Supporting Information

Synthesis, Crystal Structure, and Inherent Chirality in Hexa(tert-butylphenyl)-Substituted [6]Cycloparaphenylene

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1. Materials and General Information

All solvents for syntheses were obtained from commercial suppliers (Innochem or Acros) and used without further purification. Air-sensitive reactions were all carried out under argon. [Au_2Cl_2(dcpm)] and $PhICl_2$ were synthesized according to literature procedures.[1,2] The NMR spectra were recorded on a Bruker BioSpin (^{1}H 400 MHz, ^{13}C 100 MHz) spectrometer in $CDCl_3$ solution at 298 K. The chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to tetramethylsilane (δ = 0.00 ppm) or $CHCl_3$ (δ = 7.26 ppm). Chemical shifts for ^{13}C NMR are expressed ppm relative to $CDCl_3$ (δ = 77.0 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, m = multiplet), coupling constant (Hz), and integration. High-resolution mass spectrometry (HR-MS) analyses were carried out using MALDI-TOF-MS techniques and trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile as the matrix. UV/Vis absorption spectra were performed on a UNIC-3802 spectrophotometer. Circular dichroism (CD) spectra were performed on a CD spectrometer (JASCO, J-1500). Preparative thin-layer chromatography (PTLC) was performed using silica gel GF254 precoated plates and flash chromatography was performed on silica gel (200~300 mesh).

2. Synthetic Details

Synthesis of compound 3. The starting material **1** was synthesized according to the literature report.[3] A mixture of **1** (100 mg, 0.18 mmol, 1.0 equiv), **2** (70 mg, 0.39 mmol, 2.2 equiv), and K_2CO_3 (147 mg, 1.06 mmol, 6.0 equiv) in a round-bottomed flask was dissolved in toluene (8 mL), ethanol (2 mL), and water (2 mL). $Pd(PPh_3)_4$ (20 mg, 17 μmol, 0.1 equiv) was then added under an argon atmosphere, and the reaction mixture was heated at 100 °C for 24 h. After cooling to room temperature, the solvent was removed under reduced pressure, and the residue was extracted with CH_2Cl_2. The combined organic layers were dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (petroleum ether) to afford **3** as a white solid (87 mg, 85% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50 (d, *J* = 2.1 Hz, 1H), 7.48 (d, *J* = 2.1 Hz, 1H), 7.30 (d, *J* = 2.1 Hz, 2H), 7.26 (s, 1H), 7.24 (s, 1H), 6.97 (d, *J* = 8.4 Hz, 4H), 6.38 (d, *J* = 8.4 Hz, 4H), 1.30 (s, 18H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 149.33, 142.56, 137.90, 136.30, 133.17, 132.72, 130.11, 128.16, 124.70, 121.69, 34.39, 31.33. HR-MS (MALDI-TOF) m/z calcd. for $C_{32}H_{32}Br_2$ $[M]^+$: 576.0850, found: 576.0845.

Synthesis of compound 4. To a mixture of compound **3** (75 mg, 0.13 mmol, 1.0 equiv), KOAc (102 mg, 1.04 mmol, 8.0 equiv), $Pd(dppf)Cl_2$ (10 mg, 13.66 μmol, 0.1 equiv) and B_2pin_2 (130 mg, 0.51 mmol, 4.0 equiv) in a round-bottom flask was added 1,4-dioxane (6 mL), then, the solution was heated to 90 ℃ for 48 hours under nitrogen atmosphere. Upon cooling to room temperature, the solvent was removed under reduced pressure. The crude product was purified by column chromatography

(PE/CH_2Cl_2 = 3/1) to afford **4** as a white solid (55 mg, 63% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.80 – 7.77 (m, 2H), 7.59 (d, *J* = 1.2 Hz, 2H), 7.43 (d, *J* = 7.5 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 4H), 6.45 (d, *J* = 8.4 Hz, 4H), 1.28 (s, 18H), 1.26 (s, 24H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.29, 142.86, 140.04, 137.84, 136.62, 133.28, 131.34, 128.45, 124.31, 83.79, 34.27, 31.39, 25.11, 24.71. HR-MS (MALDI-TOF) m/z calcd. for $C_{44}H_{56}B_2O_4$ $[M]^+$: 670.4365, found: 670.4355.

Synthesis of [6]CPP-6′BuPh. A mixture of **4** (100 mg, 149 μmol, 1.0 equiv), [Au_2Cl_2(dcpm)] (130 mg, 149 μmol, 1.0 equiv), and Cs_2CO_3 (291 mg, 895 μmol, 6.0 equiv) in degassed toluene/EtOH/H_2O (8 mL/2 mL/2 mL) was stirred for 48 hours at 50 ℃ under argon atmosphere. The resulting precipitate was collected by suction filtration and washed by EtOH (50 mL). The residual solid was dried in vacuo to afford crude product **5** (135 mg, 75% yield) as a white solid, which was used without further purification.

To a suspension of **5** (135 mg, 36 μmol, 1.0 equiv) in degassed and dry DMF (20 mL) was added $PhICl_2$ (11 mmol/L in degassed and dry DMF, 10 mL, 110 μmol, 3.0 equiv) dropwise with stirring at −60 ℃ for 5 min. The reaction mixture was stirred at the same temperature for 30 min, then it was allowed to warm to 25 ℃ and stirred for 24 h. Solvent and iodobenzene (by-product) were removed under vacuum. The crude product was purified by silica gel column chromatography (hexane/CH_2Cl_2 = 20/1) to give **[6]CPP-6′BuPh** as an yellow solid (18 mg, 40% yield). This target product was characterized by ^{1}H NMR spectroscopy and high-resolution mass spectrometry (HR-MS). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ 7.82 (d, *J* = 8.3 Hz, 12H), 7.73 (d, *J* = 1.9

Hz, 6H), 7.50 (d, J = 8.3 Hz, 12H), 6.81 (dd, J = 8.7, 1.9 Hz, 6H), 6.74 (s, 6H), 1.38 (s, 54H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.68, 138.97, 138.55, 138.45, 138.42, 135.40, 131.46, 129.16, 126.12, 124.07, 34.71, 31.48. HR-MS (MALDI-TOF) m/z calcd. for $C_{96}H_{96}$ $[M]^+$: 1249.7545, found: 1249.7569.

3. ^{1}H and ^{13}C NMR Spectra and HRMS Studies

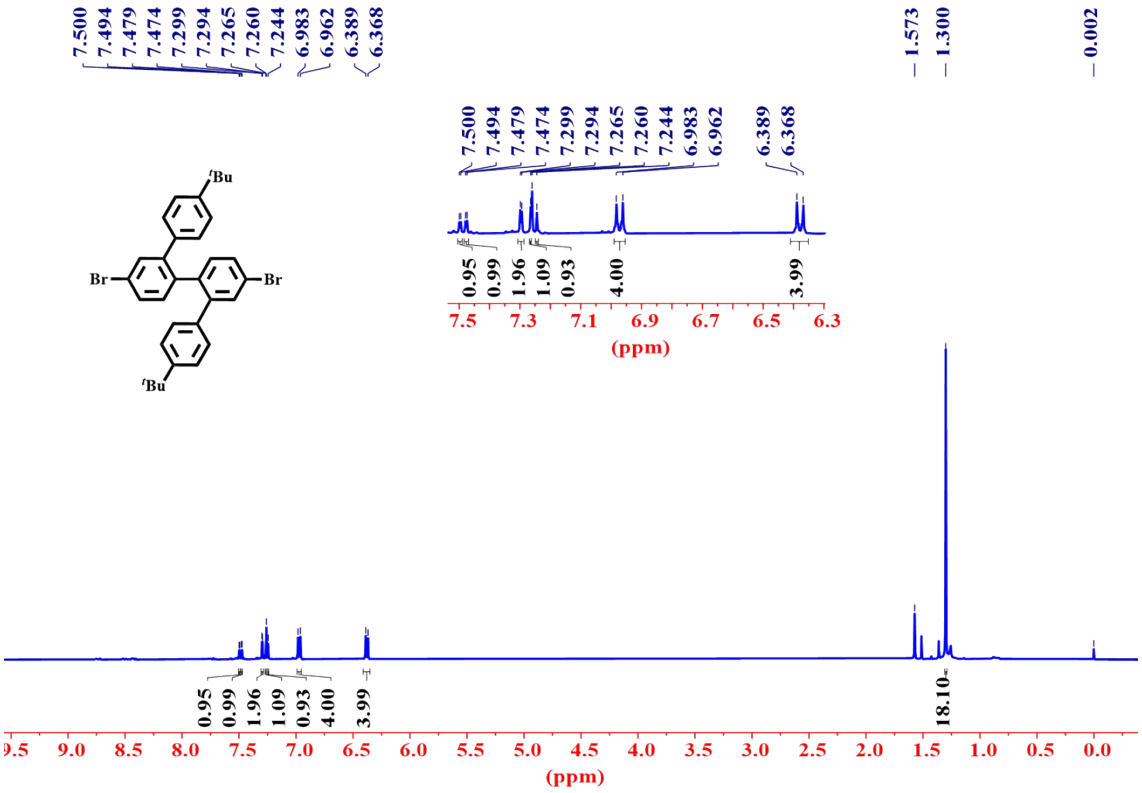


Fig. S1 ^{1}H NMR spectrum of compound **3** (400 MHz, $CDCl_3$, 298 K).

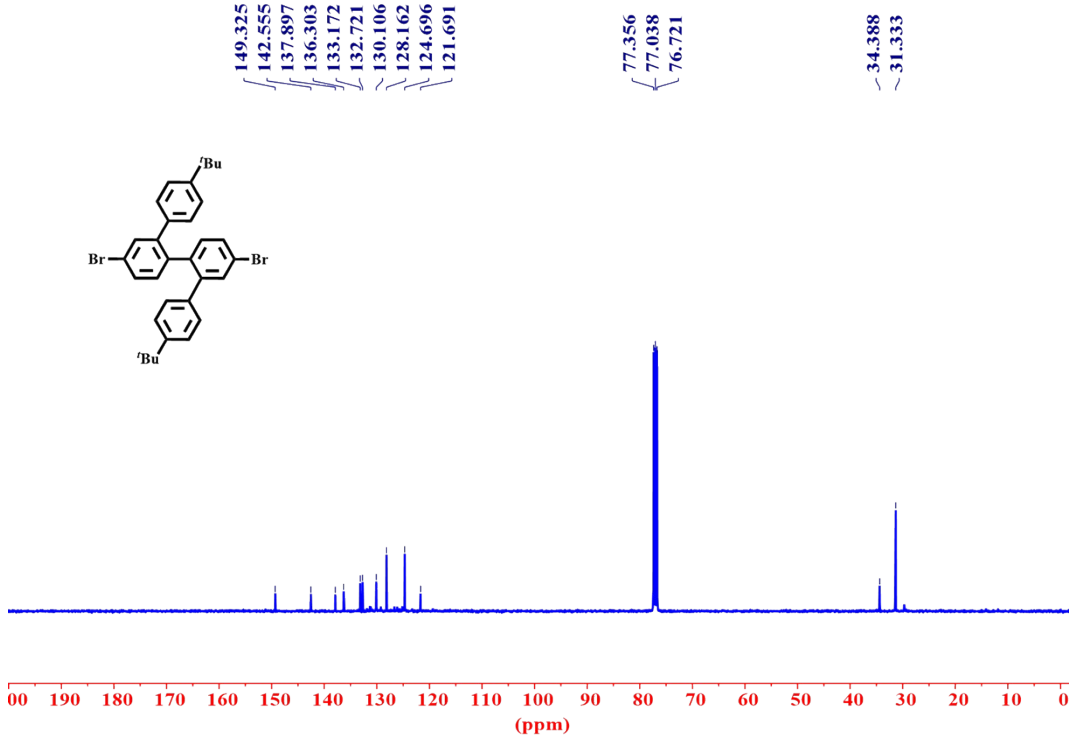


Fig. S2 ^{13}C NMR spectrum of compound **3** (100 MHz, $CDCl_3$, 298 K).

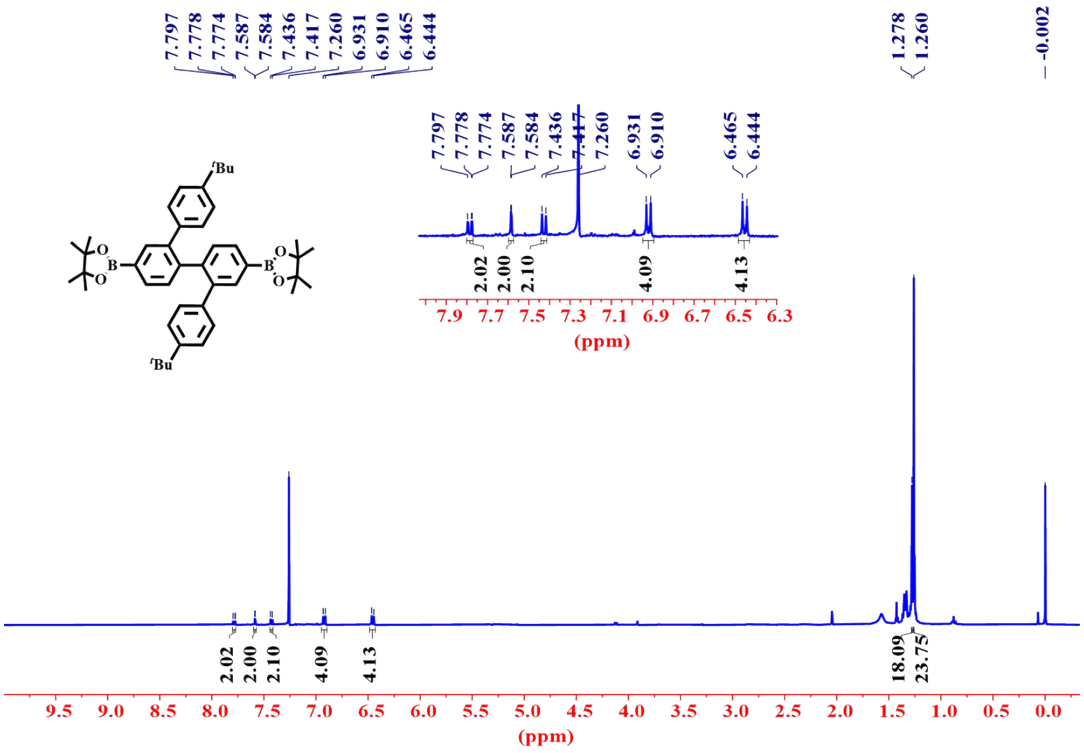


Fig. S3 ^{1}H NMR spectrum of **4** (400 MHz, $CDCl_3$, 298 K).

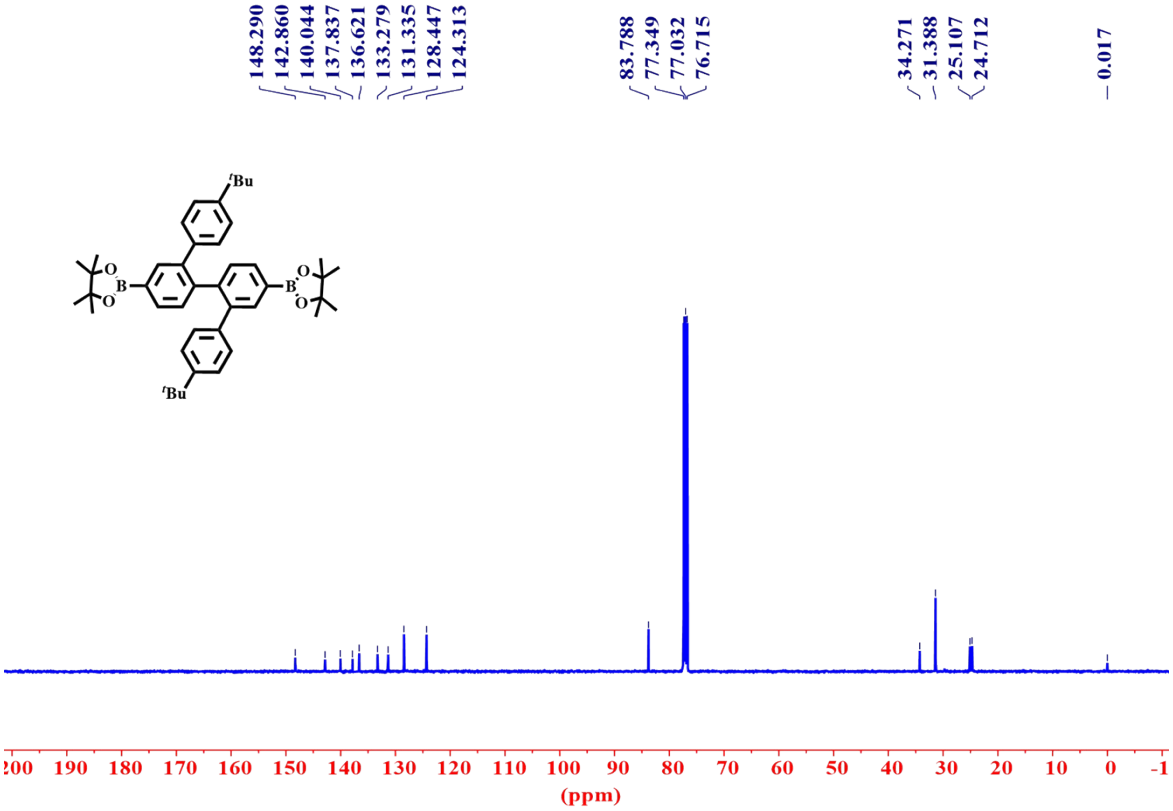


Fig. S4 ^{13}C NMR spectrum of **4** (100 MHz, $CDCl_3$, 298 K).

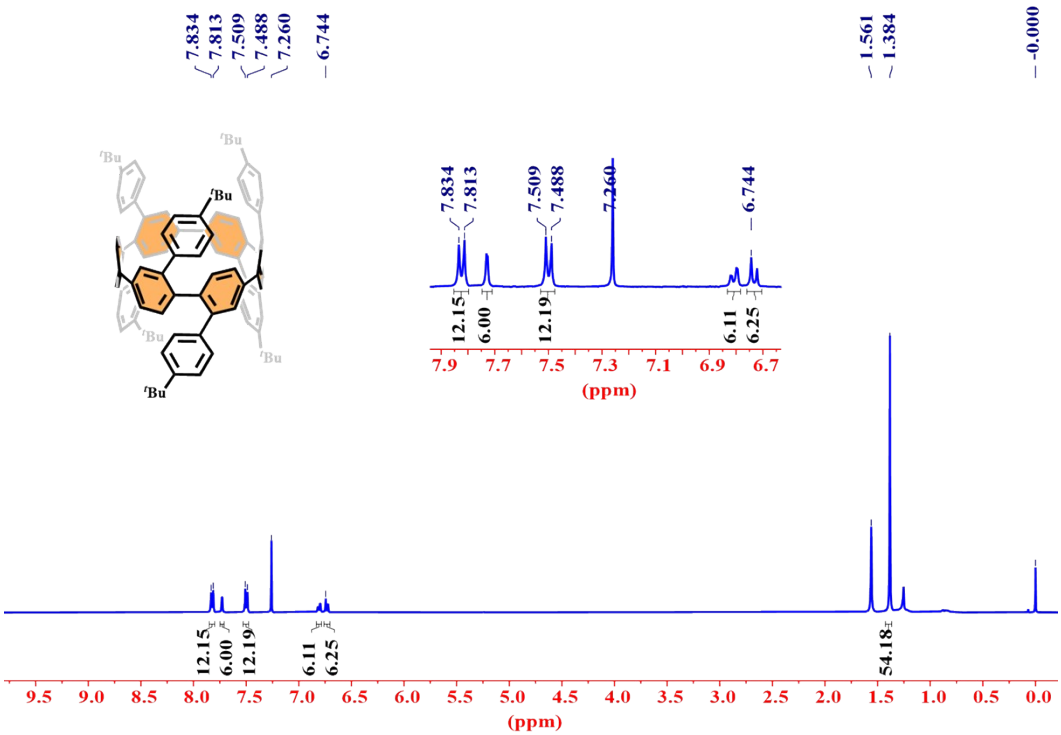


Fig. S5 ^{1}H NMR spectrum of **[6]CPP-6^{t}BuPh** (400 MHz, $CDCl_3$, 298 K).

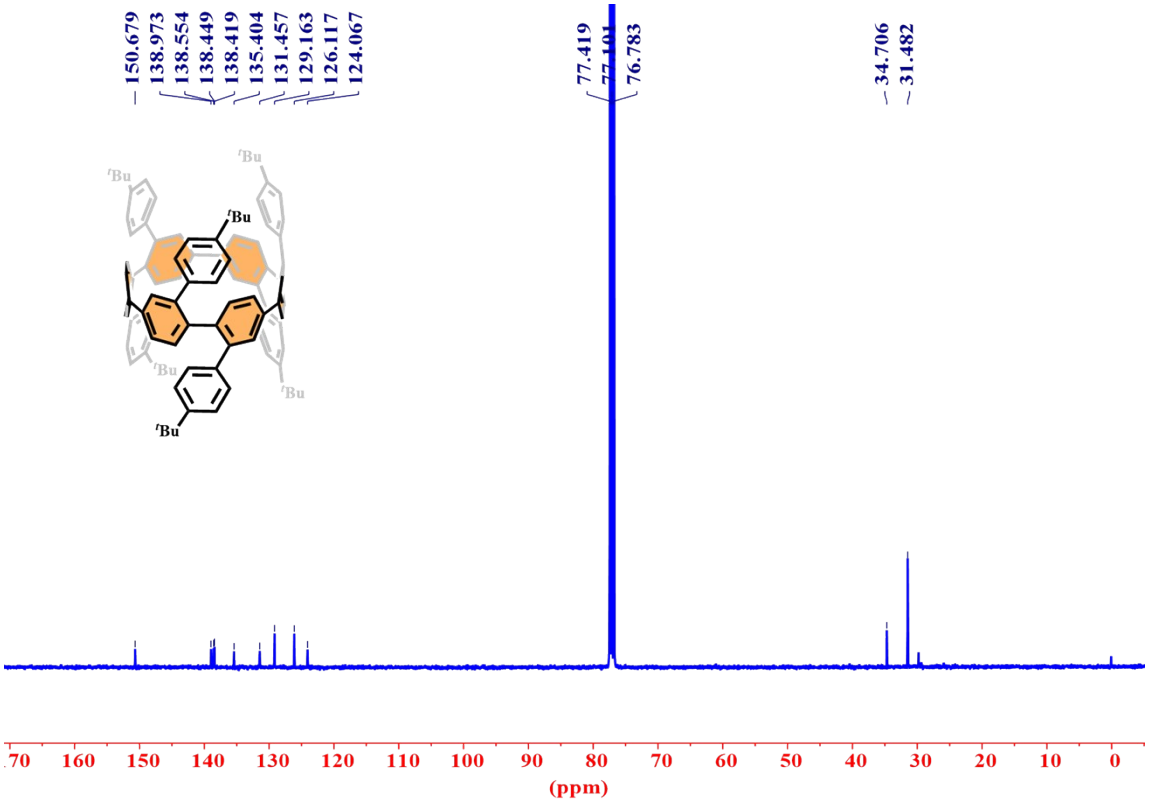


Fig. S6 ^{13}C NMR spectrum of **[6]CPP-6^{t}BuPh** (100 MHz, $CDCl_3$, 298 K).

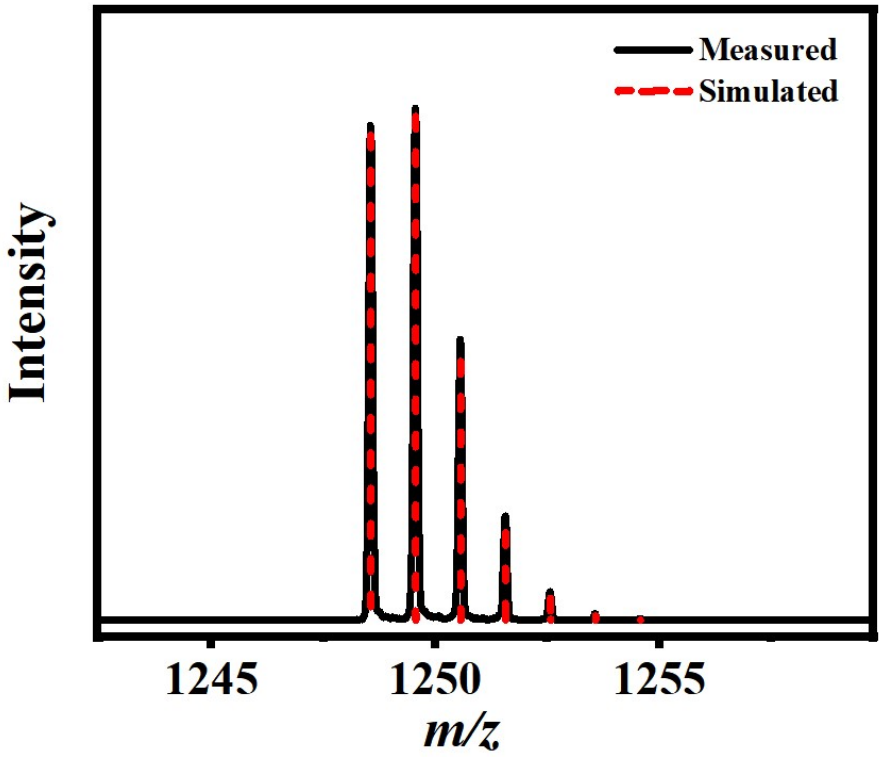


Fig. S7 MALDI-TOF MS spectrum (black solid line) and simulated data (red dash line) for **[6]CPP-6^{t}BuPh**.

4. Crystal Structures and Crystal Data

Yellow single crystals of **[6]CPP-6^{t}BuPh** suitable for X-ray diffraction were obtained by slow liquid-liquid diffusion, in which methanol was carefully layered onto a benzene solution of the compound. After standing undisturbed for approximately one week, single crystals gradually formed at the solvent interface. Data collection for [6]CPP-6tBuPh was carried out on a Bruker D8 VENTURE diffractometer at 150.0 K**.** The structures were refined using all data (based on F^2) by SHELX 2018 within Olex2. Crystallo graphic data of **[6]CPP-6^{t}BuPh** can be obtained free of charge from the Cambridge Crystallographic Data Center (CCDC number: 2521143 for **[6]CPP-6^{t}BuPh**).

Table S1. Crystal data and structure refinement for **[6]CPP-6^{t}BuPh**

Complex	[6]CPP-6^{t}BuPh
Formular	$C_{96}H_{96}$
Formular weight	1249.82
Temperature/K	150
Crystal system	triclinic
Space group	$P\bar{1}$
a / Å	14.1436
b / Å	17.1687
c / Å	20.6678
α / deg	108.502
β / deg	95.339
γ / deg	113.214
Volume/Å^3	4234.8
Z	2
ρ_{calc}g/cm^3	1.107

μ/mm^{-1}	0.322
F(000)	1522.0
Crystal size/mm^3	0.09×0.07×0.03
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	4.052 – 92.302
Index ranges	-15 ≤ h ≤ 15, -18 ≤ k ≤ 18, -22 ≤ l ≤ 22
Reflections collected	70325
Independent reflections	10913 [R_{int} = 0.1356, R_{sigma} = 0.0842]
Data/restraints/parameters	10913/231/1023
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0596, wR_2 = 0.1486
Final R indexes [all data]	R_1 = 0.1042, wR_2 = 1712

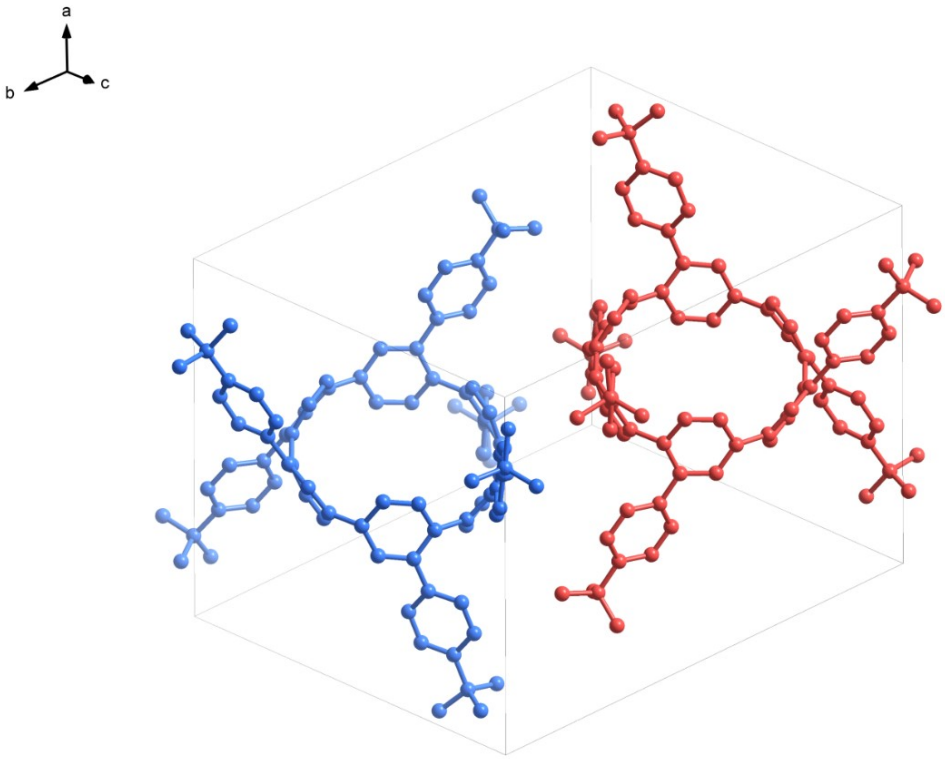


Fig. S8 Presentation of the positions for a pair of enantiomers in the crystal unit cell.

5. Chiral HPLC Analysis

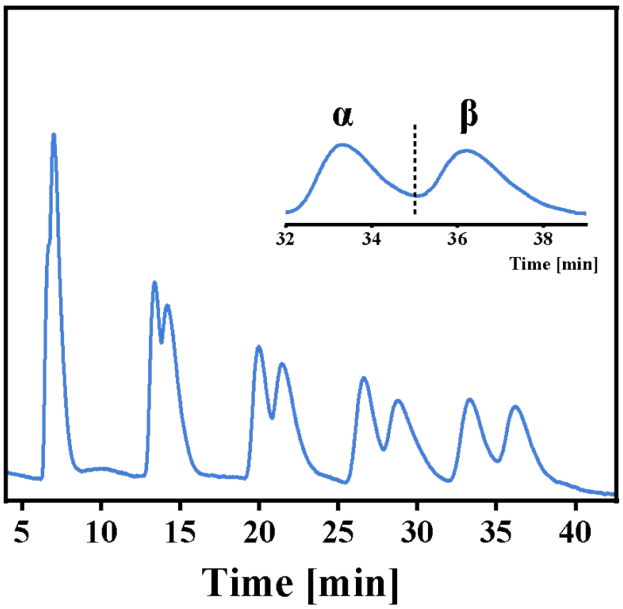


Fig. S9 Successful separation of **[6]CPP-6^{t}BuPh** equipped with CHIRALPAK IK column (10 mm I.D. × 250 mm) eluted by PE/DCM (20:1) monitored with the absorption at 350 nm.

6. Computational Details

The stationary points were obtained from the geometric optimizations at the ωb97xd[4]/6-31G(d)[5,6] level and further validated by vibrational frequency analysis (no imaginary frequency). The single-point energies of all species were taken into account by using the same functional combined with the Def2TZVP[7] basis set. As B3LYP[8] was more accurate for calculating orbital energy than ωb97xd,[9] B3LYP/Def2TZVP theoretical level was applied to identify the energy level of frontier orbitals. The excitation energies and oscillator strengths of the nanohoops were calculated with time-dependent density functional theory (TD-DFT)[10,11] at the PBE0[12]/6-311G(d,p)[13] level. Solvent effects of dichloromethane (ε = 8.93) were implicitly taken into account by applying the polarizable continuum model (PCM)[14,15] developed by Tomasi's group in the framework of the self-consistent reaction field (SCRF).[16,17] Strain energy visualization was achieved by using StrainViz.[18] The wave function analysis were implemented in Multiwfn 3.8(dev) code[19,20] and rendered by VMD 1.9.3 program.[21] All calculations were carried out with the Gaussian 16 program.[22]

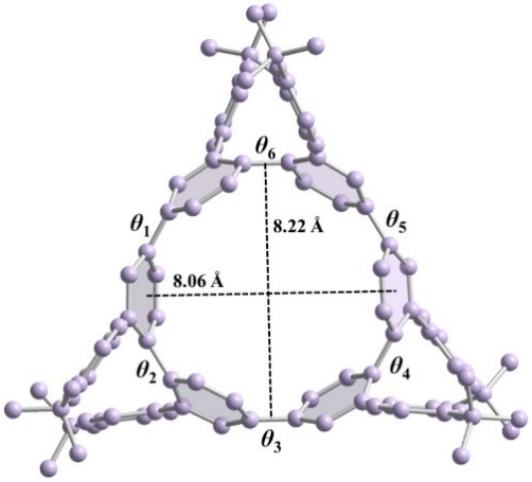


Fig. S10 The relaxed structures and calculated diameters of **[6]CPP-6^{t}BuPh**.

Table S2. The torsion angles (Unit: degree) between adjacent phenyl rings of the relaxed structures of **[6]CPP-6^{t}BuPh**.

Torsion angles (deg.)	θ_1	37
	θ_2	-37
	θ_3	37
	θ_4	-37
	θ_5	37
	θ_6	-37
	Average $\lvert\theta\rvert$	**37**

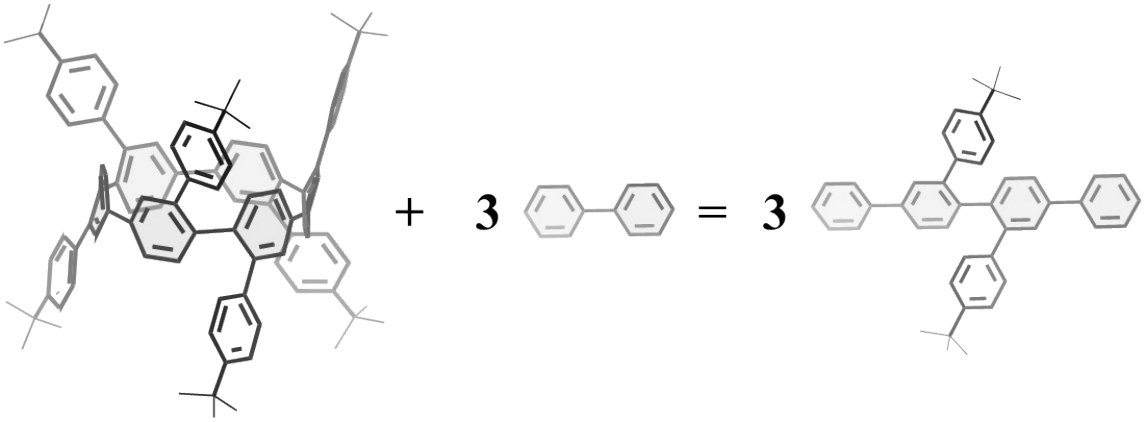


Fig. S11 The homodesmotic reactions for strain energy estimation.

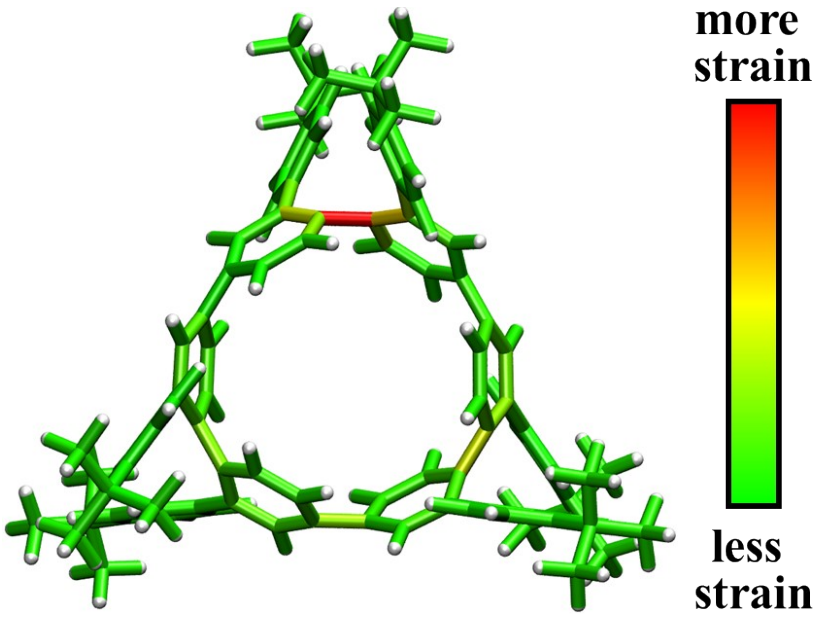
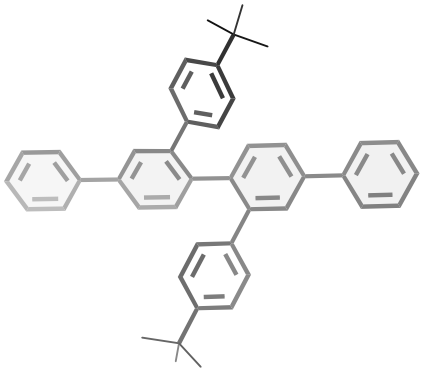
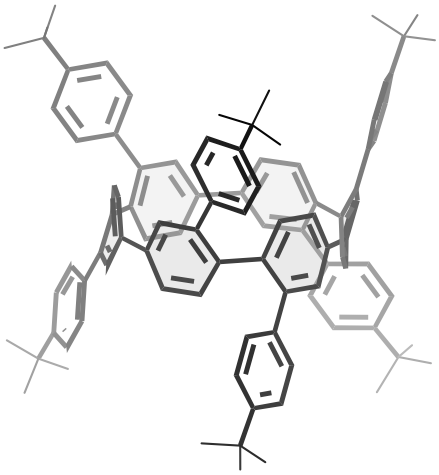


Fig. S12 StrainViz analysis of **[6]CPP-6*t*BuPh**.

Table S3. The calculated strain energies of **[6]CPP-6′BuPh** by homodesmotic reaction method.

Optimized Structure	Total Energy (Hartree)	Strain Energy (ΔH, kcal·mol^{-1})
	-463.1079622	-
	-1701.2804591	-
	-3714.3766333	**-88.38 kcal/mol**

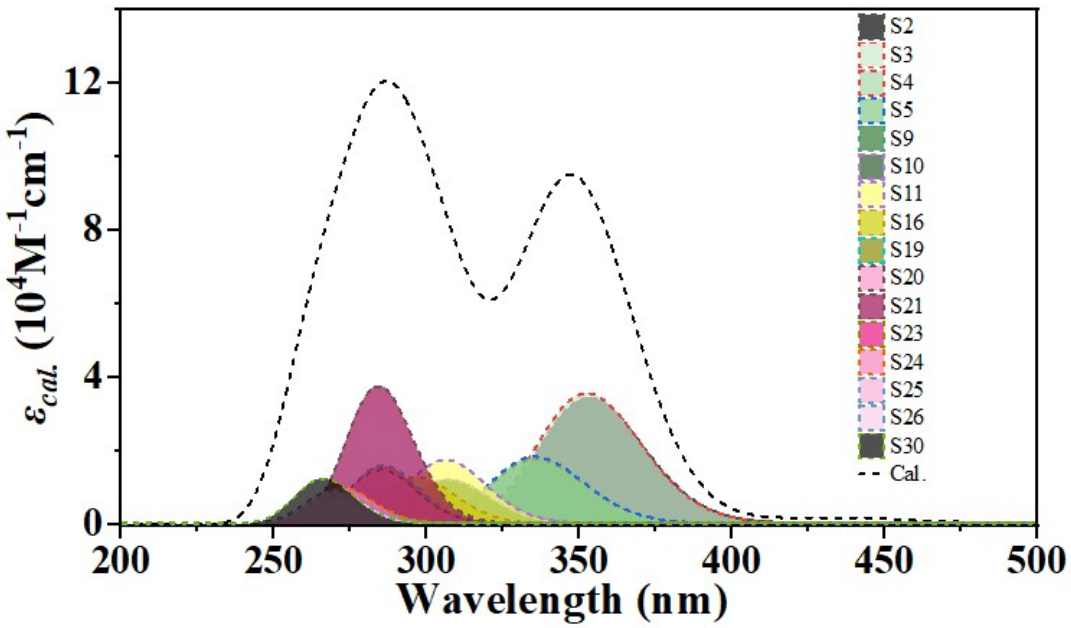


Fig. S13 Calculated (dashed lines) UV-Vis absorptions of **[6]CPP-6*t*BuPh** with separated contributions ($f > 0.1$) from different excited states. The experimental spectra were measured in dichloromethane with a concentration of 2.0×10^{-6} M at room temperature. The calculated absorption profiles were obtained by an effective Gaussian full width half maximum (FWHM) of 0.4 eV.

Table S4. Electronic transitions for **[6]CPP-6^{t}BuPh** determined by TD-DFT methods at PBE0/6-311G(d,p)/PCM(DCM) level. Only those with oscillator strengths greater than 0.02 are listed.

Excited State	Energy (eV)	Excitation (nm)	Oscillator Strength (f_{os})	Transition Type
S0→S1	2.8494	435.12	0.0274	HOMO → LUMO 97.1%
S0→S2	3.5092	353.31	0.5136	HOMO → LUMO+1 92.3%
S0→S3	3.5162	352.61	0.5293	HOMO → LUMO+2 92.0%
S0→S4	3.6922	335.8	0.2654	HOMO-1 → LUMO 93.4%
S0→S5	3.6944	335.6	0.2718	HOMO-2 → LUMO 93.7%
S0→S9	4.0366	307.15	0.1847	HOMO → LUMO+6 67.3%, HOMO-5 → LUMO 7.1%, HOMO-6 → LUMO 6.7%
S0→S10	4.0389	306.98	0.1804	HOMO → LUMO+7 66.3%, HOMO-4 → LUMO 8.2%, HOMO-7 → LUMO 6.2%
S0→S11	4.0501	306.13	0.2617	HOMO → LUMO+8 70.6%, HOMO-8 → LUMO 6.9%, HOMO-1 → LUMO+2 5.7%
S0→S13	4.1549	298.4	0.0806	HOMO-5 → LUMO 45.9%, HOMO → LUMO+4 43.9%
S0→S14	4.1633	297.8	0.0521	HOMO-4 → LUMO 26.9%, HOMO → LUMO+5 26.8%, HOMO-2 → LUMO+2 17.4%, HOMO-1 → LUMO+1 13.2%
S0→S15	4.1708	297.27	0.0296	HOMO-1 → LUMO+1 36.1%, HOMO-2 → LUMO+2 21.8%, HOMO → LUMO+5 14.4%, HOMO-4 → LUMO 14.1%
S0→S16	4.1789	296.69	0.1913	HOMO-2 → LUMO+1 46.3%, HOMO-1 → LUMO+2 42.0%
S0→S17	4.2577	291.2	0.093	HOMO-1 → LUMO+2 38.8%, HOMO-2 → LUMO+1 35.0%, HOMO-6 → LUMO 14.5%
S0→S18	4.2588	291.12	0.0805	HOMO-2 → LUMO+2 42.3%, HOMO-1 → LUMO+1 32.4%, HOMO-7 → LUMO 13.3%, HOMO → LUMO+5 5.2%
S0→S19	4.3404	285.65	0.2374	HOMO-6 → LUMO 56.2%, HOMO → LUMO+6 18.7%
S0→S20	4.3487	285.11	0.2251	HOMO-7 → LUMO 56.3%, HOMO → LUMO+7 19.1%
S0→S21	4.3623	284.22	0.5622	HOMO-8 → LUMO 75.9%, HOMO → LUMO+8 12.7%
S0→S23	4.5529	272.32	0.1297	HOMO → LUMO+11 46.9%, HOMO-3 → LUMO+2 14.8%, HOMO-5 → LUMO 6.2%, HOMO → LUMO+16 5.4%
S0→S24	4.5596	271.92	0.1507	HOMO → LUMO+10 35.5%, HOMO-3 → LUMO+1 21.0%, HOMO → LUMO+9 9.1%, HOMO → LUMO+15 5.7%, HOMO-4 → LUMO 5.3%

S0→S25	4.5928	269.95	0.1075	HOMO-3 → LUMO+1 46.6%, HOMO → LUMO+10 24.7%, HOMO-4 → LUMO+1 6.3%
S0→S26	4.5995	269.56	0.1402	HOMO-3 → LUMO+2 49.6%, HOMO → LUMO+11 18.0%, HOMO-5 → LUMO+1 8.9%, HOMO-4 → LUMO+2 7.5%
S0→S30	4.6582	266.16	0.1872	HOMO-5 → LUMO+1 34.0%, HOMO-4 → LUMO+2 29.8%, HOMO → LUMO+12 8.0%

Table S5. Cartesian coordinates of the optimized **[6]CPP-6′BuPh**.

C	2.760439	6.255589	-4.35104	H	2.200924	2.715438	-2.08787
C	2.726955	3.224974	-0.06474	H	2.888768	6.151969	-0.94766
C	2.810767	2.453105	-1.23087	H	4.066745	7.105656	-2.85887
C	2.532755	5.939695	-1.95135	H	3.879509	3.63513	5.580536
C	3.195982	6.486698	-3.04482	H	3.627073	2.173277	3.646747
C	3.884978	4.078719	4.588492	H	4.818886	1.3396	1.842439
C	3.751462	3.241705	3.490437	H	3.354373	0.590377	-2.11148
C	3.738877	3.75704	2.189271	H	3.355209	0.585167	2.111537
C	4.240985	1.641258	0.97214	H	4.821091	1.332069	-1.84232
C	3.591913	2.880591	0.99975	H	3.630693	2.167635	-3.64669
C	4.076755	0.742312	-0.08703	H	3.885556	3.629094	-5.58046
C	3.474282	1.237765	-1.2479	H	4.077924	7.099117	2.859013
C	3.476176	1.232361	1.247959	H	2.898452	6.147394	0.947742
C	4.077918	0.735955	0.087115	H	2.205114	2.712058	2.087862
C	3.596499	2.87499	-0.9997	H	1.249081	3.231311	-2.13815
C	4.243619	1.634638	-0.97205	H	3.890326	5.557675	-1.04232
C	3.744928	3.751213	-2.1892	H	4.11529	7.03288	-2.97146
C	3.756768	3.235865	-3.49037	H	1.25769	5.234229	5.507209
C	4.021424	5.460006	-4.44573	H	0.105259	4.263279	3.591737
C	3.891672	4.072671	-4.58841	H	1.223993	4.859062	1.789633
C	3.206179	6.481531	3.044923	H	1.168102	3.168006	-2.14437
C	2.542096	5.935635	1.951418	H	2.157574	2.634893	2.093674
C	2.814582	2.448748	1.230893	H	3.564311	3.478151	-1.86229
C	1.441431	3.966007	-0.12509	H	3.704917	2.00531	-3.64536
C	2.732029	3.220731	0.064748	H	5.104482	1.472745	-5.56363
C	0.722951	3.638877	-1.28245	H	8.150583	0.01866	2.921356
C	3.877481	5.131935	-2.04121	H	6.751478	0.552145	1.00227
C	4.012785	5.967399	-3.14503	H	3.423899	0.574774	2.105594
C	1.632925	5.44919	4.510238	H	3.424752	0.569353	-2.10569
C	2.770257	6.251048	4.351127	H	6.750594	0.562815	-1.00242
C	0.967557	4.902999	3.422545	H	8.150562	0.00578	-2.92153
C	1.411872	5.134748	2.115762	H	5.106876	1.464637	5.563509
C	0.6798	4.498719	0.919932	H	3.708116	1.999413	3.645266
C	0.718211	4.55592	0.937377	H	3.569798	3.472484	1.86221
C	1.383617	3.894298	-0.12707	H	2.161674	2.631458	-2.09374
C	0.661416	3.605953	-1.28955	H	1.173103	3.16612	2.144329
C	2.784055	2.404386	1.237146	H	1.23162	4.857143	-1.78966
C	2.662958	3.158203	0.0654	H	0.09859	4.263558	-3.59177
C	4.280754	1.656699	-0.99131	H	1.249495	5.236434	-5.50719
C	3.531078	2.838142	-0.98388	H	4.103965	7.039289	2.971564
C	5.120157	1.330472	-2.17196	H	3.881452	5.56374	1.042411
C	4.691326	1.581177	-3.47618	H	1.243981	3.233236	2.138129

C	6.749789	0.685096	-4.41177	H	5.156573	8.074485	-6.1181
C	5.490289	1.264962	-4.57161	H	4.40488	8.544954	-4.58878
C	7.176082	0.427795	3.09956	H	5.440574	7.102599	-4.66897
C	6.384474	0.742311	2.006367	H	4.647543	5.0288	-5.93946
C	3.506319	1.222884	1.240537	H	3.115452	5.055671	-6.82627
C	4.1421	0.743104	-0.08483	H	4.461387	6.069988	-7.3662
C	4.140929	0.74966	0.084728	H	2.123595	8.545784	-5.74957
C	3.508211	1.217328	-1.24063	H	2.974611	8.139804	-7.25449
C	6.383272	0.752405	-2.00651	H	1.61053	7.151582	-6.71207
C	7.175354	0.439137	-3.09972	H	4.388593	8.423798	-6.24968
C	5.49234	1.256258	4.571485	H	5.182341	8.025212	-4.72122
C	6.750926	0.674416	4.411625	H	3.414956	8.201516	-4.79101
C	4.693856	1.573733	3.476073	H	5.35558	4.884068	-6.80957
C	5.122273	1.322363	2.171841	H	6.313982	6.035676	-5.86687
C	3.535549	2.832538	0.983791	H	5.52682	6.553026	-7.37239
C	4.283367	1.649916	0.991207	H	2.00532	6.464479	-6.03178
C	2.667917	3.153969	-0.06547	H	2.787395	5.14032	-6.90893
C	2.787806	2.399964	-1.23722	H	2.990461	6.806592	-7.46941
C	0.667098	3.604867	1.289508	H	1.621758	7.148765	6.712191
C	1.389737	3.892075	0.127025	H	2.137057	8.542193	5.749764
C	0.711055	4.557032	-0.93739	H	2.98741	8.134783	7.254671
C	0.686865	4.497625	-0.91996	H	4.655386	5.021174	5.93951
C	1.403806	5.137022	-2.11574	H	3.123338	5.050453	6.826317
C	0.959869	4.904639	-3.42254	H	4.470888	6.062595	7.366291
C	1.62438	5.451939	-4.5102	H	4.418341	8.537774	4.588987
C	4.00315	5.973645	3.145125	H	5.451731	7.093764	4.669115
C	3.869234	5.137973	2.041292	H	5.169275	8.066034	6.11829
C	0.717215	3.639974	1.282422	H	8.443264	1.4995	-4.636
C	1.435186	3.968227	0.125067	H	7.00908	1.770101	-5.63681
C	4.012534	5.46626	4.445821	H	8.586683	1.481282	-6.39986
C	3.467541	6.831984	-5.58324	H	7.70311	0.375634	-7.75373
C	4.686274	7.686167	-5.20822	H	6.081627	0.112369	-7.10088
C	3.948866	5.675842	-6.48073	H	6.817807	1.729248	-7.04019
C	2.48289	7.71775	-6.3701	H	9.515483	0.849382	-4.54941
C	4.159252	6.346369	-5.6891	H	9.644582	0.837662	-6.31423
C	4.293407	7.833046	-5.33218	H	8.806875	2.170044	-5.49136
C	5.412864	5.926447	-6.47993	H	9.516873	0.834419	4.549239
C	2.911012	6.175938	-6.57607	H	9.645967	0.822456	6.314066
C	3.478266	6.826256	5.583358	H	8.810315	2.156152	5.491229
C	2.495024	7.713556	6.370253	H	7.006429	1.78121	5.6366
C	3.957742	5.669307	6.480806	H	8.584488	1.494852	6.399633
C	4.698362	7.67851	5.208389	H	8.441013	1.512801	4.635775
C	7.656917	0.315488	-5.5911	H	7.703806	0.363402	7.753569
C	7.940367	1.198549	-5.56056	H	6.081912	0.102643	7.100731

C	7.019748	0.656571	-6.94508	H	6.820574	1.718391	7.040069
C	8.984189	1.089239	-5.47599	H	5.347445	4.892429	6.809757
C	7.65749	0.303375	5.590938	H	6.304086	6.045556	5.867128
C	8.985958	1.075074	5.475834	H	5.515999	6.561655	7.372591
C	7.938597	1.211097	5.56035	H	2.979235	6.811197	7.469432
C	7.020864	0.645407	6.944932	H	1.994739	6.467529	6.031736
C	4.148879	6.352835	5.689209	H	2.778853	5.144607	6.908931
C	5.403099	5.934898	6.480124	H	3.401704	8.20681	4.791087
C	2.900849	6.180423	6.576091	H	4.37491	8.430623	6.249802
C	4.280707	7.839724	5.332294	H	5.169368	8.033294	4.721383

Table S6. Absorption dissymmetry factors for chiral CPP derivatives.

Compound	**λ_{abs} [nm]**	**$g_{abs}/10^{-3}$**
[6]CPP-6*t*BuPh (this work)	355	**1.05**
([7]CPPRu2,9[23]	426	**7.7**
4CzZ[6]CPP[24]	367	**5.4**
[6]CPP-12*t*BuPh[25]	313	**4.4**
diketo[6]CPP[26]	340	**1.0**
[12]PCPP[27]	334	**2.92**
SCPP[8][28]	368	**12**

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