Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Synthesis and Photophysical Properties of Helical Carbon Nanohoops with Twisted Acene Panels †

Rui Liu,[‡b] Hengxin Liu,[‡a] Can Shi,[‡a] Yunfei Wang,[a] Zhuping Chu,[a] Tianlu Wu,[a] Yaru Liu,[a] Wen-Mei Wei,[b] Ren-Hui Zheng,[d] Pingwu Du,*[c] and Dapeng Lu*[a]

[a] Inflammation and Immune Mediated Diseases Laboratory of Anhui Province, Anhui Institute of Innovative Drugs, School of Pharmacy, Anhui Medical University, 81 Meishan Road, Hefei, Anhui Province, 230032, P. R. China.

[b] School of Basic Medical Sciences, Anhui Medical University, 81 Meishan Road, Hefei, Anhui Province, 230032, P. R. China.

[c] Key Laboratory of Precision and Intelligent Chemistry, Anhui Laboratory of Advanced Photon Science and Technology, Department of Materials Science and Engineering, University of Science and Technology of China, 96 Jinzhai Road, Hefei, Anhui Province, 230026, P. R. China.

[d] Beijing National Laboratory for Molecular Sciences, State Key Laboratory for Structural Chemistry of Unstable and Stable Species, Institute of Chemistry, Chinese Academy of Sciences, Zhongguancun, Beijing 100190, P. R. China.

‡ These authors contributed equally to this work.

* Corresponding authors:

ludapeng@ahmu.edu.cn, ORCID: orcid.org/0000-0003-2283-894X
dupingwu@ustc.edu.cn, ORCID: orcid.org/0000-0002-2715-0979

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General Information

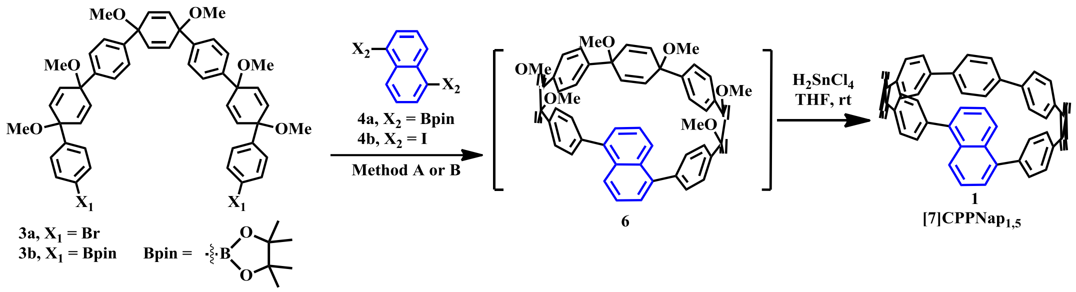
All glassware was oven-dried. Moisture and/or air sensitive reactions were carried out using standard Schlenk technique under nitrogen or argon atmosphere. Work-up and purification procedures were implemented with reagent-grade solvents under air. High resolution mass spectrometry (HR-MS) analysis were performed on an ESI-Orbitrap MS or MALDI-TOF MS. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker BioSpin (^{1}H 400 MHz, ^{13}C 100 MHz) NMR spectrometer. Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to residual peak of $CHCl_3$ (δ 7.26 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm). Coupling constants (*J*) are given in Hz. The apparent resonance multiplicity is described as s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). ^{1}H NMR data are reported in the following form: chemical shift, multiplicity, coupling constant, and integration. UV-vis absorbance and fluorescence spectra were recorded on a UV1800 spectrophotometer and an F-4700 spectrophotometer in standard quartz cuvettes, respectively. X-ray diffraction was formed on a Rigaku XtaLAB Synergy diffractometer.

Materials

All anhydrous solvents for syntheses were purchased from commercial suppliers (Energy Chemical or Innochem). The C-shaped synthon **3** (**3a,**[1] **3b**[2]), 1,5-bi-functionalized naphthalene **4** (**4a**,[3] **4b**[4]), 1,5-bi-functionalized anthracene **5** (**5a**,[5] **5b**[6]) were prepared according to previously reported procedures. Other reagents were obtained from commercial suppliers (Energy Chemical or Innochem) unless otherwise noted. Flash chromatography was performed on silica gel (300-400 mesh). Preparative thin-layer chromatography (PTLC) were performed on silica gel (GF 254) precoated plates.

Synthetic Procedures

Synthesis of [7]CPPNap$_{1,5}$ (1)

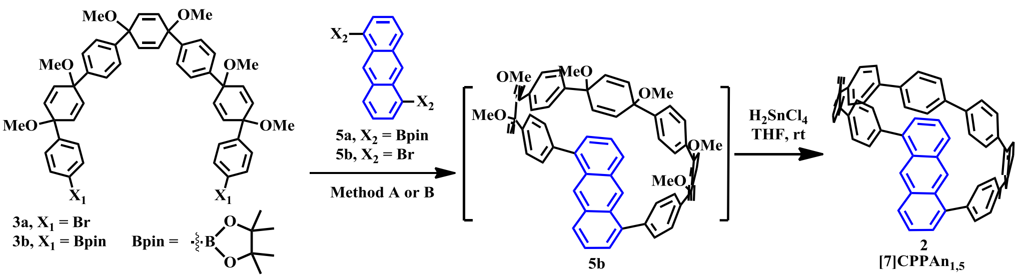


Method A: A suspension of compound **3b** (268 mg, 0.28 mmol, 1.1 equiv.), **4b** (95 mg, 0.25 mmol, 1.0 equiv.), and Cs_2CO_3 (407 mg, 1.25 mmol, 5.0 equiv.) in DMF/2-isopropanol (50 mL/5 mL) was degassed by argon for 1h at room temperature. Then, $Pd(OAc)_2$ (12 mg, 0.050 mmol, 0.2 equiv.) was added and the mixture was degassed for another 10 min. The reaction was heated up to 80 ℃ and stirred for 48 h under inert atmosphere. After cooling down to room temperature, the solvent was removed under reduced pressure. The residue was re-dissolved in CH_2Cl_2 (50 mL) and filtered through a short pad of silica gel with CH_2Cl_2 as the eluent. The filtrate was concentrated under reduced pressure to afford the crude product **6** as a gray solid, which was used for the next step without further purification.

Concentrated aqueous HCl (195 µL, 2.38 mmol) was added to a degassed solution of $SnCl_2 \cdot 2H_2O$ (268 mg, 1.19 mmol) in THF (40 mL) at room temperature, and the resulting solution was stirred at this temperature for 30 min under nitrogen atmosphere. The crude product **6** was then added to the solution, and the mixture was stirred at room temperature for 3 h. Then, the solvent was removed under reduced pressure, and the residue was re-dissolved in CH_2Cl_2 (100 mL). After washed by saturated aqueous NaCl solution, the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The solid residue was purified by silica gel column chromatography using petroleum ether/CH_2Cl_2 (*v/v*, 8:1) as the eluent to obtain [7]CPPNap$_{1,5}$ (**1**) as a yellow solid (17 mg, 10 % over two steps). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.04 (dd, J = 6.9, 2.2 Hz, 2H), 7.54 (d, J = 8.7 Hz, 4H), 7.50 (d, J = 8.7 Hz, 4H), 7.46 - 7.37 (m, 14H), 7.36 (s, 2H), 7.31 (s, 2H), 7.30 (d, J = 5.2 Hz, 2H), 7.27 (s, 3H), 7.25 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 139.77, 139.16, 139.09, 138.91, 137.93, 137.80, 137.58, 137.30, 132.03, 129.97, 128.23, 128.02, 127.55, 127.52, 127.17, 127.09, 124.91, 124.88. HR-MS (MALDI-TOF) *m/z* calcd for $C_{52}H_{34}$ $[M]^+$: 658.2661, found: 658.2737.

Method B: To a degassed solution of **3a** (158 mg, 0.18 mmol, 1.0 equiv.) and **4a** (75 mg, 0.20 mmol, 1.1 equiv.) in THF (240 mL) was added KOH in H_2O (121 mg in 10 mL, 2.16 mmol, 12.0 equiv.) and $Pd(PPh_3)_4$ (42 mg, 36 μmol, 0.2 equiv.) under argon in a 500 mL round-bottom flask. The reaction was refluxed at 80 ℃ for 48 h. The following procedures were carried out as stated in **Method A** until [7]CPPNap$_{1,5}$ (**1**) was finally obtained (8.6 mg, 7 % over two steps).

Synthesis of [7]CPPAn$_{1,5}$ (**2**)



Method A: The synthetic procedures for [7]CPPNap$_{1,5}$ (**1**) (**Method A**) was also applied for [7]CPPAn$_{1,5}$ (**2**), with **3b** (268 mg, 0.28 mmol, 1.1 equiv.), **5b** (84 mg, 0.25 mmol, 1.0 equiv.), Cs_2CO_3 (407 mg, 1.25 mmol, 5.0 equiv.), $Pd(OAc)_2$ (12 mg, 0.050 mmol, 0.2 equiv.) and DMF/2-isopropanol (50 mL/5 mL), respectively, for the cyclization reaction step, and concentrated aqueous HCl (195 μL, 2.38 mmol), $SnCl_2 \cdot 2H_2O$ (268 mg, 1.19 mmol) and THF (40 mL), respectively, for the aromatization reaction step. The product [7]CPPAn$_{1,5}$ (**2**) was finally obtained after column chromatography (petroleum ether/CH_2Cl_2, *v/v*, 8:1) as a yellow solid (9 mg, 5 % over two steps). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.70 (s, 2H), 7.67 (s, 2H), 7.57 - 7.49 (m, 12H), 7.48 - 7.41 (m, 10H), 7.37 (dd, J = 8.5, 5.3 Hz, 6H), 7.27 (d, J = 2.3 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 140.11, 139.27, 138.79, 138.03, 137.73, 137.70, 137.66, 137.27, 131.61, 129.06, 128.45, 128.15, 128.08, 127.48, 127.44, 127.09, 126.99, 126.92, 125.23, 124.71. HR-MS (MALDI-TOF) *m/z* calcd for $C_{56}H_{36}$ $[M]^+$: 708.2817, found: 708.3002.

Method B: The synthetic procedures for [7]CPPNap$_{1,5}$ (**1**) (**Method B**) was also applied for [7]CPPAn$_{1,5}$ (**2**) with **3a** (158 mg, 0.18 mmol, 1.0 equiv.), **5a** (85 mg, 0.20 mmol, 1.1 equiv.), KOH (121 mg, 2.16 mmol, 12.0 equiv.) and $Pd(PPh_3)_4$ (42 mg, 36 μmol, 0.2 equiv.) in THF/H_2O (240 mL/10 mL). [7]CPPAn$_{1,5}$ (**2**) was finally obtained with an isolated yield of 2 % over two steps (2.9 mg).

NMR Spectra

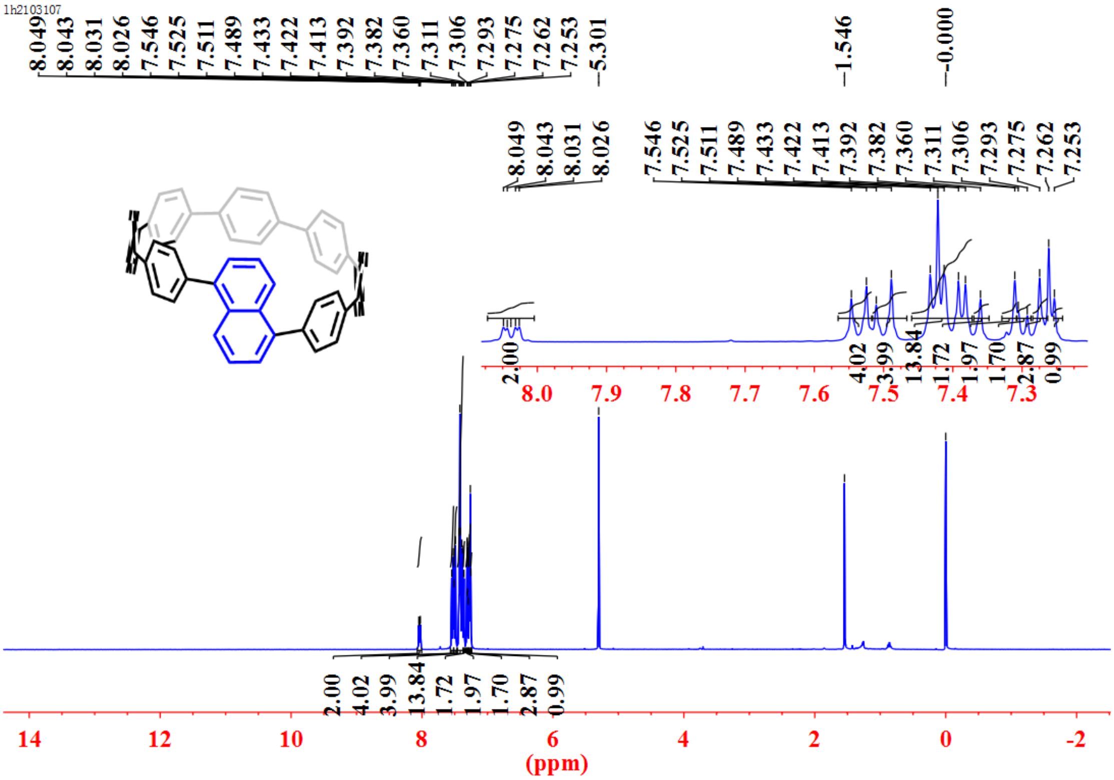


Fig. S1 ^{1}H NMR spectrum of [7]CPPNap$_{1,5}$ (**1**) (400 MHz, $CDCl_3$, 298 K).

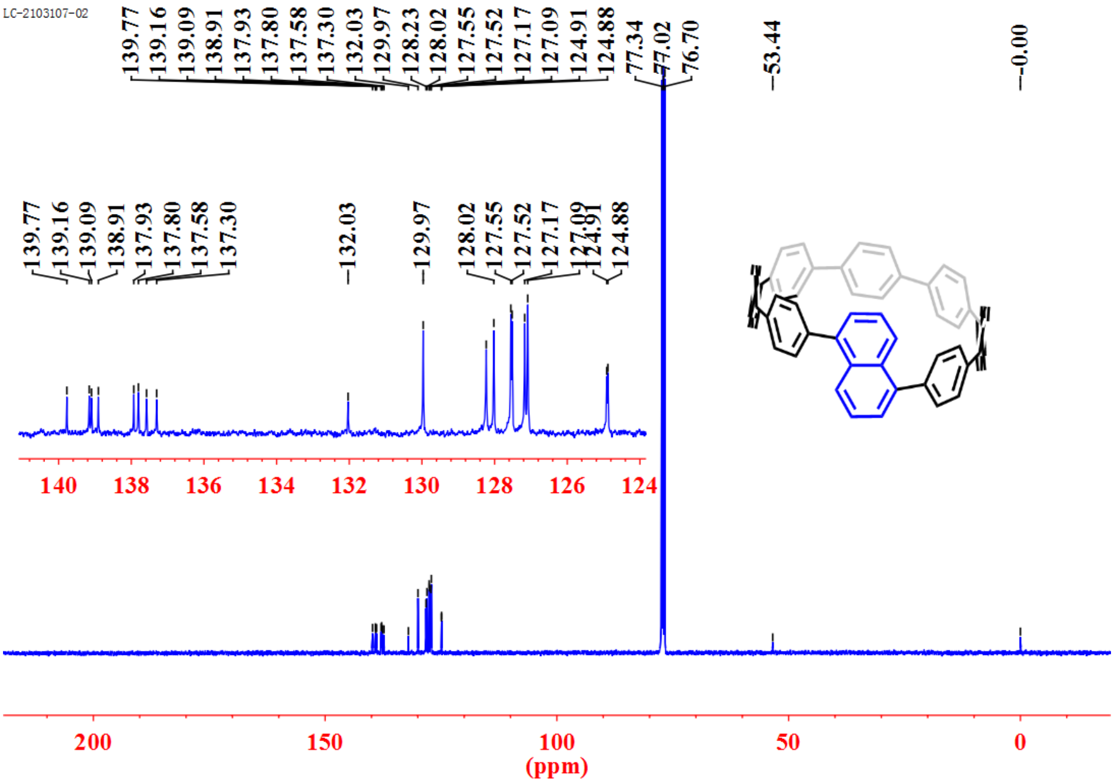


Fig. S2 ^{13}C NMR spectrum of [7]CPPNap$_{1,5}$ (**1**) (100 MHz, $CDCl_3$, 298 K).

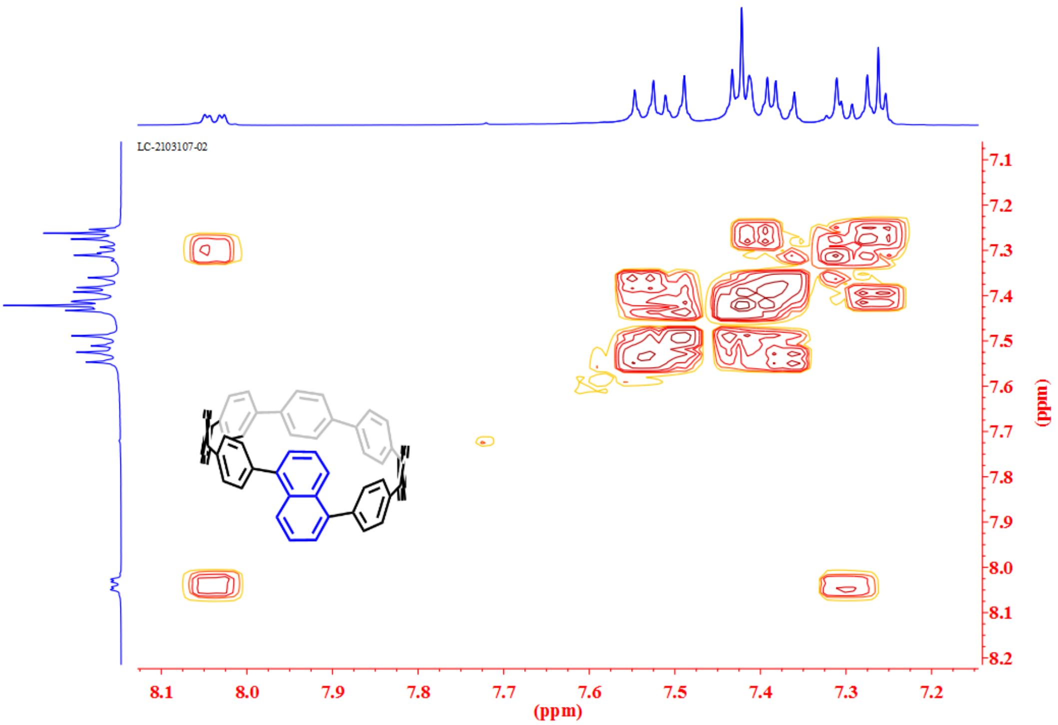


Fig. S3 The expanded 2D ^{1}H-^{1}H COSY NMR spectrum of [7]CPPNap$_{1,5}$ (**1**) (400 MHz, $CDCl_3$, 298 K).

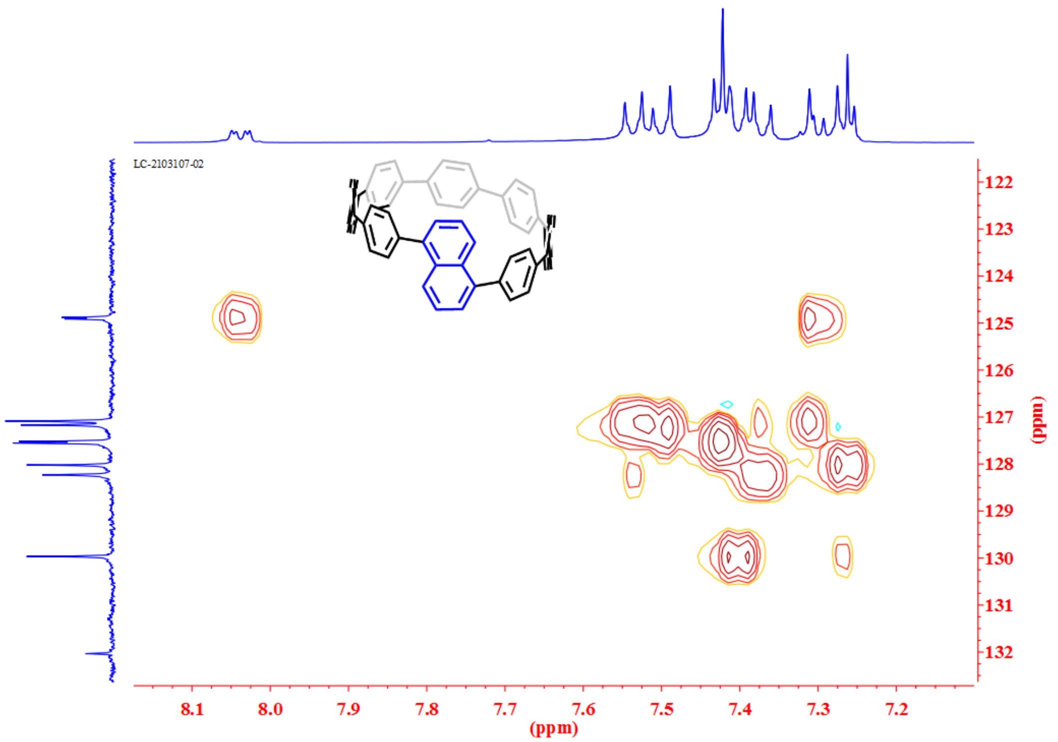


Fig. S4 The expanded 2D (H, C)-HSQC NMR spectrum of [7]CPPNap$_{1,5}$ (**1**) (400 MHz, $CDCl_3$, 298 K).

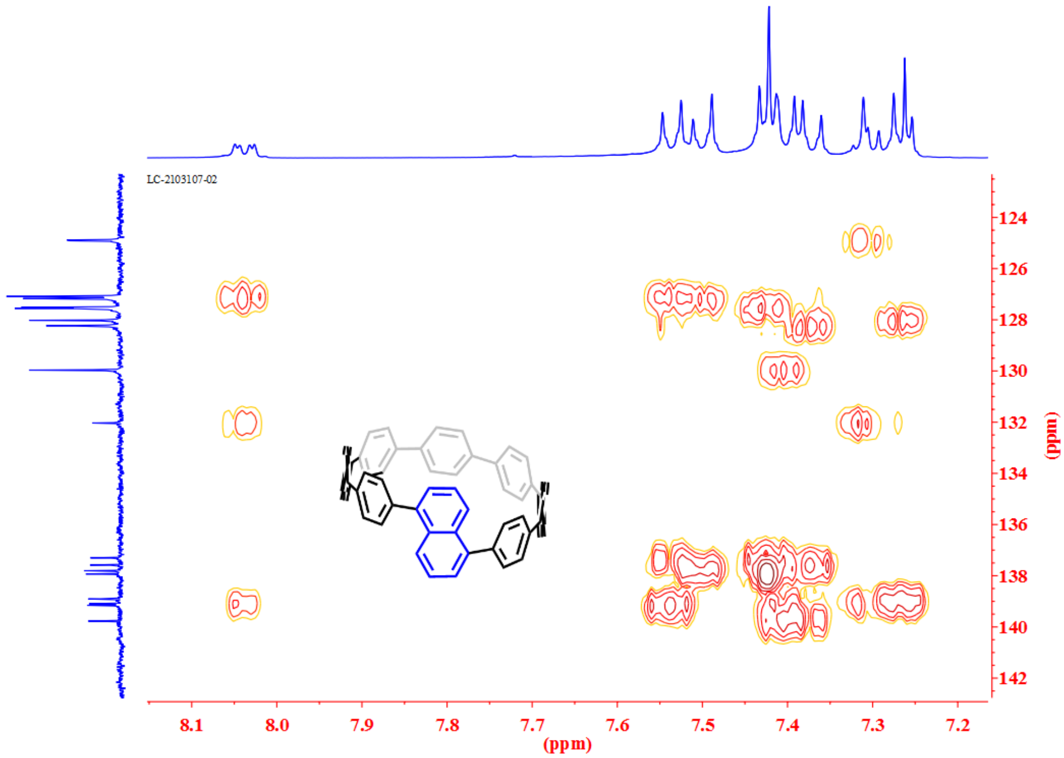


Fig. S5 The expanded 2D (H, C)-HMBC NMR spectrum of [7]CPPNap$_{1,5}$ (**1**) (400 MHz, $CDCl_3$, 298 K).

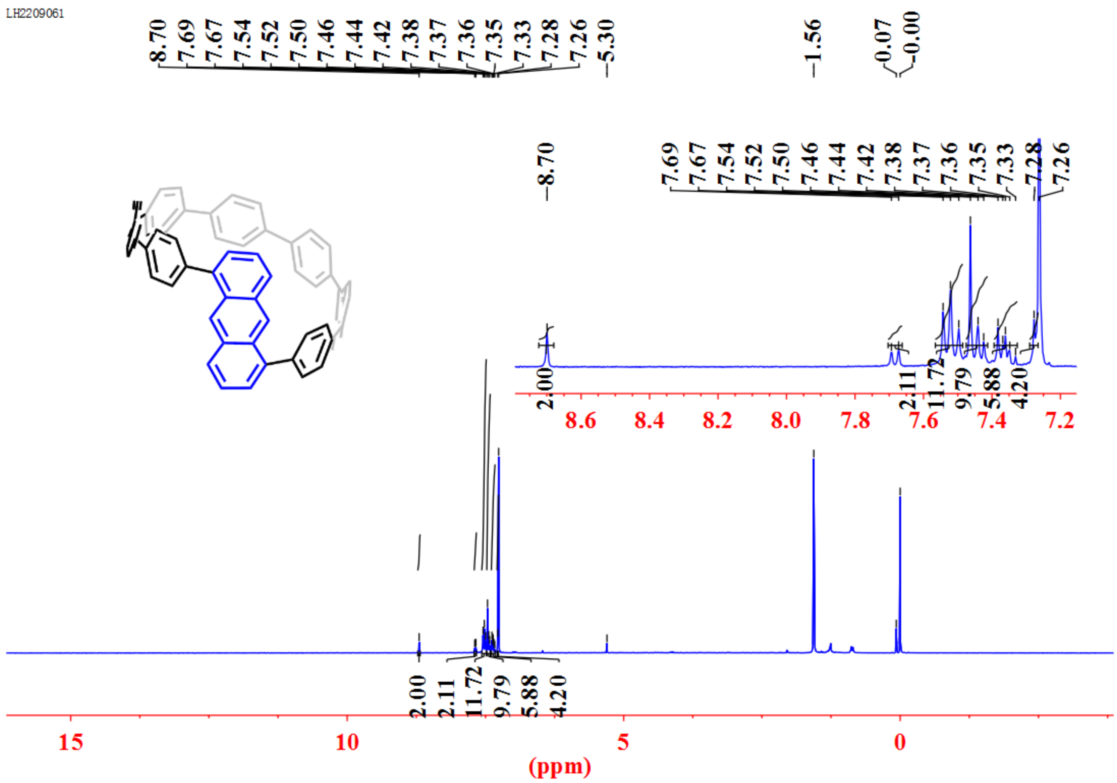


Fig. S6 ^{1}H NMR spectrum of [7]CPPAn$_{1,5}$ (**2**) (400 MHz, $CDCl_3$, 298 K).

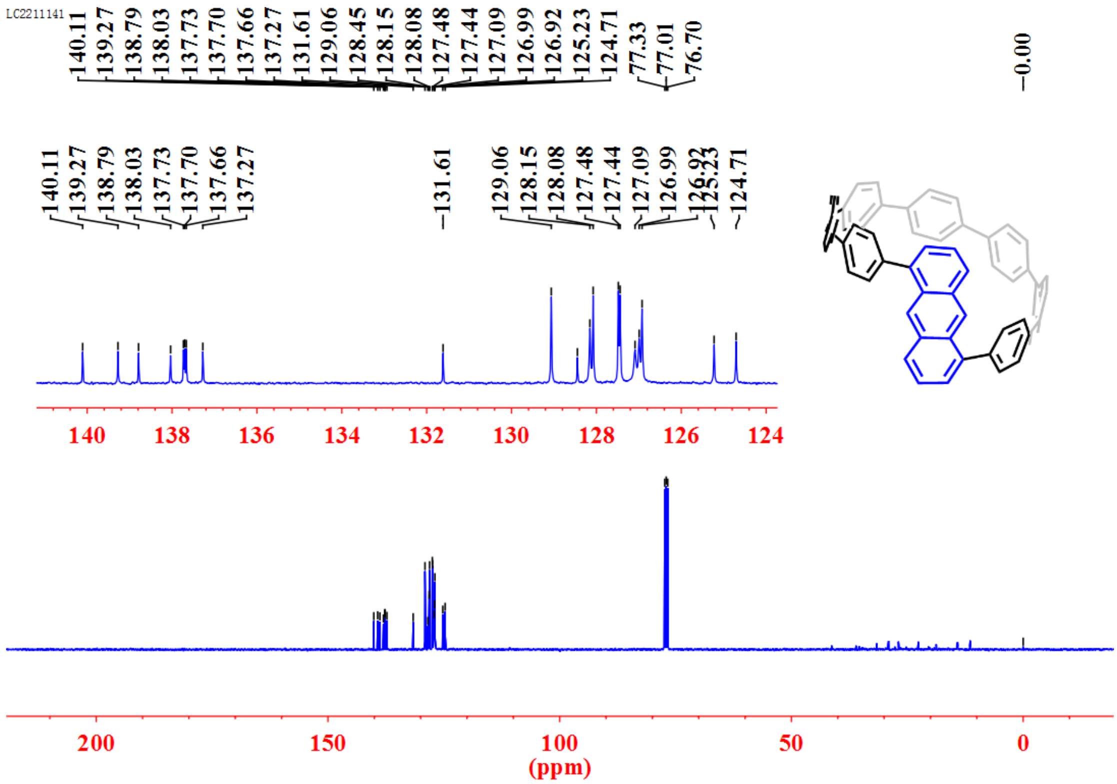


Fig. S7 ^{13}C NMR spectrum of [7]CPPAn$_{1,5}$ (**2**) (100 MHz, $CDCl_3$, 298 K).

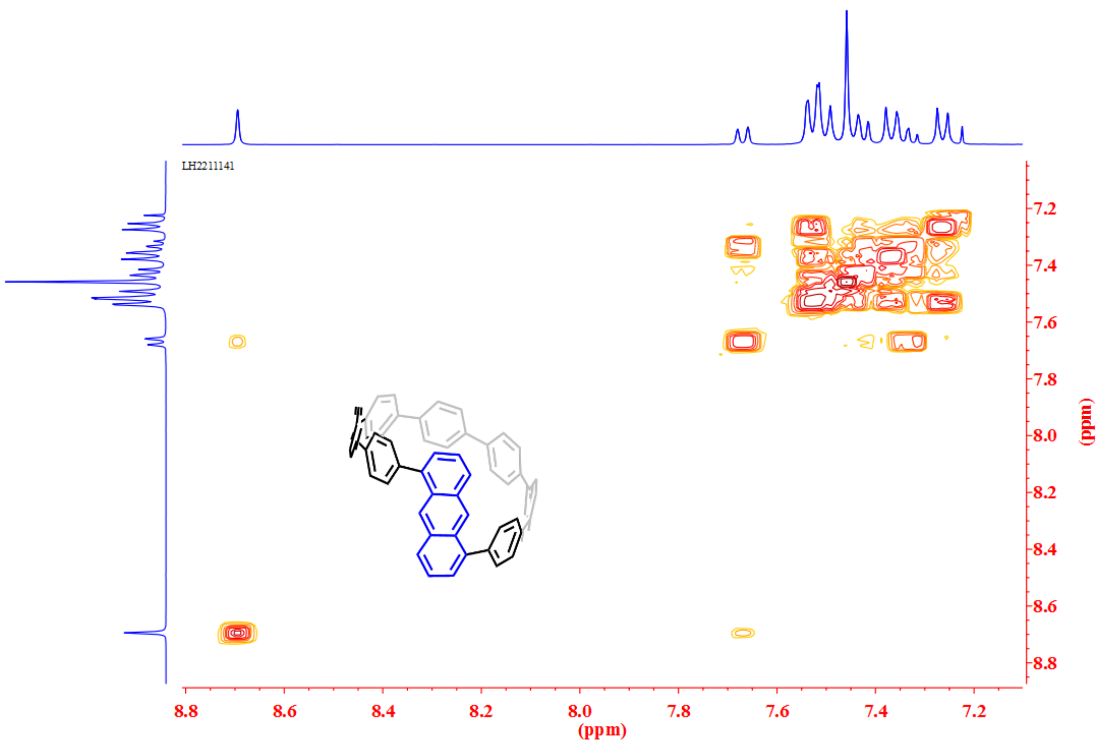


Fig. S8 The expanded 2D ^{1}H-^{1}H COSY NMR spectrum of [7]CPPAn$_{1,5}$ (**2**) (400 MHz, $CDCl_3$, 298 K).

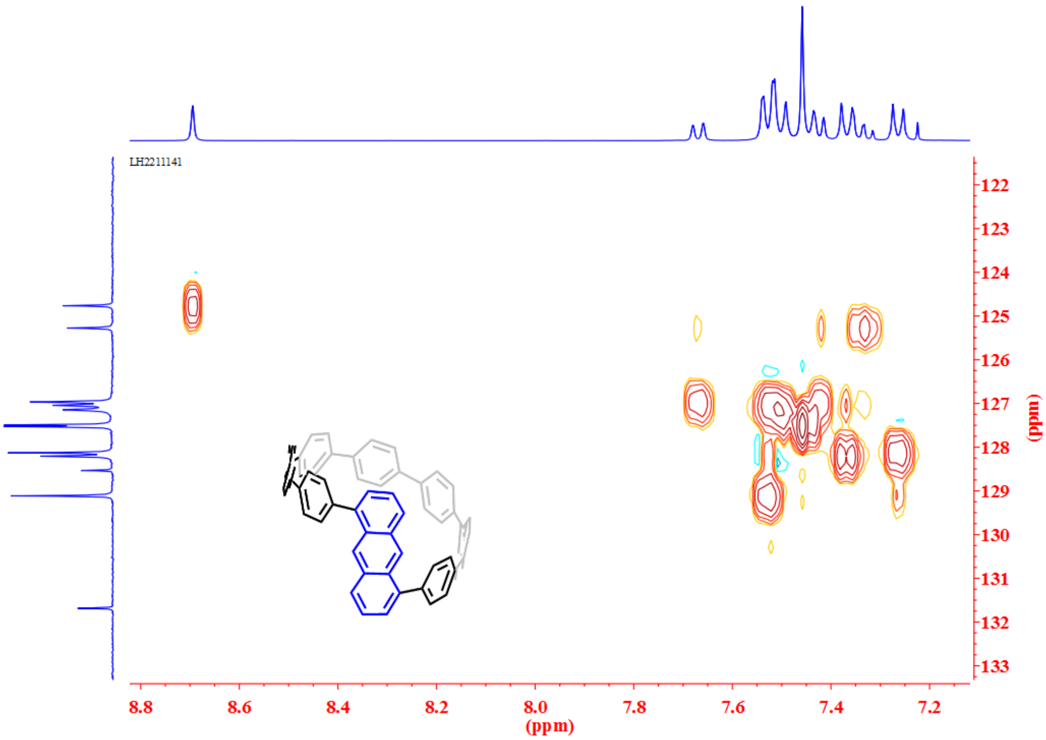


Fig. S9 The expanded 2D (H, C)-HSQC NMR spectrum of [7]CPPAn$_{1,5}$ (**2**) (400 MHz, $CDCl_3$, 298 K).

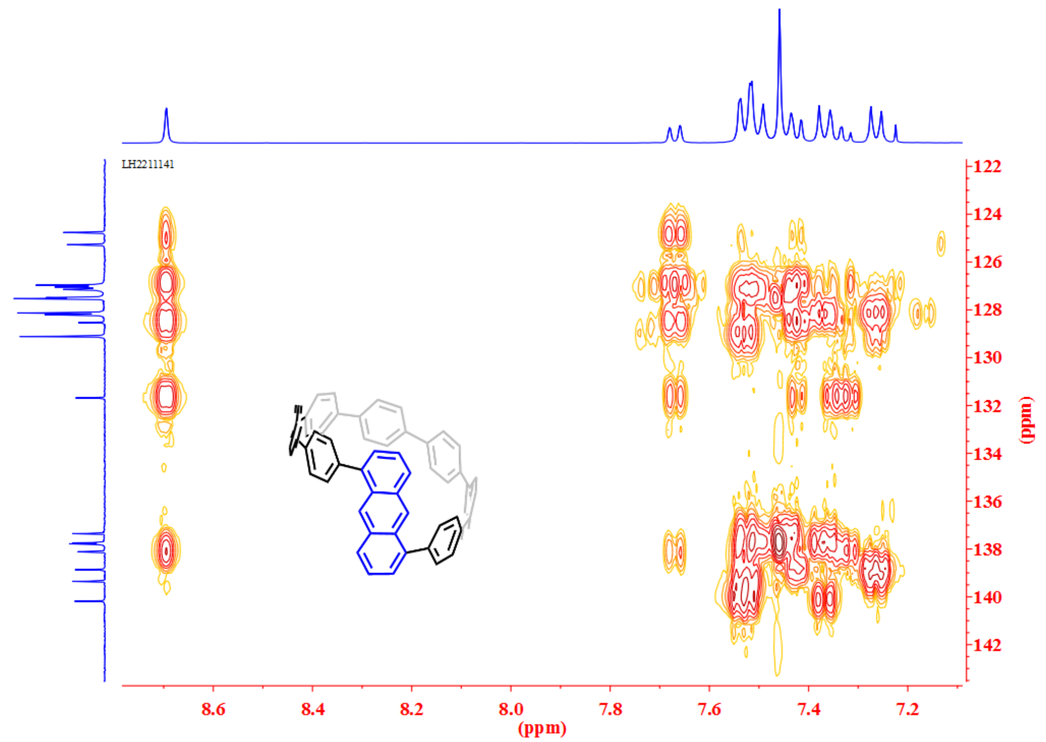


Fig. S10 The expanded 2D (H, C)-HMBC NMR spectrum of [7]CPPAn$_{1,5}$ (**2**) (400 MHz, $CDCl_3$, 298 K).

X-ray Single-Crystal Data of [7]CPPNap$_{1,5}$

Crystalline blocks of [7]CPPNap$_{1,5}$ (**1**) was obtained by slow diffusion of cyclohexane into a chloroform solution at room temperature. After a one-week period, yellow crystals suitable for X-ray diffraction were formed.

Preliminary data on the space group and unit cell dimensions as well as intensity data were collected on a Rigaku XtaLAB Synergy diffractometer under nitrogen gas flow at 120.00(10) K using Cu Kα radiation (λ = 1.54178 Å). Reflection intensities were corrected for absorption by the multi-scan method. The structure was solved by direct methods using intrinsic phasing implemented in SHELXT with the Olex2.[7, 8] The model was refined applying the full-matrix least-squares method using SHELXL.[9] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed at calculated positions and refined using a riding model. Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre (CCDC) as deposit NO. 2258729.

Table S1 Crystal data and structure refinements of [7]CPPNap$_{1,5}$.

CCDC	2258729
Empirical formula	$C_{58}H_{46}$
Formula weight	742.95
Temperature/K	120.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.8357(18)
b/Å	8.5815(6)
c/Å	18.3082(18)
α/°	90
β/°	111.006(13)
γ/°	90
Volume/Å^3	2029.3(4)
Z	2
ρ_{calc}g/cm^3	1.216
μ/mm^{-1}	0.517
F(000)	788.0
Crystal size/mm^3	0.12 × 0.12 × 0.08
Radiation	Cu Kα (λ = 1.54178)
2θ range for data collection/ °	6.944 to 133.192
Index ranges	$-13 \le h \le 16$, $-10 \le k \le 7$, $-21 \le l \le 21$

Reflections collected	6881
Independent reflections	3574 [R_{int} = 0.0438, R_{sigma} = 0.0549]
Data/restraints/parameters	3574/483/523
Goodness-of-fit on F^2	1.570
Final R indexes [I>=2σ (I)]	R_1 = 0.1476, wR_2 = 0.4000
Final R indexes [all data]	R_1 = 0.1902, wR_2 = 0.4510
Largest diff. peak/hole / e $Å^{-3}$	0.97/-0.50

Photophysical Properties

The fluorescence quantum yield, Φ_f, was calculated according to the following equation eq. S1[10] by using quinine sulfate (aqueous solution) as the standard:

$$\Phi_f = \Phi_{std} \left(\frac{I_{unk}}{A_{unk}}\right)\left(\frac{A_{std}}{I_{std}}\right)\left(\frac{\eta_{unk}}{\eta_{std}}\right)^2 \qquad \text{eq. S1}$$

where Φ_{std} is the fluorescence quantum yield of the standard; I_{unk} and I_{std} are the integrated emission intensities of the sample and the standard, respectively; A_{unk} and A_{std} are the absorbance of the sample and the standard, respectively, at the excitation wavelength λ_{ex}; and η_{unk} and η_{std} are the refraction indexes of the solvent used in the sample and the standard solutions, respectively.

Computational Details

The stationary points were obtained from the geometric optimizations at the CAM-B3LYP[11]/6-311G(d,p)[12] level. Vibrational frequency analyses were carried out to determine the nature of these structures. The single-point energies of all species were taken into account by using the same functional combined with the def2-TZVP[13] basis set. The optimized scale factors for calculating the vibrational harmonic and fundamental frequencies and the zero-point energies was 0.953.[14] The excitation energies and oscillator strengths of the nanohoops were calculated with time-dependent density functional theory (TD-DFT)[15, 16] at the PBE0/6-311G(d,p) level. Solvent effects of chloroform (ε = 4.7113) were implicitly taken into account in the process of computing the structures and properties by applying the polarizable continuum model (PCM)[17, 18] developed by Tomasi's group in the framework of the self-consistent reaction field (SCRF).[19, 20] All calculations were carried out with the Gaussian 16 program.[21] Strain energy visualization was achieved by using StrainViz.[22] The wave function analyses were carried out by means of the Multiwfn 3.8 code,[23] and visualizations of the isosurface maps were realized with VMD software.[24]

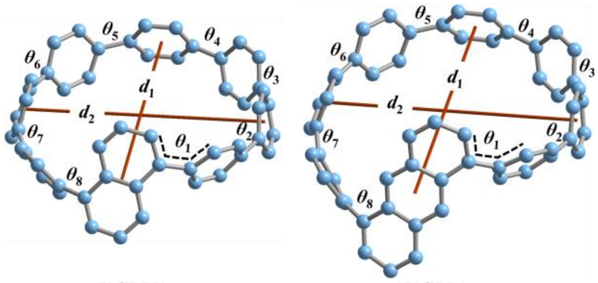


Fig. S11 The relaxed structures and calculated diameters of [7]CPPNap$_{1,5}$ and [7]CPPAn$_{1,5}$.

Table S2. Diameters (d, in Å) and dihedral angles (θ, in degrees) of [7]CPPNap$_{1,5}$ and [7]CPPAn$_{1,5}$.

		[7]CPPNap$_{1,5}$	[7]CPPAn$_{1,5}$
Diameters (d, in Å)	d_1	10.96	11.35
	d_2	11.01	11.22
	Average d	10.99	11.29
Dihedral angles (θ, in degree)	θ_1	36	32
	θ_2	-38	-43
	θ_3	27	24
	θ_4	-36	-38
	θ_5	31	29
	θ_6	-32	-34
	θ_7	42	41
	θ_8	-58	-59
	Average $\lvert \theta \rvert$	37.5	37.5

Table S3. The rate constant k_{298} and half-life at room temperature from theoretical data by kinetic analyses. $\Delta G^{\ddagger}$ were converted to k_{298} using the Eyring equation and calculated by TSTcalculator.[25] The very short half-life suggested the rapid racemization which made the isolation of pure enantiomers at ambient temperature unfeasible.[26]

	$\Delta G^{\ddagger}$ (kcal·mol^{-1})	**k_{298} (sec^{-1})**	**Half-life $t_{1/2}$ (hr)**
[7]CPPNap$_{1,5}$ (TS)	5.89	3.01×10^{8}	6.39×10^{-13}
[7]CPPNap$_{1,5}$ (TS')	10.04	2.78×10^{5}	6.93×10^{-10}
[7]CPPAn$_{1,5}$ (TS)	7.77	1.26×10^{7}	1.53×10^{-11}
[7]CPPAn$_{1,5}$ (TS')	15.70	1.99×10^{1}	9.68×10^{-6}

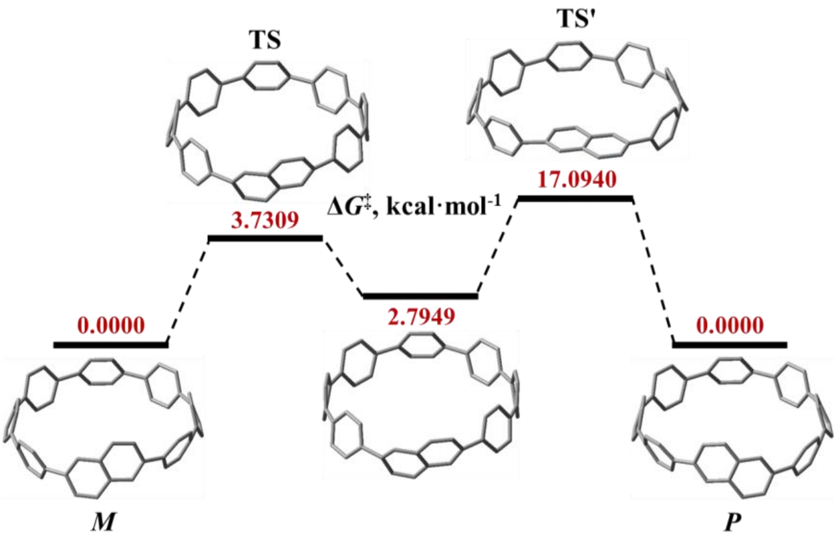
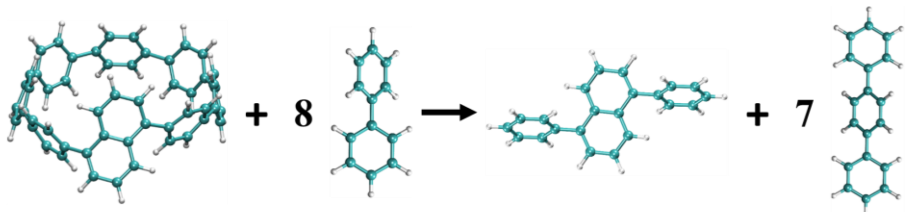
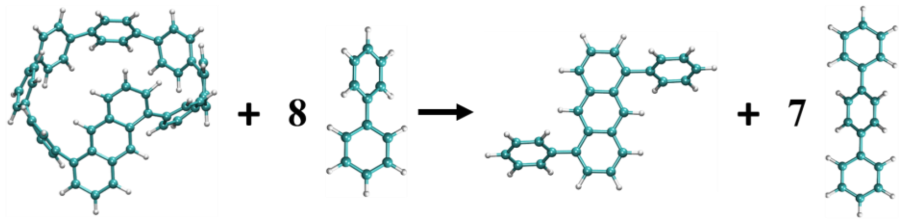


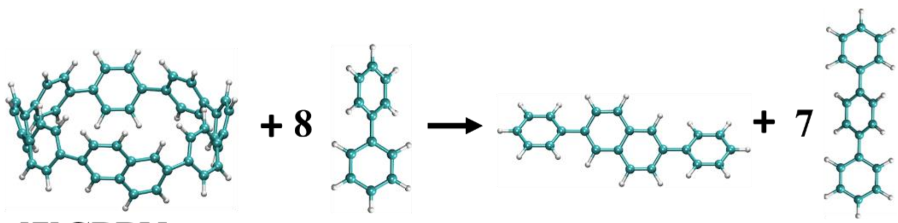
Fig. S12 The calculated racemization pathway and energy barriers of [7]CPPNap$_{2,6}$.



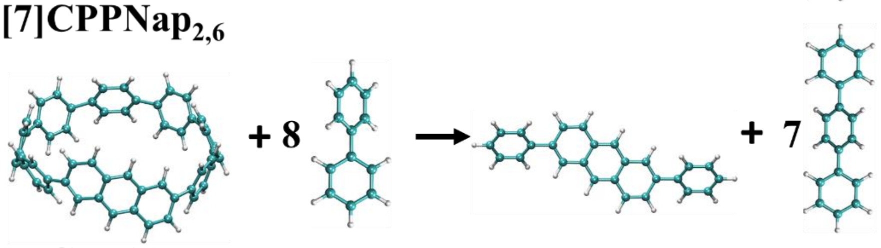
[7]CPPNap$_{1,5}$



[7]CPPAn$_{1,5}$



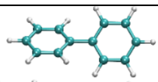
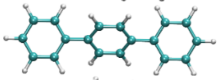
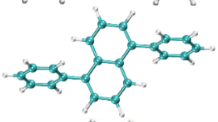
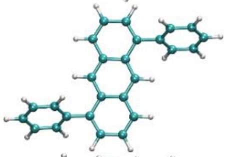
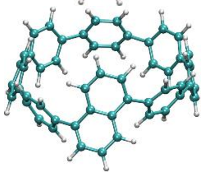
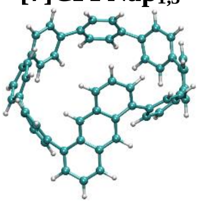
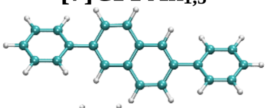
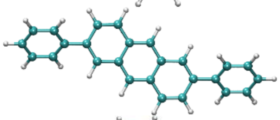
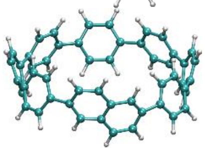
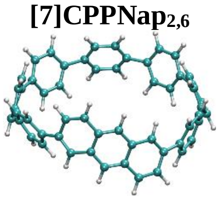
[7]CPPNap$_{2,6}$



[7]CPPAn$_{2,6}$

Fig. S13 The homodesmotic reactions for strain energy estimation.

Table S4. The calculated strain energies of [7]CPPNap$_{1,5}$, [7]CPPAn$_{1,5}$, [7]CPPNap$_{2,6}$, and [7]CPPAn$_{2,6}$ by homodesmotic reaction method.

Optimized Structure	**Total Energy (Hartree)**	**Strain Energy (ΔH, kcal mol^{-1})**
	-463.0163834	-
	-693.9390130	-
	-847.4909187	-
	-1001.0455463	-
 **[7]CPPNap$_{1,5}$**	-2000.8160616	**-73.343933559**
 **[7]CPPAn$_{1,5}$**	-2154.3763257	**-69.806973444**
	-847.4996402	-
	-1001.0537606	-
 **[7]CPPNap$_{2,6}$**	-2000.8318070	**-68.93636607**
 **[7]CPPAn$_{2,6}$**	-2154.3913551	**-65.530430043**

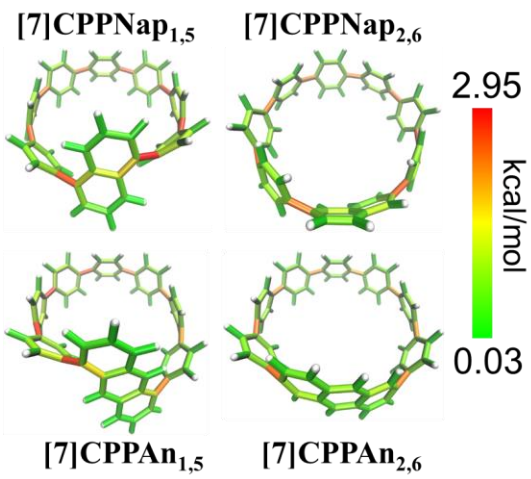


Fig. S14 Visualization of the total strain of [7]CPPNap$_{1,5}$, [7]CPPAn$_{1,5}$, [7]CPPNap$_{2,6}$, and [7]CPPAn$_{2,6}$ by StrainViz.

Table S5. Strain energy determined by StrainViz.

Strain Type (kcal/mol)	[7]CPPNap$_{1,5}$	[7]CPPAn$_{1,5}$	[7]CPPNap$_{2,6}$	[7]CPPAn$_{2,6}$
Total	**74**	**71**	**70**	**67**
Bond	2	2	2	3
Angle	6	6	4	6
Dihedral	65	63	64	58

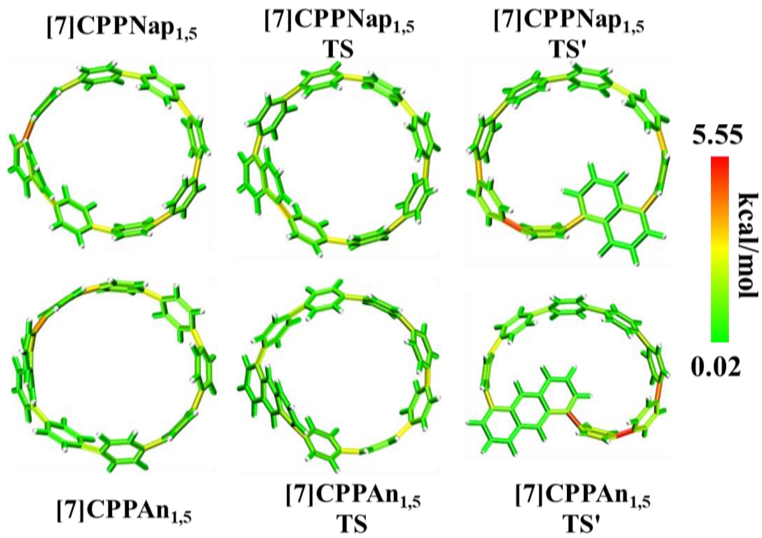


Fig. S15 Visualization of the total strain of [7]CPPNap$_{1,5}$, [7]CPPAn$_{1,5}$, and their two transitional states by StrainViz.

Table S6. The strain energy of [7]CPPNap$_{1,5}$, [7]CPPAn$_{1,5}$, and their two transitional states determined by StrainViz.

Strain Type (kcal/mol)	[7]CPPNap$_{1,5}$	[7]CPPNap$_{1,5}$ (TS)	[7]CPPNap$_{1,5}$ (TS')	[7]CPPAn$_{1,5}$	[7]CPPAn$_{1,5}$ (TS)	[7]CPPAn$_{1,5}$ (TS')
Total	**74**	**80**	**83**	**71**	**79**	**85**
Bond	2	3	6	2	6	4
Angle	6	7	8	6	9	13
Dihedral	65	69	69	63	64	67

Table S7. Electronic transitions for [7]CPPNap$_{1,5}$ determined by TD-DFT methods at PBE0/6-311G(d,p) level.

Excited State	Energy (eV)	Excitation (nm)	Oscillator Strength (f_{os})	Transition Type
$S_0 \rightarrow S_1$	3.2744	378.65	0.1024	HOMO→LUMO (0.781)
				HOMO-1→LUMO+1 (0.187)
$S_0 \rightarrow S_2$	3.5566	348.6	1.0573	HOMO→LUMO+1 (0.527)
				HOMO-1→LUMO (0.413)
$S_0 \rightarrow S_3$	3.659	338.85	0.5454	HOMO-1→LUMO+1 (0.436)
				HOMO-1→LUMO (0.267)
				HOMO→LUMO (0.127)
				HOMO→LUMO+1 (0.115)
$S_0 \rightarrow S_4$	3.675	337.37	0.2613	HOMO→LUMO+1 (0.32)
				HOMO-1→LUMO+1 (0.308)
				HOMO-1→LUMO (0.278)
				HOMO→LUMO (0.05)
$S_0 \rightarrow S_5$	4.0978	302.56	0.3666	HOMO→LUMO+2 (0.821)
				HOMO-2→LUMO (0.091)
$S_0 \rightarrow S_6$	4.1261	300.49	0.0997	HOMO-2→LUMO (0.669)
				HOMO→LUMO+2 (0.073)
				HOMO→LUMO+3 (0.069)
				HOMO-1→LUMO+3 (0.068)
$S_0 \rightarrow S_7$	4.17	297.32	0.0391	HOMO-1→LUMO+2 (0.256)
				HOMO→LUMO+3 (0.24)
				HOMO-2→LUMO+1 (0.198)
				HOMO-2→LUMO (0.102)
$S_0 \rightarrow S_8$	4.2186	293.9	0.0381	HOMO-1→LUMO+2 (0.429)
				HOMO-3→LUMO (0.15)
				HOMO→LUMO+3 (0.118)
$S_0 \rightarrow S_9$	4.2356	292.72	0.1614	HOMO-2→LUMO+1 (0.426)
				HOMO-4→LUMO+1 (0.081)
				HOMO-1→LUMO+3 (0.071)
				HOMO-1→LUMO+2 (0.068)
				HOMO→LUMO+3 (0.059)
$S_0 \rightarrow S_{10}$	4.3189	287.07	0.2082	HOMO→LUMO+3 (0.42)
				HOMO-2→LUMO+1 (0.241)
				HOMO→LUMO+4 (0.072)
$S_0 \rightarrow S_{11}$	4.3354	285.98	0.1167	HOMO-3→LUMO (0.622)
				HOMO-1→LUMO+2 (0.164)
$S_0 \rightarrow S_{12}$	4.3747	283.41	0.1131	HOMO→LUMO+4 (0.282)
				HOMO-1→LUMO+3 (0.261)
				HOMO-3→LUMO+1 (0.119)
				HOMO-1→LUMO+5 (0.079)

$S_0 \rightarrow S_{13}$	4.4068	281.35	0.106	HOMO-3→LUMO+1 (0.238) HOMO→LUMO+4 (0.144) HOMO-1→LUMO+3 (0.102) HOMO→LUMO+5 (0.097) HOMO-1→LUMO+4 (0.065)

Table S8. Electronic transitions for [7]CPPAn$_{1,5}$ determined by TD-DFT methods at PBE0/6-311G(d,p) level.

Excited State	Energy (eV)	Excitation (nm)	Oscillator Strength (f_{os})	Transition Type
$S_0 \rightarrow S_1$	2.8985	427.75	0.1643	HOMO→LUMO (0.958)
$S_0 \rightarrow S_2$	3.3397	371.24	0.3802	HOMO-1→LUMO (0.494) HOMO→LUMO+1 (0.311) HOMO-1→LUMO+1 (0.132)
$S_0 \rightarrow S_3$	3.4663	357.68	0.0543	HOMO→LUMO+1 (0.469) HOMO-1→LUMO (0.444)
$S_0 \rightarrow S_4$	3.5385	350.39	0.4661	HOMO-2→LUMO (0.878)
$S_0 \rightarrow S_5$	3.6185	342.64	0.32	HOMO→LUMO+2 (0.807)
$S_0 \rightarrow S_6$	3.6728	337.57	0.3276	HOMO-1→LUMO+1 (0.755) HOMO→LUMO+1 (0.148)
$S_0 \rightarrow S_7$	3.8316	323.58	0.1327	HOMO-5→LUMO (0.385) HOMO→LUMO+5 (0.254) HOMO→LUMO+4 (0.151)
$S_0 \rightarrow S_8$	3.9871	310.96	0.5886	HOMO-1→LUMO+2 (0.645) HOMO-2→LUMO+1 (0.237)
$S_0 \rightarrow S_9$	4.0015	309.84	0.0419	HOMO-2→LUMO+1 (0.663) HOMO-1→LUMO+2 (0.258)
$S_0 \rightarrow S_{10}$	4.1204	300.9	0.2817	HOMO-3→LUMO (0.562) HOMO-2→LUMO+2 (0.272)
$S_0 \rightarrow S_{11}$	4.162	297.9	0.0833	HOMO→LUMO+3 (0.432) HOMO-4→LUMO (0.188) HOMO-2→LUMO+2 (0.141) HOMO-3→LUMO (0.134)
$S_0 \rightarrow S_{12}$	4.24223	292.26	0.0186	HOMO-4→LUMO (0.615) HOMO→LUMO+3 (0.081) HOMO-3→LUMO (0.072) HOMO→LUMO+4 (0.053)
$S_0 \rightarrow S_{13}$	4.2831	289.47	0.0254	HOMO→LUMO+3 (0.263) HOMO-2→LUMO+2 (0.223) HOMO→LUMO+4 (0.141) HOMO→LUMO+5 (0.121) HOMO-3→LUMO (0.097)

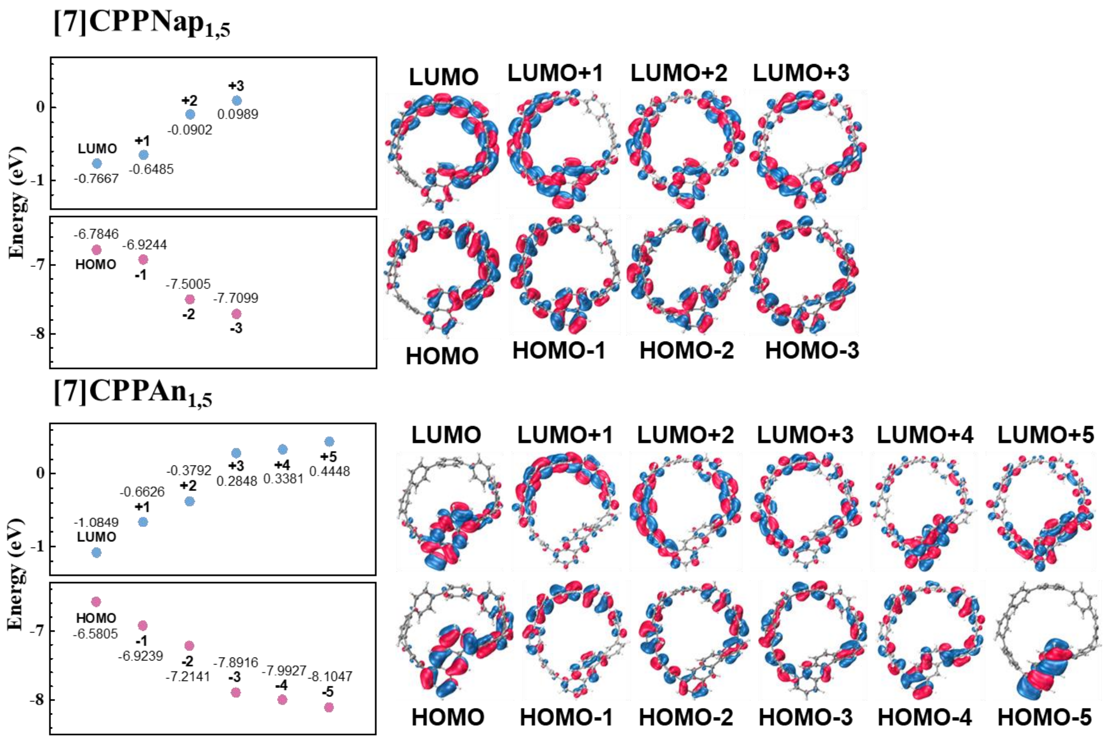


Fig. S16 Left: the calculated frontier molecular orbital profiles and the energy of [7]CPPNap$_{1,5}$ and [7]CPPAn$_{1,5}$ at the CAM-B3LYP/6-311G(d,p) level. The blue and red dots represent the unoccupied and occupied states, respectively. Right: the calculated isosurfaces for different molecular orbitals of [7]CPPNap$_{1,5}$ and [7]CPPAn$_{1,5}$.

Table S9. Hole-electron distributions of the crucial excited states for [7]CPPNap$_{1,5}$ and [7]CPPAn$_{1,5}$. Blue and red regions represent the distributions the holes and the electrons, respectively.

[7]CPPNap$_{1,5}$	**S_2**	**S_3**	**S_4**	**S_5**	**S_{10}**
					
***f*os** → $\boldsymbol{f_{os}}$	1.0573	0.5454	0.2613	0.3666	0.2082
S_r (a.u.)	0.8499	0.65996	0.66409	0.81427	0.86754
D index(Å)	0.528	4.283	4.572	1.825	1.735
Δσ(Å)	0.003	0.65	-0.66	0.267	0.071
t index(Å)	-3.441	0.632	0.919	-2.073	-2.408

[7]CPPAn$_{1,5}$	**S_2**	**S_4**	**S_5**	**S_6**	**S_8**	**S_{10}**
						
f	0.3802	0.4661	0.32	0.3276	0.5886	0.2817
S_r (a.u.)	0.83897	0.69744	0.74898	0.80863	0.85566	0.81379
D index(Å)	1.215	2.746	2.437	2.179	0.874	2.37
Δσ(Å)	0.157	-1.33	1.017	-0.108	0.082	-0.693
t index(Å)	-3.204	-0.649	-1.028	-2.197	-3.245	-1.579

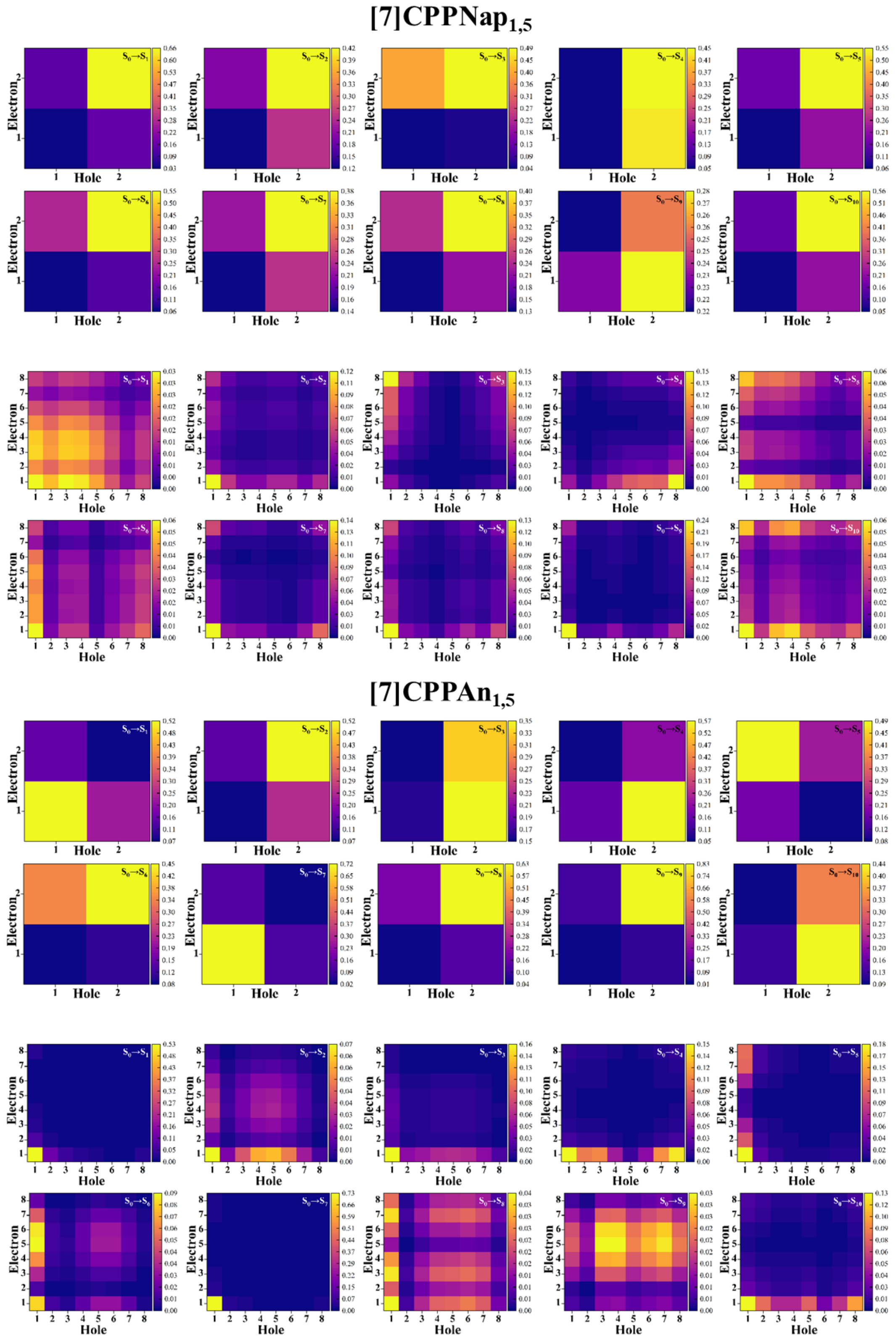


Fig. S17 IFCT heat maps based on fragments for the crucial excited states of [7]CPPNap$_{1,5}$ and [7]CPPAn$_{1,5}$, where X-axis represents the hole position, Y-axis represents the electron position, and the axis values represent the fragment numbers.

Table S10. Cartesian coordinates of the optimized species.

(*M*)-[7]CPPNap$_{1,5}$							
C	-0.814571	-5.318011	-0.097026	C	-4.108384	-1.055905	2.622442
C	1.371699	-5.596432	-1.348095	C	-4.044666	-2.806519	0.947511
C	0.656962	-5.519235	-0.149116	C	-4.857696	-1.985864	0.094883
C	2.714299	-4.873649	0.948799	C	-5.441536	-2.481120	-1.098268
C	1.388909	-5.266853	1.012525	C	-2.560710	-3.787420	-0.782591
C	2.702194	-5.213222	-1.409476	C	-3.221387	-3.940232	0.438918
C	4.504424	-3.772424	-0.368940	C	-1.592429	-5.640527	1.018979
C	3.365043	-4.724550	-0.277795	C	-2.777230	-4.968425	1.277927
C	5.307981	-3.450400	0.730709	C	-1.382974	-4.464804	-1.044587
C	5.225895	-1.701935	-1.397322	H	0.860130	-5.870998	-2.263369
C	4.574517	-2.920252	-1.473097	H	3.192979	-4.532898	1.857877
C	5.829571	-1.280128	-0.211357	H	0.878712	-5.220892	1.966718
C	5.952925	-2.226079	0.810861	H	3.198908	-5.206042	-2.372316
C	6.228907	1.088544	-1.015174	H	5.358930	-4.123067	1.578561
C	5.967894	0.181796	0.016807	H	5.126626	-1.009170	-2.223600
C	5.079859	2.025098	1.310294	H	3.987832	-3.133940	-2.357168
C	5.490686	0.706417	1.219405	H	6.485899	-1.971092	1.719545
C	5.822880	2.410206	-0.921670	H	6.675759	0.739628	-1.938912
C	4.199569	4.029998	0.147875	H	4.573835	2.347455	2.211541
C	5.133801	2.874906	0.203913	H	5.292402	0.042585	2.051708
C	3.740618	4.692354	1.291269	H	5.966472	3.063640	-1.774090
C	2.297819	4.938358	-1.043573	H	4.291944	4.609768	2.220540
C	3.504057	4.261540	-1.040421	H	1.724120	4.965082	-1.961185
C	1.732219	5.413978	0.141201	H	3.829469	3.783446	-1.955517
C	2.530981	5.369947	1.288336	H	2.168708	5.799063	2.215201
C	-0.478663	5.973102	-0.947156	H	0.018426	6.439486	-1.789503
C	0.259718	5.613876	0.185409	H	-2.275993	4.276319	1.992127
C	-1.795023	4.793195	1.170482	H	0.073805	4.846580	2.185187
C	-0.453373	5.120287	1.279825	H	-2.336760	5.842026	-1.989870
C	-1.817953	5.637520	-1.060416	H	-4.731491	4.386610	1.531798
C	-3.649449	4.071247	-0.300900	H	-4.222137	1.486073	-2.410035
C	-2.472282	4.940798	-0.040411	H	-2.890645	3.510154	-2.230587
C	-4.621561	3.761732	0.652842	H	-6.107194	2.381103	1.323002
C	-4.372092	2.138607	-1.558911	H	-4.823187	0.839972	2.025352
C	-3.616815	3.291336	-1.457755	H	-6.609600	-2.039734	-2.821381
C	-5.204289	1.719476	-0.517786	H	-6.558868	0.404730	-2.440656
C	-5.394566	2.611533	0.540527	H	-3.120646	-2.946713	2.859106
C	-4.668582	-0.186170	1.733443	H	-3.848696	-0.722579	3.619935
C	-5.056698	-0.619588	0.440191	H	-5.352929	-3.535438	-1.328394
C	-5.588425	0.274679	-0.555750	H	-2.882215	-3.021173	-1.475635
C	-6.129669	-1.647629	-1.932893	H	-1.225727	-6.360029	1.742080

C	-6.146861	-0.259040	-1.689482	H	-3.310350	-5.177051	2.198165
C	-3.746616	-2.348961	2.209138	H	-0.822055	-4.203825	-1.933479

(*P*)-[7]CPPNap$_{1,5}$

C	3.647462	4.073659	-0.301446	C	6.130622	-1.643993	-1.931986
C	1.815001	5.638728	-1.061295	C	5.588149	0.277607	-0.554067
C	2.469823	4.942604	-0.041172	C	5.056625	-0.617463	0.441464
C	0.450903	5.121375	1.279161	C	4.668075	-0.185380	1.735018
C	1.792700	4.794909	1.169777	C	4.370799	2.140469	-1.558221
C	0.475547	5.973611	-0.948024	C	5.203157	1.722238	-0.516819
C	-1.735014	5.413665	0.140704	C	4.619832	3.765243	0.652342
C	-0.262579	5.614256	0.184680	C	5.393321	2.615245	0.540702
C	-2.533556	5.369340	1.288005	C	3.615183	3.293029	-1.457836
C	-3.506562	4.260214	-1.040421	H	2.333596	5.843340	-1.990849
C	-2.300690	4.937718	-1.043894	H	-0.075989	4.847723	2.184705
C	-4.201627	4.028290	0.148035	H	2.273955	4.278497	1.991544
C	-3.742767	4.691034	1.291266	H	-0.021821	6.439554	-1.790449
C	-5.824215	2.407483	-0.920929	H	-2.171362	5.798770	2.214757
C	-5.135151	2.872680	0.204474	H	-3.831909	3.781978	-1.955470
C	-5.490634	0.704074	1.220199	H	-1.727320	4.964775	-1.961698
C	-5.080604	2.023020	1.310932	H	-4.293834	4.608261	2.220673
C	-6.229534	1.085618	-1.014235	H	-5.968370	3.060712	-1.773411
C	-5.828665	-1.282739	-0.210539	H	-5.291847	0.040462	2.052563
C	-5.967735	0.179069	0.017727	H	-4.574647	2.345716	2.212111
C	-5.951281	-2.228849	0.811634	H	-6.676385	0.736414	-1.937861
C	-4.573332	-2.922223	-1.472834	H	-6.484196	-1.974274	1.720473
C	-5.225232	-1.704213	-1.396750	H	-3.987076	-3.135687	-2.357245
C	-4.502334	-3.774362	-0.368710	H	-5.126736	-1.011457	-2.223142
C	-5.305789	-3.452849	0.731175	H	-5.356350	-4.125684	1.578911
C	-2.699654	-5.213918	-1.410138	H	-3.196469	-5.206395	-2.372922
C	-3.362568	-4.726106	-0.278093	H	-0.875906	-5.223234	1.965860
C	-1.386092	-5.268684	1.011636	H	-3.190284	-4.535937	1.857738
C	-2.711618	-4.875806	0.948317	H	-0.857531	-5.870410	-2.264717
C	-1.369035	-5.596629	-1.349175	H	1.229098	-6.360786	1.740425
C	0.817330	-5.318235	-0.098302	H	2.883996	-3.020122	-1.476258
C	-0.654135	-5.519959	-0.150226	H	0.824549	-4.203745	-1.934564
C	1.595427	-5.640840	1.017575	H	3.313140	-5.177019	2.196863
C	2.562863	-3.786716	-0.783406	H	5.354645	-3.532439	-1.328556
C	1.385460	-4.464677	-1.045657	H	3.848321	-0.723599	3.621040
C	3.223543	-3.939565	0.438044	H	3.121883	-2.947802	2.858763
C	2.779929	-4.968370	1.276678	H	6.558619	0.408760	-2.438807
C	5.442714	-2.478174	-1.097934	H	6.610770	-2.035405	-2.820666
C	4.858468	-1.983762	0.095360	H	4.822053	0.840471	2.028008
C	4.045902	-2.805520	0.947304	H	4.221374	1.487526	-2.409133

C	4.108223	-1.056094	2.623325	H	4.729973	4.390962	1.530680
C	3.747370	-2.349078	2.209212	H	6.106585	2.386136	1.322904
C	6.147038	-0.255527	-1.687860	H	2.889108	3.511268	-2.230932

[7]CPPNap$_{1,5}$ (TS)

C	-3.279051	4.289514	-0.207836	C	-6.272307	-0.952759	-2.026881
C	-1.397759	5.543115	0.943182	C	-5.739154	0.773571	-0.389484
C	-1.961565	4.978398	-0.206508	C	-5.416853	-0.285997	0.542550
C	0.239226	5.059221	-1.219253	C	-5.336530	-0.125030	1.950233
C	-1.121050	4.832757	-1.312893	C	-4.763000	2.756203	0.957690
C	-0.031857	5.761897	1.040996	C	-5.193201	2.164996	-0.236041
C	2.276461	5.158732	0.171810	C	-3.889243	3.874567	-1.394625
C	0.828549	5.435145	-0.011247	C	-4.797579	2.834036	-1.406225
C	3.191813	5.225167	-0.883878	C	-3.820467	3.774351	0.969325
C	3.860775	3.766826	1.357539	H	-2.019054	5.750083	1.806050
C	2.690096	4.505482	1.333561	H	0.865968	4.805966	-2.064998
C	4.665354	3.652649	0.221945	H	-1.503462	4.411543	-2.232714
C	4.364278	4.487481	-0.859101	H	0.375746	6.125493	1.977150
C	6.108310	1.809570	1.191011	H	2.946106	5.792456	-1.773995
C	5.529923	2.450930	0.090688	H	4.067127	3.152063	2.224622
C	5.789336	0.388909	-1.150657	H	2.020637	4.446015	2.182798
C	5.490227	1.739571	-1.110043	H	5.008273	4.494644	-1.730727
C	6.409723	0.457721	1.149725	H	6.240243	2.349019	2.121696
C	5.853246	-1.762278	0.069735	H	5.592058	-0.156920	-2.064691
C	6.141276	-0.305506	0.008084	H	5.070725	2.202608	-1.994287
C	5.876255	-2.594035	-1.054847	H	6.769873	-0.026900	2.049582
C	4.420498	-3.389993	1.143585	H	6.439181	-2.299212	-1.932802
C	5.202228	-2.251207	1.203591	H	3.812712	-3.636481	2.004003
C	4.256934	-4.095174	-0.051101	H	5.174233	-1.654237	2.106253
C	5.096257	-3.738740	-1.112852	H	5.075729	-4.308387	-2.034277
C	2.294818	-5.393410	0.856687	H	2.776579	-5.511520	1.819432
C	3.018270	-4.898452	-0.232295	H	0.515177	-4.986908	-2.519642
C	0.999836	-5.107434	-1.558490	H	2.889876	-4.552555	-2.353809
C	2.361731	-4.878733	-1.466727	H	0.380249	-5.833022	1.675171
C	0.927297	-5.596551	0.770623	H	-0.993295	-3.511420	-1.915045
C	-1.209958	-4.985625	-0.364909	H	-3.888347	-5.122961	1.719910
C	0.232149	-5.340460	-0.414534	H	-1.836915	-6.331061	1.196813
C	-1.640983	-3.910584	-1.145721	H	-3.026202	-2.321267	-1.399992
C	-3.263666	-4.770625	0.907305	H	-5.520207	-2.912780	-1.652444
C	-2.094511	-5.456702	0.610534	H	-4.903330	-1.016661	3.830166
C	-3.594789	-3.584412	0.243740	H	-3.874481	-3.029101	2.818511
C	-2.803898	-3.226246	-0.850460	H	-6.608085	1.142631	-2.301142
C	-5.634952	-1.902324	-1.281516	H	-6.704687	-1.205817	-2.987118
C	-5.174119	-1.586400	0.020430	H	-5.686096	0.782783	2.411468

C	-4.482490	-2.546985	0.835600	H	-5.078730	2.382356	1.915336
C	-4.914530	-1.145136	2.754636	H	-3.581685	4.295048	-2.343552
C	-4.403096	-2.325172	2.188277	H	-5.114120	2.466274	-2.371912
C	-6.263665	0.390138	-1.604064	H	-3.429355	4.088359	1.928837

[7]CPPNap$_{1,5}$ (TS')

C	5.972006	0.513568	0.168639	C	3.853202	-5.739437	0.116719
C	5.522650	2.771834	-0.901472	C	4.507233	-3.415607	0.017282
C	5.559334	1.946291	0.228545	C	3.122617	-3.055881	-0.128615
C	3.996798	3.473522	1.281130	C	2.734094	-1.695528	-0.233398
C	4.858054	2.393991	1.351525	C	5.697132	-1.526984	-1.110874
C	4.650365	3.847648	-0.977042	C	5.444521	-2.250609	0.053537
C	2.508807	4.888686	-0.094501	C	6.023854	-0.277314	1.322499
C	3.788823	4.154103	0.080644	C	5.745568	-1.634674	1.267600
C	1.861778	5.535335	0.963380	C	5.950929	-0.164568	-1.054287
C	0.403351	4.906379	-1.291312	H	6.113330	2.524567	-1.775059
C	1.767975	4.672473	-1.257969	H	3.370424	3.691423	2.137056
C	-0.277972	5.367224	-0.163203	H	4.863798	1.812144	2.263026
C	0.496430	5.769892	0.929605	H	4.584005	4.403856	-1.904915
C	-2.590640	5.127421	-1.172376	H	2.417270	5.790717	1.858188
C	-1.741273	5.127616	-0.061484	H	-0.155562	4.596627	-2.165671
C	-3.465966	3.943047	1.158345	H	2.233306	4.185808	-2.106262
C	-2.251005	4.605147	1.128568	H	0.016372	6.205544	1.798037
C	-3.809367	4.467355	-1.141384	H	-2.266350	5.588343	-2.098094
C	-5.210854	2.660862	-0.049068	H	-3.755325	3.434791	2.069420
C	-4.227720	3.775241	0.000069	H	-1.632719	4.594270	2.017467
C	-5.869393	2.184752	1.090312	H	-4.407391	4.429282	-2.044268
C	-5.717264	0.551040	-1.122806	H	-5.942864	2.810842	1.971741
C	-5.252055	1.853153	-1.186875	H	-5.584819	-0.087865	-1.986889
C	-6.158506	-0.000001	0.082468	H	-4.776897	2.186769	-2.100811
C	-6.333907	0.880560	1.155391	H	-6.752626	0.518853	2.087307
C	-6.145802	-2.377657	-0.802280	H	-6.715093	-2.108016	-1.684337
C	-6.031665	-1.471367	0.258018	H	-4.050648	-3.330157	2.262112
C	-4.671932	-3.111255	1.403804	H	-5.317843	-1.287205	2.277693
C	-5.399050	-1.934085	1.413234	H	-5.453670	-4.182290	-1.694883
C	-5.424468	-3.561328	-0.807531	H	-2.828204	-5.110498	2.073939
C	-3.269979	-4.609999	0.022400	H	-0.901357	-4.290965	-2.377988
C	-4.550129	-3.875952	0.240698	H	-3.308022	-4.342979	-2.114883
C	-2.421935	-4.954624	1.081868	H	-0.414651	-4.996125	1.811152
C	-1.316450	-4.514805	-1.402229	H	1.780423	-6.203035	-0.056382
C	-2.692304	-4.551006	-1.249327	H	1.143986	-0.310614	-0.505029
C	-0.476614	-4.532711	-0.288783	H	-0.586449	-2.063819	-0.596582
C	-1.042618	-4.904911	0.932036	H	5.888714	-5.014011	0.252344
C	2.532078	-5.422871	-0.029724	H	4.151509	-6.776788	0.210779

C	2.121601	-4.071218	-0.158795	H	3.476505	-0.916949	-0.167905
C	0.758544	-3.685173	-0.329806	H	5.524309	-1.990207	-2.075471
C	1.430154	-1.351884	-0.419773	H	6.148428	0.183746	2.294002
C	0.450589	-2.350293	-0.476874	H	5.626149	-2.187514	2.192352
C	4.848029	-4.733559	0.140504	H	5.966073	0.390432	-1.983375

(*M*)-[7]CPPAn$_{1,5}$

C	-0.354228	5.028345	1.482655	C	6.093723	2.881574	-0.862568
C	0.365881	5.689978	0.486113	C	6.592471	1.605541	-1.070502
C	-1.695986	5.887693	-0.768937	C	5.414700	2.260095	1.336206
C	-0.358636	6.203248	-0.594044	C	4.379999	4.290202	0.351937
C	-1.693365	4.717591	1.310792	C	5.389632	3.199933	0.304132
C	-3.568696	4.276746	-0.252609	C	3.682824	4.604157	-0.816423
C	-2.361903	5.053031	0.133153	C	2.627258	5.409476	1.600017
C	-3.589597	3.711839	-1.528354	C	3.871999	4.800764	1.551206
C	-5.404837	2.807804	0.344624	C	1.843613	5.539552	0.449722
C	-4.549192	3.859740	0.650230	C	2.443766	5.216850	-0.768762
C	-5.297596	2.123702	-0.868567	H	0.166656	4.626836	2.343091
C	-4.430463	2.656155	-1.825581	H	-2.207431	6.231213	-1.660592
C	-5.003997	-0.272154	0.949843	H	0.147132	6.790257	-1.351590
C	-5.421241	-0.365128	-0.374560	H	-2.182133	4.084521	2.041512
C	-5.843957	0.767834	-1.175548	H	-2.853385	4.017259	-2.261299
C	-6.619373	-0.791489	-2.879318	H	-6.130268	2.491447	1.084014
C	-6.459583	0.526968	-2.368958	H	-4.611083	4.322393	1.628557
C	-3.546907	-2.315438	3.648304	H	-4.336839	2.162558	-2.784870
C	-4.162416	-1.280296	3.025703	H	-5.104160	0.658138	1.488499
C	-4.152795	-2.556003	0.913516	H	-7.133397	-0.933483	-3.822200
C	-4.452619	-1.354887	1.630451	H	-6.775141	1.364198	-2.980677
C	-4.713714	-2.703415	-0.352708	H	-3.339701	-2.276624	4.710770
C	-5.401557	-1.662439	-0.982380	H	-4.446106	-0.386943	3.569883
C	-6.054021	-1.846080	-2.239227	H	-4.618476	-3.649136	-0.873586
C	-3.049100	-3.405481	2.886135	H	-6.088366	-2.841330	-2.667347
C	-2.367079	-4.405461	0.760411	H	-2.369828	-4.093935	3.372067
C	-3.279152	-3.525355	1.542400	H	-2.238389	-3.057826	-0.911846
C	-1.809704	-3.924052	-0.426924	H	-0.087854	-6.851342	1.375799
C	-0.565200	-6.029384	0.854476	H	-2.224050	-6.005438	2.195028
C	-1.777198	-5.544988	1.321871	H	-0.141188	-3.926746	-1.747031
C	0.090379	-5.409237	-0.212557	H	1.973867	-5.454306	1.676304
C	-0.609896	-4.420546	-0.904673	H	3.829974	-4.670071	-2.812726
C	2.386371	-5.325482	0.682967	H	1.561023	-5.517832	-2.581693
C	1.558400	-5.477144	-0.430246	H	4.211157	-4.564084	1.453783
C	3.437070	-4.842246	-1.818113	H	4.560614	-2.646401	-2.661489
C	2.147192	-5.332122	-1.688971	H	7.193708	-1.637341	1.370521
C	3.667419	-4.817491	0.552969	H	6.230580	-3.853578	1.095104

C	5.235649	-3.409828	-0.765694	H	5.548185	-0.460531	-2.400665
C	4.178031	-4.454593	-0.695466	H	5.787624	0.244637	1.908837
C	5.179047	-2.464642	-1.792372	H	6.177842	3.611839	-1.658544
C	6.631645	-1.857656	0.470254	H	7.046626	1.366066	-2.025095
C	6.077773	-3.118755	0.313971	H	4.900736	2.467542	2.266185
C	6.380468	-0.843091	-0.457713	H	4.042056	4.242324	-1.771237
C	5.743628	-1.210448	-1.644237	H	2.230617	5.718409	2.560171
C	5.921721	0.988245	1.132948	H	4.417601	4.652008	2.475464
C	6.417156	0.601676	-0.113635	H	1.878952	5.314825	-1.687253

(*P*)-[7]CPPAn$_{1,5}$

C	0.356030	5.030195	1.483103	C	-6.093242	2.883884	-0.862971
C	-0.363477	5.691134	0.485545	C	-6.592495	1.607890	-1.070257
C	1.699269	5.887935	-0.768162	C	-5.414289	2.263163	1.336021
C	0.361831	6.203917	-0.594192	C	-4.378217	4.292280	0.350395
C	1.695035	4.718770	1.312050	C	-5.388541	3.202308	0.303270
C	3.570920	4.276203	-0.250763	C	-3.680194	4.604673	-0.817997
C	2.364287	5.053306	0.134433	C	-2.625908	5.412563	1.598080
C	3.592485	3.712293	-1.527037	C	-3.870903	4.804213	1.549207
C	5.405732	2.805659	0.346674	C	-1.841468	5.541001	0.448285
C	4.550408	3.857911	0.652468	C	-2.441011	5.216963	-0.770299
C	5.298884	2.122656	-0.866999	H	-0.165350	4.629554	2.343619
C	4.432904	2.656390	-1.824424	H	2.211196	6.231025	-1.659684
C	5.002534	-0.273915	0.949329	H	-0.143064	6.791005	-1.352223
C	5.420925	-0.366530	-0.374716	H	2.183259	4.086101	2.043441
C	5.844710	0.766686	-1.174735	H	2.857126	4.018733	-2.260391
C	6.620760	-0.791805	-2.878814	H	6.130076	2.487988	1.086590
C	6.461091	0.526455	-2.367839	H	4.611932	4.319638	1.631245
C	3.543448	-2.318066	3.646138	H	4.339858	2.163675	-2.784215
C	4.158889	-1.282475	3.024114	H	5.102185	0.656239	1.488289
C	4.151316	-2.557751	0.911636	H	7.135137	-0.933366	-3.821568
C	4.450525	-1.356869	1.629161	H	6.777331	1.363913	-2.978883
C	4.713599	-2.704859	-0.354089	H	3.335530	-2.279626	4.708481
C	5.401794	-1.663621	-0.982940	H	4.441932	-0.389179	3.568703
C	6.054835	-1.846628	-2.239614	H	4.619023	-3.650498	-0.875210
C	3.046591	-3.408042	2.883378	H	6.089381	-2.841669	-2.668196
C	2.365804	-4.408054	0.757472	H	2.367383	-4.096907	3.368816
C	3.277264	-3.527250	1.539670	H	2.236140	-3.061224	-0.915539
C	1.807803	-3.927210	-0.429952	H	0.087012	-6.853430	1.375351
C	0.563920	-6.031792	0.853146	H	2.223555	-6.007513	2.192655
C	1.776462	-5.547411	1.319443	H	0.138710	-3.930549	-1.749172
C	-0.092363	-5.411926	-0.213443	H	-1.973427	-5.452364	1.677843
C	0.607838	-4.423942	-0.906829	H	-3.834866	-4.673206	-2.809748
C	-2.387214	-5.324799	0.684915	H	-1.566603	-5.522647	-2.580671

C	-1.560897	-5.478811	-0.429331	H	-4.209677	-4.559846	1.457139
C	-3.440887	-4.844229	-1.815389	H	-4.560208	-2.645077	-2.658848
C	-2.151234	-5.335149	-1.687323	H	-7.196096	-1.634260	1.370786
C	-3.667753	-4.815464	0.555925	H	-6.234047	-3.850890	1.096522
C	-5.236548	-3.407670	-0.763093	H	-5.546879	-0.458965	-2.399379
C	-4.179545	-4.453541	-0.692445	H	-5.787893	0.248228	1.909727
C	-5.179283	-2.463004	-1.790296	H	-6.177346	3.613728	-1.659307
C	-6.633367	-1.854899	0.471017	H	-7.046835	1.368266	-2.024716
C	-6.079899	-3.116315	0.315463	H	-4.900191	2.470770	2.265873
C	-6.380695	-0.840663	-0.456776	H	-4.038728	4.241622	-1.772576
C	-5.743363	-1.208550	-1.642919	H	-2.229906	5.722333	2.558213
C	-5.921806	0.991434	1.133440	H	-4.416980	4.656692	2.473368
C	-6.417134	0.604424	-0.113096	H	-1.875621	5.313304	-1.688554

[7]CPPAn$_{1,5}$ (TS)

C	-1.496289	-4.915862	1.615107	C	-6.773360	-0.766330	-0.747949
C	-2.406008	-5.369159	0.657386	C	-6.755553	0.601760	-0.973286
C	-0.530327	-6.211665	-0.618639	C	-5.853496	-0.421686	1.421941
C	-1.895611	-6.119542	-0.406245	C	-5.697188	-2.704793	0.483810
C	-0.129804	-5.012771	1.405606	C	-6.219443	-1.315026	0.413994
C	1.722272	-5.149574	-0.241288	C	-5.177250	-3.282073	-0.675778
C	0.374431	-5.563260	0.227636	C	-4.441074	-4.336654	1.764525
C	1.805416	-4.632740	-1.534468	C	-5.394685	-3.333290	1.697137
C	3.928882	-4.228315	0.180000	C	-3.759715	-4.757524	0.618737
C	2.838503	-4.992794	0.582278	C	-4.230135	-4.288484	-0.609470
C	3.933853	-3.568086	-1.052561	H	-1.852523	-4.345970	2.464337
C	2.876466	-3.854411	-1.922754	H	-0.166657	-6.719779	-1.504223
C	4.996592	-1.246970	0.735650	H	-2.572614	-6.560434	-1.128538
C	4.998548	-1.262251	-0.656571	H	0.543065	-4.519235	2.096667
C	4.820779	-2.444712	-1.481878	H	0.962989	-4.734868	-2.206747
C	5.616496	-1.157055	-3.398996	H	4.766309	-4.129921	0.857615
C	5.201827	-2.373329	-2.792591	H	2.842207	-5.432259	1.573219
C	5.376248	1.075638	3.576489	H	2.840368	-3.367881	-2.888534
C	5.307395	-0.085237	2.879056	H	4.965720	-2.171789	1.291552
C	4.980470	1.197164	0.795113	H	5.913264	-1.159636	-4.440702
C	5.090091	-0.062349	1.468277	H	5.104053	-3.252607	-3.418008
C	5.097559	1.179148	-0.591863	H	5.591789	1.070299	4.637969
C	5.209092	-0.008935	-1.316126	H	5.443850	-1.042084	3.369610
C	5.539238	0.005256	-2.704784	H	5.150152	2.102046	-1.148373
C	5.054959	2.305060	2.940342	H	5.750563	0.956244	-3.179938
C	3.954697	3.534566	1.110130	H	4.942198	3.188038	3.557886
C	4.775827	2.387439	1.604665	H	4.897885	4.021973	-0.769690
C	4.029494	4.157620	-0.139955	H	0.962397	4.818749	2.074988
C	1.834675	4.670807	1.450519	H	2.766460	3.427711	2.895380

C	2.865295	3.880505	1.917743	H	3.037381	5.326832	-1.630600
C	1.824803	5.133642	0.134691	H	-0.079154	6.883909	1.143440
C	2.977250	4.927143	-0.624684	H	-1.650259	4.080028	-2.579590
C	-0.418439	6.283788	0.306878	H	0.720568	4.268943	-2.145905
C	0.504246	5.527535	-0.420700	H	-2.463639	6.740836	0.680693
C	-1.326416	4.744977	-1.790067	H	-3.740066	4.064082	-2.920197
C	0.031906	4.849343	-1.543573	H	-5.739370	3.686405	1.559314
C	-1.776350	6.194448	0.046507	H	-3.993865	5.308598	1.171755
C	-3.642903	4.760468	-0.882395	H	-5.400199	2.358792	-2.497278
C	-2.267068	5.325770	-0.935025	H	-5.403422	1.579231	1.957343
C	-4.167106	3.994628	-1.927576	H	-7.148488	-1.418988	-1.527406
C	-5.307766	3.756111	0.568405	H	-7.118041	0.979785	-1.921977
C	-4.320647	4.698507	0.339551	H	-5.433850	-0.795942	2.346812
C	-5.640978	2.813022	-0.407082	H	-5.397660	-2.843669	-1.640792
C	-5.134094	3.031560	-1.691366	H	-4.164855	-4.736062	2.733504
C	-5.836047	0.942016	1.197484	H	-5.842820	-2.975631	2.616511
C	-6.184471	1.478121	-0.044581	H	-3.744248	-4.602732	-1.524558

[7]CPPAn$_{1,5}$ (TS')

C	3.384874	3.892854	1.257095	C	-3.470847	4.726795	-1.150888
C	3.030834	4.557208	0.082077	C	-4.649786	3.997355	-1.134744
C	5.046663	3.665406	-0.930425	C	-3.109189	4.191681	1.144197
C	3.935392	4.494391	-0.981716	C	-1.194123	5.140044	-0.118523
C	4.485735	3.056727	1.302889	C	-2.630168	4.766586	-0.034292
C	6.108056	1.605240	0.109352	C	-0.460418	4.776843	-1.249663
C	5.292602	2.851179	0.180452	C	0.907678	5.565512	1.012437
C	6.237355	0.932361	-1.109365	C	-0.476972	5.614733	0.983862
C	6.642601	-0.478746	1.225501	C	1.633705	5.042417	-0.061561
C	6.464322	0.896617	1.262235	C	0.923909	4.730153	-1.222369
C	6.503627	-1.182111	0.029641	H	2.720158	3.924041	2.111455
C	6.437449	-0.439261	-1.148539	H	5.686410	3.600443	-1.802254
C	3.756294	-1.535752	0.004301	H	3.736498	5.050850	-1.890306
C	4.548642	-2.676394	0.008421	H	4.635186	2.459733	2.192580
C	5.994011	-2.587915	0.033305	H	6.021489	1.446392	-2.037358
C	6.080571	-5.006627	0.039022	H	6.756060	-1.022694	2.156239
C	6.725150	-3.732592	0.051783	H	6.479678	1.395755	2.223127
C	0.294926	-0.395861	-0.293081	H	6.371878	-0.954108	-2.100103
C	1.639581	-0.371702	-0.150135	H	4.208031	-0.557167	0.048563
C	1.710549	-2.861698	-0.138160	H	6.693595	-5.899864	0.055157
C	2.374309	-1.590761	-0.083819	H	7.807592	-3.686495	0.067624
C	2.501289	-4.013976	-0.094348	H	-0.279710	0.520077	-0.355287
C	3.898973	-3.950724	-0.027459	H	2.185606	0.563152	-0.097428
C	4.726752	-5.116476	-0.003580	H	2.021857	-4.986327	-0.131652
C	-0.371797	-1.643486	-0.347180	H	4.254856	-6.092330	-0.023593

C	-0.689183	-3.994550	-0.251427	H	-1.451203	-1.644353	-0.432516
C	0.277517	-2.848920	-0.260791	H	-1.132434	-3.845330	-2.345604
C	-1.492145	-4.173654	-1.377463	H	-2.858770	-5.143336	2.074020
C	-2.490676	-4.888757	1.087493	H	-0.539574	-4.462429	1.843643
C	-1.160617	-4.513297	0.956368	H	-3.459563	-4.462672	-2.114888
C	-3.386203	-4.726504	0.022492	H	-4.425923	-3.679132	2.283682
C	-2.822660	-4.534189	-1.242787	H	-7.110392	-2.744096	-1.724495
C	-5.044922	-3.529309	1.409246	H	-5.599525	-4.640246	-1.722808
C	-4.782384	-4.241830	0.235885	H	-5.934907	-1.814502	2.285504
C	-6.537121	-2.952369	-0.828531	H	-6.191298	-0.641092	-2.010249
C	-5.673052	-4.036065	-0.826497	H	-6.731511	2.229250	1.947046
C	-5.913368	-2.452115	1.410816	H	-7.432119	-0.097967	2.051981
C	-6.787207	-0.587251	0.054529	H	-5.498969	1.669861	-2.114865
C	-6.552086	-2.045054	0.237886	H	-4.548617	2.923716	2.061577
C	-6.366137	-0.011634	-1.146984	H	-3.171455	5.221280	-2.067618
C	-6.619527	1.608838	1.065594	H	-5.241843	3.938100	-2.040437
C	-7.022461	0.283989	1.124173	H	-2.495514	4.206848	2.036321
C	-5.969888	2.116846	-0.065213	H	-0.976766	4.410472	-2.128377
C	-5.965172	1.311912	-1.205480	H	1.427834	5.882718	1.908709
C	-4.284336	3.460540	1.159251	H	-1.008774	5.971847	1.857886
C	-5.035632	3.271833	-0.002878	H	1.450417	4.328746	-2.079706

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