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Supporting Information

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Expanded porphyrin with a split personality: A Hückel-Möbius aromaticity switch

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Experimental details

NMR Spectroscopy. ^{1}H NMR spectra were recorded on a high-field spectrometer (^{1}H frequency 500.13 MHz), equipped with a broadband inverse gradient probehead. Spectra were referenced to the residual solvent signals (chloroform-*d*, 7.24 ppm, methanol-d_4 3.30 ppm) or to TMS (hexane-d_{14}) Two-dimensional NMR spectra were recorded with 2048 data points in the t_2 domain and up to 1024 points in the t_1 domain, with a 1 s recovery delay.

The spectra in limonene were recorded as follows: a saturated solution of **1** in limonene (undeuterated, racemic or enantiopure, 500 μL) was placed in a standard 5 mm NMR and TMS (10 μL) was added. An inset containing DMSO-d_6 was introduced to the tube and the sample was capped. An initial spectrum was recorded with a sweep width of ca. 30 ppm to cover all resonances and the spectrum was referenced against TMS. Subsequently, a spectrum was recorded in the range 16-18 ppm using a weak pulse for excitation. This enabled a high S/N ratio to be achieved for the weak NH signal of **1**.

Estimation of thermodynamic parameters and extrapolated chemical shifts. The chemical shift of proton *i* observed at temperature *T* was assumed to be a weighted average of the corresponding chemical shifts of the two exchanging forms **1**-H and **1**-M:

$$\delta^i(T) = p_{\mathrm{H}}(T)\delta^i_{\mathrm{H}} + p_{\mathrm{M}}(T)\delta^i_{\mathrm{M}} = \frac{K(T)}{1+K(T)}\left(\delta^i_{\mathrm{H}} - \delta^i_{\mathrm{M}}\right) + \delta^i_{\mathrm{M}}$$

where $\delta_{\mathrm{H}}{}^i$ and $\delta_{\mathrm{M}}{}^i$ are the chemical shifts of signal *i* in **1**-H and **1**-M, respectively, and

$$K(T) = \frac{p_{\mathrm{H}}}{p_{\mathrm{M}}} = \exp\left(\frac{\Delta S}{R} - \frac{\Delta H}{RT}\right)$$

is identical for all peaks. Values of ΔH, ΔS, $\delta_{\mathrm{A}}{}^i$ and $\delta_{\mathrm{B}}{}^i$ were obtained using weighted nonlinear least-squares, by minimizing the quantity

$$R = \sum_{i,j}\left(\delta^i(T_j)^{\mathrm{calc}} - \delta^i(T_j)^{\mathrm{exptl}}\right)^2 \left|\delta^i_{\mathrm{H}} - \delta^i_{\mathrm{M}}\right|,$$

where *i* and *j* index peaks and temperature values, respectively. The Solver add-on of MS Excel® was used for all calculations and the SolverAid macro [1] was employed to estimate the errors of ΔH and ΔS. Errors of the extrapolated shifts $\delta_{\mathrm{A}}{}^i$ and $\delta_{\mathrm{B}}{}^i$ could not be determined for the LS scheme used (for any chosen $\delta_{\mathrm{A}}{}^k$ and $\delta_{\mathrm{B}}{}^k$, not all terms $\delta_i(T_j)$ are dependent, only those with $i = k$).

UV-vis spectroscopy. Electronic spectra were recorded on a diode-array spectrophotometer. To obtain the low-temperature spectrum of **1**, a 10 mm cell containing the $CHCl_3$ solution was incubated in acetone bath at –70 °C. The cell was quickly removed from the bath and placed immediately in the optical path of the spectrophotometer to record the spectrum.

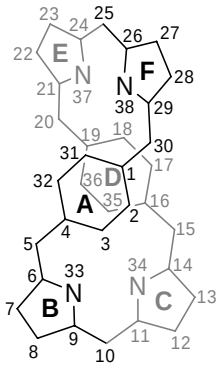
Computational chemistry. Tautomers of **1**-H and **1**-M used for the quantum chemical calculations were selected arbitrarily as 33,38-*H* in each case (calculations were performed before the X-ray structure was available). Density functional theory calculations were performed using GAUSSIAN03.[2] Geometry optimizations were carried out within unconstrained C_1 symmetry, with starting coordinates preoptimized using semiempirical methods. Becke's three-parameter exchange functional[3] with the gradient-corrected correlation formula of Lee, Yang, and Parr (B3LYP)[4] were used with the 6-31G** basis set. Absolute ^{1}H shielding values were calculated at the GIAO-RHF/6-31G** level of theory using the B3LYP geometries. The chemical shift values were subsequently calculated relative to tetramethylsilane (TMS, absolute shielding: 31.75 ppm). The shifts were then averaged over the observed symmetry of **1** in solution (D_2 with phenylene rings freely rotating).

Synthesis

General. Unless noted otherwise, all reagents and solvents were used as received. Dichloromethane was distilled from calcium hydride, and tetrahydrofuran was distilled from sodium/benzophenone ketyl in the atmosphere of nitrogen.

1,4-Bis(mesitylhydroxymethyl)benzene (2). To a 250 mL round-bottomed flask equipped with a stirring bar, 1,4-dibromobenzene (3 g, 12.71 mmol) was introduced followed by dry tetrahydrofuran (150 mL). The mixture was purged with nitrogen and the reaction vessel was sealed with rubber septa. The reaction mixture was then cooled to –90 °C and *n*-buthyllithium (2.5 M in hexane, 11.2 mL, 2.2 equiv.) was slowly added with stirring, while keeping the reaction temperature below –78 °C. When the addition was complete, the reaction was cooled to –90 °C and mesitylaldehyde (4.13 mL, 2.2 equiv.) was added dropwise from a syringe. The reaction was allowed to warm up to room temperature and the mixture was poured into aqueous ammonium chloride, and extracted with chloroform. Combined organic extracts were dried with anhydrous sodium sulfate and the solvent was removed under reduced pressure. The crude product was purified by crystallization from hexane to yield 1.28 g (27%) of white powder.

10,25-Diphenyl-5,15,20,30-tetramesityl-A,D-di-*p*-benzi[28]hexaphyrin(1.1.1.1.1.1) (1). A three necked 1 L round-bottomed flask equipped with a stirring bar and nitrogen inlet was charged with freshly distilled dichloromethane (500 mL). Dicarbinol **2** (375 mg, 1 mmol), pyrrole (139 μL, 2 mmol), and benzaldehyde (102 μL, 1 mmol) were added to the solution and nitrogen was bubbled through the stirred reaction mixture for 15 min. Boron trifluoride diethyl etherate (50 μL) was then added and the reaction was protected from light. After 2 hours of stirring, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 655.4 mg, 2 mmol) was added and the reaction was stirred for 5 minutes. The solvent was then removed under reduced pressure. The crude residue, containing a number of expanded benziporphyrin macrocycles was chromatographed on a grade II basic alumina column (35 mm × 20 cm) using dichloromethane as the eluent. The fraction containing **1** eluted as the first bluish-violet, band. This fraction was collected and freed from solvent on a rotary evaporator. Subsequent column chromatography (silica gel, benzene, 35 mm × 30 cm) yielded hexaphyrin **1** as the first fraction. The crude product was further purified by column chromatography (grade II basic alumina, 1% ethyl acetate in hexane). **1** eluted as the major green fraction preceded by a small amount of yellowish impurity. Yield: 28 mg (5%). The product may be additionally purified by crystallization from heptane or methanol. UV-vis ($CHCl_3$, ca. 203 K) λ_{max} [nm] (log ε, ε in $M^{-1}cm^{-1}$): 383 (4.75). 569 (4.85), 678 (4.22), 739 (4.25); UV-vis (hexane, 293 K) λ_{max} [nm] (log ε, ε in $M^{-1}cm^{-1}$): 439 (4.78), 590 (4.49); ^{1}H NMR (500 MHz, $CDCl_3$, 293 K) δ 12.26 (bs, 2H, NH), 7.42 (d, 4H, ^3J = 7.3 Hz, *o*-Ph), 7.36 (t, 4H, ^3J = 7.3 Hz, *m*-Ph), 7.29 (t, 2H, ^3J = 7.3 Hz, *p*-Ph), 7.10 (s, 8H, 2,3,17,18,31,32,35,36-H) 6.87 (s 4H, 3-Mes), 6.84 (s, 4H, 5-Mes), 6.57 (d, 4H, ^3J = 5.0 Hz, 8,12,23,27-H), 6.47 (d, 4H, ^3J = 5.0 Hz, 7,13,22,28-H) 2.28 (s, 12H, 4-Mes), 1.98 (s, 12H, 6-Mes), 1.91(s, 12H, 2-Mes); ^{13}C NMR ($CDCl_3$, 298 K, 126 MHz, partial assignment from HMQC and HMBC spectra) δ 160.21, 149.09 (α-pyrrole), 138.48 (*i*-Ph), 137.87, 137.48, 137.40, 137.10 (1/3/5-Mes), 136.87 (1/3/5-Mes), 132.43 (p_2), 131.45 (*o*-Ph), 130.59 (phenylene), 128.85, 128.31 (p_1), 128.17 (5/3-Mes), 128.04 (*m*-Ph), 127.94 (3/5-Mes), 126.55 (*p*-Ph), 108.13, 21.09 (4-Mes-Me), 20.59 (2-Mes-Me), 20.38 (6-Mes-Me). HRMS (ESI+): *m*/*z* 1113.5856 [M+H$^+$], calcd for $C_{82}H_{73}N_4^+$: 1113.5830.



Scheme S1. Numbering scheme for the macrocycle of **1**.

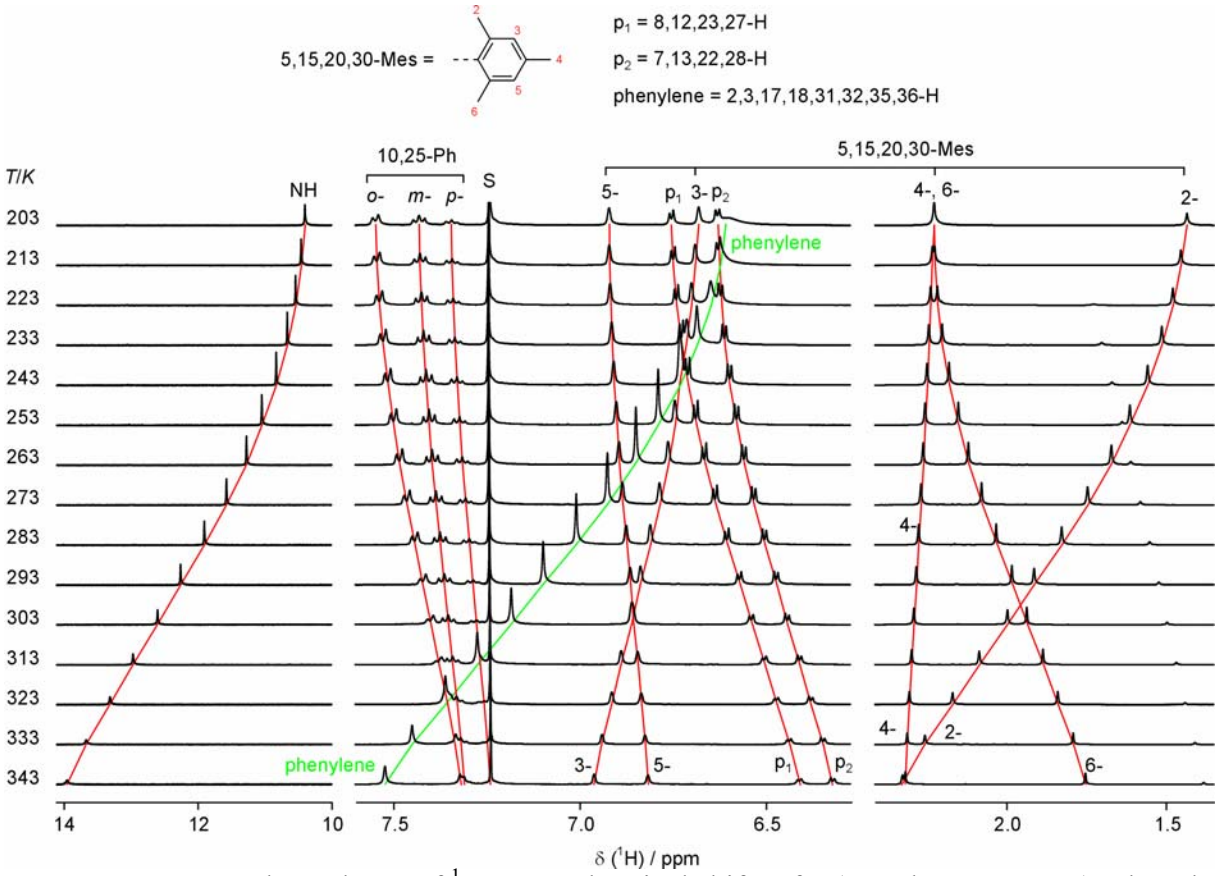


Figure S1. Temperature dependence of ^{1}H NMR chemical shifts of **1** ($CDCl_3$, 203-343 K). Phenylene rotation decelerates at lower temperatures leading to noticeable broadening of the phenylene signal.

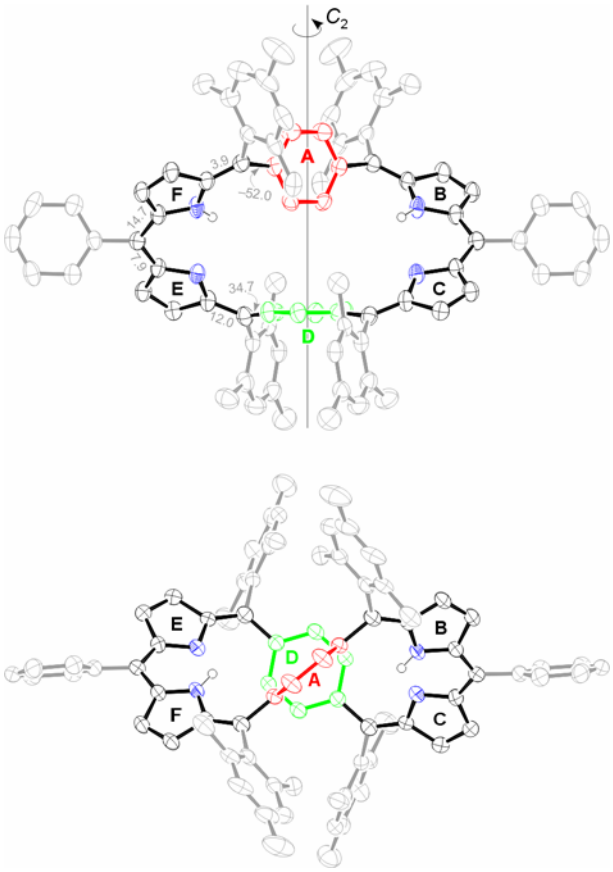


Figure S2. X-ray crystal structure of **1** with thermal ellipsoids at the 50% probability level and the meso substituents included.

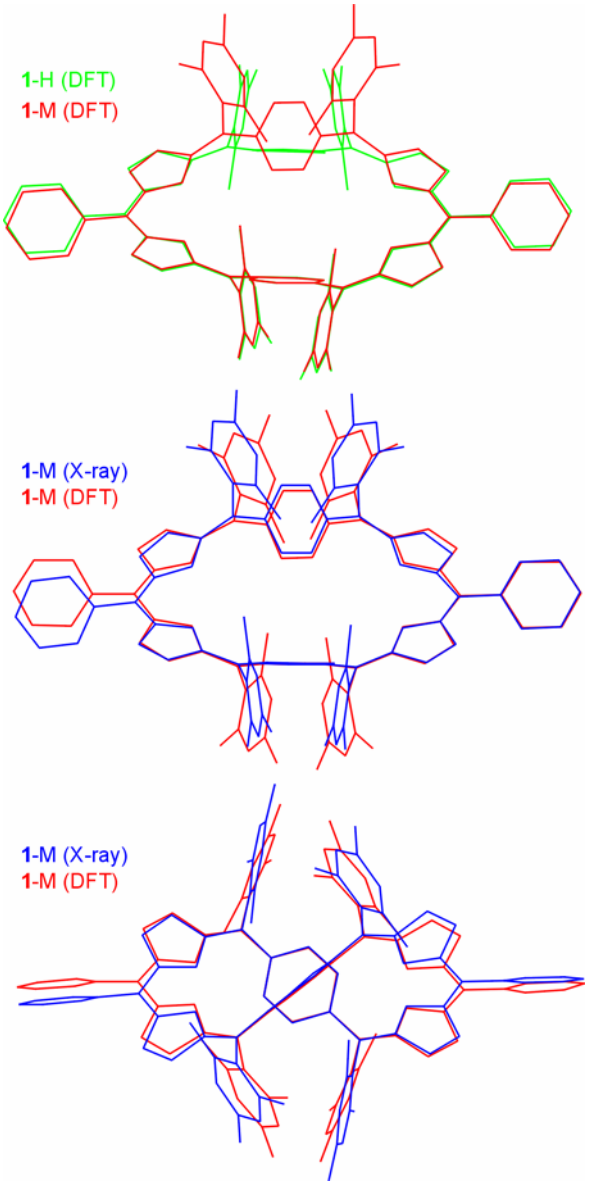


Figure S3. Comparison of calculated and experimental geometries of **1**. In each pair, the phenylene ring perpendicular to the symmetry axis was used as the reference for the overlay.

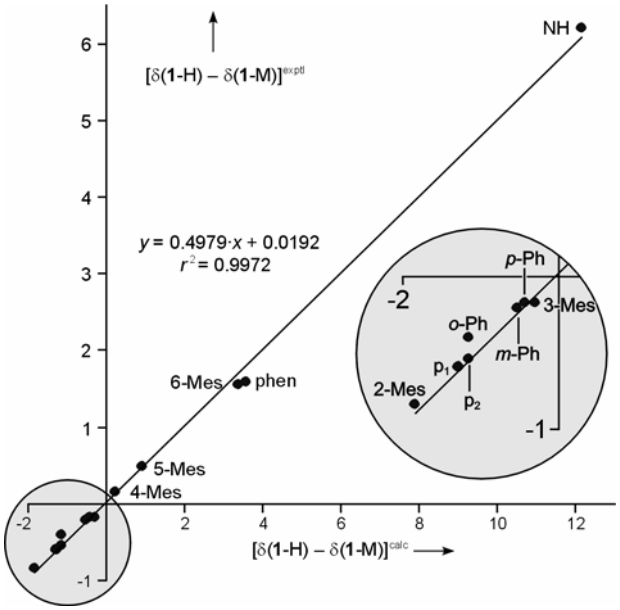


Figure S4. Chemical shift differences between conformers **1**-H and **1**-M: correlation between calculated and experimental values.

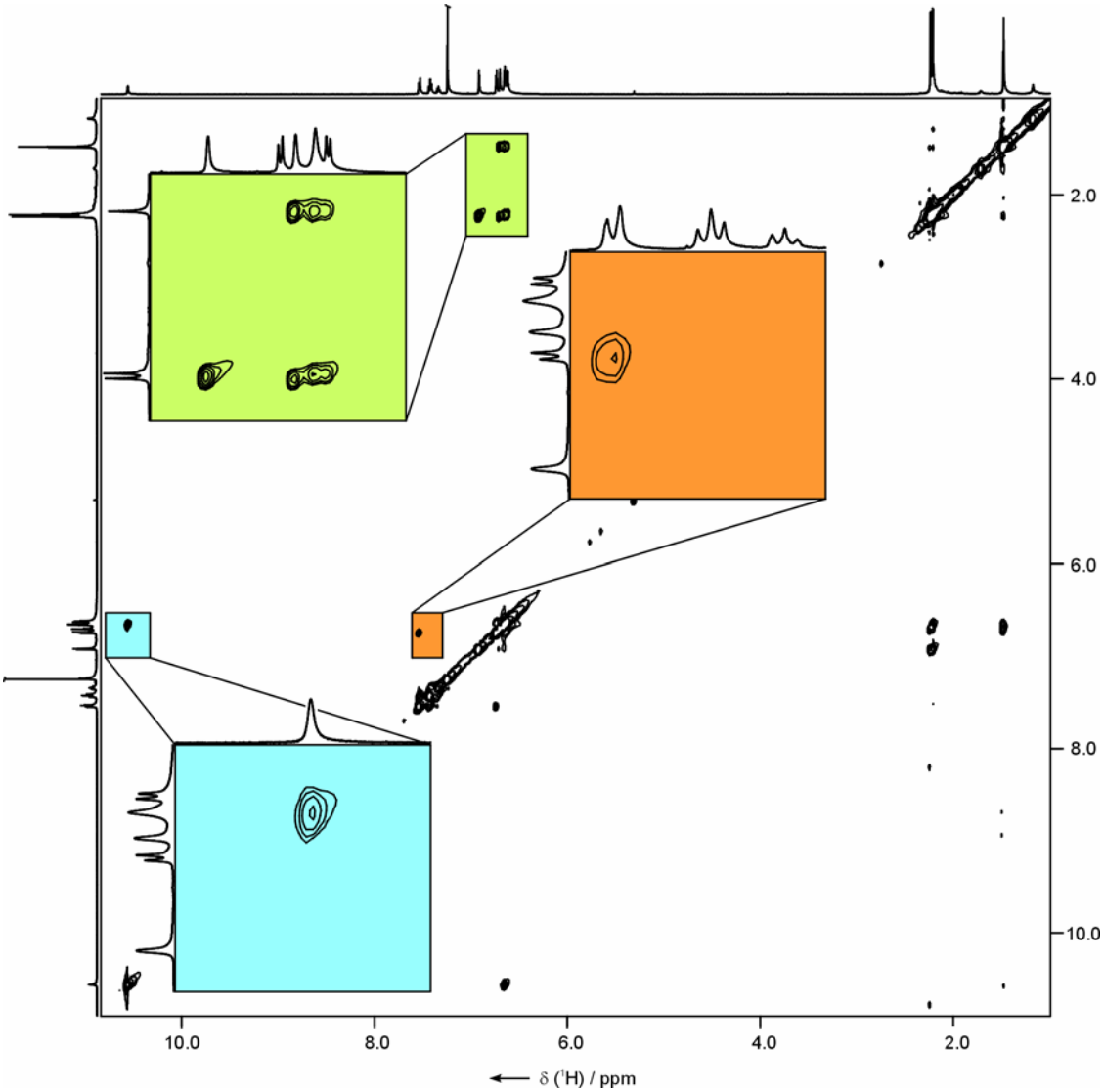


Figure S5. ^{1}H NOESY spectrum of **1** (500 MHz, $CDCl_3$, 223 K, τ_M = 500 ms). The observed NOE's are positive (in phase with the diagonal). The assignment of peaks is given in Figure S1. A ^{1}H ROESY spectrum (500 MHz, $CDCl_3$, 323 K, τ_{SL} = 300 ms) provided essentially the same structural information. No exchange between *ortho*-Mes signals (*meta*-Mes signals) was observed in either case.

Animation S1. Animated version of Figure 1. The airplane closely follows the surface of the π system showing that the surface is indeed one-sided.

The animation is available as a separate file
moebiusmovie.wmv
(Windows Media Video format)

Table S1. Experimental ^{1}H NMR chemical shifts (ppm) for **1** in $CDCl_3$ as a function of temperature.

T/K	NH	phenylene	ortho	meta	para	3-Mes	5-Mes	p_1	p_2	4-Mes	2-Mes	6-Mes
343	13.96	7.52	7.32	7.30	7.25	6.96	6.82	6.41	6.32	2.32	2.33	1.75
333	13.67	7.45	7.34	7.31	7.25	6.94	6.83	6.44	6.35	2.31	2.26	1.79
323	13.31	7.36	7.36	7.33	7.26	6.92	6.84	6.47	6.38	2.31	2.17	1.84
313	12.97	7.28	7.38	7.34	7.27	6.89	6.85	6.51	6.41	2.30	2.09	1.89
303	12.60	7.18	7.40	7.35	7.28	6.86	6.86	6.54	6.44	2.29	2.00	1.94
293	12.26	7.10	7.42	7.36	7.29	6.84	6.87	6.57	6.47	2.28	1.91	1.98
283	11.91	7.01	7.44	7.38	7.30	6.81	6.88	6.61	6.51	2.28	1.83	2.03
273	11.58	6.93	7.47	7.39	7.31	6.79	6.89	6.64	6.53	2.27	1.75	2.08
263	11.28	6.85	7.48	7.40	7.32	6.76	6.90	6.67	6.56	2.26	1.67	2.12
253	11.05	6.79	7.50	7.41	7.32	6.75	6.90	6.69	6.58	2.26	1.61	2.15
243	10.83	6.73	7.52	7.41	7.33	6.73	6.91	6.71	6.60	2.25	1.56	2.18
233	10.67	6.69	7.53	7.42	7.34	6.71	6.92	6.73	6.61	2.24	1.51	2.20
223	10.54	6.65	7.54	7.43	7.34	6.70	6.92	6.74	6.62	2.24	1.48	2.22
213	10.46	6.62	7.55	7.43	7.34	6.69	6.92	6.75	6.63	2.23	1.45	2.23
203	10.40	6.60	7.55	7.43	7.34	6.68	6.92	6.75	6.63	2.23	1.44	2.23

Table S2. Calculated ^{1}H NMR chemical shifts (ppm) for **1** in $CDCl_3$ obtained in a least-squares minimization. Extrapolated values are in italics.

	Chemical shift (ppm)													
T/K	NH	phen.	ortho	meta	para	3-Mes	5-Mes	p_1	p_2	4-Mes	2-Mes	6-Mes	ΔG [J/mol]	*K*
463	*15.83*	*8.01*	*7.20*	*7.23*	*7.19*	*7.11*	*6.77*	*6.23*	*6.16*	*2.37*	*2.80*	*1.50*	-8.06E+03	8.11E+00
443	*15.68*	*7.97*	*7.20*	*7.24*	*7.20*	*7.10*	*6.77*	*6.24*	*6.17*	*2.36*	*2.77*	*1.52*	-6.88E+03	6.48E+00
423	*15.49*	*7.92*	*7.22*	*7.25*	*7.20*	*7.08*	*6.78*	*6.26*	*6.19*	*2.36*	*2.72*	*1.54*	-5.71E+03	5.07E+00
403	*15.24*	*7.86*	*7.23*	*7.26*	*7.21*	*7.07*	*6.78*	*6.29*	*6.21*	*2.35*	*2.66*	*1.58*	-4.54E+03	3.87E+00
383	*14.91*	*7.77*	*7.25*	*7.27*	*7.22*	*7.04*	*6.79*	*6.32*	*6.24*	*2.35*	*2.57*	*1.62*	-3.36E+03	2.88E+00
363	*14.49*	*7.66*	*7.28*	*7.28*	*7.23*	*7.01*	*6.81*	*6.36*	*6.28*	*2.34*	*2.47*	*1.68*	-2.19E+03	2.07E+00
343	13.96	7.53	7.32	7.30	7.24	6.97	6.82	6.41	6.32	2.32	2.34	1.75	-1.02E+03	1.43E+00
333	13.65	7.45	7.34	7.31	7.25	6.94	6.83	6.44	6.35	2.32	2.26	1.79	-4.30E+02	1.17E+00
323	13.32	7.37	7.36	7.33	7.26	6.92	6.84	6.47	6.38	2.31	2.18	1.84	1.57E+02	9.43E-01
313	12.97	7.28	7.38	7.34	7.27	6.89	6.85	6.51	6.41	2.30	2.09	1.89	7.43E+02	7.52E-01
303	12.61	7.18	7.40	7.35	7.28	6.86	6.86	6.54	6.44	2.29	2.00	1.94	1.33E+03	5.90E-01
293	12.25	7.09	7.43	7.36	7.29	6.83	6.87	6.57	6.47	2.28	1.91	1.98	1.92E+03	4.55E-01
283	11.90	7.00	7.45	7.38	7.30	6.81	6.88	6.61	6.50	2.27	1.82	2.03	2.50E+03	3.45E-01
273	11.58	6.92	7.47	7.39	7.31	6.78	6.89	6.64	6.53	2.27	1.74	2.08	3.09E+03	2.56E-01
263	11.29	6.84	7.49	7.40	7.32	6.76	6.90	6.67	6.56	2.26	1.67	2.12	3.68E+03	1.86E-01
253	11.04	6.78	7.50	7.41	7.32	6.74	6.90	6.69	6.58	2.25	1.61	2.15	4.26E+03	1.32E-01
243	10.83	6.73	7.52	7.42	7.33	6.72	6.91	6.71	6.60	2.25	1.55	2.18	4.85E+03	9.07E-02
233	10.67	6.69	7.53	7.42	7.33	6.71	6.92	6.73	6.61	2.24	1.51	2.20	5.44E+03	6.04E-02
223	10.55	6.65	7.54	7.43	7.34	6.70	6.92	6.74	6.62	2.24	1.48	2.22	6.02E+03	3.88E-02
213	10.46	6.63	7.54	7.43	7.34	6.70	6.92	6.75	6.63	2.24	1.46	2.23	6.61E+03	2.39E-02
203	10.40	6.62	7.55	7.43	7.34	6.69	6.92	6.75	6.63	2.24	1.45	2.24	7.20E+03	1.41E-02
183	*10.34*	*6.60*	*7.55*	*7.43*	*7.34*	*6.69*	*6.92*	*6.76*	*6.64*	*2.24*	*1.43*	*2.25*	8.37E+03	4.08E-03
163	*10.32*	*6.60*	*7.55*	*7.43*	*7.34*	*6.69*	*6.93*	*6.76*	*6.64*	*2.24*	*1.43*	*2.25*	9.54E+03	8.75E-04
143	*10.32*	*6.60*	*7.55*	*7.43*	*7.34*	*6.68*	*6.93*	*6.76*	*6.64*	*2.23*	*1.43*	*2.25*	1.07E+04	1.22E-04

Table S3. Crystal data and structure refinement for **1**.

Empirical formula	$C_{85}H_{75}Cl_9N_4$	
Formula weight	1470.53	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Pccn*	
Unit cell dimensions	a = 11.9506(3) Å	α= 90°.
	b = 29.0104(8) Å	β= 90°.
	c = 21.5417(6) Å	γ = 90°.
Volume	7468.3(3) Å^3	
Z	4	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.386 mm^{-1}	
F(000)	3060	
Crystal size	0.20 × 0.15 × 0.15 mm^3	
Theta range for data collection	2.64 to 25.00°.	
Index ranges	$-14 \le h \le 13$, $-32 \le k \le 34$, $-25 \le l \le 25$	
Reflections collected	41798	
Independent reflections	6577 [R(int) = 0.0909]	
Completeness to θ = 25.00°	99.9%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9444 and 0.9268	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6577 / 0 / 485	
Goodness-of-fit on F^2	1.074	
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0971, $wR2$ = 0.2543	
R indices (all data)	$R1$ = 0.1509, $wR2$ = 0.3093	
Largest diff. peak and hole	0.773 and –0.841 e·Å^{-3}	

Table S4. Cartesian coordinates for the DFT-optimized structure of **1-H** (B3LYP/6-31G**, XYZ format).

```
158
XYZ file for :
  H        1.31112        6.83313       -6.49945
  H        1.07817        4.25112       -6.48951
  H        1.61524        1.99713       -6.55319
  H       -1.83979       -2.40093       -6.31782
  H       -1.30487       -4.63591       -6.07051
  H       -1.52293       -7.21891       -5.82856
  H       -0.29325        6.82611       -5.76925
  C        0.77964        6.79014       -5.54271
  C        1.23363        4.30415       -5.41343
  C        1.63271        1.82516       -5.47318
  H        0.11775       -7.11587       -5.19274
  H        1.02634        7.69416       -4.97961
  C       -1.85232       -2.13291       -5.25783
  H        2.55459        1.28818       -5.22670
  H        0.80160        1.15515       -5.22658
  C       -0.94140       -7.07688       -4.91127
  C       -1.41941       -4.59389       -4.98956
  H       -2.79044       -1.60892       -5.05032
  H       -1.04343       -1.41589       -5.08145
  C        1.13528        5.54216       -4.77051
  C        1.53230        3.13017       -4.71926
  H       -1.13771       -7.92687       -4.25235
  C       -1.70273       -3.36389       -4.39273
  C       -1.28176       -5.76687       -4.24047
  C        1.35459        5.58220       -3.39240
  C        1.75660        3.19021       -3.32214
  H        4.54751        3.35527       -3.14475
  H        1.27931        6.53321       -2.87046
  C       -1.87544       -3.30086       -2.98982
  C       -1.45145       -5.68385       -2.85856
  H       -4.65656       -3.47691       -2.72621
  H       -9.85385        0.43399       -2.30690
  C        1.66424        4.43222       -2.65522
  H       10.10499        0.13841       -1.97390
  C        2.07624        1.94223       -2.55596
  C        4.54617        2.54028       -2.43573
  H       -1.34874       -6.58483       -2.25648
  H       -7.38992        0.33805       -2.16766
  H        7.64206       -0.00765       -2.10513
  H       -0.59084        2.38718       -2.40430
  H        2.30021       -0.79876       -2.38378
  C        1.01117        0.94121       -2.37547
  C       -2.17880       -1.99285       -2.32200
  C       -1.75080       -4.47584       -2.21673
  C       -0.34585        1.33119       -2.34916
  H        0.49421       -2.43580       -2.30965
  C        1.27618       -0.44678       -2.33331
  C        0.24918       -1.37880       -2.29580
  H       -2.40188        0.73815       -2.26817
  C       -1.37287        0.40117       -2.28065
  C       -4.63689       -2.58890       -2.11022
  C       -1.10785       -0.98683       -2.26249
  C        3.35801        1.78327       -2.07631
  H        6.64588        2.33134       -1.84768
  C        5.61786        2.00832       -1.78518
  C       -3.44905       -1.78587       -1.82164
  C       -9.37334        0.34202       -1.33766
  H       -6.72319       -2.26093       -1.51727
  C       -5.68320       -1.96490       -1.51176
  C       -7.98338        0.28205       -1.25996
  C        9.51453        0.18641       -1.06419
  C        8.12357        0.11538       -1.13989
  C        1.88049        4.55226       -1.16211
  N        3.79457        0.82230       -1.17307
  C        5.14946        0.91733       -0.94740
  N       -3.80648       -0.72186       -1.00184
  H        2.94336        4.50228       -0.90058
  H      -11.22989        0.34901       -0.23558
  H        1.49429        5.50726       -0.79333
  C       -5.12558       -0.80488       -0.80550
  C       -1.92655       -4.46581       -0.71282
  C      -10.14692        0.29903       -0.17504
  H        1.38423        3.74726       -0.61334
  H       -2.98370       -4.41583       -0.43135
  H        3.23226        0.27030       -0.52134
  H       11.22988        0.34948        0.23566
  C       10.14691        0.29945        0.17512
  H       -1.50776       -5.37379       -0.27059
  C       -7.32799        0.17009       -0.01963
  H       -1.43680       -3.60379       -0.25059
  C        7.32799        0.17139        0.01971
  C        5.84803        0.10636       -0.05403
  C       -5.84803        0.10613        0.05412
  H        1.50897       -5.37372        0.26992
  H        1.43895       -3.60372        0.24985
  H        2.98587       -4.41569        0.43064
  H       -3.23227        0.27019        0.52142
  C       -9.51454        0.18607        1.06428
  H       -1.38138        3.74523        0.61427
  C        1.92773       -4.46570        0.71211
  H       -1.49051        5.50523        0.79318
  C        5.12561       -0.80463        0.80563
  C       -8.12457        0.11410        1.13998
  H       -2.94054        4.50320        0.89848
  C        9.37333        0.34346        1.33773
  C       -5.14949        0.91716        0.94745
  C        7.98336        0.28243        1.26104
  N        3.80651       -0.72166        1.00197
  C       -1.87767        4.55123        1.16201
  N       -3.79460        0.82219        1.17313
  H        6.72329       -2.25959        1.51746
  C        5.68328       -1.96461        1.51194
  H      -10.10499        0.13708        1.97398
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  C        3.44913       -1.78565        1.82081
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  H        1.35100       -6.58468        2.25587
  C       -3.35808        1.78222        2.07633
  C        1.75198       -4.47667        2.21602
  H        2.40185        0.73834        2.26823
  C        1.10789       -0.98668        2.26262
  C       -4.54727        2.53920        2.43571
  C        2.17988       -1.99366        2.32218
  C        1.37285        0.40132        2.28073
  H       -0.49411       -2.43672        2.30985
  C       -0.24912       -1.37871        2.29595
  C       -1.27616       -0.44773        2.33342
  C        0.34580        1.33130        2.35019
  H       -2.30018       -0.79975        2.38391
  C       -1.01121        0.94028        2.37552
  H        0.59075        2.38731        2.40429
  H        4.65671       -3.47660        2.72646
  C       -2.07632        1.94226        2.55596
  C       -1.66342        4.43127        2.65512
  H       -1.27657        6.53228        2.87026
  C        1.45268       -5.68466        2.85790
  C        1.87557       -3.30065        2.98906
  H       -4.54864        3.35422        3.14470
  C       -1.35281        5.58129        3.39225
  C       -1.75673        3.18928        3.32210
  H        1.13003       -7.92664        4.24779
  C        1.28299       -5.76764        4.23982
  C        1.70287       -3.36363        4.39297
  C       -1.13550        5.54132        4.77036
  H       -1.00164        7.69333        4.96838
  C        0.94368       -7.07763        4.91068
  C       -1.53443        3.13032        4.71921
  C        1.41959       -4.59362        4.98886
  H       -0.11346       -7.11264        5.20215
  H        2.78950       -1.60859        5.05048
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  H       -2.55764        1.28831        5.22674
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  H       -0.80464        1.15434        5.22762
  C       -0.78291        6.79035        5.54351
  C       -1.23580        4.30434        5.41433
  C       -1.63578        1.82433        5.47419
  H        1.53223       -7.22460        5.82197
  H        0.28496        6.81138        5.79804
  H        1.30505       -4.63660        6.06980
  H       -1.33739        6.84636        6.48623
  H        1.83888       -2.40158        6.31802
  H       -1.08134        4.25036        6.49041
  H       -1.61932        1.99735        6.55319
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Table S5. Cartesian coordinates for the DFT-optimized structure of **1-M** (B3LYP/6-31G**, XYZ format).

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XYZ file for :
  H       -0.21838        5.11011       -7.71244
  H       -0.98284        6.57839       -7.08907
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  H        0.70779        6.24604       -6.72273
  H        2.67528       -6.69205       -6.56098
  H       -0.79938        3.11135       -6.55594
  H        1.34536       -7.45257       -5.69194
  C        2.35123       -7.03451       -5.57183
  H        1.10766       -4.61609       -5.74902
  C       -0.69192        5.03168       -5.60277
  C       -0.92543        3.65720       -5.62390
  H        3.01443       -7.84789       -5.26442
  H       -1.12990        1.06694       -5.51074
  H        0.44033       -2.46175       -5.23098
  C        1.65687       -4.72195       -4.81683
  C        2.36146       -5.90531       -4.56820
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  C       -1.53863        1.45726       -4.57500
  H       -2.60401        1.20326       -4.54599
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  C        0.85966       -2.41277       -4.22227
  H        1.49332       -1.52248       -4.15772
  C        1.63678       -3.66891       -3.90095
  H       -1.06516        0.92113       -3.74589
  H       -4.28900        3.57126       -3.51274
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  H        0.03213       -2.26352       -3.51900
  H        3.60604       -6.92528       -3.14765
  C       -1.22716        5.04245       -3.21688
  C       -1.46874        3.64794       -3.25894
  H        4.80112       -2.78701       -3.16094
  C       -4.32732        2.84913       -2.70967
  H       -6.45247        2.33327       -2.54166
  C        2.36051       -3.78811       -2.69067
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  H        6.72394       -1.26709       -2.10203
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  C        2.33165       -2.65301       -1.70184
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  H       -2.34276        5.60740       -1.44654
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  H       -9.87655       -1.63021       -0.78060
  H       -0.60045        5.59099       -1.21486
  C        3.85249       -5.16645       -1.13502
  H        4.08434       -6.22383       -0.97901
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  C        0.48403        2.72206       -1.21328
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  C        1.12281       -2.52835       -0.87850
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  H       10.07313       -1.51494        0.25935
  C        9.45919       -0.62016        0.21658
  H        7.25040        2.55648        0.08366
  C        7.86837        1.66471        0.13241
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  H       -3.56620       -4.58517        0.08308
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  H       -1.10618       -4.63185        0.62296
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  H       -1.03235       -0.33069        0.62248
  C       -4.11684       -4.96621        0.94850
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  C       -1.85962       -4.72661        4.61117
  H        2.59729        0.50286        4.57110
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  C        1.41242        2.31873        4.68231
  C        1.14755        5.08854        4.94246
  H        1.05903        6.16849        5.04266
  C       -2.66448       -7.01732        5.32020
  H       -0.52930       -2.53953        5.06946
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  H        1.07432        0.33298        5.45348
  C        1.04887        2.89847        5.90459
  H       -3.10996       -6.71105        6.27324
  C        0.91206        4.27839        6.05769
  H        0.86867        2.24812        6.75734
  H       -0.53285        5.24015        7.35232
  C        0.50400        4.88217        7.38119
  H        1.13176        5.74167        7.63881
  H        0.57875        4.15426        8.19366
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