Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Phenanthrene cyclocarbonylation – Core post-synthetic modification of phenanthriporphyrin

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Supporting Information

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Materials

Chemicals and solvents like methanol were of at least pure grade and used without further purification unless otherwise specified. Dichloromethane was distilled over CaH_2. Toluene was dried for 48 hours over anhydrous magnesium sulfate. Toluene was filtered through a short (4 cm) column with active, basic Al_2O_3 immediately before use. 5,6-Dimethoxyphenanthriporphyrin **1** and azaacenephenatriporphyrinoid **2** were synthesized according to the previously described procedures.[1,2]

Instrumentation

NMR spectroscopy

NMR spectra were measured on Bruker Avance III 500 MHz and Bruker Avance III 600 MHz spectrometers. ^{1}H and ^{13}C shifts were referenced to the residual resonances of deuterated dichloromethane – 5.32 ppm, 54.0, and chloroform – 7.24 ppm.

Electronic spectroscopy

UV-Vis absorption spectra were recorded in CH_2Cl_2 solutions on Varian Carry-50 Bio spectrophotometers.

Mass Spectrometry

Mass spectra (High Resolution and Accurate Mass) were recorded on Bruker apex ultra FT-ICR using the electrospray technique.

X-ray crystallography

The X-ray diffraction data for **6** were collected on Xcalibur PX diffractometer with an Onyx detector (Cu-Kα radiation, λ= 1.54184 Å). Single crystals suitable for the SC-XRD experiment were obtained by slow solvent evaporation: dichloromethane/methanol. The data were collected at 110(2) K. Data reduction and analysis were carried out with the CrysAlis 'RED' program.[3] Structures were solved with direct methods using the SHELXT program and refined using all F^2 data, as implemented by the SHELXL program.[4]

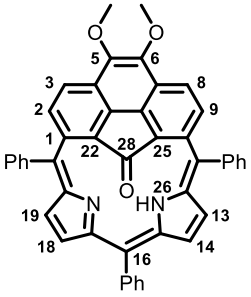
DFT calculations

Geometry optimizations were carried out within unconstrained C_1 symmetry in vacuo, with starting preoptimized models using Gaussian 16 software.[5] Calculations were performed at the B3LYP/6-31G(d,p) level of theory.[6,8] Harmonic frequencies were calculated using analytical second derivatives as verification of local minimum achievement with no negative frequencies observed. NMR shifts were calculated for optimized structures using the GIAO method and B3LYP/6-31G(d,p) set with TMS shieldings as a reference. Relative

energies were calculated including zero-point correction. Charge distributions were derived from population analysis using the NBO program.[6] The anisotropy of the Induced Current Density (AICD) plots were produced using the output file from Gaussian 09 calculations, CSGT method, iop(10/93=1).[7]

Synthesis

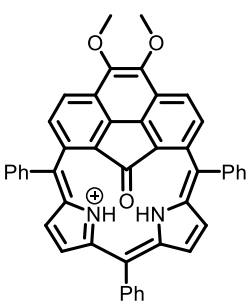
Ketophenathriporphyrin (7).



In a 120 mL high-pressure vessel equipped with magnetic stirring, a small amount of iodine (ca. 15 mg, 0.059 mmol) was dissolved in dry toluene (30 mL). The solution was degassed by bubbling N_2 for 15 minutes, then 11,16,21-triphenyl-5,6-dimethoxyphenanthriporphyrin **1** (30 mg, 0.032 mmol) and $[Fe(CO)_5]$ (1.5 ml, 11.4 mmol) were added. The solution was then refluxed for 1.5 h. After that, the solution was cooled, filtered through a piece of cotton – residue on the cotton was washed with $CHCl_3$ (stabilized with EtOH) – and evaporated under reduced pressure. The claret residue was dissolved in a small amount of dichloromethane and filtered through a short (3 cm) layer of basic, deactivated Al_2O_3 (5 ml H_2O/100 g), and the solvent was evaporated. The mixture was purified by column chromatography on silica gel with *n*-hexane/ dichloromethane as the eluent (7:3 v/v with 1% of TEA). The first green fraction that eluted was unreacted phenanthriporphyrin **1** (ca. 9.0 mg, 30% recovery). The desired product eluted as the second blue fraction, which subsequently, was recrystallized from dichloromethane/methanol yielding a blue solid. Yield: 19.7 mg (63%).

^{1}H NMR (600 MHz, CD_2Cl_2, 300 K): δ 11.28 (br, 1H, 27-NH), 7.51–7.43 (m, 10H, 11,21-Ph {7.46-*o*-Ph}), 7.41–7.33 (m, 5H, 16-*m*, *p*-Ph and 3,8-H {7.39 (d, 2H, ^3J = 8.8 Hz, 3,8-H}), 7.32–7.29 (m, 2H, 16-*o*-Ph), 6.79 (d, 2H, ^3J = 8.8 Hz, 2,9-H), 6.62 (d, 2H, ^3J = 5.2 Hz, 13,19-H), 6.27 (d, 2H, ^3J = 5.2 Hz, 14,18-H), 3.94 (s, 6H, 5,6-OCH_3). **^{13}C NMR** (151 MHz, CD_2Cl_2, 300 K): δ 201.9 (C=O), 162.5 (12,20), 152.7 (15,17), 147.8 (5,6), 140.9, 138.4, 136.2 (1,10), 133.6 (13,19), 133.5 (4,7), 133.1 (2,9), 132.9, 132.6 (11,21-Ph), 132.0 (16-*o*-Ph), 131.4 (11,21), 129.5 (14,18), 128.7 (11,21-Ph), 128.68 (11,21- Ph), 128.6 (16-*m*-Ph), 127.9 (16-*p*-Ph), 124.9 (3,8), 124.88, 124.4, 114.1 (16), 61.6 (5,6-OCH_3). **HRMS** (ESI) *m/z*: 659.2322 $[M+H]^+$, calcd for $C_{46}H_{31}N_2O_3^+$: 659.2329. **UV-Vis** (CH_2Cl_2, 298 K), λ_{max} (log ε) 355 (4.7), 360 (4.7), 445 (3.7), 480 (3.65), 555 (3.7), 600 (3.9), 720 (3.8).

Monocationic form of ketophenathriporphyrin (7-H$^+$).

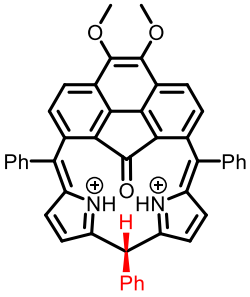


7 was dissolved in CD_2Cl_2 in an NMR tube. Then, gaseous hydrogen chloride was bubbled through the solution, which resulted in **7-H$^+$** and a change of color from blue to pale orange. An addition of a nitrogen base (i.e. TEA; 2,4,6-collidine, $NH_{3(g)}$) reversed the reaction.

^{1}H NMR (600 MHz, CD_2Cl_2, 300 K): δ 14.91 (br, 2H, 26,27-NH), 7.51–7.39 (m, 11H, {7.42 (m(d), 2H, 3,8-H}), 7.37 (m, 4H, 11,21-*o*-Ph), 7.31 (m, 2H, 16-*o*-Ph), 6.66 (d, 2H, ^3J = 8.6 Hz, 2,9-H), 6.46 (d, 2H, ^3J = 5.4 Hz, ^4J = 0.9 Hz, 13,19-H), 6.14 (d, 2H, ^3J = 5.4 Hz, ^4J = 0.9 Hz, 14,18-H), 3.96 (s, 6H, 5,6-OCH_3). **^{13}C NMR** (151 MHz, CD_2Cl_2, 300 K): δ 201.8 (C=O), 159.0, 147.9, 147.0, 139.5, 138.4, 136.7, 136.1, 133.6 (2,9), 132.6 (11,21-*o*-Ph), 132.5, 132.3 (16-*o*-Ph), 132.2

(13,19), 130.1, 129.7, 129.3 (14,18), 128.9, 128.8, 126.8, 126.0 (3,8), 111.9 (16), 61.5 (5,6-OCH_3). **UV-Vis** (CH_2Cl_2, 298 K): λ_{max} 373, 462, 595, 830.

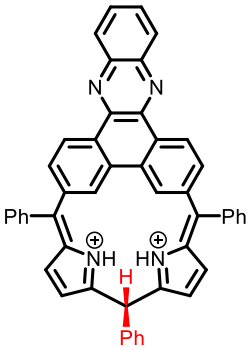
Isoketophenanthriporphyrin (7-H_2^{2+}).



7 was dissolved in CD_2Cl_2 in NMR tube. The solution was titrated with TFA (or $HBF_4{\cdot}Et_2O$) to give **7-H_2^{2+}** (the color of the solution changed from blue to khaki). An addition of a nitrogen base (i. e. TEA; 2,4,6-collidine) reversed the reaction.

^{1}H NMR (600 MHz, CD_2Cl_2, 300 K): δ 10.53 (br, 2H, 26,27-NH), 8.53 (d, 2H, ^3J = 8.4 Hz, 3,8-H) 7.95 (tt, 2H, ^3J = 7.0 Hz, ^4J = 1.8 Hz, 11,21-*p*-Ph), 7.91 (d, 2H, ^3J = 8.4 Hz, 2,9-H), 7.80–7.73 (m, 10H, {7.78 (4H, 11,21-*m*-Ph)}, {7.76 (4H, 11,21-*o*- Ph)}, {7.75 (m(dd), 2H, 13,19-H)}), 7.60–7.52 (m, 5H, 16-Ph, {7.56 (2H, 16-*o*-Ph)}, {7.55 (16-*m*- Ph}), 7.49 (dd, 2H, ^3J = 4.9 Hz, ^4J = 2.0 Hz, 14,18-H), 5.74 (s, 1H, 16-H), 4.34 (s, 6H, 5,6-OCH_3). **^{13}C NMR** (151 MHz, CD_2Cl_2, 300 K): δ 189.7 (C=O), 162.0 (11,21), 158.3 (15,17), 150.1 (5,6), 145.3 (12,20), 144.3 (13,19), 137.9, 137.3 (11,21-*p*-Ph), 137.2 (11,21-*m*-Ph), 137.1, 136.7, 135.0 (2,9), 132.0 (16-*ipso*-Ph), 131.0, 130.8 (11,21-*o*-Ph), 130.4 (16-*o*-Ph), 130.38, 130.35, 128.7 (16-*m*-Ph), 128.0 (3,8), 125.2 (14,18), 63.0 (5,6-OCH_3), 46.7 (16). **UV-Vis** (CH_2Cl_2, 298 K): λ_{max} 375, 401, 460, 530-710.

Isoazaacenephenatriporphyrinoid (2-H_2^{2+}).



2 was dissolved in CD_2Cl_2 in an NMR tube. The solution was titrated with $BF_3{\cdot}Et_2O$ to give **2-H_2^{2+}** (the color of the solution changed from green to orange). An addition of a nitrogen base (i. e. TEA; 2,4,6-collidine) reversed the reaction.

*__2-H_2^{2+}__ precipitates out of the solution after a few minutes.

^{1}H NMR (600 MHz, CD_2Cl_2, 300 K): δ 11.34 (br, 2H, NH), 9.64 (d, 2H, ^3J = 8.0 Hz, 3,8-H), 8.89 (AA'BB', 2H), 8.77 (br, 2H, 22,25-H), 8.48 (AA'BB', 2H), 8.12 (d, 2H, ^3J = 8.4 Hz, 2,9-H), 8.00 (t, 2H, ^3J = 7.3 Hz, 11,21-*p*-Ph), 7.90–7.85 (m, 6H, {7.88 (2H, 14,18-H)}, {7.86 (4H, 11,21-*o*- Ph)}), 7.81 (m(t), 4H, 11,21-*m*-Ph), 7.59 (d, 2H, ^3J = 4.3 Hz, 13,19-H), 7.57–7.49 (m, 5H,16-Ph), 6.12 (br, 1H, 16-H). **^{13}C NMR** (151 MHz, CD_2Cl_2, 300 K, based on HSQC and HMBC correlations): δ 168.6 (11,21), 144.6 (14,18), 142.8 (16-Ph), 137.5 (11,21-*p*-Ph), 137.3 (AA'BB', second spin system has not been detected), 136.8 (11,21-*o*-Ph), 135.3 (22,25), 134.1 (2,9), 130.7 (11,21-*m*-Ph), 130.2 (16-Ph), 129.0 (16-Ph), 127.9 (3,8), 126.6 (13,19), 46.4 (16).

NMR spectra

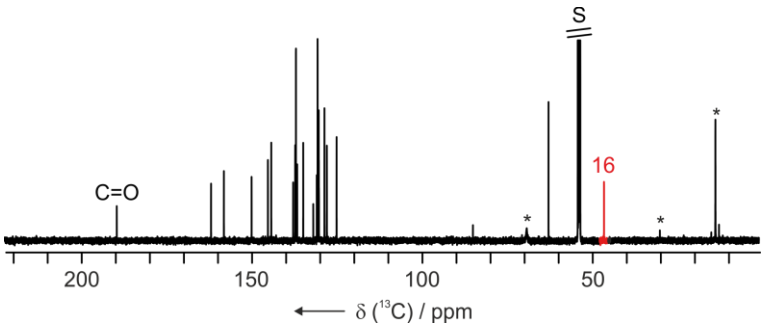


Figure S1. ^{13}C NMR spectrum of **7-H$_2^{2+}$** (151HMz, CD_2Cl_2, 300 K).

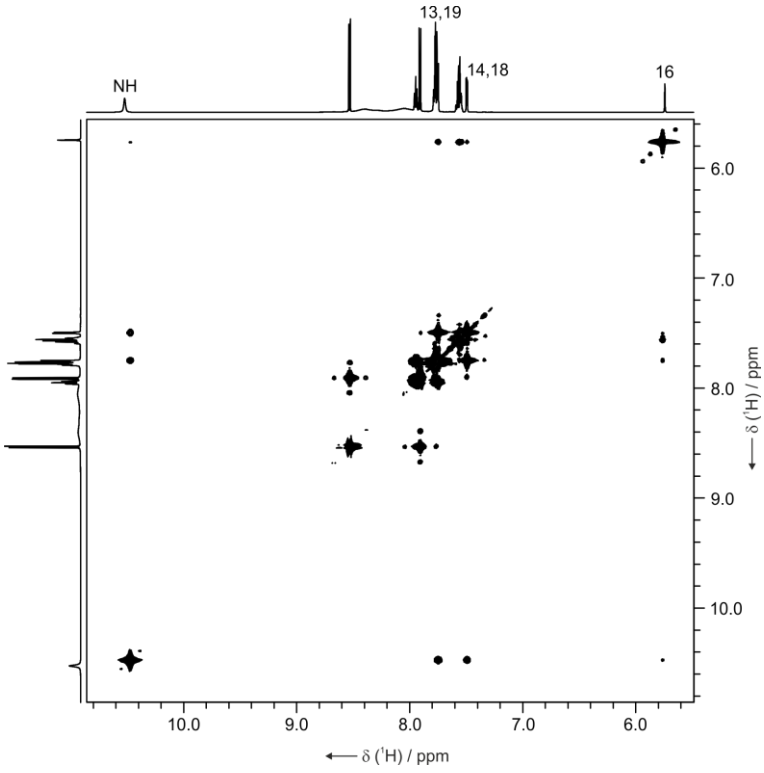


Figure S2. Part of the ^{1}H-^{1}H COSY spectrum of **7-H$_2^{2+}$** (600 MHz, CD_2Cl_2, 300 K).

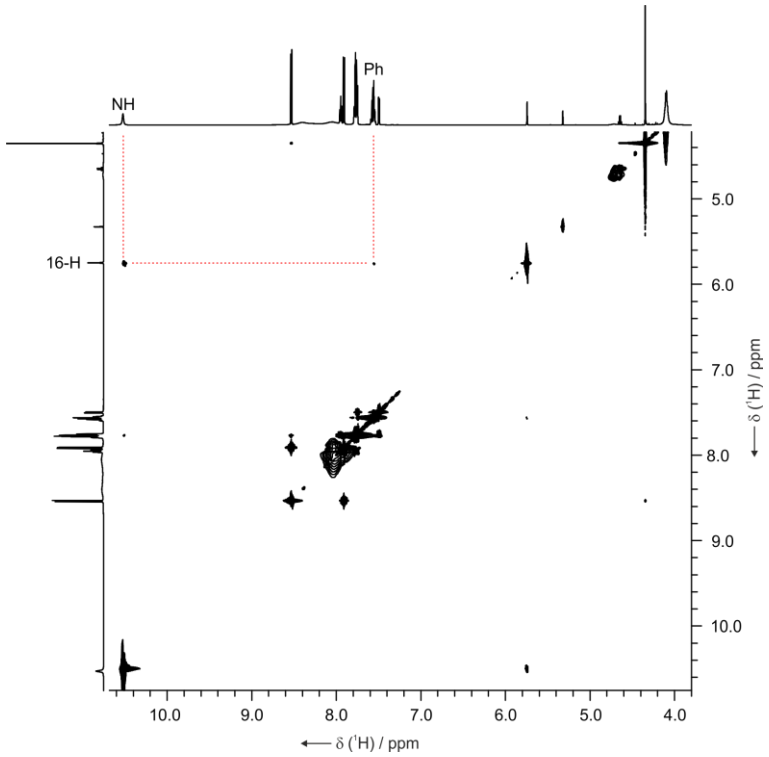


Figure S3. ^{1}H-^{1}H NOESY spectrum of **7-H$_2^{2+}$** (600 MHz, CD_2Cl_2, 300 K).

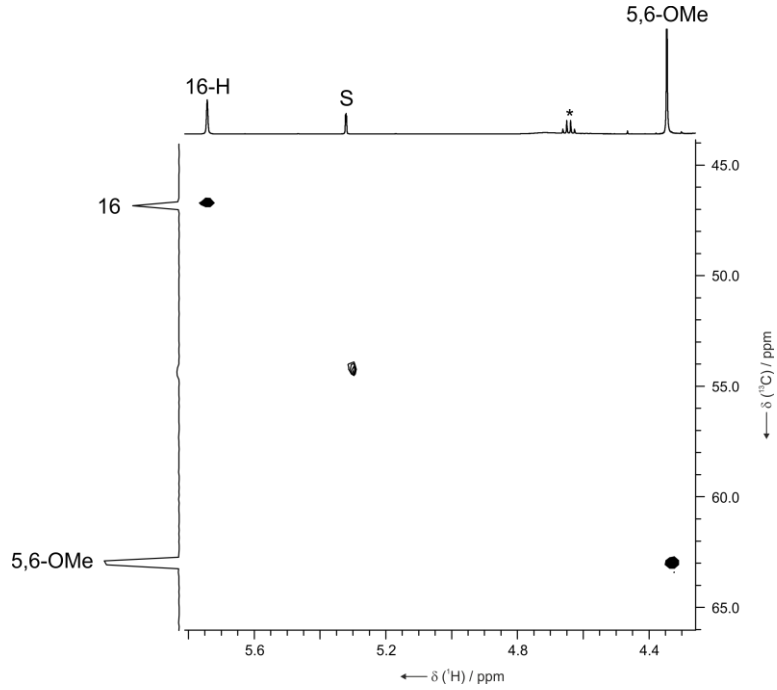


Figure S4. Part of the ^{1}H-^{13}C HSQC spectrum of **7-H$_2^{2+}$** (600 MHz, CD_2Cl_2, 300 K).

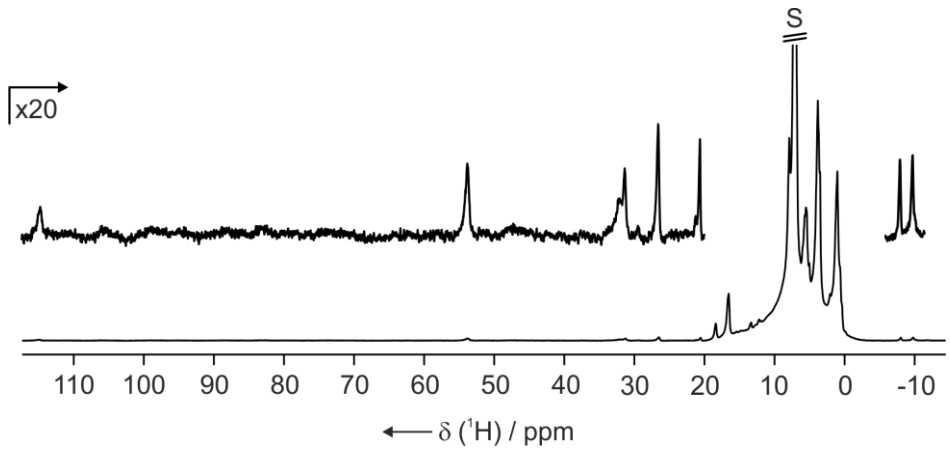
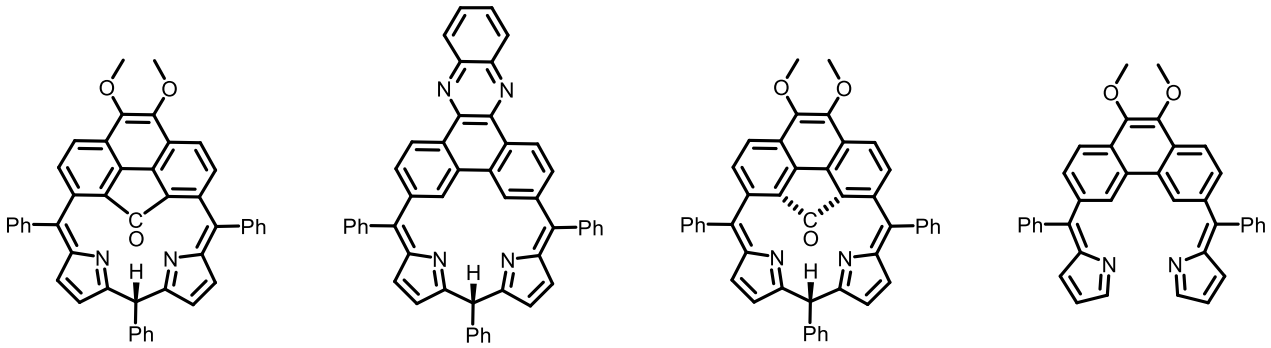


Figure S5. Paramagnetic ^{1}H NMR spectrum for a crude mixture in the reaction of **1** with $Fe(CO)_5$.

Schemes



Scheme S1. Considered neutral structures of **1-iso**, **2-iso**, **7-iso**, and **9** treated as standards for modification of charge distribution due to protonation.

DFT figures

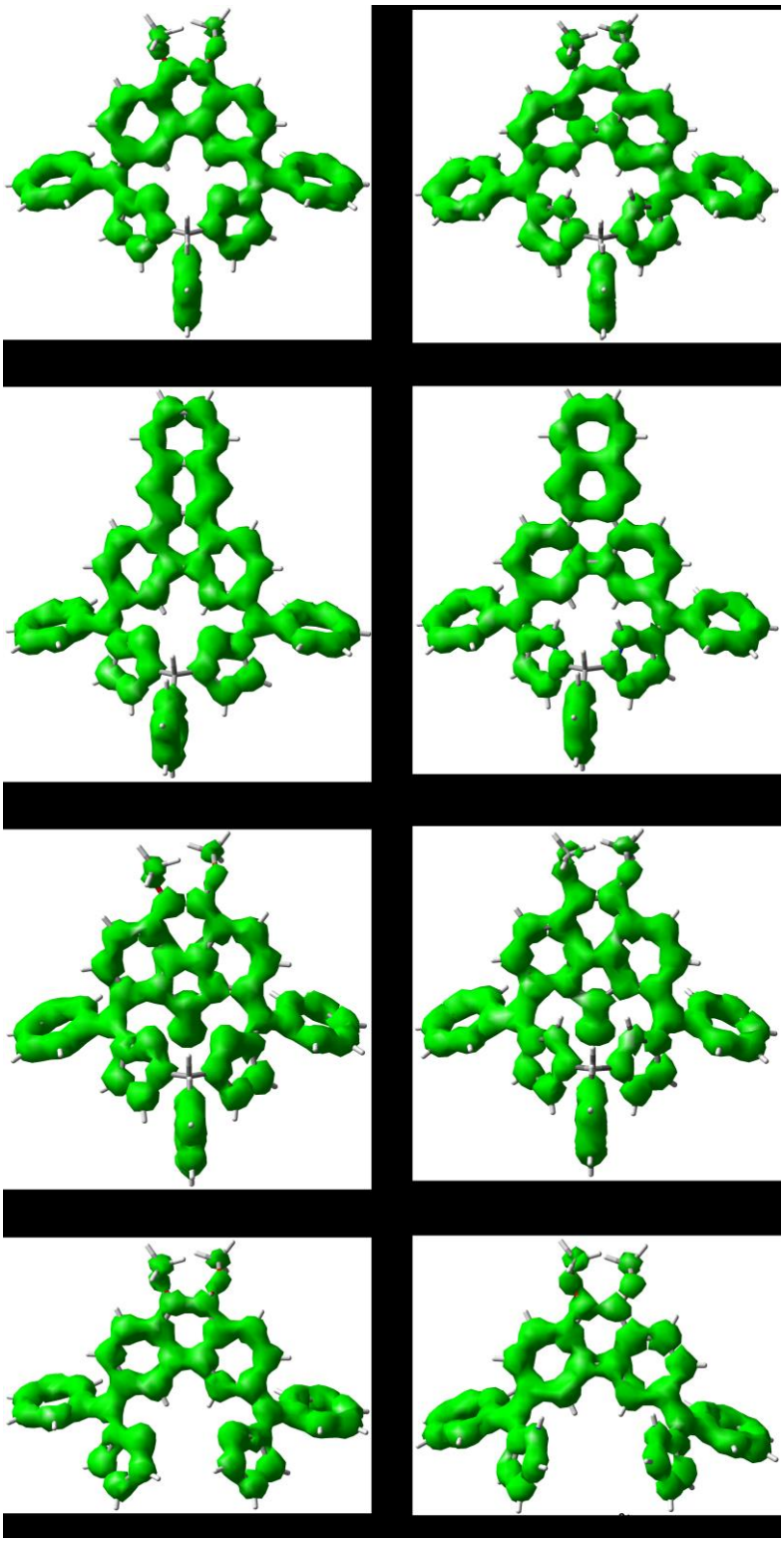


Figure S6. AICD plots of **1-iso**, **1-H$_2^{2+}$**, **2-iso**, **2-H$_2^{2+}$**, **7-iso**, **7-H$_2^{2+}$**, **9**, and **9-H$_2^{2+}$** at an isosurface value of 0.06 e/a.u.^{3}.

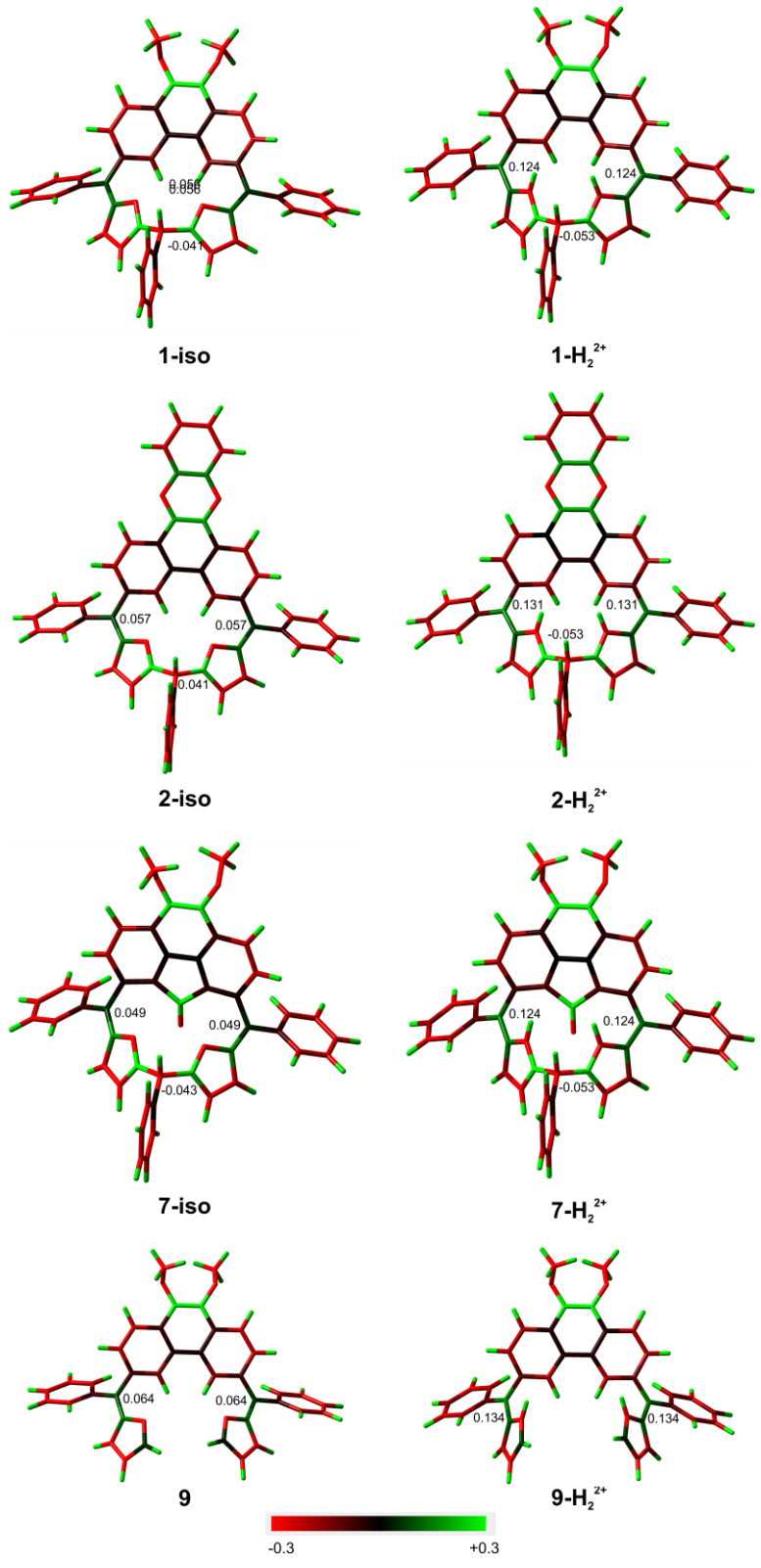


Figure S7. Partial charge distribution (NBO) of **1-iso**, **1-H$_2^{2+}$**, **2-iso**, **2-H$_2^{2+}$**, **7-iso**, **7-H$_2^{2+}$**, **9**, and **9-H$_2^{2+}$**. Color range from −0.3 e (red) to 0.3 e (green).

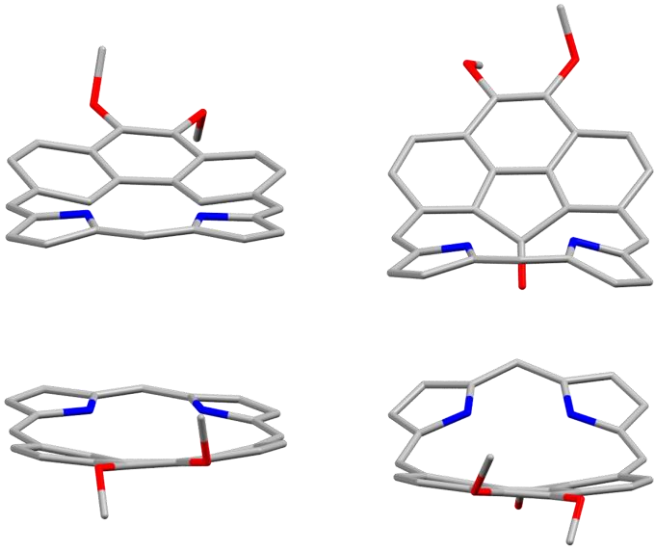


Figure S8. Dihedral angles between planes defined by dipyrromethene and phenanthrene units for **1** (11.9°) (left - DFT) and **7** (36.1°) (right - X-ray structure).

Mass spectra

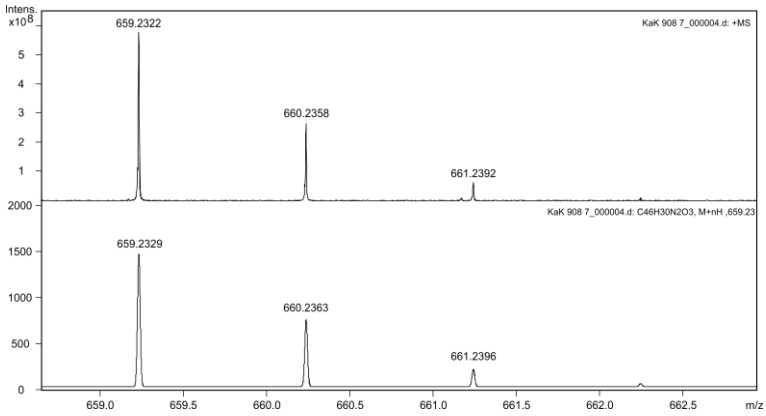


Figure S9. HRMS (ESI) of **7**: *m/z*: 659.2322 $[M+H]^+$, calcd for $C_{46}H_{31}N_2O_3^+$: 659.2329.

UV-Vis spectra

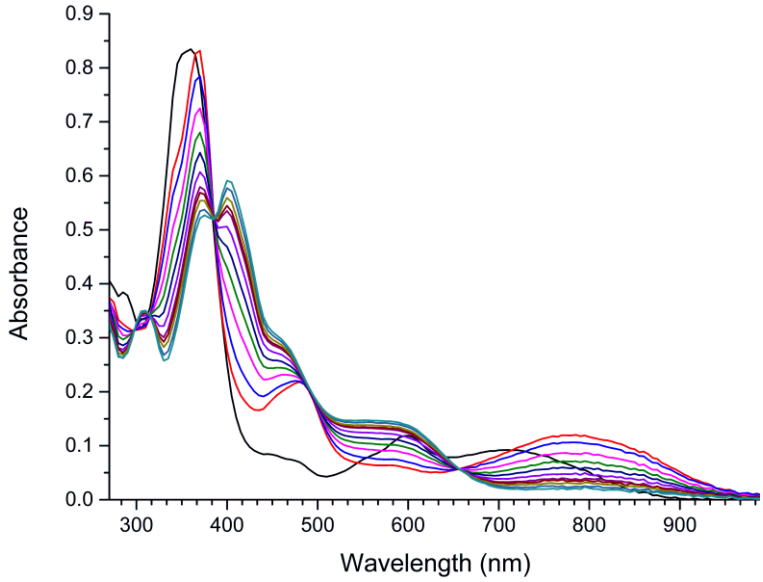


Figure S10. Electronic absorption spectra recorded during titration of **7** with a diluted solution of TFA (in dichloromethane – v/v 1:300, 298 K): black – **7**, red – **7**-$\mathbf{H}^+$, turquoise – **7**-$\mathbf{H_2}^{2+}$.

X-ray structure

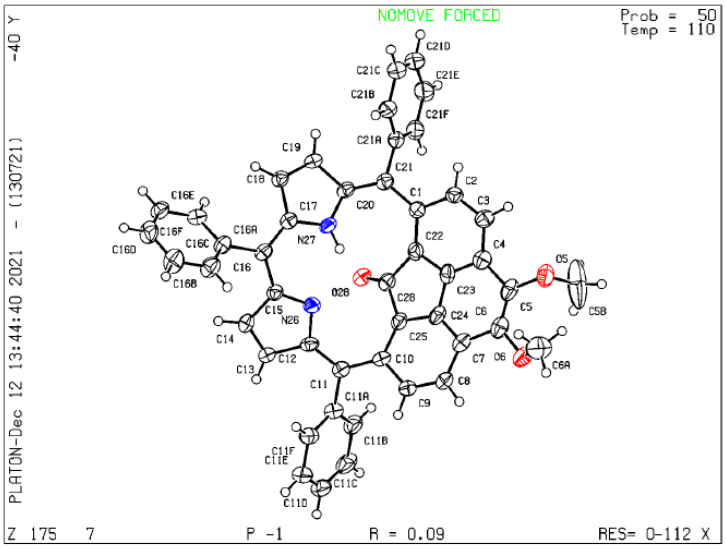


Fig. S11 Molecular structure of **7** (ORTEP plot).

Tables

Table S1. Comparison of chemical shifts for **7** and **7-H_2^{2+}** (600 MHz, CD_2Cl_2, 300 K).

Position	7				7-H_2^{2+}			
	^{1}H NMR		^{13}C NMR		^{1}H NMR		^{13}C NMR	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
2,9	6.56	6.79	128.9	133.1	8.05	7.91	132.4	135.0
3,8	7.19	7.39	119.8	124.9	8.90	8.53	127.1	128.0
5,6-OCH_3	3.81	3.94	56.0	61.6	4.50	4.34	57.9	63.0
13,19	6.38	6.62	128.3	133.6	7.81	7.75	139.3	144.3
14,18	6.03	6.27	123.7	129.5	7.93	7.49	117.7	125.2
16	-	-	114.6	114.1	3.86	5.74	51.5	46.7
CO	-	-	196.9	201.9	-	-	185.6	189.7
26,27 (NH)	12.22	11.28	-	-	6.66	10.53	-	-

Table S2. ^{1}H NMR chemical shifts (ppm) of the porphyrin skeleton for (**1**, **1-H_2^{2+}**, **2**, **1-H_2^{2+}**, **7** and **7-H_2^{2+}**) using the GIAO method (Calc. - calculated, Exp. – experimental, ND – not detected).

Position	1 [8]		1-H_2^{2+} [8]		2 [2]		2-H_2^{2+}		7		7-H_2^{2+}		8 [9**]	
	Calc.	Exp.	Calc.	[(a)]Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
2,9	5.42	5.94	8.42	8.09	6.79	6.87	8.28	8.12	6.56	6.79	8.05	7.91	7.60 (**2**) 8.66 (**9**)	7.65 (**2**) 8.07 (**9**)
3,8	6.54	6.94	9.36	8.76	8.58	8.51	10.42	9.64	7.19	7.39	8.90	8.53	8.46 (**3**) 8.63 (**8**)	8.33 (**3**) 8.38 (**8**)
5,6-OCH_3	3.53	3.71	4.57	4.31	-	-	-	-	3.81		4.50	4.34	4.14	4.16
13,19	5.09	5.59	7.86	7.85	6.28	6.41	7.78	7.59	6.38	6.62	7.81	7.75	5.97 (**13**) 7.08 (**19**)	6.94 (**13**) 7.11 (**19**)
14,18	4.70	5.24	7.60	7.63	5.94	6.10	7.84	7.88	6.03	6.27	7.93	7.49	6.91 (**14**) 6.85 (**18**)	6.19 (**14**) 6.56 (**18**)
16	-	-	6.22	5.50	-	-	4.41	6.12	-	6.12	3.86	5.74	-	-
22,25	20.18	16.70	6.88	7.23	12.85	12.01	8.22	8.77	-	-	-	-	8.62 (**22**) 9.11 (**25**)	8.65 (**22**) 8.99 (**25**)
26,27 (NH)	20.28	16.70	7.00	10.00	13.15	ND	7.50	11.34	12.22	11.28	6.66	10.53	11.04	11.12

*Standard measurement in $CDCl_3$ or CD_2Cl_2 at 300 K [(a) CD_2Cl_2, 250 K].

**The original numbering of the compound is different, and the comparison takes into account the change in the numbering and shows the same type of atom.

Table S3. Crystal data and structure refinement for **7**.

Identification code	7
Empirical formula	$C_{46}H_{30}N_2O_3$
Formula weight	658.72
Temperature/K	110(2)
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	11.109(3)
b/Å	11.704(3)
c/Å	13.820(4)
α/°	81.76(4)
β/°	71.15(3)
γ/°	75.07(3)
Volume/Å^3	1639.5(9)
Z	2
ρ_{calc}g/cm^3	1.334
μ/mm^{-1}	0.660
F(000)	688.0
Crystal size/mm^3	0.200 × 0.110 × 0.090
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.774 to 157.082
Index ranges	−14 ≤ h ≤ 13, −14 ≤ k ≤ 13, −15 ≤ l ≤ 17
Reflections collected	12222
Independent reflections	6771 [R_{int} = 0.0622, R_{sigma} = 0.0999]
Data/restraints/parameters	6771/0/466
Goodness-of-fit on F^2	0.963
Final R indexes [I>=2σ (I)]	R_1 = 0.0893, wR_2 = 0.2353
Final R indexes [all data]	R_1 = 0.1315, wR_2 = 0.2593
Largest diff. peak/hole / e Å^{-3}	0.86/−0.45

Table S4. DFT calculated Cartesian coordinates for **1-iso**.

C	-0.99777800	-4.57667900	0.93899500
C	0.37855300	-4.65797300	0.96452800
C	1.19762500	-3.55479800	0.54005000
C	-1.66438300	-3.36621900	0.54098900
C	-0.88230600	-2.27236800	0.08200200
C	0.56585500	-2.37314700	0.06727400
C	-1.53054200	-1.08746700	-0.28920200
C	1.36476300	-1.29188900	-0.32683700
O	-1.78359700	-5.62772400	1.35894500
O	1.01953200	-5.80555400	1.37703200
C	-1.76638200	-6.77616700	0.49914700
C	0.89876800	-6.09543800	2.77821800
C	-3.07231200	-3.21503600	0.61465400
C	-3.67849600	-2.01990600	0.28207400
C	-2.90632800	-0.90987900	-0.16065600
C	2.61367200	-3.59384800	0.60130200
C	2.75245600	-1.29838300	-0.20593500
C	3.37233100	-2.49576500	0.24780000
C	-3.49433300	0.40725600	-0.46587700
C	3.50864600	-0.07440600	-0.52812900
C	-2.77178700	1.57496100	-0.28994900
N	-1.54550700	1.62338900	0.39567700
C	-1.08349100	2.84246800	0.25770000
C	-1.99416300	3.68377000	-0.52346700
C	-3.05956200	2.89827700	-0.84037800
C	2.95167300	1.17987600	-0.34682600
N	1.75470600	1.39356600	0.35946500
C	1.46278900	2.66523200	0.23112600
C	3.40784100	2.45242900	-0.90280900
C	2.46620600	3.37569200	-0.56638600
C	0.22990100	3.22912600	0.94636500

C	0.33621800	4.71010700	1.28489700
C	0.39581400	5.71117600	0.30219400
C	0.37653700	5.10552500	2.62826600
C	0.49207500	7.05815400	0.65227300
C	0.53096000	7.43433800	1.99584100
C	0.47278200	6.45170100	2.98373100
C	4.88078100	-0.21119700	-1.07308500
C	5.93447700	0.59141300	-0.59809500
C	5.16274800	-1.15886200	-2.07534100
C	7.22048000	0.46288300	-1.12052000
C	7.47993500	-0.46865500	-2.12683900
C	6.44607600	-1.27896300	-2.60232000
C	-4.87971800	0.46067400	-0.99217600
C	-5.80964100	1.39182900	-0.49411200
C	-7.10823700	1.44271900	-0.99851100
C	-7.50374100	0.56606100	-2.00980800
C	-6.59425200	-0.36968700	-2.50858200
C	-5.29946400	-0.42872100	-1.99950800
H	-2.44860100	-7.50094200	0.94764400
H	-2.12348800	-6.51396000	-0.50382100
H	-0.76211000	-7.20377100	0.43001400
H	1.47663000	-7.00564200	2.94980700
H	1.31825600	-5.27969000	3.37839800
H	-0.14526800	-6.25807400	3.05992000
H	-3.66306200	-4.05009600	0.97324300
H	-4.75326700	-1.91666900	0.38840400
H	3.09071500	-4.50194900	0.95163300
H	4.45236100	-2.53741300	0.34233700
H	-1.85672600	4.72587400	-0.77298600
H	-3.91793000	3.16545000	-1.44034300
H	4.28387400	2.60096600	-1.51814000
H	2.46869800	4.42748800	-0.81299500
H	0.36677600	5.43801400	-0.74834600
H	0.33173000	4.34700200	3.40530400
H	0.53665700	7.81420700	-0.12662200
H	0.60584300	8.48289900	2.26871000
H	0.50213200	6.73056900	4.03322100
H	5.73887800	1.29965500	0.19994200
H	4.36168600	-1.78773200	-2.45034700
H	8.02220800	1.08535800	-0.73407500
H	8.48216300	-0.56854700	-2.53312000
H	6.64008000	-2.00568200	-3.38577300
H	-5.50976700	2.05862400	0.30727500
H	-7.81392300	2.16259600	-0.59433600
H	-8.51565200	0.60605300	-2.40216000
H	-6.89436600	-1.05437300	-3.29644900
H	-4.59487100	-1.15448000	-2.39277500
H	0.20071700	2.67004200	1.88677900
H	-0.95244600	-0.25380800	-0.64719300
H	0.90190800	-0.39573400	-0.70142200

Table S5. DFT calculated Cartesian coordinates for **2-iso**.

C	2.94183300	1.45407000	0.13678900
C	4.17449600	0.72336600	0.43355200
C	4.17448000	-0.72338800	0.43359900
C	2.94180700	-1.45408800	0.13686100
C	1.77903100	-0.73400700	-0.21859900
C	1.77903700	0.73398900	-0.21861300
C	2.88107500	2.86073700	0.21478600
C	1.69854500	3.54026200	-0.02384400
C	0.52061100	2.83276700	-0.36919500
C	0.60742200	1.44563400	-0.49881500
C	2.88103400	-2.86075200	0.21491500
C	1.69850400	-3.54027200	-0.02372600
C	0.52059300	-2.83277600	-0.36915700
C	0.60742300	-1.44565300	-0.49883600
N	5.27597000	1.41154700	0.71000100
C	6.40240300	0.71709000	0.98967700
C	6.40238700	-0.71712300	0.98972800
N	5.27593900	-1.41157400	0.71009800
C	-0.78019500	3.50189600	-0.57709900
C	-1.97148400	2.86370200	-0.28732500

C	-0.78394100	4.87975800	-1.12518500
C	-1.59867000	5.88131100	-0.56572700
C	-1.60331200	7.17260400	-1.09096200
C	-0.79600800	7.48877300	-2.18452500
C	0.02514000	6.50731600	-2.74492700
C	0.03930800	5.21950300	-2.21555600
N	-2.04060300	1.64604300	0.41391700
C	-3.29758700	1.27751000	0.40463000
C	-4.14510000	2.24658500	-0.29816700
C	-3.31927200	3.24611900	-0.70839100
C	-3.71351000	0.00003100	1.14227700
C	-3.29758700	-1.27747200	0.40459000
N	-2.04061400	-1.64603000	0.41392800
C	-1.97149700	-2.86367600	-0.28735500
C	-3.31927600	-3.24603200	-0.70850000
C	-4.14509600	-2.24648700	-0.29827600
C	-0.78021500	-3.50189900	-0.57709300
C	-0.78396300	-4.87974800	-1.12519300
C	-1.59875600	-5.88129100	-0.56580600
C	-1.60339400	-7.17257400	-1.09105800
C	-0.79601900	-7.48875200	-2.18456800
C	0.02519700	-6.50731100	-2.74489500
C	0.03935900	-5.21950500	-2.21550700
C	-5.16477700	0.00001000	1.60431600
C	-6.24575600	-0.00005400	0.70836800
C	-7.56225700	-0.00008100	1.16984200
C	-7.82663400	-0.00004700	2.54039200
C	-6.76346100	0.00000900	3.44288900
C	-5.44813500	0.00003400	2.97618300
H	3.78189900	3.39664400	0.49073700
H	1.66810100	4.61949600	0.08146500
H	-0.28662400	0.91902500	-0.78202500
H	3.78184500	-3.39665500	0.49091400
H	1.66803600	-4.61950000	0.08163000
H	-0.28659100	-0.91904600	-0.78214900
H	-2.20894200	5.64277400	0.29881000
H	-2.23182100	7.93429900	-0.63898300
H	-0.79985700	8.49502900	-2.59300300
H	0.65604100	6.74591900	-3.59608500
H	0.67697000	4.45977200	-2.65599000
H	-5.21431600	2.18527600	-0.43950400
H	-3.58089900	4.11878200	-1.28965100
H	-3.58089800	-4.11865700	-1.28981900
H	-5.21430100	-2.18512700	-0.43968100
H	-2.20907800	-5.64275100	0.29869500
H	-2.23195600	-7.93425800	-0.63913400
H	-0.79986500	-8.49500300	-2.59305800
H	0.65615700	-6.74592100	-3.59600800
H	0.67707300	-4.45978800	-2.65588700
H	-6.05954300	-0.00008200	-0.36151000
H	-8.38194500	-0.00013200	0.45688100
H	-8.85139900	-0.00006300	2.90000800
H	-6.95522300	0.00003200	4.51208100
H	-4.62625200	0.00007100	3.68728900
C	7.60529100	-1.41290500	1.28888800
C	7.60532400	1.41286900	1.28878400
C	8.75228600	-0.71091300	1.57412200
C	8.75230300	0.71087000	1.57406900
H	7.57952500	-2.49768600	1.28292800
H	7.57958300	2.49764900	1.28274500
H	9.67112500	-1.24242000	1.80299200
H	9.67115400	1.24237300	1.80290000
H	-3.07676700	-0.00000300	2.03266700

Table S6. DFT calculated Cartesian coordinates for **2-H_2^{2+}**.

C	-2.92261000	-1.44960000	0.09291400
C	-4.13814700	-0.71775000	0.44049900
C	-4.13818100	0.71758400	0.44049300
C	-2.92267200	1.44949300	0.09291000
C	-1.77339400	0.73611100	-0.33465200
C	-1.77337400	-0.73616200	-0.33467600
C	-2.86837000	-2.85661100	0.19531000
C	-1.70518800	-3.55190900	-0.07343500

C	-0.53861000	-2.85691100	-0.49004100
C	-0.62304800	-1.46338100	-0.65250400
C	-2.86850500	2.85650700	0.19532700
C	-1.70535000	3.55185900	-0.07339100
C	-0.53872800	2.85691300	-0.48995300
C	-0.62307700	1.46337800	-0.65240300
N	-5.22370700	-1.41191100	0.76832000
C	-6.33638900	-0.72340000	1.09102000
C	-6.33642100	0.72313800	1.09102000
N	-5.22377100	1.41169800	0.76831000
C	0.73984000	-3.53807800	-0.70685100
C	1.94886000	-2.86888400	-0.41357500
C	0.77700400	-4.89513500	-1.22764400
C	1.76559500	-5.81716200	-0.80004500
C	1.79405000	-7.10654000	-1.31388700
C	0.85296500	-7.49991600	-2.27187400
C	-0.13075400	-6.60343700	-2.70609600
C	-0.18143200	-5.31937600	-2.18239900
N	2.04126500	-1.73324100	0.40490000
C	3.30670100	-1.24877900	0.42299200
C	4.08359600	-2.06713600	-0.42095700
C	3.25897700	-3.06653600	-0.92361400
C	3.64917000	0.00012700	1.22935800
C	3.30671000	1.24898800	0.42301900
N	2.04123100	1.73339300	0.40497700
C	1.94875600	2.86904100	-0.41351000
C	3.25884700	3.06675000	-0.92357100
C	4.08352500	2.06737300	-0.42093200
C	0.73968900	3.53815500	-0.70678300
C	0.77678000	4.89520100	-1.22759200
C	1.76537800	5.81725300	-0.80005100
C	1.79378500	7.10662700	-1.31390100
C	0.85264200	7.49998200	-2.27184100
C	-0.13107800	6.60348000	-2.70601200
C	-0.18170400	5.31941900	-2.18231200
C	5.06424200	0.00008200	1.80414900
C	5.21839400	0.00000700	3.19572400
C	6.48944300	-0.00007400	3.77086000
C	7.62342800	-0.00008100	2.95902900
C	7.48092600	0.00001200	1.57034100
C	6.21060300	0.00008900	0.99471800
H	1.29284500	1.43220800	1.01256400
H	-3.76026600	-3.37517400	0.52707200
H	-1.66976700	-4.62507400	0.07531300
H	0.23599600	-0.95276200	-1.06331200
H	-3.76043200	3.37501800	0.52708700
H	-1.66997900	4.62502400	0.07536200
H	0.23605300	0.95278800	-1.06305400
H	2.46564500	-5.53003400	-0.02335500
H	2.53767800	-7.81283500	-0.96027600
H	0.88076000	-8.50759200	-2.67423000
H	-0.85240100	-6.90985400	-3.45584900
H	-0.92846000	-4.61932200	-2.53984700
H	5.13341600	-1.93664300	-0.62909900
H	3.53224300	-3.82745000	-1.63963300
H	3.53206800	3.82768000	-1.63959200
H	5.13332500	1.93689100	-0.62920700
H	2.46547000	5.53014800	-0.02339000
H	2.53742100	7.81293700	-0.96033600
H	0.88039500	8.50765800	-2.67420200
H	-0.85276600	6.90987900	-3.45573400
H	-0.92872100	4.61934600	-2.53974300
H	4.34223800	0.00003900	3.83940100
H	6.59080400	-0.00014000	4.85121400
H	8.61290000	-0.00018200	3.40425900
H	8.35917900	0.00003600	0.93282100
H	6.12753000	0.00013600	-0.08773500
H	2.96490400	0.00008800	2.08945800
H	1.29272900	-1.43185300	1.01220000
C	-7.52460500	1.42048400	1.43930800
C	-7.52454500	-1.42079900	1.43930000
C	-8.65479400	-0.71290200	1.76901000
C	-8.65482400	0.71253500	1.76901500
H	-7.50482000	-2.50498400	1.43319500
H	-7.50492800	2.50467000	1.43321000
H	-9.56543600	1.23961200	2.03452200

H	-9.56538500	-1.24001900	2.03451000

Table S7. DFT calculated Cartesian coordinates for **7**.

C	4.89387700	0.39126000	-0.89606600
C	4.80408000	-0.99389800	-0.88542600
C	3.61400600	-1.66548800	-0.40899300
C	3.78341600	1.21846000	-0.47488800
C	2.67360300	0.55464600	0.03400100
C	2.59223700	-0.85537800	0.06698900
C	1.46118100	1.13376600	0.45746600
C	1.31736300	-1.27030000	0.50393900
O	6.01612200	1.03571800	-1.36975900
O	5.84450800	-1.78812200	-1.31422800
C	7.18516700	0.89412700	-0.54983000
C	6.12911400	-1.71566800	-2.71946000
C	3.64571800	2.62953300	-0.55668200
C	2.44676400	3.22250200	-0.20367800
C	1.28642600	2.50724900	0.27361700
C	3.31523000	-3.05580700	-0.41517100
C	0.98216500	-2.62473000	0.38819500
C	2.05935500	-3.49134400	-0.03725200
C	0.02621600	3.26436000	0.39123700
C	-0.35728600	-3.22029300	0.50636400
C	-1.22975400	2.77338800	0.07894100
N	-1.53731200	1.47638500	-0.32362100
C	-2.86737500	1.43194500	-0.47351300
C	-3.47425000	2.75263100	-0.24301000
C	-2.46830600	3.56771500	0.13707800
C	-1.54338700	-2.59471800	0.16308500
N	-1.74316300	-1.29388200	-0.28246000
C	-3.07412700	-1.03582200	-0.49871400
C	-2.87155700	-3.20152800	0.15576900
C	-3.77483200	-2.28719500	-0.27789800
C	-3.62572500	0.22850500	-0.68597700
C	-5.09529800	0.30653400	-0.95408100
C	-5.99833800	0.78129900	0.01197000
C	-5.60786000	-0.12798000	-2.18687900
C	-7.36692600	0.83173500	-0.25247400
C	-7.86144600	0.40077000	-1.48508700
C	-6.97765300	-0.08260600	-2.45042100
C	-0.41409600	-4.65539700	0.92232300
C	-0.92373600	-5.66049400	0.08303800
C	0.08316200	-5.03004400	2.18290200
C	-0.95579700	-6.99240600	0.49891200
C	-0.47324300	-7.34610800	1.75931800
C	0.04844800	-6.35947000	2.59912600
C	0.16632200	4.69676700	0.79149500
C	-0.25466700	5.74998700	-0.03797400
C	-0.10216500	7.07845400	0.36126600
C	0.47463500	7.37927900	1.59551800
C	0.90814200	6.34243900	2.42509400
C	0.76486400	5.01616900	2.02320100
H	7.96828400	1.48111600	-1.03363700
H	7.00302200	1.29051400	0.45605900
H	7.49473900	-0.15262200	-0.47868000
H	6.94100600	-2.42270900	-2.90037800
H	5.25196300	-2.01147300	-3.30686100
H	6.43947700	-0.70831700	-3.01038600
H	4.46062900	3.23545200	-0.93828900
H	2.35244800	4.29371000	-0.33807500
H	4.05900000	-3.77066300	-0.75109300
H	1.84616900	-4.55113700	-0.11283900
H	-4.52391600	2.99206900	-0.32731600
H	-2.54137400	4.60035800	0.44250900
H	-3.07310700	-4.21527300	0.46479000
H	-4.84174600	-2.41481100	-0.38325500
H	-5.62127000	1.09822700	0.97963800
H	-4.92051100	-0.49541800	-2.94325300
H	-8.04861000	1.19882600	0.50954200
H	-8.92742900	0.43883300	-1.68960000
H	-7.35242400	-0.42091500	-3.41229400
H	-1.28111400	-5.39338300	-0.90682400
H	0.48743700	-4.26518900	2.83913700

H	-1.35037800	-7.75416200	-0.16748400
H	-0.49767600	-8.38250100	2.08288800
H	0.42703500	-6.62527600	3.58189500
H	-0.68811500	5.52026700	-1.00618900
H	-0.42899700	7.87801900	-0.29737800
H	0.59181500	8.41321300	1.90647700
H	1.35894400	6.56708300	3.38743500
H	1.10400400	4.21265200	2.67000900
C	0.63781500	-0.01300300	1.00960100
O	-0.29888500	0.04549000	1.78709400
H	-1.10883000	-0.50174100	-0.26066000

Table S8. DFT calculated Cartesian coordinates for **7-iso**.

C	-4.56222400	0.47194300	1.46996400
C	-4.48487300	-0.91818100	1.48124000
C	-3.36642600	-1.61957500	0.89494600
C	-3.50287800	1.28520100	0.91942000
C	-2.43157100	0.59436600	0.35377100
C	-2.36985100	-0.82243800	0.33284100
C	-1.29140900	1.15906800	-0.22544300
C	-1.18288300	-1.26805500	-0.25625300
O	-5.63325700	1.13111500	2.03087500
O	-5.49202500	-1.68410900	2.02422000
C	-6.87901100	0.97092400	1.33610700
C	-5.62329700	-1.59414200	3.45159700
C	-3.39478300	2.69976100	0.87624300
C	-2.26566100	3.28755400	0.32411500
C	-1.16293700	2.54765700	-0.21725400
C	-3.12839900	-3.01706900	0.82416600
C	-0.92576600	-2.63842000	-0.27326900
C	-1.95343500	-3.48746100	0.25555800
C	0.05679500	3.25522400	-0.66314800
C	0.35363900	-3.22167200	-0.73230000
C	1.29582700	2.76636700	-0.32314200
N	1.45028700	1.68868100	0.56157900
C	2.71413400	1.35692100	0.52128400
C	3.48608100	2.23303400	-0.37043700
C	2.60129500	3.12907000	-0.87806600
C	1.54281100	-2.62825200	-0.38093300
N	1.59865800	-1.55965000	0.52632600
C	2.82714300	-1.11352100	0.49521300
C	2.87572700	-2.85871000	-0.94125500
C	3.67538500	-1.89686900	-0.41329000
C	3.17939400	0.13198400	1.30632300
C	4.60859500	0.19221900	1.82643700
C	5.73179600	0.25166200	0.98642000
C	4.82541600	0.18919800	3.21125200
C	7.02253200	0.30590800	1.51358600
C	7.21965100	0.30201200	2.89487900
C	6.11407300	0.24335400	3.74316100
C	0.30901100	-4.45156200	-1.55403700
C	1.19579900	-5.51963800	-1.32181100
C	-0.64271100	-4.58482200	-2.58284600
C	1.14727500	-6.66970000	-2.10761600
C	0.21133100	-6.77817300	-3.13743100
C	-0.68402000	-5.73169000	-3.37120600
C	-0.10123900	4.49242400	-1.45960900
C	0.68285800	5.63288700	-1.20358500
C	0.52806100	6.78962600	-1.96552700
C	-0.41366200	6.83230900	-2.99488500
C	-1.20800200	5.71238700	-3.25228300
C	-1.06079700	4.55820800	-2.48761900
H	-7.60809900	1.57545100	1.87890000
H	-6.79702700	1.33848600	0.30642800
H	-7.19591800	-0.07571100	1.32625800
H	-6.42772100	-2.27962100	3.72479800
H	-4.69555800	-1.90674600	3.94461800
H	-5.87781200	-0.57717100	3.76271900
H	-4.18191800	3.31781800	1.29455200
H	-2.18923000	4.37021100	0.33243900
H	-3.85703200	-3.71339800	1.22518300
H	-1.77839600	-4.55852600	0.23985700
H	4.54630400	2.17886500	-0.57100800

H	2.79139200	3.90327500	-1.60744200
H	3.13535800	-3.59680100	-1.68644700
H	4.72623600	-1.74232000	-0.61075400
H	5.60399100	0.25595700	-0.09105100
H	3.97039700	0.14382100	3.88054600
H	7.87509700	0.35135900	0.84179500
H	8.22446800	0.34430700	3.30484800
H	6.25225800	0.23966700	4.82063700
H	1.90466300	-5.44918500	-0.50368800
H	-1.33594900	-3.77137400	-2.77130000
H	1.83442500	-7.48661800	-1.90740400
H	0.17340100	-7.67537400	-3.74820000
H	-1.41561900	-5.80917800	-4.17010100
H	1.39515100	5.61133100	-0.38568900
H	1.13650800	7.66235300	-1.74701600
H	-0.53441100	7.73462600	-3.58707800
H	-1.94318000	5.73826100	-4.05125100
H	-1.67531000	3.68789800	-2.69435800
C	-0.50013900	-0.01418500	-0.81536900
O	0.33602800	0.03427100	-1.68887500
H	2.50301000	0.09211300	2.16466000

Table S9. DFT calculated Cartesian coordinates for **7-H_2^{2+}**.

C	-4.62400000	0.53531200	1.38773200
C	-4.54874700	-0.86832300	1.43386300
C	-3.42366700	-1.57410700	0.86256500
C	-3.52672800	1.32453400	0.87670600
C	-2.44343700	0.62604900	0.34160100
C	-2.40130200	-0.79605800	0.31868200
C	-1.28658700	1.17732000	-0.20574500
C	-1.20995400	-1.25863800	-0.23759200
O	-5.68823000	1.22598100	1.86410400
O	-5.52986100	-1.64009800	1.95876800
C	-6.97485800	0.98443100	1.23724600
C	-5.88740600	-1.43211800	3.34925200
C	-3.41011100	2.73950000	0.83289200
C	-2.26699000	3.32507700	0.30901300
C	-1.15424700	2.57911900	-0.21134700
C	-3.20562900	-2.97667100	0.80886000
C	-0.98076200	-2.64708100	-0.26083500
C	-2.03325600	-3.47525900	0.26019100
C	0.05274300	3.28891400	-0.66114600
C	0.27009800	-3.26592400	-0.72740300
C	1.32201800	2.76417400	-0.37578000
N	1.55423200	1.75788800	0.56591200
C	2.82504400	1.30635600	0.48699400
C	3.48049700	2.05218700	-0.51798100
C	2.56751800	2.95439100	-1.03870800
C	1.50169200	-2.66246900	-0.43375100
N	1.66790300	-1.66327600	0.52941900
C	2.90558100	-1.12638100	0.46017000
C	2.75579000	-2.75396500	-1.10154300
C	3.60732900	-1.80430100	-0.56159200
C	3.26646700	0.09419400	1.29683500
C	4.70614300	0.13653900	1.80207600
C	5.81550000	0.18213400	0.94440100
C	4.92111800	0.12976100	3.18593600
C	7.10876600	0.21991000	1.46501500
C	7.31176600	0.21279300	2.84590700
C	6.21481100	0.16763600	3.70596800
C	0.22613300	-4.50487800	-1.48774800
C	1.23781600	-5.48761500	-1.34449300
C	-0.83644400	-4.74893400	-2.39323300
C	1.19031400	-6.65915300	-2.08797200
C	0.14615900	-6.87149600	-2.99502500
C	-0.86399200	-5.91401800	-3.14651200
C	-0.07131700	4.53759600	-1.39723000
C	0.86872000	5.58449800	-1.22504400
C	0.74609600	6.76506100	-1.94548900
C	-0.30268100	6.92317100	-2.85813700
C	-1.24258500	5.90133100	-3.03835800
C	-1.14062200	4.72587800	-2.30783000

H	-7.68131300	1.61547200	1.77452000
H	-6.93407300	1.28265500	0.18571600
H	-7.26602600	-0.06436700	1.31564600
H	-6.69349900	-2.13681600	3.54794800
H	-5.02883800	-1.66010400	3.98767100
H	-6.22255900	-0.40966800	3.52853000
H	-4.20542400	3.36074100	1.22908200
H	-2.18638400	4.40609500	0.32635700
H	-3.94980800	-3.65612300	1.20876600
H	-1.87762900	-4.54822700	0.26163700
H	4.50562900	1.92488000	-0.82674000
H	2.72735300	3.62922500	-1.86626500
H	2.95874800	-3.39791300	-1.94412200
H	4.62095400	-1.60176000	-0.86810800
H	5.68919600	0.18893700	-0.13323000
H	4.07435000	0.09479800	3.86697800
H	7.95777700	0.25498300	0.79002900
H	8.31914900	0.24231800	3.24785900
H	6.36283900	0.16182000	4.78089200
H	2.01988700	-5.34815400	-0.60633900
H	-1.60763300	-3.99882500	-2.52993300
H	1.95506700	-7.41653200	-1.95223400
H	0.11369400	-7.78746700	-3.57637800
H	-1.66789600	-6.08007500	-3.85570000
H	1.65296700	5.48399400	-0.48288400
H	1.45544700	7.57051100	-1.78747900
H	-0.39374500	7.84631100	-3.42164700
H	-2.04982900	6.02565000	-3.75229500
H	-1.85649900	3.92691300	-2.46677300
C	-0.49283100	-0.00965800	-0.76764000
O	0.45129800	0.03000700	-1.52501600
H	0.97136800	-1.43961900	1.22479700
H	0.87368700	1.47303400	1.25473400
H	2.62264500	0.06299600	2.18616800

Table S10. DFT calculated Cartesian coordinates for **9**.

C	-0.61823500	3.75053000	-0.44647300
C	0.75187800	3.71580600	-0.52383700
C	1.46464700	2.47232700	-0.41926900
C	-1.38258000	2.53742100	-0.34180200
C	-0.71483200	1.27823300	-0.28818000
C	0.74464700	1.24836700	-0.28603300
C	-1.49850400	0.10942100	-0.22992100
C	1.47744900	0.05493500	-0.14569200
O	-1.31248900	4.93797500	-0.51871500
O	1.49366300	4.87045000	-0.64548800
C	-1.14288300	5.80906500	0.60899100
C	1.37024900	5.53384600	-1.91282700
C	-2.79506000	2.58027100	-0.29504700
C	-3.53213700	1.42184800	-0.19725600
C	-2.89383500	0.15416600	-0.18478800
C	2.87820800	2.44998500	-0.43104500
C	2.87542300	0.03374700	-0.14329400
C	3.56633300	1.26653000	-0.28853000
C	-3.70963700	-1.07516900	-0.11070900
C	3.63885900	-1.21797900	0.02978500
C	-3.37530400	-2.22636500	-0.78649100
N	-2.33528100	-2.27362100	-1.73801400
C	-2.29787900	-3.51491300	-2.14650500
C	-3.28497100	-4.36756400	-1.49640000
C	-3.97059100	-3.55655900	-0.64644100
C	3.19129100	-2.44507000	-0.40714600
N	2.03427400	-2.60631600	-1.19665900
C	1.91055200	-3.89633700	-1.37072200
C	3.76819500	-3.75907700	-0.11540600
C	2.95594000	-4.67045400	-0.71539800
C	4.95648600	-1.12446900	0.71522600
C	6.11172600	-1.69322700	0.15112000

C	5.07313800	-0.45325400	1.94629200
C	7.34066000	-1.60735600	0.80516200
C	7.43695600	-0.95666800	2.03560300
C	6.29826500	-0.38081300	2.60445100
C	-4.93537800	-1.03035100	0.72746800
C	-6.16761600	-1.50826400	0.24645700
C	-7.30943500	-1.46595800	1.04578600
C	-7.24188100	-0.94863800	2.33996700
C	-6.02670900	-0.46141400	2.82756400
C	-4.88822900	-0.49048200	2.02641700
H	-1.76713000	6.68295600	0.41298200
H	-1.48218200	5.31979700	1.52968000
H	-0.09872800	6.11447800	0.71997700
H	2.02767400	6.40404900	-1.86439600
H	1.69675900	4.87600700	-2.72659300
H	0.34024500	5.85480700	-2.09213300
H	-3.28421400	3.54562200	-0.34703700
H	-4.61503900	1.47338900	-0.16370600
H	3.40824200	3.38878100	-0.53908500
H	4.65049500	1.27237100	-0.29994900
H	-3.42740200	-5.42780100	-1.66284100
H	-4.75973300	-3.83024800	0.03866200
H	4.63707300	-3.94869100	0.49771000
H	3.05006600	-5.74888400	-0.71167300
H	6.04076200	-2.18515300	-0.81322900
H	4.19122100	-0.00250300	2.39022300
H	8.22394300	-2.04447500	0.34876000
H	8.39367700	-0.89174200	2.54544200
H	6.36528900	0.12718400	3.56203600
H	-6.22605200	-1.89115500	-0.76678700
H	-8.25406400	-1.83053200	0.65296200
H	-8.13135000	-0.91711400	2.96231900
H	-5.96658200	-0.05658700	3.83355700
H	-3.94617700	-0.10994100	2.40798300
H	-1.02310900	-0.86069900	-0.23679700
H	0.96081000	-0.88627500	-0.03646500
H	-1.59194300	-3.82925700	-2.91081300
H	1.09386700	-4.30292100	-1.96091200

Table S11. DFT calculated Cartesian coordinates for **9-H_2^{2+}**.

C	-0.61685700	3.74176200	-0.52005500
C	0.75849400	3.70303300	-0.65261700
C	1.46411700	2.45550200	-0.52121500
C	-1.36961200	2.52214300	-0.39562500
C	-0.71032300	1.25313700	-0.37357900
C	0.75254800	1.22222200	-0.39195400
C	-1.51008000	0.09870100	-0.29506200
C	1.50440000	0.04049400	-0.25740900
O	-1.32557300	4.89975900	-0.54674000
O	1.51436100	4.81864000	-0.81555700
C	-1.04390600	5.87163300	0.49178000
C	1.26798800	5.61888900	-1.99891600
C	-2.77872700	2.58699100	-0.27006200
C	-3.53037700	1.44667900	-0.11800800
C	-2.90662000	0.16997900	-0.15230800
C	2.87995000	2.46045600	-0.49352100
C	2.90806200	0.05657300	-0.18363600
C	3.58823400	1.29980300	-0.29517100
C	-3.72378500	-1.04067000	-0.01086800
C	3.67553500	-1.17252600	0.04831200
C	-3.50271800	-2.14684300	-0.84782500
N	-2.83424300	-2.05852300	-2.07671400
C	-2.83115000	-3.26075900	-2.68266300
C	-3.44466500	-4.19882000	-1.83838100
C	-3.87054500	-3.51363100	-0.70680200
C	3.35844000	-2.35237300	-0.64487400
N	2.62721400	-2.36954400	-1.84036000
C	2.53176000	-3.63187800	-2.29937300
C	3.66735600	-3.71174000	-0.36261900
C	3.14577300	-4.49846000	-1.38269500
C	4.78799700	-1.15550600	0.98549300
C	5.94981300	-1.93864800	0.76599500

C	4.72765000	-0.34036500	2.14414400
C	6.99681000	-1.91552900	1.67750300
C	6.90644500	-1.12539600	2.82859100
C	5.77009200	-0.34076300	3.05964400
C	-4.78639500	-1.07572500	0.98163600
C	-5.99605600	-1.77698200	0.74474000
C	-6.99370400	-1.80535600	1.70988100
C	-6.80619900	-1.14894400	2.93112500
C	-5.62156200	-0.44558800	3.18069000
C	-4.62734600	-0.39359500	2.21441800
H	-1.69882600	6.71660400	0.28335200
H	-1.28427000	5.44800200	1.47145300
H	0.00059500	6.18687300	0.46932900
H	1.95570900	6.46048400	-1.92796400
H	1.49021600	5.03283700	-2.89564300
H	0.23652800	5.97342400	-2.03218100
H	-3.25141700	3.56084900	-0.29430300
H	-4.60755800	1.51344600	-0.01593700
H	3.39188400	3.40808400	-0.60478500
H	4.67127800	1.32271100	-0.25477400
H	-3.55521000	-5.25302700	-2.04610800
H	-4.34611400	-3.93496200	0.16636700
H	4.16953100	-4.05507700	0.52958300
H	3.19225900	-5.57410400	-1.46933300
H	6.04630500	-2.50971600	-0.15041000
H	3.83994700	0.25188900	2.33610600
H	7.89204100	-2.49769900	1.48642800
H	7.72599500	-1.11190500	3.54010700
H	5.70242200	0.26620400	3.95620800
H	-6.16728300	-2.24025600	-0.22027900
H	-7.92576200	-2.32242400	1.50795000
H	-7.58757000	-1.17540900	3.68402500
H	-5.47889800	0.05767200	4.13106400
H	-3.70230000	0.13418100	2.41805500
H	-1.04471400	-0.88033800	-0.27197800
H	0.99768900	-0.90767600	-0.11700100
H	2.36799300	-1.53784700	-2.35205900
H	-2.55524500	-1.18611100	-2.50351100
H	-2.41773700	-3.39138900	-3.67327300
H	2.05638900	-3.85343300	-3.24487800

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