

Supporting Information

for

NH Tautomerism of N-Confused Porphyrin: Solvent/Substituent Effects and Isomerization Mechanism

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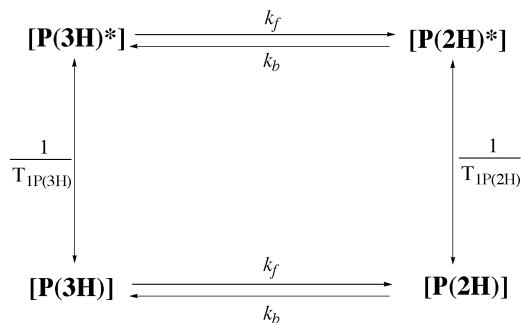
References

EXPERIMENTAL

General. Commercially available solvents and reagents were used without further purification unless otherwise mentioned. CDCl_3 (Isotec. Inc.) for NMR measurements was neutralized and the stabilizer was excluded with Alumina column. Pyridine- d_5 (Aldrich) and DMF- d_7 (Aldrich) were used as received. NCPs were synthesized from freshly distilled arylaldehydes and pyrrole by the reported procedure.¹⁻⁴

Saturation Transfer Experiment⁵ The determination of the rate constant for NCP tautomerism was conducted on a JEOL α -500 spectrometer (operating at 500.00 MHz for ^1H) with a spin saturation transfer method. The spin relaxation times were estimated by an inversion recovery method.

In this experiment, mainly we used the signal of inner CH. The tautomerism kinetics are shown in the Scheme below, where $[\mathbf{3H}]$ and $[\mathbf{3H}^*]$ are the lower and upper spin-state populations for the inner CH of tautomer- $\mathbf{3H}$, and $[\mathbf{2H}]$ and $[\mathbf{2H}^*]$ are those for the inner CH of tautomer- $\mathbf{2H}$, respectively. $T_{1,3\mathbf{H}}$ and $T_{1,2\mathbf{H}}$ are the spin lattice relaxation times for the inner CH of $\mathbf{2-3H}$ and $\mathbf{2-2H}$, and k_f , k_b are rate constants of the tautomerism.



Here, the signals of $\mathbf{2-2H}$ were saturated. With a sufficiently long duration of the decoupler r.f. pulse, the spin states of the $\mathbf{2-2H}$ can be saturated; *i.e.*, $[\mathbf{2H}] = [\mathbf{2H}^*]$. Over time, the saturated spin population is transferred to the signal of $\mathbf{2-2H}$ through the NH tautomerism, resulting in partial loss of net magnetization of the $\mathbf{P(3H)}$ signal from its thermal equilibrium value. Then, k_f were calculated according to eq. 1.

$$k_f = \frac{1}{T_{1P(3H)}} \left(\frac{I_0}{I} - 1 \right) \quad (1)$$

I_0 is the signal intensity in the thermal equilibrium, and I is that in saturation.

Synthesis of NCPs. NCTPP (**2a**),^{1a} NCTTP (**2b**),^{1b} NCT(3,5-di-*tert*-Bu)PP (**2f**),³ and NCTMP (**2h**)³ were synthesized according to the reported method.

NC-TAP (2c**):**⁴ ^1H NMR (CDCl_3): δ –4.80 (s, 1H), 4.09 (m, 12H), 7.28 (m, 4H), 7.39 (d, J = 8.5 Hz, 4H), 8.06 (d, J = 8.5 Hz, 2H), 8.08 (d, J = 8.5 Hz, 2H), 8.27 (d, J = 8.5 Hz, 2H), 8.33

(d, $J = 8.5$ Hz, 2H), 8.57 (m, 4H), 8.69 (s, 1H), 8.90 (d, $J = 4.5$ Hz, 1H), 8.95 (d, $J = 4.5$ Hz, 1H); UV/vis (CH_2Cl_2): λ_{\max} [nm] = 736, 681(sh), 592, 549, 515, 443; FAB-MS m/z = 735.0 (calcd. for $\text{C}_{48}\text{H}_{39}\text{N}_4\text{O}_4$ [$\text{M} + \text{H}]^+$ 735.2971).

NC-T(*p*Cl)PP (2d):⁴ ^1H NMR (CDCl_3): δ –5.05 (s, 1H), –2.46 (bs, 2H), 7.75 (m, 4H), 7.84 (m, 4H), 8.08 (m, 4H), 8.24 (d, $J = 8.0$ Hz, 2H), 8.28 (d, $J = 8.0$ Hz, 2H), 8.55 (m, 3H), 8.61 (d, $J = 5.0$ Hz, 1H), 8.73 (s, 1H), 8.91 (d, $J = 4.5$ Hz, 1H), 8.95 (d, $J = 5.0$ Hz, 1H); UV/vis (CH_2Cl_2): λ_{\max} [nm] = 728, 668 (sh), 585, 542, 510, 441; FAB-MS m/z = 750.8 (calcd. for $\text{C}_{44}\text{H}_{27}\text{Cl}_4\text{N}_4$ [$\text{M} + \text{H}]^+$ 751.0990).

NC-T(*p*CF₃)PP (2e):⁴ ^1H NMR (CDCl_3): δ –5.09 (s, 1H), –2.48 (bs, 2H), 8.05 (m, 4H), 8.11 (d, $J = 8.0$ Hz, 2H), 8.14 (d, $J = 8.0$ Hz, 2H), 8.29 (m, 4H), 8.44 (d, $J = 8.0$ Hz, 2H), 8.47 (d, $J = 8.5$ Hz, 2H), 8.52 (d, $J = 4.5$ Hz, 1H), 8.54 (d, $J = 5.0$ Hz, 1H), 8.57 (d, $J = 4.5$ Hz, 1H), 8.61 (d, $J = 5.0$ Hz, 1H), 8.76 (s, 1H), 8.93 (d, $J = 4.5$ Hz, 1H), 8.97 (d, $J = 5.0$ Hz, 1H); UV/vis (CH_2Cl_2): λ_{\max} [nm] = 725, 664 (sh), 581, 540, 510, 440; FAB-MS m/z = 887.0 (calcd. for $\text{C}_{48}\text{H}_{26}\text{F}_{12}\text{N}_4$ [$\text{M} + \text{H}]^+$ 887.2044).

NC-T(2,6-diMe)PP (2g): Methanesulfonic acid catalyst did not work well in this synthesis. Thus, $\text{BF}_3\cdot\text{OEt}_2$ was used instead. To a solution of 2,6-dimethylbenzaldehyde (940 mg, 7.01 mmol) and pyrrole (0.486 mL, 7.00 mmol) in CHCl_3 (100 mL), $\text{BF}_3\cdot\text{OEt}_2$ (0.18 mL, 1.46 mmol) was added and stirred for 3 h. After addition of DDQ (1.33 g, 5.86 mmol) and Et_3N (2 mL), the reaction mixture was stirred for further 30 min. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on alumina and silica gel columns. The yellow-red fraction containing crude **2g** was recrystallized from a $\text{CH}_2\text{Cl}_2/\text{MeOH}$ solution to afford a violet crystal; yield 44 mg (0.061 mmol, 4%). ^1H NMR (CDCl_3): δ –4.86 (s, 1H), –2.03 (s, 1H), –1.98 (s, 1H), 1.97 (m, 24H), 7.44 (m, 8H), 7.55 (m, 4H), 8.34 (d, $J = 5.0$ Hz, 1H), 8.36 (d, $J = 5.0$ Hz, 2H), 8.40 (d, $J = 4.5$ Hz, 1H), 8.57 (d, $J = 4.0$ Hz, 2H), 8.83 (s, 1H); ^{13}C NMR (CDCl_3): δ 21.70, 101.30, 114.91, 116.74, 122.32, 124.27, 125.12, 125.22, 127.06, 127.12, 127.15, 127.33, 127.84, 128.3, 128.35, 128.64, 133.86, 133.93, 134.45, 136.31, 136.76, 138.65, 138.72, 138.83, 139.10, 139.46, 139.52, 139.59, 139.61, 140.58, 140.60, 149.89, 155.88, 157.05, 157.50. UV/vis (CH_2Cl_2): λ_{\max} [nm] = 720, 655, 570, 532, 502, 434; FAB-MS m/z = 726.4 (calcd. for $\text{C}_{52}\text{H}_{46}\text{N}_4$ [$\text{M}]^+$ 726.3722).

Table S1. Crystallographic Data of **2a** and **2b**

	2a from CHCl ₃ -MeOH	2a from THF-MeOH	2a from DMF-MeOH	2b from CH ₂ Cl ₂ -hexane
CCDC number	1575545	1575546	1575559	1575565
formula	C ₄₄ H ₃₀ N ₄ ·CHCl ₃	C ₄₄ H ₃₀ N ₄ ·H ₂ O	C ₄₄ H ₃₀ N ₄ ·2C ₃ H ₇ NO	C ₄₈ H ₃₈ N ₄
FW	734.09	632.73	760.91	670.82
color	violet	violet	green	purple
habit	prism	prism	prism	prism
crystal system	triclinic	triclinic	triclinic	monoclinic
space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ /c
<i>a</i> , Å	9.6121(6)	8.7618(8)	12.6211(12)	14.3901(5)
<i>b</i> , Å	14.2479(7)	13.5724(11)	13.1779(16)	8.4196(3)
<i>c</i> , Å	14.6368(10)	14.6798(10)	13.5445(18)	15.7484(6)
α , deg	107.630(3)	74.067(3)	98.691(5)	90
β , deg	101.505(3)	85.926(2)	116.169(5)	95.333(3)
γ , deg	97.424(2)	73.962(2)	92.716(3)	90
<i>V</i> , Å ³	1833.0(2)	1613.3(2)	1982.2(4)	1899.80(12)
<i>Z</i>	2	2	2	2
radiation (λ , Å)		Mo (0.7107)		
<i>T</i> , °C	-150.0	-150.0	-150.0	-150.0
<i>D_c</i> , g/cm ³	1.330	1.303	1.275	1.173
μ , cm ⁻¹	0.289	0.079	0.079	0.069
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0741	0.0790	0.0698	0.0587
<i>wR</i> ₂ (obs data)	0.2216	0.1784	0.1923	0.1600
GOF	1.042	1.006	0.939	0.970
independent refs	7027	6116	6894	3725
refs (<i>I</i> > 2σ(<i>I</i>))	5645	3373	3582	2201
parameters	469	449	577	237

Table S2. Selected Structural Data of **2a** and **2b**

	2a from CHCl ₃ -MeOH	2a from THF-MeOH	2a from DMF-MeOH ^a	2b from CH ₂ Cl ₂ -hexane	
bond length (Å)					
N1–C1	1.429(4)	1.441(5)	1.422(5)	1.422(4)	1.431(3)
N1–C3	1.314(5)	1.333(4)	1.343(5)	1.343(5)	1.315(3)
N2–C6	1.380(3)	1.371(4)	1.367(4)	1.375(4)	1.366(2)
N2–C9	1.371(3)	1.376(4)	1.382(4)	1.375(4)	1.373(2)
N3–C11	1.372(4)	1.390(4)	1.387(4)	1.380(4)	1.376(3)
N3–C14	1.380(3)	1.373(4)	1.379(5)	1.387(4)	1.373(3)
N4–C16	1.370(3)	1.369(4)	—	—	—
N4–C19	1.372(4)	1.373(4)	—	—	—
N2···N4	4.365(4)	4.268(3)	4.175(4)	4.191(4)	4.312(2)
N3···C2	3.979(4)	4.083(4)	4.067(4)	4.072(6)	4.011(3)
bond angles (°)					
∠C1–N1–C3	106.2(2)	107.3(3)	109.3(3)	109.3(3)	107.36(18)
∠C6–N2–C9	110.9(2)	110.4(3)	106.5(3)	106.3(3)	111.10(16)
∠C11–N3–C14	105.3(2)	108.2(3)	108.8(3)	110.0(3)	107.28(17)
∠C16–N4–C19	111.3(2)	110.3(3)	—	—	—
mean deviation (Å)	0.224	0.209	0.040	0.028	0.075
dihedral angles (°) between the least square core-plane					
pyrrole 1	−23.68	−15.16	5.35	0.83	8.95
pyrrole 2	8.01	11.80	1.33	2.80	2.19
pyrrole 3	8.87	−15.93	5.35	0.83	8.95
pyrrole 4	12.27	11.00	—	—	—

^a In the asymmetric unit, there are two independent half molecules of **2a**, in which the confused pyrrole and normal one are disordered.

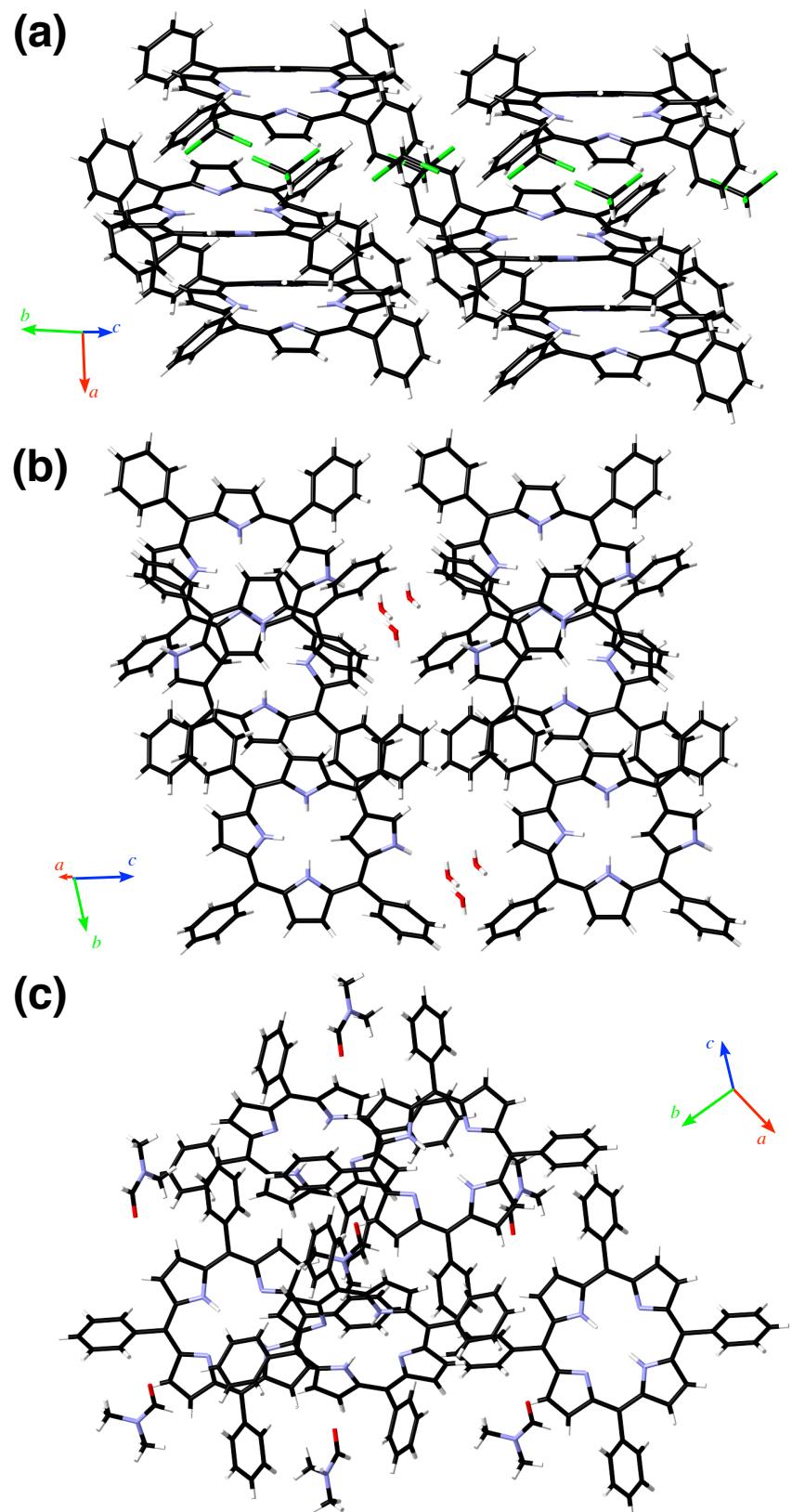


Figure S1. Crystal packing diagrams of **2a** prepared from a) $\text{CHCl}_3\text{-MeOH}$, b) $\text{THF}\text{-MeOH}$, and c) $\text{DMF}\text{-MeOH}$.

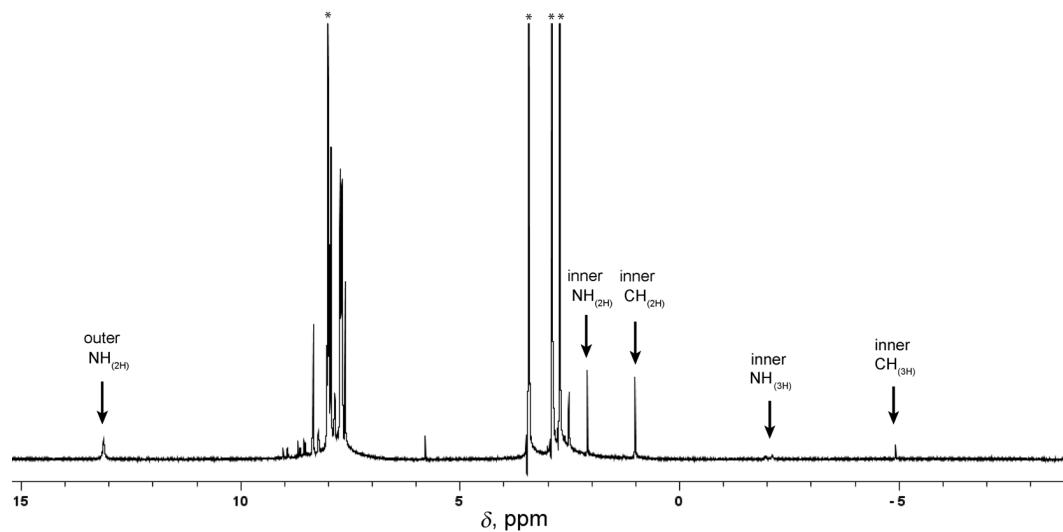


Figure S2. ^1H NMR spectrum of **2a** in $\text{DMF}-d_7$ measured with 600 MHz NMR spectrometer at room temperature.

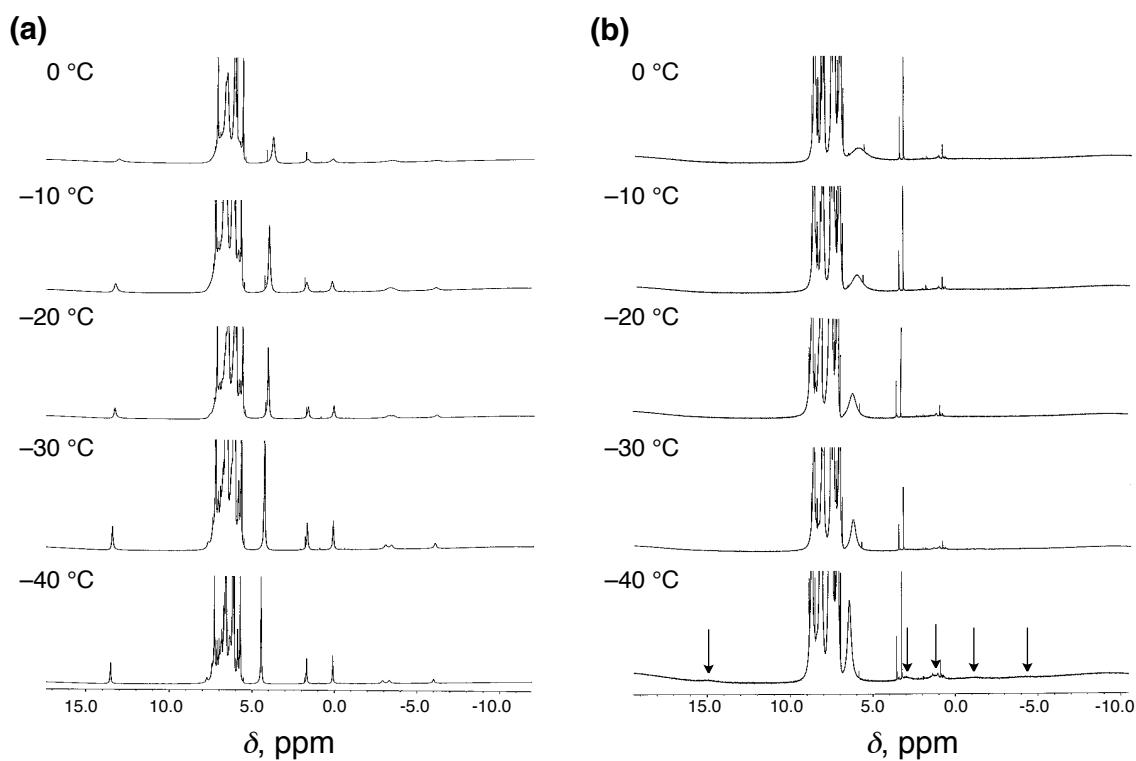


Figure S3. ^1H NMR spectrum of **2a** in $\text{pyridine}-d_5$ at various temperatures: (a) 20 mM and (b) 10 mM. Arrows in the spectrum (b: -40 °C) indicate the broadened signals of **2a**.

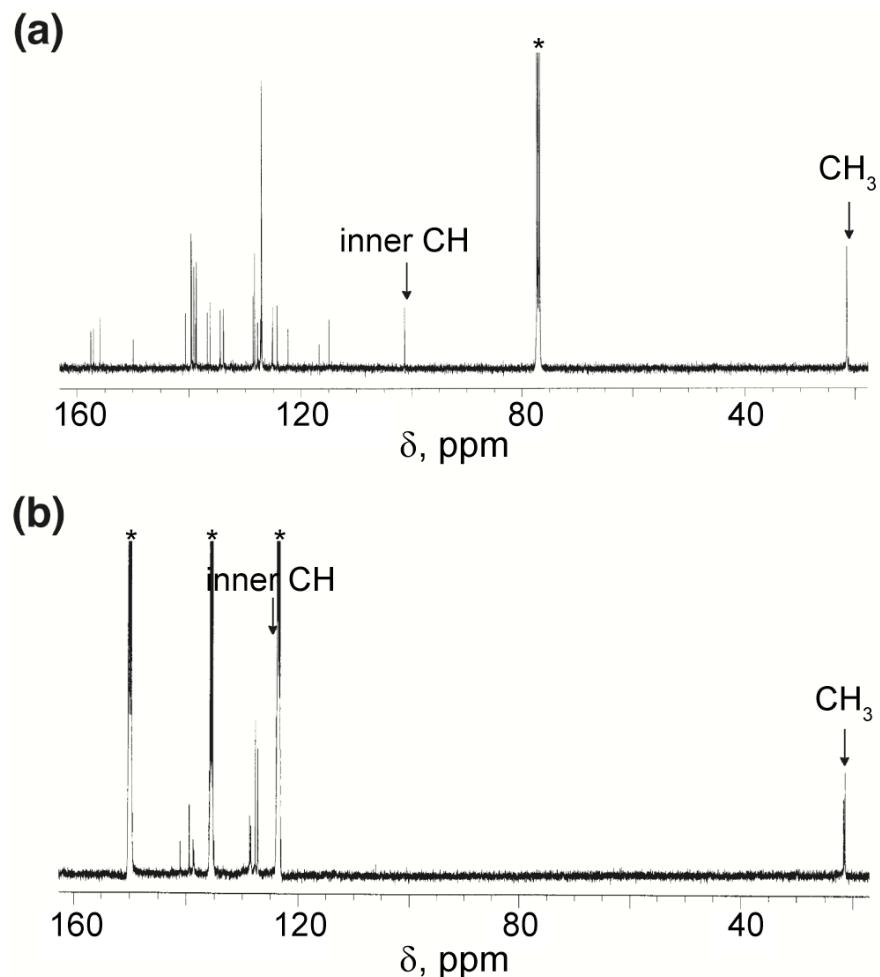
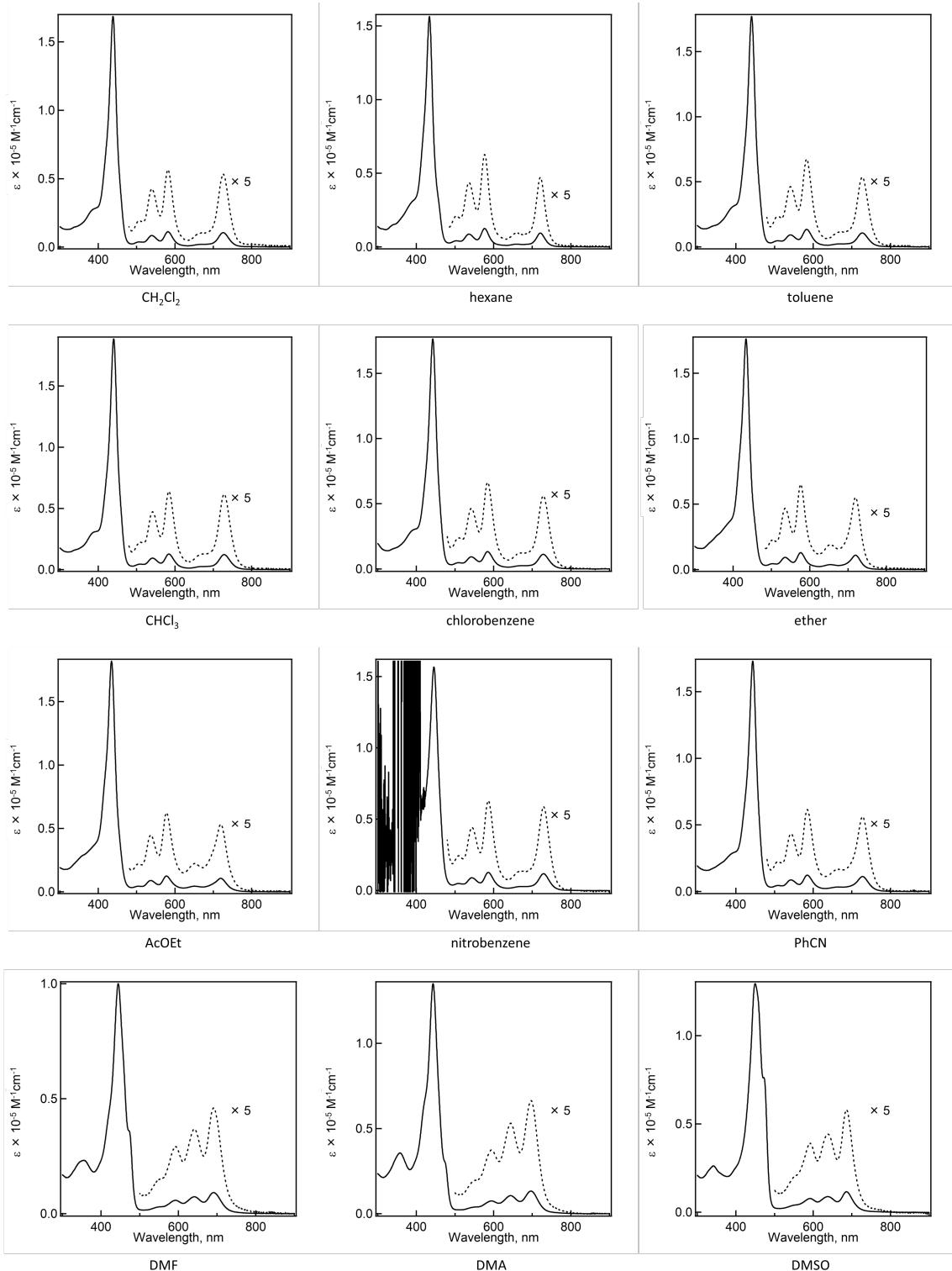


Figure S4. ^{13}C NMR spectra of **2g** at room temperature: (a) CDCl_3 and (b) pyridine- d_5 .

* solvents.



(continue)

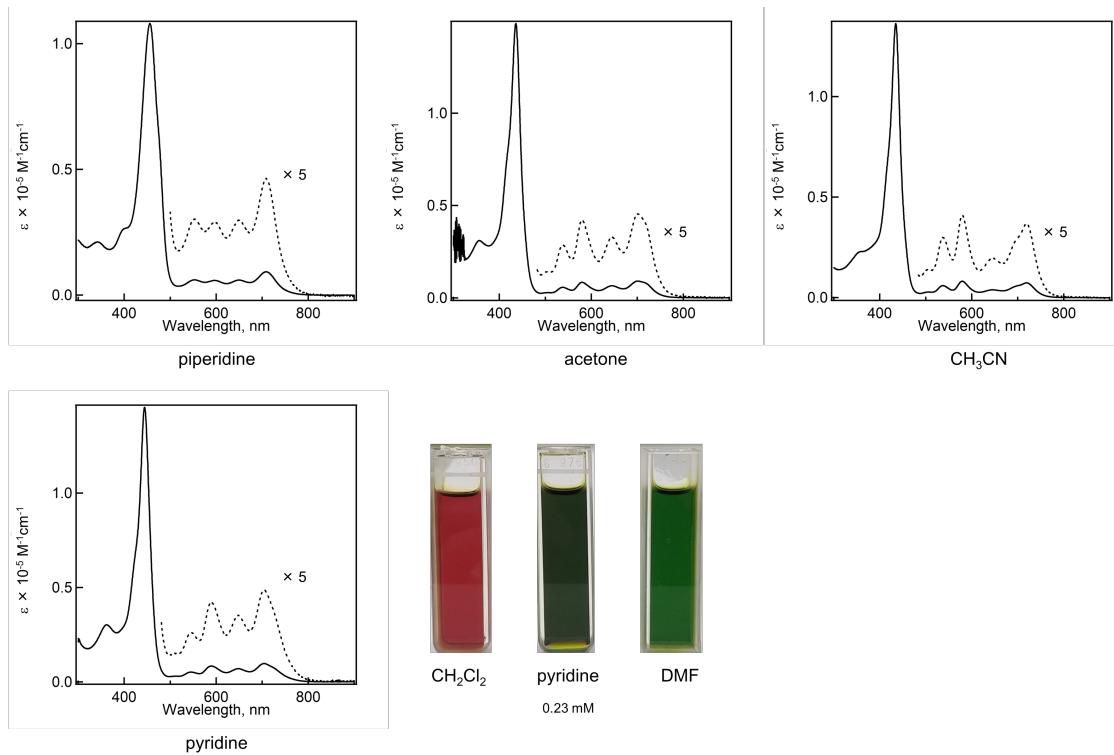


Figure S5. Absorption spectra of **2a** in various solvents.

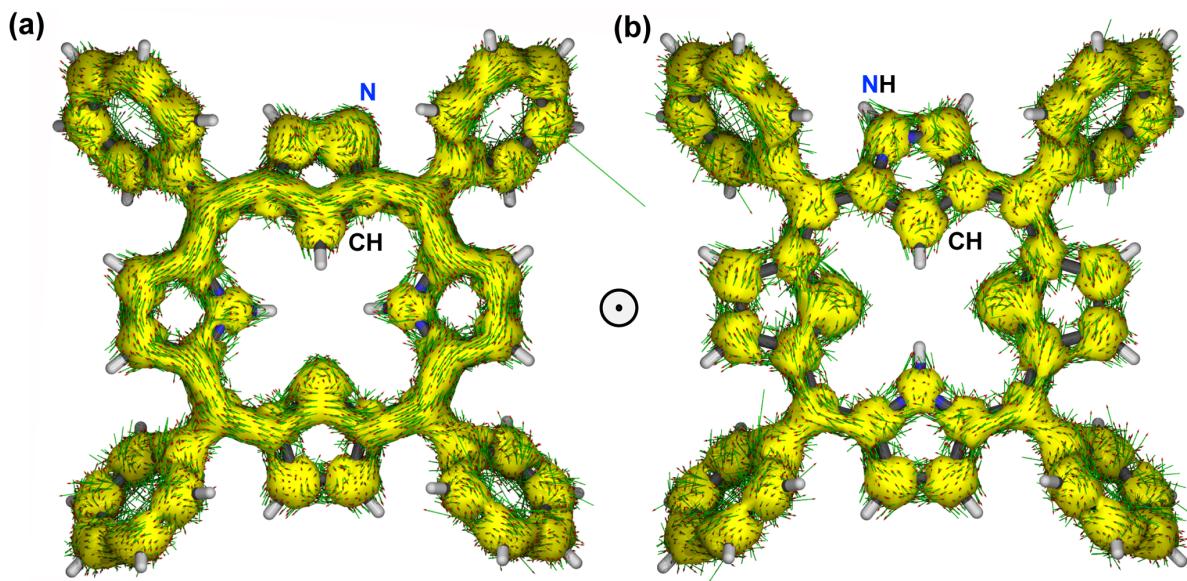


Figure S6. ACID plots of (a) **2a-3H** and (b) **2a-2H** obtained by CSGT-B3LYP/6-31G** level calculations. Isosurface value is set at 0.07.

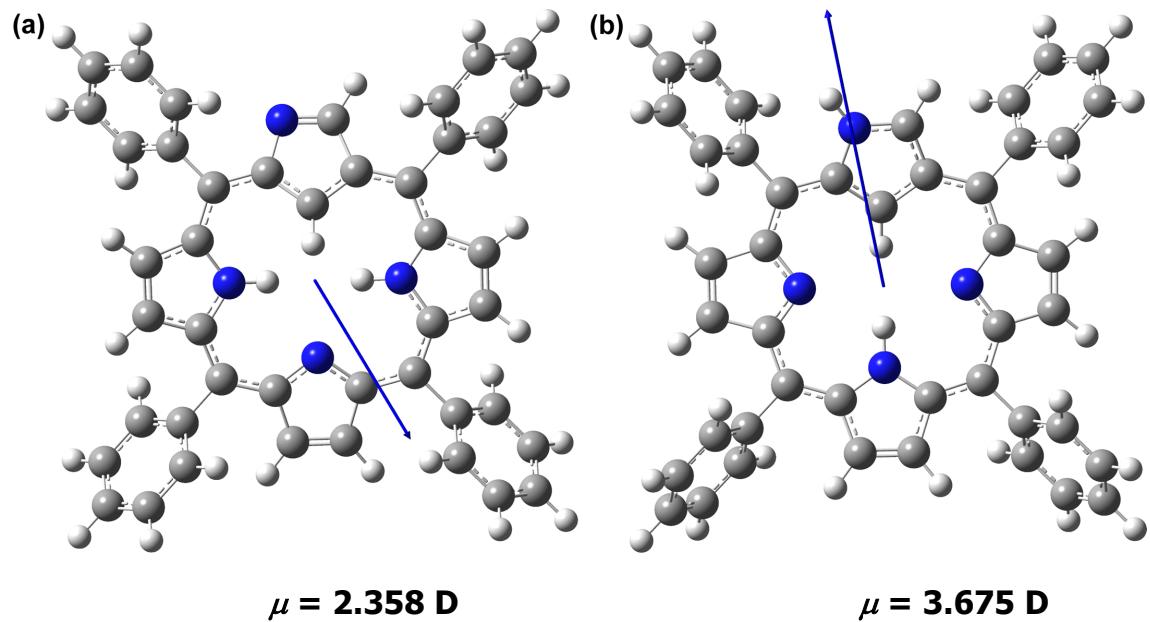


Figure S7. Caluculated dipole moments of (a) **2a-3H** and (b) **2a-2H** at the B3LYP/6-31G(d,p) level.

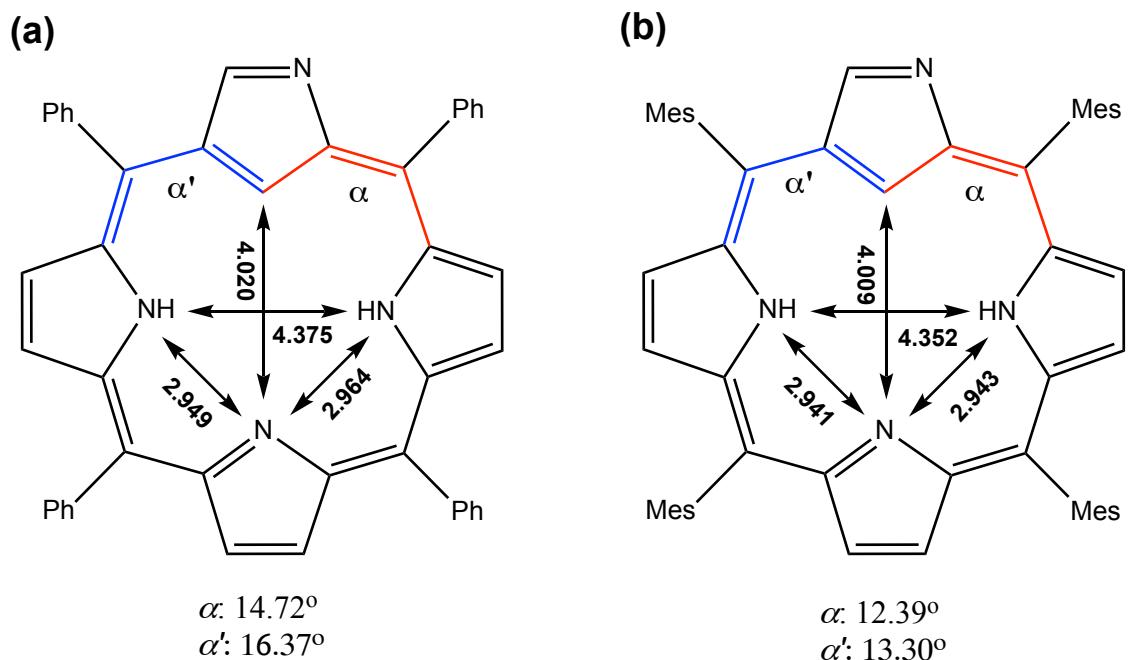


Figure S8. Comparison of $N\cdots N$ and $C\cdots N$ distances (\AA) in the optimized structures of **2a-3H** and **2g-3H** at the B3LYP/6-31G(d,p) level. α and α' denote dihedral angles shown in red and blue, respectively.

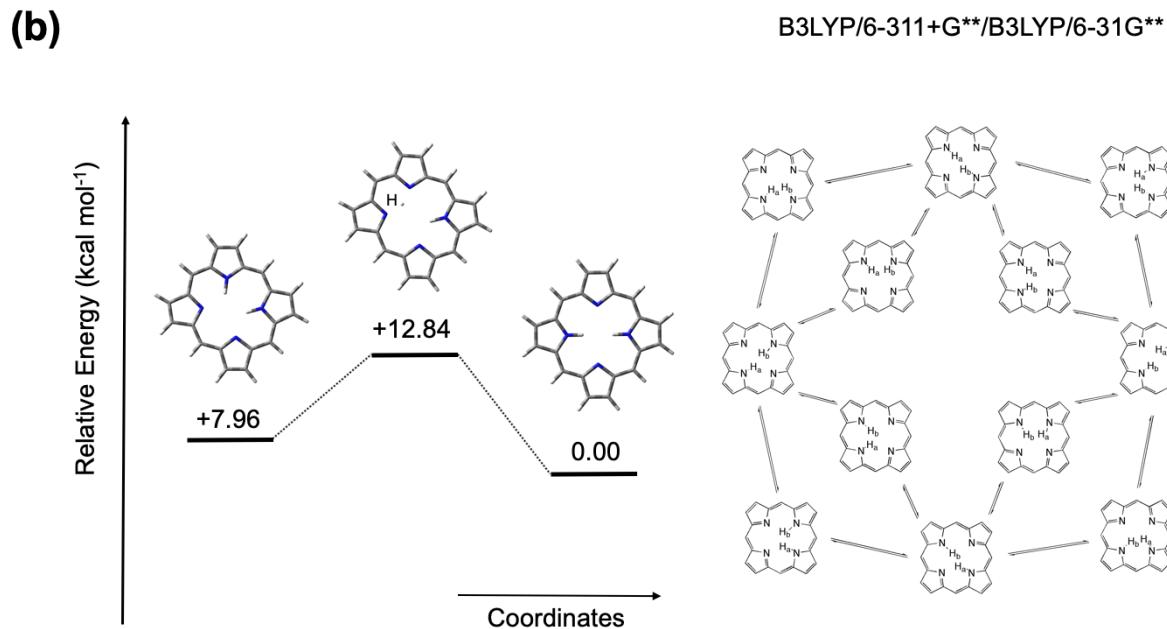
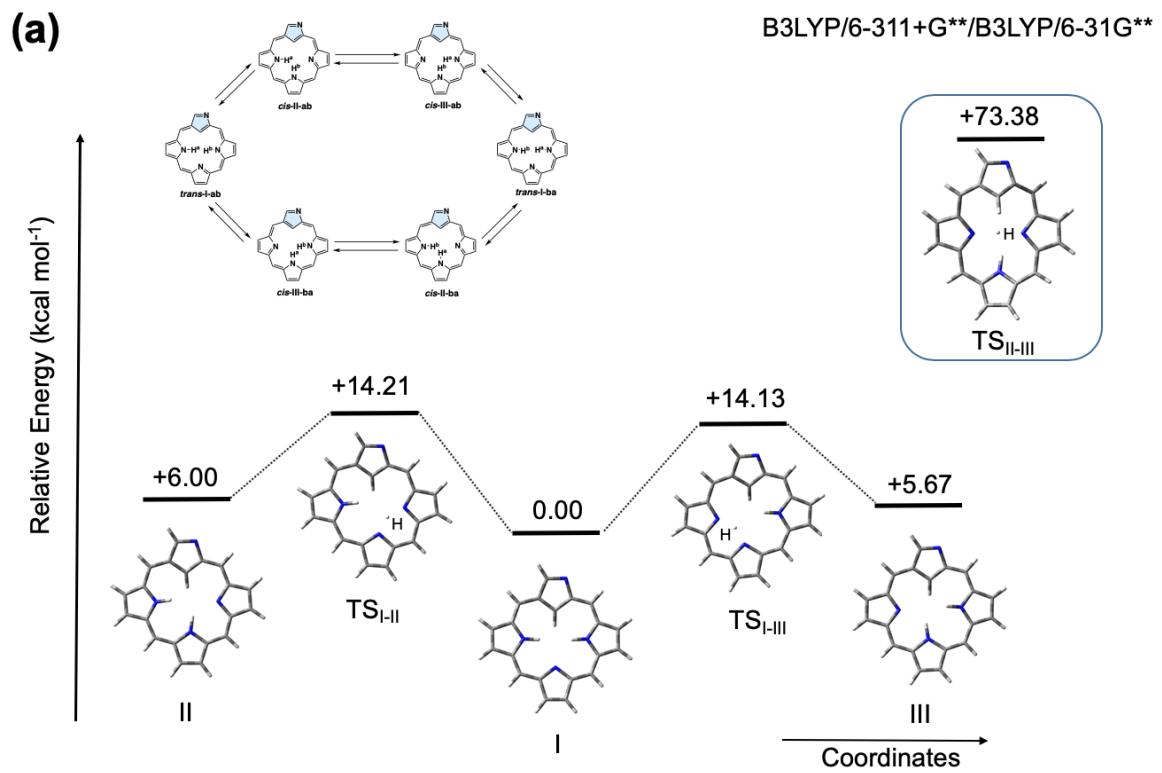
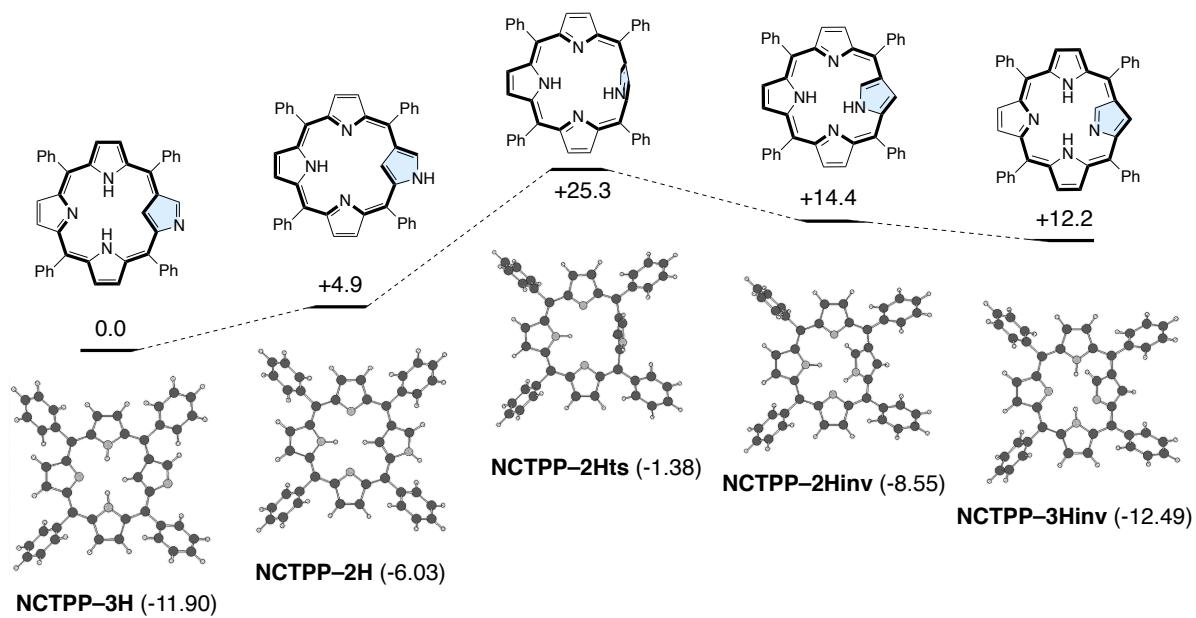


Figure S9. Energy profiles of inner-core NH tautomerism: (a) NCP and (b) Porphine.

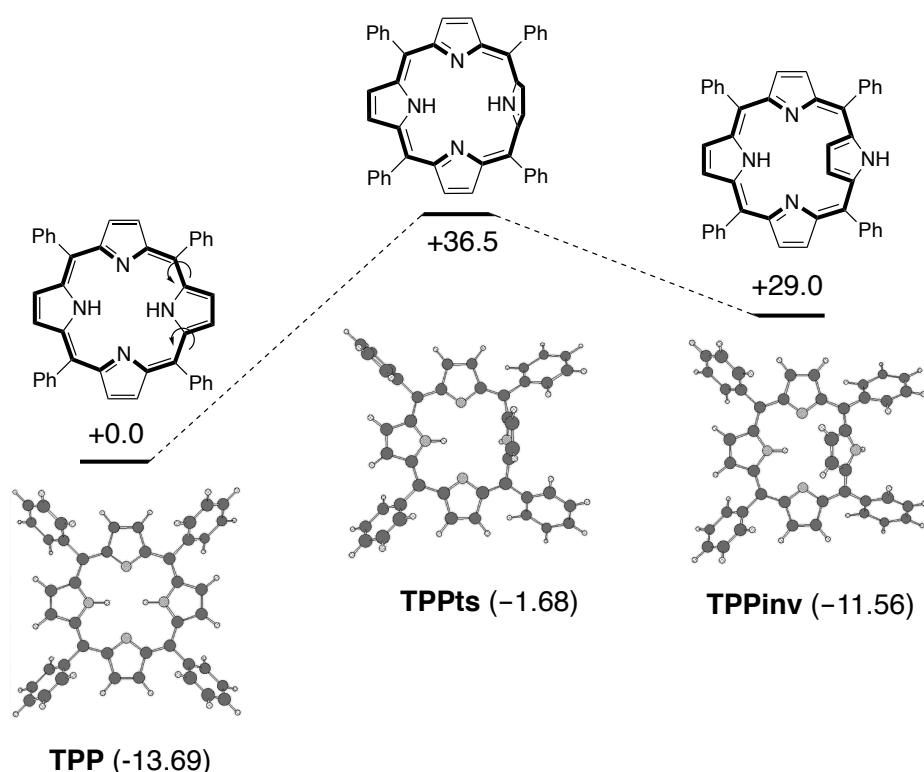
(a)

B3LYP/6-311++G**//B3LYP/6-31G**



(b)

B3LYP/6-311++G**//B3LYP/6-31G**

**Figure S10.** Energy profiles of pyrrole rotation: a) NCTPP (**2a**) and b) TPP (in kcal/mol).⁷

Cartesian coordinates for 2a-3H

Num.	Symbol	X	Y	Z
1	C	2.725914	1.278755	0.1532
2	C	4.126713	0.964473	0.419859
3	C	4.22047	-0.38409	0.452896
4	C	2.877947	-0.90131	0.202316
5	N	1.979741	0.126495	0.064858
6	C	2.273048	2.606495	-0.01106
7	C	2.616195	-2.28835	0.088868
8	C	1.342538	-2.86673	-0.07143
9	C	1.010954	-4.23662	-0.33132
10	C	-0.35566	-4.33935	-0.40125
11	C	-0.92253	-3.04116	-0.18583
12	N	0.15287	-2.18686	-0.01389
13	C	-2.27924	-2.67268	-0.13899
14	C	-2.70462	-1.3215	-0.07844
15	C	-4.00674	-0.86715	0.421526
16	N	-4.1136	0.430703	0.465915
17	C	-2.87826	0.933094	-0.01044
18	C	-2.01032	-0.12901	-0.35221
19	C	-2.64506	2.326023	-0.04442
20	C	-1.34454	2.869946	-0.16044
21	C	-0.96937	4.213469	-0.46914
22	C	0.40375	4.29514	-0.46806
23	C	0.924907	3.002385	-0.1515
24	N	-0.15947	2.176793	0.003219
25	C	-5.38149	-4.69075	-0.97362
26	C	-4.40416	-3.6972	-0.99208
27	C	-3.30656	-3.7482	-0.11364
28	C	-3.22804	-4.82215	0.791657
29	C	-4.20738	-5.81367	0.810539
30	C	-5.28643	-5.75337	-0.07338
31	C	-5.96038	5.046433	0.287318
32	C	-6.02584	3.956445	-0.58363
33	C	-4.95608	3.071564	-0.68402
34	C	-3.78915	3.264435	0.077023
35	C	-3.74017	4.362078	0.954855
36	C	-4.81532	5.243249	1.059846
37	C	3.772086	-3.23942	0.109179
38	C	4.752874	-3.20154	-0.89581

39	C	5.823993	-4.09458	-0.88348
40	C	5.934997	-5.04434	0.133561
41	C	4.967003	-5.09484	1.137789
42	C	3.895298	-4.20166	1.1247
43	C	3.286053	3.706716	-0.06411
44	C	4.256428	3.743779	-1.0792
45	C	5.193944	4.774863	-1.13417
46	C	5.179513	5.789272	-0.17533
47	C	4.219817	5.766316	0.838026
48	C	3.280862	4.736241	0.891553
49	H	4.913991	1.686104	0.577304
50	H	5.09998	-0.98137	0.640279
51	H	1.733404	-5.02688	-0.46507
52	H	-0.9314	-5.22756	-0.61179
53	H	0.123131	-1.19661	0.187953
54	H	-1.07615	-0.04029	-0.88648
55	H	-1.66892	5.002296	-0.69924
56	H	1.006095	5.163875	-0.68425
57	H	-0.05239	1.209114	0.275041
58	H	-6.21606	-4.63643	-1.66652
59	H	-4.47371	-2.87887	-1.70163
60	H	-2.40562	-4.86026	1.498696
61	H	-4.13315	-6.62868	1.524699
62	H	-6.91463	3.794461	-1.18653
63	H	-5.01236	2.224731	-1.35788
64	H	-2.86274	4.505671	1.576871
65	H	-4.76062	6.078121	1.752548
66	H	4.664527	-2.46972	-1.69283
67	H	6.569276	-4.05163	-1.67254
68	H	5.047909	-5.82634	1.936721
69	H	3.149493	-4.23735	1.913109
70	H	4.264083	2.960811	-1.83104
71	H	5.932829	4.787939	-1.93024
72	H	4.204354	6.548123	1.591951
73	H	2.54167	4.716317	1.686548
74	H	-4.79974	-1.51349	0.782176
75	H	-6.04925	-6.52616	-0.05769
76	H	-6.79811	5.733171	0.367071
77	H	5.910122	6.591695	-0.21775
78	H	6.769268	-5.73959	0.143423

Cartesian coordinates for 2a-2H

Num.	Symbol	X	Y	Z
1	C	3.061121	-0.34115	0.05003
2	C	3.880999	1.77922	0.179836
3	C	2.441645	1.852187	0.070721
4	N	1.995904	0.541998	0.013777
5	C	3.032933	-1.73589	-0.01563
6	C	1.691469	3.027486	0.022921
7	C	0.264503	3.102334	-0.05963
8	C	-0.47828	4.353951	-0.23606
9	C	-1.78887	4.013912	-0.26903
10	C	-1.84414	2.560236	-0.1127
11	N	-0.56239	2.046589	-0.00851
12	C	-3.01091	1.798677	-0.08364
13	C	-2.99479	0.35707	-0.05283
14	C	-4.08001	-0.45385	0.346824
15	N	-3.68272	-1.73754	0.335242
16	C	-2.33466	-1.82697	-0.05552
17	C	-1.91783	-0.52808	-0.31073
18	C	-1.63525	-3.07516	-0.06218
19	C	-0.24026	-3.13848	-0.10059
20	C	0.541659	-4.36261	-0.26694
21	C	1.844148	-3.98745	-0.26233
22	C	1.849102	-2.53259	-0.08606
23	N	0.598073	-2.04654	-0.01014
24	C	-4.33756	2.471297	-0.05354
25	C	-2.44188	-4.32424	0.007616
26	C	2.446047	4.321912	0.050024
27	C	2.330026	5.193999	1.144655
28	C	3.023293	6.404076	1.172273
29	C	3.84584	6.766893	0.104134
30	C	3.968334	5.911621	-0.99185
31	C	3.273528	4.7018	-1.0188
32	C	4.349696	-2.4499	-0.01921
33	C	4.714842	-3.28384	1.050292
34	C	5.935881	-3.95811	1.047862
35	C	6.816846	-3.81223	-0.0253
36	C	6.46666	-2.9886	-1.09615
37	C	5.24426	-2.31571	-1.09327
38	C	4.250504	0.470787	0.165919

39	C	-3.49568	-4.55099	-0.89927
40	C	-2.1951	-5.2969	0.994165
41	C	-2.96467	-6.45735	1.062461
42	C	-4.26402	-5.71277	-0.82925
43	C	-4.00173	-6.67036	0.152172
44	C	-5.33965	2.120783	-0.97778
45	C	-4.63729	3.453128	0.90861
46	C	-5.88806	4.068286	0.937884
47	C	-6.58822	2.740356	-0.95062
48	C	-6.86783	3.716334	0.007806
49	H	4.527022	2.639194	0.263708
50	H	1.020469	0.262244	0.03514
51	H	-0.04767	5.339413	-0.33804
52	H	-2.63548	4.668041	-0.41829
53	H	-4.24304	-2.5297	0.611797
54	H	-0.93969	-0.25026	-0.64559
55	H	0.142184	-5.35698	-0.40521
56	H	2.714433	-4.61679	-0.37823
57	H	1.69546	4.911829	1.979464
58	H	2.924076	7.061641	2.031303
59	H	4.600514	6.188041	-1.83098
60	H	3.361854	4.043715	-1.87808
61	H	4.035022	-3.39426	1.889832
62	H	6.201237	-4.59388	1.887846
63	H	7.142234	-2.87358	-1.9391
64	H	4.969211	-1.68506	-1.93342
65	H	5.251121	0.073507	0.236628
66	H	-3.68801	-3.82159	-1.68062
67	H	-1.40196	-5.12531	1.714302
68	H	-2.75877	-7.19301	1.83459
69	H	-5.06186	-5.87395	-1.54855
70	H	-5.12105	1.374559	-1.73526
71	H	-3.88483	3.715336	1.644977
72	H	-6.09988	4.818486	1.694368
73	H	-7.34132	2.465154	-1.68355
74	H	-5.07447	-0.17162	0.658188
75	H	-4.60079	-7.57441	0.207634
76	H	7.767682	-4.33719	-0.02739
77	H	4.385714	7.709105	0.125414
78	H	-7.84145	4.196995	0.030763

Cartesian coordinates for 2g-3H

Num.	Symbol	X	Y	Z
1	C	2.722512	1.285662	0.062704
2	C	4.145918	0.969909	0.143963
3	C	4.244018	-0.37936	0.132396
4	C	2.880883	-0.89593	0.04414
5	N	1.97222	0.133272	0.014719
6	C	2.262984	2.619297	0.011679
7	C	2.619195	-2.28377	-0.02742
8	C	1.344052	-2.86763	-0.11912
9	C	1.00396	-4.25646	-0.22843
10	C	-0.36503	-4.358	-0.26208
11	C	-0.9225	-3.04026	-0.17843
12	N	0.158465	-2.17787	-0.11005
13	C	-2.27781	-2.67761	-0.13149
14	C	-2.71279	-1.33392	-0.12008
15	C	-4.04916	-0.8732	0.278303
16	N	-4.16145	0.425202	0.290931
17	C	-2.89133	0.921855	-0.1008
18	C	-2.00827	-0.14356	-0.37839
19	C	-2.64801	2.308455	-0.10492
20	C	-1.35169	2.858204	-0.13993
21	C	-0.99198	4.241549	-0.21209
22	C	0.37905	4.339844	-0.17511
23	C	0.91476	3.016323	-0.07326
24	N	-0.15824	2.162041	-0.06696
25	C	-4.93457	-5.2179	-1.09134
26	C	-3.99029	-4.19178	-1.195
27	C	-3.29426	-3.78046	-0.0376
28	C	-3.56216	-4.39986	1.20235
29	C	-4.52078	-5.41718	1.259627
30	C	-5.21906	-5.84149	0.126499
31	C	-5.92879	5.116664	0.101442
32	C	-5.43593	4.671711	-1.12723
33	C	-4.38628	3.750947	-1.21383
34	C	-3.80191	3.267421	-0.02621
35	C	-4.2884	3.694949	1.225542
36	C	-5.34032	4.614492	1.265249
37	C	3.784471	-3.23781	-0.01548
38	C	4.400779	-3.61737	-1.2268

39	C	5.468781	-4.52047	-1.19351
40	C	5.947614	-5.05605	0.004867
41	C	5.322094	-4.66836	1.192819
42	C	4.250495	-3.76945	1.205949
43	C	3.277811	3.731638	0.037896
44	C	3.835104	4.209679	-1.16754
45	C	4.773538	5.245731	-1.11947
46	C	5.175367	5.824619	0.087418
47	C	4.613453	5.334621	1.268919
48	C	3.669979	4.301462	1.267497
49	H	4.94378	1.696458	0.196544
50	H	5.138267	-0.98419	0.173589
51	H	1.725393	-5.0586	-0.27479
52	H	-0.95577	-5.25838	-0.34714
53	H	0.143324	-1.18048	0.055054
54	H	-1.05704	-0.06159	-0.87966
55	H	-1.70795	5.046305	-0.29019
56	H	0.97643	5.238568	-0.21218
57	H	-0.02916	1.172264	0.092659
58	H	-5.46109	-5.53728	-1.98803
59	H	-4.72673	-5.88854	2.218095
60	H	-5.87983	5.047721	-2.04655
61	H	-5.71116	4.943573	2.23368
62	H	5.937293	-4.8125	-2.13086
63	H	5.675502	-5.07632	2.137367
64	H	5.202645	5.607377	-2.05144
65	H	4.91678	5.765664	2.220514
66	H	-4.86849	-1.51936	0.577311
67	C	-3.71483	3.14849	2.511065
68	H	-3.91237	2.073819	2.587093
69	H	-2.62934	3.283742	2.564552
70	H	-4.16061	3.641153	3.379327
71	C	-3.90145	3.29103	-2.57017
72	H	-2.84592	3.536665	-2.73105
73	H	-3.99435	2.205039	-2.67716
74	H	-4.48094	3.759934	-3.36979
75	C	-7.0853	6.085955	0.171912
76	H	-7.14326	6.707199	-0.72688
77	H	-8.04175	5.556006	0.263558
78	H	-7.00019	6.74977	1.037967
79	C	3.095678	3.808696	2.576427

80	H	2.010738	3.954043	2.618999
81	H	3.276307	2.737841	2.716151
82	H	3.53979	4.34102	3.421577
83	C	3.44109	3.616151	-2.50115
84	H	3.691275	2.551317	-2.55579
85	H	2.362606	3.695951	-2.67382
86	H	3.953405	4.12658	-3.32088
87	C	6.167303	6.963546	0.110645
88	H	5.664046	7.930741	-0.01315
89	H	6.712439	7.000528	1.05842
90	H	6.898918	6.874571	-0.69828
91	C	3.927684	-3.06431	-2.55208
92	H	2.868925	-3.2831	-2.72599
93	H	4.034569	-1.975	-2.5915
94	H	4.50169	-3.49049	-3.37902
95	C	3.612823	-3.38177	2.520897
96	H	3.659727	-2.30001	2.684721
97	H	2.553897	-3.66003	2.55263
98	H	4.115844	-3.87341	3.357674
99	C	7.123721	-6.00382	0.018675
100	H	8.069916	-5.46024	0.133926
101	H	7.056288	-6.71447	0.848006
102	H	7.189399	-6.57439	-0.91254
103	C	-2.84267	-3.98095	2.465091
104	H	-1.77858	-4.23877	2.42806
105	H	-2.90098	-2.89906	2.621294
106	H	-3.276	-4.47349	3.339388
107	C	-3.72265	-3.55307	-2.5393
108	H	-4.00372	-2.49472	-2.54495
109	H	-2.66046	-3.59814	-2.80199
110	H	-4.28854	-4.05593	-3.32776
111	C	-6.27073	-6.92155	0.220192
112	H	-6.06323	-7.61188	1.043121
113	H	-7.26449	-6.49199	0.398466
114	H	-6.3311	-7.50339	-0.70453

Cartesian coordinates for NCP-I

Num.	Symbol	X	Y	Z
1	C	1.037441	2.809800	-0.057092
2	C	0.597224	4.199740	-0.106512
3	C	-0.755758	4.174423	-0.112052
4	C	-1.143862	2.768695	-0.064464
5	N	-0.039238	1.963066	-0.036728
6	C	2.390963	2.456392	-0.021636
7	C	-2.485899	2.365353	-0.036452
8	C	-2.980107	1.062671	0.022765
9	C	-4.335054	0.597716	0.053697
10	C	-4.311252	-0.775032	0.079316
11	C	-2.944545	-1.206777	0.074626
12	N	-2.188092	-0.052671	0.051724
13	C	-2.438264	-2.505242	0.052909
14	C	-1.078738	-2.844948	0.075415
15	C	-0.496700	-4.144811	-0.290464
16	N	0.803108	-4.133057	-0.303690
17	C	1.179873	-2.811014	0.053921
18	C	0.038465	-2.035060	0.325189
19	C	2.518569	-2.417468	0.020352
20	C	2.976394	-1.097804	0.053560
21	C	4.325115	-0.620770	0.082738
22	C	4.301815	0.754359	0.075213
23	C	2.934045	1.170733	0.029664
24	C	2.181126	0.028343	0.030388
25	N	1.251157	5.059739	-0.130383
26	H	-1.441211	5.009343	-0.141187
27	H	-5.203659	1.238415	0.050333
28	H	-5.158592	-1.443427	0.107487
29	H	0.032235	-1.072849	0.805341
30	H	5.193910	-1.260518	0.117226
31	H	5.147769	1.424367	0.094184
32	H	-1.061076	-5.031438	-0.560540
33	H	3.103719	3.272826	-0.032438
34	H	3.263272	-3.195741	-0.101237
35	H	-3.169477	-3.300757	-0.047200
36	H	-3.228044	3.154788	-0.060254
37	H	-1.186826	0.026072	-0.057840
38	H	1.180149	0.073689	-0.099514

Cartesian coordinates for NCP-II

Num.	Symbol	X	Y	Z
1	C	2.043726	2.369731	-0.023890
2	C	1.985447	3.796343	-0.099406
3	C	0.666909	4.165030	-0.142328
4	C	-0.146334	2.981942	-0.092240
5	N	0.736127	1.922774	-0.026764
6	C	3.157037	1.539018	0.039256
7	C	-1.544116	2.976366	-0.086133
8	C	-2.441804	1.908528	-0.026292
9	C	-3.865499	1.954824	0.117737
10	C	-4.341546	0.664608	0.162226
11	C	-3.233942	-0.229994	0.056406
12	N	-2.109914	0.575096	-0.046889
13	C	-3.181492	-1.622839	0.053136
14	C	-1.991357	-2.367146	0.059454
15	C	-1.839926	-3.800049	-0.258242
16	N	-0.600122	-4.186383	-0.280882
17	C	0.167253	-3.026444	0.024971
18	C	-0.674457	-1.933284	0.265996
19	C	1.560238	-3.037562	-0.000009
20	C	2.404822	-1.914740	0.062928
21	C	3.859338	-1.995853	0.050937
22	C	4.321034	-0.717705	0.076213
23	C	3.141755	0.134639	0.085702
24	C	2.005199	-0.610577	0.090411
25	N	2.848995	4.443684	-0.118086
26	H	0.267373	5.166036	-0.202975
27	H	-4.440321	2.865140	0.195842
28	H	-5.367600	0.353776	0.288923
29	H	-0.314603	-0.999353	0.649407
30	H	4.433439	-2.911207	0.028555
31	H	5.346697	-0.377420	0.069547
32	H	-2.653890	-4.481097	-0.485427
33	H	4.123445	2.029911	0.033839
34	H	2.035822	-4.004266	-0.131467
35	H	-4.130250	-2.147074	0.005222
36	H	-1.998426	3.959784	-0.103075
37	H	0.585276	0.919566	0.046286
38	H	-1.237491	0.203670	-0.386250

Cartesian coordinates for NCP-III

Num.	Symbol	X	Y	Z
1	C	0.06568	2.984674	-0.089014
2	C	-0.781589	4.145259	-0.147131
3	C	-2.087953	3.74043	-0.113436
4	C	-2.107842	2.310877	-0.033643
5	N	-0.788387	1.900355	-0.028534
6	C	1.459810	3.018637	-0.073679
7	C	-3.198889	1.454188	0.028388
8	C	-3.147560	0.048483	0.083415
9	C	-4.308017	-0.831455	0.072198
10	C	-3.818043	-2.098383	0.061693
11	C	-2.365244	-1.984389	0.082041
12	N	-1.995917	-0.667270	0.103441
13	C	-1.492436	-3.079299	0.027575
14	C	-0.093660	-3.024533	0.037065
15	C	0.854428	-4.108093	-0.271237
16	N	2.092494	-3.711297	-0.272448
17	C	2.050783	-2.321189	0.032763
18	C	0.723120	-1.913648	0.257104
19	C	3.212195	-1.544836	0.020482
20	C	3.227025	-0.147307	0.037519
21	C	4.308905	0.767702	0.183823
22	C	3.802696	2.049880	0.156871
23	C	2.387111	1.972190	-0.018013
24	C	2.087444	0.632338	-0.077568
25	N	-0.409491	5.156789	-0.208497
26	H	-2.969294	4.363016	-0.140856
27	H	-5.340984	-0.51429	0.054991
28	H	-4.372310	-3.026123	0.042722
29	H	0.359630	-0.982112	0.642185
30	H	5.338327	0.477066	0.328886
31	H	4.353963	2.971144	0.268461
32	H	1.231695	0.250790	-0.447139
33	H	0.587655	-5.134596	-0.501404
34	H	1.887707	4.013984	-0.076892
35	H	4.164354	-2.058943	-0.043329
36	H	-1.958945	-4.054666	-0.081054
37	H	-4.177531	1.919797	0.015132
38	H	-0.607389	0.904089	0.063836

Cartesian coordinates for NCP-TS_{I,II}

Num.	Symbol	X	Y	Z
1	C	2.534432	1.895200	-0.016476
2	C	2.713762	3.317756	-0.081187
3	C	1.470508	3.860463	-0.137197
4	C	0.501674	2.782262	-0.102788
5	N	1.187934	1.580230	-0.035165
6	C	3.520509	0.920947	0.054443
7	C	-0.862112	3.100418	-0.108519
8	C	-2.000464	2.299693	-0.040673
9	C	-3.375696	2.687105	0.064773
10	C	-4.139351	1.543925	0.129392
11	C	-3.264246	0.415211	0.074345
12	N	-1.988852	0.936325	-0.026170
13	C	-3.517624	-0.955277	0.098211
14	C	-2.494510	-1.912982	0.122888
15	C	-2.595875	-3.328488	-0.268204
16	N	-1.440371	-3.921383	-0.327784
17	C	-0.487610	-2.929967	0.031422
18	C	-1.120030	-1.727658	0.350713
19	C	0.880770	-3.171172	-0.030886
20	C	1.925732	-2.241580	0.035545
21	C	3.304822	-2.672258	0.033092
22	C	4.093024	-1.561828	0.080135
23	C	3.199840	-0.438857	0.088387
24	C	1.894617	-0.857345	0.074380
25	N	3.667059	3.824748	-0.081100
26	H	1.204443	4.905924	-0.192228
27	H	-3.723729	3.708317	0.097322
28	H	-5.212139	1.481421	0.232325
29	H	-0.616983	-0.899264	0.814329
30	H	3.615158	-3.706582	0.004256
31	H	5.171251	-1.504850	0.088882
32	H	-3.515240	-3.842855	-0.528473
33	H	4.559845	1.222712	0.064455
34	H	1.180607	-4.200926	-0.195431
35	H	-4.551904	-1.274911	0.031112
36	H	-1.063478	4.164749	-0.143118
37	H	-1.183114	0.381218	-0.263948
38	H	1.169601	0.278024	0.010292

Cartesian coordinates for NCP-TS_{I,III}

Num.	Symbol	X	Y	Z
1	C	-0.544335	2.773371	-0.091082
2	C	-1.528782	3.838069	-0.130177
3	C	-2.764143	3.277701	-0.096830
4	C	-2.565180	1.856506	-0.036567
5	N	-1.215659	1.559739	-0.039866
6	C	0.812125	3.111156	-0.081341
7	C	-3.540039	0.869974	0.025913
8	C	-3.200042	-0.484473	0.074356
9	C	-4.080027	-1.619830	0.073186
10	C	-3.279102	-2.720192	0.054074
11	C	-1.903603	-2.273228	0.062422
12	N	-1.890506	-0.885934	0.081302
13	C	-0.847675	-3.185816	0.012602
14	C	0.522639	-2.919179	0.051970
15	C	1.626952	-3.822863	-0.302609
16	N	2.785636	-3.232521	-0.279137
17	C	2.522578	-1.884493	0.084415
18	C	1.146722	-1.708192	0.337274
19	C	3.525206	-0.914574	0.048798
20	C	3.250973	0.455659	0.042199
21	C	4.108886	1.590478	0.148481
22	C	3.329590	2.727172	0.113341
23	C	1.964384	2.325439	-0.027194
24	C	1.971760	0.962594	-0.067544
25	N	-1.276786	4.887529	-0.175042
26	H	-3.724674	3.770714	-0.107441
27	H	-5.158882	-1.575413	0.069348
28	H	-3.578002	-3.758333	0.039011
29	H	0.653380	-0.872424	0.797574
30	H	5.180083	1.537300	0.270302
31	H	3.663086	3.750794	0.190451
32	H	1.525221	-4.865080	-0.587107
33	H	0.998015	4.178884	-0.090273
34	H	4.556035	-1.236940	-0.038365
35	H	-1.152503	-4.220434	-0.116225
36	H	-4.583290	1.157551	0.023499
37	H	-1.179989	0.256221	0.018924
38	H	1.176924	0.406384	-0.337323

Cartesian coordinates for NCP-TS_{II-III}

Num.	Symbol	X	Y	Z
1	C	-3.121314	-1.066564	0.240209
2	C	-4.419999	0.796800	0.249577
3	C	-3.103497	1.138738	-0.206816
4	C	-2.400616	-0.016737	-0.238644
5	N	-2.469376	-2.269587	0.362883
6	C	-2.407658	2.310619	-0.413843
7	C	-1.006715	2.440047	-0.354781
8	C	-0.523581	3.786750	-0.477609
9	C	0.793620	3.774470	-0.190972
10	C	1.167006	2.420603	0.103421
11	C	0.049285	1.553106	-0.040834
12	N	2.514570	2.229846	0.422771
13	C	3.130428	1.006464	0.663436
14	C	4.417075	0.556071	0.092102
15	C	4.400412	-0.709565	-0.196437
16	N	3.096417	-1.143765	0.182536
17	C	2.400486	-0.147249	0.866362
18	C	2.459975	-2.215940	-0.396581
19	C	1.067988	-2.418392	-0.381098
20	C	0.624536	-3.766120	-0.523416
21	C	-0.681033	-3.801102	-0.153496
22	C	-1.097802	-2.457425	0.090781
23	C	-0.010892	-1.563849	-0.064347
24	C	-4.425695	-0.551067	0.536145
25	N	-5.224628	1.499242	0.403763
26	H	-1.513933	-0.120711	-0.698796
27	H	-1.151203	4.628768	-0.728271
28	H	1.482214	4.605475	-0.158957
29	H	1.426726	-0.223359	1.308153
30	H	1.271239	-4.589170	-0.788387
31	H	-1.337369	-4.656189	-0.087585
32	H	-5.238004	-1.124058	0.956317
33	H	5.262985	1.190707	-0.149592
34	H	-2.958922	3.234346	-0.527345
35	H	3.131019	3.115285	0.299979
36	H	3.050819	-2.96250	-0.917099
37	H	-3.031481	-3.158957	0.615511
38	H	0.070639	-0.018727	-0.015524

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