0.925247
H	6.922904	-2.732139	-0.147396

H	4.934602	-4.584089	-0.245853
H	2.374125	-4.485934	-0.273542
H	5.015742	4.527818	0.186134
H	6.969354	2.647613	0.156026
H	3.262900	0.633053	-0.024435
H	2.419755	4.496296	0.224753
H	6.947202	-0.073702	0.034264

D2

C	-5.704711	2.458005	0.057891
C	-4.742196	3.405033	0.103136
C	-3.451375	2.683325	0.063284
N	-3.650418	1.332769	0.010059
C	-4.994799	1.166295	0.014087
C	-4.709255	-3.401733	-0.111105
C	-5.686617	-2.452014	-0.069578
C	-5.039821	-1.155846	-0.012263
N	-3.679248	-1.375862	0.015563
C	-3.417440	-2.733809	-0.054600
C	1.099432	-2.867169	0.110507
N	0.017724	-3.588822	-0.250624
C	-1.057757	-2.875195	0.117943
C	-0.655747	-1.616799	0.823879
C	0.694139	-1.617170	0.824244
C	-1.099424	2.867185	-0.110695
N	-0.017771	3.588866	0.250412
C	1.057770	2.875153	-0.117950
C	0.655790	1.616673	-0.823732
C	-0.694099	1.617071	-0.824206
C	5.704711	-2.457992	-0.057964
C	4.742176	-3.404997	-0.103350
C	3.451374	-2.683260	-0.063510
N	3.650416	-1.332745	-0.010167
C	4.994830	-1.166272	-0.014103
C	4.709221	3.401733	0.111377
C	5.686611	2.452019	0.069855
C	5.039838	1.155869	0.012419
N	3.679268	1.375867	-0.015470
C	3.417441	2.733801	0.054747
H	-6.788387	2.558019	0.063075
H	-4.824695	4.488866	0.155033
H	-4.801492	-4.483980	-0.169068
H	-6.767158	-2.574887	-0.088258
H	-3.048355	-0.567233	0.000355

H	-1.316374	-0.885545	1.286887
H	1.374929	-0.896608	1.269092
H	1.316423	0.885333	-1.286595
H	-1.374862	0.896458	-1.269011
H	6.788385	-2.558032	-0.063091
H	4.824658	-4.488827	-0.155334
H	4.801447	4.483977	0.169410
H	6.767147	2.574914	0.088612
H	3.048386	0.567226	-0.000365
N	-2.312800	3.343994	0.134192
N	2.275840	3.366996	0.110949
N	2.312765	-3.343914	-0.134545
N	-2.275879	-3.367023	-0.110853
N	-5.659136	0.006146	-0.007037
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E1

C	-2.387060	1.557807	0.000013
C	-2.477239	0.150085	0.000013
N	-0.000039	1.483906	0.000443
C	-1.129759	2.222149	0.000129
C	2.477232	0.150198	0.000034
C	2.386983	1.557916	0.000007
C	1.129648	2.222200	0.000124
C	0.693177	3.603142	-0.000158
C	-0.693350	3.603111	-0.000175
C	-3.638971	-0.751559	-0.000208
C	-3.133682	-2.022392	-0.000139
C	-1.661518	-1.891066	0.000028
N	-1.347512	-0.600598	0.000133
N	1.347544	-0.600541	0.000191
C	1.661612	-1.890993	0.000035
C	3.133782	-2.022248	-0.000176
C	3.639008	-0.751390	-0.000200
C	-0.699125	-2.947612	0.000065
C	0.699268	-2.947581	0.000064
H	-3.300110	2.156855	-0.000221
H	-0.000016	0.421846	0.000490
H	3.300004	2.157007	-0.000239
H	1.344305	4.476009	-0.000393
H	-1.344517	4.475949	-0.000427
H	-4.687780	-0.454934	-0.000361
H	-3.694874	-2.957064	-0.000238
H	3.695020	-2.956892	-0.000320

H	4.687803	-0.454713	-0.000364
H	-1.147927	-3.947036	-0.000014
H	1.148114	-3.946986	-0.000023

E2

C	-2.334750	-0.412290	-0.263491
N	-0.327118	1.400303	-0.516541
C	-1.605174	1.770784	-0.284879
C	2.227730	0.743872	0.192129
C	0.569869	2.314307	-0.034104
C	-0.223292	3.504520	0.294679
C	-1.545757	3.170364	0.158867
C	-3.183134	-1.460741	0.361538
C	-2.389166	-2.552483	0.489788
C	-1.061888	-2.172458	-0.068428
N	-1.140326	-0.932429	-0.598858
N	1.346326	-0.263552	0.247884
C	1.993623	-1.416548	0.040223
C	3.441525	-1.151681	-0.070128
C	3.588981	0.203906	0.038562
C	1.307662	-2.651564	-0.097685
H	-0.130424	0.373467	-0.612341
H	0.197049	4.437457	0.665202
H	-2.418144	3.781231	0.383316
H	-4.207766	-1.311581	0.698157
H	-2.610360	-3.513474	0.951043
H	4.223255	-1.895300	-0.224756
H	4.503425	0.791705	-0.021525
H	1.950744	-3.528891	-0.258304
N	-2.622582	0.906693	-0.225434
N	1.841884	2.050050	0.203383
N	0.012510	-2.943143	0.014821

F1

C	-3.399874	-0.562853	-0.006936
C	0.807868	-3.124880	-0.076569
C	3.236240	1.126231	0.045701
C	-1.339012	2.386567	0.104953
C	-2.549171	3.014487	-0.289769
C	-3.547512	2.032171	-0.335642
C	-2.961061	0.782495	0.023935
N	-1.656840	1.076139	0.325849
C	-2.534963	-1.661733	0.008971
C	-2.832215	-3.055139	0.158407

C	-1.650796	-3.768278	0.139336
C	-0.560766	-2.851351	-0.027434
N	-1.137071	-1.587904	-0.088532
C	1.888351	-2.217609	-0.084667
C	3.288989	-2.525897	-0.179483
C	4.001530	-1.340901	-0.139954
C	3.062055	-0.268388	-0.018113
N	1.812026	-0.852981	0.009109
C	2.163429	2.034092	0.130083
C	2.165315	3.483420	0.031456
C	0.845964	3.881452	0.023083
C	0.063033	2.671013	0.135035
N	0.872725	1.595023	0.213872
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H	1.079823	-4.181998	-0.086653
H	4.255528	1.512819	-0.015448
H	-2.656352	4.060655	-0.569534
H	-4.578609	2.169649	-0.656717
H	-0.996859	0.449941	0.764804
H	-3.835314	-3.452906	0.304233
H	-1.531497	-4.843428	0.263247
H	-0.690109	-0.829701	-0.593055
H	3.689471	-3.533837	-0.274774
H	5.082155	-1.219793	-0.194060
H	1.024557	-0.201843	0.147253
H	3.047764	4.118333	-0.046087
H	0.459134	4.896996	-0.050889

F2

C	1.309358	2.367221	-0.184677
C	2.493400	2.950802	0.360470
C	3.463533	1.953056	0.450760
C	2.886388	0.724623	-0.015944
N	1.637976	1.067587	-0.466399
C	2.487446	-1.556689	0.006478
C	2.796991	-2.949047	-0.162675
C	1.621412	-3.670865	-0.157173
C	0.519639	-2.767283	0.027803
N	1.086208	-1.492880	0.105065
C	-1.771118	-2.211195	0.084726
C	-3.174876	-2.519690	0.243919
C	-3.889207	-1.342182	0.207874
C	-2.953728	-0.259961	0.015829
N	-1.703230	-0.844988	-0.054838

C	-2.163170	1.910034	-0.163577
C	-2.214907	3.357940	0.035462
C	-0.916748	3.806588	0.020267
C	-0.088713	2.635516	-0.217961
N	-0.868930	1.539847	-0.358685
H	2.583656	3.976910	0.711663
H	4.458945	2.036605	0.881453
H	0.986592	0.455008	-0.935292
H	3.809387	-3.319170	-0.309771
H	1.493220	-4.742309	-0.295886
H	0.626259	-0.734135	0.596332
H	-3.550088	-3.530602	0.388326
H	-4.963314	-1.204295	0.312165
H	-0.940363	-0.187207	-0.279064
H	-3.123491	3.933404	0.204942
H	-0.563555	4.827033	0.161846
N	3.332019	-0.535602	0.053431
N	-0.764539	-3.080475	0.076618
N	-3.183996	1.048733	-0.033222

G1

C	5.096361	0.628959	-0.000248
C	4.671499	1.918162	-0.000235
C	3.207633	1.869020	-0.000014
N	2.758785	0.590034	0.000048
C	3.890233	-0.188353	-0.000079
C	1.543854	-4.311762	0.000124
C	2.858141	-3.883217	0.000024
C	2.850377	-2.460495	0.000007
N	1.530365	-2.061897	-0.000017
C	0.707015	-3.158392	0.000089
C	3.938205	-1.582525	-0.000038
C	0.682785	4.778928	0.000482
C	-0.683581	4.778846	0.000403
C	-1.135991	3.413359	-0.000012
N	-0.000267	2.623805	-0.000174
C	1.135355	3.413492	0.000088
C	2.484382	3.077071	0.000044
C	-2.484962	3.076737	-0.000160
C	-3.937900	-1.583137	-0.000048
C	-0.706473	-3.158512	0.000107
N	-1.529970	-2.062140	0.000012
C	-2.849925	-2.460936	0.000020
C	-2.857476	-3.883672	0.000185

C	-1.543141	-4.312019	0.000186
C	-3.890164	-0.188970	-0.000134
N	-2.758845	0.589650	-0.000137
C	-3.207973	1.868544	-0.000166
C	-4.671858	1.917393	-0.000212
C	-5.096450	0.628128	-0.000145
H	6.116362	0.245968	-0.000373
H	5.268490	2.829791	-0.000329
H	1.186818	-5.338398	0.000174
H	3.756826	-4.496806	-0.000018
H	1.304556	-1.064956	0.000006
H	4.926750	-2.046449	-0.000453
H	1.352660	5.636804	0.000752
H	-1.353553	5.636646	0.000592
H	-0.000226	1.611016	-0.000363
H	3.124779	3.962668	0.000208
H	-3.125515	3.962219	-0.000028
H	-4.926368	-2.047214	0.000020
H	-1.304271	-1.065178	-0.000061
H	-3.756067	-4.497400	0.000279
H	-1.185958	-5.338606	0.000267
H	-5.269057	2.828889	-0.000264
H	-6.116386	0.244953	-0.000138

G2

C	4.982376	0.624028	0.000820
C	4.554111	1.905831	0.000679
C	3.082890	1.848464	0.000265
N	2.632262	0.566769	0.000181
C	3.771273	-0.203059	0.000457
C	1.567557	-4.226864	-0.000728
C	2.866174	-3.770840	-0.000413
C	2.827911	-2.337780	0.000036
N	1.495748	-1.970042	0.000050
C	0.701157	-3.085492	-0.000429
C	0.680611	4.654445	-0.000911
C	-0.680428	4.654474	-0.000928
C	-1.137795	3.281904	-0.000400
N	0.000058	2.479856	-0.000236
C	1.137918	3.281842	-0.000334
C	-0.701269	-3.085466	-0.000366
N	-1.495817	-1.970001	-0.000149
C	-2.828009	-2.337683	0.000086
C	-2.866314	-3.770753	-0.000055

C	-1.567713	-4.226817	-0.000372
C	-3.771268	-0.202910	0.000445
N	-2.632253	0.566843	0.000092
C	-3.082847	1.848580	0.000328
C	-4.554038	1.905989	0.000560
C	-4.982351	0.624201	0.000727
H	5.991795	0.217494	0.001098
H	5.117504	2.836849	0.000825
H	1.227689	-5.259691	-0.001045
H	3.788083	-4.347179	-0.000452
H	1.258709	-0.974175	-0.000034
H	1.374963	5.491417	-0.001275
H	-1.374726	5.491491	-0.001315
H	-0.000004	1.466837	0.000882
H	-1.258783	-0.974127	-0.000332
H	-3.788249	-4.347050	0.000081
H	-1.227866	-5.259651	-0.000529
H	-5.117414	2.837018	0.000611
H	-5.991787	0.217713	0.000949
N	-2.415097	2.997227	-0.000159
N	2.415229	2.997167	0.000002
N	3.869781	-1.526078	0.000352
N	-3.869853	-1.525953	0.000398

H1

C	4.262045	3.385847	0.287646
C	2.949021	3.796862	0.239124
C	2.173035	2.617444	-0.094713
N	2.980830	1.543785	-0.209256
C	4.258916	1.956237	0.021933
C	5.309023	-2.619715	-0.146330
C	6.056041	-1.458823	-0.067171
C	5.143957	-0.348490	-0.041863
N	3.883230	-0.890941	-0.096121
C	3.914648	-2.257260	-0.135324
C	5.336052	1.040901	0.041529
C	2.762664	-3.063758	-0.108449
C	-5.309019	2.619736	0.146407
C	-6.056026	1.458839	0.067211
C	-5.143933	0.348513	0.041850
N	-3.883209	0.890973	0.096110
C	-3.914643	2.257290	0.135380
C	-2.762659	3.063786	0.108512
C	-5.336029	-1.040876	-0.041602

C	-0.784546	-2.426075	0.340564
N	0.280333	-3.210212	-0.054575
C	1.486293	-2.575636	0.229937
C	1.137916	-1.373592	0.924327
C	-0.236052	-1.293470	0.993409
C	-1.137962	1.373551	-0.924210
C	0.236004	1.293408	-0.993330
C	0.784534	2.426037	-0.340553
N	-0.280324	3.210203	0.054587
C	-1.486301	2.575636	-0.229875
N	-2.980822	-1.543808	0.209235
C	-4.258905	-1.956229	-0.022020
C	-4.262044	-3.385830	-0.287785
C	-2.949027	-3.796866	-0.239241
C	-2.173038	-2.617471	0.094669
H	5.140129	3.998416	0.492053
H	2.569714	4.809475	0.376709
H	5.682339	-3.642472	-0.163635
H	7.141119	-1.377041	-0.027567
H	3.093792	-0.226349	-0.199644
H	6.354230	1.416840	0.157897
H	2.880101	-4.119472	-0.366871
H	-5.682343	3.642490	0.163749
H	-7.141103	1.377050	0.027612
H	-3.093756	0.226385	0.199566
H	-2.880086	4.119503	0.366927
H	-6.354208	-1.416804	-0.157994
H	0.197349	-4.023995	-0.650356
H	1.845780	-0.674028	1.357653
H	-0.835463	-0.516561	1.456879
H	-1.845855	0.673973	-1.357473
H	0.835391	0.516470	-1.456782
H	-0.197314	4.024010	0.650330
H	-5.140130	-3.998379	-0.492244
H	-2.569728	-4.809478	-0.376858

H2

C	4.194831	3.291716	0.398569
C	2.898610	3.742525	0.366344
C	2.096977	2.622747	-0.108261
N	2.882594	1.543994	-0.320765
C	4.156579	1.887440	-0.005546
C	5.197736	-2.547188	-0.159049
C	5.912388	-1.373227	-0.091214

C	4.969124	-0.272204	-0.088942
N	3.717737	-0.847403	-0.146607
C	3.786011	-2.214477	-0.150556
C	-5.197730	2.547192	0.159188
C	-5.912381	1.373233	0.091314
C	-4.969114	0.272212	0.088951
N	-3.717727	0.847410	0.146598
C	-3.786005	2.214484	0.150631
C	-0.715580	-2.462822	0.375908
N	0.364866	-3.198178	-0.066611
C	1.552736	-2.560167	0.263652
C	1.183454	-1.418370	1.060246
C	-0.186815	-1.368240	1.121361
C	-1.183489	1.418316	-1.060135
C	0.186779	1.368182	-1.121293
C	0.715570	2.462806	-0.375920
N	-0.364862	3.198187	0.066596
C	-1.552742	2.560158	-0.263595
N	-2.882599	-1.544005	0.320740
C	-4.156573	-1.887428	0.005458
C	-4.194815	-3.291678	-0.398749
C	-2.898596	-3.742492	-0.366511
C	-2.096977	-2.622746	0.108193
H	5.092459	3.837807	0.683951
H	2.539491	4.743645	0.603521
H	5.577478	-3.566698	-0.153727
H	6.991965	-1.247095	-0.040181
H	2.919634	-0.197686	-0.275642
H	-5.577475	3.566701	0.153930
H	-6.991960	1.247101	0.040309
H	-2.919615	0.197688	0.275554
H	0.326400	-3.986620	-0.701607
H	1.880298	-0.747636	1.551989
H	-0.806004	-0.644822	1.642890
H	-1.880352	0.747552	-1.551812
H	0.805950	0.644733	-1.642801
H	-0.326374	3.986664	0.701548
H	-5.092436	-3.837749	-0.684193
H	-2.539472	-4.743597	-0.603739
N	-5.195466	-1.028610	-0.013511
N	-2.740671	3.032381	0.115693
N	5.195474	1.028624	0.013454
N	2.740677	-3.032375	-0.115622

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