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Supplementary Information for:

Tubularenes

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Experimental section

General considerations. All reactions were performed in oven-dried or flame-dried round bottom flasks, unless otherwise noted. The flasks were fitted with Teflon magnetic stir bar, rubber septa and/or reflux condenser, under a positive pressure of nitrogen, unless otherwise noted. Anhydrous and anaerobic THF, diethyl ether, hexane, dichloromethane, and benzene were dried and deoxygenated on dual high-performance columns within a Glass Contour 800L Solvent Purification System. Anhydrous and anaerobic *ortho*-dichlorobenzene was purchased from Sigma Aldrich (sure-seal bottle).

^{1}H and ^{13}C NMR spectra were recorded on Bruker Avance III 400 MHz or Bruker Avance III 600 MHz. Chemical shifts for protons are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) and are reference to residual protium in the NMR solvent ($CHCl_3$: δ 7.26; CH_2Cl_2: δ 5.32; $(CH_3)_2SO$: δ 2.50; and CH_3OH: δ 4.78, 3.31). Chemical shifts for carbon are reported in ppm downfield from TMS and are referenced to the carbon resonances of the solvent ($CHCl_3$: δ 77.0; CH_2Cl_2: δ 54.0; $(CH_3)_2SO$: δ 39.51; and CH_3OH: δ 49.1. Data is presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constants in Hertz, and integration. Some ^{1}H NMR and ^{13}C NMR were recorded at high temperatures to enhance signal resolution in the aromatic region. Resonances corresponding to the numerous aromatic carbon atoms in the reported compounds sometimes overlap, thereby reducing the number of observed resonances.

High-resolution mass spectrometry (HRMS) was performed on a (1) Thermo Scientific Q-Exactive Oribtrap instrument equipped with a Dionex Ultimate 3000 (RSLC) inlet system, and electrospray (ESI) and atmospheric pressure chemical (APCI) ionization sources; or (2) a Bruker Daltonics UltrafleXtreme MALDI TOF/TOF MS instrument using dithranol (DIT) matrix.

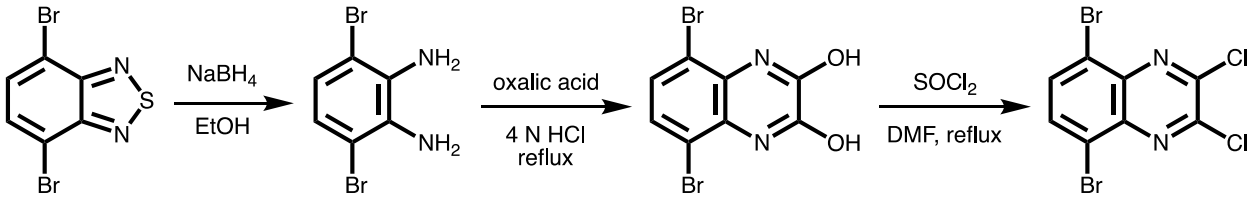
Absorption spectra were obtained on a Cary 60 UV-Vis spectrophotometer and emission spectra were recorded in a HORIBA Jobin Yvon Fluoromax-3 spectrofluorometer.

Electrochemical data (cyclic voltammetry and differential pulse voltammetry) were recorded on a CHI760E bipotentiostat using a three-electrode cell setup with a 1 mm diameter glassy carbon working electrode, Pt wire counter electrode, and Ag wire as reference electrode. All measurements were done under a dinitrogen atmosphere and at room temperature. A 0.1 M

solution of tetrabutylammonium hexafluorophosphate, [*n*-Bu_4N][PF_6], in *ortho*-dichlorobenzene was used as the supporting electrolyte. Data was referenced to Fc/Fc^+ by introducing ferrocene in the same solution. The energy level values of the lowest unoccupied molecular orbitals (LUMO) were calculated according to the following equation: $E_{LUMO} = [E_{1/2}(\text{first reduction}) - 4.80]$ eV.

Single crystal data for tubular[4,8,8,8]arene (**1**) was collected on a Bruker X8 Prospector Ultra diffractometer equipped with an APEX II CCD detector and an IμS microfocus Cu Kα X-ray source (λ = 1.54178 Å). Temperature was maintained using an Oxford Cryosystem nitrogen flow apparatus. Single crystals of **1** suitable for X-ray structure analysis were coated with Paratone N-oil and mounted on MiTeGen Kapton loops (polyimide). Data for compound **1** was collected at 150 K. Raw data were integrated and corrected for Lorentz and polarization effects using Bruker APEX3.[1] Absorption corrections were applied using SADABS.[2] Space group assignments were determined by examination of systematic absences, E-statistics, and successive refinement of the structures. The program PLATON[3, 4] was employed to confirm the absence of higher symmetry for any of the crystals. The positions of the heavy atoms were determined using intrinsic phasing methods using the program SHELXT[5] and SHELXL[6] with Olex2[7] interface. Successive cycles of least-square refinement followed by difference Fourier syntheses revealed the positions of the remaining non-hydrogen atoms. Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were added in idealized positions. Crystallographic data for **1** is given in Table S1. The cavity size of **1** was calculated from the solvent accessible volume calculator in Olex2. By employing this functionality, we found a discrete pocket within the interior of **1** of 265.9 $Å^3$ (Probe 1.2 Å, grid 0.25 Å).

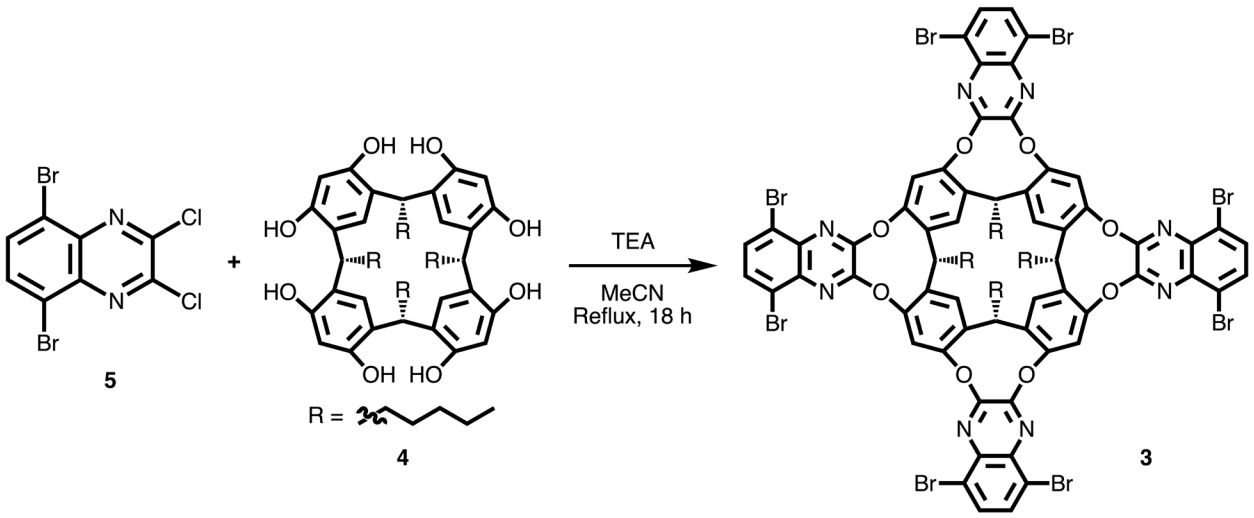
Synthesis details. Compounds **S1**,[8] **S2**,[9] and **4**[10] were obtained according to published procedures.



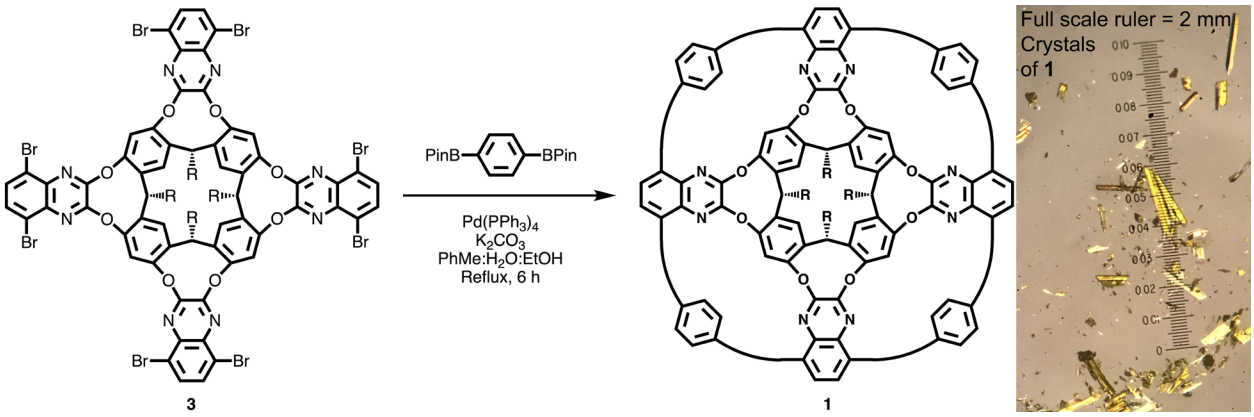
S1 **S2** **S3** **5**

Compound **S3**. A 500 mL round bottom flask was loaded with 10 g (37.6 mmol) of **S2** in 150 mL of 4 N HCl. The first portion of oxalic acid (2.5 g, 27.8 mmol) was added and the reaction mixture was refluxed for 6 h. Then a second portion of oxalic acid (2.5 g, 27.8 mmol) was added and the mixture refluxed overnight (~12 h). The solution mixture was cooled down to room temperature and vacuum filtered. The filtrate was washed several times with copious amounts of deionized water and dried in air to obtain a brown solid. The product was used in the next step without further purifications. Yield: 52% (6.3 g, 19.7 mmol). ^{1}H NMR (400 MHz, DMSO-*d*$_6$, 20 °C): 7.32 (2H, s), 11.03 (2H, s).

Compound **5**. A 500 mL flask was loaded with 5 g (15.6 mmol) of **S3** in 100 mL of thionyl chloride. After stirring for 5 min at room temperature, 1 mL of dimethyl formamide (DMF) was added dropwise. The reaction mixture was refluxed for 5 h and then cooled down to room temperature. The reaction mixture was dried under vacuum (caution: thionyl chloride has a very strong odor, consider setting up the rotary evaporator in a well-ventilated hood). The solid was washed several times with copious amounts of deionized water and 100 mL of MeOH, subsequently it was dried in air. The pure product (pale yellow solid) was obtained by flash column using a pure DCM. Yield: 63% (3.5 g, 9.9 mmol). ^{1}H NMR (400 MHz, DMSO-*d*$_6$, 20 °C): 8.20. ^{13}C NMR (100 MHz, DMSO-*d*$_6$, 20 °C): 121.3, 135.0, 138.7, 146.9. $C_8H_3N_2Br_2Cl_2$, HRMS (calculated): 354.80346, HRMS (exp.): 354.80278.

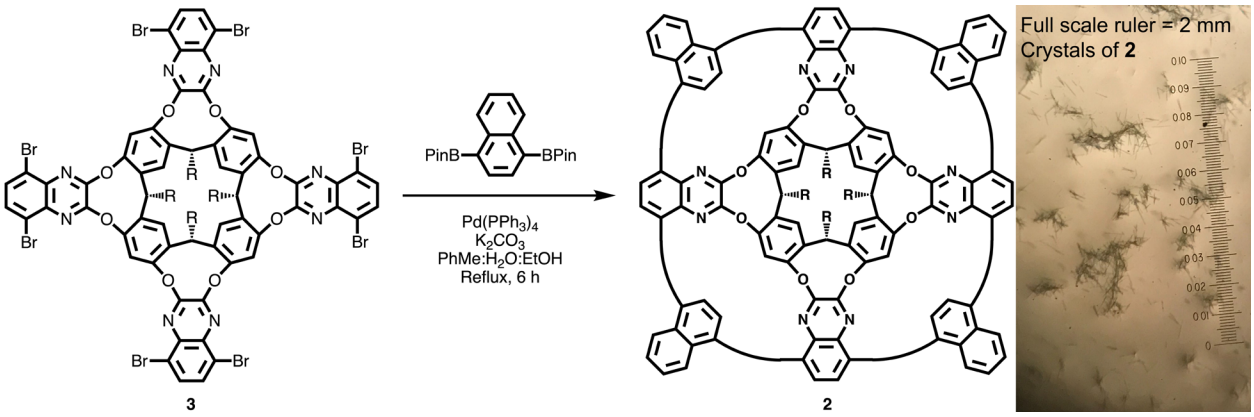


Compound **3**. A 500 mL round bottom flask was loaded with 1.5 g of **4** (2 mmol) and 2.9 g of **5** (8.2 mmol, 4.1 eq) in 100 mL of acetonitrile. Triethylamine (TEA, 5.6 mL, 40 mmol, 20 eq) was added to the latter solution dropwise over 10 min. The reaction mixture was refluxed overnight (~12 h). The reaction mixture was cooled down to room temperature followed by removal of solvent under vacuum. A brown solid was obtained and washed with 200 mL of MeOH. This brown solid was dried in air. The pure product (beige powder) is obtained after passing the crude product through a flash column starting with DCM/Hexanes (1:1) and moving to pure DCM as the eluent. Yield: 57% (2.17 g, 1.14 mmol). ^{1}H NMR (400 MHz, DMSO-*d*$_6$, 100 °C): 0.67 (12H, broad), 1.07 (24H, broad), 2.10 (8H, broad), 3.63 (4H, t), 7.05 (4H, s), 7.42 (4H, s), 7.84 (8H, s). ^{13}C NMR (100 MHz, DMSO-*d*$_6$, 100 °C): 12.9, 21.2, 25.5, 29.9, 30.1, 36.4, 112.9, 119.8, 124.4, 130.9, 132.2, 135.8, 148.3, 151.7. $C_{80}H_{64}Br_8N_8O_8$, HRMS ([(M+H)/z]$^+$ calculated): 1904.8305, HRMS (exp.): 1904.8298.



3 1

Tubular[4,8,8,8]arene (**1**). A Pyrex Schlenk flask was loaded with 0.3 g of **3** (0.16 mmol), 0.3 g of 1,4-benzenediboronic acid bis(pinacol) ester (0.9 mmol, 5.6 eq), and 1.2 g of K_2CO_3 in 250 mL of toluene, 25 mL of water and 25 mL of EtOH. The reaction mixture was degassed for 30 min while stirring vigorously at room temperature. To this mixture, 0.18 g of $Pd(PPh_3)_4$ (0.16 mmol, 1 eq) was added. This amount of catalyst forms 8 C-C bonds, thus representing ~0.12 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. Then, the reaction mixture was refluxed under N_2 atmosphere overnight (~12 h). This reaction was repeated three times. The solvent was removed under vacuum and the resulting dark black solid passed through a flash column using 70% DCM in hexanes. The final product was purified using 40% DCM in hexanes by preparatory TLC. Yield: 1.3% (0.011 g, 0.006 mmol). High quality crystals were grown by slow evaporation of a DCM/MeCN (1:1) solution of **1**. ^{1}H NMR (400 MHz, CD_2Cl_2, 20 °C): 0.96 (12H, t), 1.41 (24H, m), 2.34 (8H, q), 5.80 (4H, t), 6.78 (8H, s), 7.40 (4H, s), 7.74 (4H, s), 8.11 (8H, s), 8.75 (8H, s). ^{13}C NMR (100 MHz, CD_2Cl_2, 20 °C):14.5, 23.3, 28.3, 30.3, 32.5, 34.5, 117.4, 124.3, 128.3, 129.4, 134.6, 136.1, 137.1, 139.2, 139.8, 150.2, 152.0. $C_{104}H_{80}N_8O_8$, HRMS ([M/z]$^+$ calculated): 1569.6172, HRMS (exp.): 1569.6179.



Tubular[4,8,8,12]arene (**2**). A Pyrex Schlenk flask was loaded with 0.3 g of **3** (0.16 mmol), 0.34 g of 1,4-naphthalenediboronic acid bis(pinacol) ester (0.9 mmol, 5.6 eq), and 1.2 g of K_2CO_3 in 250 mL of toluene, 25 mL of water and 25 mL of EtOH. The reaction mixture was degassed for 30 min while stirring vigorously at room temperature. To this mixture, 0.18 g of $Pd(PPh_3)_4$ (0.16 mmol, 1 eq) was added. This amount of catalyst forms 8 C-C bonds, thus representing ~0.12 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. Then, the reaction mixture was refluxed under N_2 atmosphere overnight (~12 h). This reaction was repeated three times. The solvent was removed under vacuum and the resulting dark black solid passed through a flash column using 70% DCM in hexanes. The final product was purified using 50% DCM in hexanes by preparatory TLC. Yield: 0.8% (0.007 g, 0.004 mmol). ^{1}H NMR (400 MHz, CD_2Cl_2, 20 °C): 0.88 (24H, t), 2.08 (16H, q), 5.45 (4H, t), 5.98 (4H, s), 6.55 (8H, s), 7.07 (4H, s), 7.62 (8H, m), 8.30 (8H, s), 8.41 (8H, m). ^{13}C NMR (100 MHz, CD_2Cl_2, 20 °C):14.4, 23.2, 28.1, 30.2, 32.3, 32.5, 116.5, 123.8, 125.1, 130.2, 133.1, 133.4, 136.6, 138.3, 139.5, 141.3, 150.1, 151.5. $C_{120}H_{88}N_8O_8$, HRMS ($[M/z]^+$ calculated): 1769.6798, HRMS (exp.): 1769.6634.

Computational details. All calculations were carried out using Gaussian 16 software package.[11] Four different hybrid functionals, long-range corrected (ωB97XD),[12] meta-GGA (M06-2X),[13] meta-NGA (MN15),[14] and GGA (B3LYP)[15] of density functional theory (DFT) were used for all optimizations and subsequent studies. The frequency calculations were carried out for all optimized structures to ensure the absence of any imaginary frequencies for the ground state molecules. The intrinsic reaction coordinate (IRC) calculation is carried out, in addition to the presence of one imaginary frequency, for the transition state structures. In order to include the dispersion effects, the D3 version of Grimme with Becke-Johnson damping factors (D3BJ) were used for the B3LYP functional.[16] The double-zeta quality basis set (6-31G*) was used for all calculations. The implicit solvation effects were included using the integral equation formalism variant of the polarizable continuum model (IEF-PCM) with standard parameters of dichloromethane (CH_2Cl_2).[17] The gauge-independent atomic orbital (GIAO) method[18] was used for ^{1}H NMR chemical shift calculations. The calculated chemical shieldings were scaled with ^{1}H NMR chemical shift of tetramethylsilane (TMS) calculated at the same level of theory. The DFT calculated ^{1}H NMR chemical shifts assisted in assigning the experimental spectra. The analysis of TD-DFT studies was carried out using GaussSum 3.0 software.[19]

Table S1. Crystallographic data for tubular[4,8,8,8]arene **1**.

	Tubular[4,8,8,8]arene (**1**)
CCDC Number	1994725
Chemical formula	$C_{104}H_{80}N_8O_8 \cdot C_2H_3N$
Formula weight	1610.81
Space group	*Pnma*
***a* (Å)**	16.087 (3)
***b* (Å)**	25.358 (5)
***c* (Å)**	21.354 (4)
α (deg)	90
β (deg)	90
γ (deg)	90
***V* (Å^3)**	8711 (3)
Z	4
μ (mm^{-1})	0.623
T (K)	150
***R*1[a] (*wR*2[b])**	0.079 (0.253)
Reflections	8540
Radiation type	Cu $K\alpha$

[a]$R1 = [\Sigma w(F_o - F_c)^2/\Sigma wF_o^2]^{1/2}$; [b]$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}]$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2,0) + 2(F_c^2)]/3$

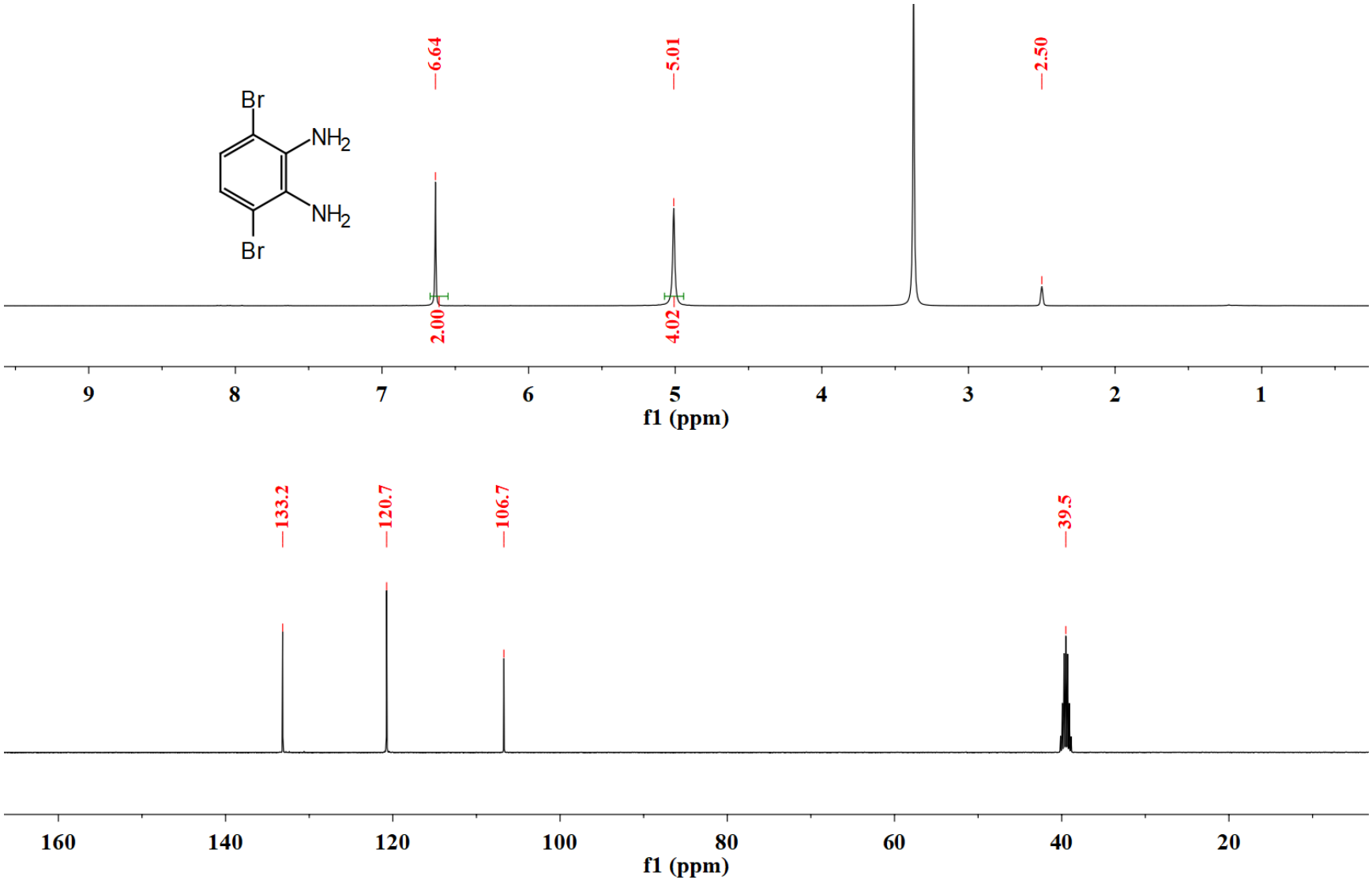


Figure S1. ^{1}H and ^{13}C NMR spectra of compound **S2**. Data collected in DMSO-*d*$_6$ at 20 °C.

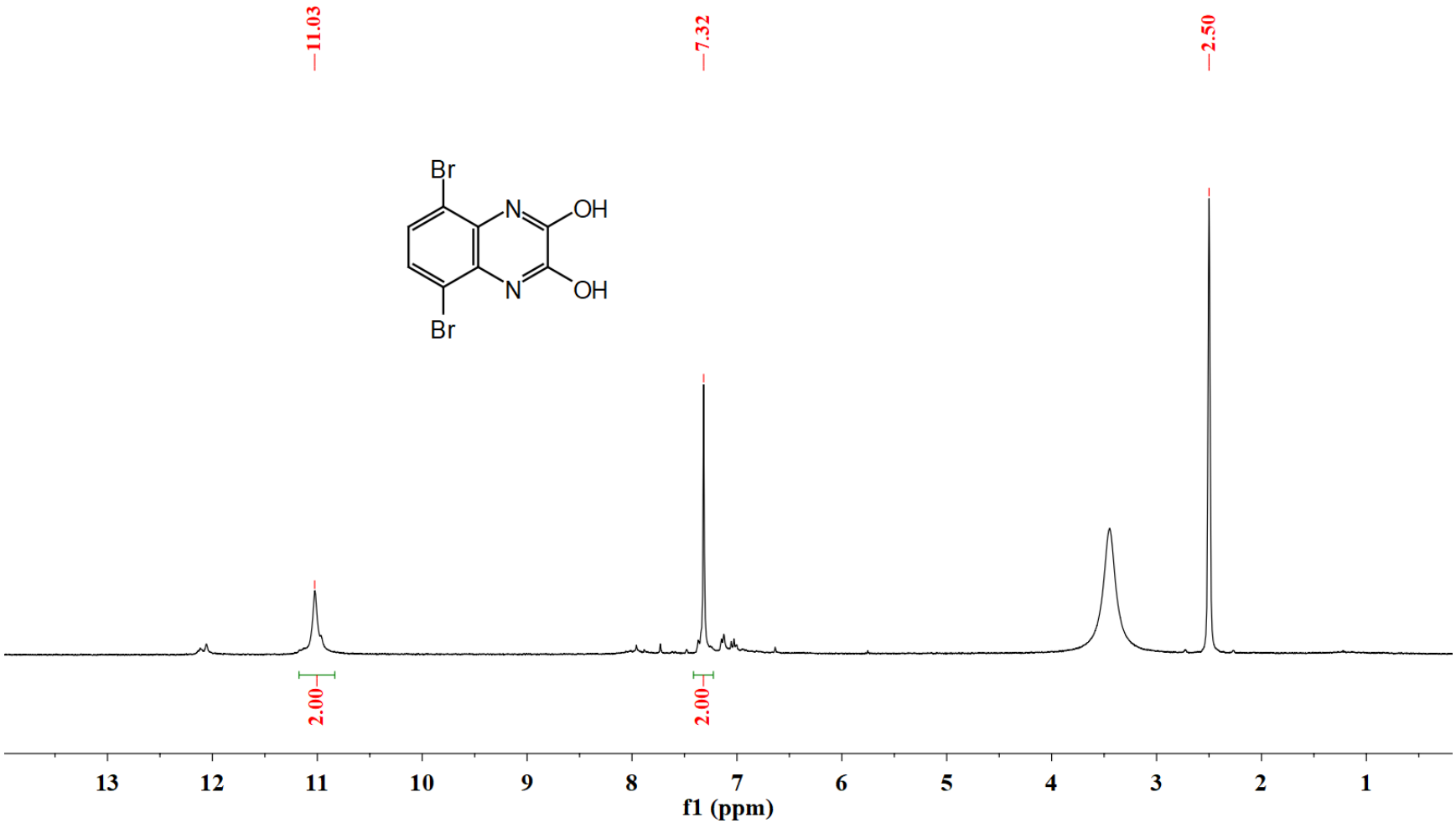


Figure S2. ^{1}H NMR spectrum of compound **S3**. Data collected in DMSO-d_6 at 20 °C.

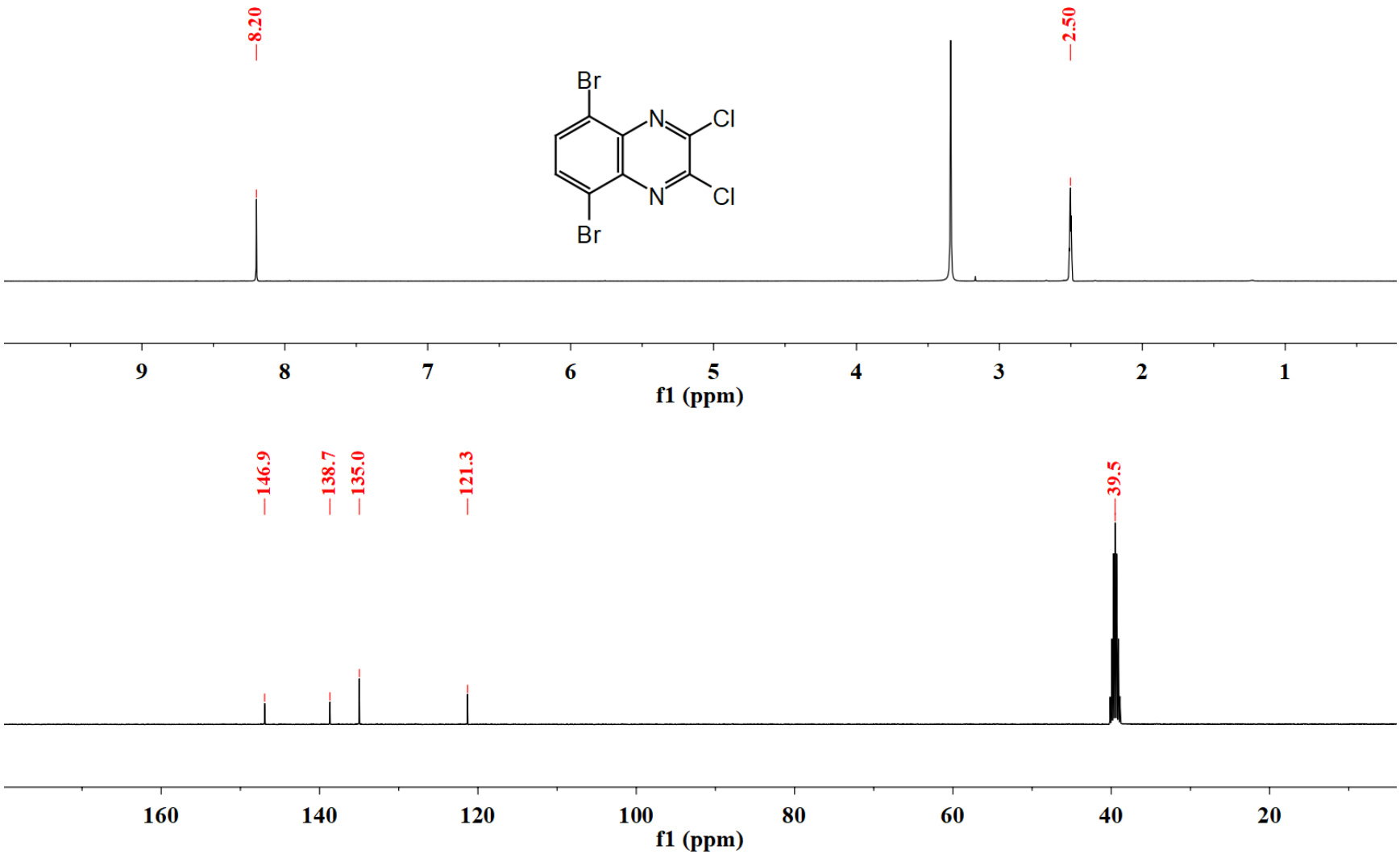


Figure S3. ^{1}H and ^{13}C NMR spectra of compound **5**. Data collected in DMSO-d_6 at 20 °C.

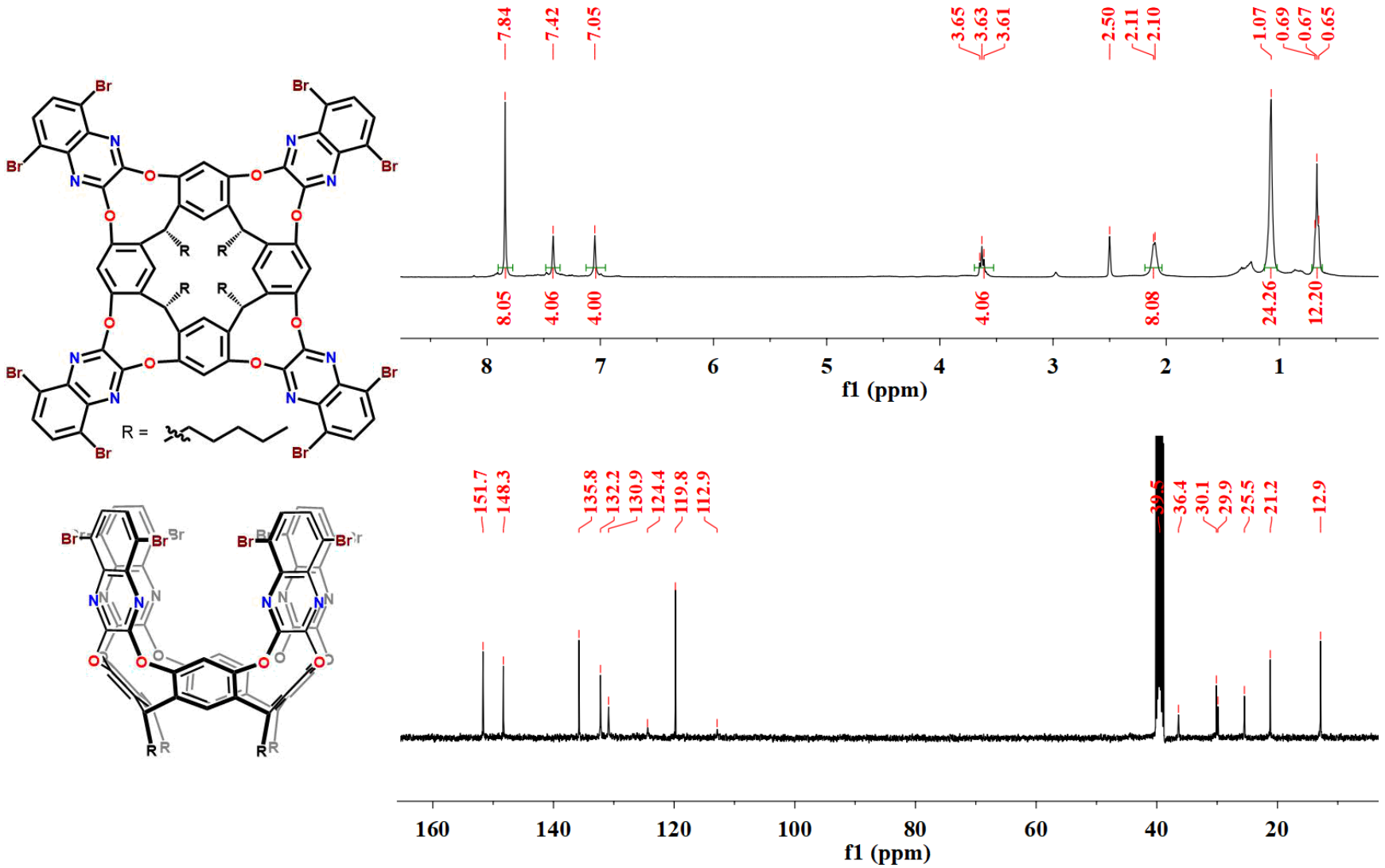


Figure S4. ^{1}H and ^{13}C NMR spectra of compound **3**. Data collected in DMSO-d_6 at 100 °C.

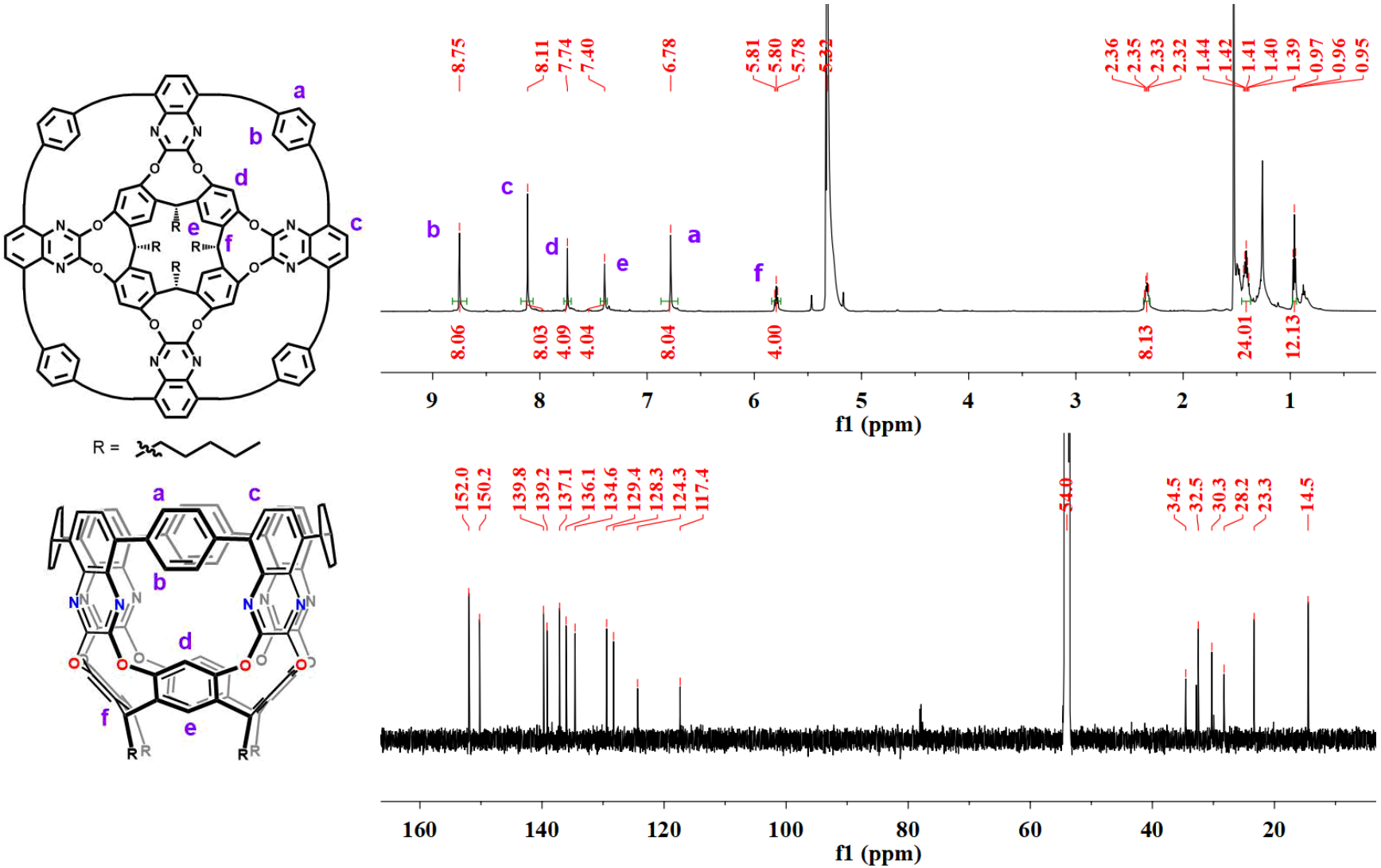


Figure S5. ^{1}H and ^{13}C NMR spectra of tubularene **1**. Data collected in CD_2Cl_2 at 20 °C.

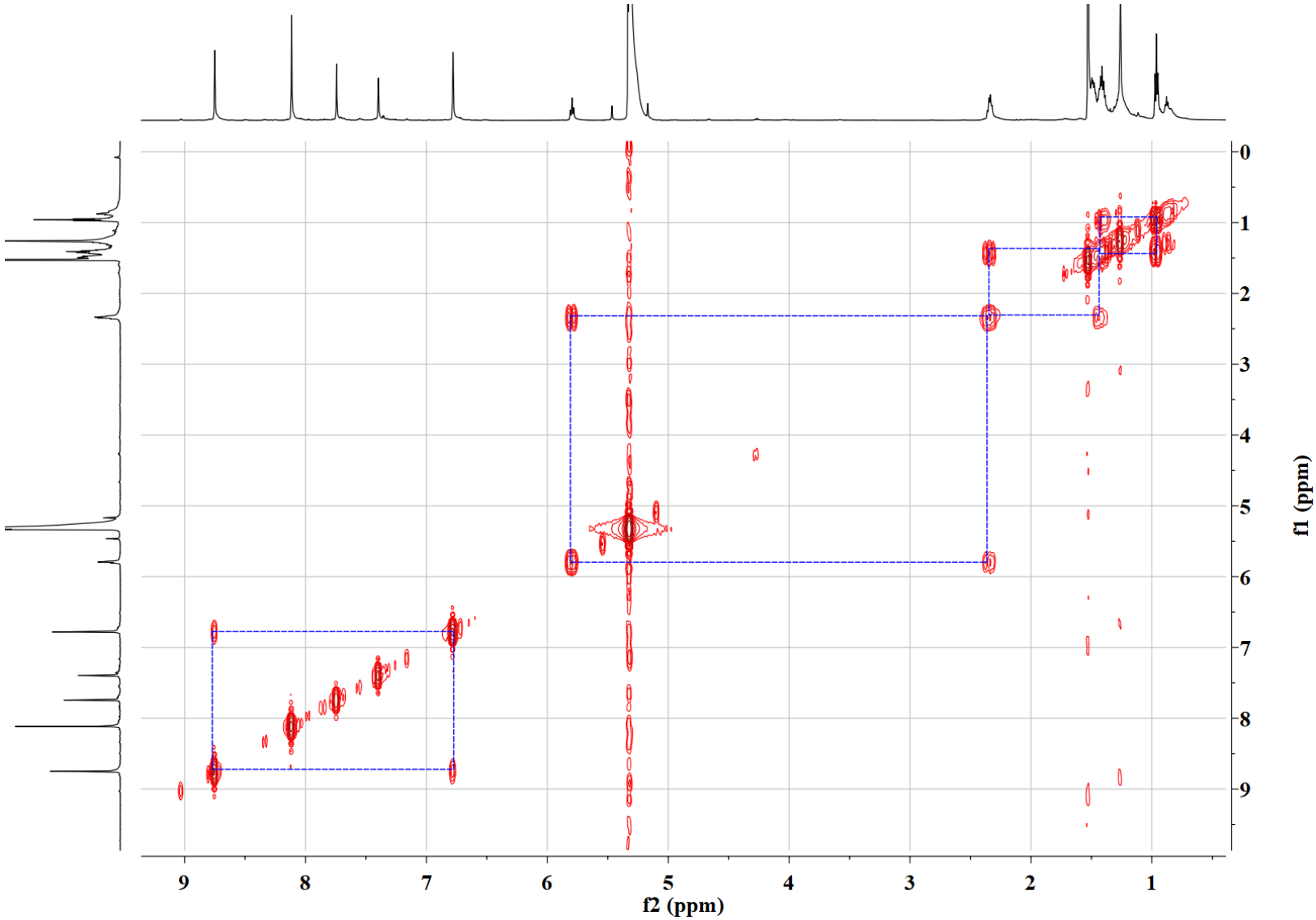


Figure S6. COSY NMR spectrum of tubularene **1**. Data collected in CD_2Cl_2 at 20 °C.

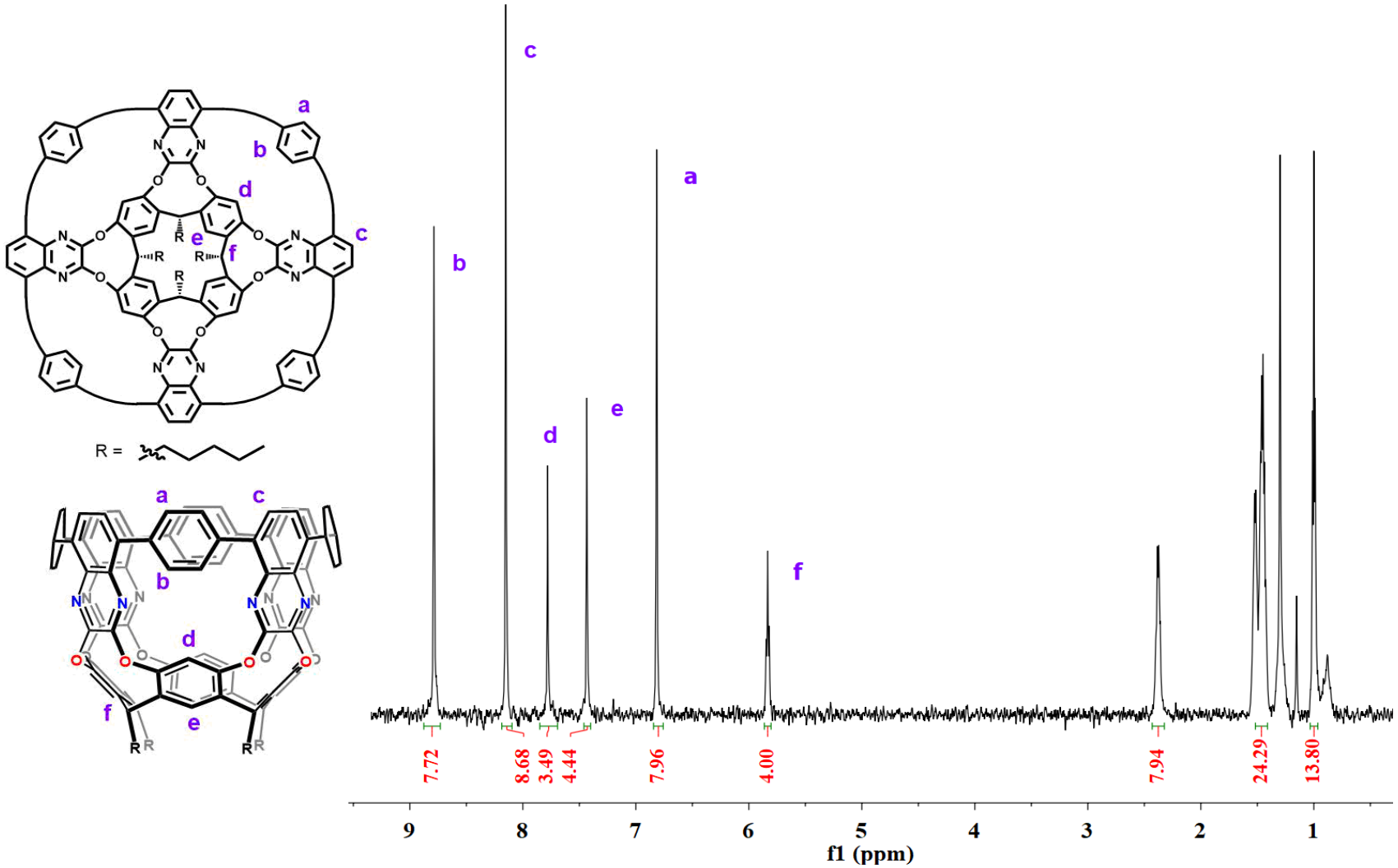


Figure S7. DOSY NMR spectrum of tubularene **1**. Shown above is one of the many regular ^{1}H NMR spectrum collected during a DOSY experiment to show the slowly-diffusing species. Data collected in CD_2Cl_2 at 20 °C.

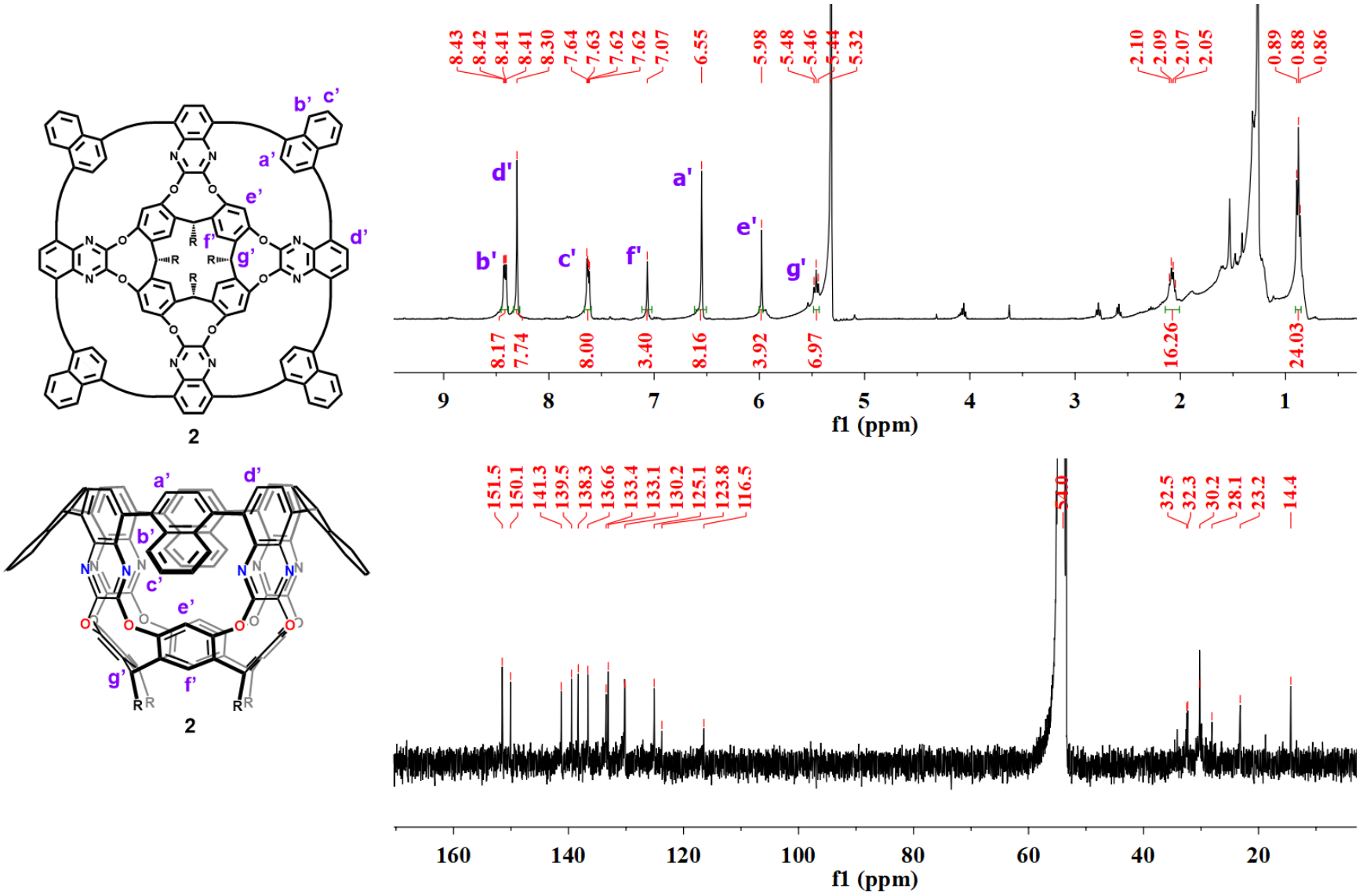


Figure S8. ^{1}H and ^{13}C NMR spectra of tubularene **2**. Data collected in CD_2Cl_2 at 20 °C.

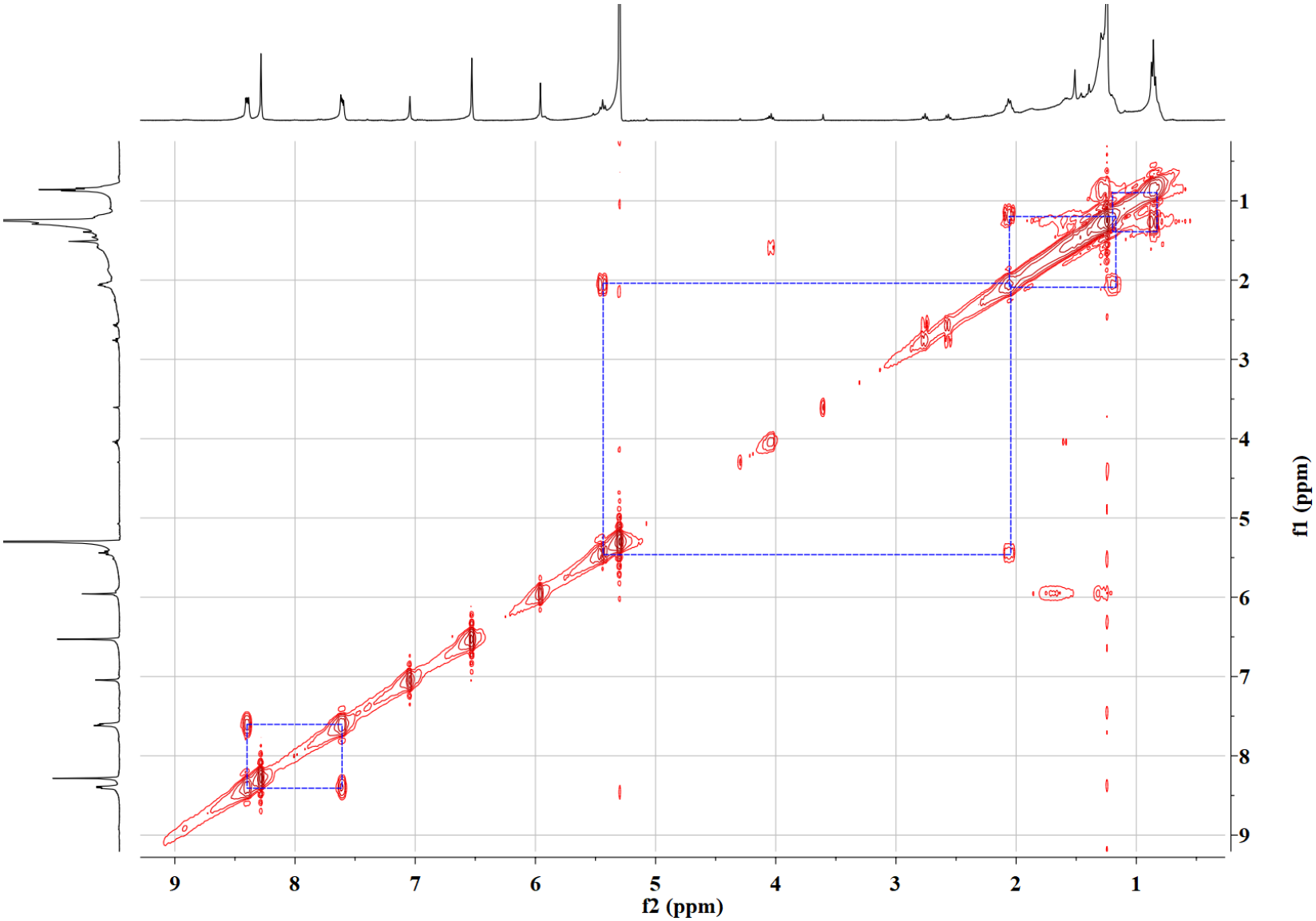


Figure S9. COSY NMR spectrum of tubularene **2**. Data collected in CD_2Cl_2 at 20 °C.

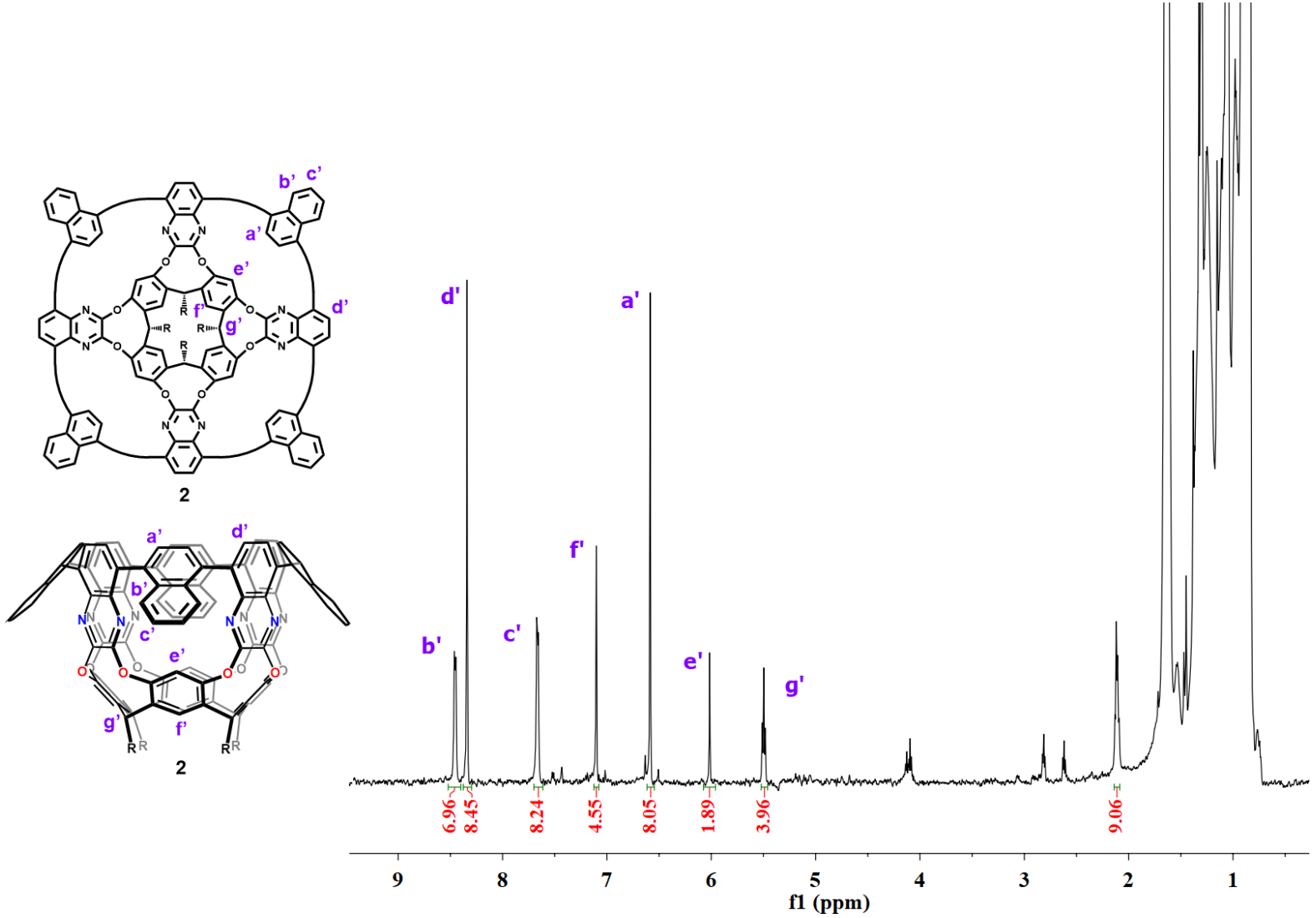


Figure S10. DOSY NMR spectrum of tubularene **2**. Shown above is one of the many regular ^{1}H NMR spectrum collected during a DOSY experiment to show the slowly-diffusing species. Data collected in CD_2Cl_2 at 20 °C.

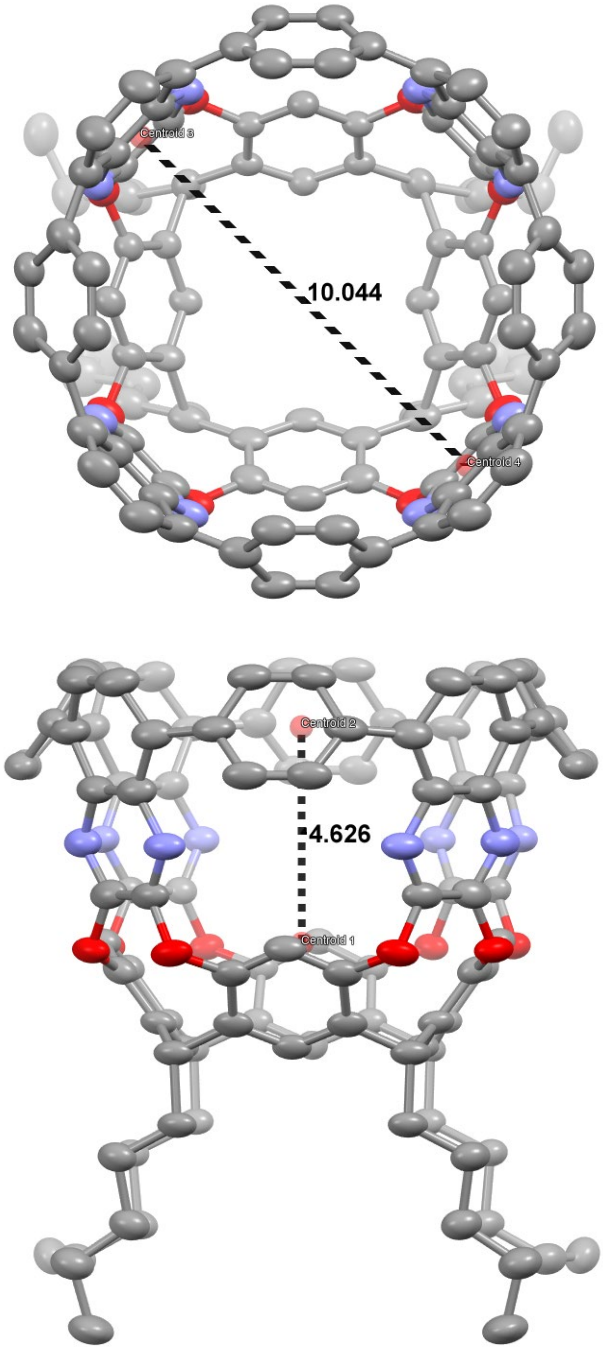


Figure S11. Interior cavity measurements of tubularene **1**. Calculated volume ≈ 360 Å^3. *Top*: Diameter (10.044 Å). Defined as the distance from centroid-to-centroid of two opposing pyrazinic rings. *Bottom*: Height (4.626 Å). Defined as the distance between *i*) centroid 1 (resulting from the four top carbon atoms of each of the aromatic rings making up the resorcin[4]arene fragment), and *ii*) centroid 2 (resulting from the *para* carbons in the top eight-member aromatic ring).

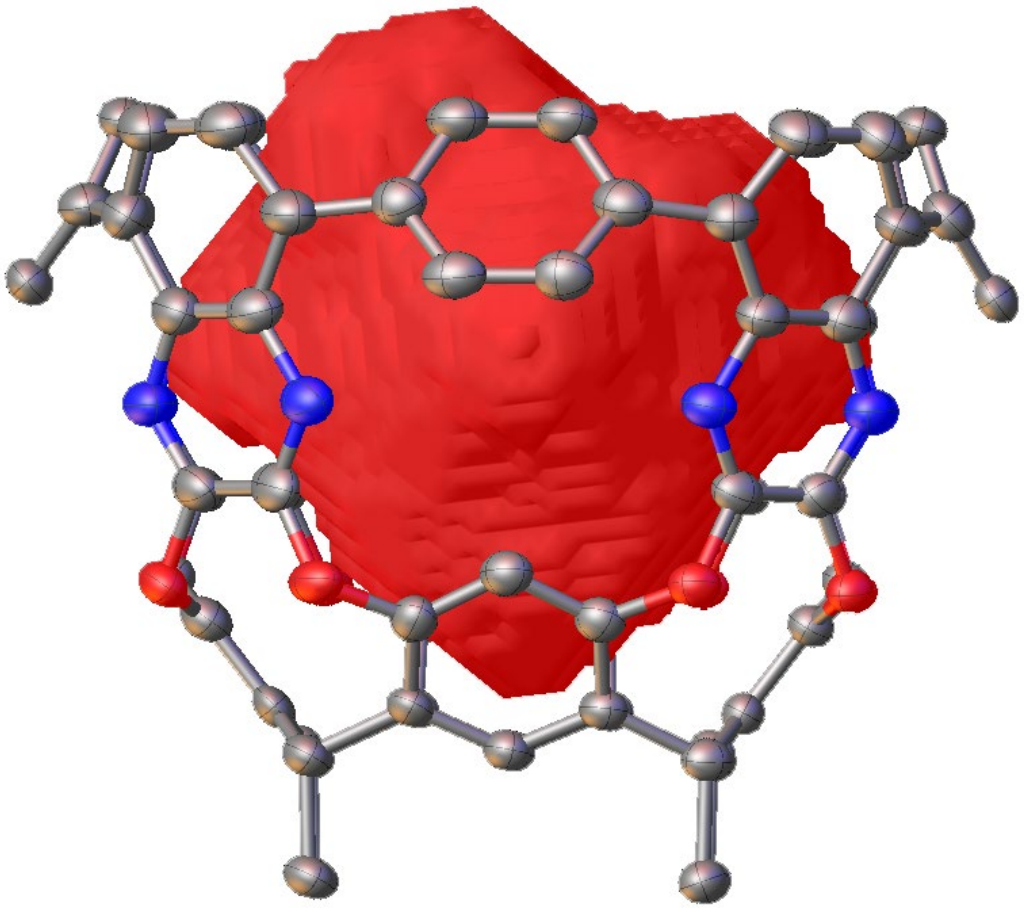


Figure S12. Surface (in red) of the solvent accessible volume (265.9 $Å^3$) of tubularene **1** calculated in Olex2.

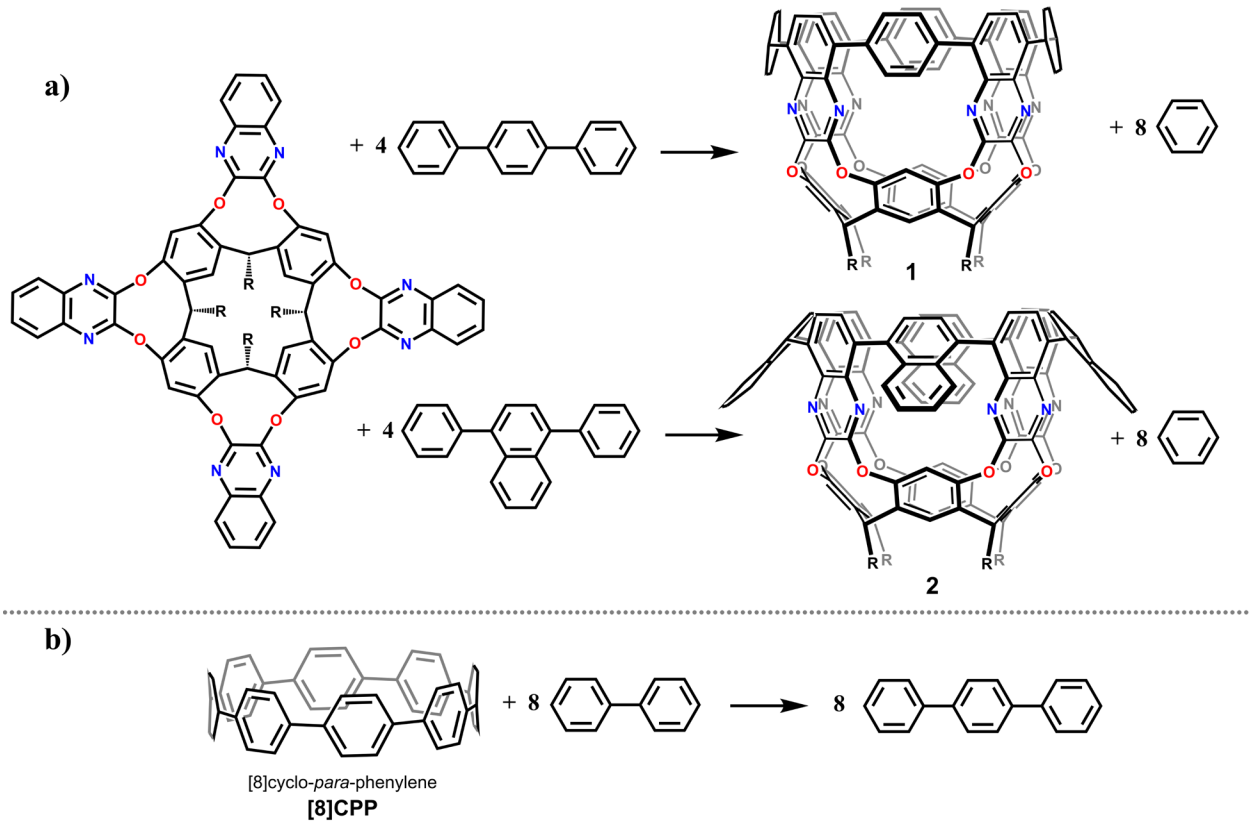


Figure S13. Homodesmotic reactions for the calculation of strain energies of a) tubularene **1** and **2** and b) **[8CPP]**.

Table S2. Strain energies (ΔH, in kcal/mol) of **1**, **2**, and **[8]CPP** calculated at DFT/6-31G* level of theory based on homodesmotic reactions as described in *Figure S13*.

	B3LYP	B3LYP-D3BJ	M062X	MN15	ωB97XD
1	92.4	86.6	89.2	86.4	90.5
2	87.4	76.7	81.6	78.1	81.4
[8]CPP	71.9	69.3	72.7	70.9	72.4

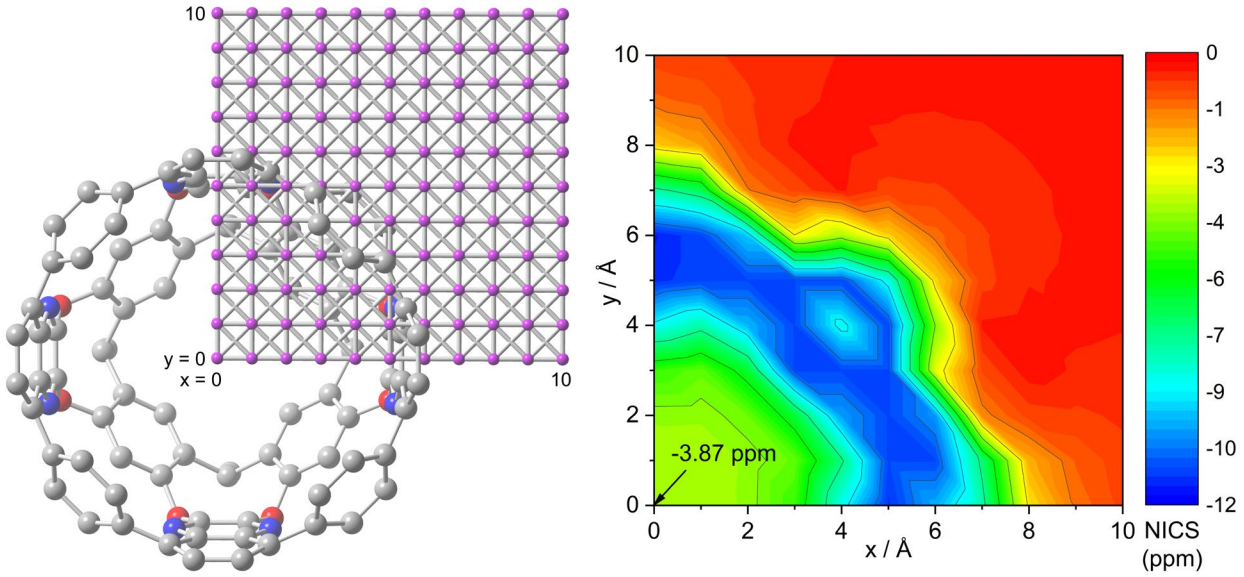


Figure S14. Nucleus-independent chemical shifts (NICS) in **1**. The origin of the grid shown in the left hand side starts at the geometric center of the [8]CPP-like nanoring in **1**. At the origin, NICS = –3.87 ppm. NCIS were calculated at the MN15/6-31G*+PCM(CH_2Cl_2) level of theory.

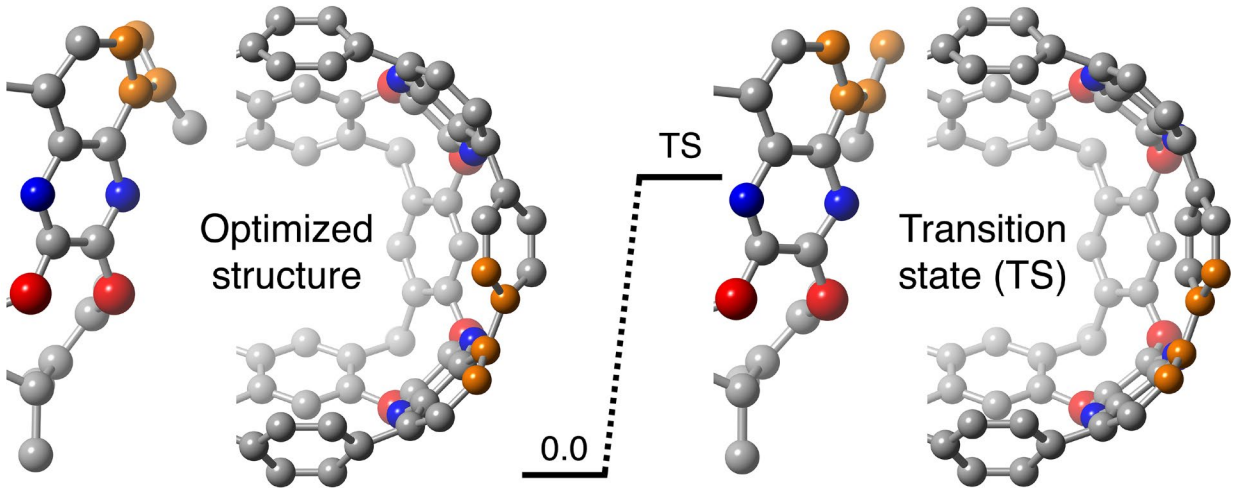
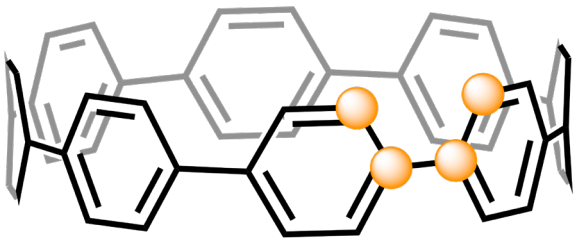


Figure S15. Dihedral angle (θ) change between the highlighted aromatic rings of the (left) DFT optimized strucure of tubularene **1** and (right) transition state (TS) during ring flipping (θ was measured between the highlighted atoms). The hydrogens and the rest of the molecule's atoms are omitted for clarity.

Table S3. DFT calculated thermochemistry of ring flipping in **1**. Provided below are the relative energy (ΔE+ZPE), enthalpy (ΔH), and Gibbs free energy (ΔG) for the rotation of one of the phenyl groups (as described in *Figure S15*) using DFT/6-31G*+PCM(CH_2Cl_2), in kcal/mol.

	B3LYP-D3BJ		M062X		MN15		*ω*B97XD	
	1	TS	**1**	TS	**1**	TS	**1**	TS
ΔE+ZPE	0.0	26.9	0.0	29.6	0.0	28.6	0.0	30.0
ΔH	0.0	26.4	0.0	29.2	0.0	28.2	0.0	29.5
ΔG	0.0	27.6	0.0	30.1	0.0	29.2	0.0	30.9
θ (°)	–38.2	13.6	–39.2	12.8	–38.6	12.4	–41.1	13.5

Table S4. DFT calculated thermochemistry of ring flipping in **[8]CPP**. Provided below are the relative energy (ΔE+ZPE), enthalpy (ΔH), and Gibbs free energy (ΔG) for the rotation of one of the phenyl groups using DFT/6-31G*+PCM(CH_2Cl_2), in kcal/mol. Dihedral angle (θ) is determined by the highlighted atoms.



[8]cyclo-*para*-phenylene

[8]CPP

	B3LYP-D3BJ		M062X		MN15		*ω*B97XD	
	[8]CPP	TS	**[8]CPP**	TS	**[8]CPP**	TS	**[8]CPP**	TS
ΔE+ZPE	0.0	2.7	0.0	3.2	0.0	2.9	0.0	3.6
ΔH	0.0	2.2	0.0	2.7	0.0	2.4	0.0	3.2
ΔG	0.0	3.3	0.0	3.7	0.0	3.5	0.0	4.2
θ (°)	30.0	–0.3	31.3	–0.6	30.0	–0.7	33.8	–0.6

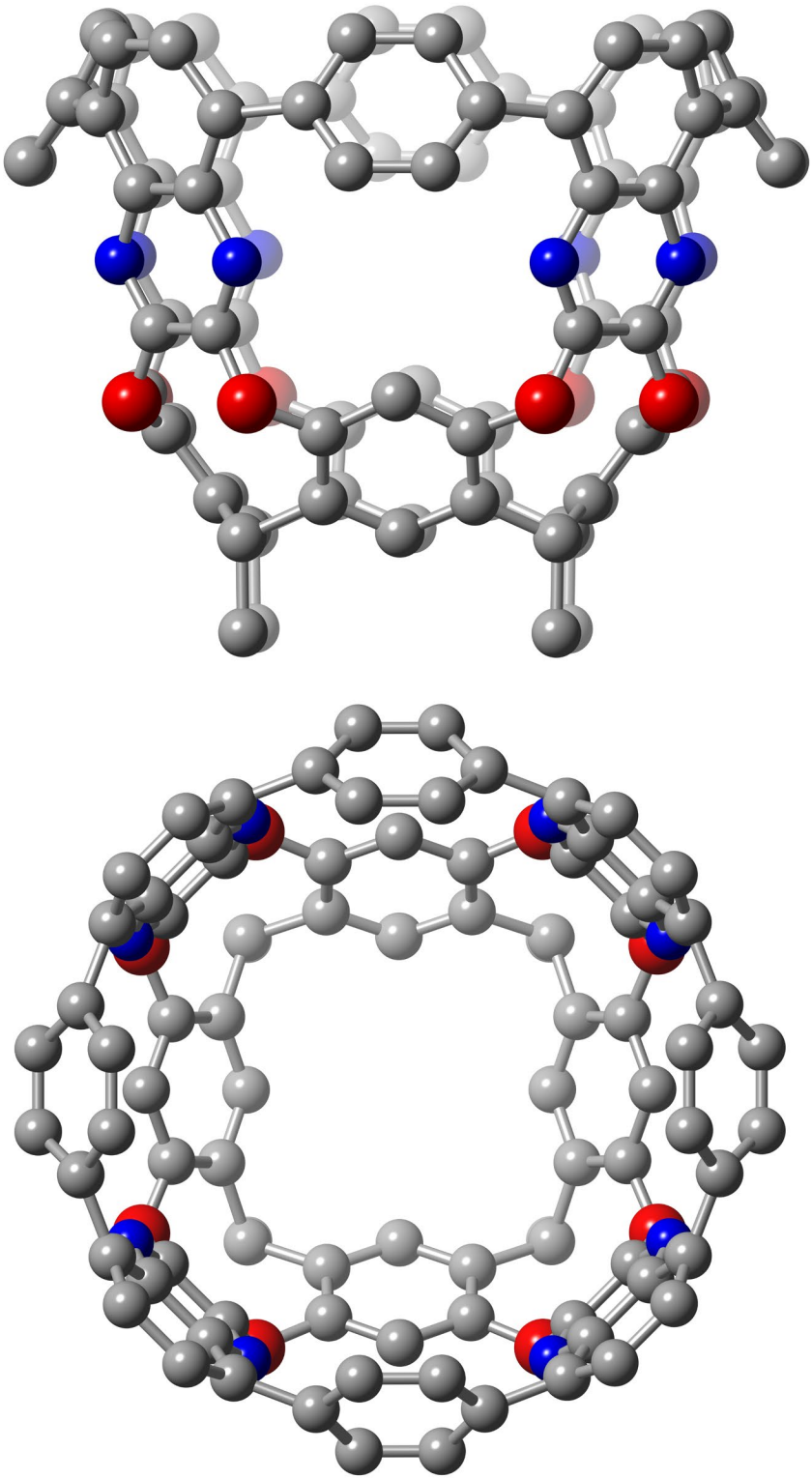


Figure S16. DFT optimized structure of tubularene **1** at the MN15/6-31G*+PCM(CH_2Cl_2) level of theory.

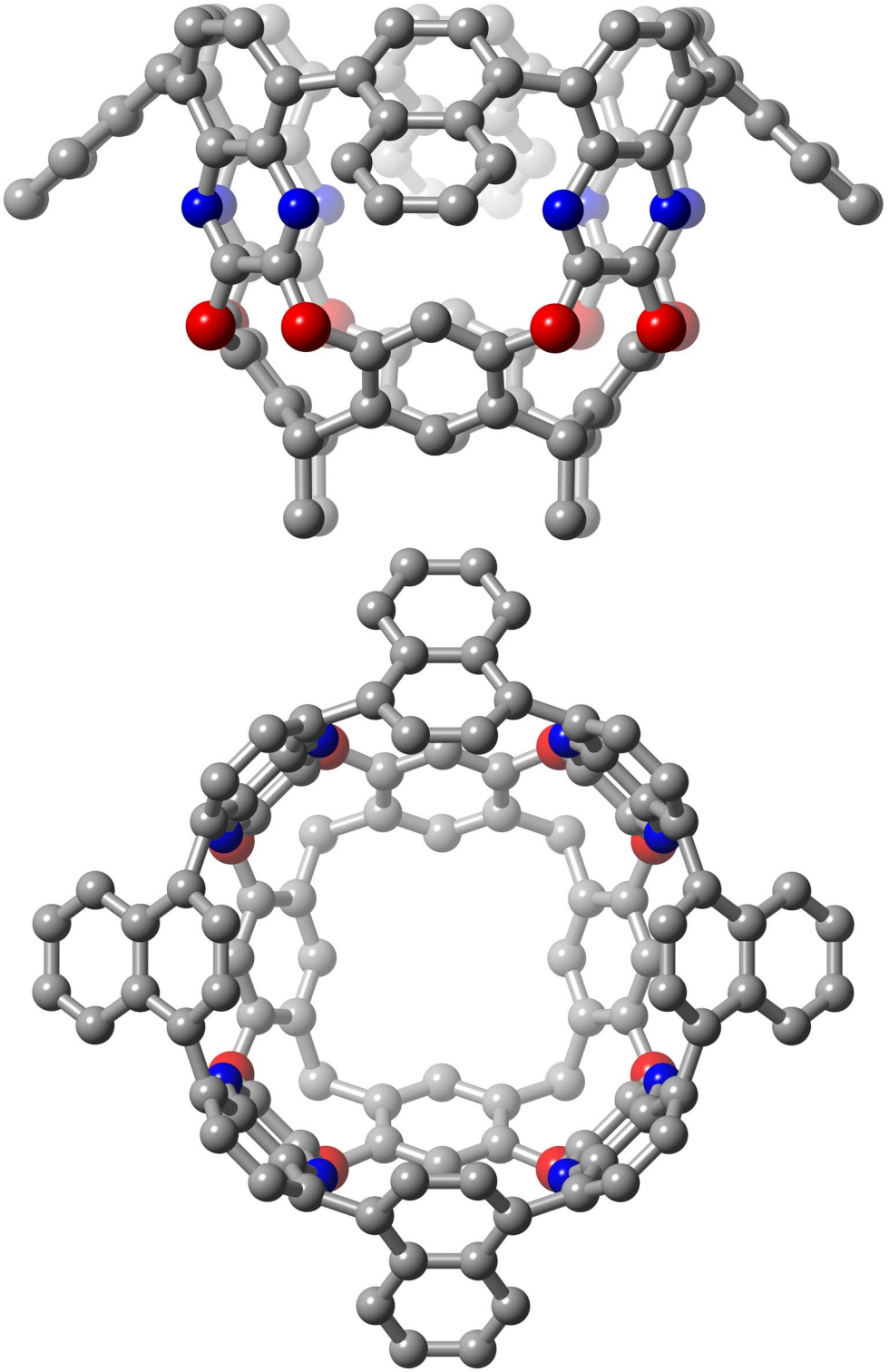


Figure S17. DFT optimized structure of tubularene **2** at the MN15/6-31G*+PCM(CH_2Cl_2) level of theory.

Table S5. Calculated absorption energies (λ, nm), oscillator strengths (*f*), and main contributions with its percentages at time-dependent (TD) DFT/6-31G*+PCM(CH_2Cl_2) level of theory. Except for the HOMO-to-LUMO transition, only major and intense transitions are provided. H and L stands for HOMO and LUMO, respectively.

	1			**2**		
	λ (nm)	*f*	Major contributes	λ (nm)	*f*	Major contributes
B3LYP-D3BJ	507.9	0.000	H→L (94%)	504.4	0.000	H→L (88%)
	451.3	0.296	H→L+1 (90%)	466.7	0.337	H-1→L (22%)
						H→L+1 (67%)
	451.2	0.296	H→L+2 (90%)	466.6	0.336	H-2→L (22%)
	414.7	0.139	H-1→L (91%)			H→L+2 (67%)
	414.6	0.139	H-2→L (91%)			
M062X	381.2	0.000	H→L (68%)	380.3	0.000	H→L (62%)
						H-2→L+2 (14%)
						H-1→L+1 (15%)
	348.8	0.636	H-1→L (33%)	355.5	0.718	H-1→L (38%)
			H→L+1 (47%)			H→L+1 (46%)
	348.7	0.636	H-2→L (33%)	355.4	0.719	H-2→L (38%)
			H→L+2 (47%)			H→L+2 (46%)
	284.5	0.287	H-16→L+1 (11%)	282.1	0.144	H-20→L+2 (10%)
			H-15→L+2 (11%)			H-19→L+1 (10%)
			H-14→L (18%)			H-18→L (13%)
			H→L+8 (10%)			H→L+8 (12%)
MN15	417.4	0.000	H→L (74%)	416.8	0.000	H→L (68%)
						H-2→L+2 (13%)
						H-1→L+1 (13%)
	379.3	0.540	H-2→L (28%)	388.4	0.593	H-1→L (38%)
			H→L+1 (10%)			H→L+1 (50%)
			H→L+2 (48%)			
				388.2	0.593	H-2→L (38%)
						H→L+2 (50%)
	379.2	0.540	H-1→L (28%)	300.9	0.282	H-2→L+3 (15%)
			H→L+1 (48%)			H-2→L+4 (15%)
			H→L+2 (10%)			H→L+5 (23%)
	296.8	0.184	H-14→L (20%)	300.9	0.280	H-1→L+3 (15%)
			H→L+8 (17%)			H-1→L+4 (15%)
						H→L+6 (23%)
***ω*B97XD**	366.5	0.000	H→L (54%)	364.2	0.000	H→L (49%)
						H-1→L+1 (15%)
						H-2→L+2 (15%)
	340.8	0.591	H-2→L+3 (12%)	343.1	0.747	H-1→LUMO (29%)
			H-1→L (32%)			H→L+1 (40%)
			H→L+1 (43%)			
	340.7	0.590	H-2→L (32%)	343.0	0.747	H-2→L (29%)
			H-1→L+3 (12%)			H→L+2 (40%)
			H→L+2 (43%)			
	285.5	0.363	H-14→L (18%)	287.2	0.214	H-17→L+3 (12%)
	266.5	0.174	H-2→L+3 (18%)	279.9	0.318	H-1→L+4 (11%)
			H-1→L (19%)			
			H→L+11 (11%)			
	266.4	0.174	H-2→L (20%)	279.8	0.317	H-2→L+4 (11%)
			H-1→L+3 (18%)			
			H→L+12 (11%)			
	260.7	0.154	H-2→L+1 (27%)			
			H-1→L+2 (27%)			

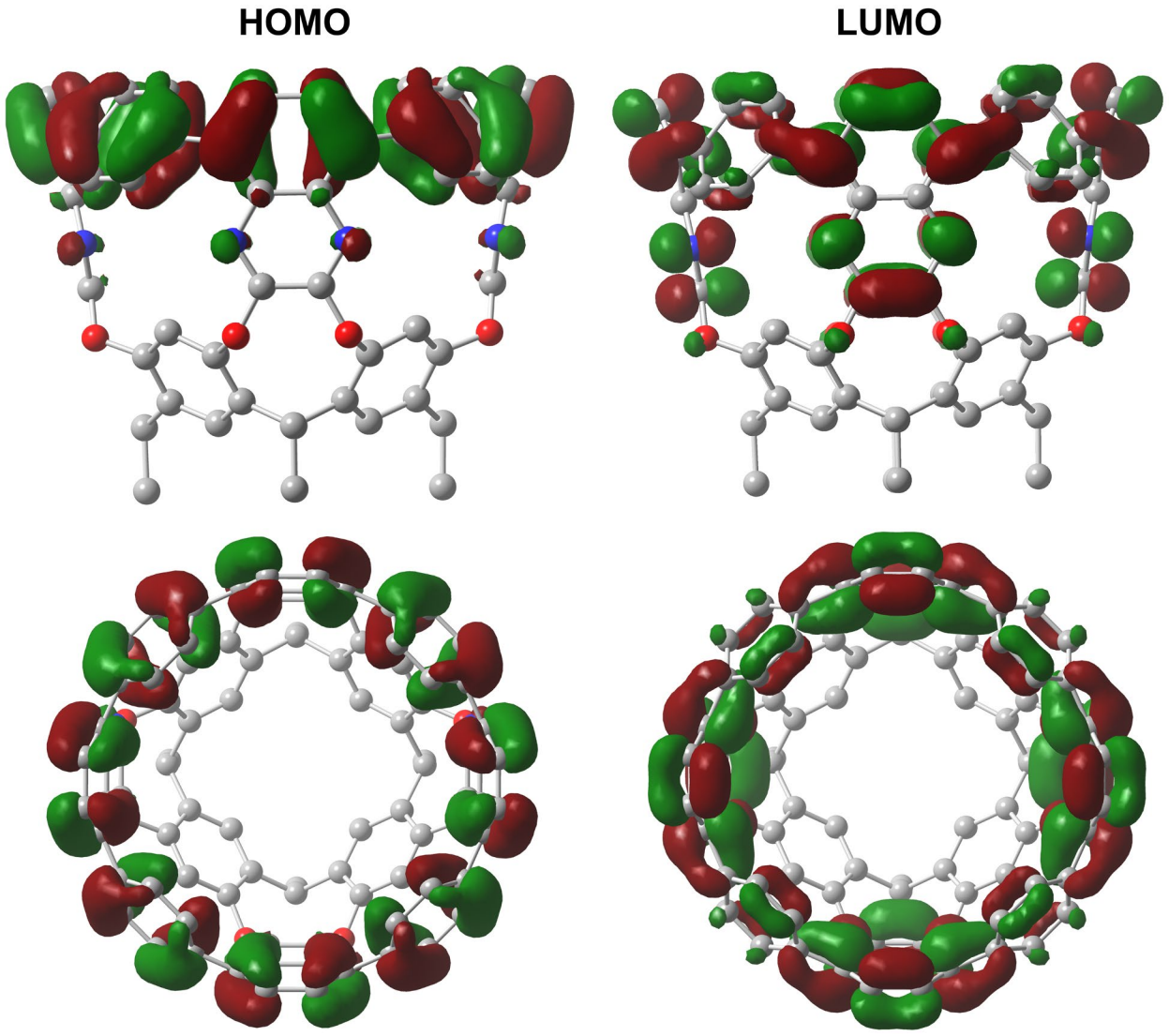


Figure S18. HOMO and LUMO (±0.02 au) of tubularene **1** calculated by DFT at the MN15/6-31G*+PCM(CH_2Cl_2) level of theory.

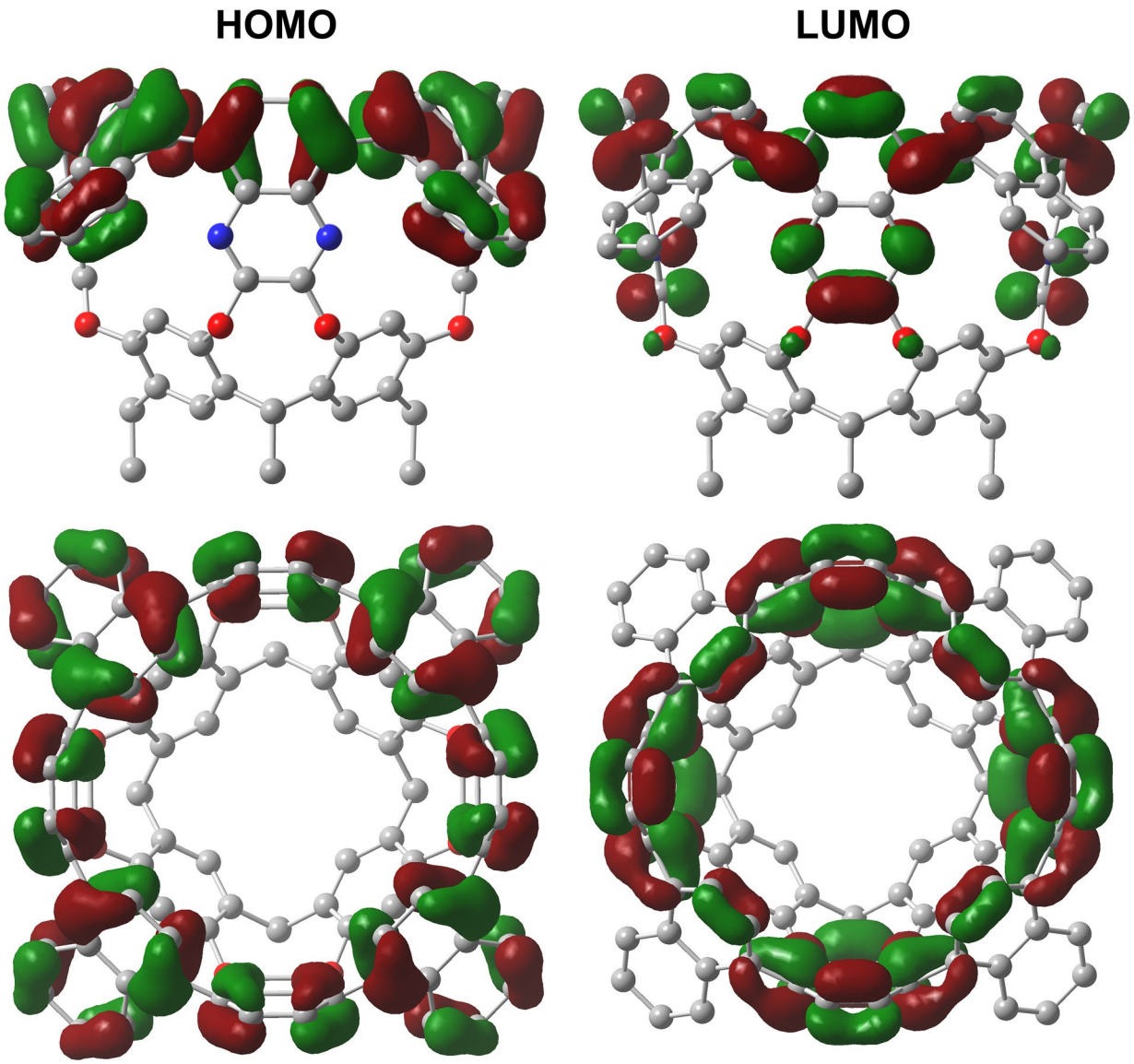


Figure S19. HOMO and LUMO (±0.02 au) of tubularene **2** calculated by DFT at the MN15/6-31G*+PCM(CH_2Cl_2) level of theory.

Table S6. Calculated HOMO and LUMO energy levels for tubularene **1** and **2** at different levels of theory.

	B3LYP	B3LYP-D3BJ	M062X	MN15	*ω*B97XD	**Exp.**
			[8]CPP			
LUMO	–1.70	–1.69	–0.90	–1.08	0.09	–1.92[20]
HOMO	–5.10	–5.10	–6.36	–5.84	–7.01	–5.16[20]
			1			
LUMO	–2.42	–2.48	–1.69	–1.85	–0.76	–2.79
HOMO	–5.42	–5.43	–6.72	–6.20	–7.36	–5.36
			2			
LUMO	-2.3	-2.4	-1.6	-1.8	-0.7	–2.63
HOMO	-5.3	-5.3	-6.6	-6.1	-7.2	–5.27

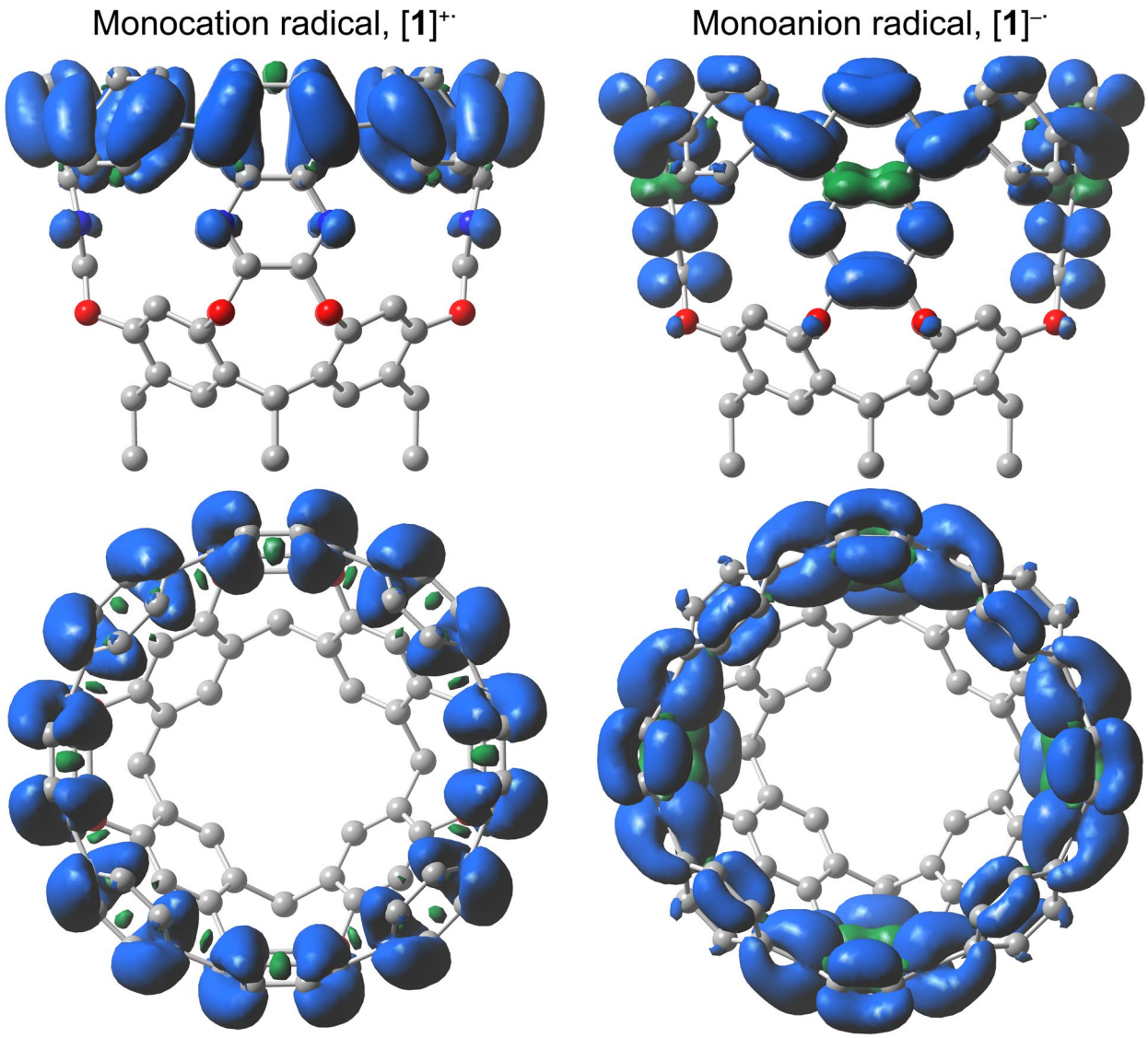


Figure S20. Spin density distribution plots (±0.0004 au) in the ground state of radical monocation and monoanion of tubularene **1** calculated by DFT at the *ω*B97XD/6-31G*+PCM(CH_2Cl_2) level of theory.

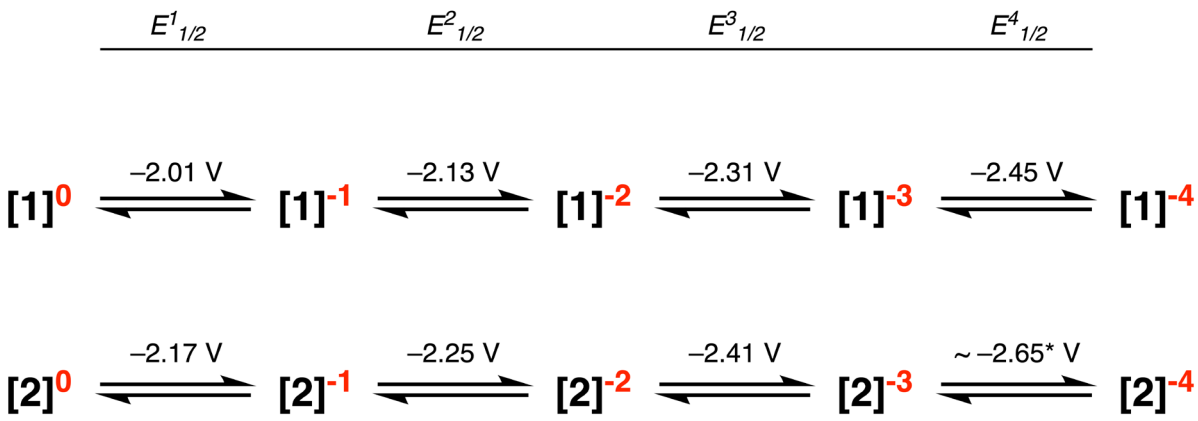
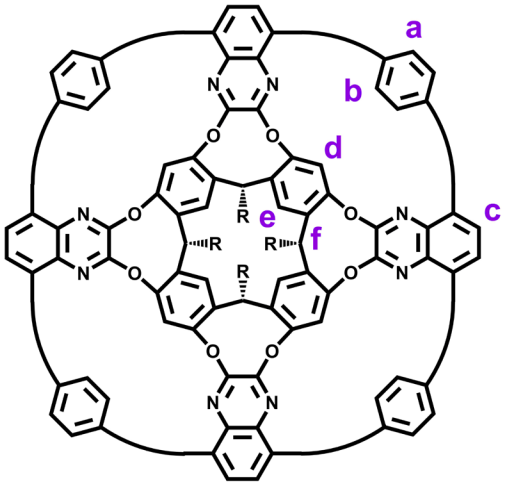
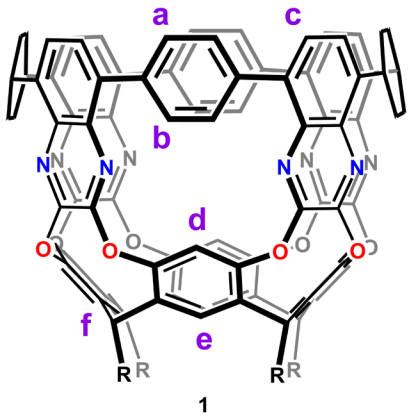


Figure S21. Electron transfer series for tubularenes **1** and **2**. The fourth reduction event in **2** coincides with the onset of solvent (*ortho*-dichlorobenzene) reduction. Nonetheless, a shoulder, marked with an asterisk in Figure 2e, is observed in the differential pulsed voltammogram of **2** at around –2.65 V.

Table S7. Calculated ^{1}H NMR of tubularene **1** by DFT/6-31G*+PCM(CH_2Cl_2) level of theory.



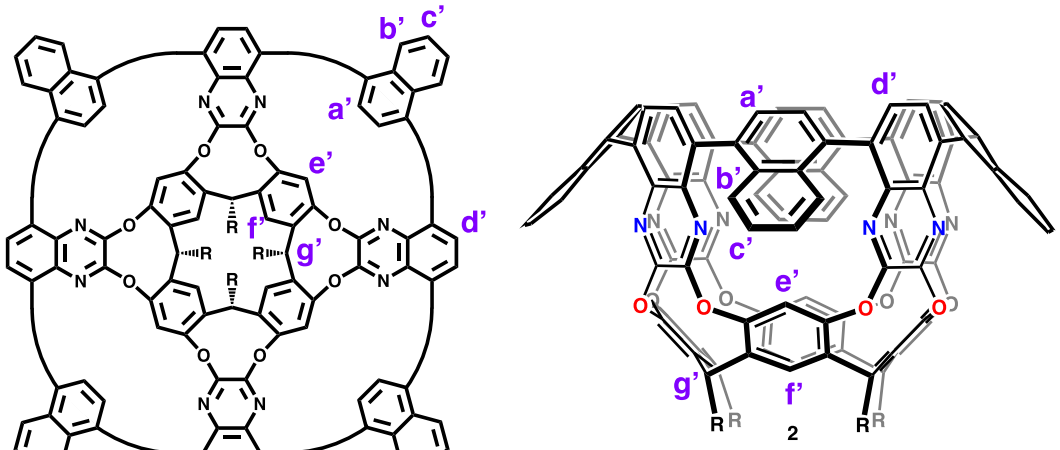
1



1

	B3LYP-D3BJ	M062X	MN15	*ω*B97XD	**Exp.**
a	6.9	7.4	7.3	6.9	**6.78**
b	8.8	9.4	9.1	8.9	**8.75**
c	8.1	8.8	8.6	8.3	**8.11**
d	7.9	8.4	8.3	8.0	**7.74**
e	7.8	8.4	8.3	8.0	**7.40**
f	5.8	5.9	6.0	5.8	**5.80**

Table S8. Calculated ^{1}H NMR of tubularene **2** by DFT/6-31G*+PCM(CH_2Cl_2) level of theory.



	B3LYP-D3BJ	M062X	MN15	ωB97XD	**Exp.**
a'	6.7	7.3	7.2	6.8	**6.55**
b'	8.5	9.1	9.0	8.7	**8.42**
c'	7.7	8.4	8.2	7.9	**7.63**
d'	8.3	8.4	8.8	8.5	**8.30**
e'	6.2	6.7	6.6	6.3	**5.98**
f'	7.5	8.2	8.1	7.7	**7.07**
g'	5.5	5.7	5.8	5.5	**5.46**

Cartesian Coordinates of all optimized molecules (MN15/6-31G*+PCM(CH_2Cl_2)

1

Zero-point correction= 1.160199 (Hartree/Particle)
Thermal correction to Energy= 1.229519
Thermal correction to Enthalpy= 1.230463
Thermal correction to Gibbs Free Energy= 1.070518
Sum of electronic and zero-point Energies= -4415.829816
Sum of electronic and thermal Energies= -4415.760496
Sum of electronic and thermal Enthalpies= -4415.759552
Sum of electronic and thermal Free Energies= -4415.919498

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C	7.30105900	1.51476900	3.14909600
C	8.04637400	1.66016400	1.94095300
C	9.09127100	3.50902300	2.80439000
C	10.81205100	5.89653600	5.00130500
H	9.88580600	6.08546100	4.45213100
C	11.34435500	7.24750100	5.49116600
H	12.27880000	7.16357800	6.05643300
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C	11.26100300	4.52356800	2.91316300
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C	14.02902300	4.61450100	3.31187700
C	13.14412900	5.21439300	4.21044800
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C	16.40292400	2.30177900	3.82220200
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C	16.00508200	3.60667700	5.78317300
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C	16.72723700	-0.78647800	7.00393200
C	16.27586300	-2.96906300	6.46686300
C	15.53079600	-3.11432900	7.67532800
C	15.97899700	-0.93246000	8.21758300
C	16.49044100	2.70208500	8.12330600
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C	16.97093500	4.08148600	8.58646300
H	16.30822400	4.89582000	8.27467400
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C	13.68332700	0.61481800	9.69307200
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C	6.83578000	-0.17207000	0.98371900
C	13.49978900	-1.89728200	-1.13340300
C	14.60743800	-2.52052400	-0.52340600
C	15.93875000	-5.29223500	5.99005300
C	15.20260300	-5.43568000	7.18371400
H	12.84639100	5.19842600	11.00422500
H	17.96417200	4.28817200	8.17477200
H	15.72343000	6.81637000	3.31031300
H	10.60582600	7.72523200	6.14314600
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C	15.34038600	-1.90045100	0.47654400
C	16.37575100	-4.05585100	5.54053600
C	14.87232600	-4.34879900	7.97826200
C	9.69300000	-3.00040900	9.62600900
C	7.43065000	-1.72817200	8.38111500
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C	6.10986500	-0.11343500	4.67397800
C	5.90655700	0.65126200	5.83625100
C	6.16474300	0.11631300	7.09813000
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C	6.61497600	-2.01785300	6.09738600
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C	12.14445700	-3.24706300	10.38773700
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H	10.39134100	-4.98029400	8.05895300

2

Zero-point correction= 1.346408 (Hartree/Particle)
Thermal correction to Energy= 1.427163
Thermal correction to Enthalpy= 1.428107
Thermal correction to Gibbs Free Energy= 1.244698
Sum of electronic and zero-point Energies= -5029.487353
Sum of electronic and thermal Energies= -5029.406598
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C	11.78554700	2.59218600	2.47430800
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H	15.29750400	5.01859300	5.47296600
H	16.79608200	4.72076700	4.58583100
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C	16.06012000	0.99796100	4.40918200
C	16.47811000	-0.05784100	5.21708600
H	16.83647200	-0.98845600	4.78054700
C	16.47031000	0.12903500	6.59811500
C	16.05864100	1.33145000	7.18571400
C	15.63360500	2.35093200	6.33161600
H	15.30094100	3.29116900	6.76713100
C	16.31010300	-2.00833500	7.66918900
C	15.86684700	-4.20391800	7.18981400
C	15.10256100	-4.31386400	8.38978300
C	15.54262600	-2.11909600	8.87532000
C	16.08199700	1.50094900	8.69879300
H	16.79404000	0.76635000	9.08396800
C	16.56655600	2.88815600	9.13408500
H	15.91443200	3.69927300	8.79295400
H	16.61483100	2.94060400	10.22665100
C	14.72426100	1.13865500	9.28512600
C	14.47011500	-0.15999800	9.74256600
C	13.24546300	-0.52489900	10.29889000
H	13.08325500	-1.53109500	10.68173000
C	12.25220100	0.44805400	10.39512700
C	12.45058200	1.76236100	9.95501700
C	13.68994800	2.07044300	9.39087100
H	13.86343200	3.08413800	9.03538900
C	10.11180600	-0.62724600	10.47146300
C	9.14388600	-2.67657000	10.13843900
C	8.03619600	-2.05105900	9.49244600
C	8.99828900	0.00149400	9.82259900
C	11.34572500	2.80036600	10.09677000

H	10.68166200	2.44265100	10.88802900
C	11.87267600	4.17545000	10.52140700
H	12.55029300	4.62307700	9.78655800
H	11.03631200	4.86759300	10.66356300
C	10.51348100	2.85553000	8.82289200
C	9.34860300	2.08854400	8.69976600
C	8.55171600	2.12695900	7.55708200
H	7.63067900	1.54971300	7.49856100
C	8.94164200	2.96226300	6.51200300
C	10.09620800	3.75147700	6.57982000
C	10.86792600	3.66237700	7.73984600
H	11.77398300	4.26111100	7.80952500
O	8.11647000	3.12303100	5.40401200
O	9.57900700	3.33368300	3.10491000
O	14.04298500	2.09733400	1.78462100
O	16.16362700	0.89941600	3.02570900
O	16.99005100	-0.85161700	7.43636100
O	15.52794400	-1.06291300	9.73475700
O	11.05843500	0.16306100	11.04924700
O	8.93535900	1.36193300	9.81142300
C	8.05604800	-4.80317800	9.92750600
C	6.96096200	-4.18472900	9.28800000
C	5.71790700	-1.53399200	2.66549300
C	6.47287100	-1.42505200	1.47852300
C	13.18620600	-3.28837700	-0.49515200
C	14.28155200	-3.90654000	0.14418300
C	15.53112800	-6.54100200	6.77124400
C	14.77538800	-6.64974000	7.95770400
H	12.41951800	4.09012300	11.46611500
H	17.56686600	3.07725900	8.73109700
H	15.41732600	5.49998600	3.77734900
H	10.27309800	6.52166600	6.52087600
N	13.38610800	0.07554100	0.90134600
N	15.54567300	-1.14381600	2.16349800
N	16.42780800	-3.00606900	6.85060500
N	14.93750000	-3.22064000	9.19119900
N	10.18684100	-1.91607900	10.58377900
N	8.02633100	-0.69601700	9.32432200
N	7.15019000	1.17783700	4.64099600
N	8.63967700	1.39209500	2.29970700
C	7.54651000	-0.55541900	1.37148400
C	6.00814900	-0.77730200	3.78962700
C	12.77411500	-2.00698700	-0.16559800
C	15.00598200	-3.26675600	1.13729700
C	15.97936800	-5.31792400	6.29836500
C	14.43939600	-5.53955000	8.71599200
C	9.20724200	-4.10205700	10.24932600
C	6.97545800	-2.84175400	8.94652400
C	5.30060900	-0.57622100	6.30279200
C	4.62563400	0.66857300	6.18035400
C	4.20012900	1.35684700	7.29053300
C	4.44330300	0.83762900	8.58724300
C	5.10566600	-0.35622400	8.73981700
C	5.54614500	-1.10043200	7.61191600
C	10.81892600	-0.34092600	-0.67138000
C	11.58606100	0.57700100	-1.43882200
C	11.06820100	1.79190600	-1.81689800
C	9.75379400	2.15752100	-1.43074000
C	8.99162400	1.29854400	-0.67669800
C	9.49198500	0.02824000	-0.28153600
C	17.14334200	-4.29264700	4.18777100
C	18.38776400	-4.00675800	4.81226000
C	19.34673200	-3.25857200	4.17360500
C	19.10150700	-2.74397500	2.87539800
C	17.90342300	-2.99067700	2.25024900
C	16.89564800	-3.77243200	2.87740400
C	12.95174600	-4.89667400	10.77284200
C	14.02266600	-4.63715600	11.67063800
C	13.79635400	-4.06030100	12.89670600
C	12.48066900	-3.69880800	13.28206800
C	11.42581000	-3.92362800	12.43126400
C	11.62349600	-4.53174200	11.16187900
C	6.22103500	-2.35717900	7.75532000
C	5.73265200	-1.31495500	5.15271800
C	6.16218100	-2.61674800	5.33784000
H	6.48137300	-3.20057400	4.47845900
C	6.40358700	-3.13177200	6.62396300
H	6.90053100	-4.09447200	6.71086400
C	11.33937900	-1.62010400	-0.28663800
C	8.70108200	-0.88674600	0.48817100
C	9.15838400	-2.18457700	0.62940900
H	8.56860900	-2.89916700	1.19755700
C	10.46210700	-2.54707000	0.24662800
H	10.83146500	-3.52834600	0.53291800
C	15.64822000	-4.05306200	2.22911500
C	16.14075200	-5.08811600	4.83396000
C	15.06523400	-5.52034400	4.07894900
H	14.29971400	-6.13572200	4.54427800
C	14.82167800	-5.00874900	2.79188100
H	13.87705500	-5.24772200	2.31036400
C	13.17048200	-5.51580600	9.49847300
C	10.52965700	-4.79027900	10.27190900
C	12.06678700	-5.95213600	8.78784300
H	12.20922100	-6.43682300	7.82552500
C	10.76178700	-5.59355900	9.17000200
H	9.94413500	-5.81429600	8.48882300
H	4.44528300	1.05910300	5.18160700
H	5.29809800	-0.76215200	9.73012400
H	12.59351900	0.28816200	-1.72883700
H	7.98308500	1.57030000	-0.37419200
H	18.56588900	-4.40445900	5.80856600
H	17.70513000	-2.59923200	1.25529300
H	10.41327300	-3.64877000	12.71712800
H	15.02829000	-4.91650400	11.36535300
H	11.66401700	2.47574500	-2.41575700
H	9.35008100	3.11935600	-1.73598000
H	19.86628200	-2.15552300	2.37529200
H	20.29799100	-3.06137100	4.66093100
H	14.62547800	-3.88183800	13.57639700
H	12.30914200	-3.24540000	14.25483200
H	4.10114900	1.38650400	9.46070200
H	3.67302700	2.30062600	7.17776200
H	14.32603500	-7.60918600	8.20346700
H	15.64031600	-7.42007200	6.14023800
H	8.05057500	-5.88482600	10.04096500
H	6.14643100	-4.80940200	8.92857200
H	6.29670500	-2.14302700	0.68081500
H	4.98388900	-2.33259300	2.74508500
H	12.56585100	-3.88517600	-1.15987200
H	14.47058300	-4.96018700	-0.04807800

1 (Anion Radical)

Zero-point correction= 1.156318 (Hartree/Particle)
Thermal correction to Energy= 1.225876
Thermal correction to Enthalpy= 1.226821
Thermal correction to Gibbs Free Energy= 1.065829
Sum of electronic and zero-point Energies= -4415.937981
Sum of electronic and thermal Energies= -4415.868422
Sum of electronic and thermal Enthalpies= -4415.867478
Sum of electronic and thermal Free Energies= -4416.028470

C	8.35222800	3.35486700	4.01780000
C	7.30871600	1.50404700	3.14697800
C	8.05870000	1.64739200	1.94002000
C	9.09959000	3.50016700	2.80592200
C	10.81517400	5.88375500	5.00380200
H	9.88815200	6.06995100	4.45486700
C	11.34396700	7.23682700	5.49205600
H	12.27758800	7.15461400	6.05899700
H	11.53307400	7.89581200	4.63805900
C	11.76350100	5.19747200	4.03041800
C	11.26652600	4.51957600	2.91065500
C	12.10627000	3.88749700	1.99584700
H	11.69753600	3.38091300	1.12455500
C	13.48194500	3.95245500	2.20557800
C	14.03433300	4.61716600	3.30686300
C	13.14852300	5.21117200	4.20842000
H	13.55581600	5.72194300	5.07884000
C	14.52310700	2.11139000	1.07470600
C	13.98604500	0.13717600	0.03942100
C	15.10658400	-0.49424000	0.65763600
C	15.64837600	1.47732500	1.69550700
C	15.54345000	4.67165700	3.50117800
H	15.99158300	4.50491600	2.51799900
C	16.03061100	6.03334000	4.00783600
H	15.63260700	6.29323600	4.99454200
H	17.12309800	6.03526600	4.08171400
C	15.99219700	3.51585200	4.38465300
C	16.40632700	2.30583200	3.81553900
C	16.82816000	1.22958800	4.59299000
H	17.16311100	0.30419500	4.13001700
C	16.84455400	1.38024800	5.97818100
C	16.43869300	2.56649900	6.60154700
C	16.00204200	3.60641500	5.77816400
H	15.67072800	4.53329400	6.24232500
C	16.71603400	-0.78644400	6.99603500
C	16.26305300	-2.96991000	6.45334200
C	15.52073000	-3.11748300	7.66460800
C	15.96793300	-0.93128500	8.20747200
C	16.47564900	2.69499700	8.11808800
H	17.19499900	1.95308900	8.47509200
C	16.96018800	4.07189200	8.58501800
H	16.29898100	4.88828800	8.27520600
H	17.02159500	4.09456100	9.67803900
C	15.12647300	2.31103000	8.71148300
C	14.88123300	0.99970000	9.13555500
C	13.66558100	0.61900100	9.70174300
H	13.50054800	-0.40194700	10.03892400
C	12.67104300	1.58533600	9.86550300
C	12.86539800	2.90994200	9.44675400
C	14.08964800	3.23478700	8.85966100
H	14.25082800	4.25729200	8.52258700
C	10.52968400	0.51618600	9.97595100
C	9.59891100	-1.56499300	9.62191000
C	8.45673900	-0.92352700	8.99111600
C	9.43973300	1.12860500	9.37254700
C	11.76010800	3.94020600	9.63068300
H	11.11006600	3.55683100	10.42156800
C	12.28627900	5.30858500	10.07632900
H	12.95278700	5.77402000	9.34178800
H	11.44977300	5.99545500	10.24348500
C	10.90889800	4.01232400	8.37078300
C	9.75128400	3.22823800	8.25601500
C	8.95769800	3.27038700	7.10781400
H	8.05854700	2.66229500	7.03813900
C	9.32025900	4.13230000	6.07445500
C	10.46111900	4.94028200	6.14547700
C	11.24423300	4.83996700	7.29742900
H	12.14416100	5.44835400	7.36910900
O	8.47286000	4.31024500	4.98132100
O	9.90050700	4.59469000	2.66095300
O	14.35706700	3.45267200	1.24492700
O	16.50343100	2.24374900	2.42813400
O	17.38684500	0.38106200	6.77904300
O	15.94743100	0.10176400	9.09512100
O	11.51639900	1.28866500	10.56302300
O	9.34234400	2.50907700	9.36209200
C	8.54393200	-3.72219300	9.25075800
C	7.45939900	-3.11283900	8.65238100
C	6.11791700	-0.33525100	2.17995900
C	6.86276100	-0.19813000	0.99300800
C	13.52310400	-1.88222800	-1.16304600
C	14.63010600	-2.50575600	-0.55251700
C	15.90686400	-5.28722200	5.96802300
C	15.18300700	-5.43564300	7.16655000
H	12.84673900	5.20795600	11.01186900
H	17.95452100	4.27837800	8.17511800
H	15.72655600	6.82163500	3.31132600
H	10.60395400	7.71321100	6.14354200
H	5.38010100	-1.13200200	2.23914900
H	6.67632700	-0.89789800	0.18102000
H	12.91191800	-2.46608600	-1.84756900
H	14.83290600	-3.54801400	-0.78824000
H	16.01572900	-6.15321100	5.31843500
H	14.76492500	-6.41170500	7.40147100
H	8.54552000	-4.80410400	9.37466600
H	6.62399600	-3.72425000	8.31453600
N	13.72144100	1.45210500	0.29791800
N	15.90561000	0.22133000	1.50327800
N	16.83423200	-1.76555500	6.15359300
N	15.38722800	-2.05143800	8.50524600
N	10.61576500	-0.80204400	10.10472300
N	8.41905600	0.43172200	8.88938500
N	7.50786000	2.38291800	4.17131600
N	8.96419100	2.66386100	1.82374700
C	7.91609200	0.69769300	0.87896200
C	6.40305700	0.40530600	3.32073700
C	13.09773700	-0.61531100	-0.79407600
C	15.35865200	-1.88874600	0.45270600
C	16.35727500	-4.05285300	5.52257400

C	14.85555500	-4.35102100	7.97116400
C	9.69431400	-2.99134800	9.63759300
C	7.43342400	-1.72088400	8.39112700
C	6.27191300	-1.49480300	4.86557600
C	6.09730800	-0.10926900	4.67636300
C	5.96366500	0.67198400	5.83958800
C	6.22906300	0.13996200	7.09822300
C	6.65378400	-1.19828200	7.25611800
C	6.52836000	-2.02609100	6.11970000
H	6.36547400	-2.14434900	3.99796200
H	5.73115700	1.72797800	5.75632600
H	6.20141500	0.79477300	7.96095800
H	6.81073400	-3.07361600	6.19171600
C	10.74178600	-1.21778100	-0.57273600
C	11.66914600	-0.21768000	-0.90924700
C	11.18279200	1.09615700	-1.02713000
C	9.89288100	1.42145500	-0.60848300
C	9.04542100	0.44506700	-0.05472100
C	9.45871300	-0.89363200	-0.15530000
H	11.07472200	-2.24866300	-0.48295000
H	11.84428100	1.88834800	-1.36049300
H	9.57950400	2.45945100	-0.62615100
H	8.82668100	-1.68070800	0.24789400
C	15.58879700	-4.34446900	3.21862700
C	16.54850900	-3.77810100	4.07374700
C	17.40257100	-2.80484700	3.52459900
C	17.15619100	-2.26563900	2.26236700
C	16.04879600	-2.68346400	1.50366300
C	15.34407400	-3.80893900	1.96200900
H	14.91760100	-5.10996700	3.59947300
H	18.21000900	-2.39755500	4.12297000
H	17.77718800	-1.45060600	1.90696300
H	14.48840000	-4.17131000	1.39796600
C	12.51839600	-5.01393700	8.30967900
C	13.65132900	-4.36050600	8.83457400
C	13.43678100	-3.53099000	9.95132800
C	12.15020700	-3.18699600	10.35552100
C	11.01185400	-3.64906200	9.65753900
C	11.23723200	-4.67921900	8.71896600
H	12.63321100	-5.67890200	7.45635000
H	12.02746500	-2.47459000	11.16252000
H	14.28267100	-3.07978300	10.45813200
H	10.39326400	-5.09591300	8.17466100

1 (Cation Radical)

Zero-point correction= 1.158671 (Hartree/Particle)
Thermal correction to Energy= 1.228353
Thermal correction to Enthalpy= 1.229297
Thermal correction to Gibbs Free Energy= 1.067756
Sum of electronic and zero-point Energies= -4415.638970
Sum of electronic and thermal Energies= -4415.569288
Sum of electronic and thermal Enthalpies= -4415.568343
Sum of electronic and thermal Free Energies= -4415.729885

C	8.35590200	3.36444000	4.00689400
C	7.31924600	1.51647400	3.13213900
C	8.05323700	1.67559500	1.91990800
C	9.09489700	3.52426200	2.78860800
C	10.81473400	5.90076500	5.00281800
H	9.88688700	6.09145900	4.45701300
C	11.34888900	7.25044900	5.49421100
H	12.28690500	7.16605700	6.05344800
H	11.53198400	7.91101500	4.64069100
C	11.75928700	5.21032700	4.02788200
C	11.26158200	4.53872700	2.90484600
C	12.10029200	3.90703800	1.98901700
H	11.69319700	3.41085000	1.11100000
C	13.47570400	3.96266200	2.20381500
C	14.02932500	4.61947500	3.30938000
C	13.14390400	5.21498300	4.21036000
H	13.55179700	5.72275200	5.08217800
C	14.50590600	2.11711400	1.07635600
C	13.95513600	0.14185400	0.05049500
C	15.06479600	-0.49661500	0.67883500
C	15.62273700	1.47526000	1.70624100
C	15.53858400	4.67093900	3.50659500
H	15.98808400	4.50221700	2.52444100
C	16.02683400	6.03298500	4.01141300
H	15.62391200	6.29915100	4.99445400
H	17.11873000	6.03183400	4.09069400
C	15.98447900	3.51540700	4.39239200
C	16.39159800	2.30218800	3.82442600
C	16.81497000	1.22619500	4.60190500
H	17.15138000	0.30230300	4.13769800
C	16.83527800	1.38164800	5.98573500
C	16.44076900	2.57078500	6.60944800
C	16.00439600	3.61072900	5.78548700
H	15.68590300	4.54264700	6.24776600
C	16.70789200	-0.78186300	7.01632500
C	16.21576000	-2.95523400	6.47862100
C	15.49779000	-3.10125700	7.69753700
C	15.97868200	-0.92702100	8.24327500
C	16.49107400	2.70470400	8.12582500
H	17.21705500	1.96864700	8.48146900
C	16.96959500	4.08549900	8.58717900
H	16.30260300	4.89799000	8.28026800
H	17.03918500	4.10969300	9.67938700
C	15.14640800	2.31577800	8.72622100
C	14.90928200	1.00721900	9.16158400
C	13.69624700	0.62230200	9.72659600
H	13.54419400	-0.39376400	10.08132900
C	12.69749100	1.58292000	9.86292300
C	12.87521100	2.90681800	9.44619100
C	14.10332200	3.23414600	8.86664500
H	14.26147100	4.25545500	8.52702700
C	10.57621600	0.47852700	9.95613700
C	9.65358600	-1.58084400	9.55063200
C	8.54676400	-0.96012200	8.90914700
C	9.45642900	1.10465000	9.31406900
C	11.76493500	3.93426200	9.62296600
H	11.11219800	3.55619700	10.41434400
C	12.28851800	5.30307400	10.07080800
H	12.96054600	5.76734000	9.34140500
H	11.44980600	5.98815200	10.23061100
C	10.91996400	4.00765000	8.35791000
C	9.77221000	3.21847600	8.22184300
C	8.96750400	3.26608500	7.08623000
H	8.06542500	2.66326700	7.01428900
C	9.32622900	4.13902300	6.06124900

C	10.46314600	4.95221600	6.14098100
C	11.24620100	4.85041400	7.29281400
H	12.13580500	5.47170600	7.37216800
O	8.48269000	4.31663900	4.97004200
O	9.89457200	4.61694600	2.65444700
O	14.34919800	3.45819200	1.24477500
O	16.47940400	2.23767300	2.43802900
O	17.37116100	0.37849500	6.79304100
O	15.97234400	0.10552200	9.12117200
O	11.51688300	1.26466600	10.53390600
O	9.38016900	2.45741400	9.32292500
C	8.61243500	-3.73675900	9.20817400
C	7.52460200	-3.12494500	8.59344700
C	6.12488600	-0.32086700	2.15541500
C	6.84455800	-0.15894700	0.95744300
C	13.47892200	-1.88203100	-1.14506800
C	14.56915700	-2.51469900	-0.52004400
C	15.81102600	-5.27995500	5.96981200
C	15.09621100	-5.42300600	7.15532300
H	12.84027500	5.20149500	11.01080000
H	17.95959400	4.29486800	8.16961900
H	15.72898000	6.81831100	3.30931100
H	10.61355100	7.72549600	6.15158600
H	5.39231900	-1.12215400	2.21574800
H	6.64338900	-0.84156800	0.13553200
H	12.87274600	-2.45933200	-1.83882600
H	14.76683400	-3.55793600	-0.75438000
H	15.93571100	-6.14594300	5.32604500
H	14.69643300	-6.40218700	7.40227000
H	8.59665600	-4.81554700	9.33269300
H	6.70110600	-3.74411200	8.24939200
N	13.69942900	1.45923800	0.30363300
N	15.86432200	0.21426000	1.52742600
N	16.78843100	-1.75899300	6.16653000
N	15.38229000	-2.04080800	8.54312200
N	10.66684800	-0.81425800	10.03893900
N	8.50283300	0.39642900	8.79178600
N	7.52593900	2.38181900	4.16807700
N	8.95819500	2.69180000	1.80439100
C	7.90195900	0.73451200	0.85103500
C	6.42200500	0.41250400	3.29607900
C	13.06511800	-0.60654700	-0.78532300
C	15.30177900	-1.89522300	0.48311600
C	16.27102800	-4.03287000	5.52931700
C	14.81104500	-4.33287800	7.99473800
C	9.75581700	-3.01776300	9.59706200
C	7.51331700	-1.75458500	8.30324900
C	6.34602600	-1.50775500	4.81347200
C	6.14790000	-0.12443600	4.65060900
C	5.97852000	0.64754700	5.81837300
C	6.25976000	0.11303500	7.06932100
C	6.70027000	-1.22144300	7.19991100
C	6.61009900	-2.04796000	6.06142500
H	6.44953700	-2.14237300	3.93785900
H	5.71119200	1.69458800	5.73890700
H	6.20338200	0.75121300	7.94311300
H	6.91091200	-3.09001900	6.12394600
C	10.70022200	-1.18735700	-0.62289700
C	11.64544000	-0.19184600	-0.92295900
C	11.17716600	1.13086900	-1.02852800
C	9.88776800	1.46573200	-0.61965500
C	9.02334100	0.48913100	-0.09150000
C	9.41687000	-0.85412800	-0.21589400
H	11.01595800	-2.22475900	-0.55205200
H	11.85057600	1.91872400	-1.34632400
H	9.58586100	2.50688000	-0.62844700
H	8.76930500	-1.64152000	0.16053300
C	15.56721200	-4.37649900	3.22343000
C	16.48950100	-3.76816500	4.09869200
C	17.32838400	-2.76753800	3.56357500
C	17.08932600	-2.24285100	2.29958300
C	15.99146500	-2.68361300	1.53270800
C	15.32027700	-3.83989000	1.97027300
H	14.92171600	-5.17209000	3.58488200
H	18.12704200	-2.35291700	4.16699600
H	17.70394200	-1.42532900	1.94176800
H	14.48818100	-4.22978600	1.39082400
C	12.54841800	-5.14285700	8.49450600
C	13.66451600	-4.35494300	8.89142400
C	13.45893400	-3.46563900	9.98485200
C	12.18457400	-3.13395100	10.38904900
C	11.04828200	-3.67453500	9.72158900
C	11.27637900	-4.81232700	8.89833900
H	12.66510700	-5.89992300	7.72594200
H	12.04754100	-2.40790600	11.17983900
H	14.30911100	-2.99656900	10.46278500
H	10.43891700	-5.32145500	8.43260100

1 (Phenyl Rotation Transition State)

Zero-point correction= 1.159183 (Hartree/Particle)
Thermal correction to Energy= 1.227920
Thermal correction to Enthalpy= 1.228864
Thermal correction to Gibbs Free Energy= 1.070302
Sum of electronic and zero-point Energies= -4415.801400
Sum of electronic and thermal Energies= -4415.732663
Sum of electronic and thermal Enthalpies= -4415.731719
Sum of electronic and thermal Free Energies= -4415.890281

C	8.49860400	3.23616700	3.92432900
C	7.52485600	1.38879200	3.01137800
C	8.23642900	1.59548600	1.79819300
C	9.21702900	3.45104100	2.70341700
C	10.80703400	5.88149200	4.98976500
H	9.87616900	6.04838400	4.44080400
C	11.30002700	7.24313700	5.49043200
H	12.24137700	7.18260200	6.04687300
H	11.46148100	7.91515300	4.64160500
C	11.77626200	5.22547800	4.01479800
C	11.31565800	4.55987700	2.87333500
C	12.18108200	3.95785700	1.96649100
H	11.80017600	3.46323400	1.07639100
C	13.54903500	4.03416800	2.20633900
C	14.07161300	4.68713000	3.32892800
C	13.15772700	5.25276100	4.22066500
H	13.54030400	5.74918600	5.11035700
C	14.57917300	2.18960800	1.10552700

C	14.08241600	0.22913200	0.04309900
C	15.18231000	-0.38923000	0.69724600
C	15.67800000	1.55732900	1.77066300
C	15.57475500	4.76284900	3.56116400
H	16.04896000	4.60009800	2.58941200
C	16.02683800	6.13378900	4.07484400
H	15.59191900	6.39543800	5.04542800
H	17.11594800	6.15027100	4.18505200
C	16.01692300	3.61443700	4.45802600
C	16.42130100	2.39927400	3.89306400
C	16.83944900	1.32164900	4.66875400
H	17.17469500	0.39676800	4.20713000
C	16.85485000	1.47770700	6.05197000
C	16.46139000	2.66808200	6.67450700
C	16.03342800	3.71237800	5.85131700
H	15.71849000	4.64602600	6.31294400
C	16.73674100	-0.69991400	7.05505100
C	16.35122200	-2.88398800	6.53835700
C	15.62436500	-3.06162700	7.74680300
C	16.01568700	-0.87502800	8.27950000
C	16.50196800	2.78563400	8.19233600
H	17.24027400	2.05903600	8.54246500
C	16.94768500	4.16995900	8.67449800
H	16.26287800	4.97106200	8.37658700
H	17.01319400	4.18103000	9.76721100
C	15.16241000	2.35999200	8.77873300
C	14.94958200	1.04376100	9.20511500
C	13.73898200	0.63080200	9.75152200
H	13.60523400	-0.39193600	10.09544200
C	12.71778700	1.56594600	9.87982300
C	12.86791400	2.89549200	9.47009500
C	14.09611700	3.25249500	8.90831300
H	14.23315500	4.27700700	8.56848100
C	10.65694700	0.37588000	9.89971200
C	9.77720200	-1.69591400	9.50223900
C	8.68459400	-1.09345200	8.82091600
C	9.55492100	0.97728400	9.20896100
C	11.73383800	3.90074200	9.62501800
H	11.06612300	3.50320100	10.39438200
C	12.21920900	5.27514600	10.09736100
H	12.90892400	5.75347500	9.39388600
H	11.36512400	5.94665000	10.23237300
C	10.92370700	3.96633900	8.33686100
C	9.82279000	3.12144600	8.15832900
C	9.04495900	3.14314000	7.00510700
H	8.17516700	2.49965200	6.90410600
C	9.39102700	4.04358300	6.00283700
C	10.47976700	4.91441200	6.11993500
C	11.23400500	4.84295600	7.29386700
H	12.08550700	5.51053700	7.40740200
O	8.57680100	4.18755500	4.88404100
O	9.95133300	4.58695500	2.59071700
O	14.43336000	3.53481100	1.25793800
O	16.51140600	2.33766100	2.50796300
O	17.38443000	0.47889800	6.85979500
O	16.01684700	0.15480700	9.17019100
O	11.53895600	1.19670800	10.52451300
O	9.44700000	2.32643300	9.23647600
C	8.57276600	-3.75431000	9.59151100
C	7.51964500	-3.18364300	8.84955400
C	6.13619800	-0.22465100	1.91755100
C	6.79451900	0.04184300	0.70081500
C	13.94125700	-1.64556800	-1.42576000
C	15.01155800	-2.28532900	-0.73794600
C	16.39597200	-5.24067800	6.18067500
C	15.71070100	-5.42279400	7.41569000
H	12.74050300	5.17672300	11.05483100
H	17.93398700	4.40816800	8.26336700
H	15.73645600	6.91284700	3.36266000
H	10.55187300	7.69072800	6.15264900
H	5.31911900	-0.94212200	1.92227600
H	6.42083800	-0.43209100	-0.20135800
H	13.49902400	-2.16677200	-2.27019800
H	15.28471500	-3.29367100	-1.03963700
H	16.60880900	-6.12026100	5.57784600
H	15.50106300	-6.44049200	7.73310900
H	8.45361900	-4.76930300	9.95739000
H	6.65364400	-3.79855500	8.61633100
N	13.78409900	1.53228500	0.31467100
N	15.93535800	0.29541100	1.60516300
N	16.85393000	-1.66401000	6.19316700
N	15.43895200	-1.99973700	8.58284700
N	10.78249000	-0.91493100	9.98682400
N	8.63592000	0.25401300	8.64206600
N	7.72590200	2.20327100	4.08195300
N	9.12526300	2.62346300	1.70530900
C	8.01271000	0.71952400	0.67092300
C	6.61282900	0.28077900	3.12188200
C	13.30417300	-0.52871000	-0.90771000
C	15.50760800	-1.75790100	0.43325000
C	16.55005000	-3.98260300	5.64278100
C	15.10250500	-4.36657100	8.07619500
C	9.81566900	-3.12898700	9.68183400
C	7.63982200	-1.92187800	8.27830300
C	6.96315900	-1.75569600	4.53984400
C	6.50532200	-0.38826800	4.42484300
C	6.20608800	0.32175900	5.60504800
C	6.45511800	-0.21460700	6.85950800
C	7.01839300	-1.49696800	7.01693800
C	7.21766900	-2.31226100	5.83847600
H	5.79890200	1.32258800	5.52341100
H	6.24138100	0.37383700	7.74392300
C	10.90189600	-1.32755800	-0.70297800
C	11.83594000	-0.26130500	-1.01577200
C	11.32786300	1.02121800	-1.13357000
C	10.01438400	1.34177600	-0.72816000
C	9.14344900	0.38325000	-0.23633600
C	9.54438000	-1.00948800	-0.34846800
H	11.98713000	1.82917700	-1.42949300
H	9.71908100	2.38480100	-0.71689400
C	15.10995200	-3.52363100	3.72941700
C	16.47171800	-3.65017400	4.18702700
C	17.50156600	-3.28877900	3.35189900
C	17.24363800	-2.73903800	2.06363000
C	15.95733300	-2.55330100	1.61687900
C	14.85224100	-2.97465500	2.44224800
H	18.52848500	-3.35985400	3.69979000
H	18.07935200	-2.40230200	1.45630800
C	12.67863800	-5.11753300	8.17377800
C	13.80348400	-4.45950000	8.81291100
C	13.54745500	-3.71460200	9.95149000
C	12.23231600	-3.39067400	10.34937800
C	11.12288900	-3.84018400	9.65213000
C	11.33892600	-4.83716900	8.61669000

H	12.09925000	-2.69347800	11.16888400
H	14.37379900	-3.26304600	10.48842400
C	7.81967400	-3.59187600	5.90552200
H	8.12238100	-3.99429500	6.86192600
C	7.33421500	-2.51875900	3.40648100
H	7.26200600	-2.08402700	2.41933800
C	7.85712700	-3.79851900	3.51092800
H	8.12185500	-4.34562300	2.61108100
C	8.10124100	-4.34123600	4.77362300
H	8.55946100	-5.32012700	4.87825500
C	11.27930800	-2.70266800	-0.68522400
H	12.30102800	-2.98080100	-0.89270000
C	8.66876100	-2.09609600	-0.06482600
H	7.63312100	-1.90729700	0.16994900
C	9.06259000	-3.41277500	-0.11297600
H	8.33843900	-4.20039900	0.07951200
C	10.40013300	-3.72225800	-0.41141000
H	10.74371000	-4.75254300	-0.42575800
C	13.49525500	-2.81019200	2.03662400
H	13.27454700	-2.37124200	1.07084300
C	13.99789700	-3.88050600	4.54727800
H	14.16951300	-4.27644100	5.54117200
C	12.70073500	-3.73026900	4.11724800
H	11.87904900	-4.02517700	4.76725600
C	12.44509500	-3.18612800	2.84044400
H	11.42305900	-3.05445500	2.49005000
C	12.83207200	-6.01389200	7.07527900
H	13.81560200	-6.21094600	6.67746600
C	10.27520700	-5.52142600	7.96273800
H	9.25778700	-5.37018700	8.28680200
C	11.77735900	-6.65748400	6.47455000
H	11.95812600	-7.33940400	5.64867300
C	10.47338700	-6.41941300	6.94037400
H	9.62283200	-6.93641400	6.50314000

Cavitand (Vase Form)

Zero-point correction= 0.919067 (Hartree/Particle)
Thermal correction to Energy= 0.976738
Thermal correction to Enthalpy= 0.977682
Thermal correction to Gibbs Free Energy= 0.827868
Sum of electronic and zero-point Energies= -3497.816275
Sum of electronic and thermal Energies= -3497.758604
Sum of electronic and thermal Enthalpies= -3497.757660
Sum of electronic and thermal Free Energies= -3497.907474

C	8.58280500	3.06192500	4.18250900
C	8.22770400	0.86868700	3.69184900
C	8.97161800	1.01087500	2.48974500
C	9.33364500	3.20693100	2.96274300
C	10.73977300	5.87032200	4.98757600
H	9.80568400	6.00493500	4.43392500
C	11.21213900	7.25512800	5.44631600
H	12.14836600	7.21934300	6.01464300
H	11.37795200	7.90187300	4.57845300
C	11.71729700	5.22153000	4.01489800
C	11.24467700	4.53768900	2.88833800
C	12.10228000	3.98245600	1.94772200
H	11.71121400	3.46537400	1.07806200
C	13.47340800	4.08756900	2.15205000
C	14.01007300	4.73066500	3.27366100
C	13.10342800	5.28690400	4.18236700
H	13.49655700	5.79078900	5.06402700
C	14.37278000	2.19195800	1.13811700
C	13.55537300	0.16932600	0.49907900
C	14.58162600	-0.48449400	1.23254400
C	15.43952500	1.52957600	1.84436400
C	15.51767100	4.79570300	3.48972600
H	15.97697400	4.62538000	2.51141200
C	15.98254400	6.16688100	3.99117200
H	15.56051700	6.43149400	4.96718300
H	17.07312200	6.18162300	4.08873000
C	15.98007800	3.65172300	4.38604600
C	16.37182900	2.43312400	3.81849400
C	16.81031200	1.36307800	4.58767100
H	17.11818000	0.43257100	4.12285300
C	16.84457000	1.51332500	5.96933800
C	16.45853400	2.70147300	6.60087400
C	16.02687100	3.74858700	5.77959700
H	15.71475400	4.68069400	6.24753100
C	16.53875900	-0.63742700	6.86591300
C	15.68366900	-2.60594300	6.11630500
C	14.95044400	-2.75452800	7.32426800
C	15.79449500	-0.78777200	8.09024300
C	16.50542500	2.81785700	8.12068400
H	17.22187000	2.06596400	8.46467800
C	17.00413400	4.18737000	8.59337500
H	16.34555800	5.01015100	8.29343200
H	17.07471800	4.20424500	9.68592200
C	15.16032200	2.43920200	8.73121800
C	14.91394700	1.12249300	9.13709400
C	13.69960000	0.73148100	9.68952800
H	13.53505000	-0.29522000	9.99844000
C	12.70327800	1.68796400	9.83484900
C	12.88792000	3.02419800	9.45942000
C	14.12428700	3.36366700	8.90286300
H	14.28950700	4.39333900	8.59027800
C	10.63099200	0.55731600	9.72270500
C	9.91247700	-1.42346500	8.86950200
C	8.71546300	-0.80265100	8.42204900
C	9.43933400	1.19684900	9.22596300
C	11.76067900	4.03226100	9.65614200
H	11.13387100	3.63990100	10.46247800
C	12.26762200	5.41218500	10.08811400
H	12.89721100	5.89305900	9.33108600
H	11.42070900	6.07843300	10.28195300
C	10.87532300	4.09540200	8.41693300
C	9.70706500	3.32927300	8.32970800
C	8.89931000	3.34246800	7.19819200
H	8.00706600	2.72749300	7.14912400
C	9.26758700	4.14481000	6.12613400
C	10.40675800	4.95795000	6.16199800
C	11.19303100	4.89810900	7.31608200
H	12.09877400	5.50117500	7.35858500
O	8.47148900	4.16099400	4.98309800
O	9.86845000	4.43404800	2.70063100
O	14.33811800	3.55374500	1.19780400
O	16.36810600	2.33039100	2.43233100
O	17.32423600	0.46913500	6.75467300
O	15.94169100	0.19077500	9.02522700

O	11.49365700	1.34009200	10.42435100
O	9.32771300	2.54267400	9.41653200
C	9.15015500	-3.53212700	7.96882100
C	7.95031200	-2.91701800	7.53718000
C	7.89292100	-1.47324100	3.20488500
C	8.63537200	-1.33185600	2.00753500
C	12.66263600	-1.97635000	-0.16289900
C	13.67651700	-2.62780400	0.58006800
C	14.78140300	-4.69920300	5.31483800
C	14.05126500	-4.84732300	6.51866600
H	12.86147900	5.32497100	11.00399600
H	17.99547900	4.39054100	8.17518500
H	15.68380400	6.94596300	3.28228200
H	10.45453700	7.71655500	6.08823400
H	7.48678800	-2.44542100	3.47175500
H	8.79135200	-2.19707300	1.36851300
H	11.93073900	-2.56979700	-0.70463700
H	13.70763500	-3.71383100	0.60411600
H	14.70633000	-5.46402500	4.54643300
H	13.42486300	-5.72412000	6.65965200
H	9.30528600	-4.59133300	7.78165700
H	7.19620300	-3.51236100	7.02899900
N	13.46934800	1.53725800	0.47824500
N	15.53641600	0.23791200	1.90077600
N	16.48595700	-1.51329000	5.91140700
N	15.02705600	-1.80854400	8.31340400
N	10.86721600	-0.70462800	9.54163100
N	8.50784900	0.53927000	8.60940800
N	8.04562600	1.93488400	4.53276600
N	9.51959000	2.21823600	2.14454000
C	9.16657600	-0.11201900	1.65284200
C	7.69039900	-0.39340100	4.03479200
C	12.60133300	-0.60096100	-0.20528500
C	14.62208900	-1.89752000	1.26515700
C	15.58459400	-3.59862300	5.11415200
C	14.13231800	-3.89297900	7.50825300
C	10.11527600	-2.80143900	8.62569500
C	7.73351100	-1.57513600	7.75973200
H	11.83990000	-0.07030000	-0.77056300
H	15.41402300	-2.36867300	1.84065000
H	9.75132800	0.02482400	0.74795200
H	7.13668100	-0.47308400	4.96556900
H	16.16172600	-3.45899900	4.20419100
H	13.58952000	-3.98042100	8.44547400
H	6.82172500	-1.07387500	7.44627100
H	11.04416100	-3.24603200	8.97183500

Cavitand (Kite Form)

Zero-point correction= 0.918730 (Hartree/Particle)
Thermal correction to Energy= 0.976469
Thermal correction to Enthalpy= 0.977413
Thermal correction to Gibbs Free Energy= 0.828386
Sum of electronic and zero-point Energies= -3497.811242
Sum of electronic and thermal Energies= -3497.753503
Sum of electronic and thermal Enthalpies= -3497.752559
Sum of electronic and thermal Free Energies= -3497.901585

C	8.89874700	4.36298500	4.65115300
C	6.64818900	4.45625500	5.01337200
C	6.52761000	5.43858100	3.99643700
C	8.78995900	5.40858700	3.65937700
C	10.95334500	6.31925300	5.79823200
H	9.90484800	6.47380000	5.51238300
C	11.40484600	7.61424000	6.47836000
H	12.45577400	7.56706900	6.78651800
H	11.29784100	8.45284300	5.78407900
C	11.76250600	6.03874100	4.53792500
C	11.19408700	5.79984000	3.28185600
C	11.99220100	5.50190600	2.18263300
H	11.53383200	5.33000800	1.21457000
C	13.37293600	5.40950500	2.31970500
C	13.98846900	5.63984500	3.55492400
C	13.14947100	5.92166500	4.63334100
H	13.60328800	6.01913000	5.62119100
C	15.04419900	4.28592000	0.89941700
C	16.72156700	3.60586400	-0.49974800
C	17.08297900	2.57497400	0.40574500
C	15.37864100	3.19699800	1.78887300
C	15.48695500	5.50607500	3.79558100
H	15.98647300	5.38303800	2.82586100
C	16.07128300	6.77705500	4.41738300
H	15.61803100	6.99955100	5.39038200
H	17.15341700	6.67994100	4.55962000
C	15.72586800	4.24728400	4.61998900
C	15.25897400	3.02392200	4.12328700
C	15.35947700	1.84252800	4.84312900
H	14.99377900	0.90718900	4.43492100
C	15.93363700	1.89559000	6.10462800
C	16.41966300	3.08656200	6.65832300
C	16.31186900	4.24890700	5.88915000
H	16.67524200	5.18695600	6.29974700
C	17.18184100	0.17492200	7.09424900
C	19.09632000	-0.80883900	6.33786200
C	19.49371300	-1.05960000	7.67678800
C	17.61155000	-0.02187400	8.46002800
C	16.94635800	3.06212500	8.08778200
H	17.78993700	2.36113500	8.13250700
C	17.48540100	4.40946700	8.57511100
H	16.70552100	5.17974000	8.58585000
H	17.86795900	4.30734300	9.59489000
C	15.83728200	2.54296500	8.99427200
C	15.84163300	1.27387200	9.58353500
C	14.77168200	0.84463600	10.36104800
H	14.79782000	-0.13870100	10.81839100
C	13.66247500	1.66298600	10.54498400
C	13.61102000	2.94063900	9.97679500
C	14.69923700	3.32505500	9.19285700
H	14.64007600	4.28207100	8.67137700
C	11.36059700	1.09867900	11.22208000
C	9.30996700	0.76976800	12.18094500
C	8.66744200	1.06725900	10.95116800
C	10.70317700	1.33824500	9.95751200
C	12.41208700	3.87391500	10.09066300
H	11.70850000	3.45022800	10.81903600
C	12.81790300	5.24473400	10.63802000
H	13.54191900	5.74560800	9.98490400
H	11.94401100	5.89754800	10.74209600

C	11.72107300	3.92890100	8.73382900
C	11.27823000	2.73039500	8.16052600
C	10.71378100	2.67593500	6.89469900
H	10.37492600	1.73586600	6.47437200
C	10.60429400	3.85920800	6.17924300
C	11.02818700	5.09009600	6.69539300
C	11.57539900	5.09835700	7.98179200
H	11.91821200	6.04000600	8.40173800
O	10.12897000	3.82260100	4.87517000
O	9.84676700	5.93579700	2.99643200
O	14.05660200	5.18146400	1.13814000
O	14.60708200	3.01837500	2.89728800
O	15.96371500	0.74791000	6.88542400
O	16.91283600	0.39853600	9.54139700
O	12.70232300	1.14974300	11.39930000
O	11.48546600	1.55062200	8.86272900
C	7.15171600	0.44205000	13.21622200
C	6.51274600	0.74416700	11.98929400
C	4.26277400	4.52464500	5.37384100
C	4.13929000	5.50127500	4.35606400
C	18.50402400	2.91581800	-1.97782800
C	18.86496200	1.89020700	-1.07076700
C	21.10252500	-1.88178400	5.53249900
C	21.49887600	-2.13749000	6.86759600
H	13.28135400	5.12718700	11.62195200
H	18.30098300	4.75905900	7.93223300
H	15.88392400	7.63025600	3.75883600
H	10.79791000	7.82025300	7.36710700
H	3.37434400	4.18142600	5.89715900
H	3.15688100	5.89661700	4.11151800
H	19.06577400	3.03480000	-2.90060300
H	19.69782900	1.23386100	-1.30848400
H	21.73805100	-2.20796000	4.71354400
H	22.43504900	-2.65614800	7.05678900
H	6.54840600	0.19975200	14.08716000
H	5.42759400	0.72900500	11.93283700
N	15.69558900	4.46197000	-0.21164500
N	16.37128500	2.39803700	1.56122500
N	17.90827100	-0.17897000	6.08298500
N	18.72693500	-0.63432800	8.72532400
N	10.67215500	0.81032800	12.28620700
N	9.41421000	1.34919500	9.83931800
N	7.87531000	3.93055500	5.31530700
N	7.63256700	5.90864600	3.34340500
C	5.24933000	5.95423200	3.67785600
C	5.49716000	4.00825300	5.70061800
C	17.45273200	3.76173400	-1.70085700
C	18.16751600	1.72001800	0.10466900
C	19.91999700	-1.22694500	5.26799600
C	20.71242000	-1.73413600	7.92407500
C	8.52549600	0.45492200	13.31536200
C	7.25627100	1.05324700	10.87180000
H	20.99410700	-1.91311700	8.95764500
H	19.58508300	-1.01942600	4.25575200
H	6.79730800	1.28506300	9.91498900
H	9.04155600	0.23174800	14.24462400
H	5.18427800	6.70560100	2.89627300
H	5.62548900	3.25512100	6.47275800
H	18.41593600	0.94097500	0.81968400
H	17.15707500	4.55899600	-2.37658900

[8]CPP

Zero-point correction= 0.648710 (Hartree/Particle)
Thermal correction to Energy= 0.683557
Thermal correction to Enthalpy= 0.684501
Thermal correction to Gibbs Free Energy= 0.583833
Sum of electronic and zero-point Energies= -1845.437811
Sum of electronic and thermal Energies= -1845.402965
Sum of electronic and thermal Enthalpies= -1845.402021
Sum of electronic and thermal Free Energies= -1845.502688

C	0.03983700	5.54785400	-0.05608000
C	1.50757200	5.33940500	0.05535700
C	2.36545600	5.36840800	-1.05782500
C	3.56326300	4.65983200	-1.05732700
C	3.95031600	3.89426800	0.05617000
C	4.84043100	2.70881300	-0.05530700
C	4.78412100	1.94698800	-1.23199300
C	5.13058100	0.60082600	-1.23240500
C	5.54785000	-0.03983800	-0.05612200
C	5.81544000	0.77552800	1.05718100
C	5.46843400	2.12333800	1.05761700
C	3.20278300	4.05337000	1.23264600
C	2.00648000	4.76120400	1.23221900
C	-0.60081800	5.13060600	-1.23237700
C	-1.94697900	4.78414400	-1.23198300
C	-2.70881500	4.84043700	-0.05530300
C	-3.89427000	3.95031900	0.05614800
C	-4.05339400	3.20278800	1.23262200
C	-4.76122800	2.00648600	1.23218300
C	-5.33940100	1.50757300	0.05531000
C	-5.54785000	0.03983800	-0.05612200
C	-5.81544000	-0.77552800	1.05718100
C	-5.46843400	-2.12333800	1.05761700
C	-5.13058000	-0.60082700	-1.23240600
C	-4.78412100	-1.94698800	-1.23199300
C	-4.84043100	-2.70881400	-0.05530700
C	-3.95031600	-3.89426800	0.05617000
C	-3.20278300	-4.05337000	1.23264600
C	-2.00648000	-4.76120400	1.23221900
C	-1.50757200	-5.33940500	0.05535800
C	-0.03983700	-5.54785400	-0.05608000
C	0.77554000	-5.81542500	1.05722100
C	2.12335000	-5.46842100	1.05763800
C	2.70881500	-4.84043700	-0.05530300
C	3.89427000	-3.95032000	0.05614900
C	4.05339400	-3.20278900	1.23262200
C	4.76122800	-2.00648600	1.23218300
C	5.33940100	-1.50757400	0.05531000
C	5.36838000	-2.36545300	-1.05787600
C	4.65980600	-3.56326200	-1.05736600
C	1.94697900	-4.78414400	-1.23198200
C	0.60081800	-5.13060700	-1.23237700
C	-2.36545600	-5.36840800	-1.05782500
C	-3.56326200	-4.65983200	-1.05732700
C	-5.36838000	2.36545300	-1.05787700
C	-4.65980600	3.56326100	-1.05736600
C	-2.12335000	5.46842100	1.05763700

C	-0.77554000	5.81542400	1.05722000
H	2.05105800	5.88102400	-1.96493400
H	4.16447500	4.63092600	-1.96405300
H	4.31119900	2.36558800	-2.11715300
H	4.91833300	0.00636000	-2.11782100
H	6.22084700	0.33045200	1.96382500
H	5.60867900	2.70839600	1.96453600
H	3.47293700	3.48318600	2.11826400
H	1.37627700	4.72364800	2.11755900
H	-0.00634400	4.91837500	-2.11779200
H	-2.36557200	4.31123800	-2.11715400
H	-3.48323100	3.47294800	2.11825200
H	-4.72369300	1.37628600	2.11752600
H	-6.22084700	-0.33045200	1.96382500
H	-5.60867900	-2.70839600	1.96453600
H	-4.91833300	-0.00636000	-2.11782200
H	-4.31119900	-2.36558800	-2.11715300
H	-3.47293700	-3.48318600	2.11826400
H	-1.37627700	-4.72364800	2.11755900
H	0.33047200	-6.22081800	1.96387500
H	2.70841700	-5.60864900	1.96455400
H	3.48323100	-3.47294800	2.11825300
H	4.72369300	-1.37628600	2.11752600
H	5.88097400	-2.05105100	-1.96499600
H	4.63087800	-4.16447000	-1.96409400
H	2.36557200	-4.31123800	-2.11715400
H	0.00634400	-4.91837600	-2.11779200
H	-2.05105800	-5.88102500	-1.96493400
H	-4.16447500	-4.63092600	-1.96405300
H	-5.88097400	2.05105000	-1.96499700
H	-4.63087800	4.16447000	-1.96409400
H	-2.70841700	5.60864900	1.96455300
H	-0.33047200	6.22081800	1.96387500

Biphenyl

Zero-point correction= 0.182734 (Hartree/Particle)
Thermal correction to Energy= 0.191651
Thermal correction to Enthalpy= 0.192595
Thermal correction to Gibbs Free Energy= 0.148222
Sum of electronic and zero-point Energies= -462.542805
Sum of electronic and thermal Energies= -462.533888
Sum of electronic and thermal Enthalpies= -462.532943
Sum of electronic and thermal Free Energies= -462.577316

C	-0.69309600	-1.50168300	-0.13779200
C	0.69995000	-1.49885800	-0.13304600
C	1.41601600	-0.30027200	-0.00242600
C	0.69572200	0.89636900	0.12246200
C	-0.69735900	0.89551300	0.11606200
C	-1.39773100	-0.30401500	-0.01364600
H	-1.22946600	-2.44104000	-0.24784700
H	1.24437200	-2.43255500	-0.25782600
H	1.23665000	1.83151000	0.25159500
H	-1.23709100	1.83343000	0.22188800
H	-2.48474700	-0.30546900	-0.01799500
C	2.90082200	-0.29818700	0.00352300
C	3.61986700	0.73587200	-0.61297800
C	3.61811100	-1.33009700	0.62564900
C	5.01295700	0.73925800	-0.60714900
H	3.07796700	1.52952800	-1.12309700
C	5.01115600	-1.32917400	0.63081600
H	3.07461800	-2.12541800	1.13145300
C	5.71455800	-0.29388400	0.01458800
H	5.55172600	1.54636500	-1.09755500
H	5.54851200	-2.13463600	1.12545200
H	6.80157700	-0.29227800	0.01882600

p-Terphenyl

Zero-point correction= 0.264084 (Hartree/Particle)
Thermal correction to Energy= 0.277694
Thermal correction to Enthalpy= 0.278638
Thermal correction to Gibbs Free Energy= 0.222715
Sum of electronic and zero-point Energies= -693.236870
Sum of electronic and thermal Energies= -693.223260
Sum of electronic and thermal Enthalpies= -693.222316
Sum of electronic and thermal Free Energies= -693.278239

C	-2.28664600	-1.22714600	0.00735100
C	-0.88711500	-1.21041400	0.09280800
C	-0.18255600	-0.01152900	0.09007000
C	-0.84931100	1.21907500	0.00459200
C	-2.24902900	1.20245200	-0.07773800
C	-2.95342700	0.00346100	-0.07777400
C	-3.03793400	-2.50639000	0.00463400
C	-2.52360200	-3.63908500	-0.64307600
C	-3.22813900	-4.84066800	-0.64755500
C	-4.46318300	-4.93241700	-0.00518100
C	-4.98641200	-3.81286100	0.64227200
C	-4.27992200	-2.61236600	0.64759700
H	-0.34715300	-2.15101100	0.17850000
H	0.90426000	-0.02669800	0.13718000
H	-2.79124300	2.14439900	-0.12620500
H	-4.03795900	0.01722600	-0.16276000
H	-1.57451600	-3.56538400	-1.16983000
H	-2.81573300	-5.70503300	-1.16226500
H	-5.01396500	-5.86954700	-0.00912800
H	-5.94414800	-3.87642400	1.15301200
H	-4.67973800	-1.75044800	1.17764100
C	-0.09749300	2.49800100	-0.00087500
C	1.05899000	2.65563700	0.77685400
C	-0.52553200	3.57864700	-0.78579100
C	1.76630400	3.85563200	0.76941700
H	1.38866600	1.83608400	1.41195100
C	0.17972900	4.77980500	-0.79265600
H	-1.40497100	3.46299300	-1.41577000
C	1.32929300	4.92317400	-0.01527800
H	2.65623900	3.96009600	1.38525100
H	-0.16429200	5.60290000	-1.41419400
H	1.88063900	5.85996300	-0.02097700

Benzene

Zero-point correction= 0.101216 (Hartree/Particle)
Thermal correction to Energy= 0.105635

Thermal correction to Enthalpy= 0.106579
Thermal correction to Gibbs Free Energy= 0.073739
Sum of electronic and zero-point Energies= -231.849069
Sum of electronic and thermal Energies= -231.844650
Sum of electronic and thermal Enthalpies= -231.843706
Sum of electronic and thermal Free Energies= -231.876547

C	-0.36800500	0.38218900	0.00005600
C	1.02718600	0.38212400	0.00048000
C	1.72478900	1.59031500	-0.00003400
C	1.02725900	2.79866100	-0.00105000
C	-0.36784200	2.79872500	-0.00150700
C	-1.06548900	1.59045600	-0.00092500
H	-0.91168400	-0.55948800	0.00049000
H	1.57076400	-0.55961400	0.00127000
H	2.81215100	1.59033300	0.00031800
H	1.57105900	3.74026800	-0.00146800
H	-0.91153700	3.74039600	-0.00227900
H	-2.15285100	1.59057400	-0.00126000

References

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