

Electronic Supplementary Information:

Size-Dependent Fluorescence Properties of [*n*]Cycloparaphenylenes (*n* = 8 - 13), Hoop-Shaped π -Conjugated Molecules

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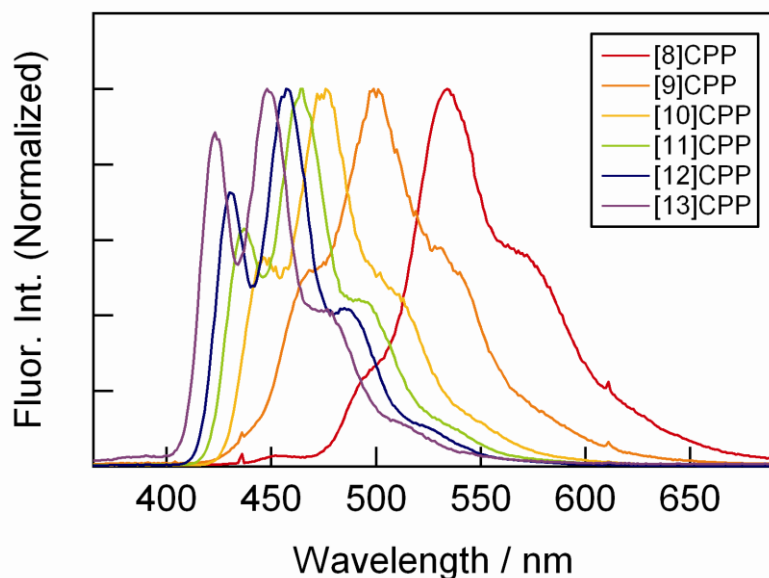


Fig. S1. Fluorescence spectra of [*n*]CPPs in 2-methyltetrahydrofuran at 77 K. The samples were excited at 350 nm.

Table S1. Fluorescence peaks (λ_{fl}) and lifetime (τ_{fl}) of [*n*]CPPs in 2-methyltetrahydrofuran at 77 K.

<i>n</i>	λ_{fl} / nm ^a	τ_{fl} / ns ^b
8	503(sh), 534, 562(sh)	20.4
9	472(sh), 500, 531(sh)	14.1
10	446, 476, 506(sh), ~544(sh)	7.8
11	437, 465, 490(sh), ~529(sh)	4.7
12	430, 458, 485, ~521(sh)	3.2
13	423, 448, 474(sh), ~509(sh)	2.3

^a (sh) denotes a shoulder peak. ^b Excitation: 370 nm. Estimation error: <5%

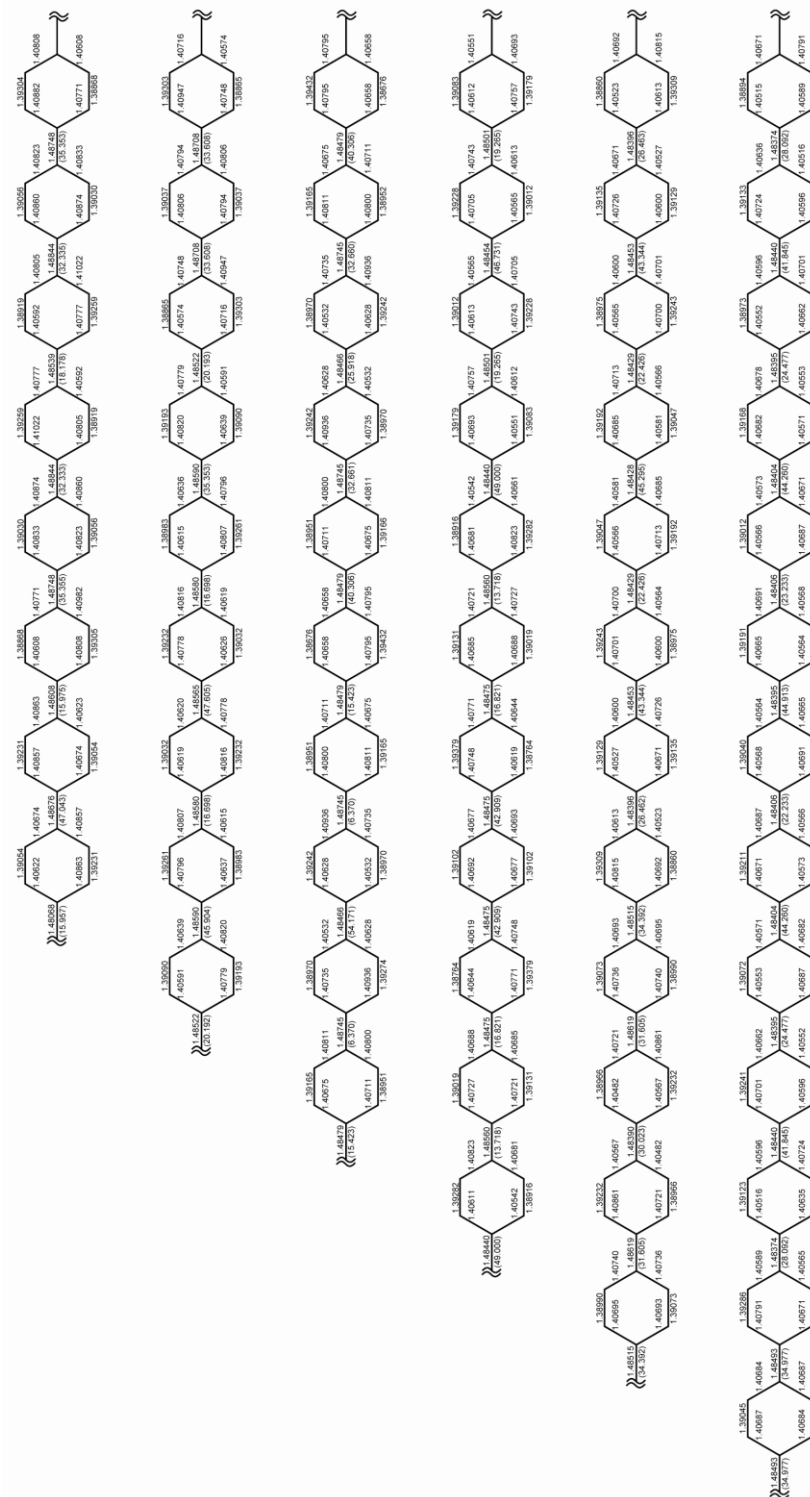


Fig. S2. Structures of CPPs in the ground state estimated by density functional theory at B3LYP/6-31G(d) level. Numbers indicate bond length. Numbers in parentheses are dihedral angle.

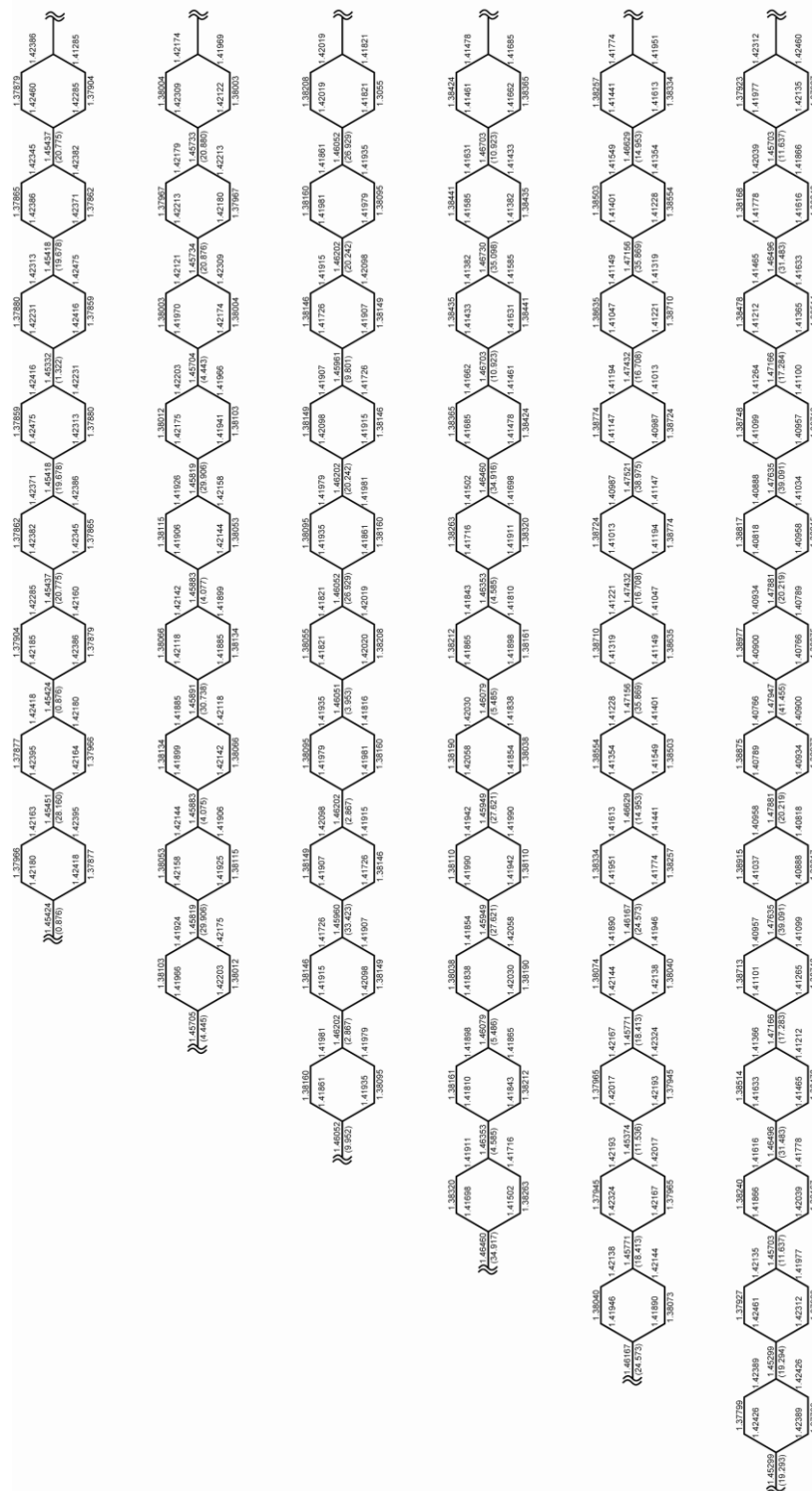


Fig. S3. Structures of CPPs in the S_1 state estimated by density functional theory at B3LYP/6-31G(d) level. Numbers indicate bond length. Numbers in parentheses are dihedral angle.