Supporting Information for

Cycloparaphenylene Double Nanohoop: Structure, Lamellar Packing and Encapsulation of C₆₀ in the Solid State

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General

The silica-gel column chromatography was performed using Merck 60 silica gel (40–63 µm). The gel permeation chromatography (GPC) was performed on Shimadzu SPD-M40 with Dr. Maisch ReproGel 500 GPC polystyrene columns (length = 600 mm, ID = 20 mm, eluent = CHCl₃). The nuclear magnetic resonance (NMR) measurements were performed on NMR spectrometers operating at 400 or 500 MHz proton frequencies at 25 °C. Standard pulse sequences were used. Chemical shifts (δ) are reported in parts per million (ppm) relative to the solvent residual peak (¹H and ¹³C NMR, respectively): CDCl₃ (δ = 7.26 and 77.16 ppm) and CD₂Cl₂ (δ = 5.32 and 53.84 ppm). High-resolution mass spectrometry (HRMS) was performed by the mass-spectrometry service at the University of Zurich and measured as HR-ESI-MS (TOF) or HR-APCI-MS (TOF). For all reactions performed at elevated temperatures, oil bath was used as a heat source.

Materials

Anhydrous solvents and chemical reagents were purchased from commercial sources and were used without further purification unless stated otherwise. The reactions were performed under N₂ atmosphere unless stated otherwise. Compounds ⁴¹, ⁵² and ⁷³ were prepared according to the methods reported in the literature.
Synthesis

To a solution of 7 (2.69 g, 6.67 mmol) in anhydrous THF (70 mL), n-BuLi (1.6 M in hexanes, 4.17 mL, 6.67 mmol) was added over 15 min at −78 °C and the mixture was stirred at −78 °C for additional 1 h. Trisopropylborate (3.08 mL, 13.3 mmol) was then added, and the resultant mixture was slowly warmed to room temperature overnight. The reaction was quenched with aq. HCl (1 M), and the mixture was stirred for 30 min before it was extracted with Et2O. The combined organic layers were washed with brine, dried over anhydrous MgSO4 and concentrated under reduced pressure. The crude product was washed with n-hexane and then filtered to afford 6 in 58% yield (1.43 g, 3.87 mmol) as a white solid. This material was used directly in the next step without further purification.

A mixture of 4 (222 mg, 0.379 mmol), 6 (350 mg, 0.948 mmol), Pd(PPh3)4 (43.8 mg, 0.038 mmol) and sodium hydroxide (75.8 mg, 1.90 mmol) in a 10:1 mixture of 1,4-dioxane and H2O (10.5 mL) was stirred at 80 °C for 16 h. The reaction mixture was diluted with DCM, washed with water and brine, dried over anhydrous MgSO4 and concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography using n-hexane/DCM (3:1 v/v) as an eluent to afford 3 in 60% yield (223 mg, 0.227 mmol) as a colorless oil. 1H NMR (400 MHz, CD2Cl2, ppm): δ 8.11 (d, J = 8.4 Hz, 1H), δ 7.92 (d, J = 8.4 Hz, 1H), 7.58 (d, J = 8.3 Hz, 1H), 7.53–7.47 (m, 4H), 7.43–7.33 (m, 7H), 7.20 (s, 1H), 7.15 (s, 1H), 3.47 (t, J = 7.0 Hz, 2H), 2.93 (t, J = 7.1 Hz, 2H), 2.75 (t, J = 7.6 Hz, 4H), 2.61 (t, J = 7.4 Hz, 4H), 1.69–1.62 (m, 4H), 1.56–1.48 (m, 4H), 1.46–1.32 (m, 12H), 1.29–1.18 (m, 12H), 0.93–0.83 (m, 12H). 13C NMR (101 MHz, CD2Cl2, ppm): δ 200.0, 141.3, 141.2, 141.1, 140.6, 140.5, 140.44, 140.35, 140.0, 139.74, 139.67, 139.65, 134.2, 134.0, 133.6, 133.43, 133.37, 132.7, 132.6, 132.2, 132.1, 131.3, 130.3, 129.6, 129.5, 129.2, 129.12, 129.06, 129.01, 128.98, 128.93, 128.86, 126.7, 123.6, 123.5, 41.0, 36.1, 32.8, 32.1, 31.93, 31.86, 31.614, 31.605, 30.51, 30.50, 29.6, 29.54, 29.48, 29.4, 29.0, 23.0, 22.94, 22.90, 14.28, 14.26, 14.2 (five carbon resonances could not be determined because of signal overlap). HRMS (ESI) m/z: [M + H]+ Calcd for C61H72Br2O 979.4023; Found 979.4012.
To a solution of 3 (216 mg, 0.220 mmol) in a 3:1 mixture of DCM and EtOH (6 mL), sodium borohydride (25 mg, 0.66 mmol) was added at room temperature and the resultant mixture was stirred at room temperature for 16 h. The mixture was then diluted with DCM, washed with water and brine, dried over anhydrous MgSO₄ and concentrated under reduced pressure to afford the desired alcohol intermediate as a colorless oil, which was used directly in the next step.

To a hot (90 °C) solution of the alcohol intermediate in toluene (2 mL), a catalytic amount of p-toluenesulfonic acid monohydrate was added and the resultant mixture was stirred at 90 °C for 30 min before it was passed through Florisil® using DCM as an eluent to afford the desired hydro-precursor as a colorless oil, which was used directly in the next step.

To a solution of the hydro-precursor in a 1:1 mixture of DCM and toluene (10 mL), p-chloranil (162 mg, 0.661 mmol) was added at room temperature and the resultant pale-yellow mixture quickly changed color to yellow, then green, finally brown. This mixture was stirred at room temperature overnight. After removal of the solvents under reduced pressure, the crude product was purified by silica-gel column chromatography using n-hexane/DCM (6:1 v/v) as an eluent to afford 1 in 63% yield (133 mg, 69.1 µmol) as a yellow solid. ¹H NMR (400 MHz, CD₂Cl₂, ppm): δ 9.35 (s, 4H), 8.49 (d, J = 7.8 Hz, 4H), 8.08 (t, J = 7.8 Hz, 2H), 7.86 (d, J = 8.0 Hz, 8H), 7.55–7.53 (m, 12H), 7.23 (s, 4H), 2.77 (t, J = 8.0 Hz, 8H), 2.69 (t, J = 8.0 Hz, 8H), 1.72–1.64 (m, 8H), 1.61–1.53 (m, 8H), 1.46–1.34 (m, 24H), 1.32–1.23 (m, 24H), 0.94–0.90 (m, 12H), 0.87–0.83 (m, 12H). ¹³C NMR (101 MHz, CDCl₃, ppm): δ 141.2, 141.0, 140.5, 140.4, 140.2, 139.8, 133.6, 132.2, 131.3, 130.6, 129.8, 126.4, 125.4, 124.9, 124.1, 123.7, 122.9, 36.2, 32.9, 32.1, 31.9, 31.6, 30.5, 29.6, 29.4, 23.1, 22.9, 14.3 (two carbon resonances could not be determined because of signal overlap). HRMS (APCI) m/z: [M + H]⁺ Calcd for C₁₂₂H₁₃₈Br₄ 1919.7605; Found 1919.7610.
A mixture of 5 (670 mg, 1.03 mmol), bis(pinacolato)diboron (1.04 g, 4.11 mmol), Pd$_2$(dba)$_3$ (47 mg, 0.051 mmol), XPhos (98 mg, 0.21 mmol), dry potassium acetate (807 mg, 8.23 mmol) and anhydrous 1,4-dioxane (20 mL) was stirred at 110 °C for 20 h. After the addition of water, the mixture was extracted with DCM. The combined organic layers were washed with brine, dried over anhydrous MgSO$_4$ and concentrated under reduced pressure. The crude product was washed with n-hexane and then filtered to afford 2 in 92% yield (792 mg, 0.949 mmol) as a white solid. $^1$H NMR (500 MHz, CD$_2$Cl$_2$, ppm): δ 7.71 (d$_{AA\cdotXX\cdot}$, $J = 8.2$ Hz, 4H), 7.56 (d$_{AA\cdotXX\cdot}$, $J = 8.5$ Hz, 4H), 7.46 (d$_{AA\cdotXX\cdot}$, $J = 8.4$ Hz, 4H), 7.43 (d$_{AA\cdotXX\cdot}$, $J = 8.1$ Hz, 4H), 6.14 (d$_{AA\cdotXX\cdot}$, $J = 10.5$ Hz, 4H), 6.10 (d$_{AA\cdotXX\cdot}$, $J = 10.5$ Hz, 4H), 3.44 (s, 6H), 3.43 (s, 6H), 1.32 (s, 24H). $^{13}$C NMR (125 MHz, CD$_2$Cl$_2$, ppm): δ 147.1, 143.2, 144.2, 135.1, 133.9, 133.7, 127.3, 126.9, 125.8, 84.2, 75.2, 75.0, 52.22, 52.20, 25.1 (the resonance of the quaternary carbon atom bound to Bpin could not be observed, a feature often observed for this class of compounds). HRMS (ESI) m/z: [M + Na]$^+$ Calcd for C$_{52}$H$_{60}$B$_2$O$_8$ 857.4367; Found 857.4376.

A mixture of 1 (133 mg, 69.1 µmol), 2 (127 mg, 0.152 mmol), SPhos Pd G3 (5.4 mg, 6.9 µmol), aq. K$_3$PO$_4$ (2 M, 3.5 mL, 7.0 mmol) and 1,4-dioxane (35 mL) was stirred at 80 °C for 24 h. After the addition of water, the mixture was extracted with DCM. The combined organic layers were washed with brine, dried over anhydrous MgSO$_4$ and concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography using DCM/Et$_2$O (1:1 v/v) as an eluent to afford the macrocyclic precursor in a mixture with impurities that could not be identified.
A mixture of sodium (104 mg, 4.52 mmol), naphthalene (387 mg, 3.02 mmol) and anhydrous THF (6 mL) was stirred at room temperature for 18 h before use. To a solution of the macrocyclic precursor in anhydrous THF (5 mL), the freshly prepared solution of sodium naphthalenide (4.4 mL, 2.2 mmol) was added at −78 °C and the resultant mixture was stirred at −78 °C for 2 h. A solution of iodine in THF (1 M, 2 mL) was then added at −78 °C and the resultant mixture was stirred at −78 °C for 15 min before the addition of saturated aq. Na₂S₂O₃. The mixture was extracted with DCM and the organic layer was washed with brine, dried over anhydrous MgSO₄ and concentrated under reduced pressure. The crude product was loaded on recycling GPC (eluent: CHCl₃) to afford CPP-bPP in 31% yield (54 mg, 21 µmol) as an orange solid.

1H NMR (500 MHz, CDCl₃, ppm): δ 9.27 (s, 4H), 8.66 (d, J = 7.8 Hz, 4H), 8.18 (t, J = 7.8 Hz, 2H), 7.87 (dₓₓₓₓ, J = 7.7 Hz, 8H), 7.64–7.52 (m, 48H), 7.39 (dₓₓₓₓ, J = 7.8 Hz, 8H), 7.29 (s, 4H), 7.01 (s, 4H), 2.66 (t, J = 8.1 Hz, 8H), 2.60 (t, J = 8.1 Hz, 8H), 1.55–1.48 (m, 16H), 1.26–1.13 (m, 48H), 0.76–0.72 (m, 24H). 13C NMR (125 MHz, CDCl₃, ppm): δ 141.6, 141.0, 140.6, 140.5, 140.2, 140.0, 138.8, 138.7, 138.6, 138.4, 138.1, 138.0, 137.6, 131.9, 131.2, 131.0, 130.2, 130.1, 129.8, 127.7, 127.62, 126.57, 127.5, 126.8, 126.3, 126.2, 125.3, 124.9, 124.1, 122.9, 33.1, 32.8, 31.69, 31.67, 31.6, 31.5, 29.4, 29.2, 22.7, 22.6, 14.2, 14.1. HRMS (APCI) m/z: [M + H]⁺ Calcd for C₁₉₄H₁₈₆ 2516.4627; Found 2516.4631.

Figure S1. MALDI-TOF MS of CPP-bPP (ionization: reflector positive, matrix: DCTB). DCTB = trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile.
X-Ray Crystallography

Qualified single crystals of CPP-bPP were obtained by slow vapor diffusion of CH$_3$CN into a CHCl$_3$ or toluene solution at room temperature. Qualified single crystals of CPP-bPP$\supseteq$C$_{60}$ were obtained by slow vapor diffusion of CH$_3$CN into a toluene solution of the mixture of CPP-bPP and C$_{60}$ at room temperature.

Single-crystal X-ray diffraction study of compound CPP-bPP obtained from CHCl$_3$/CH$_3$CN (CPP-bPP-c) was performed at BL-17A beamline in KEK, and the data processing was performed on the XDS software. The structure was solved by the direct method with SHELXT program and refined by full-matrix least-squares methods using the SHELXL program suite running on the Yadokari-XG 2009 software program. Disordered parts of CPP-bPP were restrained by SIMU, DFIX, and DANG. Disordered solvent molecules were modeled with 6 CHCl$_3$ molecules restrained by SIMU, DFIX, and DANG. Non-hydrogen atoms were analyzed anisotropically, and hydrogen atoms were input at the calculated positions and refined with a riding model.

Single-crystal X-ray diffraction study of compound CPP-bPP obtained from toluene/CH$_3$CN (CPP-bPP-t) was performed at BL41XU beamline in SPring-8, and the data processing was performed on the XDS software. The structure was solved by the direct method with SHELXT program and refined by full-matrix least-squares methods using the SHELXL program suite running on the Yadokari-XG 2009 software program. Compound CPP-bPP was partly restrained by DFIX, and disordered parts were restrained by SIMU, DFIX, and DANG. Disordered solvent molecules were modeled with 9 toluene molecules restrained by SIMU, DFIX, DANG, FLAT, and AFIX 66. Non-hydrogen atoms were analyzed anisotropically, and hydrogen atoms were input at the calculated positions and refined with a riding model.

One level-A alert was suggested by the PLATON/CIF check program. The level-A alert indicated a lack of high-angle diffractions to result in a small sin$\theta_{\text{max}}$/wavelength value below 0.550 (0.5035). This level-A alert from insufficient numbers of diffractions is unavoidable for highly complex structures with the disordered structures, because the disorders are present with solvent molecules, alkyl group conformations and phenylene orientations. Nonetheless, the monochromated synchrotron source allowed us to refine the diffraction data with a resolution of $\sim$0.99 Å, which afforded reliable structures suitable for the present discussion and conclusions.

Single-crystal X-ray diffraction study of the 1:1 CPP-bPP$\supseteq$C$_{60}$ complex was performed at BL-17A beamline in KEK, and the data processing was performed on the XDS software. The structure was solved by the direct method with SHELXT program and refined by full-matrix least-squares methods using the SHELXL program suite running on the Yadokari-XG 2009 software program. Compound CPP-bPP was
partly restrained by SIMU and DFIX, and disordered parts were restrained by SIMU, DFIX, and DANG. C_{60} was modeled as a rigid model with AFIX 6 and restrained by SIMU. Disordered solvent molecules were modeled with 5 toluene molecules restrained by SIMU, DFIX, DANG, and AFIX 66. Non-hydrogen atoms were analyzed anisotropically, and hydrogen atoms were input at the calculated positions and refined with a riding model. One level-A alert was suggested by the PLATON/CIF check program. The level-A alert indicated a lack of high-angle diffractions to result in a small $\sin \theta_{\text{max}}/\lambda$ value below 0.550 (0.5030). This level-A alert from insufficient numbers of diffractions is unavoidable for highly complex structures with the disordered structures, because the disorders are present with solvent molecules, C_{60} molecules, alkyl group conformations and phenylene orientations. Nonetheless, the monochromated synchrotron source allowed us to refine the diffraction data with a resolution of ~1.00 Å, which afforded reliable structures suitable for the present discussion and conclusions.

Crystallographic data were deposited in the Cambridge Crystallographic Data Centre [CCDC 2104607 (CPP-bPP-c), 2104608 (CPP-bPP-t) and 2104609 (CPP-bPP$\supset$C_{60})]. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data of CPP-bPP-c (CCDC 2104607)

| Property                  | Value                      |
|---------------------------|----------------------------|
| Empirical formula         | C_{197}H_{189}Cl_{9}       |
| Formula weight            | 2875.52                    |
| Temperature               | 95(2) K                    |
| Crystal system            | triclinic                  |
| Space group               | P$\bar{1}$                 |
| Unit cell dimensions      | $a = 14.410(3)$ Å, $a = 72.04(3)^\circ$ |
|                          | $b = 16.800(3)$ Å, $\beta = 72.01(3)^\circ$ |
|                          | $c = 18.907(4)$ Å, $\gamma = 79.00(3)^\circ$ |
| Volume                    | 4118.0(18) Å³             |
| Z                         | 1                          |
| Density (calculated)      | 1.160 g cm⁻³               |
| Absorption coefficient    | 0.385 mm⁻¹                 |
| $F(000)$                  | 1524                       |
| Crystal size              | 0.050 × 0.010 × 0.010 mm³  |
| $\theta$ range for data collection | 1.623° to 31.560°         |
Index ranges

-16<=h<=16, -19<=k<=19, -21<=l<=21

Reflections collected

122574

Independent reflections

13345 [R(int) = 0.1880]

Completeness to θ = 31.560

98.3 %

Data / restraints / parameters

13345 / 554 / 1200

Goodness-of-fit on F^2

1.089

Final R indices [I > 2sigma(I)]

R_1 = 0.1082, wR_2 = 0.2755

R indices (all data)

R_1 = 0.2386, wR_2 = 0.3483

Largest diff. peak and hole

0.439 and -0.305 e•Å^-3

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**Table S2.** Crystal data of CPP-\(\cdot\)PP-t (CCDC 2104608)

| Property                              | Value                          |
|---------------------------------------|-------------------------------|
| Empirical formula                     | C_{239.5}H_{238}              |
| Formula weight                        | 3116.28                       |
| Temperature                           | 100(2) K                      |
| Crystal system                        | triclinic                     |
| Space group                           | P-1                           |
| Unit cell dimensions                  |                               |
| a = 14.290(3) Å                       | a = 65.62(3)°                 |
| b = 19.430(3) Å                       | β = 70.47(3)°                 |
| c = 20.890(4) Å                       | γ = 87.59(3)°                 |
| Volume                                | 4948(2) Å^3                   |
| Z                                      | 1                             |
| Density (calculated)                  | 1.046 g cm^-3                 |
| Absorption coefficient                | 0.056 mm^-1                   |
| F(000)                                | 1675                          |
| Crystal size                          | 0.040 × 0.020 × 0.010 mm^3    |
| θ range for data collection           | 1.140° to 20.637°             |
| Index ranges                          | -14<=h<=14, -19<=k<=19, -20<=l<=20 |
| Reflections collected                 | 68675                         |
| Independent reflections               | 10465 [R(int) = 0.1290]       |
| Completeness to θ = 20.637            | 98.9 %                        |
| Data / restraints / parameters        | 10465 / 1459 / 1549           |
Goodness-of-fit on $F^2$ 1.667
Final $R$ indices [$I > 2\sigma(I)$] $R_1 = 0.1291$, $wR_2 = 0.2961$
$R$ indices (all data) $R_1 = 0.1943$, $wR_2 = 0.3310$
Largest diff. peak and hole 0.279 and $-0.189$ e$\cdot \text{Å}^{-3}$

Table S3. Crystal data of CPP-bPP$\supset C_{60}$ (CCDC 2104609)

| Property                  | Value                        |
|----------------------------|------------------------------|
| Empirical formula          | C$_{289}$H$_{226}$           |
| Formula weight             | 3698.68                      |
| Temperature                | 95(2) K                      |
| Crystal system             | triclinic                    |
| Space group                | $P\bar{1}$                   |
| Unit cell dimensions       | $a = 13.780(3)$ Å, $\alpha = 65.04(3)^\circ$  |
|                           | $b = 19.900(4)$ Å, $\beta = 73.33(3)^\circ$  |
|                           | $c = 20.900(4)$ Å, $\gamma = 89.81(3)^\circ$ |
| Volume                     | 4931(2) Å$^3$                |
| Z                          | 1                            |
| Density (calculated)       | 1.245 g cm$^{-3}$            |
| Absorption coefficient     | 0.116 mm$^{-1}$              |
| $F(000)$                   | 1960                         |
| Crystal size               | 0.040 × 0.020 × 0.020 mm$^3$ |
| $\theta$ range for data collection | 1.434$^\circ$ to 26.919$^\circ$ |
| Index ranges               | $-13\leq h\leq 13$, $-19\leq k\leq 19$, $-20\leq l\leq 20$ |
| Reflections collected      | 84698                        |
| Independent reflections    | 10312 [$R(\text{int}) = 0.0858$] |
| Completeness to $\theta = 26.919$ | 98.1 %                      |
| Data / restraints / parameters | 10312 / 1353 / 1661          |
| Goodness-of-fit on $F^2$   | 2.066                        |
| Final $R$ indices [$I > 2\sigma(I)$] | $R_1 = 0.1563$, $wR_2 = 0.4022$ |
| $R$ indices (all data)     | $R_1 = 0.2055$, $wR_2 = 0.4347$ |
| Largest diff. peak and hole | 0.379 and $-0.310$ e$\cdot \text{Å}^{-3}$ |
**Figure S2.** Packing structure of CPP.\(^1\) The thermal ellipsoids are shown at the 20% probability level.

**Figure S3.** Packing structure of CPP-PP.\(^1\) The thermal ellipsoids are shown at the 20% probability level. Solvent molecules are omitted for clarity.

**Figure S4.** Packing structure of CPP-\(^{dH}\)PP-\(^{c}\). The thermal ellipsoids are shown at the 20% probability level. Solvent molecules are omitted for clarity.
**Figure S5.** Packing structure of CPP-$b$PP-$t$, $d = 5.347$ Å. The thermal ellipsoids are shown at the 20% probability level. Solvent molecules are omitted for clarity.

**Figure S6.** Packing structure of 1:1 CPP-$b$PP$\supset$C$_{60}$ complex (C$_{60}$ molecules are omitted). The thermal ellipsoids are shown at the 20% probability level. Solvent molecules are omitted for clarity.
Figure S7. Packing structure of CPP-bPP⊃C₆₀. The thermal ellipsoids are shown at the 20% probability level. Solvent molecules are omitted for clarity. Notably, C₆₀ molecules are randomly residing inside the cavities of CPP-bPP (illustration in (a) is only a representative example). In addition, the arrangement of C₆₀ molecules as shown in (b) on the right is not realistic because the neighboring two C₆₀ molecules (highlighted in green, violet or pink) display a short C–C distance of 2.24 Å, which would give rise to a severe Pauli repulsion.

Figure S8. Distortion of the phenylene rings in the CPP loops of CPP-bPP was assessed by calculating an average value of the angles C₁–C₂–C₃ and C₂–C₃–C₄ for each phenylene ring in the solid-state structure (CHCl₃ / green, toluene / magenta).
Photophysical Properties

A. Determination of the extinction coefficient

![Figure S9](image)

Figure S9. The plot of absorbance versus concentration for the determination of the extinction coefficient of CPP-βPP at 343 nm in CHCl₃.

B. Comparison of photophysical properties of CPP-βPP and CPP-PP

![Figure S10](image)

Figure S10. UV–Vis absorption and fluorescence spectra of (a) CPP-βPP ($\lambda_{ex} = 343$ nm) and (b) CPP-βPP ($\lambda_{ex} = 338$ nm) in CHCl₃ at 25 °C.
C. Determination of the quantum yields

The quantum yield of compound CPP-\(^b\)PP was determined at the excitation wavelengths of 350 and 410 nm in CHCl\(_3\) as described by Jobin Yvon Horiba.\(^8\) Quinine sulfate (0.1 M H\(_2\)SO\(_4\)) and perylene (cyclohexane) were used as standards. The integrated fluorescence area for CPP-\(^b\)PP was 450–650 nm. The quantum yields were calculated using the following equation:

\[
\phi_x = \phi_{\text{std}} \left( \frac{\text{Grad}_x}{\text{Grad}_{\text{std}}} \right) \left( \frac{n^2}{n_{\text{std}}^2} \right)
\]

where the subscripts \(x\) and std denote the unknown and the standard, respectively, \(\phi\) is the quantum yield, Grad is the slope from the plot of integrated fluorescence intensity versus absorbance (Figures S11 and S12) and \(n\) is the refractive index. The refractive indexes of CHCl\(_3\), 0.1 M H\(_2\)SO\(_4\) and cyclohexane are 1.445, 1.332 and 1.426, respectively.

**Figure S11.** The plots of integrated fluorescence (FL) intensity versus absorbance for quinine sulfate and CPP-\(^b\)PP (excitation at 350 nm). The dotted lines are fit to the experimental data (square points).

**Figure S12.** The plots of integrated fluorescence (FL) intensity versus absorbance for perylene and CPP-\(^b\)PP (excitation at 410 nm). The dotted lines are fit to the experimental data (square points).
D. Comparison of the excitation and absorption spectra

![Figure S13. Excitation and absorption spectra of CPP-βPP in CHCl₃.](image)

E. Solvatochromism

![Figure S14. UV–Vis absorption spectra of CPP-βPP in various solvents at 25 °C.](image)

**Host–Guest Complexation**

Test of binding ability of CPP-βPP toward C₆₀ in solution by UV–Vis absorption spectroscopy

![Figure S15. UV–Vis absorption spectra of CPP-βPP in CHCl₃ at 25 °C before and after addition of C₆₀.](image)
Test of binding ability of CPP-bPP toward C₆₀ in thin film by steady-state photoluminescence (PL)

Thin films were fabricated through a stepwise process by using microscope glass substrates. The substrates were cleaned by a standard cleaning process, which involved sequential sonication in ethanol and isopropyl alcohol for 10 and 15 min, respectively, at a minimum temperature of 60 °C, then dried in a nitrogen stream. Additionally, the substrates were cleaned with oxygen plasma for 3 min with a power of 40 W before deposition. The precursor solutions were prepared by dissolving CPP-bPP (2 mg) in 1 mL of chlorobenzene and using its 1:1 mixture with C₆₀. The films were deposited by spin-coating 40 μL of the solution onto the substrate in a glovebox under inert nitrogen atmosphere by a single-step spin-coating process (4000 rpm for 20 s with a ramp of 1000 rpm s⁻¹) followed by annealing at 80 °C for 10 min to remove the residual solvent. The resultant films were used for further analysis.

Steady-state PL spectra were recorded by exciting the films deposited onto microscope glass slides. The emission between 450–850 nm and 850–1200 nm was recorded with a Fluorolog 322 spectrometer (Horiba Jobin Yvon iHR320 and a CCD) within with a bandpass of 5 nm upon excitation at 405 nm. The samples were mounted at 60° and emission recorded at 90° from the incident beam path.

![Graph](image)

**Figure S16.** Steady-state PL spectra of thin films based on CPP-bPP on microscope glass slides upon excitation at 405 nm.

**Redox Properties**

Cyclic voltammetry was performed on a Metrohm Autolab AUT84478 in a standard three-electrode configuration at a scan rate of 50 mV s⁻¹. CPP-bPP was dissolved in DCM that contained tetrabutylammonium hexafluorophosphate (Bu₄NPF₆, 0.1 M) as a supporting electrolyte. Glassy carbon
(inside diameter of 3 mm), platinum and Ag/AgCl were used as the working electrode, the counter electrode and the reference electrode, respectively. Ferrocenium/ferrocene (FeCp$_2^+$/FeCp$_2^0$) was used as a standard. Potentials were referenced to ferrocenium/ferrocene (FeCp$_2^+$/FeCp$_2^0$).

The CH$_2$Cl$_2$ solution of CPP-$b$PP showed two reversible waves, one for oxidation and one for reduction, with a half-wave potential at 0.39 V and −2.09 V versus ferrocenium/ferrocene, respectively. Based on the oxidation and reduction potentials, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energy levels of CPP-$b$PP are estimated as −5.49 eV and −3.01 eV, respectively. The obtained HOMO–LUMO gap is in an excellent agreement with that calculated from the onset of absorption (2.43 eV).

Figure S17. Cyclic voltammogram of CPP-$b$PP.

DFT Calculations

All calculations were performed with Gaussian 16, Revision A.03. The gas-phase geometry was optimized with B3LYP functional and 6-31G(d,p) basis set. Absorption spectrum was calculated at the CAM-B3LYP/6-31G(d,p) level of theory [scrf = (solvent = CHCl$_3$)].

A. Optimized geometry

Figure S18. Optimized structure of CPP-$b$PP. Hydrogen atoms are omitted for clarity.
B. Molecular orbitals

Figure S19. Selected lowest unoccupied molecular orbitals (LUMOs) of CPP-bPP.
Figure S20. Selected highest occupied molecular orbitals (HOMOs) of CPP-$\delta$PP.
C. Absorption spectrum

Optimized structure of CPP-βPP was calculated at the B3LYP/6-31G(d,p) level of DFT. Then, a time-dependent DFT calculation [TD-DFT; CAM-B3LYP/6-31G(d,p); scrf = (solvent = CHCl₃)] of 15 states was performed to calculate the UV–Vis spectra of CPP-βPP.

![Absorption spectrum](image)

| Excited State | Wavelength (nm) | Energy (eV) | Oscillator strength | Major transitions |
|---------------|----------------|-------------|--------------------|-------------------|
| 1             | 456.93         | 2.71        | 1.3447             | HOMO → LUMO (0.69) |
| 2             | 373.23         | 3.32        | 0.0175             | HOMO → LUMO+5 (0.49) |
|               |                |             |                    | HOMO-7 → LUMO (0.32) |
|               |                |             |                    | HOMO-5 → LUMO (0.19) |
| 3             | 336.88         | 3.68        | 0.8242             | HOMO-1 → LUMO+1 (0.62) |
|               |                |             |                    | HOMO-4 → LUMO+4 (0.10) |
| 4             | 334.29         | 3.71        | 1.1550             | HOMO-2 → LUMO+2 (0.61) |
|               |                |             |                    | HOMO-3 → LUMO+3 (0.22) |
| 5             | 317.43         | 3.91        | 3.1006             | HOMO → LUMO+6 (0.32) |
|               |                |             |                    | HOMO → LUMO+8 (0.23) |
|               |                |             |                    | HOMO → LUMO+3 (0.23) |
|               |                |             |                    | HOMO-5 → LUMO (0.23) |
|               |                |             |                    | HOMO → LUMO+11 (0.16) |
|               |                |             |                    | HOMO-7 → LUMO (0.17) |
| 6             | 304.94         | 4.07        | 1.6604             | HOMO → LUMO+6 (0.33) |
|               |                |             |                    | HOMO-5 → LUMO (0.28) |
|               |                |             |                    | HOMO-7 → LUMO (0.27) |
|               |                |             |                    | HOMO → LUMO+5 (0.24) |
|               |                |             |                    | HOMO → LUMO+8 (0.21) |
|               |                |             |                    | HOMO → LUMO+11 (0.17) |

Figure S21. Calculated absorption spectrum and electronic transitions for CPP-βPP.
Conductivity Measurements

Freshly prepared single crystals of CPP-bPP (obtained from toluene) and CPP-PP were picked up. A standard four-probe technique was employed with silver wires (50 µm) attached with PELCO® Silver Paste to secure a conducting pathway to the patterned electrodes. The current passes through two outside contacts, and the two inside contacts are used to measure the voltage drop without current flowing. In contrast to a two-probe measurement, this method enables to eliminate the resistance of wires and contacts. Current density–voltage (J–V) characteristic was measured with a PC-controlled source meter (2400, Keithley, Japan).

The conductivity of single crystals of CPP-bPP (obtained from toluene) and CPP-PP was calculated using the following equations:

\[ J = \sigma \cdot E \]
\[ J = \frac{I}{t \cdot w} \]
\[ E = \frac{V}{L} \]

where \( J \) is current density, \( E \) is electric field, \( t \) is the thickness of the crystal, \( w \) is the width of the crystal, \( L \) is the length of crystal between the silver wires, and \( \sigma \) is the calculated electrical conductivity.

For CPP-bPP, \( t = 11.1 \) µm, \( w = 33.4 \) µm and \( L = 707.4 \) µm.

For CPP-PP, \( t = 6.9 \) µm, \( w = 20.6 \) µm and \( L = 90.1 \) µm.

![Figure S22](image_url). The J–V curves for CPP-bPP and CPP-PP.
Copies of NMR Spectra

$^1$H (400 MHz, top) and $^{13}$C NMR (101 MHz, bottom) of 3 in CD$_2$Cl$_2$ at 25 °C
$^1$H (400 MHz, top) and $^{13}$C NMR (101 MHz, bottom) of 1 in CD$_2$Cl$_2$ at 25 °C
$^1$H (500 MHz, top) and $^{13}$C NMR (125 MHz, bottom) of 2 in CD$_2$Cl$_2$ at 25 °C
$^1$H (400 MHz, top) and $^{13}$C NMR (101 MHz, bottom) of CPP-$^3$PP in CDCl$_3$ at 25 °C
**Cartesian Coordinates**

**CPP$_b$PP (B3LYP/6-31G(d,p), gas phase)**

\[ E = -5932.604301 \text{ Hartree} \]

| Center Number | Atomic Number | Atomic Type | X      | Y      | Z      |
|---------------|---------------|-------------|--------|--------|--------|
| 1             | 6             | 0           | -3.777614 | -3.483938 | 0.273285 |
| 2             | 6             | 0           | -1.179587 | -4.930875 | 0.116918 |
| 3             | 6             | 0           | 0.028735  | -5.615553 | 0.061050 |
| 4             | 6             | 0           | 1.232340  | -4.920771 | 0.045282 |
| 5             | 6             | 0           | -1.232121 | -0.657584 | 0.033823 |
| 6             | 6             | 0           | -2.437980 | -1.422391 | 0.111646 |
| 7             | 6             | 0           | -2.461010 | -2.790424 | 0.182466 |
| 8             | 6             | 0           | -1.213840 | -3.525696 | 0.148865 |
| 9             | 6             | 0           | 1.256353  | -3.515333 | 0.077012 |
| 10            | 6             | 0           | 2.497085  | -2.770210 | 0.034312 |
| 11            | 6             | 0           | 2.460497  | -1.401522 | -0.005722 |
| 12            | 6             | 0           | 1.246210  | -0.645882 | 0.006984 |
| 13            | 6             | 0           | 0.010849  | -1.360096 | 0.052968 |
| 14            | 6             | 0           | 0.017955  | -2.794496 | 0.102892 |
| 15            | 6             | 0           | -0.009984 | 2.916140  | -0.166226 |
| 16            | 6             | 0           | -0.004162 | 1.483380  | -0.081119 |
| 17            | 6             | 0           | 1.238417  | 0.782583  | -0.024962 |
| 18            | 6             | 0           | 2.441883  | 1.551862  | 0.027621 |
| 19            | 6             | 0           | 2.466959  | 2.922360  | -0.006164 |
| 20            | 6             | 0           | 1.221632  | 3.649960  | -0.149996 |
| 21            | 6             | 0           | -1.248091 | 3.631291  | -0.270704 |
| 22            | 6             | 0           | -2.488689 | 2.884003  | -0.264750 |
| 23            | 6             | 0           | -2.452878 | 1.519702  | -0.145672 |
| 24            | 6             | 0           | -1.239415 | 0.768276  | -0.057559 |
| 25            | 6             | 0           | 1.186484  | 5.048087  | -0.294413 |
| 26            | 6             | 0           | -0.022162 | 5.728723  | -0.382633 |
| 27            | 6             | 0           | -1.225635 | 5.034676  | -0.350472 |
| 28            | 6             | 0           | -3.814103 | 3.559561  | -0.369732 |
|   | 6 | 0 | -4.778282 | 3.370327 | 0.631835 |
|---|---|---|------------|----------|----------|
| 30 | 6 | 0 | -6.041266 | 3.947358 | 0.531594 |
| 31 | 6 | 0 | -6.400314 | 4.732874 | -0.576486 |
| 32 | 6 | 0 | -5.432109 | 4.927997 | -1.574785 |
| 33 | 6 | 0 | -4.165412 | 4.355624 | -1.473126 |
| 34 | 6 | 0 | -4.100811 | -4.336922 | 1.342334 |
| 35 | 6 | 0 | -5.359284 | -4.928032 | 1.437557 |
| 36 | 6 | 0 | -6.041266 | -4.697249 | 0.465154 |
| 37 | 6 | 0 | -6.014384 | -3.856117 | -0.610134 |
| 38 | 6 | 0 | -4.760209 | -3.258785 | -0.702592 |
| 39 | 6 | 0 | -7.775753 | 5.304757 | -0.643514 |
| 40 | 6 | 0 | -8.259137 | 6.014760 | 0.465959 |
| 41 | 6 | 0 | -9.579517 | 6.456928 | 0.583795 |
| 42 | 6 | 0 | -10.473053 | 6.158416 | -0.466828 |
| 43 | 6 | 0 | -9.970667 | 5.517166 | -1.609744 |
| 44 | 6 | 0 | -8.647672 | 5.084818 | -1.733485 |
| 45 | 6 | 0 | -11.947712 | 6.346754 | -0.366907 |
| 46 | 6 | 0 | -12.639655 | 5.799685 | 0.725342 |
| 47 | 6 | 0 | -14.025802 | 5.727019 | 0.737661 |
| 48 | 6 | 0 | -14.797341 | 6.208592 | -0.335806 |
| 49 | 6 | 0 | -14.108903 | 6.840956 | -1.386323 |
| 50 | 6 | 0 | -12.715841 | 6.901023 | -1.404680 |
| 51 | 6 | 0 | -16.239241 | 5.861220 | -0.395786 |
| 52 | 6 | 0 | -16.975501 | 5.596662 | 0.772670 |
| 53 | 6 | 0 | -18.168395 | 4.886067 | 0.728284 |
| 54 | 6 | 0 | -18.703743 | 4.424898 | -0.488844 |
| 55 | 6 | 0 | -18.076044 | 4.878717 | -1.664139 |
| 56 | 6 | 0 | -16.867160 | 5.565850 | -1.619019 |
| 57 | 6 | 0 | -7.713061 | -5.289125 | 0.526611 |
| 58 | 6 | 0 | -8.576457 | -5.114074 | 1.631214 |
| 59 | 6 | 0 | -9.895621 | -5.557361 | 1.506280 |
| 60 | 6 | 0 | -10.401475 | -6.169258 | 0.348661 |
| 61 | 6 | 0 | -9.514075 | -6.425777 | -0.718315 |
| 62 | 6 | 0 | -8.198179 | -5.970351 | -0.599633 |
| 63 | 6 | 0 | -11.874712 | -6.370815 | 0.255164 |
| 64 | 6 | 0 | -12.579740 | -5.810575 | -0.822004 |
|   |   |   |          |          |          |
|---|---|---|----------|----------|----------|
| 65| 6 | 0 | -13.966619 | -5.754349 | -0.825038 |
| 66| 6 | 0 | -14.725887 | -6.265160 | 0.243582  |
| 67| 6 | 0 | -14.024009 | -6.907933 | 1.278656  |
| 68| 6 | 0 | -12.630220 | -6.952871 | 1.287141  |
| 69| 6 | 0 | -16.171646 | -5.936957 | 0.315535  |
| 70| 6 | 0 | -16.918006 | -5.673707 | -0.846730 |
| 71| 6 | 0 | -18.119302 | -4.978373 | -0.790257 |
| 72| 6 | 0 | -18.652246 | -4.531657 | 0.433294  |
| 73| 6 | 0 | -18.011802 | -4.984966 | 1.601846  |
| 74| 6 | 0 | -16.795104 | -5.657519 | 1.544721  |
| 75| 6 | 0 | -19.670957 | 3.296458  | -0.493037 |
| 76| 6 | 0 | -19.640244 | 2.364100  | -1.545920 |
| 77| 6 | 0 | -20.149293 | 1.081043  | -1.390652 |
| 78| 6 | 0 | -20.703231 | 0.661826  | -0.168850 |
| 79| 6 | 0 | -20.924198 | 1.652545  | 0.804954  |
| 80| 6 | 0 | -20.428249 | 2.942857  | 0.641375  |
| 81| 6 | 0 | -19.632194 | -3.414400 | 0.449472  |
| 82| 6 | 0 | -19.599520 | -2.482624 | 1.502777  |
| 83| 6 | 0 | -20.123220 | -1.204654 | 1.353910  |
| 84| 6 | 0 | -20.694568 | -0.790498 | 0.138403  |
| 85| 6 | 0 | -20.916482 | -1.782934 | -0.833463 |
| 86| 6 | 0 | -20.405570 | -3.068175 | -0.676270 |
| 87| 6 | 0 | -9.990595  | 7.226714  | 1.820585  |
| 88| 6 | 0 | -8.233682  | 4.341445  | -2.983934 |
| 89| 6 | 0 | -9.925507  | -7.165111 | -1.973529 |
| 90| 6 | 0 | -8.156531  | -4.406314 | 2.900132  |
| 91| 6 | 0 | 3.820911   | -3.457221 | 0.017005  |
| 92| 6 | 0 | 3.778485   | 3.615078  | 0.131449  |
| 93| 6 | 0 | 3.997730   | 4.616882  | 1.093159  |
| 94| 6 | 0 | 5.253579   | 5.195924  | 1.261557  |
| 95| 6 | 0 | 6.351967   | 4.796294  | 0.482484  |
| 96| 6 | 0 | 6.126366   | 3.803490  | -0.487505 |
| 97| 6 | 0 | 4.871251   | 3.228512  | -0.660846 |
| 98| 6 | 0 | 4.236218   | -4.290975 | 1.068951  |
| 99| 6 | 0 | 5.502546   | -4.871391 | 1.069106  |
|100| 6 | 0 | 6.403796   | -4.649516 | 0.015385  |
|   |   |   | 5.978137 | -3.834765 | -1.045769 |
|---|---|---|---|---|---|
| 101| 6 | 0 | 4.715265 | -3.246010 | -1.042938 |
| 102| 6 | 0 | 7.723074 | 5.356633 | 0.645433 |
| 103| 6 | 0 | 8.438698 | 5.710908 | -0.508776 |
| 104| 6 | 0 | 9.782451 | 6.093915 | -0.507440 |
| 105| 6 | 0 | 10.462695 | 6.115153 | 0.732570 |
| 106| 6 | 0 | 9.727616 | 5.825969 | 1.893193 |
| 107| 6 | 0 | 8.381216 | 5.453026 | 1.892825 |
| 108| 6 | 0 | 11.943377 | 6.243140 | 0.843978 |
| 109| 6 | 0 | 12.632003 | 5.283056 | 1.606362 |
| 110| 6 | 0 | 14.018313 | 5.225818 | 1.619565 |
| 111| 6 | 0 | 14.795319 | 6.126128 | 0.869037 |
| 112| 6 | 0 | 14.114474 | 7.143780 | 0.180221 |
| 113| 6 | 0 | 12.720350 | 7.201925 | 0.170161 |
| 114| 6 | 0 | 16.239687 | 5.831718 | 0.695372 |
| 115| 6 | 0 | 16.845645 | 5.929387 | -0.569593 |
| 116| 6 | 0 | 18.043917 | 5.276860 | -0.844733 |
| 117| 6 | 0 | 18.681472 | 4.487379 | 0.129474 |
| 118| 6 | 0 | 18.174686 | 4.555558 | 1.440045 |
| 119| 6 | 0 | 16.983854 | 5.216794 | 1.717212 |
| 120| 6 | 0 | 7.780441 | -5.223245 | -0.000672 |
| 121| 6 | 0 | 8.715051 | -4.965615 | 1.026551 |
| 122| 6 | 0 | 10.019133 | -5.431493 | 0.854095 |
| 123| 6 | 0 | 10.448464 | -6.146470 | -0.276678 |
| 124| 6 | 0 | 9.496944 | -6.460884 | -1.270405 |
| 125| 6 | 0 | 8.192810 | -5.981322 | -1.105798 |
| 126| 6 | 0 | 11.909988 | -6.412246 | -0.394465 |
| 127| 6 | 0 | 12.660751 | -6.857128 | 0.708516 |
| 128| 6 | 0 | 14.052180 | -6.822128 | 0.698370 |
| 129| 6 | 0 | 14.757694 | -6.338900 | -0.417339 |
| 130| 6 | 0 | 14.010633 | -6.009874 | -1.561178 |
| 131| 6 | 0 | 12.619695 | -6.044585 | -1.549597 |
| 132| 6 | 0 | 16.188655 | -5.953057 | -0.344093 |
| 133| 6 | 0 | 16.660031 | -5.311122 | 0.812853 |
| 134| 6 | 0 | 17.851325 | -4.598161 | 0.805617 |
| 135| 6 | 0 | 18.642267 | -4.497987 | -0.354054 |
|   |   |   | 137          6           0       18.254830 | -5.286786 | -1.454445 |
|---|---|---|------------------|-----------|-----------|
|   |   |   | 138          6           0       17.052305 | -5.989109 | -1.453270 |
|   |   |   | 139          6           0       19.616552 | 3.391437  | -0.229804 |
|   |   |   | 140          6           0       19.389772 | 2.688740  | -1.425895 |
|   |   |   | 141          6           0       19.873598 | 1.401090  | -1.608001 |
|   |   |   | 142          6           0       20.615059  | 0.746988  | -0.607117 |
|   |   |   | 143          6           0       21.019062  | 1.530648  | 0.491582  |
|   |   |   | 144          6           0       20.527370  | 2.820286  | 0.678616  |
|   |   |   | 145          6           0       19.637105  | -3.399326 | -0.457808 |
|   |   |   | 146          6           0       20.140774  | -2.746554 | 0.682795  |
|   |   |   | 147          6           0       20.620183  | -1.443557 | 0.614154  |
|   |   |   | 148          6           0       20.652321  | -0.738238 | -0.603371 |
|   |   |   | 149          6           0       20.399271  | -1.487795 | -1.767590 |
|   |   |   | 150          6           0       19.888142  | -2.778329 | -1.695743 |
|   |   |   | 151          6           0       10.449346  | 6.394071  | -1.831264 |
|   |   |   | 152          6           0       7.725189   | 5.107377  | 3.211322  |
|   |   |   | 153          6           0       9.823042   | -7.293457 | -2.491503 |
|   |   |   | 154          6           0       8.380544   | -4.154520 | 2.258736  |
|   |   |   | 155          1           0       0.032026   | -6.700818 | 0.019885  |
|   |   |   | 156          1           0       2.166972   | -5.465499 | -0.011485 |
|   |   |   | 157          1           0       3.389393   | -0.906911 | 0.148729  |
|   |   |   | 158          1           0       3.408319   | -0.879212 | -0.042109 |
|   |   |   | 159          1           0       3.387153   | 1.040442  | 0.157814  |
|   |   |   | 160          1           0       3.399782   | 0.994953  | -0.159973 |
|   |   |   | 161          1           0       2.116796   | 5.600875  | -0.336634 |
|   |   |   | 162          1           0       3.361841   | -4.526681 | 2.115099  |
|   |   |   | 163          1           0       5.578905   | -0.392380 |
|   |   |   | 164          1           0       4.528996   | 2.766167  | 1.499229  |
|   |   |   | 165          1           0       6.773562   | 3.772714  | 1.314214  |
|   |   |   | 166          1           0       5.668229   | 5.541624  | -2.438406 |
|   |   |   | 167          1           0       3.442565   | 4.515144  | -2.267641 |
|   |   |   | 168          1           0       3.361841   | -4.526681 | 2.115099  |
|   |   |   | 169          1           0       5.574796   | -5.584612 | 2.274686  |
|   |   |   | 170          1           0       6.761328   | -3.655050 | -1.372329 |
|   |   |   | 171          1           0       4.532054   | -2.611558 | -1.544349 |
|   |   |   |                     |                     |                     |
|---|---|---|---------------------|---------------------|---------------------|
|173| 1 | 0 | -7.568343          | 6.226122            | 1.278659            |
|174| 1 | 0 | -10.666861         | 5.281959            | -2.410570           |
|175| 1 | 0 | -12.080716         | 5.344941            | 1.536753            |
|176| 1 | 0 | -14.511699         | 5.204571            | 1.554612            |
|177| 1 | 0 | -14.665825         | 7.270292            | -2.214173           |
|178| 1 | 0 | -12.212944         | 7.365811            | -2.248170           |
|179| 1 | 0 | -16.572522         | 5.882632            | 1.739188            |
|180| 1 | 0 | -18.631787         | 4.597239            | 1.665714            |
|181| 1 | 0 | -18.490527         | 4.620657            | -2.633603           |
|182| 1 | 0 | -16.357645         | 5.786023            | -2.552096           |
|183| 1 | 0 | -10.586792         | -5.354517           | 2.320187            |
|184| 1 | 0 | -7.512831          | -6.147319           | -1.425101           |
|185| 1 | 0 | -12.031330         | -5.333526           | -1.627684           |
|186| 1 | 0 | -14.463956         | -5.222720           | -1.629114           |
|187| 1 | 0 | -14.571216         | -7.358411           | 2.101789            |
|188| 1 | 0 | -12.116977         | -7.428151           | 2.118462            |
|189| 1 | 0 | -16.516767         | -5.947900           | -1.817410           |
|190| 1 | 0 | -18.592202         | -4.688701           | -1.722679           |
|191| 1 | 0 | -18.423252         | -4.737364           | 2.575369            |
|192| 1 | 0 | -16.276593         | -5.877810           | 2.472859            |
|193| 1 | 0 | -19.085881         | 2.588580            | -2.450534           |
|194| 1 | 0 | -19.975527         | 0.351048            | -2.174978           |
|195| 1 | 0 | -21.427025         | 1.391654            | 1.732142            |
|196| 1 | 0 | -20.569450         | 3.661465            | 1.443009            |
|197| 1 | 0 | -19.032673         | -2.702238           | 2.400872            |
|198| 1 | 0 | -19.948112         | -0.473252           | 2.136637            |
|199| 1 | 0 | -21.432187         | -1.526634           | -1.754837           |
|200| 1 | 0 | -20.547933         | -3.787898           | -1.476729           |
|201| 1 | 0 | -9.154582          | 7.828538            | 2.189575            |
|202| 1 | 0 | -10.831527         | 7.895190            | 1.622304            |
|203| 1 | 0 | -10.291672         | 6.562352            | 2.639889            |
|204| 1 | 0 | -9.112203          | 3.960641            | -3.512045           |
|205| 1 | 0 | -7.691479          | 4.987956            | -3.684398           |
|206| 1 | 0 | -7.577627          | 3.496582            | -2.757561           |
|207| 1 | 0 | -10.233952         | -6.481366           | -2.773933           |
|208| 1 | 0 | -9.086892          | -7.751242           | -2.361464           |

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|   |   |   | x   | y   | z   |
|---|---|---|-----|-----|-----|
| 209 | 1 | 0 | -10.760990 | -7.844427 | -1.789906 |
| 210 | 1 | 0 | -7.517455 | -3.543621 | 2.693039 |
| 211 | 1 | 0 | -9.033116 | -4.057998 | 3.453278 |
| 212 | 1 | 0 | -7.593417 | -5.066851 | 3.570318 |
| 213 | 1 | 0 | 3.178338 | 4.933046 | 1.731019 |
| 214 | 1 | 0 | 5.378065 | 5.973923 | 2.007251 |
| 215 | 1 | 0 | 6.956563 | 3.463699 | -1.099196 |
| 216 | 1 | 0 | 4.730845 | 2.466147 | -1.421506 |
| 217 | 1 | 0 | 3.564768 | -4.471225 | 1.903223 |
| 218 | 1 | 0 | 5.794643 | -5.509771 | 1.897207 |
| 219 | 1 | 0 | 6.657656 | -3.644696 | -1.871471 |
| 220 | 1 | 0 | 4.412450 | -2.615005 | -1.873481 |
| 221 | 1 | 0 | 7.922855 | 5.658808 | -1.463921 |
| 222 | 1 | 0 | 10.247152 | 5.861525 | 2.847142 |
| 223 | 1 | 0 | 12.066648 | 4.519778 | 2.131555 |
| 224 | 1 | 0 | 14.505429 | 4.411611 | 2.145972 |
| 225 | 1 | 0 | 14.679594 | 7.889910 | -0.371559 |
| 226 | 1 | 0 | 12.231909 | 7.998519 | -0.381252 |
| 227 | 1 | 0 | 16.319860 | 6.429826 | -1.377466 |
| 228 | 1 | 0 | 18.442243 | 5.310306 | -1.854573 |
| 229 | 1 | 0 | 18.654508 | 3.985802 | 2.229690 |
| 230 | 1 | 0 | 16.583328 | 5.184461 | 2.726060 |
| 231 | 1 | 0 | 10.759676 | -5.173265 | 1.605964 |
| 232 | 1 | 0 | 7.456610 | -6.210437 | -1.872733 |
| 233 | 1 | 0 | 12.142342 | -7.200701 | 1.599071 |
| 234 | 1 | 0 | 14.599008 | -7.140135 | 1.581508 |
| 235 | 1 | 0 | 14.521694 | -5.621137 | -2.436734 |
| 236 | 1 | 0 | 12.078632 | -5.687901 | -2.419718 |
| 237 | 1 | 0 | 16.025635 | -5.263271 | 1.692358 |
| 238 | 1 | 0 | 18.101640 | -4.009750 | 1.681214 |
| 239 | 1 | 0 | 18.871714 | -5.309311 | -2.347798 |
| 240 | 1 | 0 | 16.757706 | -6.537162 | -2.343868 |
| 241 | 1 | 0 | 18.703371 | 3.092790 | -2.162523 |
| 242 | 1 | 0 | 19.542968 | 0.850212 | -2.481311 |
| 243 | 1 | 0 | 21.669349 | 1.104551 | 1.249950 |
| 244 | 1 | 0 | 20.803492 | 3.364060 | 1.577712 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 245 | 1 | 0 | 20.066417 | -3.221438 | 1.655936 |
| 246 | 1 | 0 | 20.856633 | -0.931101 | 1.541078 |
| 247 | 1 | 0 | 20.503830 | -1.024351 | -2.743564 |
| 248 | 1 | 0 | 19.571316 | -3.258920 | -2.615633 |
| 249 | 1 | 0 | 9.850296  |  6.002378 | -2.657905 |
| 250 | 1 | 0 | 10.562917 |  7.471798 | -1.998488 |
| 251 | 1 | 0 | 11.448572 |  5.954482 | -1.894435 |
| 252 | 1 | 0 | 8.482567  |  4.879016 |  3.966355 |
| 253 | 1 | 0 | 7.123914  |  5.937529 |  3.601209 |
| 254 | 1 | 0 | 7.059669  |  4.244553 |  3.123047 |
| 255 | 1 | 0 | 8.952433  | -7.882781 | -2.794642 |
| 256 | 1 | 0 | 10.102187 | -6.672278 | -3.351691 |
| 257 | 1 | 0 | 10.652169 | -7.980217 | -2.306003 |
| 258 | 1 | 0 | 7.741251  | -3.299612 |  2.022074 |
| 259 | 1 | 0 | 7.849816  | -4.750020 |  3.010938 |
| 260 | 1 | 0 | 9.293309  | -3.779244 |  2.729585 |

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