

Non-empirical Anharmonic Vibrational Perturbation Theory Applied to Biomolecules: Free-Base Porphin

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SUPPORTING INFORMATION

Figure S1. The porphin molecular model and numbering of atoms.

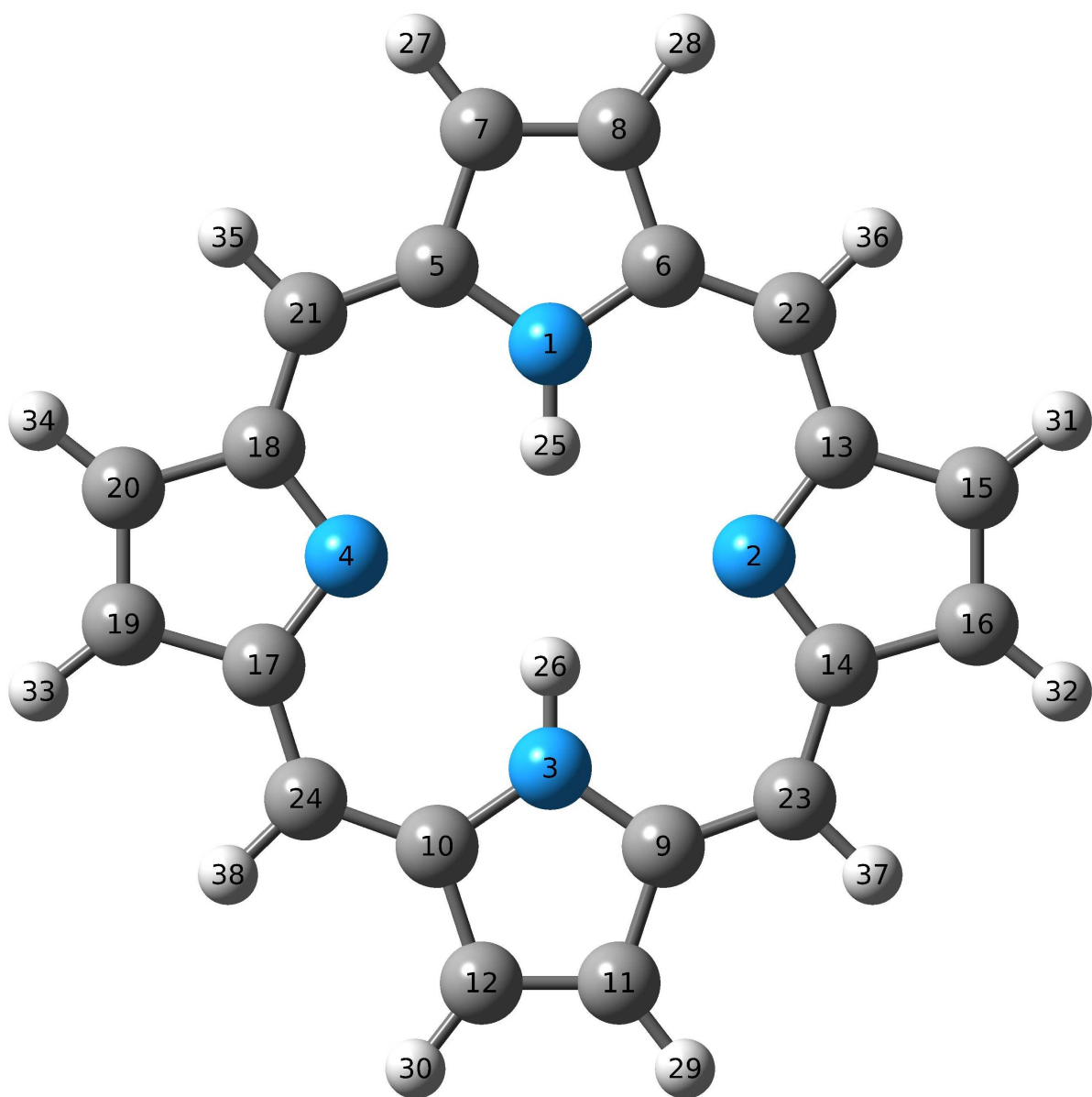


Figure S2. The base porphin molecular model and numbering of atoms used in Z-matrix with one fictitious atom.

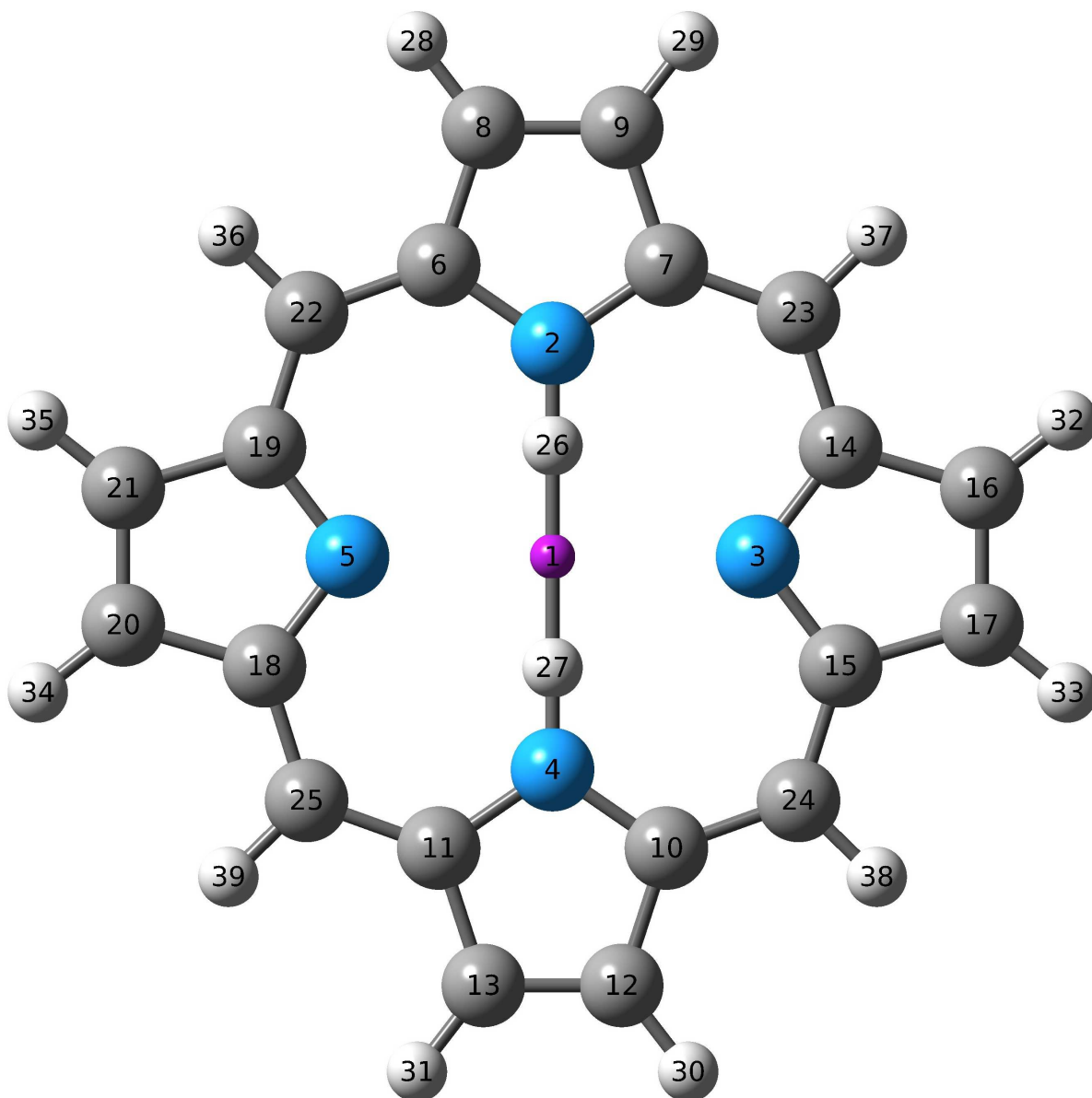


Table S1. The Definition of the Molecular Geometry of Porphin, Calculated by Means of B3LYP/6-31+G(d,p) Quantum-Mechanical Method, After Orientation of Cartesian Axes.

Center A	Type	Atom	Reference B C D			Bond Length A-B	Angle Value A-B-C	Dih.Ang. A-B-C-D
1	X							
2	N	1	1			2.11834614		
3	N	2	1	2		2.03705073	90.0	
4	N	3	1	3	2	2.11834614	90.0	180.0
5	N	4	1	4	3	2.03705073	90.0	180.0
6	C	5	2	1	5	1.37316387	124.57165994	0.0
7	C	6	2	1	3	1.37316387	124.57165994	0.0
8	C	7	6	2	7	1.43588226	106.57494361	0.0
9	C	8	7	2	6	1.43588226	106.57494361	0.0
10	C	9	4	1	3	1.37316387	124.57165994	0.0
11	C	10	4	1	5	1.37316387	124.57165994	0.0
12	C	11	10	4	11	1.43588226	106.57494361	0.0
13	C	12	11	4	10	1.43588226	106.57494361	0.0
14	C	13	3	1	2	1.36417637	127.19132199	0.0
15	C	14	3	1	4	1.36417637	127.19132199	0.0
16	C	15	14	3	15	1.46094601	111.00641295	0.0
17	C	16	15	3	14	1.46094601	111.00641295	0.0
18	C	17	5	1	4	1.36417637	127.19132199	0.0
19	C	18	5	1	2	1.36417637	127.19132199	0.0
20	C	19	18	5	19	1.46094601	111.00641295	0.0
21	C	20	19	5	18	1.46094601	111.00641295	0.0
22	C	21	6	2	1	1.39543715	125.59902964	0.0
23	C	22	7	2	1	1.39543715	125.59902964	0.0
24	C	23	10	4	1	1.39543715	125.59902964	0.0
25	C	24	11	4	1	1.39543715	125.59902964	0.0
26	H	25	1	3	4	1.10355495	90.0	180.0
27	H	26	1	5	2	1.10355495	90.0	180.0
28	H	27	8	6	2	1.08154469	124.38620228	180.0
29	H	28	9	7	2	1.08154469	124.38620228	180.0
30	H	29	12	10	4	1.08154469	124.38620228	180.0
31	H	30	13	11	4	1.08154469	124.38620228	180.0
32	H	31	16	14	3	1.08279524	125.45308505	180.0
33	H	32	17	15	3	1.08279524	125.45308505	180.0
34	H	33	20	18	5	1.08279524	125.45308505	180.0
35	H	34	21	19	5	1.08279524	125.45308505	180.0
36	H	35	22	6	2	1.08592143	115.85218841	180.0
37	H	36	23	7	2	1.08592143	115.85218841	180.0
38	H	37	24	10	4	1.08592143	115.85218841	180.0
39	H	38	25	11	4	1.08592143	115.85218841	180.0

Table S2. Cartesian Coordinates of Porphin After Orientation of Cartesian Axes.

Atom	Atomic Number	Isotope Species	Coordinates (Angstroms)			Atomic Mass
			X	Y	Z	
1	7(N)	N(14)	0.00000000	0.00000000	-2.11834614	14.00307400
2	7(N)	N(14)	0.00000000	2.03705073	0.00000000	14.00307400
3	7(N)	N(14)	0.00000000	0.00000000	2.11834614	14.00307400
4	7(N)	N(14)	0.00000000	-2.03705073	0.00000000	14.00307400
5	6(C)	C(12)	0.00000000	-1.13068667	-2.89752948	12.00000000
6	6(C)	C(12)	0.00000000	1.13068667	-2.89752948	12.00000000
7	6(C)	C(12)	0.00000000	-0.68705291	-4.26316009	12.00000000
8	6(C)	C(12)	0.00000000	0.68705291	-4.26316009	12.00000000
9	6(C)	C(12)	0.00000000	1.13068667	2.89752948	12.00000000
10	6(C)	C(12)	0.00000000	-1.13068667	2.89752948	12.00000000
11	6(C)	C(12)	0.00000000	0.68705291	4.26316009	12.00000000
12	6(C)	C(12)	0.00000000	-0.68705291	4.26316009	12.00000000
13	6(C)	C(12)	0.00000000	2.86166597	-1.08673220	12.00000000
14	6(C)	C(12)	0.00000000	2.86166597	1.08673220	12.00000000
15	6(C)	C(12)	0.00000000	4.26471050	-0.67951079	12.00000000
16	6(C)	C(12)	0.00000000	4.26471050	0.67951079	12.00000000
17	6(C)	C(12)	0.00000000	-2.86166597	1.08673220	12.00000000
18	6(C)	C(12)	0.00000000	-2.86166597	-1.08673220	12.00000000
19	6(C)	C(12)	0.00000000	-4.26471050	0.67951079	12.00000000
20	6(C)	C(12)	0.00000000	-4.26471050	-0.67951079	12.00000000
21	6(C)	C(12)	0.00000000	-2.44338466	-2.42417041	12.00000000
22	6(C)	C(12)	0.00000000	2.44338466	-2.42417041	12.00000000
23	6(C)	C(12)	0.00000000	2.44338466	2.42417041	12.00000000
24	6(C)	C(12)	0.00000000	-2.44338466	2.42417041	12.00000000
25	1(H)	H(1)	0.00000000	0.00000000	-1.10355495	1.00782522
26	1(H)	H(1)	0.00000000	0.00000000	1.10355495	1.00782522
27	1(H)	H(1)	0.00000000	-1.34720761	-5.11985997	1.00782522
28	1(H)	H(1)	0.00000000	1.34720761	-5.11985997	1.00782522
29	1(H)	H(1)	0.00000000	1.34720761	5.11985997	1.00782522
30	1(H)	H(1)	0.00000000	-1.34720761	5.11985997	1.00782522
31	1(H)	H(1)	0.00000000	5.11373586	-1.35152379	1.00782522
32	1(H)	H(1)	0.00000000	5.11373586	1.35152379	1.00782522
33	1(H)	H(1)	0.00000000	-5.11373586	1.35152379	1.00782522
34	1(H)	H(1)	0.00000000	-5.11373586	-1.35152379	1.00782522
35	1(H)	H(1)	0.00000000	-3.22032580	-3.18284546	1.00782522
36	1(H)	H(1)	0.00000000	3.22032580	-3.18284546	1.00782522
37	1(H)	H(1)	0.00000000	3.22032580	3.18284546	1.00782522
38	1(H)	H(1)	0.00000000	-3.22032580	3.18284546	1.00782522

Table S3. Internal Valence Coordinate Definition of Porphin.

Number	Description	Definition	Type
1	N-H str #1	N(1) - H(25)	Bond Stretch
2	N-C1 str #1	N(1) - C(6)	Bond Stretch
3	N-C2 str #1	N(1) - C(5)	Bond Stretch
4	C1-C3 str #1	C(6) - C(8)	Bond Stretch
5	C2-C4 str #1	C(5) - C(7)	Bond Stretch
6	C3-C4 str #1	C(8) - C(7)	Bond Stretch
7	C1-C1 str #1	C(6) - C(22)	Bond Stretch
8	C2-C2 str #1	C(5) - C(21)	Bond Stretch
9	C3-H3 str #1	C(8) - H(28)	Bond Stretch
10	C4-H4 str #1	C(7) - H(27)	Bond Stretch
11	N-H str #2	N(3) - H(26)	Bond Stretch
12	N-C1 str #2	N(3) - C(10)	Bond Stretch
13	N-C2 str #2	N(3) - C(9)	Bond Stretch
14	C1-C3 str #2	C(10) - C(12)	Bond Stretch
15	C2-C4 str #2	C(9) - C(11)	Bond Stretch
16	C3-C4 str #2	C(12) - C(11)	Bond Stretch
17	C1-C1 str #2	C(10) - C(24)	Bond Stretch
18	C2-C2 str #2	C(9) - C(23)	Bond Stretch
19	C3-H3 str #2	C(12) - H(30)	Bond Stretch
20	C4-H4 str #2	C(11) - H(29)	Bond Stretch
21	N-C1 str #3	N(2) - C(14)	Bond Stretch
22	N-C2 str #3	N(2) - C(13)	Bond Stretch
23	C1-C3 str #3	C(14) - C(16)	Bond Stretch
24	C2-C4 str #3	C(13) - C(15)	Bond Stretch
25	C3-C4 str #3	C(16) - C(15)	Bond Stretch
26	C1-C1 str #3	C(14) - C(23)	Bond Stretch
27	C2-C2 str #3	C(13) - C(22)	Bond Stretch
28	C3-H3 str #3	C(16) - H(32)	Bond Stretch
29	C4-H4 str #3	C(15) - H(31)	Bond Stretch
30	C7-H str #3	C(23) - H(37)	Bond Stretch
31	C8-H str #3	C(22) - H(36)	Bond Stretch
32	N-C1 str #4	N(4) - C(18)	Bond Stretch
33	N-C2 str #4	N(4) - C(17)	Bond Stretch
34	C1-C3 str #4	C(18) - C(20)	Bond Stretch
35	C2-C4 str #4	C(17) - C(19)	Bond Stretch
36	C3-C4 str #4	C(20) - C(19)	Bond Stretch
37	C1-C1 str #4	C(18) - C(21)	Bond Stretch
38	C2-C2 str #4	C(17) - C(24)	Bond Stretch
39	C3-H3 str #4	C(20) - H(34)	Bond Stretch
40	C4-H4 str #4	C(19) - H(33)	Bond Stretch
41	C7-H str #4	C(21) - H(35)	Bond Stretch
42	C8-H str #4	C(24) - H(38)	Bond Stretch
43	1alf C3NC4	C(6) - N(1) - C(5)	Angle Bend
44	1bet C3NH	C(6) - N(1) - H(25)	Angle Bend
45	1bet' C4NH	C(5) - N(1) - H(25)	Angle Bend
46	1alf1 NC1C3	N(1) - C(6) - C(8)	Angle Bend
47	1bet1 NC1H1	N(1) - C(6) - C(22)	Angle Bend
48	1bet1' C3C1H1	C(8) - C(6) - C(22)	Angle Bend
49	1alf2 NC2C4	N(1) - C(5) - C(7)	Angle Bend
50	1bet2 NC2H2	N(1) - C(5) - C(21)	Angle Bend
51	1bet2' C3C1H2	C(7) - C(5) - C(21)	Angle Bend
52	1alf3 C1C3C4	C(6) - C(8) - C(7)	Angle Bend
53	1bet3 C1C3H3	C(6) - C(8) - H(28)	Angle Bend
54	1bet3' C4C3H3	C(7) - C(8) - H(28)	Angle Bend
55	1alf4 C2C4C3	C(5) - C(7) - C(8)	Angle Bend
56	1bet4 C2C4H4	C(5) - C(7) - H(27)	Angle Bend
57	1bet4' C3C4H4	C(8) - C(7) - H(27)	Angle Bend
58	2alf C3NC4	C(10) - N(3) - C(9)	Angle Bend
59	2bet C3NH	C(10) - N(3) - H(26)	Angle Bend
60	2bet' C4NH	C(9) - N(3) - H(26)	Angle Bend
61	2alf1 NC1C3	N(3) - C(10) - C(12)	Angle Bend
62	2bet1 NC1H1	N(3) - C(10) - C(24)	Angle Bend
63	2bet1' C3C1H1	C(12) - C(10) - C(24)	Angle Bend
64	2alf2 NC2C4	N(3) - C(9) - C(11)	Angle Bend

65	2bet2	NC2H2	N(3) - C(9) - C(23)	Angle Bend
66	2bet2'	C3C1H2	C(11) - C(9) - C(23)	Angle Bend
67	2alf3	C1C3C4	C(10) - C(12) - C(11)	Angle Bend
68	2bet3	C1C3H3	C(10) - C(12) - H(30)	Angle Bend
69	2bet3'	C4C3H3	C(11) - C(12) - H(30)	Angle Bend
70	2alf4	C2C4C3	C(9) - C(11) - C(12)	Angle Bend
71	2bet4	C2C4H4	C(9) - C(11) - H(29)	Angle Bend
72	2bet4'	C3C4H4	C(12) - C(11) - H(29)	Angle Bend
73	3alf	C3NC4	C(14) - N(2) - C(13)	Angle Bend
74	3alf1	NC1C3	N(2) - C(14) - C(16)	Angle Bend
75	3bet1	NC1H1	N(2) - C(14) - C(23)	Angle Bend
76	3bet1'	C3C1H1	C(16) - C(14) - C(23)	Angle Bend
77	3alf2	NC2C4	N(2) - C(13) - C(15)	Angle Bend
78	3bet2	NC2H2	N(2) - C(13) - C(22)	Angle Bend
79	3bet2'	C3C1H2	C(15) - C(13) - C(22)	Angle Bend
80	3alf3	C1C3C4	C(14) - C(16) - C(15)	Angle Bend
81	3bet3	C1C3H3	C(14) - C(16) - H(32)	Angle Bend
82	3bet3'	C4C3H3	C(15) - C(16) - H(32)	Angle Bend
83	3alf4	C2C4C3	C(13) - C(15) - C(16)	Angle Bend
84	3bet4	C2C4H4	C(13) - C(15) - H(31)	Angle Bend
85	3bet4'	C3C4H4	C(16) - C(15) - H(31)	Angle Bend
86	3alfa	C23	C(9) - C(23) - C(14)	Angle Bend
87	3beta	C23-H	C(9) - C(23) - H(37)	Angle Bend
88	3beta'	C23-H	C(14) - C(23) - H(37)	Angle Bend
89	3alfa	C22	C(6) - C(22) - C(13)	Angle Bend
90	3beta	C22-H	C(6) - C(22) - H(36)	Angle Bend
91	3beta'	C22-H	C(13) - C(22) - H(36)	Angle Bend
92	4alf	C3NC4	C(18) - N(4) - C(17)	Angle Bend
93	4alf1	NC1C3	N(4) - C(18) - C(20)	Angle Bend
94	4bet1	NC1H1	N(4) - C(18) - C(21)	Angle Bend
95	4bet1'	C3C1H1	C(20) - C(18) - C(21)	Angle Bend
96	4alf2	NC2C4	N(4) - C(17) - C(19)	Angle Bend
97	4bet2	NC2H2	N(4) - C(17) - C(24)	Angle Bend
98	4bet2'	C3C1H2	C(19) - C(17) - C(24)	Angle Bend
99	4alf3	C1C3C4	C(18) - C(20) - C(19)	Angle Bend
100	4bet3	C1C3H3	C(18) - C(20) - H(34)	Angle Bend
101	4bet3'	C4C3H3	C(19) - C(20) - H(34)	Angle Bend
102	4alf4	C2C4C3	C(17) - C(19) - C(20)	Angle Bend
103	4bet4	C2C4H4	C(17) - C(19) - H(33)	Angle Bend
104	4bet4'	C3C4H4	C(20) - C(19) - H(33)	Angle Bend
105	4alfa	C21	C(5) - C(21) - C(18)	Angle Bend
106	4beta	C21-H	C(5) - C(21) - H(35)	Angle Bend
107	4beta'	C21-H	C(18) - C(21) - H(35)	Angle Bend
108	4alfa	C24	C(10) - C(24) - C(17)	Angle Bend
109	4beta	C24-H	C(10) - C(24) - H(38)	Angle Bend
110	4beta'	C24-H	C(17) - C(24) - H(38)	Angle Bend
111	N-H op.wag 1		H(25) - N(1) - C(6) - C(5)	Out of Plane
112	C-C1 op.wag1		C(22) - C(6) - N(1) - C(8)	Out of Plane
113	C-C2 op.wag1		C(21) - C(5) - N(1) - C(7)	Out of Plane
114	C-H3 op.wag1		H(28) - C(8) - C(6) - C(7)	Out of Plane
115	C-H4 op.wag1		H(27) - C(7) - C(5) - C(8)	Out of Plane
116	N-H op.wag 2		H(26) - N(3) - C(10) - C(9)	Out of Plane
117	C-C1 op.wag2		C(24) - C(10) - N(3) - C(12)	Out of Plane
118	C-C2 op.wag2		C(23) - C(9) - N(3) - C(11)	Out of Plane
119	C-H3 op.wag2		H(30) - C(12) - C(10) - C(11)	Out of Plane
120	C-H4 op.wag2		H(29) - C(11) - C(9) - C(12)	Out of Plane
121	C-C1 op.wag3		C(23) - C(14) - N(2) - C(16)	Out of Plane
122	C-C2 op.wag3		C(22) - C(13) - N(2) - C(15)	Out of Plane
123	C-H3 op.wag3		H(32) - C(16) - C(14) - C(15)	Out of Plane
124	C-H4 op.wag3		H(31) - C(15) - C(13) - C(16)	Out of Plane
125	C-C1 op.wag4		C(21) - C(18) - N(4) - C(20)	Out of Plane
126	C-C2 op.wag4		C(24) - C(17) - N(4) - C(19)	Out of Plane
127	C-H3 op.wag4		H(34) - C(20) - C(18) - C(19)	Out of Plane
128	C-H4 op.wag4		H(33) - C(19) - C(17) - C(20)	Out of Plane
129	C21-H35 wag		H(35) - C(21) - C(5) - C(18)	Out of Plane
130	C22-H36 wag		H(36) - C(22) - C(6) - C(13)	Out of Plane
131	C23-H37 wag		H(37) - C(23) - C(9) - C(14)	Out of Plane
132	C24-H38 wag		H(38) - C(24) - C(10) - C(17)	Out of Plane

133	N-C1= tors 1	C(5) - N(1) - C(6) - C(8)	Torsion
134	N-C2= tors 1	C(6) - N(1) - C(5) - C(7)	Torsion
135	C1-C3 tors 1	N(1) - C(6) - C(8) - C(7)	Torsion
136	C2-C4 tors 1	N(1) - C(5) - C(7) - C(8)	Torsion
137	C3-C4 tors 1	C(6) - C(8) - C(7) - C(5)	Torsion
138	N-C1= tors 2	C(9) - N(3) - C(10) - C(12)	Torsion
139	N-C2= tors 2	C(10) - N(3) - C(9) - C(11)	Torsion
140	C1-C3 tors 2	N(3) - C(10) - C(12) - C(11)	Torsion
141	C2-C4 tors 2	N(3) - C(9) - C(11) - C(12)	Torsion
142	C3-C4 tors 2	C(10) - C(12) - C(11) - C(9)	Torsion
143	N-C1= tors 3	C(13) - N(2) - C(14) - C(16)	Torsion
144	N-C2= tors 3	C(14) - N(2) - C(13) - C(15)	Torsion
145	C1-C3 tors 3	N(2) - C(14) - C(16) - C(15)	Torsion
146	C2-C4 tors 3	N(2) - C(13) - C(15) - C(16)	Torsion
147	C3-C4 tors 3	C(14) - C(16) - C(15) - C(13)	Torsion
148	N-C1= tors 4	C(17) - N(4) - C(18) - C(20)	Torsion
149	N-C2= tors 4	C(18) - N(4) - C(17) - C(19)	Torsion
150	C1-C3 tors 4	N(4) - C(18) - C(20) - C(19)	Torsion
151	C2-C4 tors 4	N(4) - C(17) - C(19) - C(20)	Torsion
152	C3-C4 tors 4	C(18) - C(20) - C(19) - C(17)	Torsion
153	C5-C21 tors1	N(1) - C(5) - C(21) - C(18)	Torsion
154	C6-C22 tors1	N(1) - C(6) - C(22) - C(13)	Torsion
155	C9-C23 tors2	N(3) - C(9) - C(23) - C(14)	Torsion
156	C10-C24tors2	N(3) - C(10) - C(24) - C(17)	Torsion
157	C14-C23tors3	N(2) - C(14) - C(23) - C(9)	Torsion
158	C13-C22tors3	N(2) - C(13) - C(22) - C(6)	Torsion
159	C18-C21tors4	N(4) - C(18) - C(21) - C(5)	Torsion
160	C17-C24tors4	N(4) - C(17) - C(24) - C(10)	Torsion
161	-N-C1-Ctors1	C(6) - N(1) - C(5) - C(21)	Torsion
162	-N-C2-Ctors1	C(5) - N(1) - C(6) - C(22)	Torsion
163	-N-C1-Ctors2	C(10) - N(3) - C(9) - C(23)	Torsion
164	-N-C2-Ctors2	C(9) - N(3) - C(10) - C(24)	Torsion
165	-N-C1-Ctors3	C(14) - N(2) - C(13) - C(22)	Torsion
166	-N-C2-Ctors3	C(13) - N(2) - C(14) - C(23)	Torsion
167	-N-C1-Ctors4	C(18) - N(4) - C(17) - C(24)	Torsion
168	-N-C2-Ctors4	C(17) - N(4) - C(18) - C(21)	Torsion

The Definition of the Out-of-Plane Wagging Coordinate (A-B-C-D):
A - the End Atom, B - the Apex Atom, C,D - the Anchor Atoms.

Table S4. Internal Non-redundant Local Symmetry Coordinate Definition of Porphin.

No.	Description	Definition
1	N-C1 str 1	+1.000000*(2)[N-C1 str #1]
2	N-C2 str 1	+1.000000*(3)[N-C2 str #1]
3	C1-C3 str 1	+1.000000*(4)[C1-C3 str #1]
4	C2-C4 str 1	+1.000000*(5)[C2-C4 str #1]
5	C3-C4 str 1	+1.000000*(6)[C3-C4 str #1]
6	N-H str 1	+1.000000*(1)[N-H str #1]
7	C1-C1 str 1	+1.000000*(7)[C1-C1 str #1]
8	C2-C2 str 1	+1.000000*(8)[C2-C2 str #1]
9	C3-H3 str 1	+1.000000*(9)[C3-H3 str #1]
10	C4-H4 str 1	+1.000000*(10)[C4-H4 str #1]
11	C3-H rock 1	+0.707107*(53)[1bet3 C1C3H3]-0.707107*(54)[1bet3'C4C3H3]
12	C4-H rock 1	+0.707107*(56)[1bet4 C2C4H4]-0.707107*(57)[1bet4'C3C4H4]
13	C3-H wag 1	+1.000000*(114)[C-H3 op.wag1]
14	C4-H wag 1	+1.000000*(115)[C-H4 op.wag1]
15	N1-H rock 1	+0.707107*(44)[1bet C3NH]-0.707107*(45)[1bet'C4NH]
16	N1-H wag 1	+1.000000*(111)[N-H op.wag 1]
17	Ring5 def1 1	+0.632456*(43)[1alf C3NC4]-0.511667*(46)[1alf1 NC1C3] -0.511667*(49)[1alf2 NC2C4]+0.195440*(52)[1alf3 C1C3C4] +0.195440*(55)[1alf4 C2C4C3]
18	Ring5 def2 1	-0.371748*(46)[1alf1 NC1C3]+0.371748*(49)[1alf2 NC2C4] +0.601501*(52)[1alf3 C1C3C4]-0.601501*(55)[1alf4 C2C4C3]
19	Ring5 tor1 1	+0.195440*(133)[N-C1= tors 1]+0.195440*(134)[N-C2= tors 1] -0.511667*(135)[C1-C3 tors 1]-0.511667*(136)[C2-C4 tors 1] +0.632456*(137)[C3-C4 tors 1]
20	Ring5 tor2 1	-0.601501*(133)[N-C1= tors 1]+0.601501*(134)[N-C2= tors 1] +0.371748*(135)[C1-C3 tors 1]-0.371748*(136)[C2-C4 tors 1]
21	N-C1 str 2	+1.000000*(12)[N-C1 str #2]
22	N-C2 str 2	+1.000000*(13)[N-C2 str #2]
23	C1-C3 str 2	+1.000000*(14)[C1-C3 str #2]
24	C2-C4 str 2	+1.000000*(15)[C2-C4 str #2]
25	C3-C4 str 2	+1.000000*(16)[C3-C4 str #2]
26	N-H str 2	+1.000000*(11)[N-H str #2]
27	C1-C1 str 2	+1.000000*(17)[C1-C1 str #2]
28	C2-C2 str 2	+1.000000*(18)[C2-C2 str #2]
29	C3-H3 str 2	+1.000000*(19)[C3-H3 str #2]
30	C4-H4 str 2	+1.000000*(20)[C4-H4 str #2]
31	C3-H rock 2	+0.707107*(68)[2bet3 C1C3H3]-0.707107*(69)[2bet3'C4C3H3]
32	C4-H rock 2	+0.707107*(71)[2bet4 C2C4H4]-0.707107*(72)[2bet4'C3C4H4]
33	C3-H wag 2	+1.000000*(119)[C-H3 op.wag2]
34	C4-H wag 2	+1.000000*(120)[C-H4 op.wag2]
35	N-H rock 2	+0.707107*(59)[2bet C3NH]-0.707107*(60)[2bet'C4NH]
36	N-H wag 2	+1.000000*(116)[N-H op.wag 2]
37	Ring5 Def1 2	+0.632456*(58)[2alf C3NC4]-0.511667*(61)[2alf1 NC1C3] -0.511667*(64)[2alf2 NC2C4]+0.195440*(67)[2alf3 C1C3C4] +0.195440*(70)[2alf4 C2C4C3]
38	Ring5 Def2 2	-0.371748*(61)[2alf1 NC1C3]+0.371748*(64)[2alf2 NC2C4] +0.601501*(67)[2alf3 C1C3C4]-0.601501*(70)[2alf4 C2C4C3]
39	Ring5 Tor1 2	+0.195440*(138)[N-C1= tors 2]+0.195440*(139)[N-C2= tors 2] -0.511667*(140)[C1-C3 tors 2]-0.511667*(141)[C2-C4 tors 2] +0.632456*(142)[C3-C4 tors 2]
40	Ring5 Tor2 2	-0.601501*(138)[N-C1= tors 2]+0.601501*(139)[N-C2= tors 2] +0.371748*(140)[C1-C3 tors 2]-0.371748*(141)[C2-C4 tors 2]
41	N-C1 str 3	+1.000000*(21)[N-C1 str #3]
42	N-C2 str 3	+1.000000*(22)[N-C2 str #3]
43	C1-C3 str 3	+1.000000*(23)[C1-C3 str #3]
44	C2-C4 str 3	+1.000000*(24)[C2-C4 str #3]
45	C3-C4 str 3	+1.000000*(25)[C3-C4 str #3]
46	C1-C1 str 3	+1.000000*(26)[C1-C1 str #3]
47	C2-C2 str 3	+1.000000*(27)[C2-C2 str #3]
48	C3-H3 str 3	+1.000000*(28)[C3-H3 str #3]
49	C4-H4 str 3	+1.000000*(29)[C4-H4 str #3]
50	C3-H rock 3	+0.707107*(81)[3bet3 C1C3H3]-0.707107*(82)[3bet3'C4C3H3]
51	C4-H rock 3	+0.707107*(84)[3bet4 C2C4H4]-0.707107*(85)[3bet4'C3C4H4]
52	C3-H(32)wag3	+1.000000*(123)[C-H3 op.wag3]
53	C4-H(31)wag3	+1.000000*(124)[C-H4 op.wag3]

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54 Ring5 Def1 3 +0.632456*( 73)[3alf C3NC4 ]-0.511667*( 74)[3alf1 NC1C3 ]
-0.511667*( 77)[3alf2 NC2C4 ]+0.195440*( 80)[3alf3 C1C3C4 ]
+0.195440*( 83)[3alf4 C2C4C3]
55 Ring5 Def2 3 -0.371748*( 74)[3alf1 NC1C3 ]+0.371748*( 77)[3alf2 NC2C4 ]
+0.601501*( 80)[3alf3 C1C3C4 ]-0.601501*( 83)[3alf4 C2C4C3]
56 Ring5 Tor1 3 +0.195440*(143)[N-C1= tors 3]+0.195440*(144)[N-C2= tors 3]
-0.511667*(145)[C1-C3 tors 3]-0.511667*(146)[C2-C4 tors 3]
+0.632456*(147)[C3-C4 tors 3]
57 Ring5 Tor2 3 -0.601501*(143)[N-C1= tors 3]+0.601501*(144)[N-C2= tors 3]
+0.371748*(145)[C1-C3 tors 3]-0.371748*(146)[C2-C4 tors 3]
58 C23-H str 3 +1.000000*( 30)[C7-H str #3]
59 C23-H rock 3 +0.707107*( 87)[3beta C23-H ]-0.707107*( 88)[3beta'C23-H ]
60 C22-H str 3 +1.000000*( 31)[C8-H str #3]
61 C22-H rock 3 +0.707107*( 90)[3beta C22-H ]-0.707107*( 91)[3beta'C22-H ]
62 C23-H37 wag +1.000000*(131)[C23-H37 wag]
63 C24-H38 wag +1.000000*(132)[C24-H38 wag]
64 N-C1 str 4 +1.000000*( 32)[N-C1 str #4]
65 N-C2 str 4 +1.000000*( 33)[N-C2 str #4]
66 C1-C3 str 4 +1.000000*( 34)[C1-C3 str #4]
67 C2-C4 str 4 +1.000000*( 35)[C2-C4 str #4]
68 C3-C4 str 4 +1.000000*( 36)[C3-C4 str #4]
69 C1-C1 str 4 +1.000000*( 37)[C1-C1 str #4]
70 C2-C2 str 4 +1.000000*( 38)[C2-C2 str #4]
71 C3-H3 str 4 +1.000000*( 39)[C3-H3 str #4]
72 C4-H4 str 4 +1.000000*( 40)[C4-H4 str #4]
73 C3-H rock 4 +0.707107*(100)[4bet3 C1C3H3]-0.707107*(101)[4bet3'C4C3H3]
74 C4-H rock 4 +0.707107*(103)[4bet4 C2C4H4]-0.707107*(104)[4bet4'C3C4H4]
75 C3-H(00)wag4 +1.000000*(127)[C-H3 op.wag4]
76 C4-H(00)wag4 +1.000000*(128)[C-H4 op.wag4]
77 Ring5 Def1 4 +0.632456*( 92)[4alf C3NC4 ]-0.511667*( 93)[4alf1 NC1C3 ]
-0.511667*( 96)[4alf2 NC2C4 ]+0.195440*( 99)[4alf3 C1C3C4 ]
+0.195440*(102)[4alf4 C2C4C3]
78 Ring5 Def2 4 -0.371748*( 93)[4alf1 NC1C3 ]+0.371748*( 96)[4alf2 NC2C4 ]
+0.601501*( 99)[4alf3 C1C3C4 ]-0.601501*(102)[4alf4 C2C4C3]
79 Ring5 Tor1 4 +0.195440*(148)[N-C1= tors 4]+0.195440*(149)[N-C2= tors 4]
-0.511667*(150)[C1-C3 tors 4]-0.511667*(151)[C2-C4 tors 4]
+0.632456*(152)[C3-C4 tors 4]
80 Ring5 Tor2 4 -0.601501*(148)[N-C1= tors 4]+0.601501*(149)[N-C2= tors 4]
+0.371748*(150)[C1-C3 tors 4]-0.371748*(151)[C2-C4 tors 4]
81 C21-H str 4 +1.000000*( 41)[C7-H str #4]
82 C21-H rock 4 +0.707107*(106)[4beta C21-H ]-0.707107*(107)[4beta'C21-H ]
83 C24-H str 4 +1.000000*( 42)[C8-H str #4]
84 C24-H rock 4 +0.707107*(109)[4beta C24-H ]-0.707107*(110)[4beta'C24-H ]
85 C21-H35 wag +1.000000*(129)[C21-H35 wag]
86 C22-H36 wag +1.000000*(130)[C22-H36 wag]
87 >C1-C rock 1 +0.707107*( 47)[1bet1 NC1H1 ]-0.707107*( 48)[1bet1'C3C1H1]
88 >C2-C rock 1 +0.707107*( 50)[1bet2 NC2H2 ]-0.707107*( 51)[1bet2'C3C1H2]
89 >C1-C rock 2 +0.707107*( 62)[2bet1 NC1H1 ]-0.707107*( 63)[2bet1'C3C1H1]
90 >C2-C rock 2 +0.707107*( 65)[2bet2 NC2H2 ]-0.707107*( 66)[2bet2'C3C1H2]
91 >C1-C rock 3 +0.707107*( 75)[3bet1 NC1H1 ]-0.707107*( 76)[3bet1'C3C1H1]
92 >C2-C rock 3 +0.707107*( 78)[3bet2 NC2H2 ]-0.707107*( 79)[3bet2'C3C1H2]
93 >C1-C rock 4 +0.707107*( 94)[4bet1 NC1H1 ]-0.707107*( 95)[4bet1'C3C1H1]
94 >C2-C rock 4 +0.707107*( 97)[4bet2 NC2H2 ]-0.707107*( 98)[4bet2'C3C1H2]
95 >C-C-C< X4 -0.500000*( 86)[3alfa C23 ]+0.500000*( 89)[3alfa C22 ]
-0.500000*(105)[4alfa C21 ]+0.500000*(108)[4alfa C24 ]
96 C5-C21 tors1 +1.000000*(153)[C5-C21 tors1]
97 C10-C24tors2 +1.000000*(156)[C10-C24tors2]
98 C14-C23tors3 +1.000000*(157)[C14-C23tors3]
99 C13-C22tors3 +1.000000*(158)[C13-C22tors3]
100 C17-C24tors4 +1.000000*(160)[C17-C24tors4]
101 -N-C-C1tors1 +1.000000*(161)[-N-C1-Ctors1]
102 -N-C-C2tors1 +1.000000*(162)[-N-C2-Ctors1]
103 -N-C-C1tors2 +1.000000*(163)[-N-C1-Ctors2]
104 -N-C-C2tors2 +1.000000*(164)[-N-C2-Ctors2]
105 -N-C-C1tors3 +1.000000*(165)[-N-C1-Ctors3]
106 -N-C-C2tors3 +1.000000*(166)[-N-C2-Ctors3]
107 -N-C-C1tors4 +1.000000*(167)[-N-C1-Ctors4]
108 -N-C-C2tors4 +1.000000*(168)[-N-C2-Ctors4]

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