

Electronic Supplementary Information

for

Coordination assembly and host-guest chemistry of a triply
interlocked [2]catenane

Weibin Yu,^{*a} Feng-Yi Qiu,^a Shi-Ting Luo,^a Hua-Tian Shi,^a Guozan Yuan,^{*a}, and Xianwen Wei^{*a}

Analysis and Testing Central Facility, School of Chemistry and Chemical Engineering, Anhui
University of Technology, Maanshan 243002, P. R. China.

E-mail: yuweibin@ahut.edu.cn

Table of contents

1. NMR spectra of complex 1
2. ESI-TOF-MS spectra of host-guest assemblies
3. Calculated binding constants K values based on ^1H NMR titrations
4. IR spectra of complex 1
5. Crystal data of 1

1. NMR spectra of complex 1.

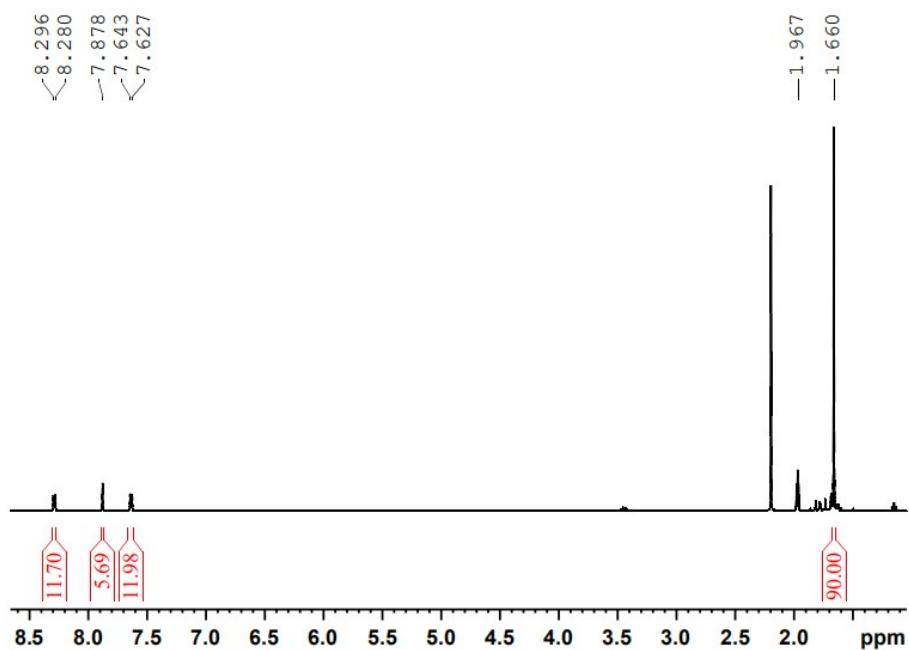


Fig. S1. The ^1H NMR spectrum of **1-monomer** at low concentration in $\text{CD}_3\text{CN-}d_3$.

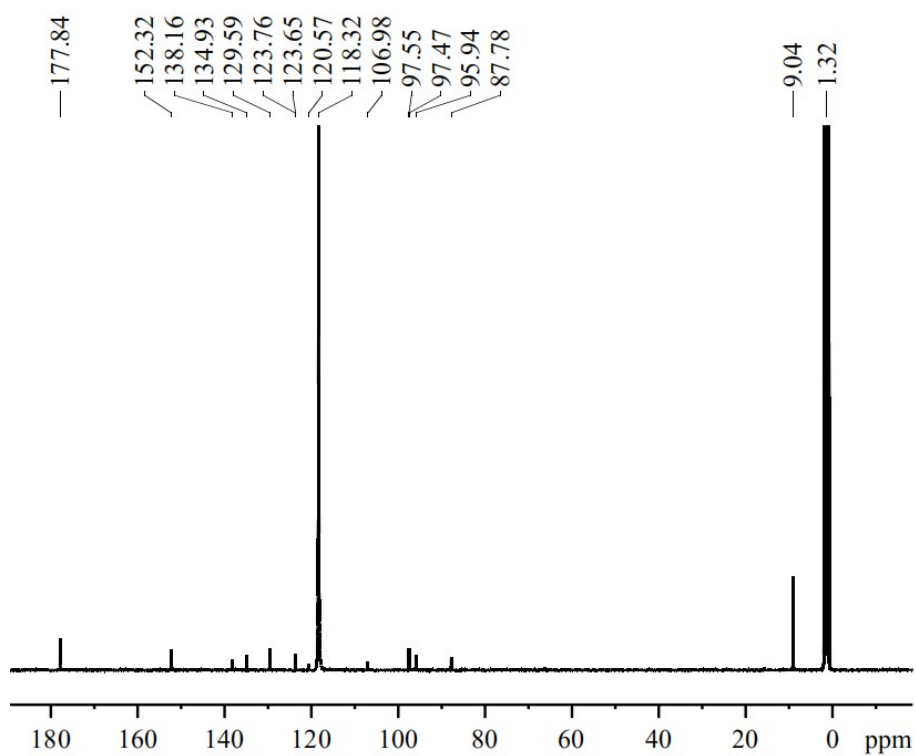


Fig. S2. The ^{13}C NMR spectrum of **1-monomer** at low concentration in $\text{CD}_3\text{CN-}d_3$.

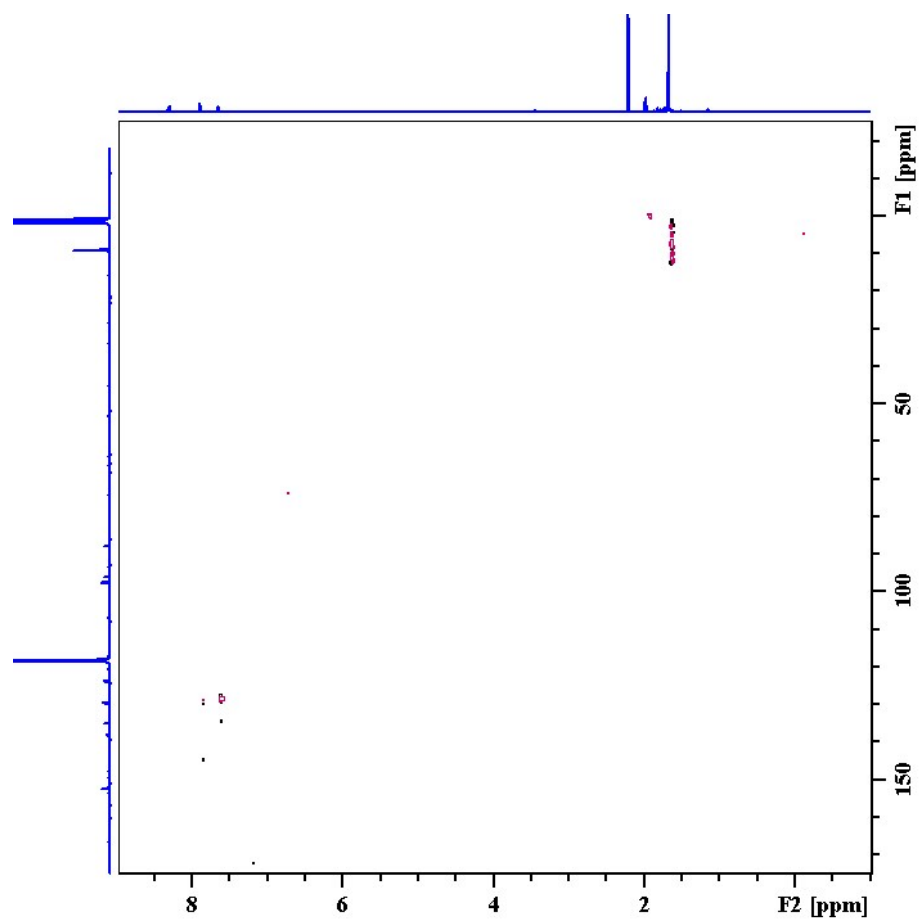


Fig. S3. The $\{^1\text{H}-^{13}\text{C}\}$ (HSQC) NMR spectrum of **1-monomer** at low concentration in $\text{CD}_3\text{CN}-d_3$.

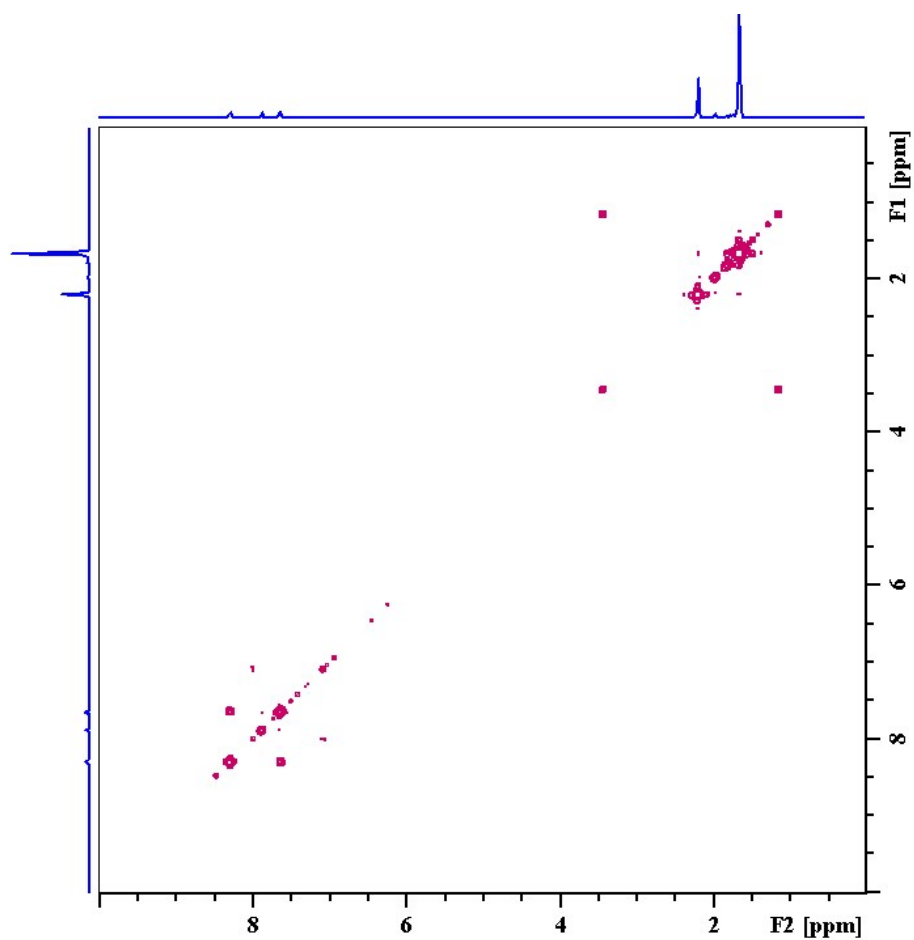


Fig. S4. The $\{^1\text{H}-^1\text{H}\}$ (COSY) NMR spectrum of **1-monomer** at low concentration in $\text{CD}_3\text{CN}-d_3$.

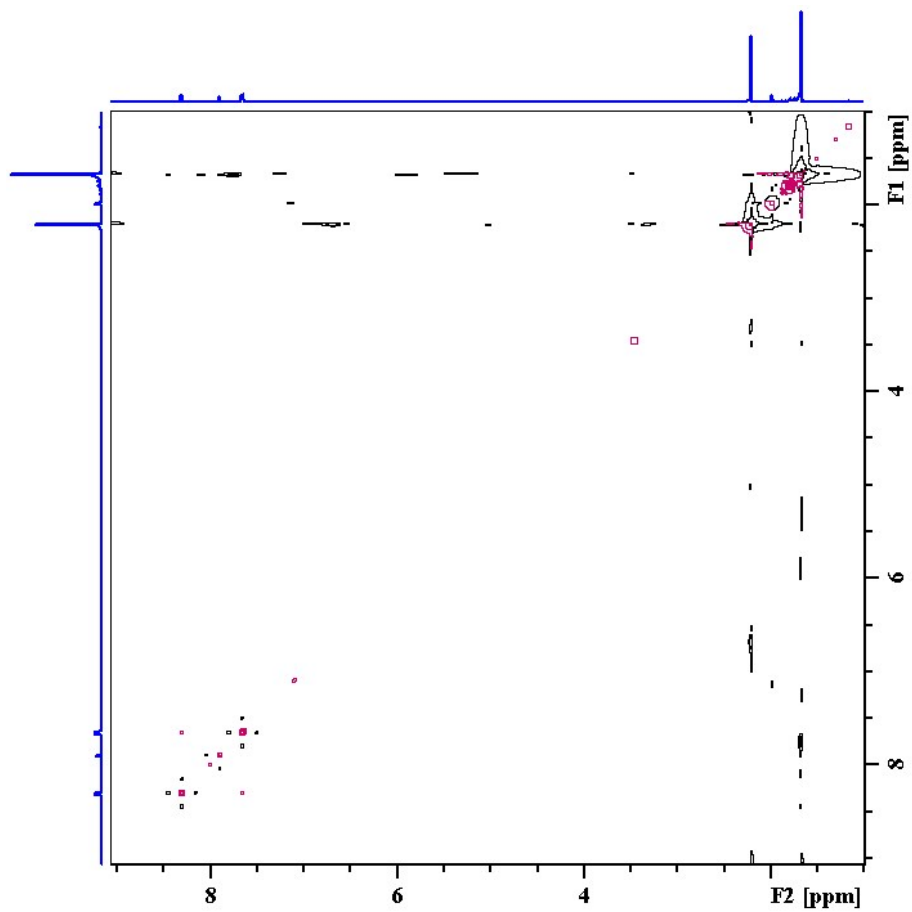


Fig. S5. The $\{^1\text{H}-^1\text{H}\}$ (NOESY) NMR spectrum of **1-monomer** at low concentration in $\text{CD}_3\text{CN}-d_3$.

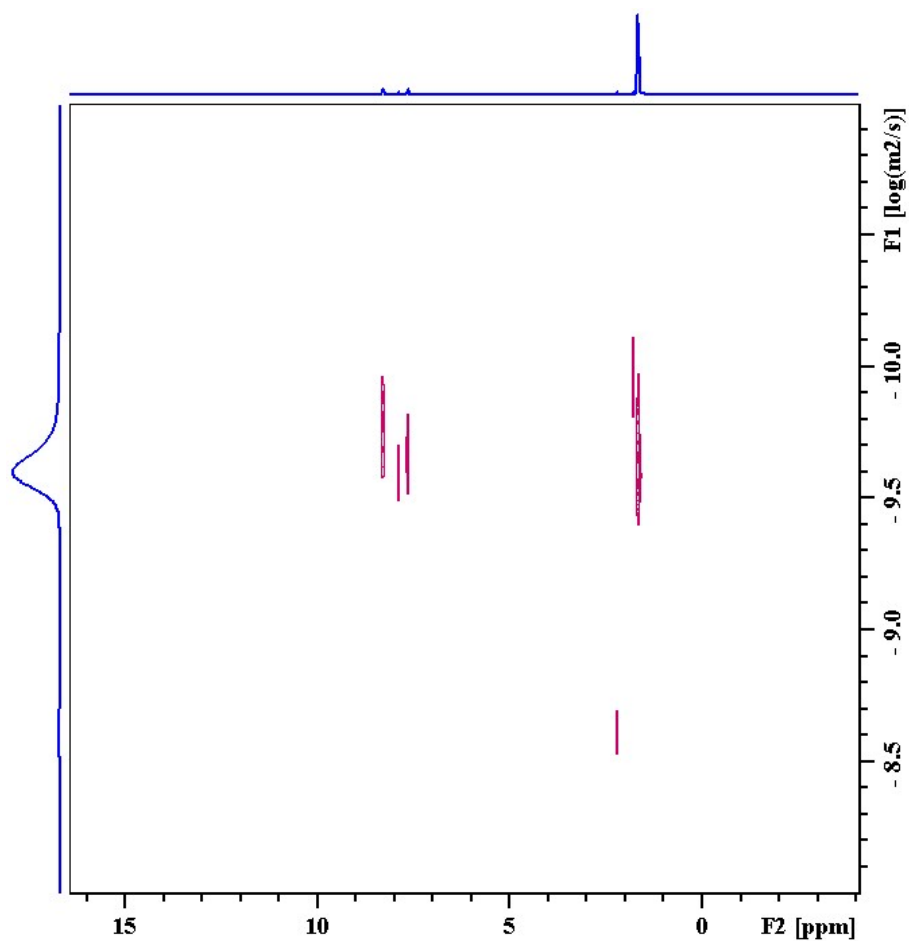


Fig. S6. The $\{^1\text{H}-^1\text{H}\}$ (DOSY) NMR spectrum of **1-monomer** at low concentration in $\text{CD}_3\text{CN}-d_3$.

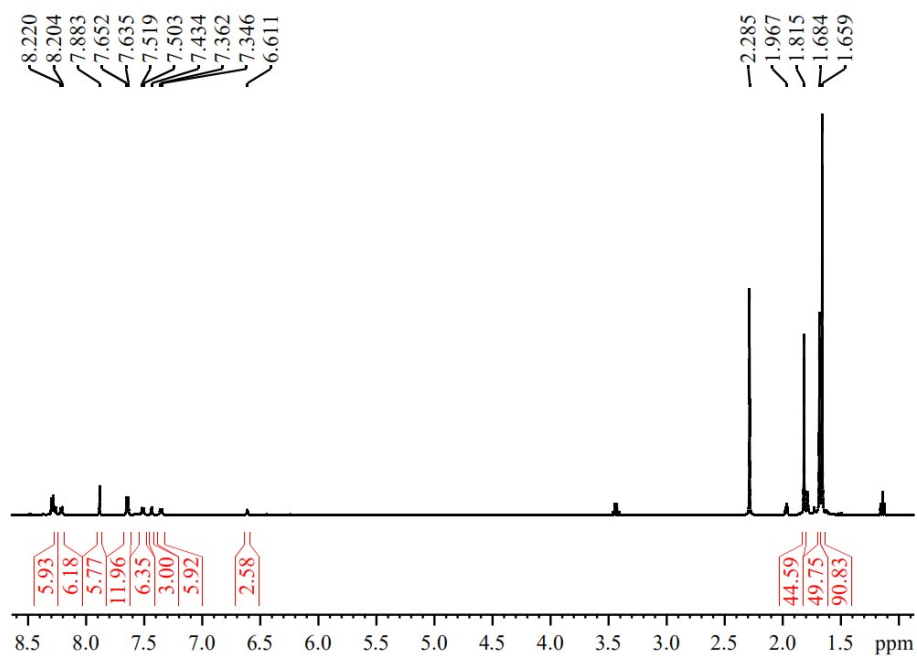


Fig. S7. The ^1H NMR spectrum of coexistence of **1-monomer** and **1-catenane** at high concentration in $\text{CD}_3\text{CN}-d_3$.

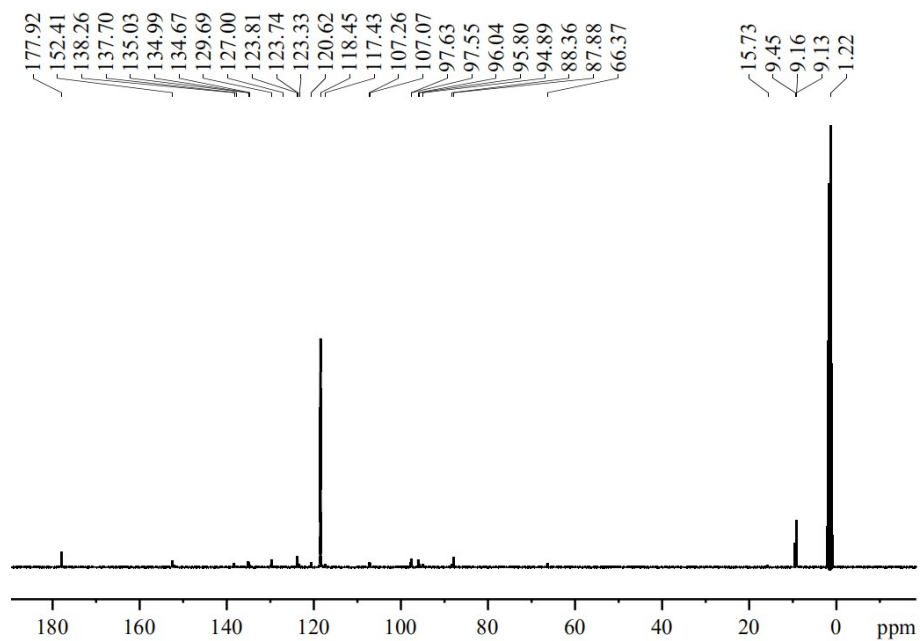


Fig. S8. The ^{13}C NMR spectrum of coexistence of **1-monomer** and **1-catenane** at high concentration in $\text{CD}_3\text{CN-}d_3$.

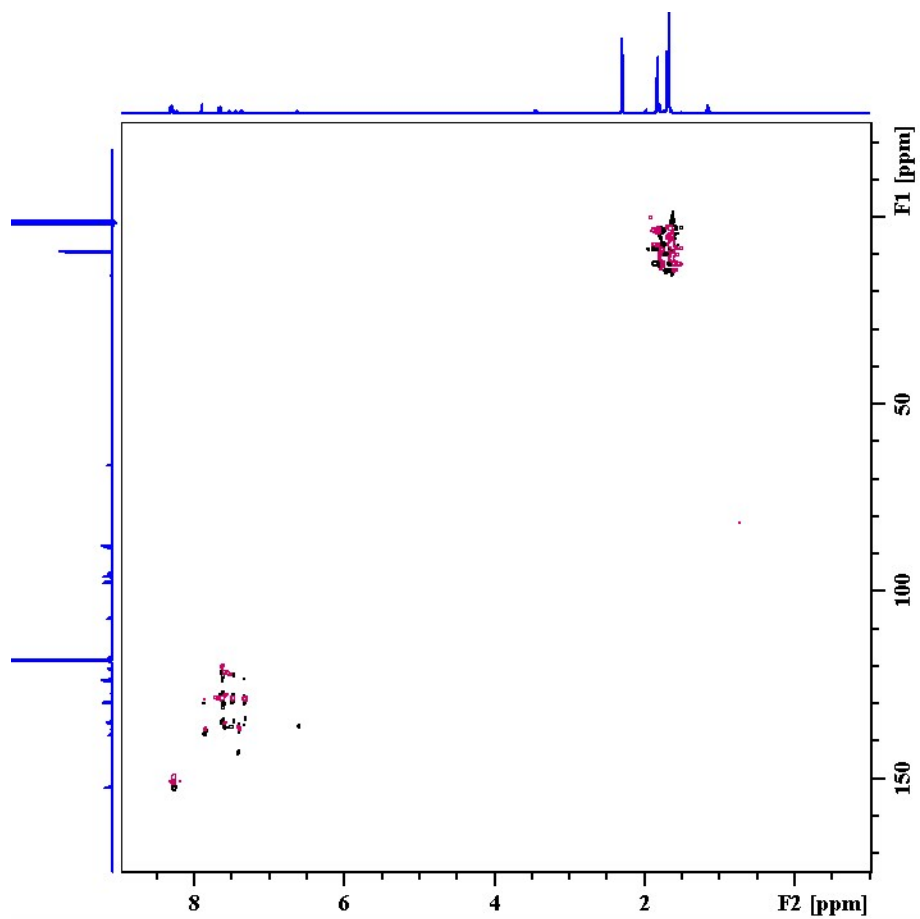


Fig. S9. The $\{^1\text{H-}^{13}\text{C}\}$ (HSQC) NMR spectrum of coexistence of **1-monomer** and **1-catenane** at high concentration in $\text{CD}_3\text{CN-}d_3$.

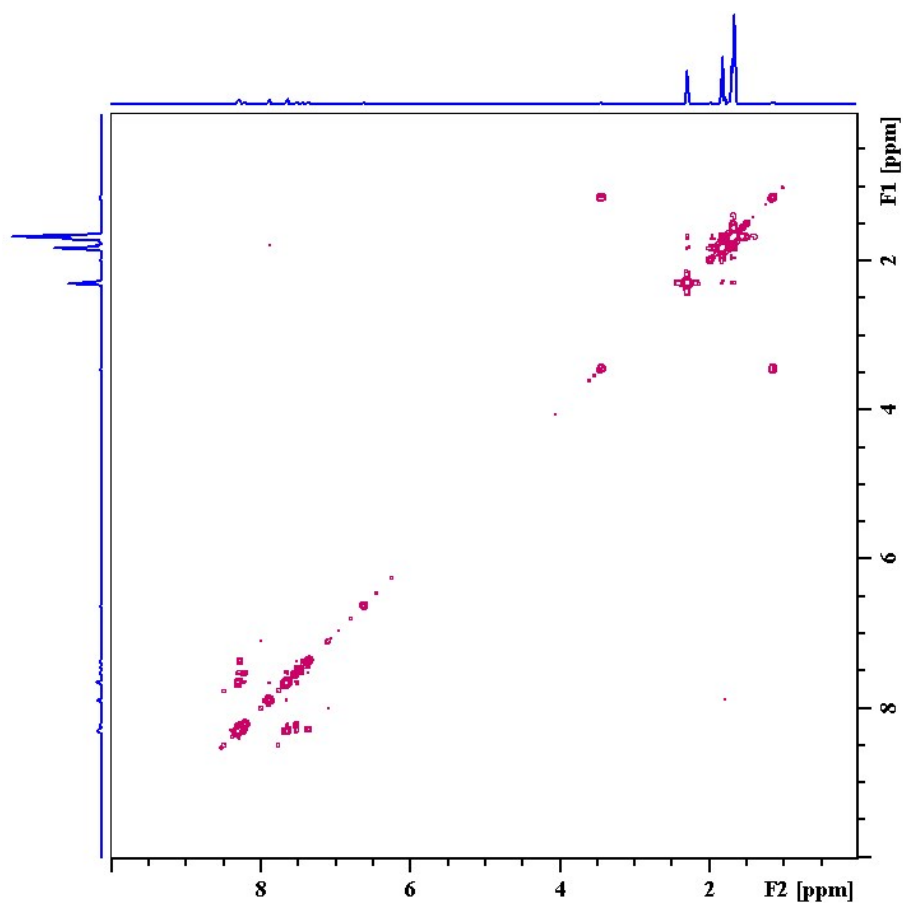


Fig. S10. The $\{^1\text{H}-^1\text{H}\}$ (COSY) NMR spectrum of coexistence of **1-monomer** and **1-catenane** at high concentration in $\text{CD}_3\text{CN}-d_3$.

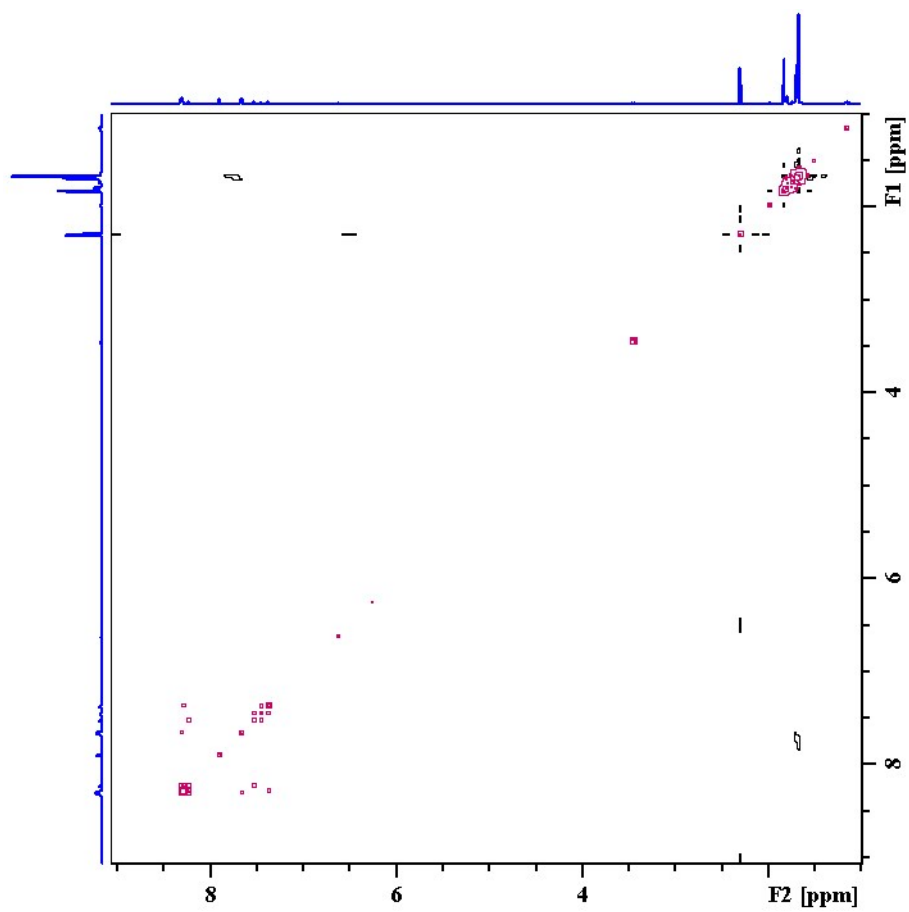


Fig. S11. The $\{^1\text{H}-^1\text{H}\}$ (NOESY) NMR spectrum of coexistence of **1-monomer** and **1-catenane** at high concentration in $\text{CD}_3\text{CN}-d_3$.

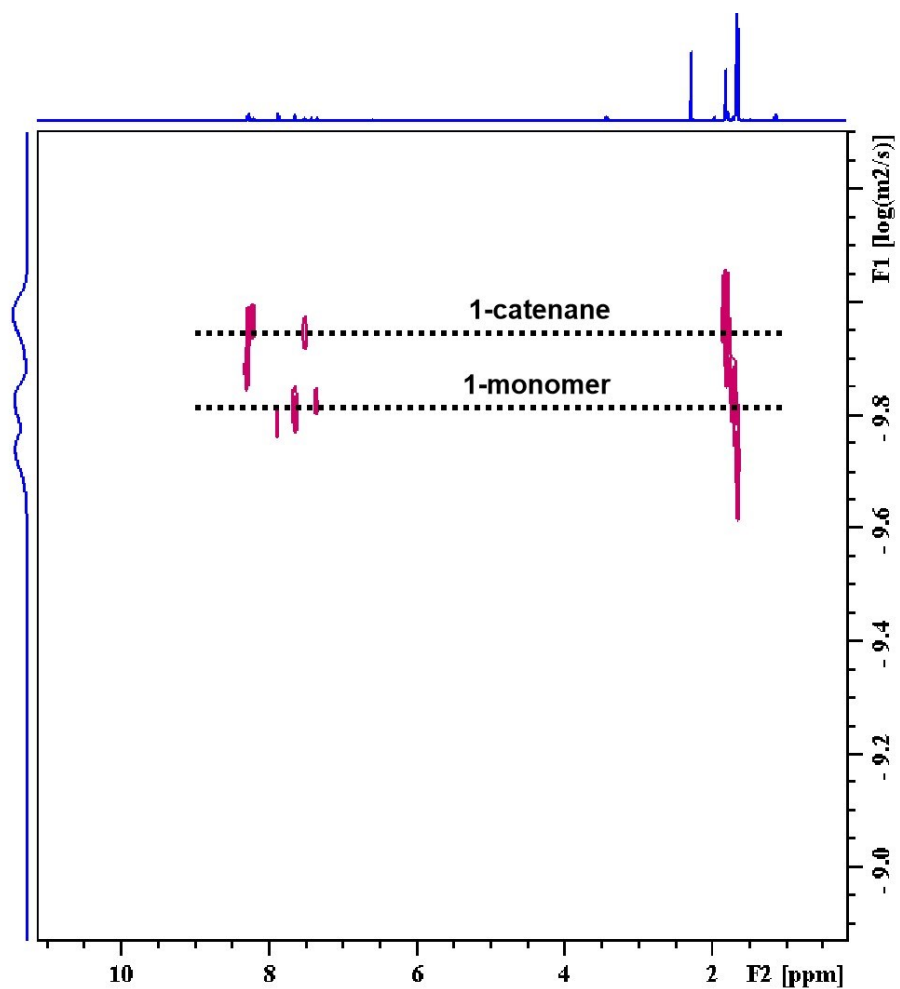


Fig. S12. The $\{^1H-^1H\}$ (DOSY) NMR spectrum of coexistence of **1-monomer** and **1-catenane** at high concentration in CD_3CN-d_3 .

2. ESI-TOF-MS spectra of host-guest assemblies.

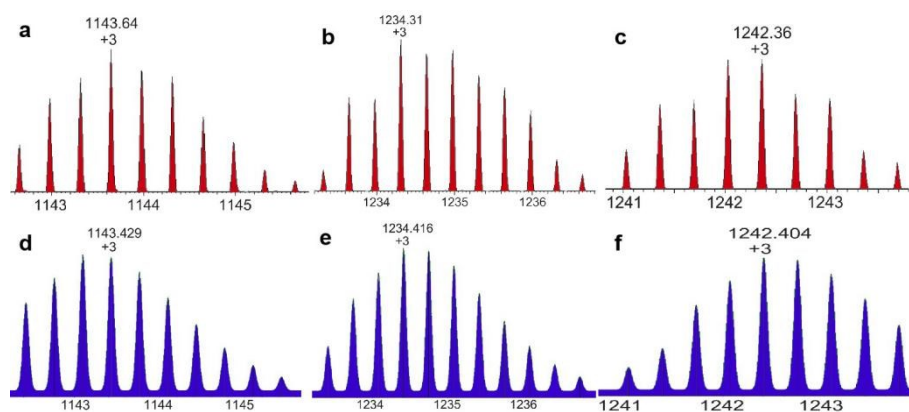


Fig. S13. ESI-TOF-MS of guests encapsulated by **1-monomer** in methanol. a) {[triphenylene □**1-monomer**] + 7CH₃OH+H₂O-3OTf}³⁺; b) {[perylene □**1-monomer**] + 6CH₃OH-3OTf}³⁺; c) {[coronene □**1-monomer**] + 3CH₃OH+4H₂O-3OTf}³⁺; d), e), and f) are simulated for a), b), and c), respectively.

3. NMR spectra of host-guest assemblies.

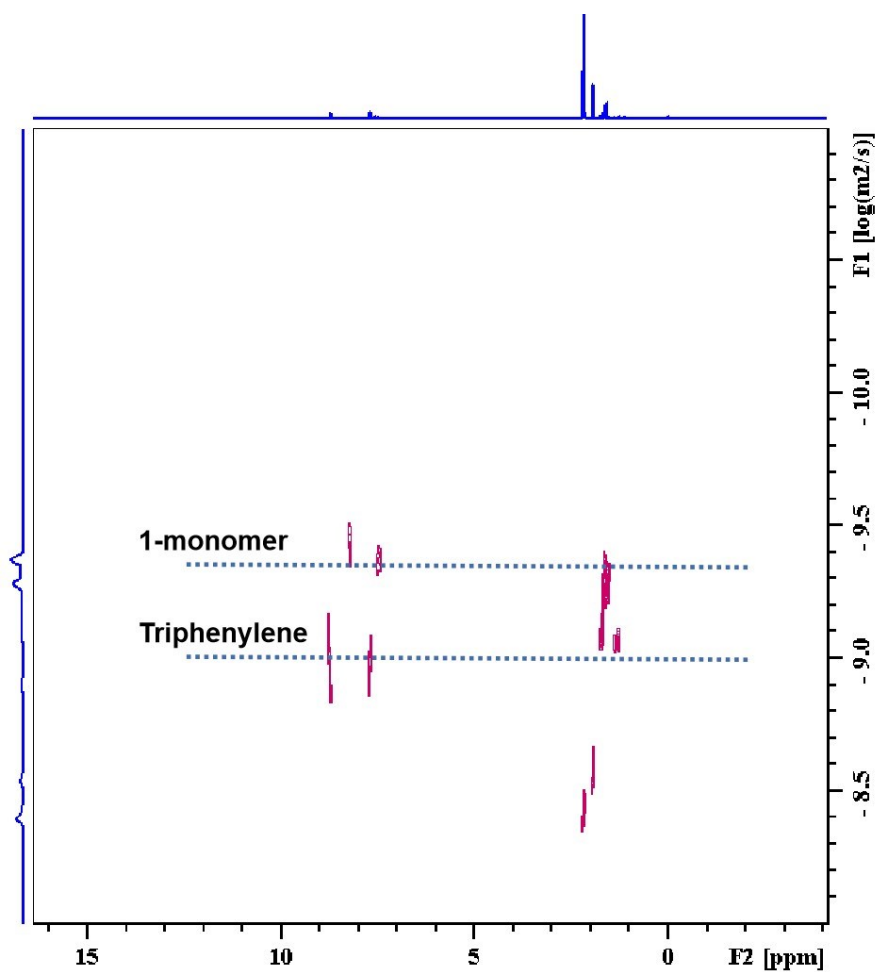


Fig. S14. The ^1H - ^1H DOSY NMR spectra of triphenylene encapsulated by **1-monomer**.

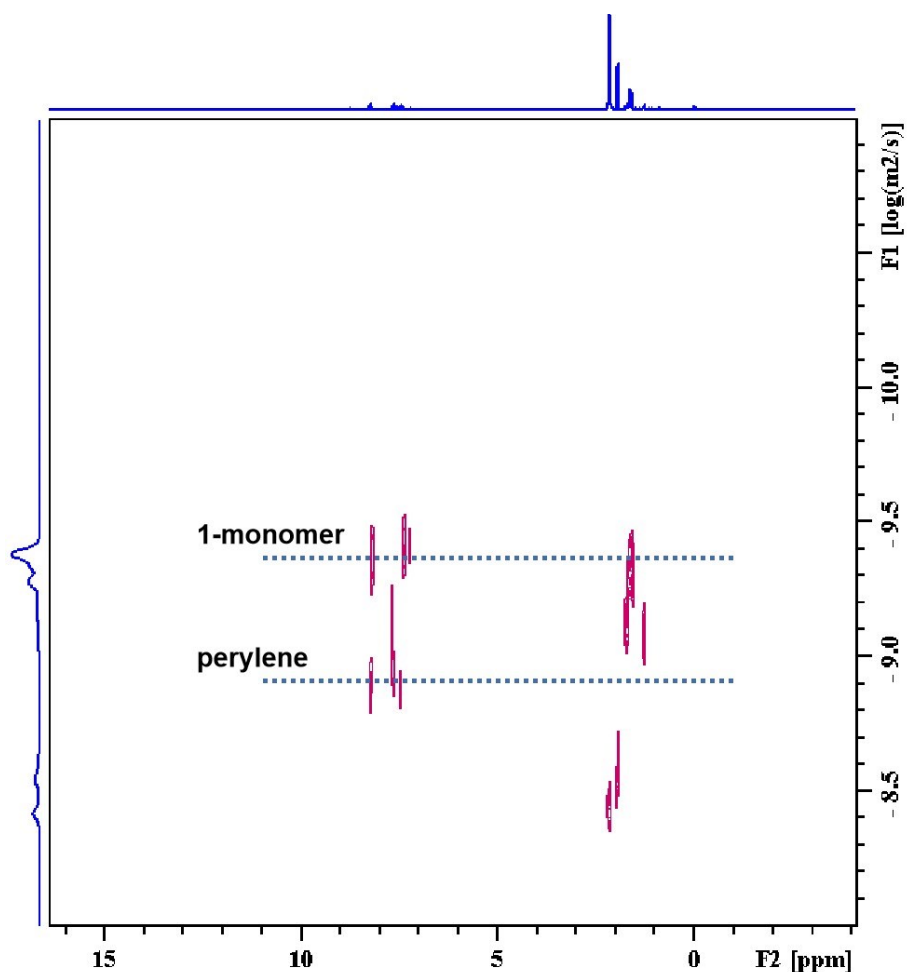


Fig. S15. The ^1H - ^1H DOSY NMR spectra of perylene encapsulated by 1-monomer.

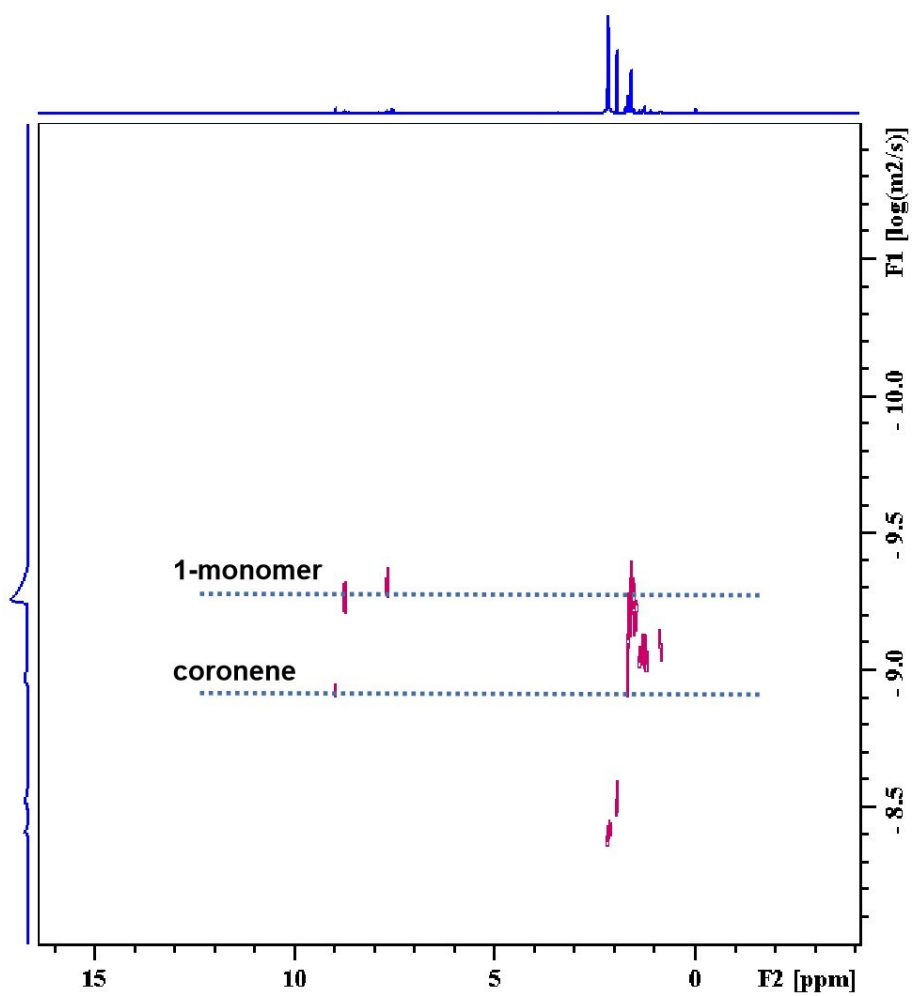


Fig. S16. The 1H - 1H DOSY NMR spectra of coronene encapsulated by **1-monomer**.

4. Calculated binding constants K values based on ^1H NMR titrations.

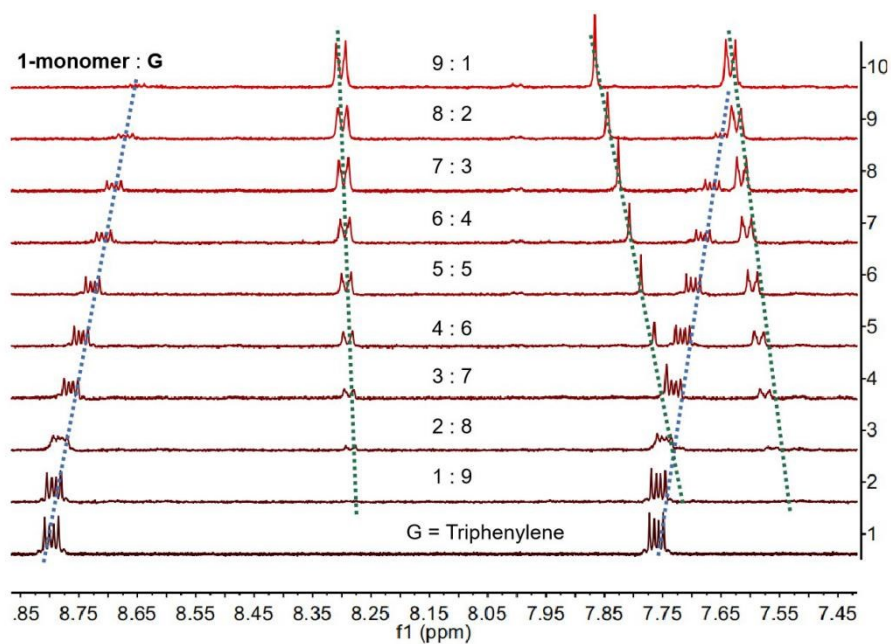


Fig. S17. Illustration of the Job's plot for determination of stoichiometry (triphenylene \square 1-monomer).

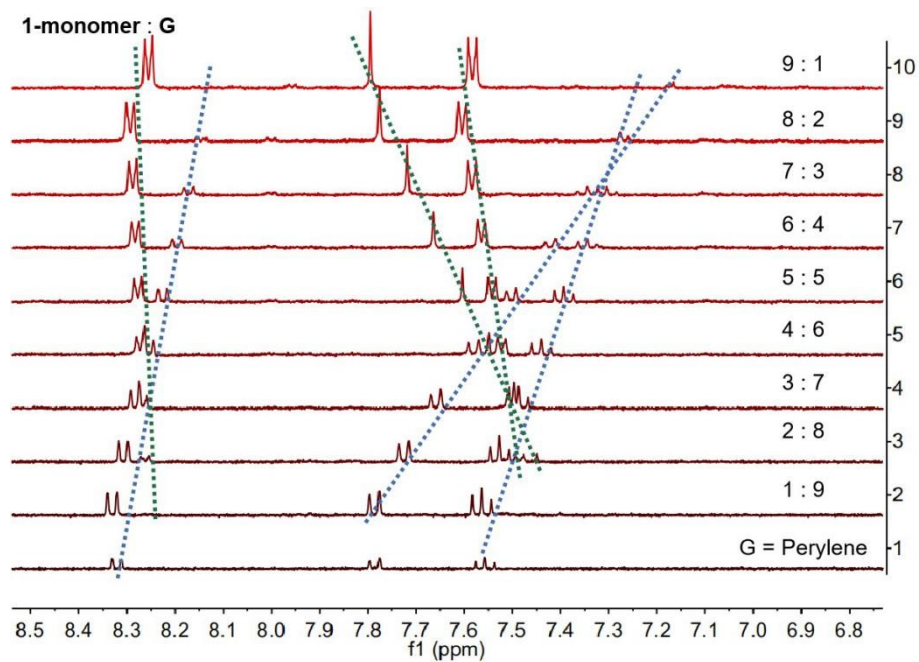


Fig. S18. Illustration of the Job's plot for determination of stoichiometry (perylene \square 1-monomer).

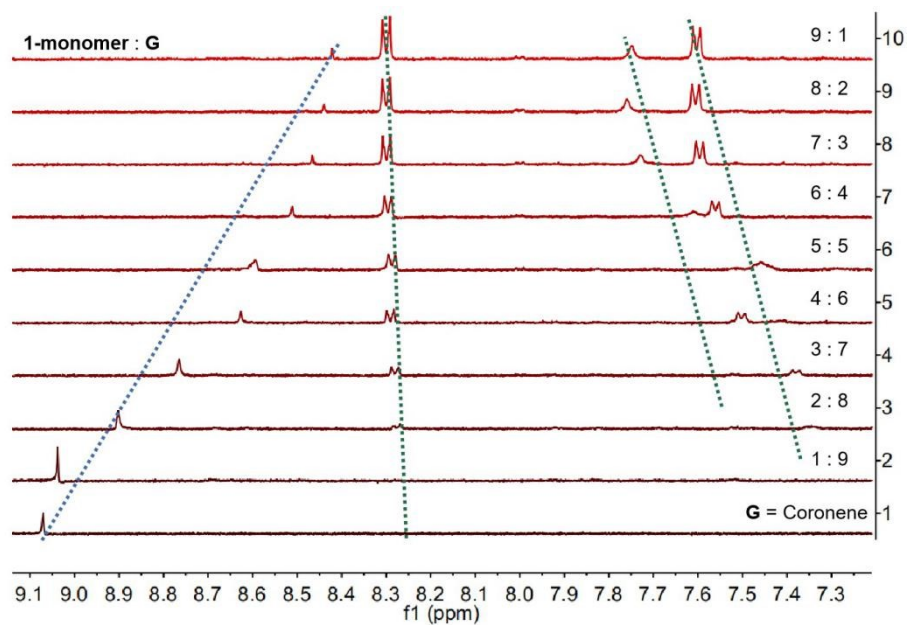


Fig. S19. Illustration of the Job's plot for determination of stoichiometry (coronene □ **1-monomer**).

5. IR spectra of complex 1.

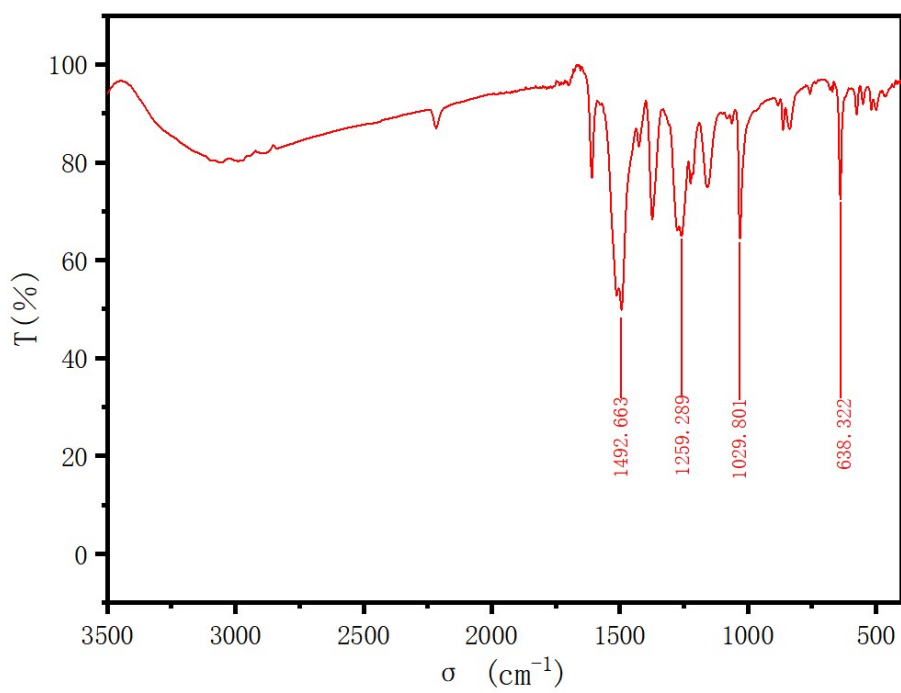


Fig. S20. IR spectra of complex 1.

6. Crystal data of 1.

Table S2. Crystal data of 1.

1	
<i>Formula</i>	C ₁₃₂ H ₁₁₉ Cl ₆ N ₆ O ₁₂ Rh ₆
<i>M_r</i>	2811.48
<i>T</i> [K]	173
<i>Crystal system</i>	Monoclinic
<i>Space group</i>	C2
<i>a</i> [Å]	41.690(5)
<i>b</i> [Å]	27.665(4)
<i>c</i> [Å]	16.596(2)
<i>α</i> [°]	90
<i>β</i> [°]	90.706(6)
<i>γ</i> [°]	90
<i>V</i> [Å ³]	19140(4)
<i>Z</i>	4
<i>ρ_{calcd}</i> [g cm ⁻³]	0.976
<i>F</i> (000)	5684
<i>Crystal size</i> [mm ³]	0.20 × 0.15 × 0.13
<i>2θ_{max}</i> [°]	77.42
<i>Reflections collected</i>	37376
<i>Independent reflections</i>	27713
<i>Parameters</i>	1487
<i>R₁</i> [<i>I</i> > 2σ(<i>I</i>)]	0.1069
<i>wR₂</i> [all data]	0.1976
<i>GOF</i>	1.070
<i>CCDC number</i>	2053030