

## Electronic Supplementary Information

### Two pyrene-based cagearene constitutional isomers: synthesis, separation, and host–guest chemistry

Yating Li,<sup>a‡</sup> Shang Li,<sup>a‡</sup> Mengbin Wang,<sup>b</sup> Li Shao,<sup>c</sup> Shuai Fang,<sup>\*a</sup> Bin Hua<sup>\*a,b</sup> and  
Feihe Huang<sup>\*a,b</sup>

<sup>a</sup>*Stoddart Institute of Molecular Science, Department of Chemistry, Zhejiang University,  
Hangzhou 310058, P. R. China. Email addresses: fangshuai123@zju.edu.cn;  
huabin@zju.edu.cn; fhuang@zju.edu.cn; Fax and Tel: +86-571-8795-3189.*

<sup>b</sup>*Zhejiang-Israel Joint Laboratory of Self-Assembling Functional Materials, ZJU-Hangzhou  
Global Scientific and Technological Innovation Center, Zhejiang University, Hangzhou  
311215, P. R. China*

<sup>c</sup>*Department of Materials Science and Engineering, Zhejiang Sci-Tech University, Hangzhou  
310018, P. R. China*

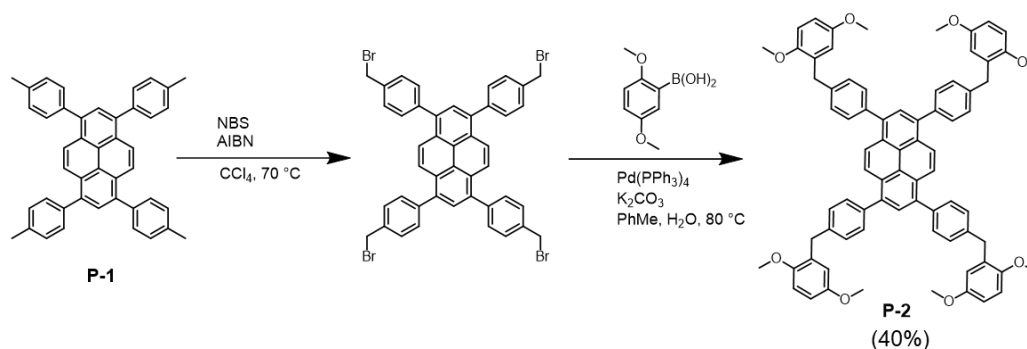
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## ***1. General information***

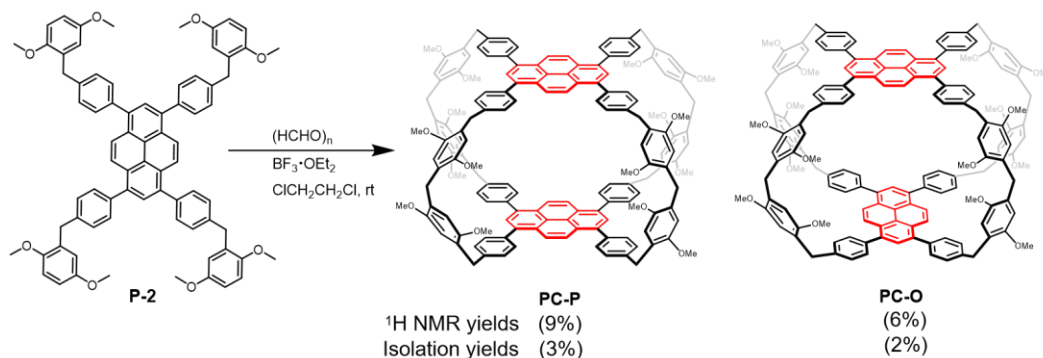
All reagents including guest compounds and solvents were purchased from commercial sources and used without further purification. **P-1** was prepared according to a reported procedure.<sup>S1</sup> NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer, a Bruker AVANCE DMX 500 spectrometer, or an Agilent DD2-600 spectrometer at ambient temperature. MALDI-TOF mass spectra were obtained on a Bruker UltrafleXtreme instrument. High performance liquid chromatography (HPLC) was operated on a reversed-phase column with Waters2695. Single crystal X-ray diffraction (SCXRD) was performed on a Bruker D8 VENTURECMOS X-ray diffractometer with graphite monochromatic Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). Melting points were obtained with a SGW X-4 INESA instrument. UV-Vis spectra were recorded on a UV-2600 spectrometer (Shimadzu Corporation, Japan) at 20 °C in a 1 cm quartz cell. Fluorescence emission spectra were collected on a RF-5301 spectrofluorophotometer, a RF-6000 spectrofluorophotometer (Shimadzu Corporation, Japan) or an Edinburgh FS1000 spectrofluorometer. Absolute fluorescence quantum yields were measured on an Edinburgh FS1000 spectrofluorometer.

## 2. Synthesis of cagearenes.



**Scheme S1** Synthetic route to **P-2**.

**P-1** (562 mg, 1.00 mmol) was added into a round bottom flask, followed by the addition of *n*-bromosuccinimide (NBS) (783 mg, 4.40 mmol), 2,2'-azobis(2-methylpropionitrile) (AIBN) (66 mg, 0.40 mmol) and carbon tetrachloride (CCl<sub>4</sub>, 15 mL). After being degassed through evacuation and nitrogen purging, the mixture was reacted at 70 °C overnight. The reaction mixture was then evaporated, extracted with DCM and washed with water. After the solvent was removed, the crude product was recrystallized in ethyl acetate/petroleum ether to obtain yellow powder. Next, the obtained powder, 2,5-dimethoxyphenylboronic acid (1201 mg, 6.60 mmol), K<sub>2</sub>CO<sub>3</sub> (607 mg, 4.40 mmol) and Pd(PPh<sub>3</sub>)<sub>4</sub> (204 mg, 0.18 mmol) were combined in a flask, and then toluene (90 mL) and distilled water (H<sub>2</sub>O, 18 mL) were added. The flask was degassed by evacuation and purging with nitrogen for three times. The reaction was stirred overnight at 80 °C under nitrogen atmosphere and then quenched with water. The organic layer was washed with water, and then dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>. After the solvent was evaporated, the crude product was purified by column chromatography (dichloromethane/petroleum ether, 1:2 v/v) and recrystallized to obtain **P-2** as pale yellow powder (443 mg, 40%). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, 298 K) δ (ppm): 8.15 (s, 4H), 7.96 (s, 2H), 7.55 (d, *J* = 8.1 Hz, 8H), 7.36 (d, *J* = 8.0 Hz, 8H), 6.84 (d, *J* = 8.8 Hz, 4H), 6.79–6.74 (m, 8H), 4.06 (s, 8H), 3.82 (s, 12H), 3.76 (s, 12H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 298 K) δ (ppm): 153.80, 151.96, 140.02, 138.86, 137.24, 131.07, 130.75, 129.72, 129.02, 128.18, 126.19, 125.38, 117.12, 111.77, 111.61, 56.30, 55.86, 35.98. MALDI-TOF MS (Figure S7): *m/z* calcd. for C<sub>76</sub>H<sub>66</sub>O<sub>8</sub>H<sup>+</sup> [M+H]<sup>+</sup> 1107.483, found 1107.483, error 0 ppm. Melting point: 123.0–123.9 °C.



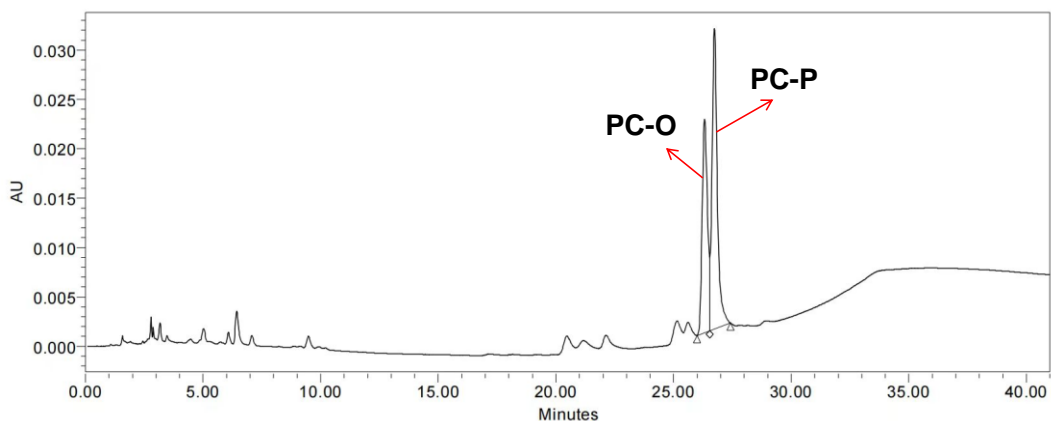
**Scheme S2** Synthetic route to **PC-P** and **PC-O**.

**P-2** (1107 mg, 1.00 mmol), paraformaldehyde (240 mg, 8.00 mmol) and anhydrous dichloroethane (DCE) (625 mL) were mixed in a flask under the nitrogen protection. Then boron trifluoride diethyl etherate (0.5 mL) was added. The reaction was detected by thin-layer chromatography, and water was added when the reactants disappeared. The organic layer was washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After concentrating the filtrate through reduced pressure distillation, the crude product was purified by column chromatography (aluminum oxide, dichloromethane/petroleum ether = 1:1) and recrystallized to obtain the product, **PC-P** (30.3 mg, 3%) and **PC-O** (20.4 mg, 2%).

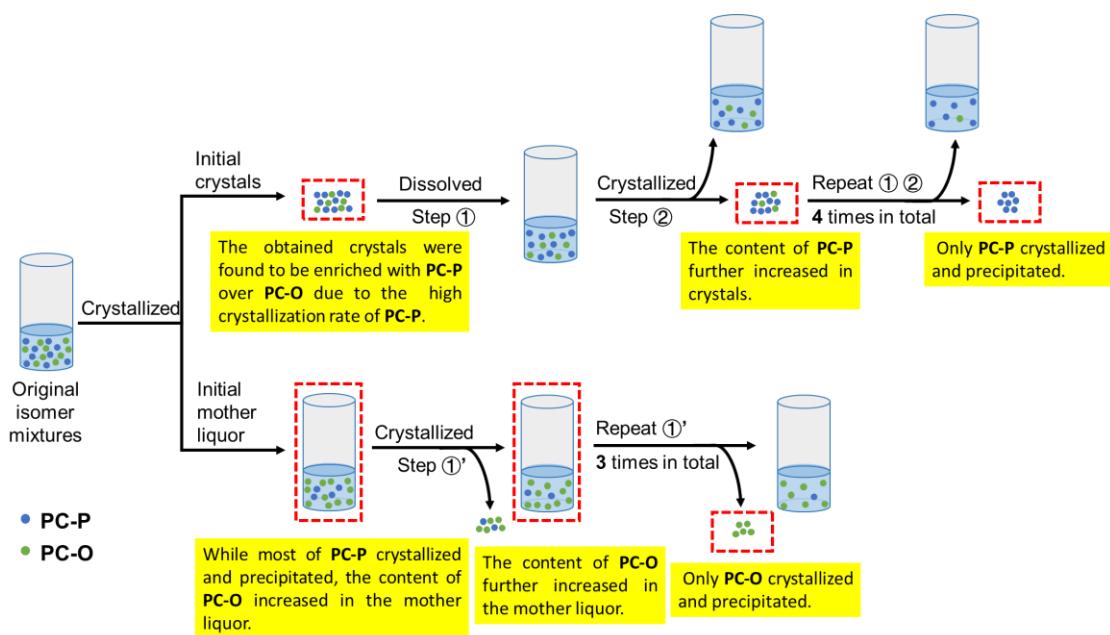
**PC-P:** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K)  $\delta$  (ppm): 7.91 (s, 8H), 7.72 (s, 4H), 7.37–7.22 (m, 32H), 7.03 (s, 8H), 6.72 (s, 8H), 3.99 (s, 16H), 3.92 (s, 8H), 3.84 (s, 24H), 3.79 (s, 24H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 298 K)  $\delta$  (ppm): 151.43, 151.19, 140.60, 138.58, 136.79, 130.56, 129.54, 128.80, 128.57, 127.77, 127.45, 125.81, 125.00, 114.83, 113.65, 56.25, 56.15, 36.10, 30.29. MALDI-TOF MS (Figure S11):  $m/z$  calcd for C<sub>156</sub>H<sub>132</sub>O<sub>16</sub>H<sup>+</sup> [M+H]<sup>+</sup>, 2261.959; found 2261.970, error 5 ppm. The solid powder of **PC-P** remains stable and does not melt at 315 °C. However, it begins to deteriorate once the temperature surpasses this threshold.

**PC-O:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 298 K)  $\delta$  (ppm): 7.92 (s, 8H), 7.74 (s, 4H), 7.34 (d,  $J$  = 7.8 Hz, 18H), 7.22 (s, 14H), 6.97 (s, 8H), 6.72 (s, 8H), 4.09 (s, 3H), 4.05 (s, 5H), 3.97 (s, 5H), 3.93 (s, 11H), 3.81 (s, 24H), 3.75 (s, 24H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, 298 K)  $\delta$  (ppm): 151.60, 151.47, 140.56, 138.65, 136.88, 130.56, 128.90, 128.44, 127.82, 127.29, 125.91, 125.01, 114.83, 114.04, 56.30, 35.99, 29.86. MALDI-TOF MS (Figure S15):  $m/z$  calcd for

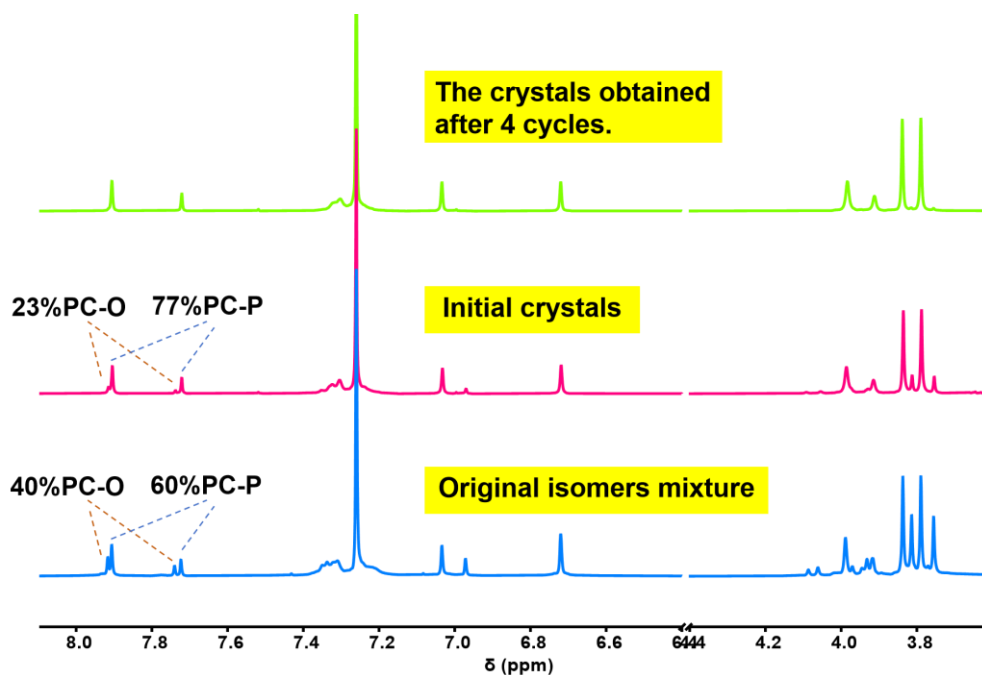
$C_{156}H_{132}O_{16}H^+ [M+H]^+$ , 2261.959; found 2261.961, error 1 ppm. The solid powder of **PC-O** remains stable and does not melt at 315 °C. However, it begins to deteriorate once the temperature surpasses this threshold.



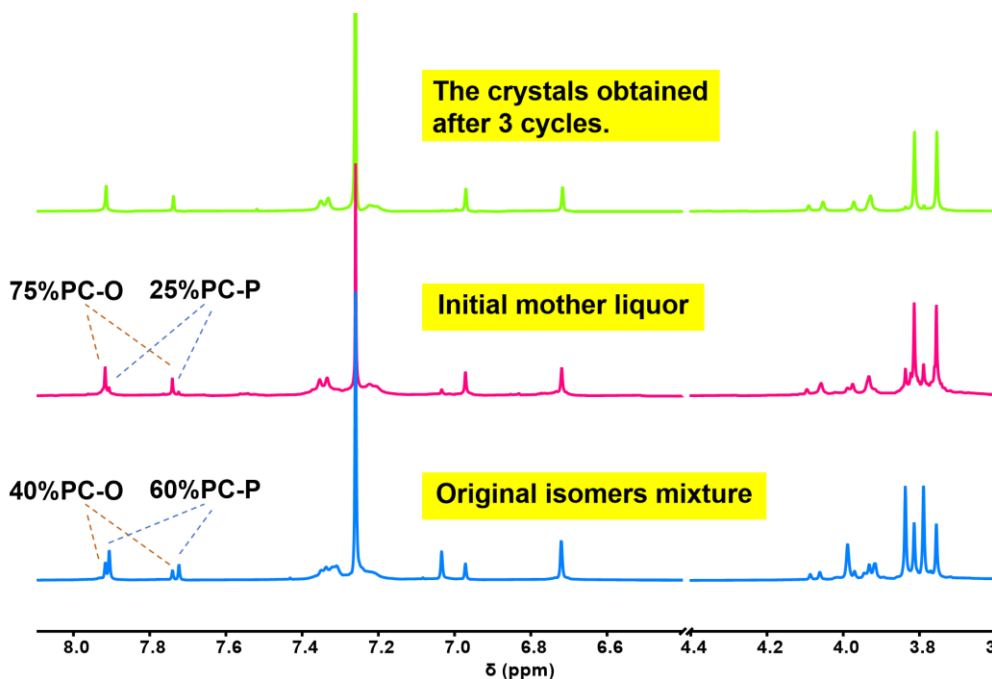
**Fig. S1** HPLC spectrum of **PC-P** and **PC-O**.



**Fig. S2** The designed process for separating **PC-P** and **PC-O**.



**Fig. S3** The changes of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ , 298 K) in the process of purifying **PC-P**. After the first crystallization purification, the content of **PC-P** within the obtained crystals increased significantly. After the fourth crystallization purification, pure **PC-P** was obtained.



**Fig. S4** The changes of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ , 298 K) in the process of purifying **PC-O**. After the first crystallization purification, the content of **PC-O** in the mother liquor increased significantly. After the third crystallization purifications, pure **PC-O** was obtained.

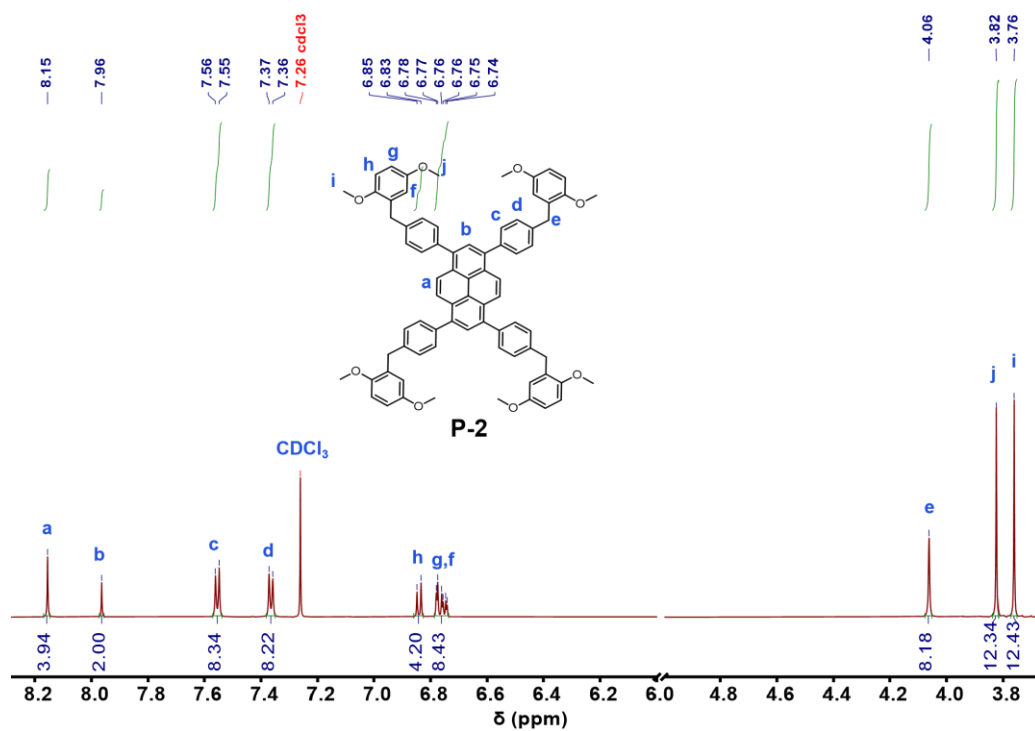


Fig. S5 <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>, 298 K) of P-2.

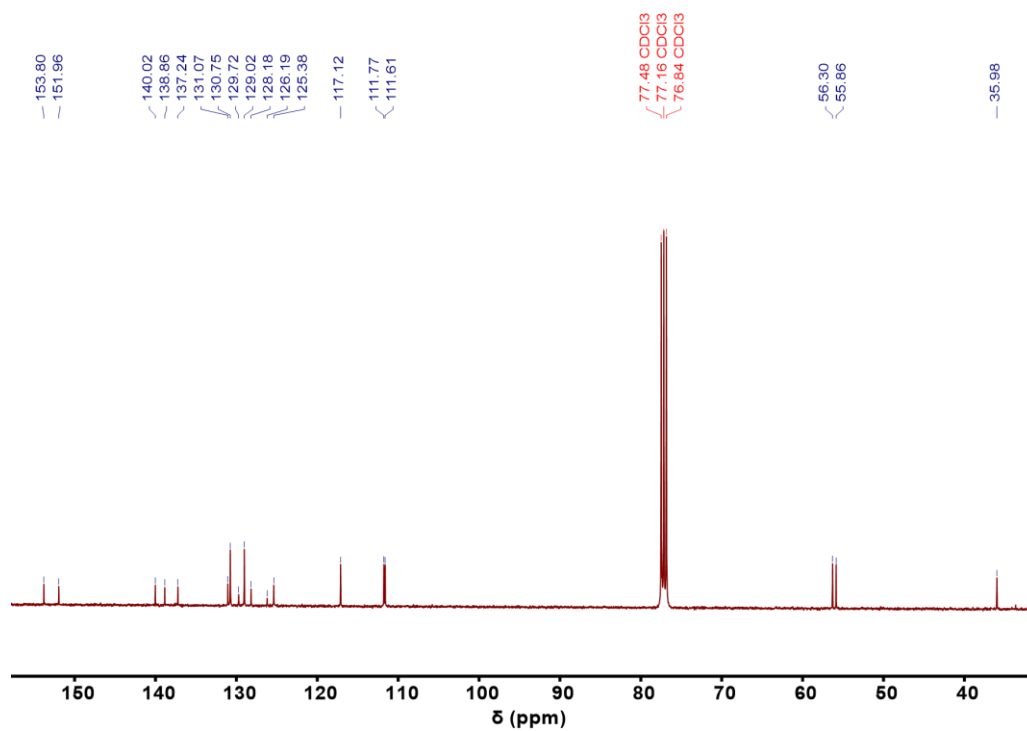


Fig. S6 <sup>13</sup>C NMR spectrum (100 MHz, CDCl<sub>3</sub>, 298 K) of P-2.

### MALDI-TOF Mass Spectrum

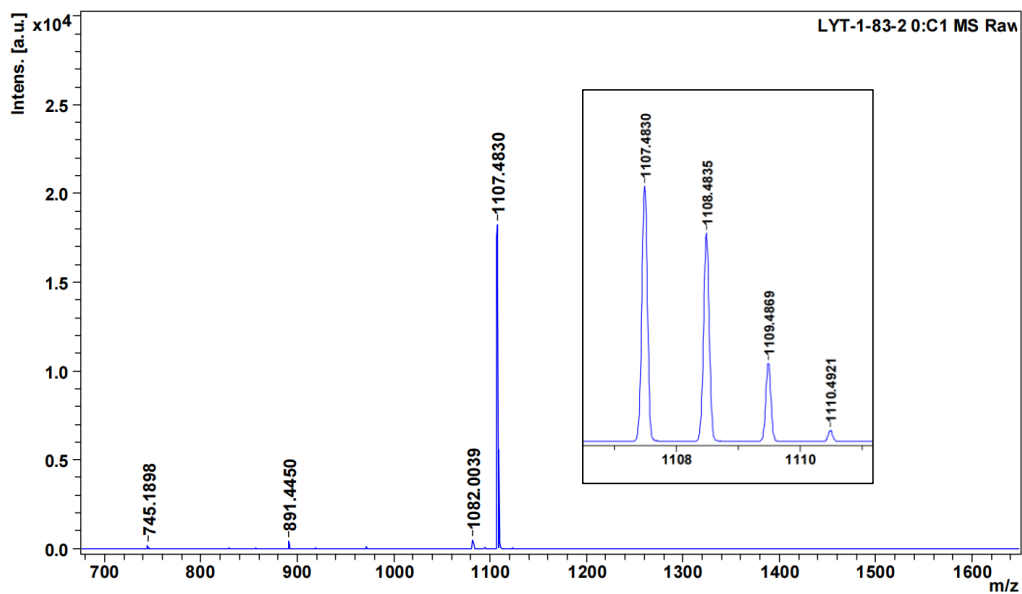


Fig. S7 MALDI-TOF MS spectrum of P-2.

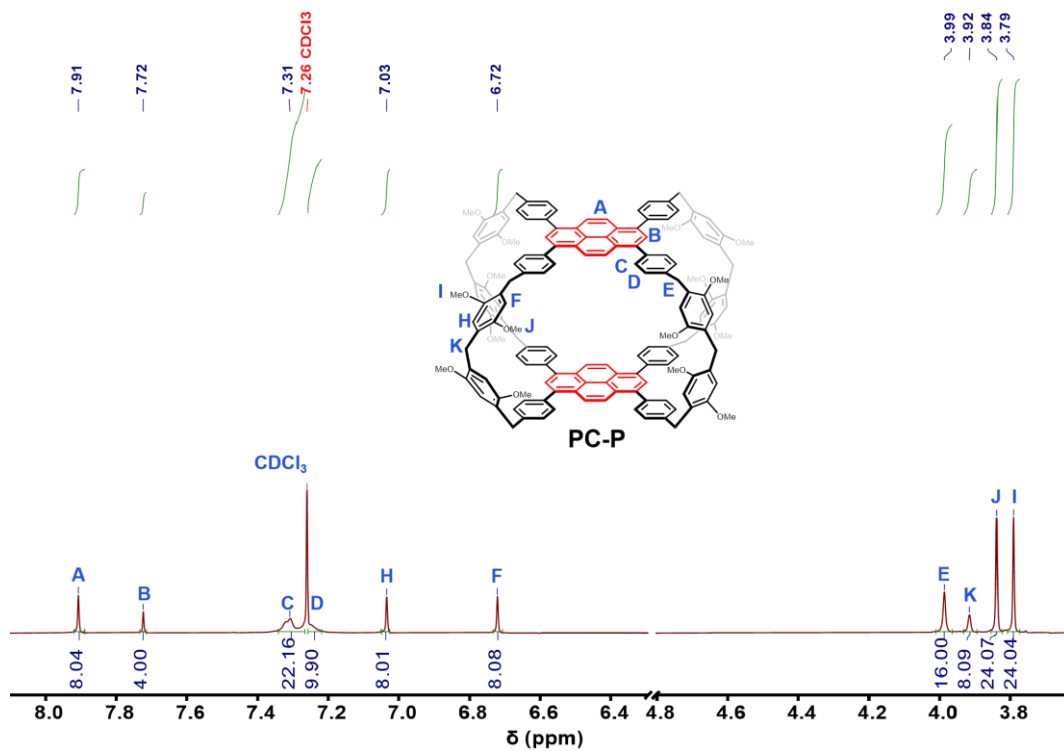


Fig. S8 Partial <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>, 298 K) of PC-P.



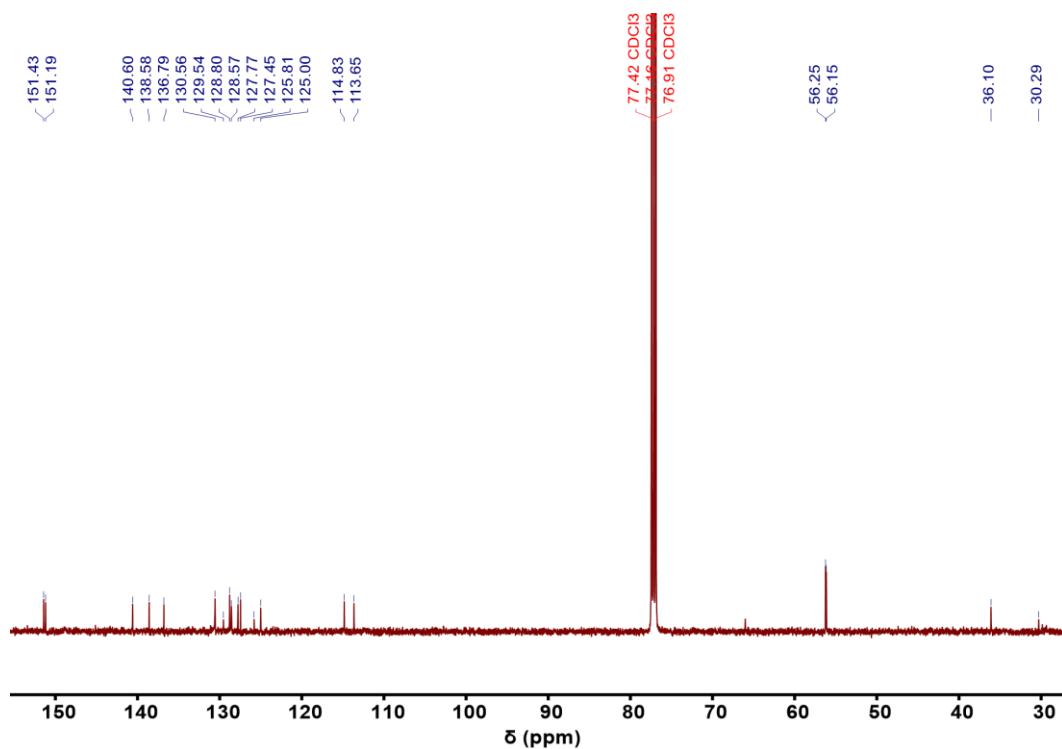


Fig. S9  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ , 298 K) of PC-P.

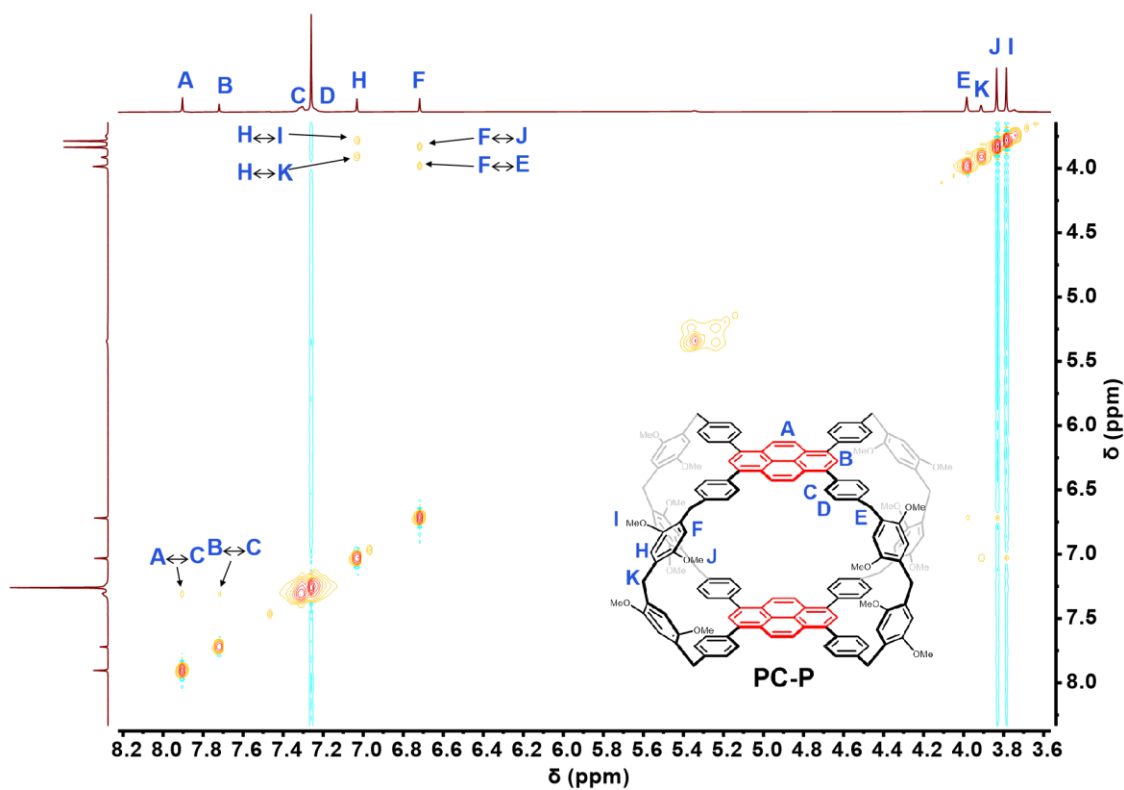


Fig. S10 Partial 2D  $^1\text{H}$ - $^1\text{H}$  NOESY spectrum (500 MHz,  $\text{CDCl}_3$ , 298 K) of PC-P.

### MALDI-TOF Mass Spectrum

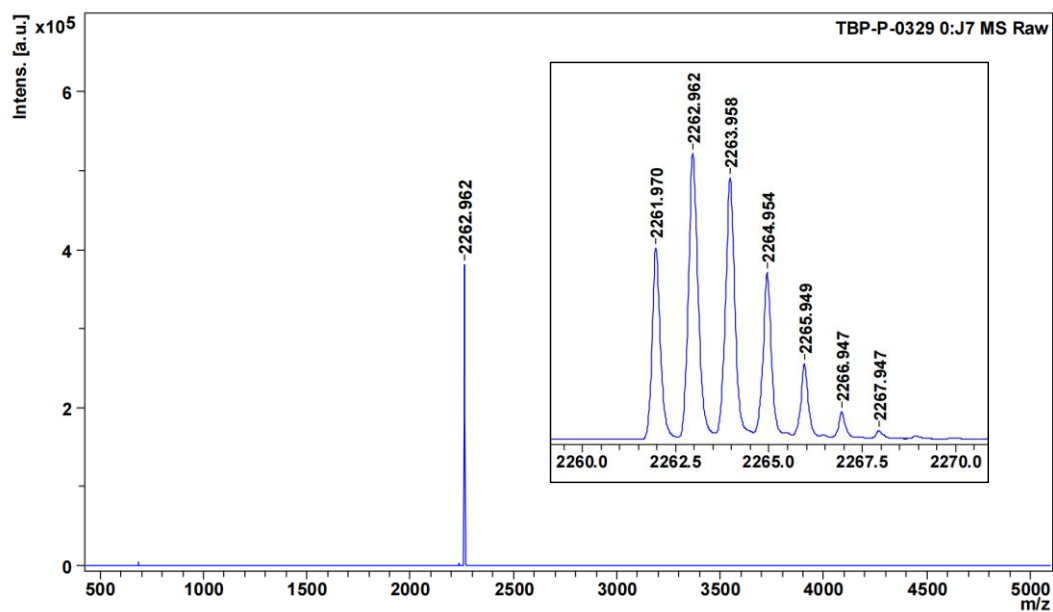


Fig. S11 MALDI-TOF MS spectrum of PC-P.

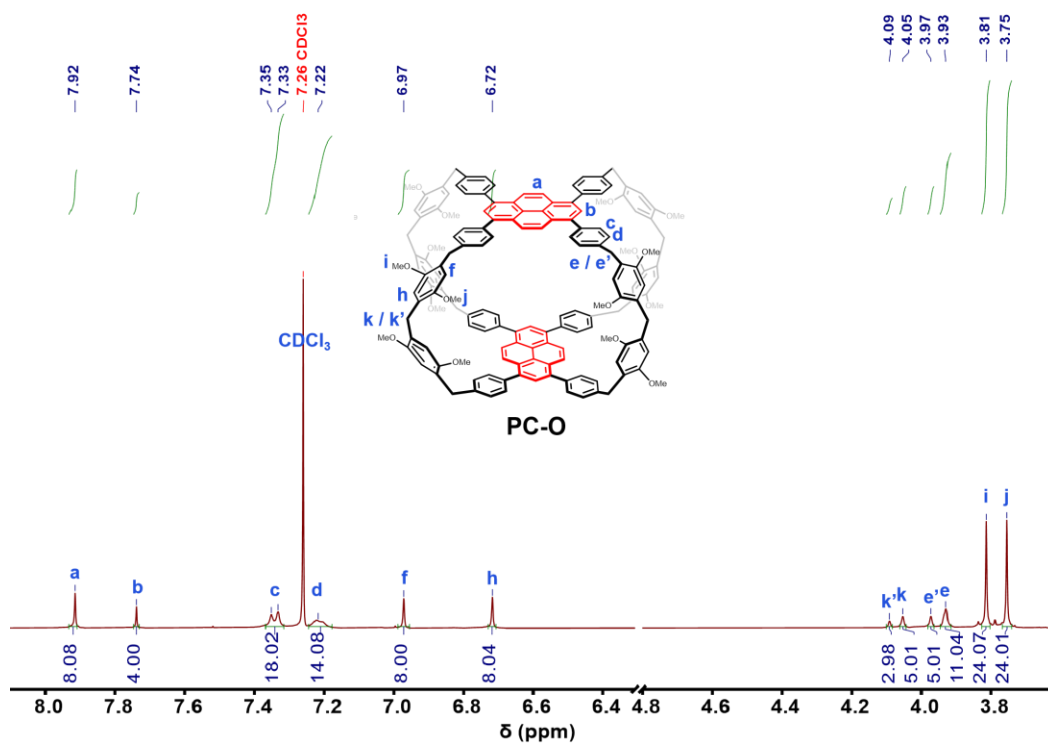


Fig. S12 Partial <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 298 K) of PC-O.

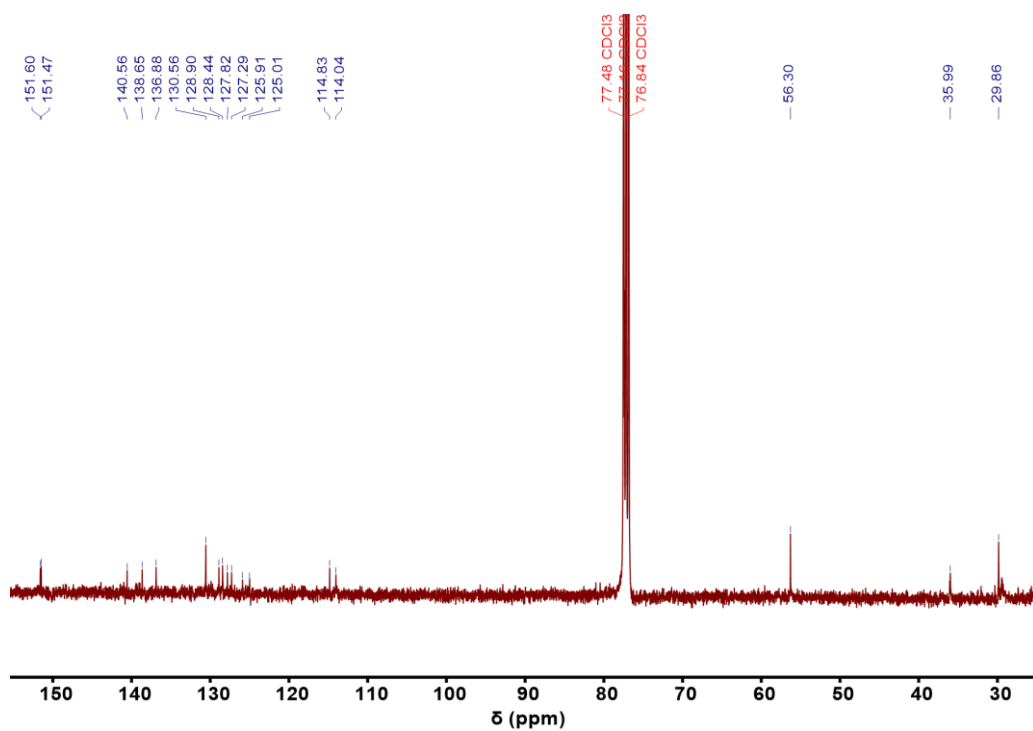


Fig. S13 The  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ , 298 K) of PC-O.

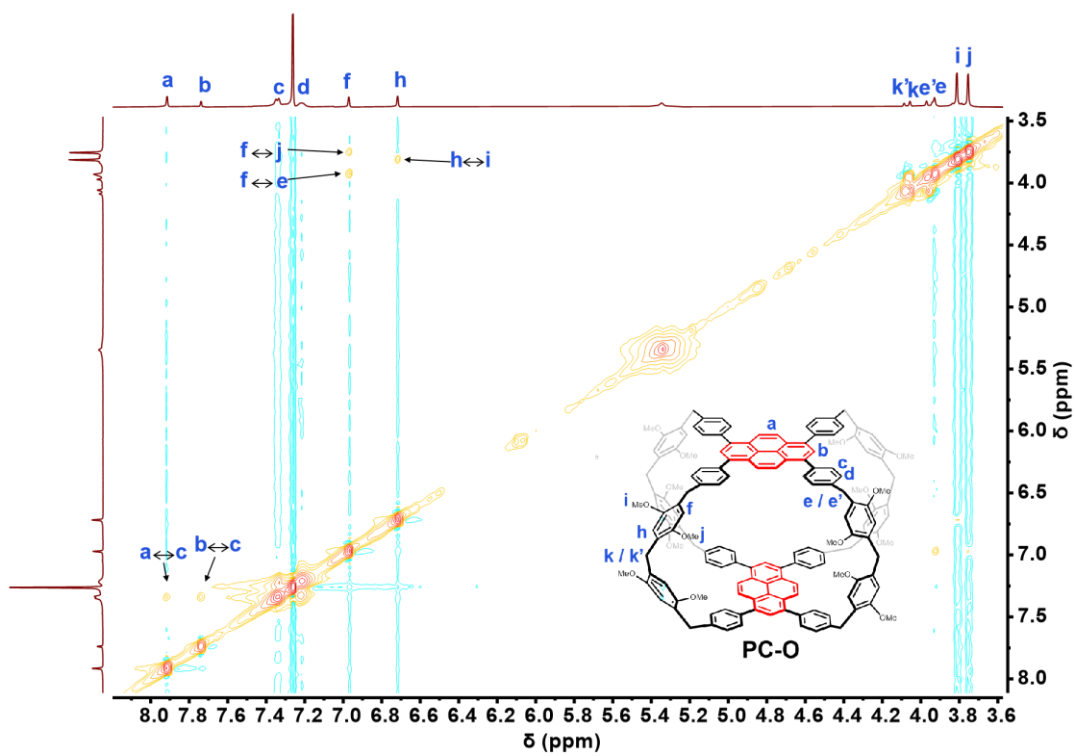


Fig. S14 Partial 2D  $^1\text{H}$ - $^1\text{H}$  NOESY spectrum (500 MHz,  $\text{CDCl}_3$ , 298 K) of PC-O.

### MALDI-TOF Mass Spectrum

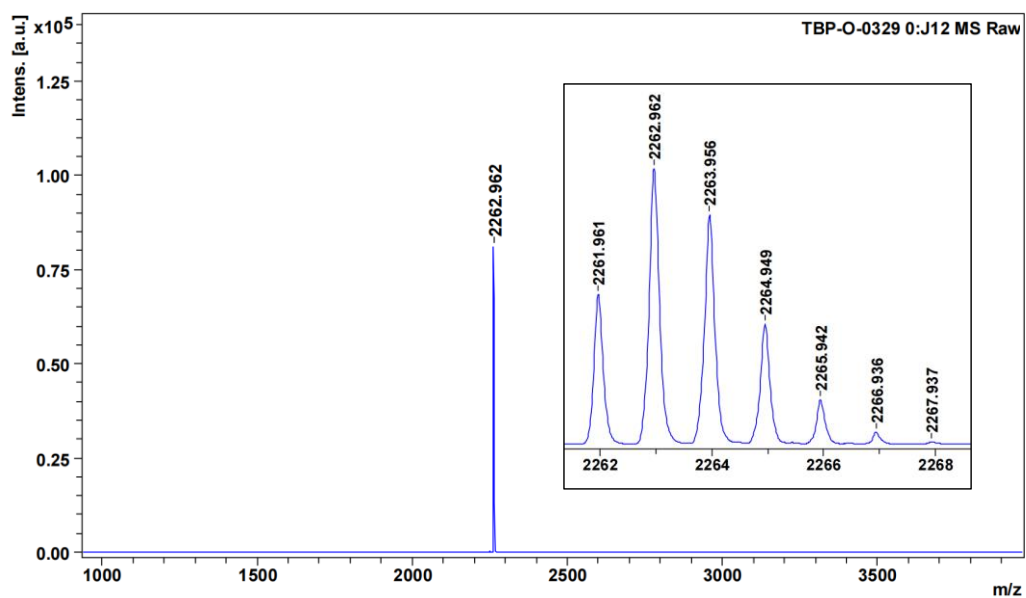


Fig. S15 MALDI-TOF MS spectrum of PC-O.

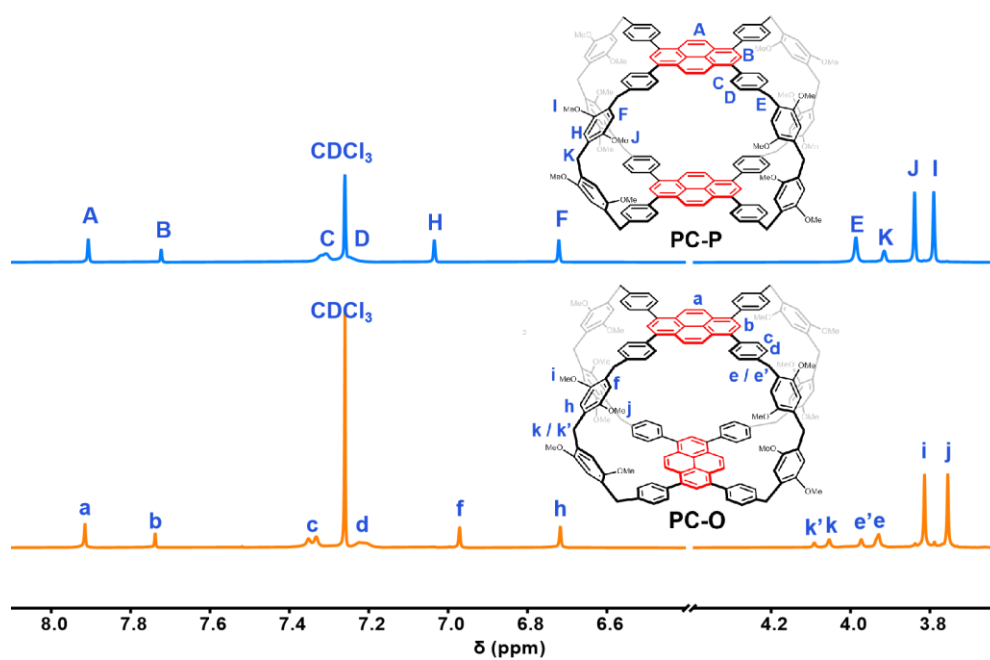


Fig. S16 The assigned <sup>1</sup>H NMR spectra of the signals for PC-P and PC-O.

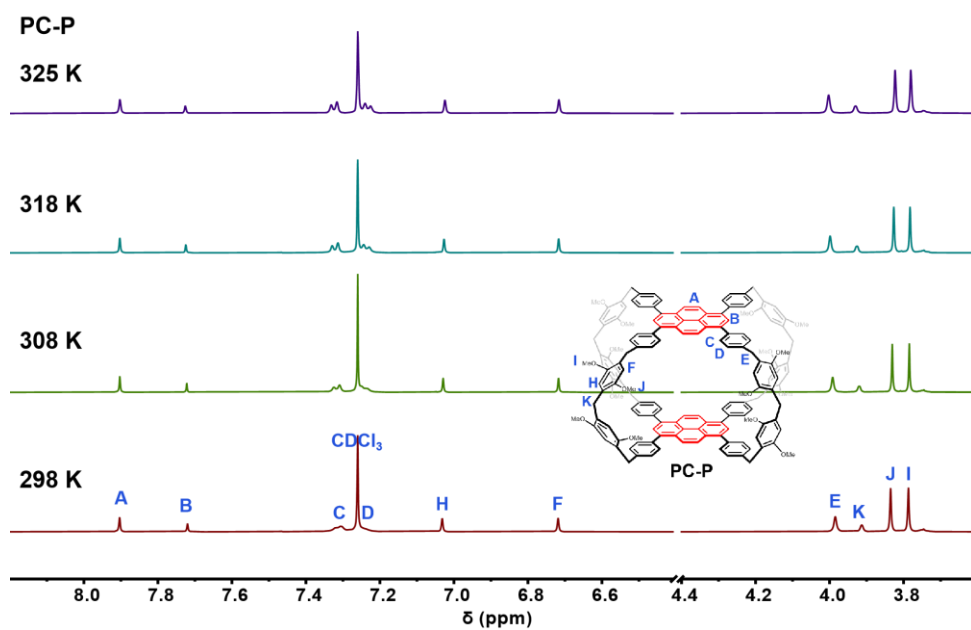


Fig. S17 Partial <sup>1</sup>H VT-NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PC-P.

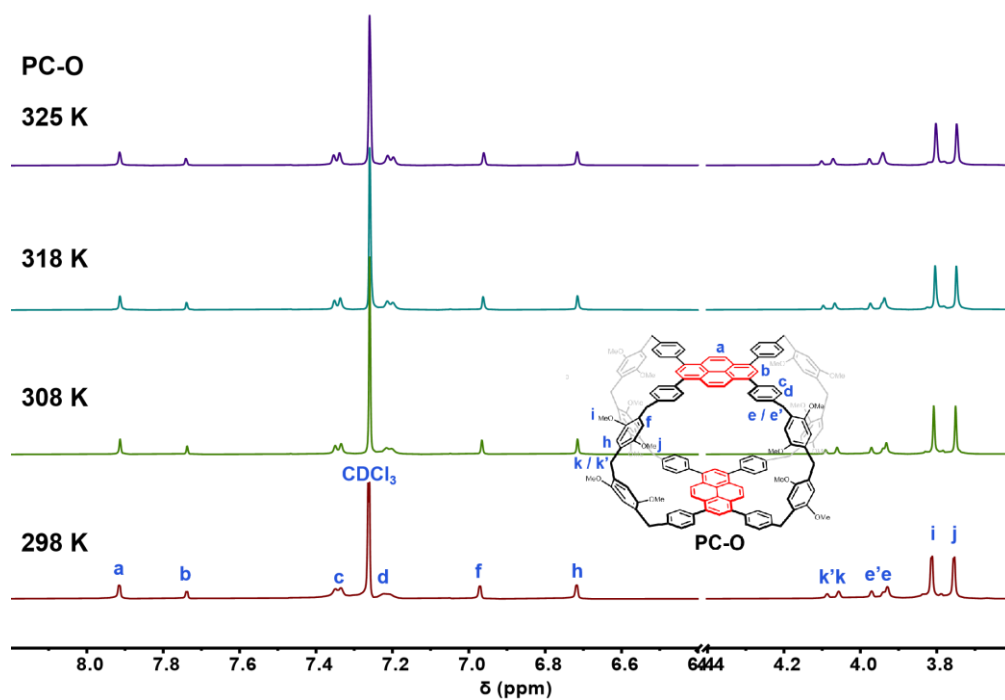
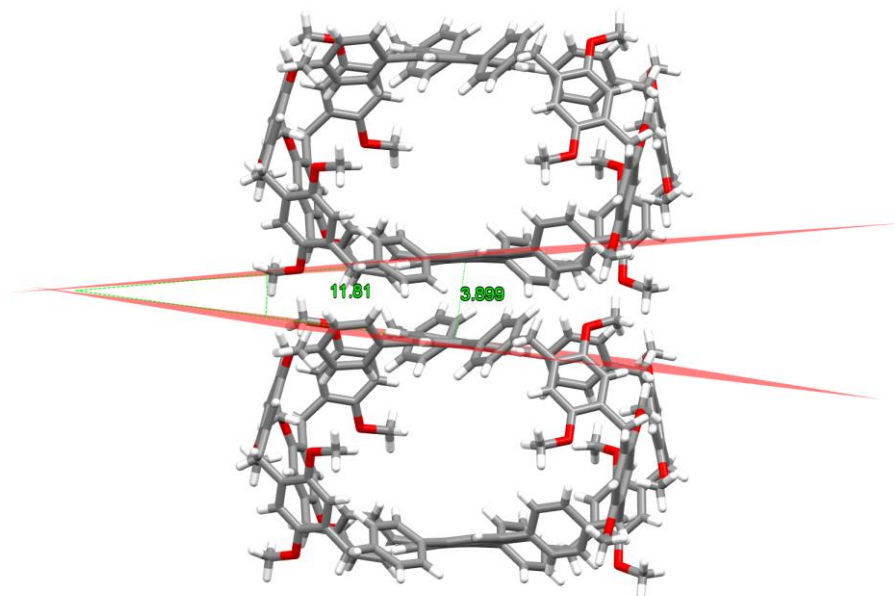


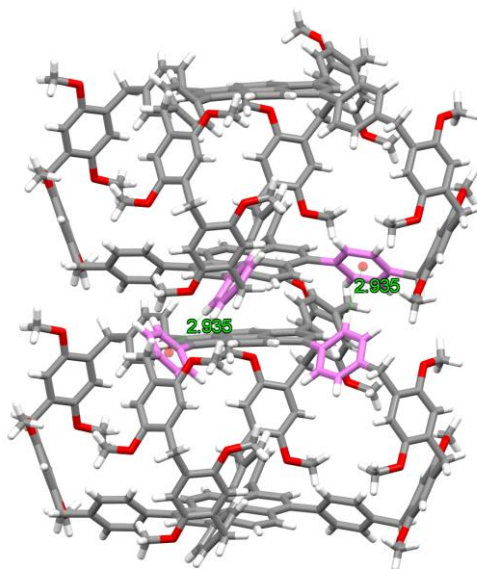
Fig. S18 Partial <sup>1</sup>H VT-NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PC-O.

### 3. X-ray single crystal diffraction data of PC-P

Single crystals were obtained by slow diffusion of isopropyl ether into a toluene solution of PC-P. CCDC: 2337817.



**Fig. S19** Illustration of  $\pi$ - $\pi$  stacking interaction between two PC-P molecules. The dihedral angle is 11.81°. Solvent molecules were omitted for clarity. Atoms color code: O (red), C (gray), H (white).

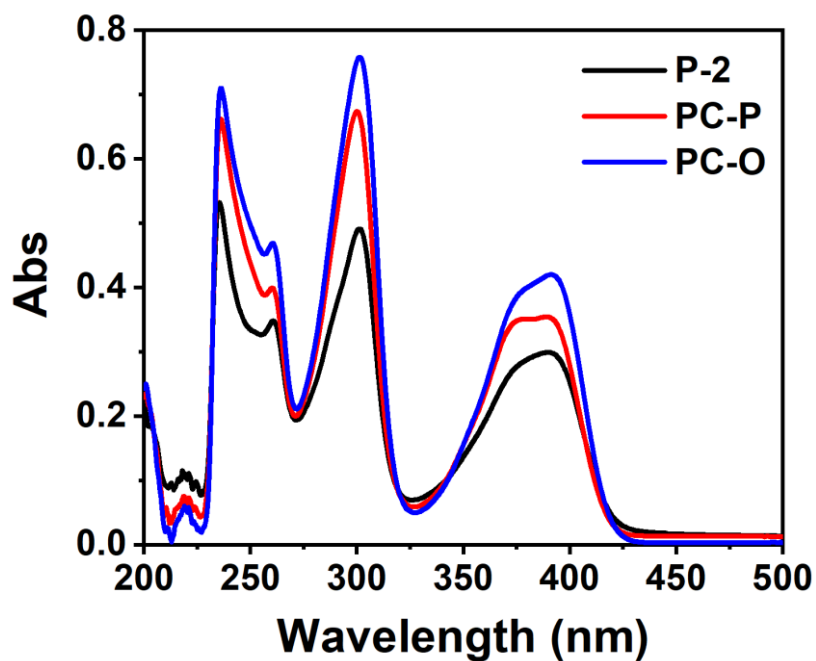


**Fig. S20** Illustration of C-H $\cdots$  $\pi$  interactions between two PC-P molecules. Solvent molecules were omitted for clarity. Atoms color code: O (red), C (gray and purple), H (white).

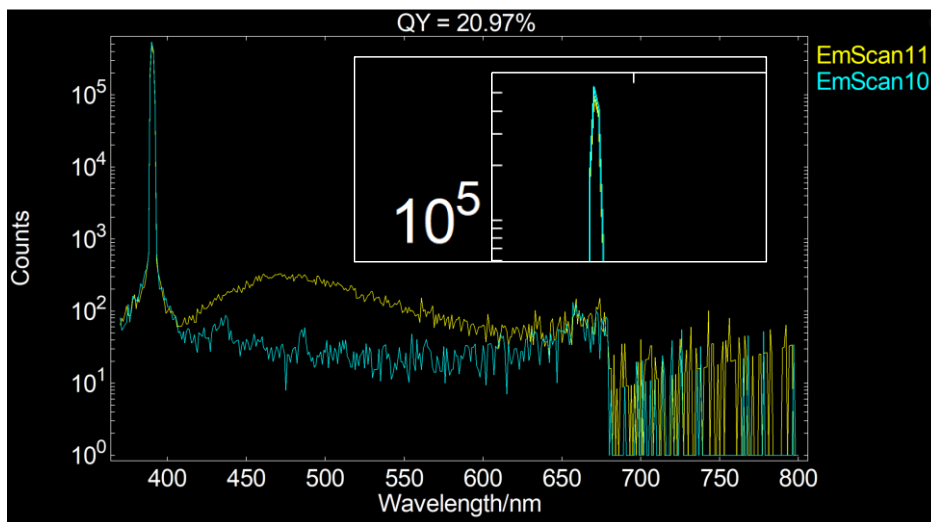
**Table S1.** Experimental crystallographic data for the crystal of **PC-P**.

Identification code	<b>PC-P</b>
Empirical Formula	C <sub>170</sub> H <sub>148</sub> O <sub>16</sub>
Formula weight	2446.88
Temperature (K)	213.00
Crystal system	orthorhombic
Space group	<i>Pbcn</i>
<i>a</i> (Å)	12.832(2)
<i>b</i> (Å)	38.948(7)
<i>c</i> (Å)	37.835(6)
$\alpha$ (°)	90
$\beta$ (°)	90
$\gamma$ (°)	90
Volume (Å <sup>3</sup> )	18910(6)
<i>Z</i>	4
$\rho_{\text{calc}}$ (g/cm <sup>3</sup> )	0.859
$\mu$ (mm <sup>-1</sup> )	0.273
<i>F</i> (000)	5184.0
Crystal size (mm <sup>3</sup> )	0.07 × 0.07 × 0.05
Radiation	GaK $\alpha$ ( $\lambda$ = 1.34139)
2 $\theta$ range for data collection (°)	6.31 to 110.266
Index ranges	-9 ≤ <i>h</i> ≤ 15, -47 ≤ <i>k</i> ≤ 39, -31 ≤ <i>l</i> ≤ 46
Reflections collected	77365
Independent reflections	17862 [ <i>R</i> <sub>int</sub> = 0.1482, <i>R</i> <sub>sigma</sub> = 0.1500]
Data/restraints/parameters	17862/36/835
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.024
Final <i>R</i> indexes [ <i>I</i> ≥ 2 $\sigma$ ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.1192, <i>wR</i> <sub>2</sub> = 0.3430
Final <i>R</i> indexes [all data]	<i>R</i> <sub>1</sub> = 0.2319, <i>wR</i> <sub>2</sub> = 0.4197
Largest diff. peak/hole (e Å <sup>-3</sup> )	0.32/-0.30

#### 4. UV-Vis absorption spectra and quantum yield calculations

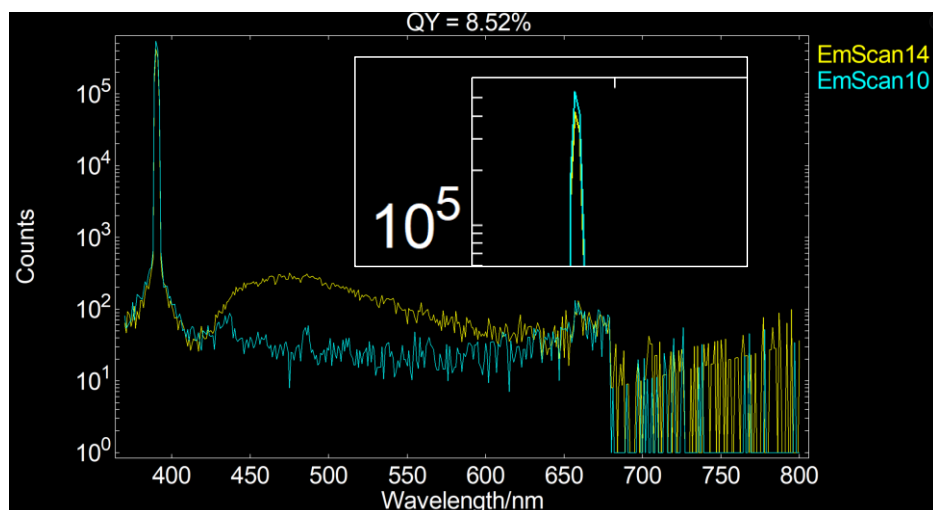


**Fig. S21** UV-Vis spectra of **P-2**, **PC-P** and **PC-O** in tetrahydrofuran ( $5.00 \times 10^{-6}$  M).

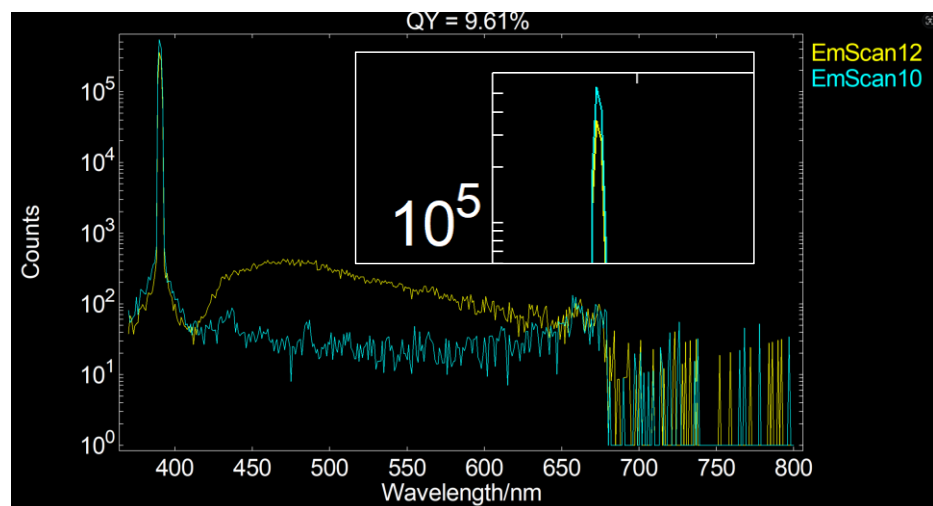


**Fig. S22** Quantum yield spectrum of **P-2** in the solid state (EmScan11: **P-2**, EmScan10: blank control). Insets: photons net absorption of **P-2**.





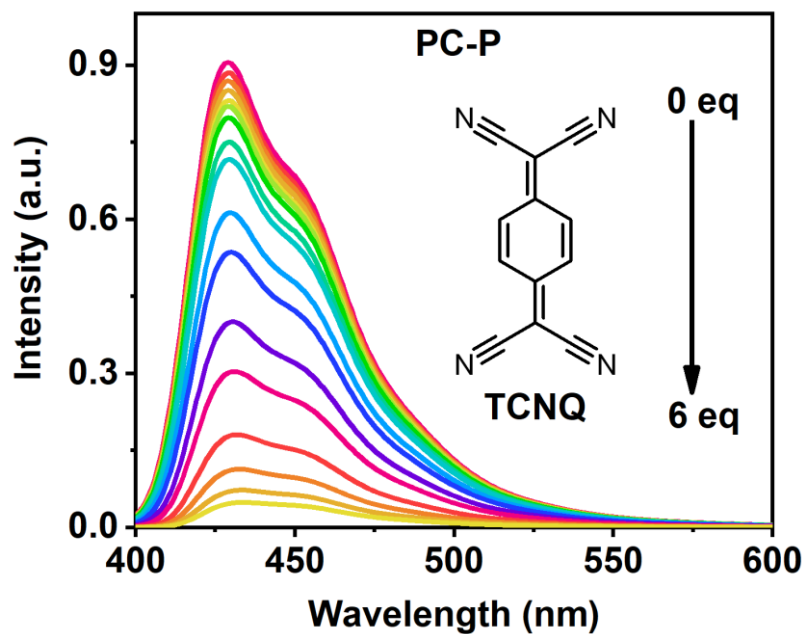
**Fig. S23** Quantum yield spectrum of **PC-P** in the solid state (EmScan14: **PC-P**, EmScan10: blank control). Insets: photons net absorption of **PC-P**.



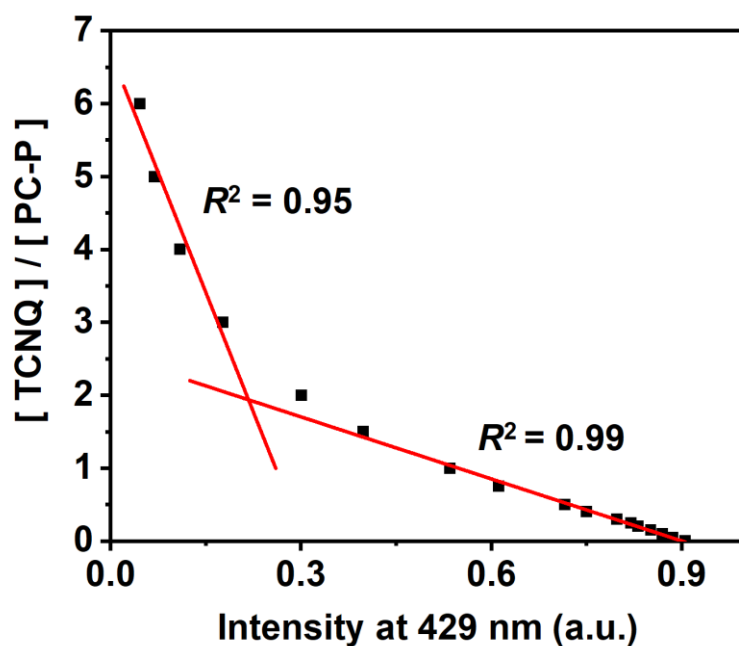
**Fig. S24** Quantum yield spectrum of **PC-O** in the solid state (EmScan12: **PC-O**, EmScan10: blank control). Insets: photons net absorption of **PC-O**.

### ***5. Investigation of host–guest complexation behavior in solution***

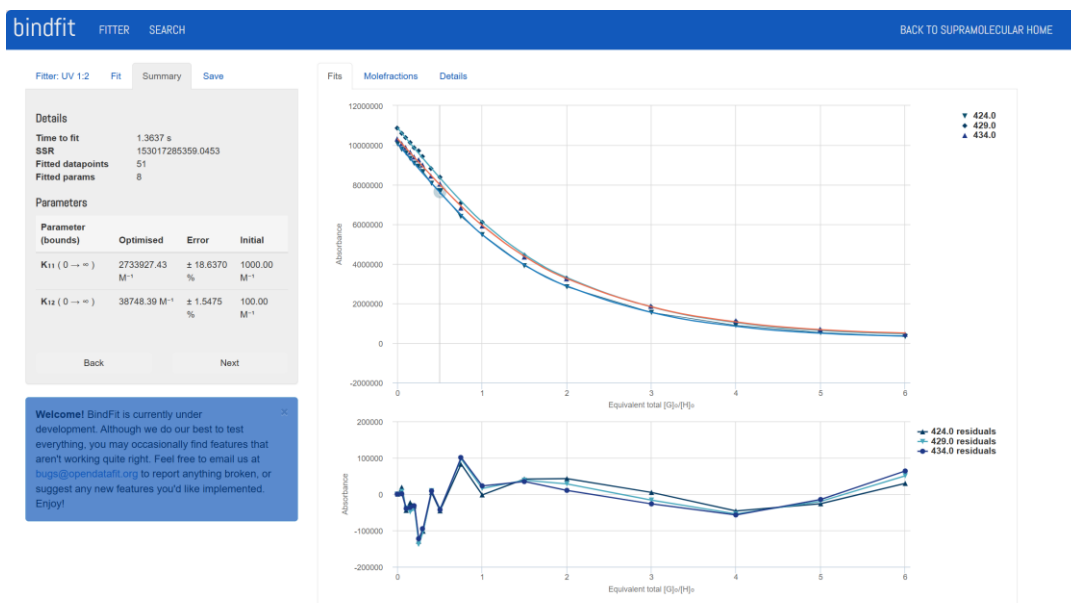
To investigate the host–guest complexation of electron-rich organic cages **PC-P** and **PC-O** with various electron-deficient guests, fluorescence titration experiments were conducted. The guests included 7,7,8,8-tetracyanoquinodimethane (**TCNQ**), tetrachloro-1,4-benzoquinone (**TCQ**), and 1,2,4,5-tetracyanobenzene (**TCB**).



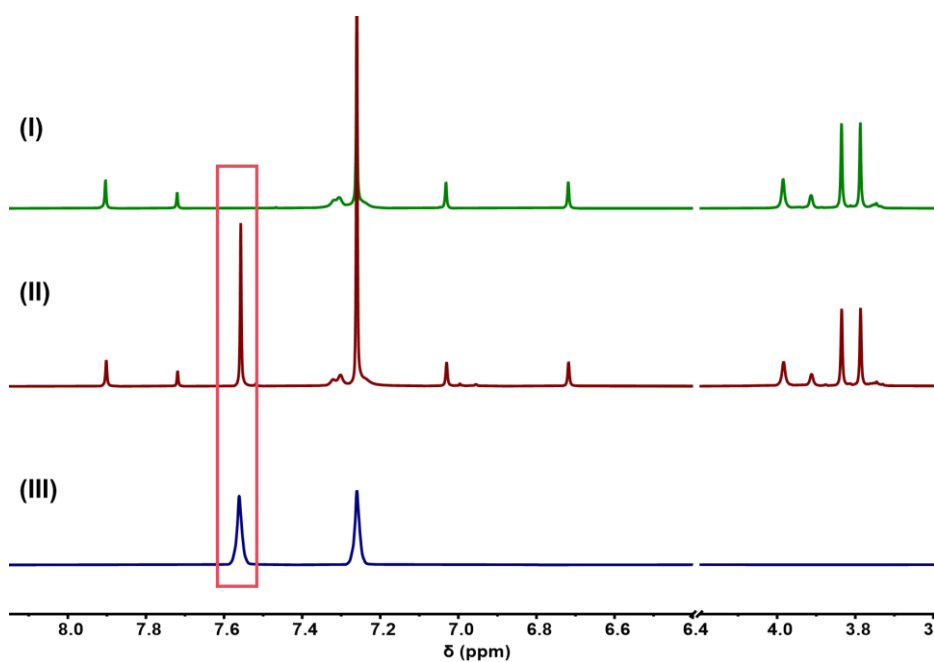
**Fig. S25** The fluorescence emission spectra of PC-P ( $1.00 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of TCNQ.



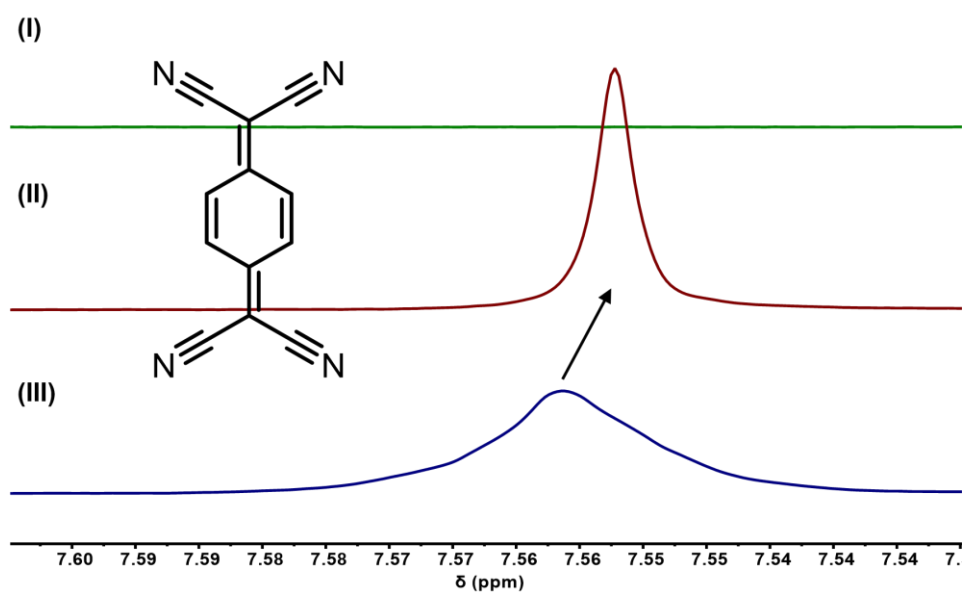
**Fig. S26** A molar ratio plot for PC-P and TCNQ, showing a 1:2 complexation stoichiometry.



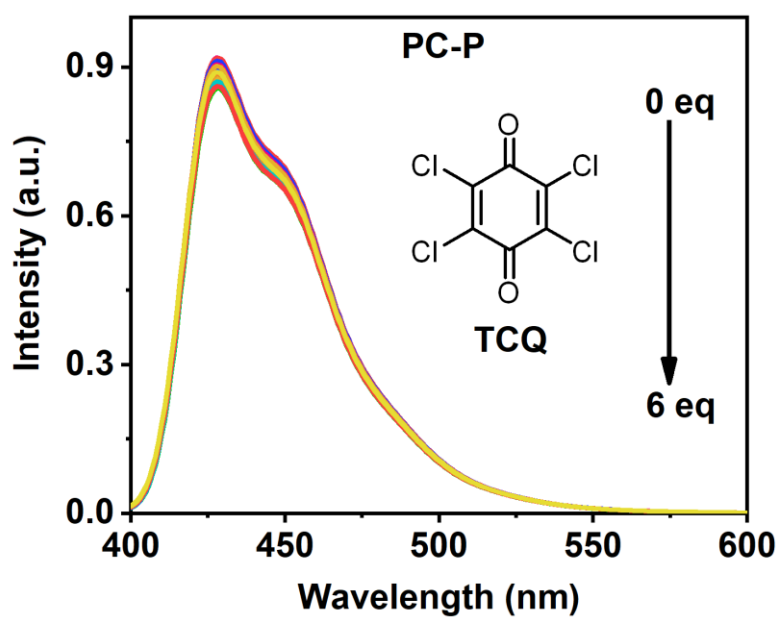
**Fig. S27** Non-linear curve-fitting graph of the complexation constants of **PC-P** and **TCNQ** using a 1:2 binding model by a non-linear curve-fitting method available at the website [www.supramolecular.org](http://www.supramolecular.org).



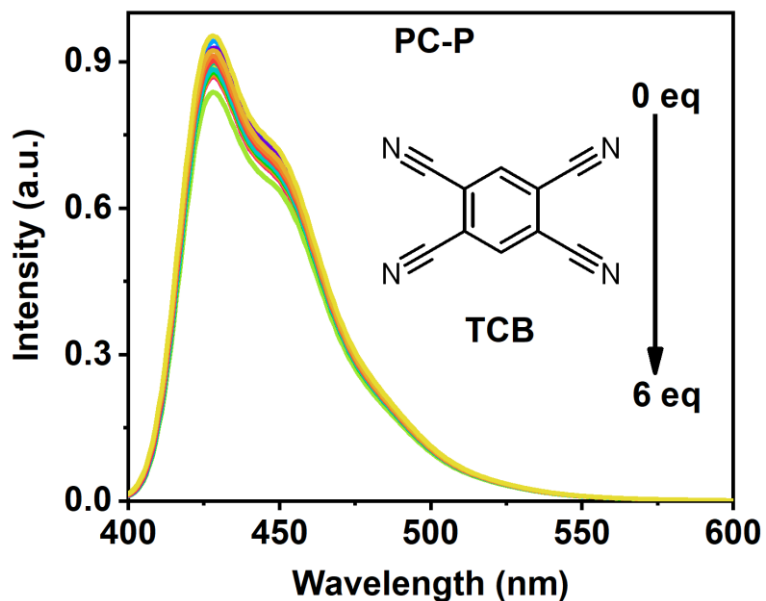
**Fig. S28** Partial <sup>1</sup>H NMR spectra (600 MHz, CDCl<sub>3</sub>, 298 K): (I) **PC-P**; (II) 0.88 mM **PC-P** and 8.8 mM **TCNQ**; (III) **TCNQ**.



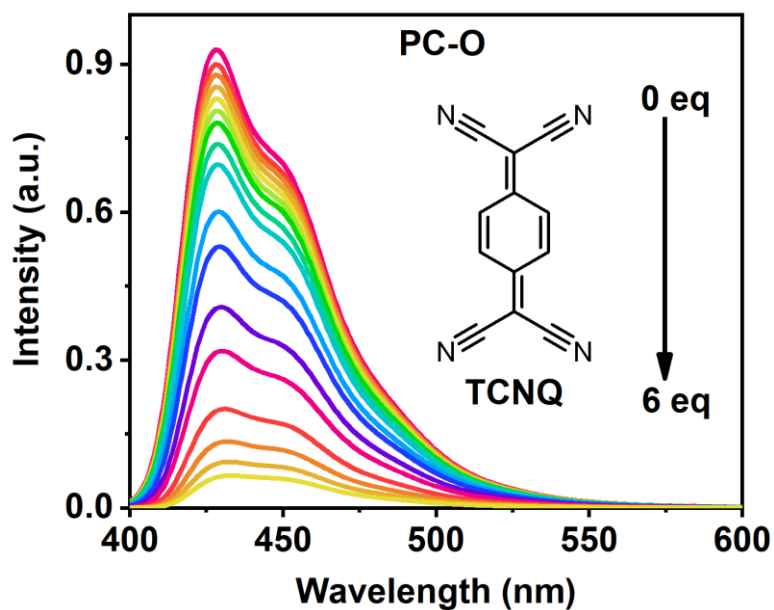
**Fig. S29** The marked region (from 7.60 ppm to 7.53 ppm) of Fig S28. The upfield shift of protons on TCNQ in the presence of PC-P suggested that the two guest molecules were in the inner space.



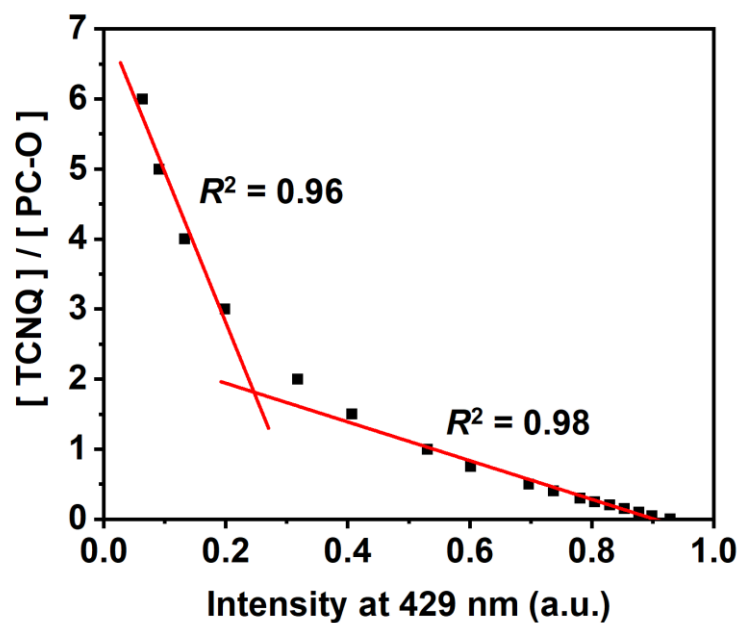
**Fig. S30** The fluorescence emission spectra of PC-P ( $1.00 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of TCQ. The curve underwent a non-significant change, which indicates that almost no complexation took place in this system.



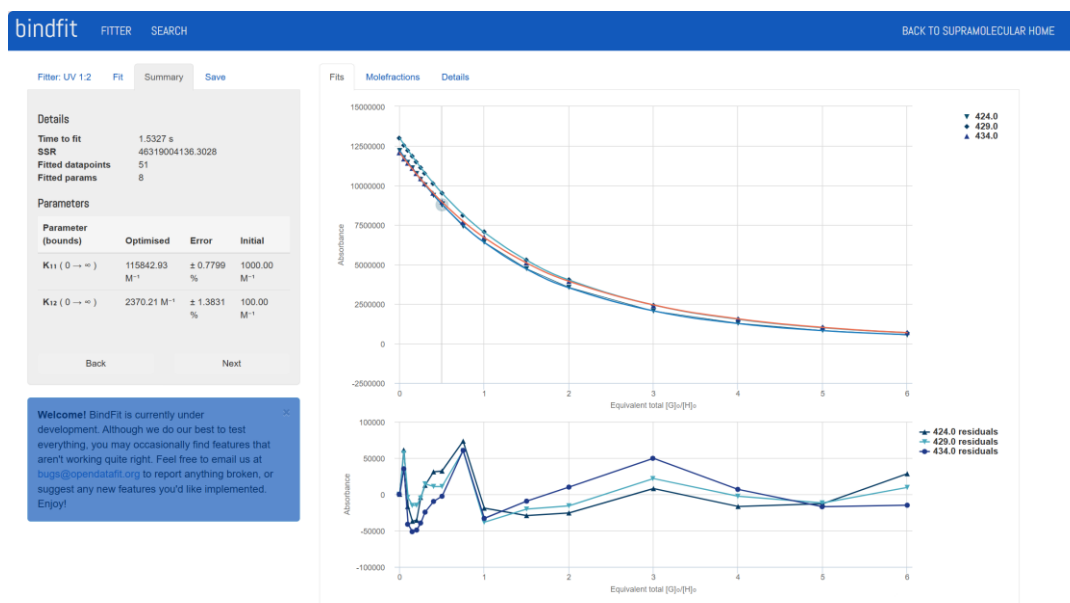
**Fig. S31** The fluorescence emission spectra of PC-P ( $1.00 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of TCB. The curve underwent a non-significant change, which indicates that almost no complexation took place in this system.



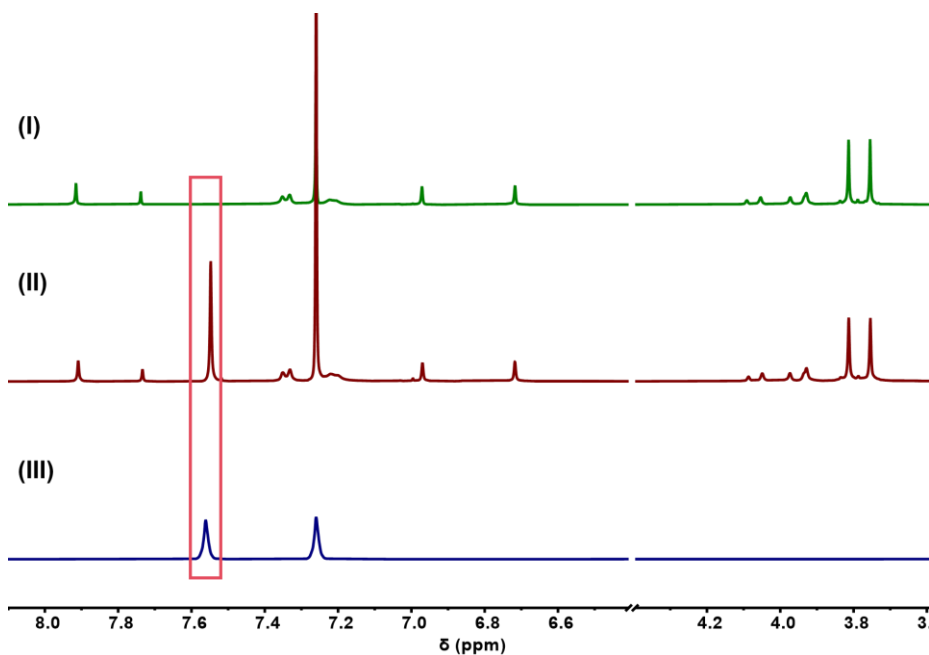
**Fig. S32** The fluorescence emission spectra of PC-O ( $1.0 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of TCNQ.



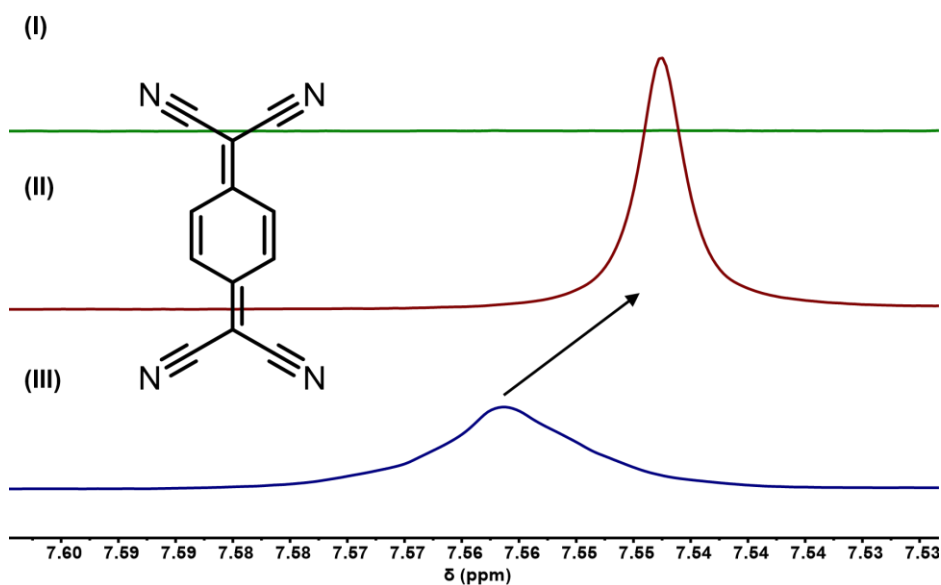
**Fig. S33** A mole ratio plot for TCNQ and PC-O, showing a 1:2 complexation stoichiometry.



**Fig. S34** Non-linear curve-fitting graph of the complexation constants of PC-O to 2TCNQ using a 1:2 binding model by a non-linear curve-fitting method available at the website [www.supramolecular.org](http://www.supramolecular.org).

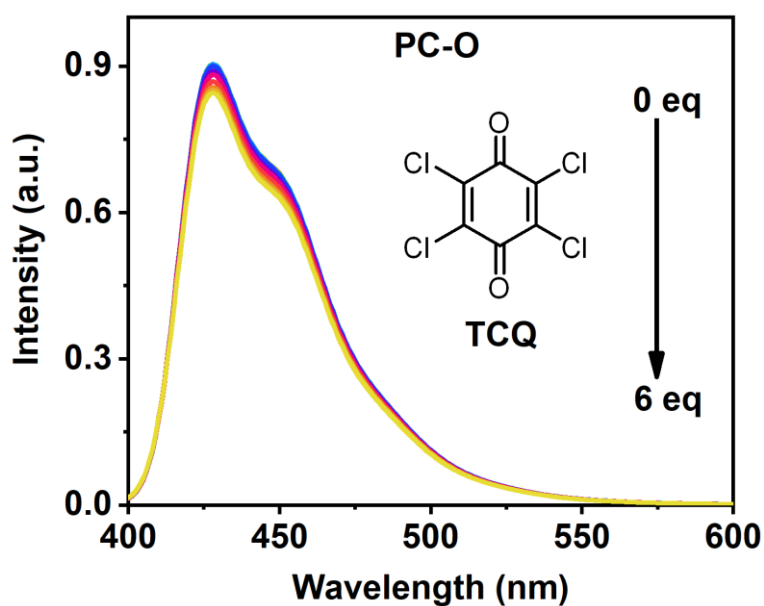


**Fig. S35** Partial <sup>1</sup>H NMR spectra (400 MHz, CDCl<sub>3</sub>, 298 K): (I) **PC-O**; (II) 0.88 mM **PC-O** and 8.8 mM **TCNQ**; (III) **TCNQ**.

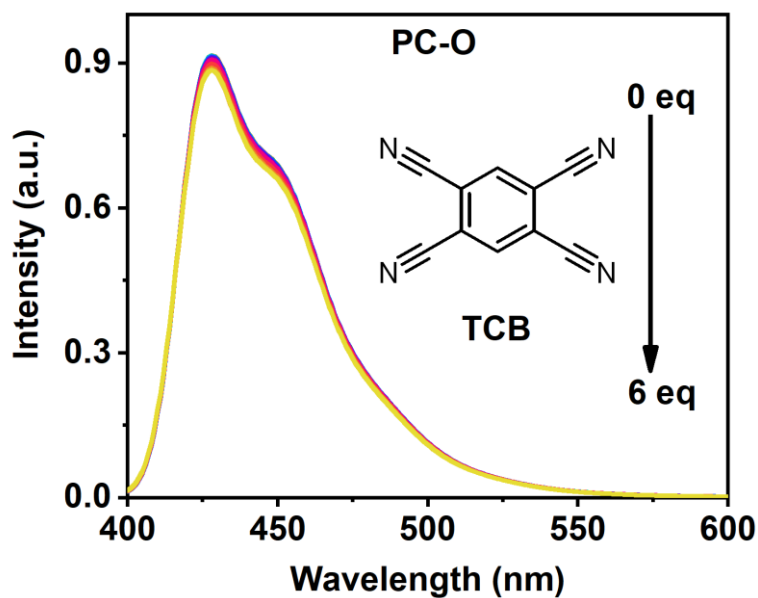


**Fig. S36** The marked region (from 7.60 ppm to 7.53 ppm) of Fig S35. The upfield shift of protons on **TCNQ** in the presence of **PC-O** suggested that the two guest molecules were in the inner space.

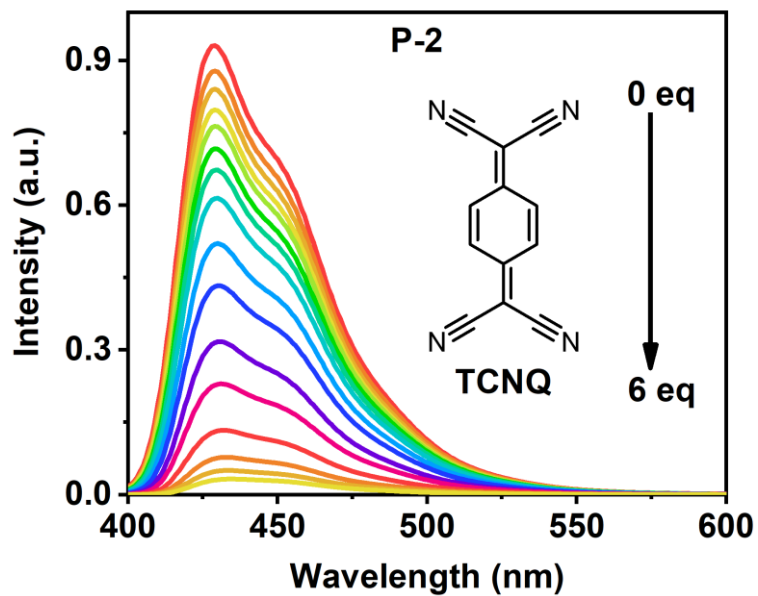




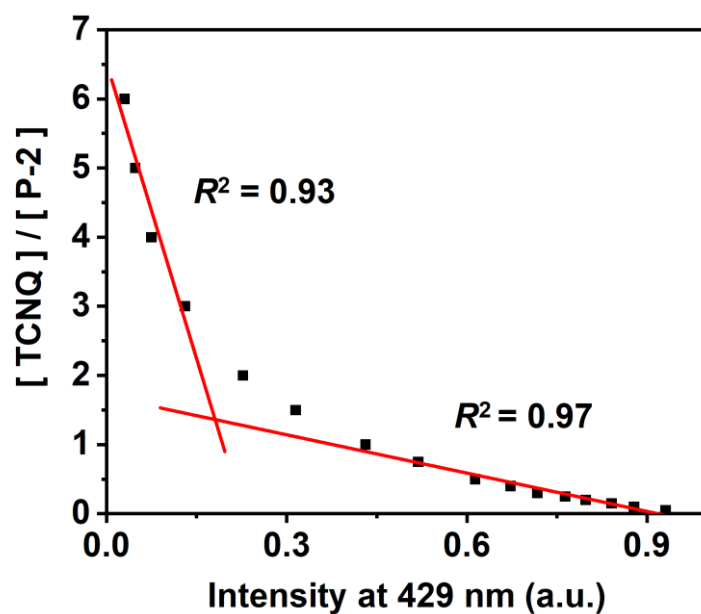
**Fig. S37** The fluorescence emission spectra of PC-O ( $1.00 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of TCQ. The curve underwent a non-significant change, which indicates that almost no complexation took place in this system.



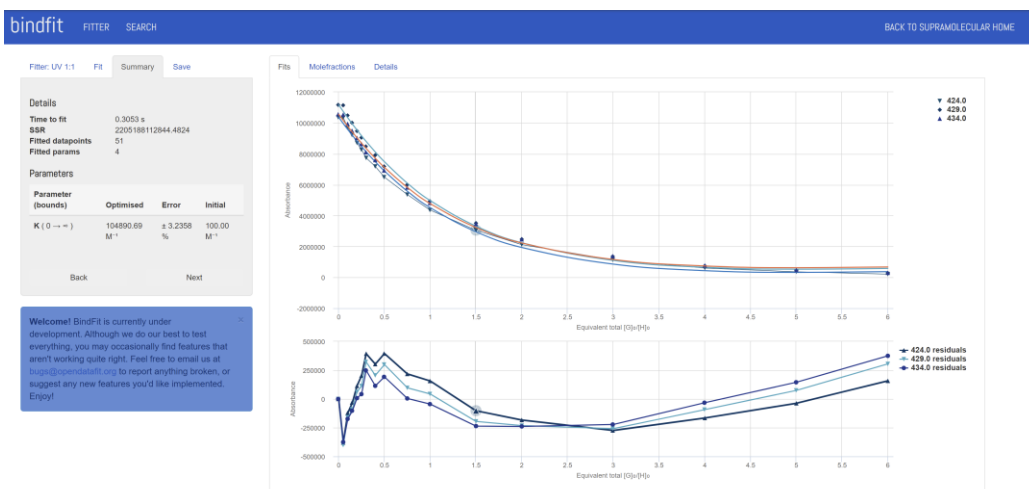
**Fig. S38** The fluorescence emission spectra of PC-O ( $1.00 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of TCB. The curve underwent a non-significant change, which indicates that almost no complexation took place in this system.



**Fig. S39** The fluorescence emission spectra of **P-2** ( $1.00 \times 10^{-5}$  M, dichloromethane) in the presence of 0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 equiv. of **TCNQ**.



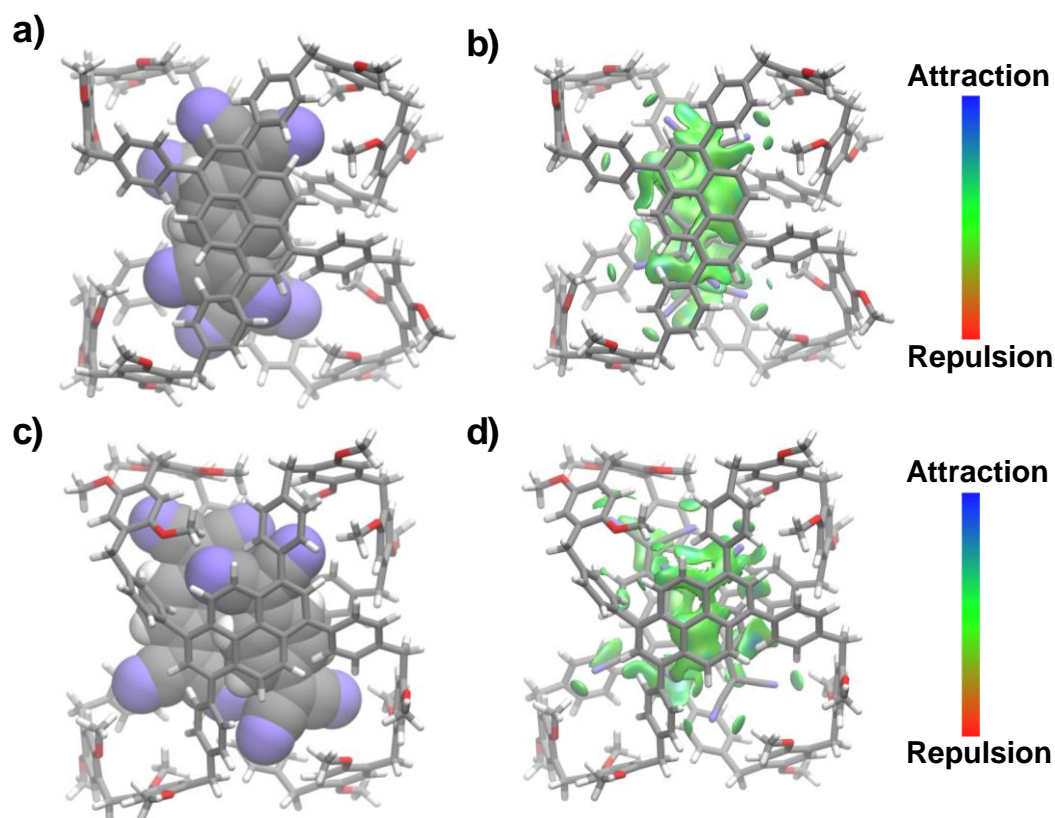
**Fig. S40** A mole ratio plot for **TCNQ** and **P-2**, showing a 1:1 complexation stoichiometry.



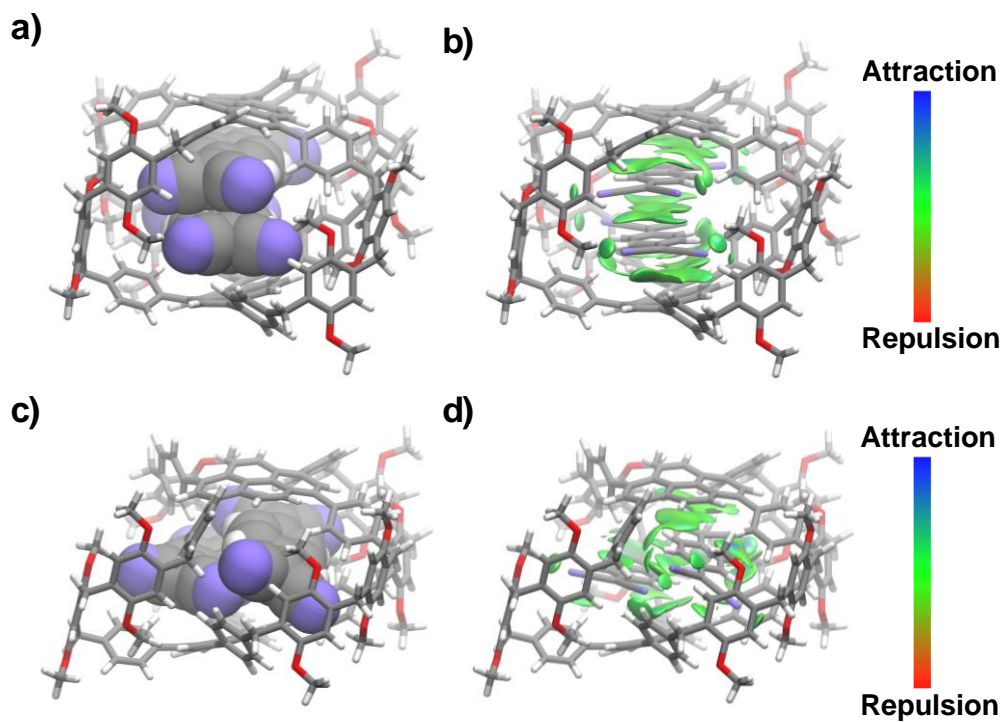
**Fig. S41** Non-linear curve-fitting graph of the complexation constants of **P-2@TCNQ** using a 1:1 binding model by a non-linear curve-fitting method available at the website [www.supramolecular.org](http://www.supramolecular.org).

## 6. Computational analysis

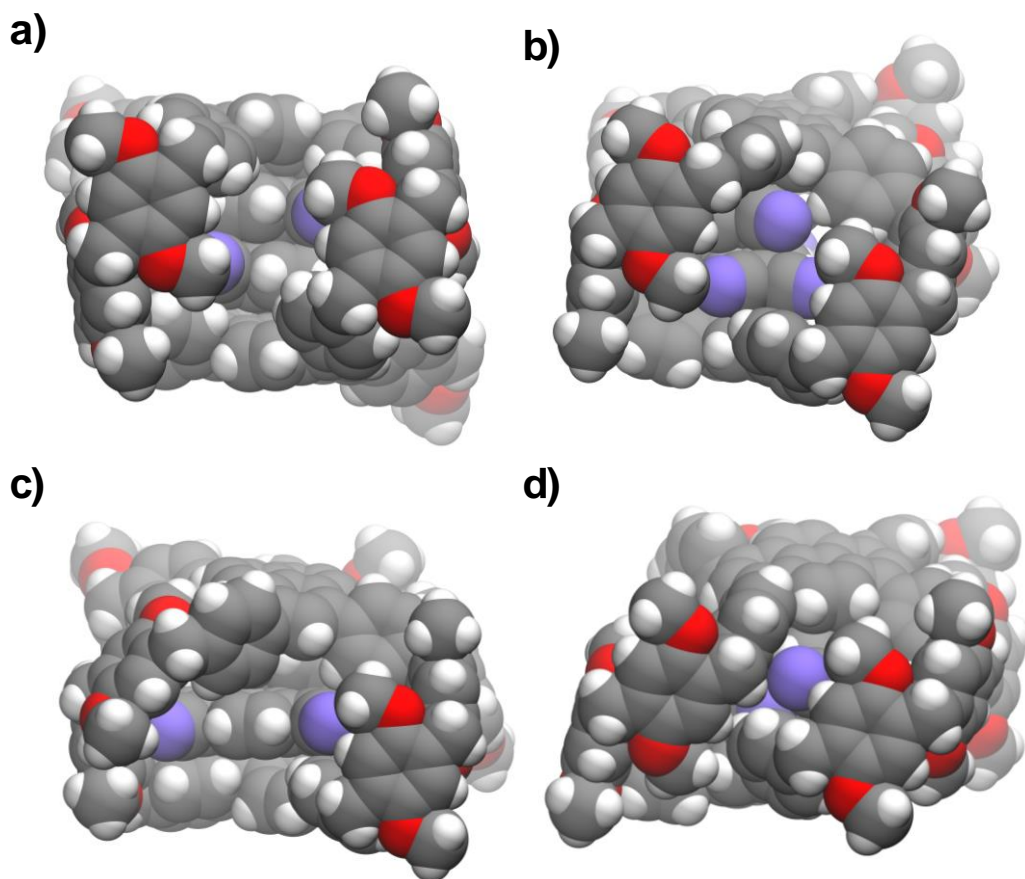
All-electron DFT calculations were carried out by the latest version of ORCA quantum chemistry software<sup>S2</sup> (Version 5.0.4). The BLYP functional<sup>S3-S5</sup> and def2-SVP basis set<sup>S6, S7</sup> were adopted for all calculations. The single point energy calculations were performed by B3LYP functional with def2-TZVP basis set. The DFT-D3 dispersion correction<sup>S8</sup> with BJ-damping was applied to correct the weak interactions to improve the calculation accuracy. The noncovalent interactions between **PC-P/PC-O** and **TCNQ** were studied by using the Independent Gradient Model (IGM) method through Multiwfn software.<sup>S9</sup> The visualization of IGM and orbitals were rendered by VMD software.<sup>S10</sup> Setting **PC-O** as the energy reference (zero), the relative single-point energy of **PC-P** was calculated to be 6.15 kcal/mol.



**Fig. S42** Top views of the calculated structures of (a) **PC-P**⊃**2TCNQ** and (c) **PC-O**⊃**2TCNQ**. The intermolecular binding isosurfaces (visual study of weak intermolecular interaction) between the cagearenes and **TCNQ** in (b) **PC-P**⊃**2TCNQ** and (d) **PC-O**⊃**2TCNQ**.  $\Delta\kappa$  inter ( $\rho$ ) = 0.009 au. Isosurfaces are colored according to a BGR scheme over the range  $-0.05 < \text{sign}(\lambda_2)\rho < +0.05$  au.



**Fig. S43** Side views of the calculated structures of (a) **PC-P $\supset$ 2TCNQ** and (c) **PC-O $\supset$ 2TCNQ**. The intermolecular binding isosurfaces (visual study of weak intermolecular interaction) between the cagearenes and **TCNQ** in (b) **PC-P $\supset$ 2TCNQ** and (d) **PC-O $\supset$ 2TCNQ**.  $\Delta\kappa$  inter ( $\rho$ ) = 0.009 au. Isosurfaces are colored according to a BGR scheme over the range  $-0.05 < \text{sign}(\lambda_2)\rho < +0.05$  au.



**Fig. S44** Side views of space-filling representations of (a, b) **PC-P=2TCNQ** and (c, d) **PC-O=2TCNQ**.

Optimized structure of **PC-P**

O	13.73860722863168	36.07393592545269	20.88916439142725
O	8.45132315714079	36.38620539286416	19.14964929800600
O	10.06306745062793	38.85727737747771	33.72393532609034
O	15.38806700918209	40.34449498120004	34.45399385809652
O	9.84074937455790	26.83764062412043	36.29435295881120
O	14.68262127837432	24.23902591800575	37.23781229985772
O	10.88090358571371	22.67490716885590	34.09257249003922
O	16.37431243355148	22.62946020269939	33.09778862929205
C	12.41922925673040	36.13922581480946	20.49612276311157
C	12.02575022483532	37.30094048665399	19.78461899600621
C	10.69670231886138	37.38344269347190	19.32768072732789
H	10.39495052429610	38.29383529252001	18.79835511730292
C	9.76452490037799	36.35687248374919	19.58215338669797
C	7.99357646696798	37.53811816947474	18.45726528560125
H	8.08489314887500	38.46010040168456	19.07559392208518
H	8.54788336678494	37.70133002074466	17.50567138022569
H	6.92623913753866	37.36313994836666	18.22636919291697
C	10.14584539151412	35.21838506765390	20.33690329532838
C	11.47786423362894	35.12926944584579	20.78227901735317
H	11.77254777336022	34.25198067518673	21.36713796727178
C	9.11719074713091	34.12282451098712	20.62318520661328
H	8.12082082707572	34.59778166937991	20.70208811504107
H	9.05794027350448	33.45186739812036	19.73743697372016
C	9.40366341015192	33.30048166096070	21.86440179073928
C	8.85545089754220	33.65889062180837	23.11582994182181
H	8.17717854675475	34.52348245648402	23.17711540645016
C	9.14358168775930	32.92347169583368	24.27629634934386
H	8.66484459536417	33.20313595131883	25.22412560996799
C	10.01320500483312	31.80244581742362	24.23861367319265

C	10.55409214509039	31.44194418422856	22.97929209949659
H	11.23774594765122	30.59091578497854	22.91009152400124
C	10.25195297279386	32.17304616527020	21.82045014155947
H	10.69686525018159	31.86556318878714	20.86192083402673
C	10.30415911644812	30.99055144265103	25.45599285632095
C	10.60400935602572	31.58614840820974	26.72559645536435
C	10.75179199157518	30.75021332505998	27.89357489031346
C	10.96457016262454	31.34183255349847	29.19503943928851
C	11.06973167884103	32.77521597617031	29.31887933623118
C	11.04681743811280	33.56283479356902	28.11540891989530
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C	10.81201953419400	32.99780480327907	26.88616841916084
H	10.82701244005954	33.63079080339470	25.99587853321416
C	11.24987634882003	33.35617589169185	30.61448506093349
C	11.31748472660396	34.82954791220224	30.82332998178793
C	10.37700303405970	35.71298824198911	30.23580093334943
H	9.55694707670736	35.30215621834765	29.63198576830399
C	10.45511675939557	37.09940040564015	30.44110043761721
H	9.70054981335057	37.75709251757600	29.98306073800610
C	11.47415791683380	37.66431010747980	31.23586105790162
C	11.57109491738418	39.18089177348778	31.43508280698863
H	10.56316452490498	39.62008647924707	31.29958355882656
H	12.22261838784010	39.61509845592479	30.64664436471398
C	12.13509908188451	39.52349006525571	32.79851730096587
C	11.36384810812148	39.24796225997267	33.95396158873966
C	9.30303591727285	38.36157916624234	34.81721856974937
H	9.80144405742374	37.49364476174284	35.30405636494513
H	9.12254779280775	39.14237644516103	35.59017716175207
H	8.33178515352879	38.03567946828876	34.40128371052311
C	11.95439854887820	39.31509257984885	35.22982501225577



H	11.39208038847763	39.03414903843855	36.12548443742478
C	13.31171889790651	39.65635840087958	35.38860692430384
C	14.06611900042053	39.99825714757670	34.23879976673684
C	16.21580480977313	40.58995537545149	33.32560366575890
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H	15.85124060586969	41.44912873735291	32.71940325195978
C	13.47342682061043	39.92793763591680	32.96036636710715
H	14.06200214903713	40.13184911851621	32.05756539967008
C	12.39352887783758	36.78540947075666	31.85017888314460
H	13.18116700416005	37.18908849906826	32.50031781593761
C	12.31128206796284	35.39885305996585	31.65672208769961
H	13.03893218039310	34.74516235839089	32.15489743449707
C	11.38697631748525	32.50421380797468	31.72461396909497
H	11.57699593540965	32.95852052172124	32.70471589080189
C	11.28577434218095	31.09865383649656	31.64768267935447
C	11.39422714801674	30.33117177099642	32.92170704262789
C	12.13817426500568	29.13051347760068	33.05365462053428
H	12.63017782157583	28.69759142212542	32.17721038138625
C	12.31788606329638	28.51664886662677	34.30498045962861
H	12.91473422210049	27.59587445141667	34.37107745413129
C	11.76238513886867	29.07099845669379	35.47830420730571
C	12.00319687661571	28.45917084432360	36.85893522456806
H	11.16885648351333	28.76560562075291	37.52205510415781
H	12.92863315962868	28.89814737814391	37.28998780672995
C	12.13506573456363	26.95035059106194	36.85355538554651
C	11.01265072053222	26.15131008331777	36.52502850459190
C	8.72484765280670	26.11958759383207	35.78604907722707
H	8.35259144007629	25.35865684797769	36.50849016409863
H	7.92874434514626	26.86523084454333	35.60540632367596

H	8.96820679443743	25.60645185432466	34.82887693549119
C	11.14447377852837	24.75273643619034	36.42556974733086
H	10.29780695398028	24.12870888081501	36.12368622604348
C	12.38147825941267	24.11696333663525	36.65000859186092
C	13.49621424490639	24.91263719216162	37.01610742531987
C	15.85612732626145	24.99803884456133	37.49364739223866
H	15.77421614538587	25.59029401235032	38.43241411599604
H	16.68240930814764	24.27061478537551	37.60126342701029
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C	13.36378763591478	26.31408017350176	37.11018290478122
H	14.22593735069879	26.94270985194534	37.36388996485232
C	12.56393853218968	22.63412220608469	36.33707300762786
H	11.59366075187759	22.11220011485354	36.42111941505633
H	13.27574538201607	22.17593809794456	37.04753191112109
C	13.10660881008177	22.52380308425541	34.91574654050294
C	12.23198584848119	22.65199213970302	33.80659002637817
C	9.97008764493129	22.94990252725017	33.03604273717860
H	8.96098662209527	22.96424119600242	33.48837960354439
H	10.17237246309886	23.93708450519548	32.56391990219819
H	9.99906522041670	22.16641062033164	32.24633896506303
C	12.75856669559638	22.78123358580247	32.50676436096592
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C	17.28579072074428	22.47610732050673	34.17776655626672
H	17.14927147141368	21.50354992700594	34.70098271787552
H	18.30017025098111	22.51191503450260	33.73915901115959
H	17.18346411251670	23.29431978806759	34.92563226132474
C	14.49272093466060	22.47402401394558	34.67686174171335
H	15.15486952102766	22.39467032593520	35.54403306902711

C	10.98897346700911	30.24359952643566	35.34754565329555
H	10.51530255000272	30.67937905148544	36.24058418248270
C	10.80790715944069	30.85879004554624	34.10174332099766
H	10.19007786618652	31.76442244672462	34.03386769337793
C	11.04983809733667	30.49982913476159	30.36821307366598
C	10.82553955029394	29.08796831759330	30.20176132814483
H	10.76596690519212	28.45105717329817	31.09044929420673
C	10.66609691832934	28.52225723959327	28.95832482786056
H	10.48970841616479	27.44349189154293	28.87160839521335
C	10.67527308507598	29.31867669941429	27.76017271248887
C	10.53551986055807	28.74012361857011	26.45962919532699
C	10.66751130491230	27.26908657635546	26.26631204016642
C	11.81447264622603	26.59965882547082	26.75988082265862
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C	11.96639009382971	25.21422820270783	26.60248639830131
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C	10.98378521598534	24.44565926870188	25.94165457629452
C	11.20321844949574	22.95687446007437	25.68645810963155
H	11.91283540948391	22.55443414332175	26.43584057727135
H	10.25025353858996	22.40537591050862	25.78289187313750
C	9.84893645585752	25.11368362900028	25.42805535102007
H	9.08700888697921	24.53016734041783	24.89335687835444
C	9.69298186938289	26.50090873708308	25.58615577106122
H	8.79201845968025	26.99893660548888	25.19910373513987
C	10.30404309435414	29.58331183775383	25.35694948975537
H	10.13303322316326	29.12330544470813	24.37470566921181
C	12.97578965740889	38.49015172859028	19.65518615587206
H	12.51906990529937	39.24628442014904	18.98820611821979
H	13.93902210369122	38.17457406971138	19.20930112141775
C	14.09848619612136	35.11526586441067	21.88003018648646

H	13.49342861554778	35.24116216379946	22.80273081666718
H	13.98856895045989	34.07124529080682	21.51465477195380
H	15.16101240781801	35.29970401601548	22.12490889951666
O	12.49800132498648	37.23921258106921	37.54257933632707
O	17.70130003012144	36.23226895069935	35.78789664587228
O	15.77439936180827	38.88423179666913	23.77898070755447
O	11.01231231508547	39.89526268788939	21.06790013831135
O	15.67206358007394	27.47544366277273	20.44376791326443
O	11.05148713401914	24.51466467734381	19.46120934540547
O	15.01165882525018	23.13227662730510	22.45566803012556
O	9.56643622379664	22.42298658843984	23.46127871312775
C	13.78611734715674	36.95438759100035	37.13024893453186
C	14.59408482021913	38.06592077675135	36.77980417239760
C	15.91103806218746	37.82685960024047	36.34344563850294
H	16.50979910348721	38.69258056452156	36.04450772761074
C	16.42548022423071	36.51818773602847	36.24138315773508
C	18.54320860387357	37.31633690994612	35.41694167397365
H	18.10901301170773	37.91063131024241	34.58178338294653
H	18.73762170353001	38.00240590084888	36.27134496440119
H	19.49925151296885	36.87085091952442	35.08525683565837
C	15.62372853341872	35.40880271543645	36.60317786922246
C	14.30763402398151	35.64796568151502	37.04423103495169
H	13.69225509868400	34.78116784983226	37.31409971961237
C	16.15359045784675	33.98519773135127	36.49024162259233
H	17.25356379003891	34.00436568198340	36.61085714695049
H	15.73697860951664	33.38136854620220	37.32031670830958
C	15.80547646619810	33.30629256797239	35.16859373387836
C	16.45179648126011	33.67369718512483	33.96552668837221
H	17.21328817149528	34.46550023325135	33.99200579581282
C	16.15207438804267	33.02507000175854	32.75768262357593

H	16.69931152597234	33.30052727298632	31.84551241188733
C	15.19269375689423	31.98059330343421	32.70185165277511
C	14.53261692617225	31.63213248672535	33.90462941778324
H	13.77975757247199	30.83795041730128	33.89573014783752
C	14.83148112832452	32.28815922455495	35.11019853449505
H	14.30138752551720	31.98853899417246	36.02725689706431
C	14.94795469402507	31.20634892861255	31.44919766880678
C	14.68084374233018	31.83292452045014	30.18948371272231
C	14.55340459697288	31.02413329192760	29.00070867543408
C	14.33586754749794	31.64692934416315	27.71509681878048
C	14.20956434659071	33.08173186089125	27.63021729640146
C	14.25793487773890	33.84609404831764	28.84762085560929
H	14.06438788731004	34.92345177383380	28.80969832758938
C	14.49715610648462	33.25153718558792	30.06256286561393
H	14.51172139560238	33.86647396419967	30.96597444020832
C	13.97610916706793	33.68719555831036	26.35630960698458
C	13.83960311623838	35.16195104500346	26.18605360099863
C	14.81851059146306	36.06117553638410	26.67513380092398
H	15.69314004205486	35.66338460304191	27.20769166075501
C	14.71536511444963	37.44317907327756	26.44439060007642
H	15.51198596954770	38.11377730029211	26.79843219939361
C	13.62873238646687	37.98319339688086	25.72763845164549
C	13.57127236269324	39.46586716356170	25.34793719723460
H	14.46252110762947	39.98272774519391	25.75233449969299
H	12.67277665742239	39.94510048409508	25.78801083469729
C	13.50756839346729	39.56367209830609	23.83170437664699
C	14.61540922991504	39.11802197687798	23.06895105072329
C	16.84863354753373	38.22025870309741	23.12788153499297
H	16.54203596387724	37.22351421431303	22.74013601255151
H	17.25779165307604	38.81746324717413	22.28254831502712

H	17.63902653295432	38.08315355805448	23.88873976794481
C	14.46436890814105	38.85923866637845	21.69369969520320
H	15.27904319686422	38.40707888647612	21.11772799174273
C	13.23372875731609	39.06526926168510	21.04358590412003
C	12.16740361565393	39.64284640834028	21.77723747688869
C	9.81918345226588	40.17443236739294	21.78635238388673
H	9.00827694463285	40.23370390628265	21.03624301301366
H	9.57990943869802	39.36790462888175	22.51457216656965
H	9.87468584001931	41.14305557975268	22.33226378602252
C	12.30572655406640	39.86633361299882	23.16357177600049
H	11.45757337579350	40.22843264535751	23.75794567426300
C	12.64423367676560	37.09110867216303	25.24834834441372
H	11.80145051753248	37.48068384761162	24.65981187213637
C	12.74807350903353	35.70995694274969	25.46649866990064
H	11.97381820256996	35.04321750940289	25.06421544665088
C	13.84175955509733	32.86333628062411	25.22659927222533
H	13.61249312930457	33.33947198678931	24.26633839872965
C	13.99601769061423	31.45977305984491	25.25862736420253
C	13.90508263310744	30.72676812516874	23.96343956577423
C	13.25796378147558	29.47429950307129	23.80589718507914
H	12.80685039402108	28.98200513544311	24.67297312973149
C	13.11076271241731	28.88118412470451	22.53973650546307
H	12.58737063954185	27.91796924592757	22.45607773702854
C	13.59384934500329	29.51351069416649	21.37394732086762
C	13.37068056833706	28.92907554356571	19.97923602945263
H	14.15858390472879	29.32801472261645	19.30864630266284
H	12.40135853857199	29.30337610087956	19.58509358039313
C	13.36538477752364	27.41543582881968	19.92970275107533
C	14.55836983598477	26.70171106288619	20.20110415273638
C	16.85692697615279	26.83326764091463	20.89416257575682

H	17.27769770095133	26.14566101632009	20.12628402915149
H	17.58918207155515	27.63568292258888	21.09995212307851
H	16.67950140377755	26.25258921364300	21.82685718041038
C	14.54951429079363	25.29359867597427	20.23222235118119
H	15.45387577635578	24.73146926812486	20.48429873899268
C	13.36740320632523	24.56456219061091	19.99650382396072
C	12.17990566628415	25.27746829049012	19.69469098933687
C	9.80797593139036	25.17894312887395	19.28446044209744
H	9.80268944767209	25.82289693920099	18.37663452693545
H	9.04465246104279	24.38743185565213	19.16434287217914
H	9.54532500671679	25.80628244660298	20.16543903637434
C	12.18961767932976	26.68790559061469	19.66680943768941
H	11.27181656865332	27.25032807659442	19.45637190654892
C	13.32248749513618	23.05503573261531	20.21830138617979
H	14.33523202867725	22.63034178134411	20.09407281201813
H	12.64829795441478	22.57983578367497	19.48253273559886
C	12.80696195607828	22.79930005984709	21.63065628932483
C	13.67392327990512	22.94491273557626	22.74344395492577
C	15.89465065661778	23.45376441427944	23.52270958296803
H	16.88931831544690	23.61711015327629	23.06758125061112
H	15.57948645631277	24.37969246109449	24.05323243015662
H	15.97071124570689	22.62795787704725	24.26486240551168
C	13.15037867120895	22.92534223964187	24.05069330476356
H	13.80637392025370	23.07665723203310	24.91632163264508
C	11.77131951596021	22.76349621521175	24.28602157287839
C	10.91277555303317	22.57147687572390	23.17743223145746
C	8.66349615946960	22.25470765889251	22.37639613821723
H	8.89096492969623	21.34012043415440	21.78457413021235
H	7.65551192042995	22.15642611029080	22.82021324780638
H	8.67461737603801	23.12979843823570	21.68856422271796

C	11.43697493815017	22.58300500489540	21.86913054047371
H	10.77886132187036	22.49103301748058	21.00012061189812
C	14.27087275983642	30.74175565504862	21.52771774917033
H	14.69048084667333	31.24155655700213	20.64126124707258
C	14.42760932553428	31.33017224273330	22.78913794676738
H	14.98195286213888	32.27393349386601	22.87444846634419
C	14.26523859856682	30.83515769976359	26.51917495162675
C	14.53452476432942	29.42663713585453	26.64791794895320
H	14.62446674535229	28.81738642210393	25.74308238452242
C	14.70563938163115	28.83117762198567	27.87490378283309
H	14.92182861636526	27.75791215537760	27.92978711660874
C	14.66282059158228	29.59064623800336	29.09631402188471
C	14.81410879460028	28.97879515687683	30.37984453479849
C	14.79651721560017	27.49593149697238	30.52540363587270
C	13.73270706429633	26.73808158403223	29.97737659549753
H	12.90663844686802	27.26255864289756	29.48516206805841
C	13.71632796617881	25.33865612913094	30.07439866753962
H	12.87529216087667	24.77897682344988	29.63828971882015
C	14.75707592024000	24.64246206506612	30.72557143939238
C	14.69384177511559	23.12684205940489	30.89478110088227
H	14.03254607761265	22.69709452781676	30.11685867681980
H	15.70013048167630	22.68598408556745	30.77154277462927
C	15.80553017323487	25.39697925078233	31.30008087879254
H	16.61100404644764	24.86861563640266	31.82829079998032
C	15.82476960822487	26.79810420635972	31.20372040080015
H	16.66258277408206	27.36551145689369	31.63439416406420
C	14.98604594741309	29.79887301286175	31.51137486053518
H	15.15184141546746	29.32146013210952	32.48585784647380
C	14.00244295055375	39.47256242986959	36.73535330451928
H	14.80763273838029	40.21895881077239	36.85910014889198



H	13.27129628257174	39.60297342606810	37.55354338239869
C	11.60915201427231	36.15576468892269	37.78098925229894
H	11.49035497926462	35.51454804532347	36.87924747623530
H	11.94661868928164	35.51667340151302	38.62744620685930
H	10.63152397701400	36.60371029699596	38.03940496632046

Optimized structure of **PC-O**

O	13.99129558644260	36.96638182252721	20.62167300129186
O	8.48023172106464	36.07798382810743	20.70524382197529
O	10.48986436788577	39.69372577625337	32.32492670236175
O	15.72349669647710	39.74050905337352	34.24405551236840
O	10.58866253276294	27.22920344080078	36.55784948592239
O	15.71703216728318	25.04370717525399	36.35030902849402
O	11.23302258557593	22.52778237709656	34.80705930169375
O	15.85799419258315	23.08127348921755	31.73791180815018
C	12.63319445449578	36.71034306730069	20.62025200743797
C	11.78633601009784	37.82538534200356	20.84354424083138
C	10.39486621201030	37.61652790293427	20.87005529487492
H	9.75701109283265	38.48227979097062	21.07458766611411
C	9.83939891168708	36.33618666460137	20.66719491592209
C	7.59343457451227	37.16494107405403	20.93533693627051
H	7.77896730191797	37.65002010241432	21.91990245294338
H	7.67335987121633	37.94059693365943	20.14121806259092
H	6.57167810267095	36.74237177049254	20.92721514879986
C	10.68275110338200	35.22879064290569	20.40732558679159
C	12.07622306785921	35.43470126690293	20.39731183140829
H	12.72130922464201	34.56725155025807	20.21199339870846
C	10.10573454096225	33.83399643804910	20.19113354416972
H	9.08278481845399	33.92852774436463	19.78052459685312
H	10.72256630293294	33.30051792667988	19.44133232868638

C	10.06946930188548	33.01752261725584	21.47855408805327
C	9.11964957196363	33.30185437357958	22.48696097800489
H	8.37739158019355	34.09218347182509	22.30900770721891
C	9.12628451006689	32.59963204714366	23.70129631366231
H	8.37435498710755	32.83020736413152	24.46932066505891
C	10.08520878885126	31.58714627728301	23.95341847649745
C	11.01853187295237	31.28861307880752	22.93491854925870
H	11.76916107149661	30.51189642868052	23.10658055882744
C	11.01143365660721	31.99676120938190	21.72125297823333
H	11.76255568989486	31.75191948398799	20.95480644654963
C	10.13349176229695	30.84944052710415	25.25078905611870
C	10.31964239003646	31.53152452481331	26.49250729712092
C	10.38917474815047	30.77331041444354	27.71854074738015
C	10.60438729869355	31.45428009880585	28.97543519099716
C	10.73004374885871	32.89344886078613	29.00513990853695
C	10.65774531567429	33.60417227579767	27.75768326025996
H	10.76757504942178	34.69087071869632	27.76626505293257
C	10.48091681183523	32.95774063252011	26.55977703985461
H	10.48034426886552	33.53529625645056	25.62882768410657
C	10.98324165401394	33.55453539966997	30.25004952656617
C	11.26197960815636	35.01667090633601	30.34161714054775
C	10.45564477805905	36.01918097624589	29.74931203281804
H	9.51094942415797	35.73836812206104	29.26398504077826
C	10.83636943530871	37.37225637008436	29.79253495838815
H	10.19100098022662	38.13441644296081	29.33104543392366
C	12.03262038662342	37.77235444868678	30.42075045394266
C	12.48224656432685	39.23308370267571	30.46708796479906
H	11.68260045371358	39.87741297100175	30.05451306100396
H	13.38048762298171	39.35602524711482	29.82848121413744
C	12.81504460799367	39.61239447724501	31.89849623724141

C	11.76717512677420	39.72476695322997	32.84501001265817
C	9.39228326149094	39.64454946221981	33.22436981793554
H	9.44304100337057	38.75340283483789	33.88899426304154
H	9.33262574564462	40.55513389636906	33.86209592298657
H	8.48000177005340	39.57913317340704	32.60298446514478
C	12.06154678809257	39.78982120888894	34.22053810069262
H	11.25925232285280	39.80013741528204	34.96564609617594
C	13.39049298805422	39.75506386342879	34.68545734888035
C	14.44065015186040	39.72850612370775	33.73421174940201
C	16.80148157768544	39.43034392392509	33.37211847934633
H	17.71260088234541	39.39772338643996	33.99886344787304
H	16.66192670845881	38.44108796771209	32.88216217506659
H	16.93900557568895	40.20246066207842	32.58211393806380
C	14.14539696301004	39.65041729056350	32.35639223565783
H	14.94910957379080	39.56441865887176	31.61479747694142
C	12.80473670310911	36.78160551491531	31.06355019525568
H	13.72183443890414	37.06931942911496	31.59485565035345
C	12.42400143677714	35.43654950941846	31.03450379801408
H	13.05329483203114	34.68601786321493	31.52393981131265
C	11.12794955349120	32.77259201918211	31.41155762093090
H	11.37973808138313	33.28082888447894	32.35077214558117
C	11.01425129037171	31.36871162547531	31.42141912961240
C	11.30638921121666	30.66227505812137	32.70008636124278
C	12.21341397040697	29.57382738699318	32.75168843948562
H	12.64722962026920	29.19457565429111	31.81979248643691
C	12.63285073762911	29.03564067938478	33.97734099919349
H	13.35648582145734	28.20833565277335	33.98467673729681
C	12.16082083402009	29.55515905615267	35.20217858987768
C	12.68226353814599	29.03213705973129	36.54054588957261
H	11.95448251697305	29.30268333766757	37.33101929000482

H	13.63074847880887	29.55849274998437	36.78218736397145
C	12.93336552072918	27.53769765488415	36.55043867940539
C	11.83474440124218	26.64325231462151	36.52651513653120
C	9.44663500902859	26.39571601488541	36.41331753761949
H	9.34759680162021	25.67440386210266	37.25554952694063
H	8.56803575657220	27.06689436016597	36.40754084559882
H	9.47359944100190	25.82177759674315	35.46009227492513
C	12.05549260083215	25.25397784051725	36.45669730526416
H	11.21799692840081	24.55053608403203	36.40503801512801
C	13.35940890771268	24.72266026599062	36.40214247119655
C	14.45914991082742	25.61561280837143	36.42698140669511
C	16.85126324481579	25.90069857257851	36.34876081913310
H	16.91753019273109	26.50473237022566	37.28102379282572
H	17.73913463913289	25.24490274233163	36.28189760444889
H	16.84558834175585	26.59475231926619	35.47840748775693
C	14.23633621878665	27.00712210816594	36.50862717204715
H	15.07840142464570	27.70977477375327	36.52090654430964
C	13.57679236686536	23.22826515883476	36.18953488811103
H	12.76965553656914	22.66086693685223	36.68617021707941
H	14.54345312984879	22.92585569370877	36.63048162453913
C	13.57610719383122	22.92572123422033	34.69533077907173
C	12.36580095975598	22.63312551278145	34.01956499134254
C	9.98973716975744	22.25881503791006	34.17281913022249
H	9.23113237877282	22.21536706083659	34.97621203074453
H	9.70968505671373	23.05950810921932	33.45187315459575
H	10.00023218199788	21.28593420339217	33.63252278663838
C	12.35848160587738	22.49216561375820	32.61494832555792
H	11.42506860676618	22.28510462484023	32.07746085832251
C	13.53520582067635	22.65098136343999	31.85927524942710
C	14.74730189886200	22.92815476766554	32.53842662218675

C	17.06839013716281	23.51999090119789	32.34047565351377
H	17.46482080697194	22.77720096256488	33.06877208945637
H	17.79865238281935	23.64659625008776	31.52004912765490
H	16.93666372624885	24.49203989115519	32.86612410793373
C	14.75777878787191	23.06079425597686	33.94008290253365
H	15.67663635965721	23.31768069827393	34.47710414979294
C	11.22542481423302	30.61035717306910	35.15491760550788
H	10.82014607991929	31.01295886475476	36.09581504700535
C	10.80963662860877	31.15789174435696	33.93115045728241
H	10.08555468296301	31.98485443814866	33.92219175919166
C	10.70575946716858	30.69346667148599	30.19832754868873
C	10.43215945834992	29.28196362096372	30.14101442853149
H	10.37429387088378	28.71776819774197	31.07994791762673
C	10.20648874606855	28.63794000682200	28.94633473631220
H	9.96706153462968	27.56922677574771	28.95176477779424
C	10.25641469459832	29.33523798948820	27.68596940659850
C	10.13693907155784	28.66703857031572	26.42209969097429
C	10.14678180653229	27.18345518231504	26.29283460338494
C	11.04902235022186	26.39910839165103	27.04999508975356
H	11.71551565181318	26.88828763850349	27.75981895807706
C	11.13937535666484	25.01093117890331	26.87951846065743
H	11.86671031563382	24.44906364904066	27.48258248432293
C	10.33305488614459	24.34529940245661	25.93455165002426
C	10.51866548253947	22.85824285993001	25.66122276996697
H	11.06514284975983	22.39734984052875	26.50791973759942
H	9.53957473599646	22.35386962145246	25.57208696124927
C	9.42542517041290	25.11742941762981	25.17249089078530
H	8.79582984536313	24.61233957826088	24.42537489544700
C	9.33104191926718	26.50684038524966	25.34820693587348
H	8.60663966495988	27.08028362483540	24.75249721033736

C	10.06528911773664	29.44610434628647	25.24786268306121
H	9.97843958208644	28.93835060619046	24.27974327189470
C	12.37731420072831	39.20881274815053	21.09146517702340
H	11.62839279439141	39.97333686593681	20.81383736312902
H	13.26566834196587	39.34457995779890	20.44715388106516
C	14.88636336051128	35.87381282780080	20.46245762349369
H	14.75511505917673	35.11147067370638	21.26244764420094
H	14.76392469990688	35.37477801270322	19.47504856655699
H	15.90758899909290	36.29344245667224	20.52759590362250
O	11.87869710698757	37.44354109318116	36.15305613536849
O	17.25274912712938	36.11916463644258	36.86601691418710
O	15.75042504742307	39.04623592375813	24.79528470701853
O	10.54432249714078	40.01833789103789	23.04752161947964
O	15.75856331002065	27.10762628336527	20.64493942910820
O	11.38332644302944	23.90583083899567	19.35221208395102
O	14.78138714356189	23.16614959179994	23.07961526367082
O	9.30402405628743	22.09928727745703	23.22778811006214
C	13.19586257626746	37.08281466043918	36.34334157666359
C	14.13313279234190	38.14378321231740	36.43601913032295
C	15.48717867096954	37.82304659886746	36.64579697167389
H	16.20472763452309	38.64881876103621	36.68931146500159
C	15.92403996151540	36.48393003901922	36.72443471914709
C	18.22436508968543	37.14661356663857	37.00393719917152
H	18.26591918870604	37.80356612600134	36.10597151677310
H	18.03132039782920	37.78413914057970	37.89542523575268
H	19.20030741567540	36.64095896860341	37.12503768197656
C	14.99081596740335	35.42563780174711	36.61120829552242
C	13.63219703215602	35.74615945017313	36.42779632883537
H	12.91781563155759	34.92067221038010	36.32076343148592
C	15.44940876117315	33.97193140420623	36.53797511663605

H	16.44808355726594	33.87659286986169	37.00231199347054
H	14.74615522918836	33.32646785943129	37.10024938648181
C	15.48788622903542	33.53345831047456	35.07821454695919
C	16.45644552319775	34.07121341706166	34.19883591628925
H	17.24523858799646	34.71837505759568	34.60823791201070
C	16.39565043115514	33.82121708388860	32.82081331049142
H	17.14946539686426	34.26121851777818	32.15174984531657
C	15.36639893687164	33.01786911108608	32.26772080414410
C	14.42582404479563	32.44521755515981	33.15715823548371
H	13.60909214223899	31.83389727441230	32.76170158383617
C	14.48693767264469	32.70054235384801	34.53734876042050
H	13.71616011741979	32.26707809121515	35.19151633631456
C	14.12554110272410	28.01113775657181	28.00950075873854
C	14.36863438947198	29.22941417063355	28.71763154160787
C	14.27280803787636	30.48793497945572	28.01383462152296
C	14.52191859579411	31.72507427849739	28.71783090464522
C	14.88853504433007	31.69319945386998	30.11514032154714
C	15.02416778776863	30.41750423362619	30.76419957768023
H	15.36012818556465	30.39114150178223	31.80740882167315
C	14.77648872340734	29.24078522058992	30.09654444564575
H	14.92409562996137	28.28347377852572	30.61069253288725
C	15.17430973459366	32.91872166520132	30.79378548324677
C	14.57673293770581	35.56481032327721	28.14564760581208
C	15.55895954227694	36.56537722461356	28.34381627034062
H	16.50802679046992	36.29787986933075	28.83032104939524
C	15.34996001835063	37.88423194763708	27.90519814103692
H	16.14144919476168	38.63619394984764	28.04213688400734
C	14.14702732856526	38.25760023794825	27.27206580371706
C	13.90857759968555	39.67599823828669	26.75808655215787
H	14.82606705243741	40.27644934471657	26.91403495780282

H	13.09693257145613	40.15477039642762	27.34469569829605
C	13.52113928751418	39.66771126451997	25.28918109799646
C	14.48041554133121	39.28813002367036	24.31797385278918
C	16.71312743694012	38.49564019121558	23.90668404510796
H	16.36005821010656	37.53932122187177	23.46051815515633
H	16.96811894731973	39.19716949818666	23.08067421922744
H	17.61999301911503	38.30198939404340	24.50887909661691
C	14.10763846983256	39.16301032662621	22.96559925887162
H	14.83077458819289	38.84476007640028	22.20794766609788
C	12.78592324643120	39.40846632384996	22.54597672794337
C	11.82634216753442	39.79311104117800	23.51483765078138
C	9.53311271567846	40.36514993482841	23.98285642688554
H	8.59775153191668	40.48300149645322	23.40440128010836
H	9.38677922429780	39.57163375162484	24.74977352798950
H	9.75751859416461	41.32244877138034	24.50474423387249
C	12.20202461588256	39.92426916275578	24.86936286743819
H	11.46578147500526	40.21230934520116	25.62968170742539
C	13.16389071488389	37.26423525073756	27.08225678802853
H	12.21654583135968	37.52699189657003	26.59088144227222
C	13.37525793076944	35.94694522136047	27.50423417725846
H	12.58312383228105	35.20564309564432	27.37599423972420
C	15.15238711740101	34.11932826681586	30.06248061775023
H	15.34749564334389	35.05555186969442	30.59854542816580
C	14.74507111869828	34.19897852353973	28.71719811001636
C	13.66153472858404	29.16100039440537	24.41947569638646
C	12.77655171571583	28.19109030965648	23.88171386650913
H	12.16125343824199	27.58864457737106	24.55962239809567
C	12.66753331988158	27.99494031862362	22.50033619684551
H	11.98452259610765	27.22187608317187	22.12202167568173
C	13.44394346291721	28.74851674492061	21.59131510466421



C	13.39708998872549	28.42846904253133	20.09487147740684
H	14.21759681312533	28.96773273957386	19.58290596912470
H	12.44059145348746	28.77920199065881	19.65433051393665
C	13.51697279131876	26.92443425957602	19.91257382598789
C	14.70445255772106	26.27644208657791	20.33352300527234
C	16.85958393548053	26.56656590014978	21.36299351282280
H	17.42275761953692	25.81615166995856	20.76406021708631
H	17.52836029055033	27.41543960684027	21.59680056696297
H	16.53160507812343	26.08908104213085	22.31253472485283
C	14.72998918600976	24.87704962425765	20.48376558306654
H	15.61131282108786	24.37326174367614	20.89332627074245
C	13.59769967950586	24.09115427426765	20.19495067661591
C	12.44549407177110	24.72958107199896	19.67025162177755
C	10.14951618605452	24.50298087259194	18.97879293296432
H	10.24066857652441	25.10085581730574	18.04451543010827
H	9.43998210128885	23.67272962917859	18.80346876681049
H	9.74821990944469	25.16008990666081	19.78243188273710
C	12.41100966549697	26.13491446003573	19.54662919039080
H	11.49734061570377	26.64520870901143	19.21802509149785
C	13.54005653668826	22.62398434436758	20.60913109038852
H	14.56722506295371	22.22951831407310	20.71757553174788
H	13.01271866829953	22.02487660832707	19.84402174362816
C	12.79191440629104	22.52607358207246	21.93718015824489
C	13.43333096964447	22.87592623210328	23.15404794293842
C	15.40919509124172	23.73333686561731	24.22346351230865
H	16.44904524281915	23.96572482422052	23.92735416889065
H	14.90222333250493	24.66920846861480	24.54753123379498
H	15.43141234135132	23.02718943079898	25.08349817503057
C	12.69305576603518	22.93173485890864	24.35063276566131
H	13.17464075700365	23.22193694354999	25.29228814221604

C	11.31155350304717	22.65953492467807	24.37413446829915
C	10.67010100533201	22.31162698892393	23.16223346834113
C	8.61677882643488	21.75341215158974	22.03324772064141
H	8.99612854937170	20.80337929585115	21.59475136239814
H	7.55370543605741	21.62505413183323	22.30919075270766
H	8.69777109580314	22.55201471823831	21.26172110541287
C	11.41562493655479	22.23145209362319	21.96722526391303
H	10.92737944002291	21.99178850148410	21.01782839751893
C	14.32633560071399	29.71203139153918	22.11903140270942
H	14.96844321648592	30.28539497677956	21.43391888806677
C	14.43441699088767	29.91884527868348	23.50524506589970
H	15.16430331477985	30.64524015825061	23.88598180465497
C	14.42356486212600	32.98872685436478	28.02069433923626
C	14.03061365766953	32.96709037563146	26.63587296189650
H	13.92697270962119	33.91671803640595	26.10015156018493
C	13.79537636455778	31.78895052947305	25.96505479814236
H	13.47037107720613	31.82279065403035	24.91963829981002
C	13.95851885824540	30.50911446560988	26.60230299009782
C	13.83152161548936	29.26999422031055	25.89496729634335
C	14.06425108238315	26.67764162435146	28.67002170899371
C	14.71064216469047	25.55376205982040	28.10056879935311
H	15.35986080943272	25.69713182533117	27.22510221011901
C	14.54701052681999	24.26904692519745	28.64411971177768
H	15.07700550340237	23.41596014723369	28.19372669319897
C	13.71893994961066	24.05348405577029	29.76506781742529
C	13.51464861954601	22.65242689918922	30.34309179322780
H	12.54036491729498	22.24923315405037	29.99377476522433
H	14.30345356135038	21.98554565117374	29.94283076524808
C	13.07826806046934	25.17325494866171	30.34058632855200
H	12.43593754898896	25.03301293071337	31.22128021044288

C	13.24732217260931	26.45940692066874	29.80823773002791
H	12.69992924510936	27.30499580948909	30.24456082875262
C	13.90167591398836	28.06678359325953	26.62320317413459
H	13.76698645570694	27.12280121778733	26.08212566517594
C	13.69789924547666	39.58302934890831	36.16999285008387
H	14.50791857472495	40.26942852874455	36.48139685820006
H	12.79303101211195	39.82683924793852	36.75861994365931
C	10.96982887551462	36.45079286903791	35.68968100792097
H	11.33985030513791	35.96166273358241	34.76210947476350
H	10.77495790625250	35.66835856892671	36.45680675952568
H	10.02030489337835	36.97361385626373	35.46918292129433

Optimized structure of **TCNQ**

N	4.19570018705460	2.22920663320875	0.00042150659487
N	-4.19581078095057	2.22911717204752	-0.00086394830780
C	-0.68603105045422	1.24283846539123	0.00000360549350
H	-1.23966862402245	2.19136678276040	0.00000441483216
N	4.19578326591366	-2.22910120792056	-0.00072707293391
C	2.84426131009905	0.00002774556914	-0.00007373756154
C	3.59433316641437	1.21885449057918	-0.00003603647995
C	0.68601857306936	-1.24282166747635	-0.00000317170961
H	1.23965728098003	-2.19134930097186	-0.00000621119161
C	-2.84427391423612	-0.00000405929080	0.00004876629780
C	0.68600051300365	1.24284974663941	-0.00003059249143
H	1.23962326111121	2.19138652856456	-0.00004903871561
C	1.43275324957245	0.00001960006770	-0.00003432426056
C	-0.68601302463045	-1.24283330964237	0.00002540526564
H	-1.23963658747223	-2.19136916916397	0.00004650405232
C	-1.43276508716062	-0.00000306157171	0.00003032482410
N	-4.19561199214218	-2.22924347098507	0.00022904394863

C	-3.59435938494929	1.21881609397605	-0.00003921257251
C	3.59435199138520	-1.21878734333804	-0.00018525734253
C	-3.59434535258545	-1.21883166844322	0.00013703225806

Optimized structure of **PC-P $\rightarrow$ 2TCNQ**

O	11.75109078060209	36.84083468503945	21.68652302622653
O	6.28051920353210	36.84685510566318	20.63479899576329
O	11.27659307984631	39.29486954600679	31.56096626982262
O	16.56558144000991	37.80541628119322	32.48580272159335
O	7.92822867105769	25.98992175214051	35.57641111681538
O	13.41279066822394	25.88536302554449	36.51991354068969
O	11.65550584848367	23.49784991013624	33.27771329066176
O	17.02764674273464	23.08583939958680	34.70601428951495
C	10.41240173418165	36.81301168306260	21.39755277644577
C	9.68892285666034	38.01021508357844	21.64817249123470
C	8.30909951646914	38.02726282757571	21.38028938309967
H	7.75423996832106	38.94610977663276	21.60444518671178
C	7.64185378502464	36.89547737253019	20.86748289292644
C	5.50737506381481	38.01812144037254	20.86673764672118
H	5.54289046975065	38.33352680093161	21.93332907150498
H	5.84670004426188	38.86896535334803	20.23510185892027
H	4.46527579587457	37.76228767627281	20.60051904899668
C	8.36948509124659	35.71174936011990	20.58745320499883
C	9.74540875023844	35.68405558755095	20.87841383871059
H	10.29587618080050	34.75150219082025	20.70497509252614
C	7.66107178516379	34.45986228900033	20.08109454280863
H	6.67094129286635	34.73909964654336	19.67621910443025
H	8.24791957054200	34.00223108381918	19.26049016052778
C	7.51337627537066	33.46185057175480	21.21899011215390
C	6.72336944224231	33.78219177786576	22.34726419506813

H	6.12575659870904	34.70478791831250	22.33589159241102
C	6.72652328028066	32.96147772828245	23.48036767900419
H	6.10977488561569	33.23114836735660	24.34821475773222
C	7.51913282348215	31.78379034094588	23.52887064528152
C	8.23254813546663	31.41949701670960	22.36186961526546
H	8.83781630429642	30.50576939564433	22.35546763611766
C	8.23935984153792	32.25445613833508	21.23481003858988
H	8.84897760726107	31.97778155419304	20.36161785537904
C	7.62410820622709	30.97845718462963	24.77113798706366
C	7.80390130628912	31.60053783743499	26.05710869582742
C	7.75544694038719	30.79054959759728	27.24846245787903
C	7.95367995395458	31.38715181065586	28.54861376762053
C	8.36141221732424	32.76814114702086	28.64219156472319
C	8.47031841064130	33.52206832948562	27.42820236301158
H	8.84594918091589	34.54817150468412	27.46799639349720
C	8.16238189515082	32.98028432117365	26.19697910169056
H	8.28667546031649	33.59445866873478	25.30000168952666
C	8.78154611087921	33.28542523678090	29.91858329686139
C	9.58080116039169	34.54219875459491	30.01609492451630
C	9.20236745242409	35.77676128944553	29.43535801302960
H	8.18583804678659	35.90293390455376	29.03854147773494
C	10.11581783630440	36.84174671320473	29.35216886526794
H	9.80644917596599	37.79054947773593	28.88935565679541
C	11.43312271634301	36.71254196267867	29.84024153403003
C	12.48178110909864	37.78886730328078	29.59555018908834
H	11.99079847259939	38.67173047266998	29.14136916086937
H	13.20535312524719	37.39262028624393	28.85562549367475
C	13.24156034781392	38.19552496221840	30.84108837391789
C	12.58311639657994	38.95577713462537	31.84069400217622
C	10.52162895221008	39.96895706227009	32.55887538292730

H	10.45733800149455	39.37528277065424	33.49782970066430
H	10.94994201572633	40.96754045956860	32.80109295949457
H	9.50512121328339	40.10312702907842	32.14514522146461
C	13.26159381144512	39.30283002000639	33.02397378969326
H	12.75127654045488	39.86131392732322	33.81771682977453
C	14.59588807399168	38.90745228357364	33.24558473529671
C	15.25613368768553	38.15799782737066	32.24223370407535
C	17.02586899639069	36.55476461229190	31.97088222877415
H	17.96529325145401	36.32061264876920	32.50573148293976
H	16.28842519575050	35.74801914714249	32.16701392161332
H	17.23827135529050	36.60454438607454	30.87952019937531
C	14.57367170203715	37.80389652577522	31.05784428959544
H	15.08486195625902	37.22305067767314	30.27889445976293
C	11.77439246672913	35.52750276688598	30.52651188927086
H	12.77178009403733	35.42423454594873	30.97845187945462
C	10.86481692614265	34.46596686248796	30.62083029990363
H	11.16889443769348	33.54959066629883	31.14116879860184
C	8.66725560150092	32.46313922028688	31.05211068127566
H	9.03985823462567	32.84923860451705	32.00768001381622
C	8.20366252107504	31.12968972894482	31.00910145657670
C	8.26510189378224	30.34946381120469	32.27471285460607
C	8.83497835349481	29.05394677611232	32.33150795327484
H	9.13589330939296	28.55136279999462	31.40718563203338
C	9.10845712179593	28.42573785012138	33.55484051673533
H	9.61495864343403	27.45175210750196	33.55396720179721
C	8.79391635305476	29.05364819223049	34.77642426273768
C	9.12109914071204	28.43035705972209	36.13289431029489
H	8.16258014684793	28.23722458883913	36.65915257017338
H	9.66476831928536	29.18409347029680	36.73886389101057
C	9.92714946256459	27.14939219647779	36.09071306231740

C	9.28440732234639	25.91623597755659	35.80978071288949
C	7.23229571374535	24.80063322513118	35.22757613818005
H	7.27454967780525	24.04038487681898	36.03946361411506
H	6.17911791164287	25.09217449388623	35.05992026572408
H	7.63682668201811	24.34423115426662	34.29655151117133
C	10.03038713147685	24.72051235962883	35.77760161054491
H	9.54771704539540	23.76416770549782	35.54627175506733
C	11.41487252154315	24.71608445419231	36.02157055001108
C	12.06459114322197	25.95138102362624	36.28212573373407
C	14.17502472189122	27.09497427407148	36.51677254301713
H	13.91598541663749	27.74568004139084	37.38187840953989
H	15.23357806334542	26.78775977834698	36.60480847835994
H	14.04282546004928	27.66578391003135	35.57460955411381
C	11.31718550823039	27.15030982130924	36.30414945928325
H	11.81378087322763	28.10875436458352	36.49769850839450
C	12.20419071246292	23.41420214812412	36.01185446031919
H	11.49096256065836	22.58126213906388	35.84848336710513
H	12.66587343545452	23.26021389393716	37.00841034194214
C	13.30673011851390	23.34888647552349	34.96573617062344
C	12.99041008728130	23.41478083407314	33.58439458755613
C	11.2766689997788	23.85676449811899	31.94730694409840
H	10.17428175974242	23.94447987382043	31.95812460849127
H	11.71145423538024	24.83299603359609	31.64988141264607
H	11.56514884237265	23.07328969322280	31.21092788163361
C	14.02429578550943	23.37460162261083	32.62362895437079
H	13.78698690995336	23.43799698174099	31.55473064894608
C	15.37353362434929	23.24847063461524	33.00444271381313
C	15.68623710396064	23.18798438800613	34.38609041005326
C	17.39360771975045	23.02178353252230	36.07901682457662
H	16.95390075923743	22.13297224972317	36.58379595169922

H	18.49620545607301	22.94363390027035	36.10552519735030
H	17.07960882028241	23.93398260662255	36.63358798565088
C	14.65503244014833	23.23634583266763	35.34483132634124
H	14.88514693641227	23.21478893539686	36.41595073805431
C	8.16875348714232	30.32014966833666	34.72720868838150
H	7.89614494406505	30.82405414105345	35.66737234600250
C	7.91894043564508	30.96068309299288	33.50713041724975
H	7.45574228531591	31.95727131109145	33.50256584921701
C	7.84758697825663	30.57175796776878	29.73652805741299
C	7.40922944688927	29.21255373580657	29.58044890089989
H	7.15805770618277	28.62974068388853	30.47335564832632
C	7.32387073257624	28.62161125117706	28.33537475116646
H	7.02749527801523	27.56874566384405	28.25270923327193
C	7.58706092632469	29.36384099130494	27.13769841419710
C	7.67993993341844	28.74556373300230	25.84173659607844
C	7.92286918925385	27.28970465465441	25.67073409878587
C	8.80799172196309	26.60118979178298	26.54091002511039
H	9.23472486349714	27.12549876316625	27.40236479186078
C	9.19615887870063	25.27968700720795	26.28377221133558
H	9.90919629508866	24.78620620777807	26.96108415985435
C	8.71450937589753	24.58449785179000	25.15510188763712
C	9.24147423588310	23.19660651712155	24.81664578166244
H	9.62812851423740	22.71616731450414	25.73645103375557
H	8.42311532794137	22.56743954914947	24.42020646423144
C	7.80104437602130	25.25021646428054	24.30496551273584
H	7.41643298454377	24.72078415315460	23.42330949595018
C	7.41375044606866	26.57316443746765	24.55689279774220
H	6.70369924449896	27.06601341607580	23.87826017076542
C	7.64012912407657	29.57145900857471	24.70218844753999
H	7.65835412918121	29.10024428344382	23.71196727305787



C	10.37767568055235	39.26910607079227	22.15731092251097
H	9.58368996019477	39.98178025453438	22.46526260779017
H	10.91214100694298	39.74932802662656	21.30988107205668
C	12.45750790578912	35.60323633387257	21.81750029988039
H	11.94074629510315	34.91713762378485	22.52048007229126
H	12.58562739516692	35.09659096544503	20.83507379318175
H	13.45382917490686	35.86277343154682	22.21989830192468
O	13.83094073027600	36.97529387175728	35.25877167959231
O	19.28962162018694	36.84313128968982	36.37249211754622
O	14.90212934669846	40.01508896261033	24.14183058671366
O	9.76057460073298	37.89504644993793	24.53963322063561
O	17.70583035110743	26.33407595823480	21.32627551524696
O	12.25917995043615	25.99647746447836	20.23671090768599
O	14.06120088355593	23.72849086777571	23.54279314337386
O	8.73259370833696	23.02105762142327	22.06669111700087
C	15.16609439749496	36.90951992871776	35.56385301807006
C	15.93519291884288	38.06255494973429	35.25682919441495
C	17.30824859710735	38.05587014926807	35.55513438414703
H	17.89653191382594	38.93894943266583	35.28009356907992
C	17.93192160516171	36.92563113445058	36.12109914457595
C	20.10131372375254	37.97798437798507	36.09603645430457
H	20.08599679952591	38.24514954218705	35.01576790656036
H	19.78257934119052	38.86736288122494	36.68377048346983
H	21.13225075540297	37.70281580994304	36.38561856215927
C	17.16664475702433	35.77099880444933	36.42239814352461
C	15.78977514651357	35.78015284584086	36.13288591911397
H	15.20816265184105	34.87267680485824	36.33610531104280
C	17.84047759122453	34.49723896539090	36.92085725589715
H	18.82967127722431	34.74689735279457	37.34689515169742
H	17.23063694016972	34.03393875070199	37.72096660669802

C	17.98588961355677	33.52167897337489	35.76113648744492
C	18.79967660038506	33.84874056560542	34.65116977987991
H	19.41449323151589	34.75901010314634	34.69124405615018
C	18.80145644992376	33.04979494860728	33.50183926005833
H	19.43927140733884	33.32419213359391	32.65070887456211
C	17.98991892766952	31.88722212535877	33.41632963430811
C	17.24342537352008	31.51935659842243	34.56116752496516
H	16.61636670539255	30.62086144238718	34.53715556703717
C	17.23314252995883	32.33199873042143	35.70505250561690
H	16.60001863590183	32.05129523757570	36.56004262815871
C	17.90459004339665	31.09625814130504	32.16164847898978
C	17.75074499565532	31.73295273757113	30.88036258090867
C	17.80206458240290	30.93542542034518	29.68056175450359
C	17.63058429529860	31.55020489986373	28.38545507536889
C	17.27322918090747	32.94561084660794	28.30225804849692
C	17.15079866830359	33.68724035388365	29.52285591160551
H	16.79973599360828	34.72263012649599	29.48546911049421
C	17.41624290634197	33.12023367802664	30.75192024914588
H	17.28464740256280	33.71904671751364	31.65720617248165
C	16.92542901372250	33.50141439100079	27.02449749931258
C	16.31290895174421	34.85327425681053	26.88023514198644
C	16.86643887652071	36.03238386808438	27.44069280861036
H	17.83430284842046	35.98568572242002	27.95834257233763
C	16.21236314785287	37.26790301299352	27.31126492911748
H	16.66657435601192	38.16784093179474	27.75306745423388
C	14.98692199186923	37.38374081654475	26.61372164077855
C	14.27941719721870	38.73852770441791	26.53811769996996
H	15.04447614694134	39.53017587224323	26.44012979557694
H	13.77489336690121	38.91536026013890	27.50970781278221
C	13.26031677932309	38.87760636587046	25.42501743418746

C	13.61264798782834	39.53195873536315	24.21836105141432
C	15.31820272347270	40.65875178479649	22.94542007400038
H	15.24619138029166	39.98234232973611	22.06451527528534
H	14.72167050224166	41.57514205821083	22.73530913625038
H	16.37571211078562	40.94485086240769	23.09538934360880
C	12.66499468590098	39.65645667976844	23.18210196880089
H	12.92870059071221	40.15855411628754	22.24370032762015
C	11.37395986359057	39.11163157580928	23.29588290894605
C	11.02839065777144	38.42922285896894	24.48842194753077
C	9.52490507324701	36.78043946086844	25.40270813095489
H	8.51273756073488	36.40892644752354	25.15659011739900
H	10.25680187460351	35.96491177092512	25.22171923705818
H	9.55182752211473	37.06514053743110	26.47707079794484
C	11.96570427419383	38.32966711047271	25.53873848592891
H	11.69130355936431	37.81773635787753	26.46985296642648
C	14.45214258443654	36.21601927930137	26.02959407052522
H	13.51427770736482	36.27095249700935	25.46245391605673
C	15.09977277024574	34.97700673843701	26.15719837998505
H	14.64715265286409	34.08875769854462	25.69621701318340
C	17.00813050473833	32.68283389017351	25.88486362511115
H	16.68714202460121	33.10458511277587	24.92587389995971
C	17.40336357905724	31.32799961580184	25.91873653965254
C	17.32889470102302	30.56665770360218	24.64138658331861
C	16.73530017932248	29.28328071641235	24.56474550705650
H	16.42714855648167	28.77188697825612	25.48107274492241
C	16.44816618781983	28.67787085684652	23.33276838057915
H	15.92211237371194	27.71440248878379	23.32119412338769
C	16.77544947986075	29.31552984088012	22.12006123358250
C	16.42767395528726	28.72331476082256	20.75448496731631
H	17.37583534292688	28.58643968781477	20.19250456230418

H	15.83676244533980	29.47476601751274	20.19100972700847
C	15.67189707514767	27.41140253987245	20.77469974841822
C	16.35926254878222	26.20442874720170	21.06615756874470
C	18.44180256742303	25.17540894082977	21.69623069837037
H	18.44542802123670	24.40987490458343	20.88838765392955
H	19.47895417195778	25.50973236409495	21.88256081588244
H	18.03696907759208	24.70873249527051	22.62198104243979
C	15.66295830169043	24.97902095205537	21.08285952982554
H	16.17852883990910	24.04390130397473	21.32933572520827
C	14.28670951885929	24.91727155500981	20.80368088318165
C	13.59388535294455	26.12345445195674	20.52012027315394
C	11.44574833124596	27.17142465586976	20.19174638730885
H	11.72731760792353	27.83349780624965	19.34248363161869
H	10.40935413312866	26.81718432161444	20.03954545109018
H	11.49521924110120	27.74370077615569	21.14088155823654
C	14.28954641718385	27.35396764794755	20.52241789168573
H	13.75739162393841	28.29073812242208	20.31762999894588
C	13.54800798952613	23.58630534681511	20.80428002479303
H	14.29076897552979	22.78128036544023	20.97635654039765
H	13.10352838039037	23.41422091039551	19.80303423144310
C	12.43762436900760	23.47822871346856	21.83934129723690
C	12.73563339445598	23.57142058357555	23.22297910853572
C	14.40350468147597	24.18291140020912	24.85355384207988
H	15.49828204362417	24.33988690961421	24.84514582935604
H	13.90573155369020	25.14487041310167	25.09346819923363
H	14.15825739952055	23.42571222236489	25.63186948770650
C	11.69688968506879	23.47863154429177	24.17432077592128
H	11.92115542284038	23.55765284702125	25.24516531015949
C	10.36063984164737	23.27249566344977	23.78227552958751
C	10.06426560745727	23.19347992470327	22.39806259742116

C	8.38344617385014	22.92267009545906	20.69150371609098
H	8.87557855416499	22.05408430284416	20.19997663041540
H	7.28703667358954	22.78403546703312	20.65653243550538
H	8.65147939721520	23.84481845712459	20.12912841215275
C	11.10045549440770	23.29295272058593	21.44818077025177
H	10.88226899862455	23.25298073340242	20.37503970975843
C	17.43014147718329	30.56633112438453	22.18787726078893
H	17.71691465345482	31.07631660100810	21.25521164588344
C	17.69213108010137	31.18493781557977	23.41682974138806
H	18.17991824979533	32.16944030643050	23.43372114135709
C	17.72722131484568	30.74562916480621	27.18886436325142
C	18.13177168451849	29.37459716467094	27.33360074531113
H	18.37378669795039	28.79523877135773	26.43597684032335
C	18.20577987485629	28.77101093804098	28.57256951580528
H	18.48432150808260	27.71271509672183	28.64539733112299
C	17.95292149022930	29.50603951898832	29.77723308901209
C	17.85883268389953	28.87578567598710	31.06606789769969
C	17.63873194080965	27.41412397650539	31.21603088225051
C	16.73981926410546	26.73030443960554	30.35652569056030
H	16.27385590706293	27.26980361654733	29.52482065763373
C	16.40052536437705	25.38979541375677	30.58172635649058
H	15.67708838143961	24.89711560771829	29.91516579248648
C	16.94992440046540	24.67060108841633	31.66377011281511
C	16.48753933878833	23.25026475028340	31.96272063992123
H	16.11582291104493	22.78089619329026	31.03114909967958
H	17.33648846624911	22.64733277360825	32.33495293494029
C	17.87012732229754	25.33651172515740	32.50597353468262
H	18.30409603402095	24.78980515573308	33.35322128789339
C	18.20560350269464	26.68003610936103	32.28862193588643
H	18.92557518736270	27.17309620173289	32.95675401479243

C	17.88810655923461	29.68824348432163	32.21546451455687
H	17.86435639590074	29.20481875943393	33.19988134285708
C	15.29589480780607	39.25183888053710	34.55553872241492
H	16.08741399898188	40.00737168836130	34.36983708252186
H	14.54987479620210	39.72677613739020	35.22539995070861
C	13.09155147715684	35.75605763090542	35.14703411822396
H	13.59770193718251	35.04129927708076	34.46540601319057
H	12.93460349694055	35.27568398768188	36.13862305035735
H	12.10852156535065	36.03192106535244	34.72316579420217
N	11.60435229108094	31.53252615580258	32.28947490763349
N	10.72845371473094	33.50091437896712	24.08691119665001
C	11.13436111236013	31.74825088860545	27.23543391392375
H	11.17582056802385	32.79313513981599	26.90884775757025
N	11.75177703658484	27.25879572516531	31.08426270976074
C	11.44829937508036	29.75275129503897	30.40442020856131
C	11.52157033680770	30.73108622860703	31.43094975336064
C	11.12417805547360	29.04377069775217	28.04022483271802
H	11.13808711783909	27.99564558016757	28.36333231056480
C	10.88578473748062	31.02518229307397	24.86254731969763
C	11.25241659396818	31.44419800053415	28.57384454491580
H	11.37645142554816	32.25124039787132	29.30223146277340
C	11.26182951945007	30.07843869581275	29.02962788311019
C	10.98024091135046	29.34646211827405	26.70359985596862
H	10.87308013442858	28.53915665378606	25.96977322705578
C	10.99292870761530	30.71308115132335	26.24914254494235
N	10.89992044709889	29.16237208245807	23.04902533313192
C	10.82318472228653	32.37399735035756	24.41369300088181
C	11.61218847512500	28.39227696157420	30.80252953175892
C	10.89340083490768	30.00376882723466	23.87132394894047
N	14.72622826084167	33.63699994605051	32.77834467204628

N	13.99194119399711	31.97217675774293	24.62438330366994
C	14.32386796672655	31.69763717919559	28.27057242127850
H	14.20169580152599	32.52357789403975	27.56114737766663
N	14.62391674621740	29.24764440354289	33.71881596393219
C	14.64978573449185	31.16904717716410	31.96673450868126
C	14.67492780320782	32.50924667037437	32.44543403657758
C	14.59068069907271	29.54348948862786	30.07696471958347
H	14.69287360383591	28.71655106598991	30.78991348129438
C	14.12322485715634	30.06932686692501	26.38945853457632
C	14.43417245143796	31.96205858696219	29.61670330093507
H	14.39653342729247	32.99711494920567	29.97312488793343
C	14.56977249716205	30.89604662396927	30.57264238398971
C	14.46269282279730	29.28018634481176	28.72998001232962
H	14.45601267002615	28.24265739301694	28.37402682029828
C	14.31635929386304	30.34438943675015	27.77389980239542
N	13.81180259673444	27.59192246626397	25.66072986013826
C	14.05717308176918	31.10176209729736	25.41415518782020
C	14.63699307937074	30.11854040806848	32.92837521161811
C	13.95534020425052	28.72363719423791	25.94804657738081

Optimized structure of **PC-O<sub>2</sub>TCNQ**

O	14.07627394140471	36.43365576067691	21.65388930886071
O	8.73233729283100	35.94697418777449	20.12956510354679
O	10.47861391761109	38.70544400568446	32.34877388438208
O	15.76254077151151	37.92766845368400	33.92424008118029
O	9.20121158292662	25.85912459769728	36.75097331496450
O	13.62394381417767	29.24774624864767	36.55382965907506
O	13.53529505351830	23.95305207880892	36.13551301513718
O	17.33337230529177	26.85989782656378	33.28002594880089
C	12.76450590604479	36.26923763039377	21.26749840569462

C	11.95867470176890	37.43552922790175	21.29987963673151
C	10.60734124896604	37.32859632310151	20.92883861374046
H	9.98927496369931	38.23115919846269	20.98971342067508
C	10.05856777916598	36.10495255885063	20.49741049367804
C	7.88841447422356	37.09095882809621	20.13254806675408
H	7.79437612699655	37.53487114925351	21.14895660148931
H	8.25560221603165	37.87872293234880	19.43749526265704
H	6.89312659472488	36.74633700774855	19.79582113867631
C	10.87274362803914	34.94901253832857	20.42096313149387
C	12.21779996361507	35.04414357181059	20.82977374554346
H	12.83211927574212	34.13624689982732	20.80208012242247
C	10.29578083067302	33.62377737482053	19.93627176497640
H	9.44941972660367	33.83443096306761	19.25379845035895
H	11.06631805035639	33.07778175050561	19.35802728899618
C	9.81906612440897	32.74482230345239	21.08545796438469
C	8.79919710395876	33.19016375964966	21.95749132253300
H	8.30647628432753	34.15047199345704	21.75612788129327
C	8.43423184709711	32.43293853004582	23.07795781010123
H	7.64862860239055	32.80123393041386	23.75276718792454
C	9.07179688402085	31.20012356882881	23.36402157719793
C	10.05340303545385	30.73099031563612	22.46176202032257
H	10.58487782385289	29.79779381981350	22.68331014394354
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C	12.29295936484801	34.38742353234599	35.09910084980218
H	12.91808999254616	33.99167416854054	34.27337756598624
H	12.20936401014002	33.61805790298903	35.89792475528599
H	11.28318585462214	34.61420503257523	34.71221060177473
N	11.79076601414443	31.12513254307311	33.41214310738426
N	11.64395934311795	30.12397747838610	25.12436670464625
C	11.63428487457267	29.53423306654726	28.71397593607299
H	11.46122875734590	30.39833314955225	28.06657737252424
N	12.18167177248621	26.60177955721984	33.82342131307983

C	11.96939625360037	28.74737041497933	32.37149483526331
C	11.86724380103448	30.03993062054139	32.96192332697685
C	12.04392412342343	27.27814307867137	30.36397809243693
H	12.20403275666780	26.41240317869098	31.01896037519937
C	11.81375019797423	28.07147981523932	26.70128570157602
C	11.68028116936392	29.70284737824350	30.08121829028758
H	11.54209231817901	30.70191927876661	30.50823640644951
C	11.90405763707510	28.58365188438942	30.95930924757836
C	11.99880672029078	27.11025236120451	28.99741765679594
H	12.13108516232829	26.11081505212298	28.56207496873504
C	11.80717060720557	28.23612555376884	28.11765269583407
N	12.18966691256126	25.74871209214226	25.59144842125961
C	11.69798984828311	29.18368376750163	25.82897068514935
C	12.10507860918831	27.60789928551621	33.21668808186460
C	12.01731020241236	26.79984179929269	26.09043404361930
N	14.27783249970289	33.69851276074940	32.32930932631093
N	11.43773779229774	35.56214313931387	24.81544026179886
C	12.90598282597013	33.82989825715607	27.57873928485043
H	12.42109586738499	34.79821841638638	27.41109526599552
N	15.03657617409545	29.51492557443441	31.18628427684101
C	14.33777513590996	31.90477299826265	30.44418621636449
C	14.28616239351860	32.87896408241848	31.48528328091968
C	14.14806076361750	31.32863936405162	28.00854921785118
H	14.60002968828034	30.34843063232216	28.19532843887288
C	12.78240679697219	33.35541946873940	25.14568536066324
C	13.34552969233051	33.50782338690728	28.83890640590951
H	13.21579542956366	34.22482116156005	29.65308306064949
C	13.96205157612437	32.23656111845480	29.11130204150499
C	13.80472841646302	31.69442253353984	26.72327459032370
H	13.99776673331444	31.01553746018337	25.88660618103075

C	13.15119116589792	32.95403545191588	26.45846324434654
N	13.43921964634640	32.14973171868014	22.93816572171129
C	12.05595742724007	34.56845459198160	24.94166271071019
C	14.73899945562767	30.59493207275623	30.82269666684276
C	13.13452203011532	32.63808936256060	23.96467709814811

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