Supporting Information

Selective Recognition and Enrichment of C_{70} over C_{60} Using an Anthracene-Based Nanotube

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1. Experimental Section

1.1. General Method

All the reagents involved in this research were commercially available and used without further purification unless otherwise noted (Bis(pinacolato)diboron, Bidepharm, 98%; Potassium phosphate tribasic, Energy-chemical, 99%; $PdCl_2$(dppf), Bidepharm, 98%; 2,6-Dibromo-4-methoxypyridine, Bidepharm, 96%; $Pd(PPh_3)_4$, Bidepharm, 98%; K_2CO_3, Energy-chemical, 99%; Extra dry N,N-Dimethylformamide (DMF) Energy-chemical, 99%; Toluene-d_8, CIL, 99.6 atom % D; Chloroform-d_1, CIL, 99.8 atom % D Dichloromethane-d_2, CIL, 99.9 atom % D). Solvents for Column chromatography (Energy-chemical, 99%) were employed as purchased without further purification. Thin-layer chromatography (TLC) was carried out on 0.25 mm Leyan silica gel plates (60F-254). Column chromatography was performed on silica gel (200-300 mesh) as the stationary phase. ^{1}H, ^{13}C NMR, 2D NMR spectra were performed on Bruker AVANCE III 500M with Prodigy Platform. Chemical shifts are reported in ppm with residual solvents or TMS (tetramethylsilane) as the internal standards. The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; dd, doublet of doublet; m, multiplet. Host-guest complexes were prepared by simply mixing the guests and hosts in 1: 1 stoichiometry in the corresponding solvent. Electrospray-ionization high-resolution mass spectrometry (ESI-HRMS) experiments were conducted on an applied Q-EXACTIVE mass spectrometry system. UV-Vis spectra were recorded on an SHIMADZU S-1700 UV-Vis spectrophotometers, using a 1 cm quartz cuvette. Fluorescent spectra were recorded on a Edinburgh FS5 spectrofluorometer, using a 1 cm quartz cuvette.

1.2. ^{1}H NMR Titration Experiments Method

The association constants for the complexes of **1** with C_{60} are small (< 10^5 M^{-1}) and the chemical exchange is fast at the NMR timescale. Thus, we used direct NMR titrations to determine their association constants in toluene.

For the complexes of **1** and C_{70} with large association constants (> 10^5 M^{-1}) and fast exchange kinetics, the association constants were determined by competitive NMR titrations and using guest C_{60} (binding constant with **1** is 2.3 $\times$ 10^4 M^{-1}) as the outgoing guest. The data from competitive titrations was nonlinearly fitted[1] according to the equations developed by Prof. Werner Nau (available from their website, http://www.jacobs-university.de/ses/wnau). All ^{1}H NMR titration experiments were repeated 3 times, and the averaged values and standard deviations are given.

1.3. Fluorescent Titration Experiments Method

The fluorescent titration experiments were conducted with excitation wavelength of 375 nm. The fluorescent intensity at 435 nm decreased with the addition of the guests, which were used for nonlinear

fitting. Nonlinear curve-fitting method was then used to obtain the association constant through the following equation:

$$I=I_0+((I_{GH}-I_0)/2/[H]_0)([H]_0+[G]_0+1/K_a-sqrt(([H]_0+[G]_0+1/K_a)^2-4[H]_0[G]_0))$$

1.4. X-Ray Single Crystallography Method

Suitable single crystals of $(\mathbf{1}+3H)^{3+}\cdot(TFA^-)_3$ were successfully obtained by slow evaporation of their saturated solutions in toluene.

Single crystal X-ray data were collected on a Bruker D8 VENTURE with Ga Kα radiation (λ = 1.34138 Å) at 100 K. The structures were solved by intrinsic phasing methods (SHELXT) and refined by full-matrix least-squares F^2 using SHELXL[2] in the OLEX2 program package.[3] All non-hydrogen atoms were refined with anisotropic thermal parameters and the hydrogen atoms were fixed at calculated positions and refined by a riding mode.

1.5. Computational Method

Geometry optimizations were performed with Gaussian 16 software package,[4] using the ωB97XD/6-31G(d)[5,6] method in vacuum. Frequency calculations were then conducted at the same computational level to confirm the nature of all located stationary points and to obtain the thermal correction to Gibbs free energy and enthalpy. Single point energy was calculated with Gaussian 16 software package using the ωB97XD/6-311++G(d,p). The total Gibbs free energy of the complex is the addition of single point energy and the thermal correction to Gibbs free energy (ZPE+$\Delta G_{0\rightarrow T}$). Non-covalent interaction (Independent gradient model based on Hirshfeld partition, IGMH) analysis[7] was carried out with Multiwfn 3.8 (dev) program[8,9] and visualized by the VMD 1.9.3 program.[10] (set isovalue = 0.008).

1.6 Synthetic Procedures

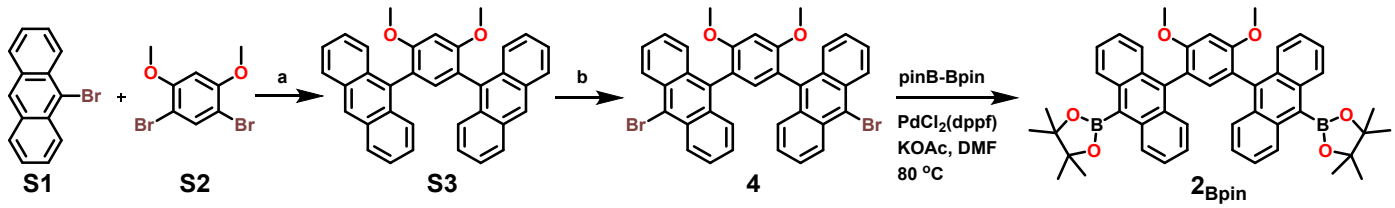


Figure S1. Synthetic procedures of $\mathbf{2}_{Bpin}$.

The synthesis of **4** has been reported previously.[11] Reagents and conditions from **S1** to **4**: a) i) Ar atmosphere, **S1**, n-BuLi, THF, -80 °C; ii) $ZnCl_2$, THF; iii) **S2**, $PdCl_2(PhCN)_2$ catalyst, THF, 80 °C; b) DBH, THF, 0 °C to room temperature. Reagents and conditions from **4** to $\mathbf{2}_{Bpin}$: **4** (1.2 g, 1.85 mmol, 1.0 equiv.), bis(pinacolato)diboron (2.8 g, 11.0 mmol, 6.0 equiv.), potassium acetate (2.4 g, 24.5 mmol, 13.0 equiv.) and $PdCl_2$(dppf) (0.3 g, 0.37 mmol, 0.2 equiv.) were dissolved in the dry DMF (500 mL) in a two-neck flask under Ar atmosphere. The resulting mixture was stirred avoiding light at 80 °C for 12 h. After the reaction, the solvents were evaporated under reduced pressure, and the residue was

poured into water. The resulting suspension was extracted with ethyl acetate (200 mL × 3). The combined organic phases were washed consecutively with brine (200 mL × 3) and dried over anhydrous Na_2SO_4. After removing the ethyl acetate, the residue was purified by column chromatography (SiO_2, Hexane / CH_2Cl_2 = 1 / 2) to give the compound **2_{Bpin}** as a light green solid (0.6 g, 43 %).

2_{Bpin}: ^{1}H NMR (500 MHz, $CDCl_3$, 298K) δ [ppm] = 8.45 (d, *J* = 8.6 Hz, 4H), 7.93 (d, *J* = 8.7 Hz, 4H), 7.48 (ddd, *J* = 8.4, 6.4, 1.4 Hz, 4H), 7.42 (ddd, *J* = 8.0, 6.6, 1.3 Hz, 4H), 7.16 (s, 1H), 6.95 (s, 1H), 3.73 (s, 6H), 1.60 (s, 24H).

2_{Bpin}: ^{13}C NMR (126 MHz, $CDCl_3$, 298K) δ [ppm] = 158.81, 136.20, 136.07, 135.58, 130.33, 128.53, 127.35, 125.29, 124.79, 119.64, 96.46, 84.37, 56.04, 25.23.

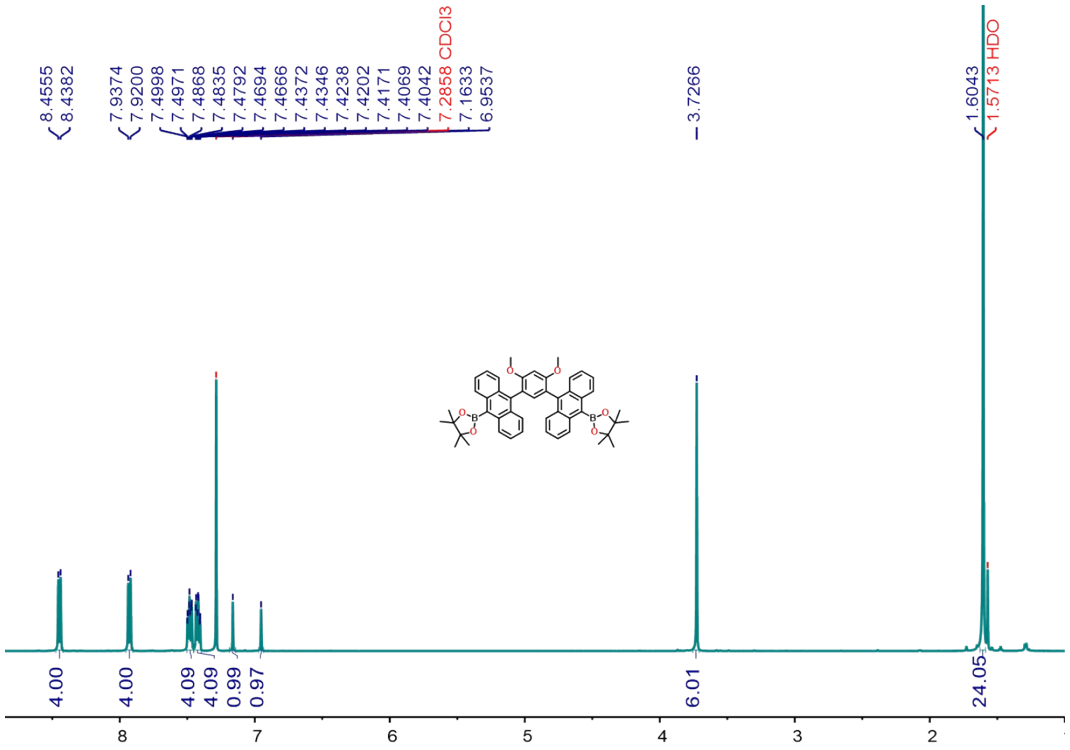


Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of **2_{Bpin}**.

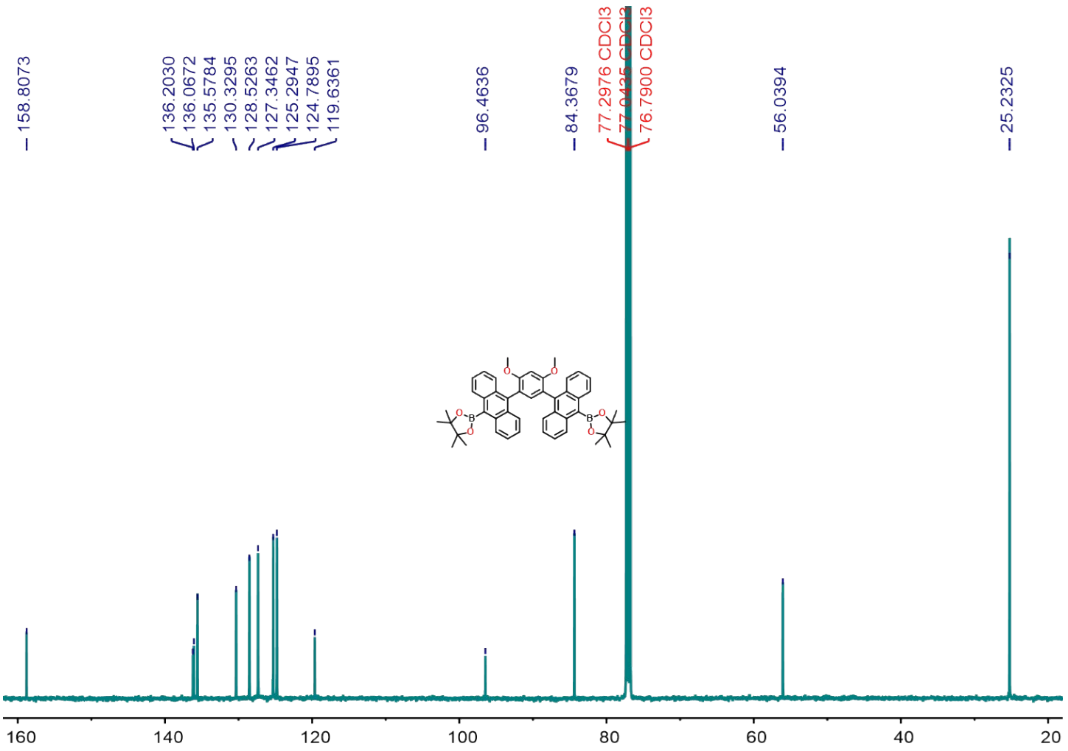


Figure S3. ^{13}C NMR spectrum (126 MHz, $CDCl_3$, 298 K) of $\mathbf{2_{Bpin}}$.

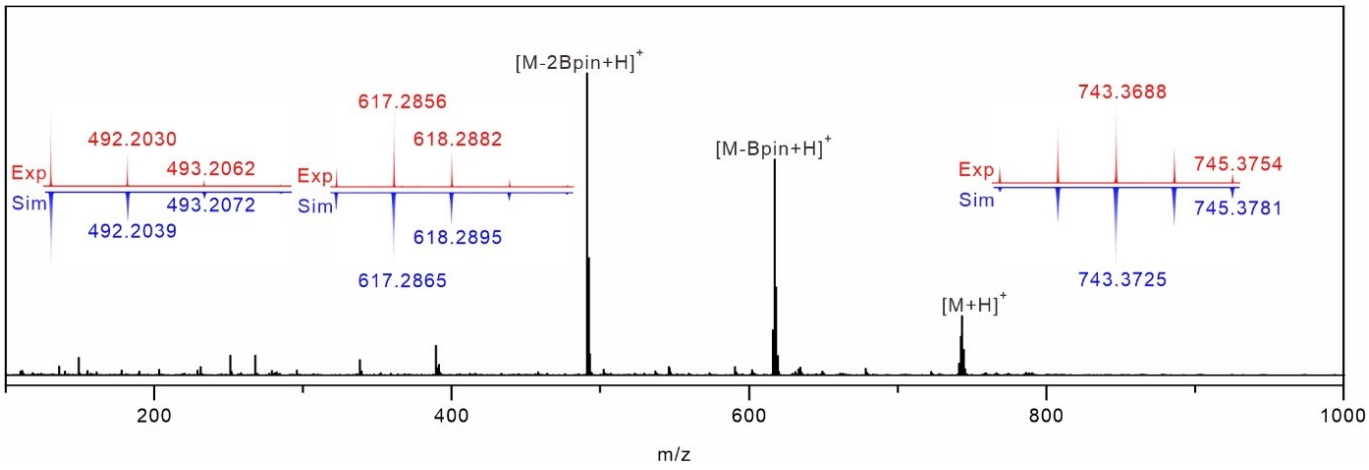


Figure S4. Experimental and simulated ESI mass spectra of $\mathbf{2_{Bpin}}$.

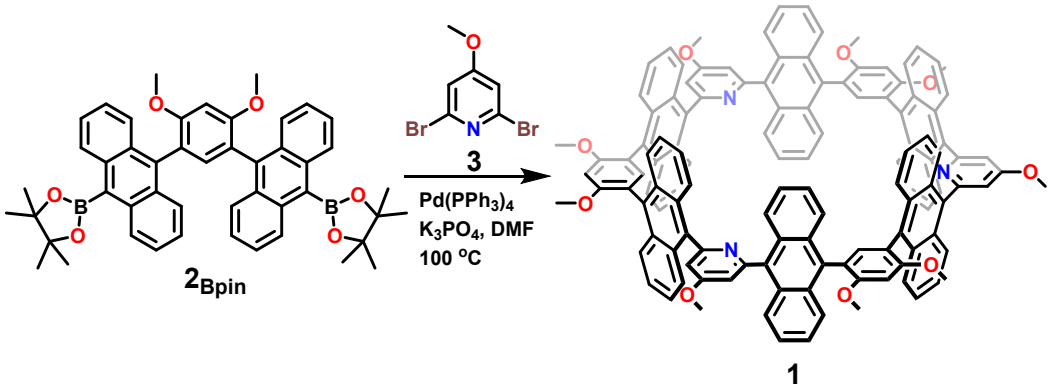


Figure S5. Synthetic procedures of nanotube **1**.

2,6-Dibromo-4-methoxypyridine **3** (0.16 g, 0.6 mmol, 1 equiv.), potassium phosphate tribasic (0.64 g, 3.0 mmol, 5 equiv.), $Pd(PPh_3)_4$ (0.14 g, 0.12 mmol, 0.2 equiv.) and $\mathbf{2_{Bpin}}$ (0.45 g, 0.6 mmol, 1 equiv.) were dissolved in the DMF (350 mL) in a two-neck flask under Ar atmosphere. The resulting mixture was stirred avoiding light at 100 °C for 24 h. After the reaction, the solvents were evaporated under reduced pressure, and the residue was poured into water. The resulting suspension was extracted with dichloromethane (100 mL × 3). The combined organic phases were washed consecutively with brine (100 mL × 3) and dried over anhydrous Na_2SO_4. After removing the dichloromethane, the residue was purified by column chromatography (SiO_2, Hexane / CH_2Cl_2 = 1 / 0 to 0 / 1) to give the compound **1** as a light yellow solid (18 mg, 5 %).

1: ^{1}H NMR (500 MHz, CD_2Cl_2, 298K) δ [ppm] = 7.93 – 7.85 (m, 24H), 7.41 (qd, *J* = 6.5, 3.2 Hz, 24H), 7.30 (s, 6H), 7.09 (s, 3H), 7.05 (s, 3H), 4.00 (s, 9H), 3.85 (s, 18H).

1: ^{13}C NMR (126 MHz, CD_2Cl_2, 298K) δ [ppm] = 166.28, 159.97, 158.80, 136.07, 135.34, 134.07, 130.37, 129.53, 126.82, 126.34, 125.31, 124.97, 119.12, 111.88, 95.86, 55.95, 55.57, 29.69.

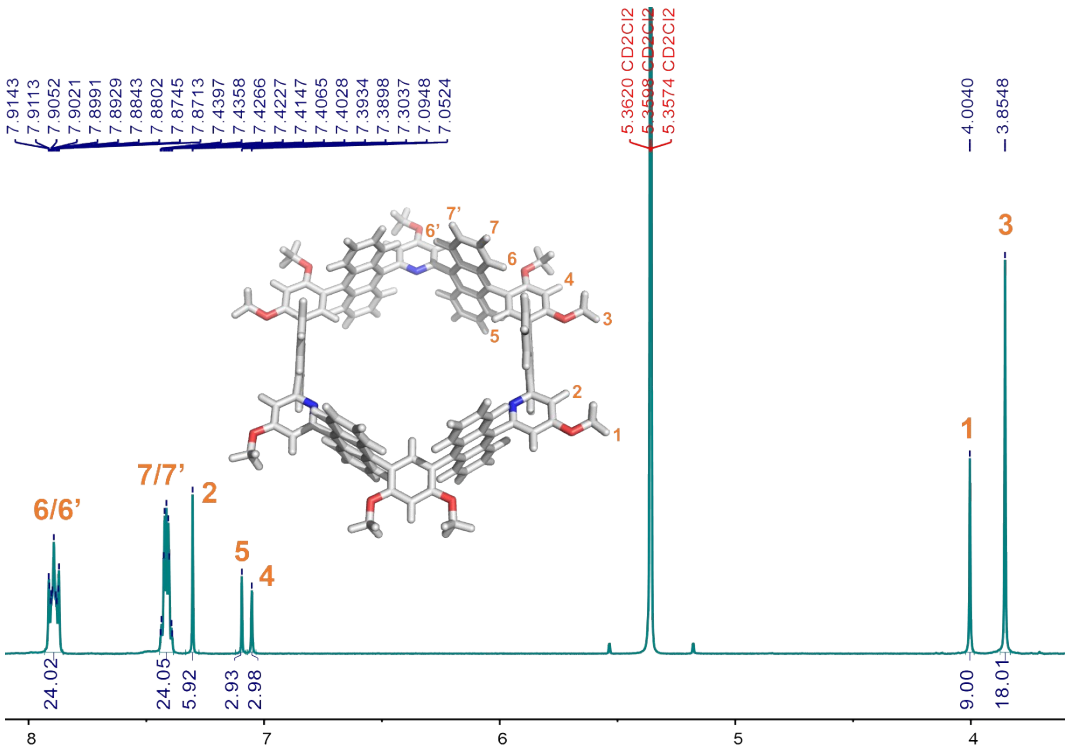


Figure S6. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of **1**.

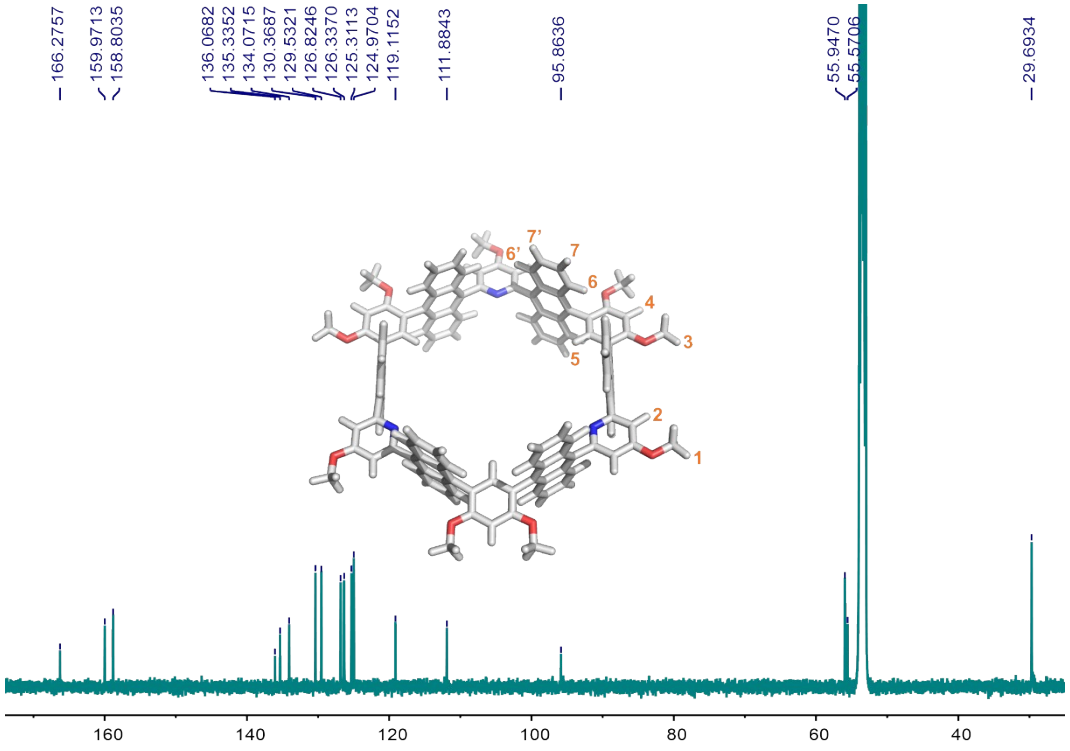


Figure S7. ^{13}C NMR spectrum (126 MHz, CD_2Cl_2, 298 K) of **1**.

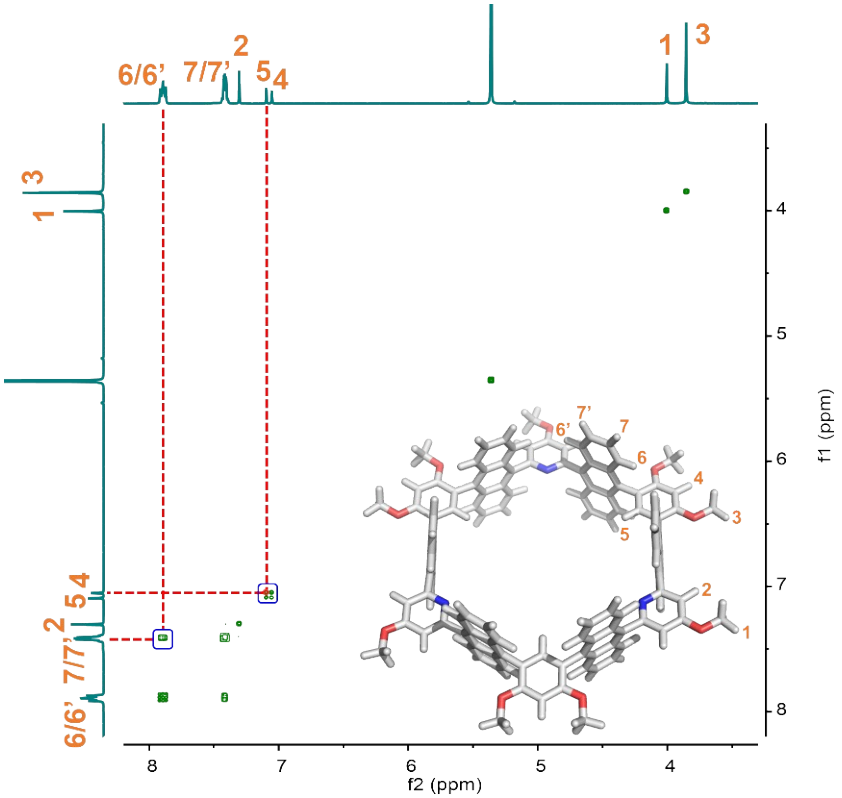


Figure S8. 2D NMR spectra of nanotubes. ^{1}H,^{1}H-COSY NMR spectrum of **1** (500 MHz, CD_2Cl_2, 298 K). The ^{1}H,^{1}H-COSY signals of protons are marked with blue boxes.

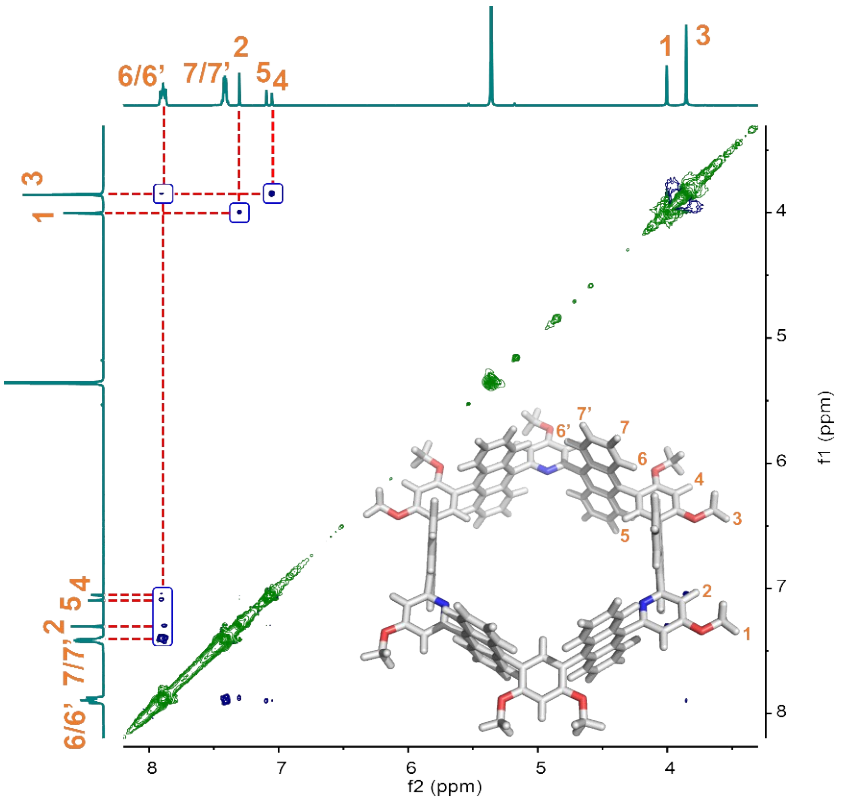


Figure S9. 2D NMR spectra of nanotubes. ^{1}H,^{1}H-ROESY NMR spectrum of **1** (500 MHz, CD_2Cl_2, 298 K). The NOE signals of protons are marked with blue boxes.

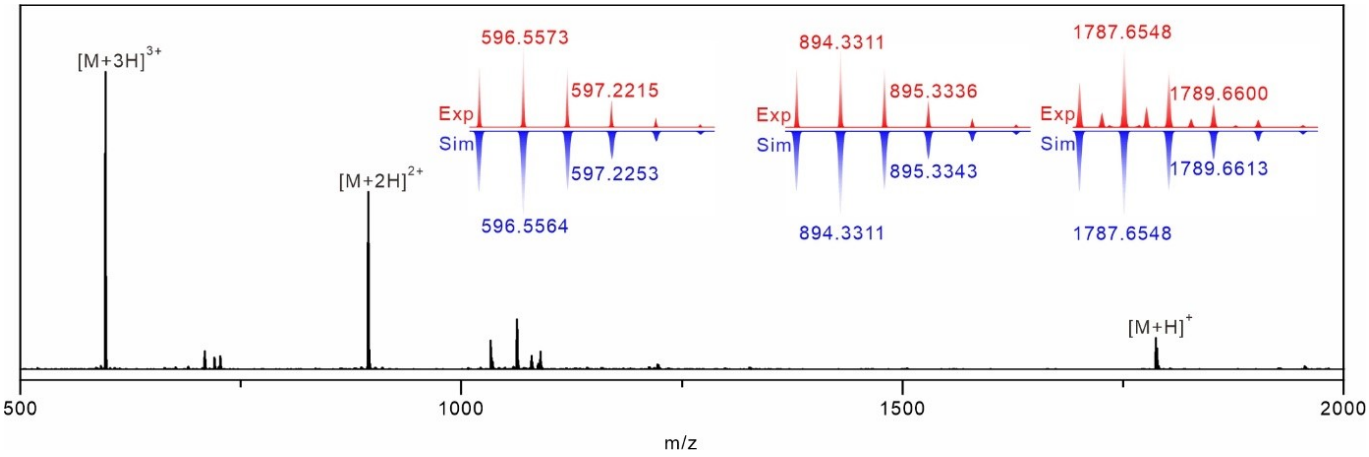


Figure S10. Experimental and simulated ESI mass spectra of **1**.

2. Optical Stimuli-Responsive Properties

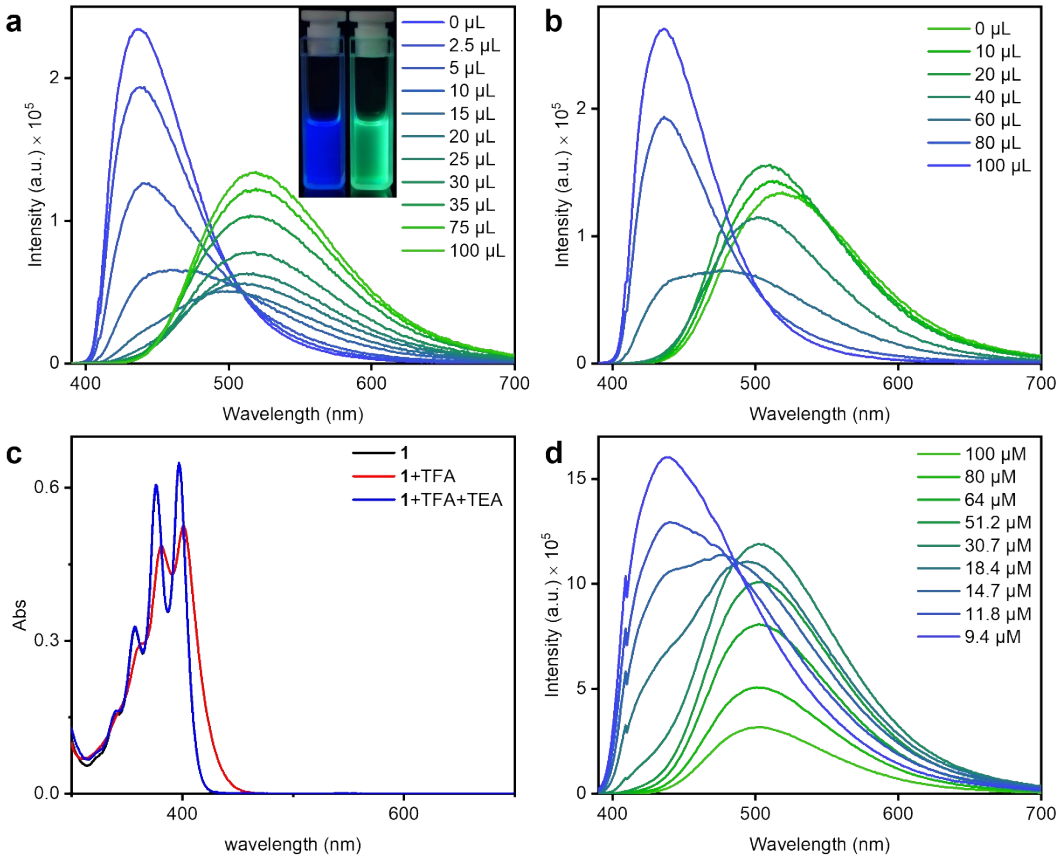


Figure S11. Fluorescence emission spectra of a) nanotube **1** (100 μM in toluene, 2.5 mL in quartz cuvette) by adding different volume of trifluoroacetic acid (TFA, 250 mM in toluene); b) **1** with excess TFA (green line, 100 μM in toluene), the spectrum shifts from 518 nm to 436 nm by adding different volume of triethylamine (TEA, 125 mM in toluene); c) UV-Vis spectra of **1** with pH-driven reversibility (5 μM in toluene, then added 100 equiv TFA, subsequently added 100 equiv TEA) and d) different concentrations of protonated nanotube **1** after adding excess TFA (100 equiv).

3. X-Ray Single Crystallography

Table S1: Crystal data and structure refinement for (**1**+3H)$^{3+}$·(TFA^{-})$_3$

entry	(**1**+3H)$^{3+}$·(TFA^{-})$_3$
Moiety formula	$C_{126}H_{87}N_3O_9$, 5($C_2HF_3O_2$), 4(C_7H_8)
Empirical formula	$C_{164}H_{124}F_{15}N_3O_{19}$
Formula weight	2725.65
Temperature/K	100.00
Crystal system	triclinic
Space group	*P-1*
a/Å	11.7820(6)
b/Å	18.0992(10)
c/Å	38.789(2)
α/°	87.108(3)
β/°	89.657(2)
γ/°	86.001(3)
Volume/Å^3	8240.8(8)
Z	2
ρ_{calc}g/cm^3	1.098
μ/mm^{-1}	0.445
F(000)	2832.0
Reflections collected	178709
Independent reflections	33623 [R_{int} = 0.0827, R_{sigma} = 0.0700]
Data/restraints/parameters	33623/477/1896
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0904, wR_2 = 0.2784
Final R indexes [all data]	R_1 = 0.1448, wR_2 = 0.3228
CCDC number	

Alert level B:

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 0.95 eA-3
PLAT230_ALERT_2_B Hirshfeld Test Diff for C04B --C04U . 7.2 s.u.

Response: The crystal has too weak diffraction to obtain high resolution data.

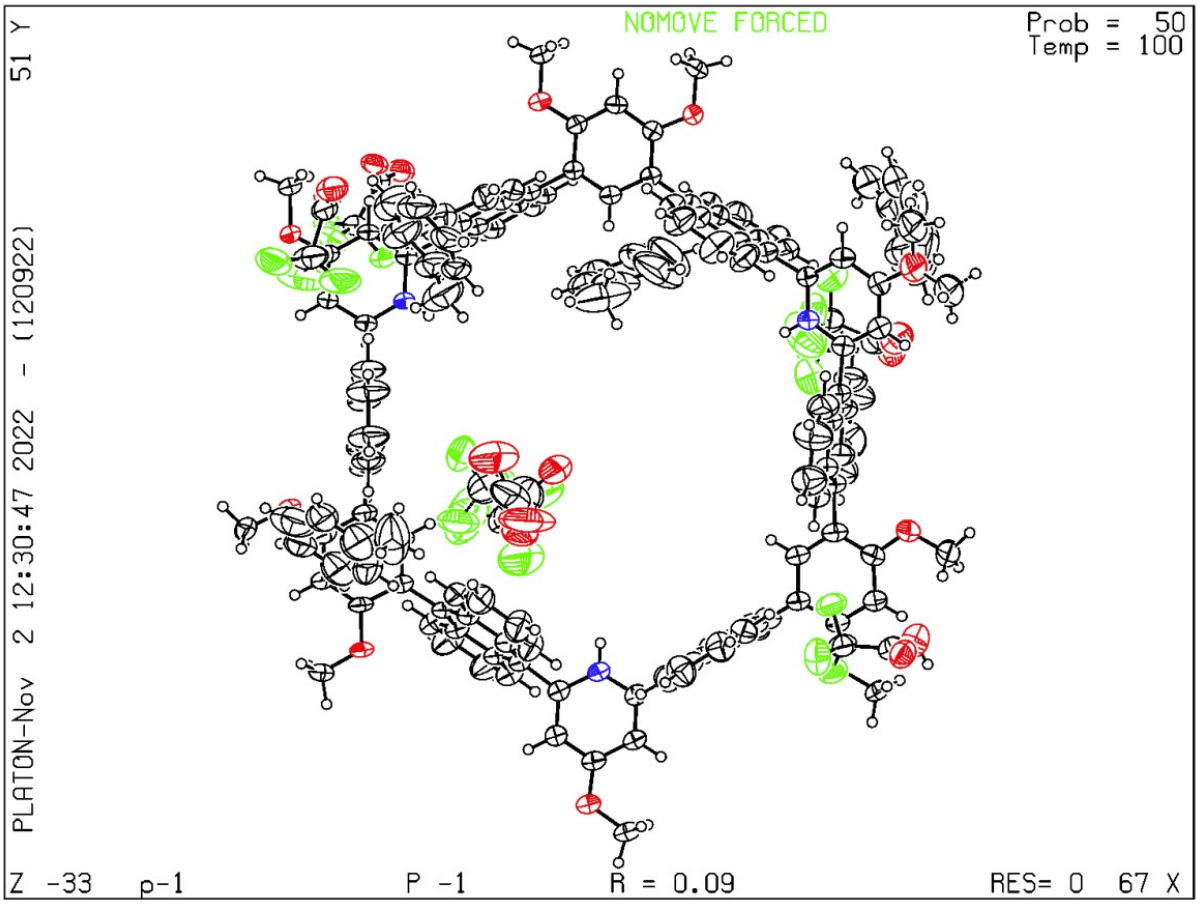
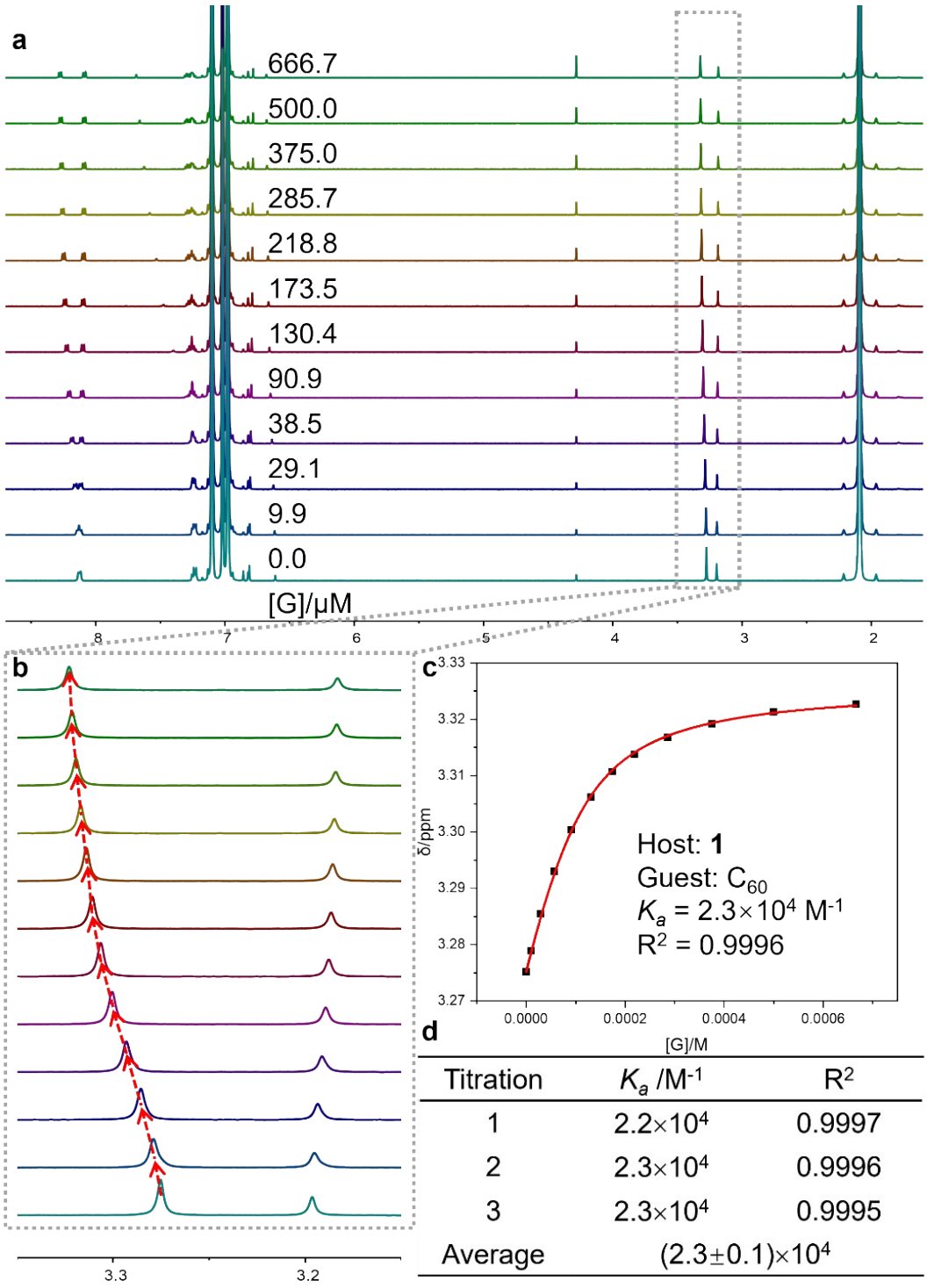


Figure S12. Crystal structure of $(\mathbf{1}+3H)^{3+}\cdot(TFA^{-})_3$.

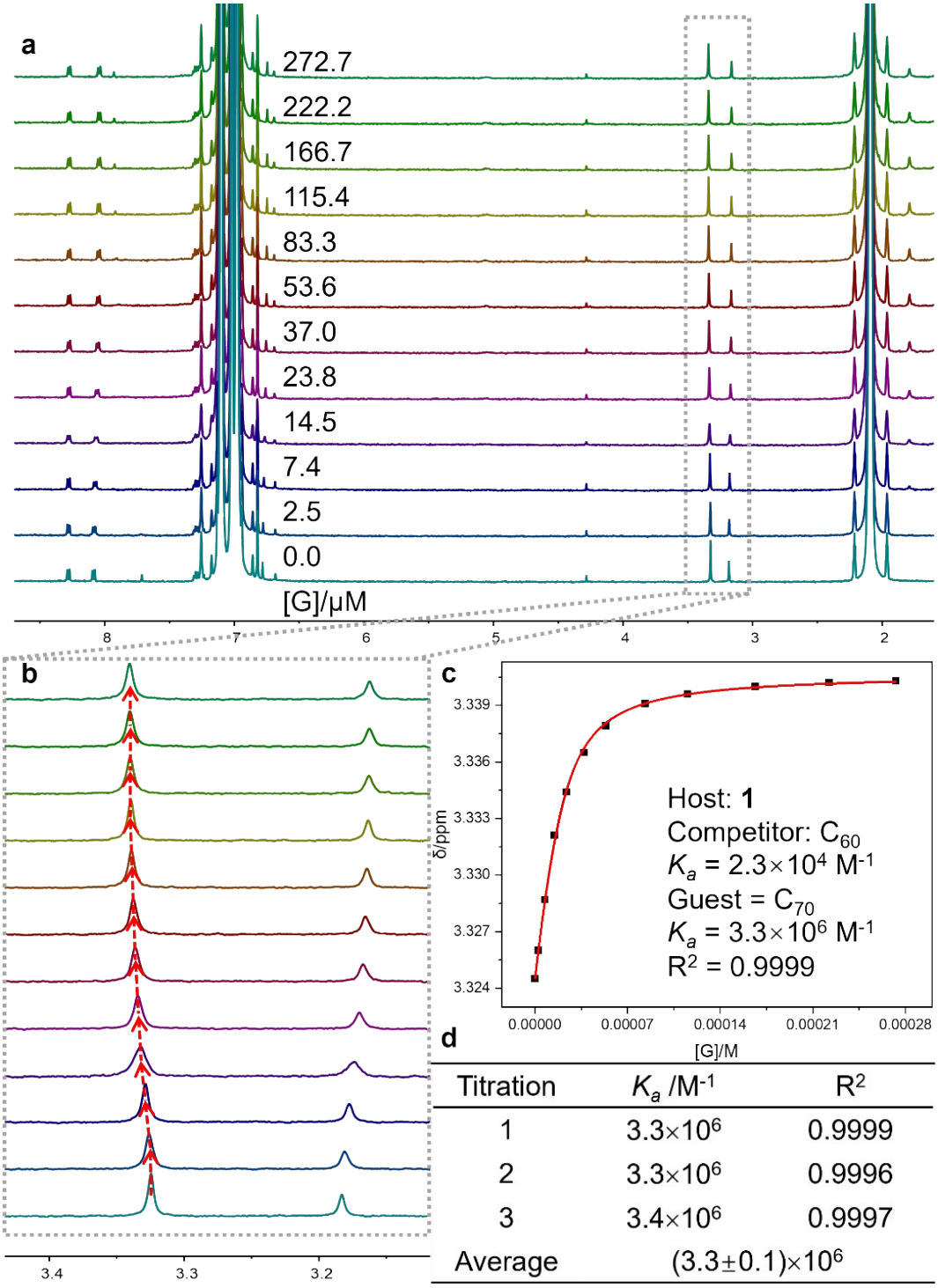
4. ^{1}H NMR Titration Experiments



d

Titration	K_a /M^{-1}	R^2
1	2.2×10^4	0.9997
2	2.3×10^4	0.9996
3	2.3×10^4	0.9995
Average	$(2.3\pm0.1)\times10^4$	

Figure S13. ^{1}H NMR titration experiments. a) ^{1}H NMR spectra (500 MHz, Toluene-d_8, 298 K) of **1** (0.1 mM) titrated by **C_{60}**, the concentration range of **C_{60}** is 0 ~ 666.7 μM; b) Enlarged region at signals of proton b and c, the changes of signals of proton c with the addition of **C_{60}** are marked with red arrow and used for nonlinear fitting; c) Nonlinear fitting for the complexation between **1** and **C_{60}** based on the NMR data. The titration experiments were repeated 3 times; d) averaged values and standard deviations are given.

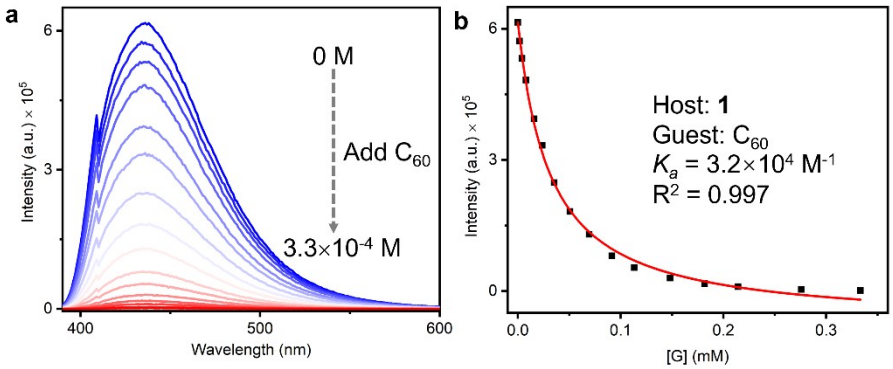


d

Titration	K_a /M^{-1}	R^2
1	3.3×10^6	0.9999
2	3.3×10^6	0.9996
3	3.4×10^6	0.9997
Average	$(3.3\pm0.1)\times10^6$	

Figure S14. ^{1}H NMR titration experiments. a) ^{1}H NMR spectra (500 MHz, Toluene-d_8, 298 K) of the mixture of **1** (0.01 mM) and **C_{60}** (1 mM, as a competitor) titrated by **C_{70}**, the concentration range of **C_{70}** is 0 ~ 272.7 μM; b) Enlarged region at signals of proton b and c, the changes of signals of proton c with the addition of **C_{70}** are marked with red arrow and used for nonlinear fitting; c) Nonlinear fitting for the complexation between **1** and **C_{70}** based on the NMR data. The titration experiments were repeated 3 times; d) averaged values and standard deviations are given.

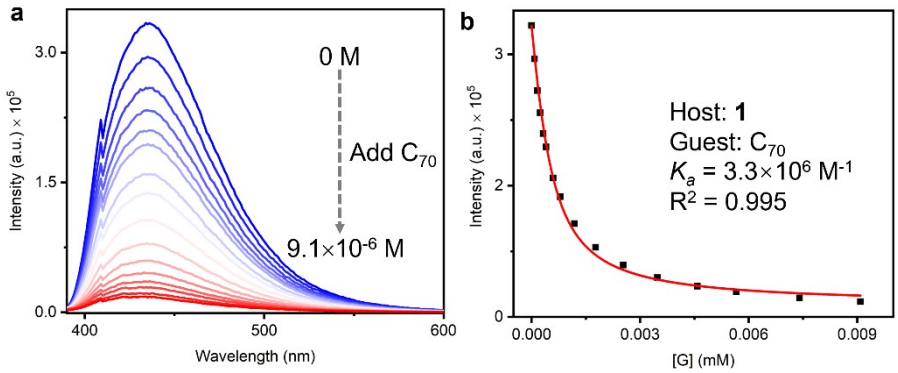
5. Fluorescent Titration Experiments



c

Titration	K_a /M^{-1}	R^2
1	3.2×10^4	0.997
2	3.3×10^4	0.998
3	3.3×10^4	0.997
Average	$(3.3\pm0.1)\times10^4$	

Figure S15. Fluorescent titration experiments. a) Fluorescent spectra ($Slit_{ex}$ = 1.0, $Slit_{em}$ = 1.0, Ex = 375 nm) of **1** (2×10^{-6} M) titrated by **C_{60}**, the concentration range of **C_{60}** is 0 ~ 3.3×10^{-4} M; b) The changes of fluorescent intensity at 435nm were used for nonlinear fitting; c) The titration experiments were repeated 3 times, and averaged values and standard deviations are given.



c

Titration	K_a /M^{-1}	R^2
1	2.8×10^6	0.997
2	3.2×10^6	0.996
3	3.3×10^6	0.995
Average	$(3.1\pm0.1)\times10^6$	

Figure S16. Fluorescent titration experiments. a) Fluorescent spectra ($Slit_{ex}$ = 1.5, $Slit_{em}$ = 1.5, Ex = 375 nm) of **1** (4×10^{-7} M) titrated by **C_{70}**, the concentration range of **C_{60}** is 0 ~ 9.1×10^{-6} M; b) The changes of fluorescent intensity at 435nm were used for nonlinear fitting; c) The titration experiments were repeated 3 times, and averaged values and standard deviations are given.

6. Job Plots and High-Resolution Mass Spectra (HRMS)

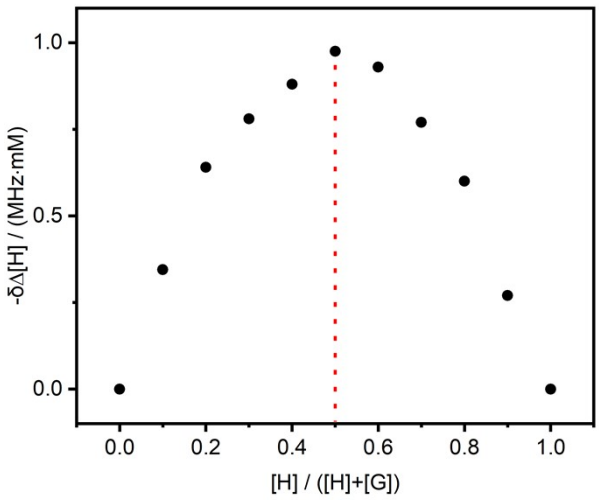


Figure S17. Job plots of **1**⊃C_{60}.

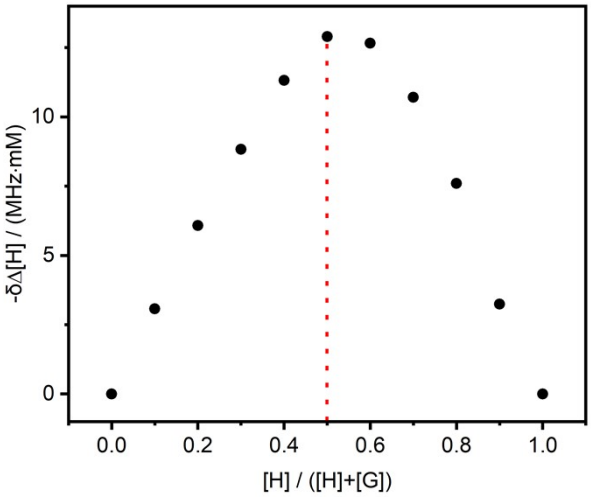


Figure S18. Job plots of **1**⊃C_{60}.

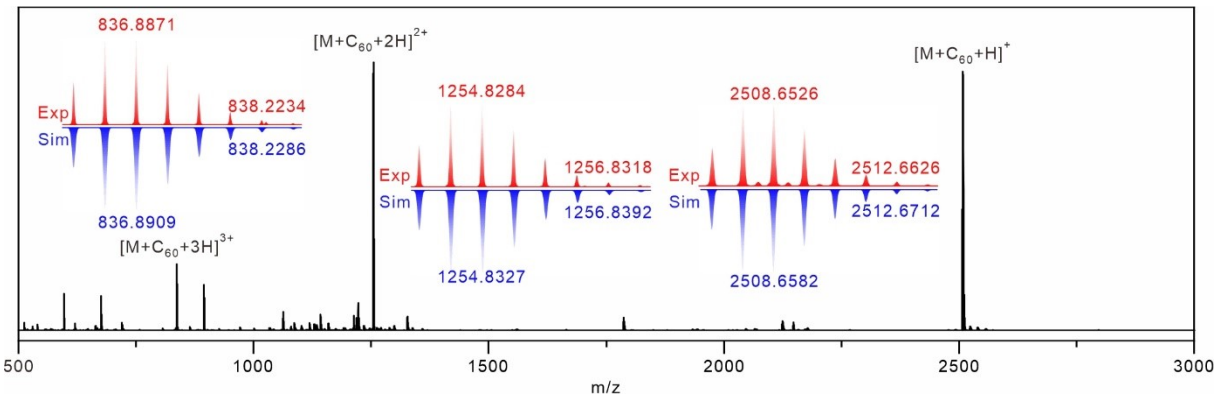


Figure S19. Experimental and simulated ESI mass spectra of **1**⊃C_{60}.

7. Computational Data

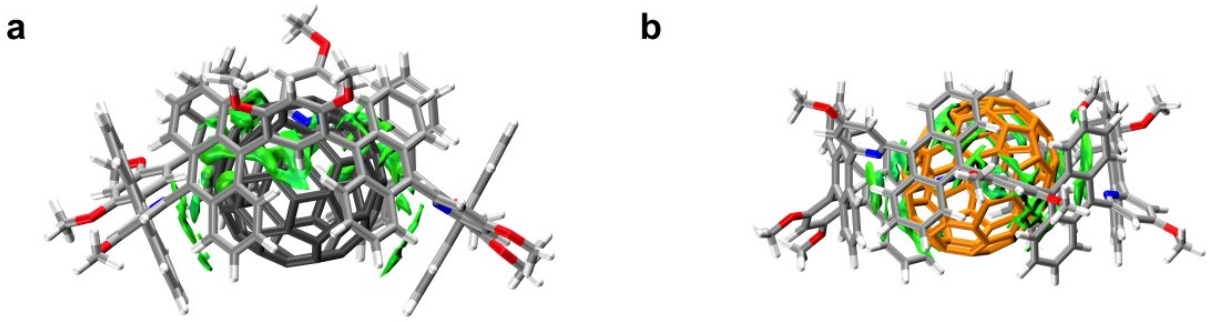


Figure S20. Side view of energy minimized structures with noncovalent interaction analysis of a) **1**⊃C_{60} and b) **1**⊃C_{70}.

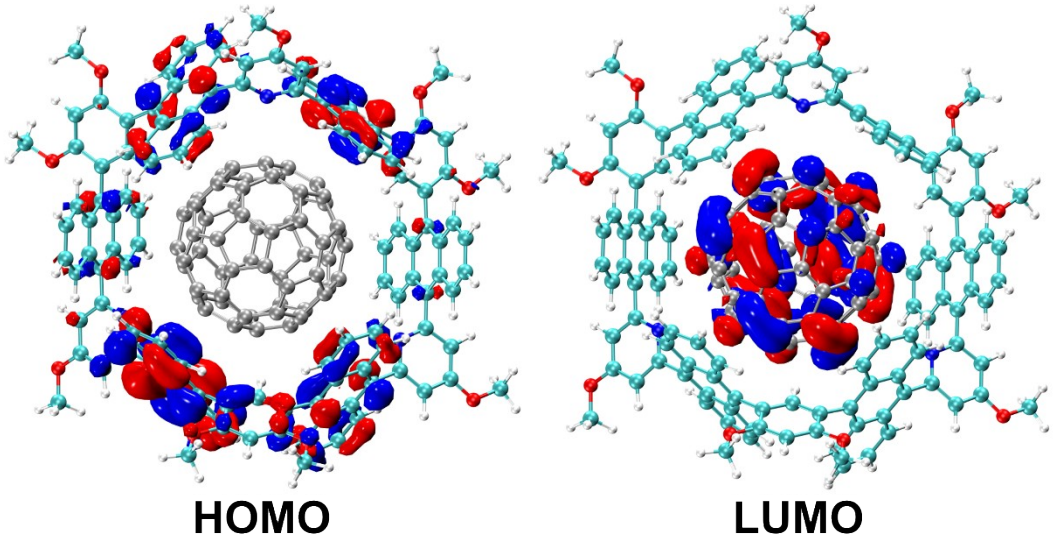


Figure S21. Analysis of frontier orbitals. Energy minimized structures and zero point energy obtained of **1**⊃C_{60} by DFT (ωB97XD/6-31G(d) and ωB97XD/6-311++G(d,p)) calculations in vacuum at 298 K. The HOMO-LUMO orbitals were calculated by Multiwfn 3.8 (dev) program and visualized by the VMD 1.9.3 program.

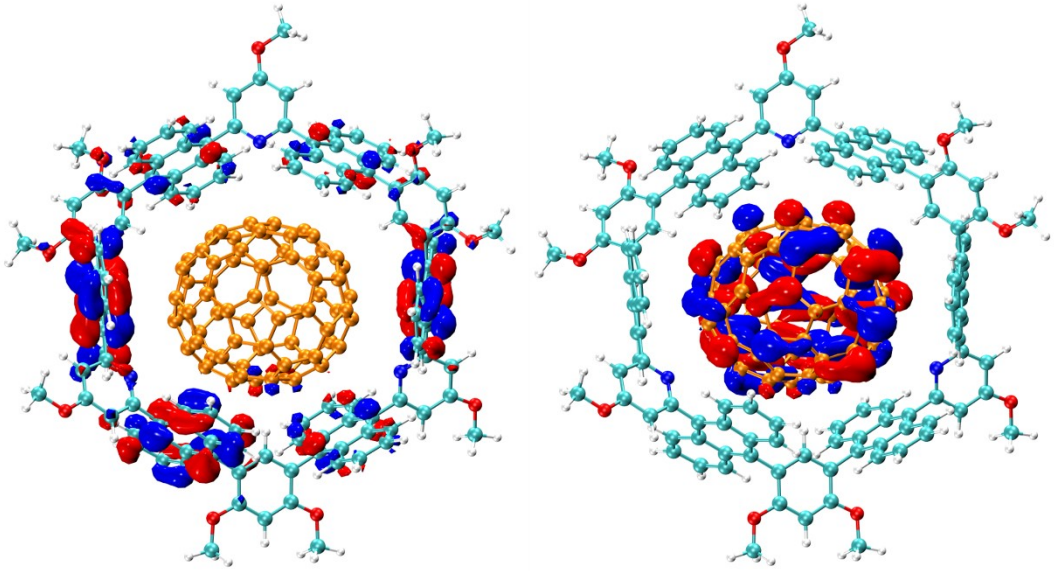


Figure S22. Analysis of frontier orbitals. Energy minimized structures and zero point energy obtained of **1**⊃C_{70} by DFT (ωB97XD/6-31G(d) and ωB97XD/6-311++G(d,p)) calculations in vacuum at 298 K. The HOMO-LUMO orbitals were calculated by Multiwfn 3.8 (dev) program and visualized by the VMD 1.9.3 program.

Table *S2*: Thermodynamic parameters of all calculated structures (298 K) Gibbs free energy (ZPE + $G_{0\rightarrow T}$) and enthalpy (ZPE + $H_{0\rightarrow T}$) are obtained after thermal correction (kJ/mol). The binding energy is defined as:

$$E_{binding} = E_{host\text{-}guest} - E_{host} - E_{guest}$$

	ΔG	ΔH	$-T\Delta S$	$\Delta E_{binding}$
C_{60}	-6000657.0	-6000489.0	-168.0	-
C_{70}	-7000987.9	-7000803.4	-184.5	-
1	-14946932.6	-14946222.3	-710.3	-
1⊃C_{60}	-20947788.2	-20946987.1	-801.2	-198.7
1⊃C_{70}	-21948156.0	-21947336.7	-819.4	-235.5

Initial molecular coordinates of **1**, C_{60}, C_{70}, **1**⊃C_{60}, and **1**⊃C_{70} were obtained after optimization with PM6

8. Stimuli-Responsive Properties

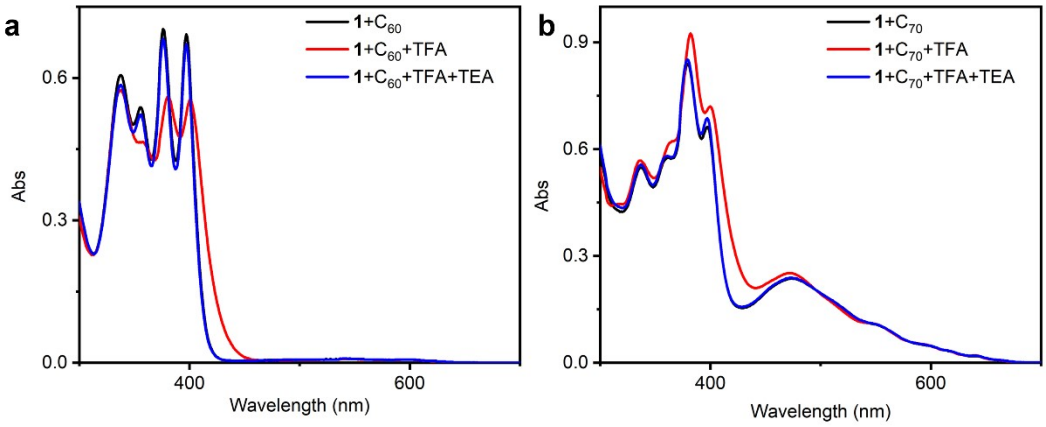


Figure S23. UV-Vis spectra of a) **1**⊃C_{60}, and b) **1**⊃C_{70} with pH-driven reversibility. The spectra were recorded with 5 μM host and/or host-guest complexes, then added 100 equiv TFA, subsequently added 100 equiv TEA.

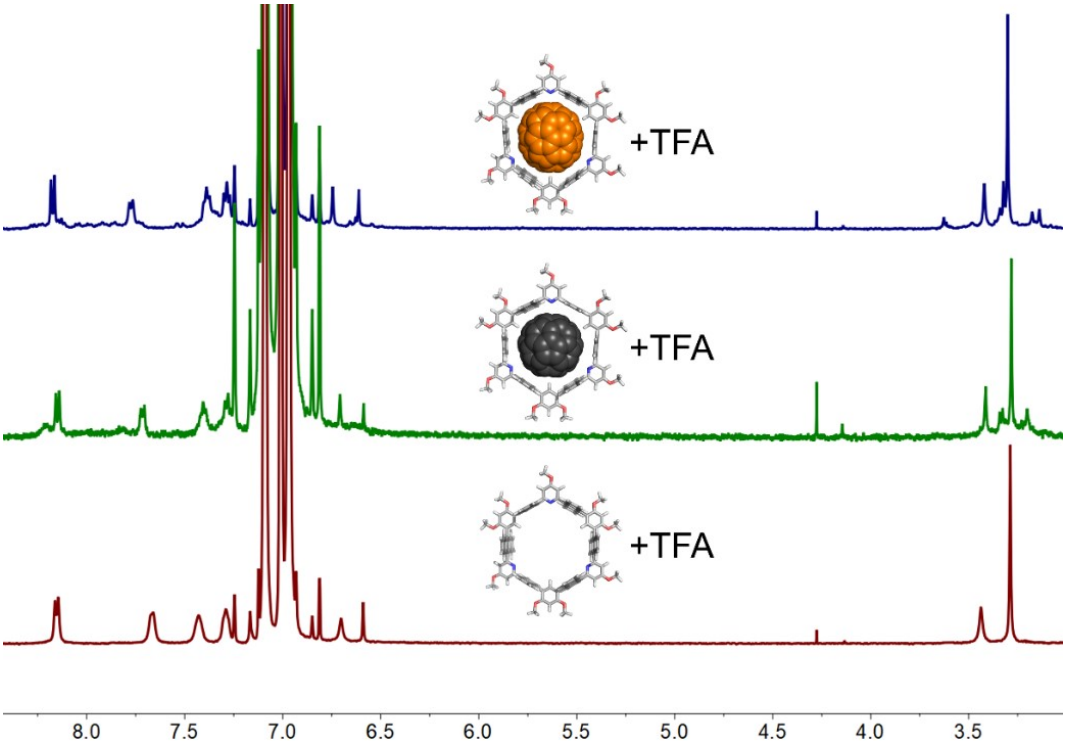


Figure S24. ^{1}H NMR spectra of nanotube **1** and host-guest complexes with excess TFA (~100 equiv).

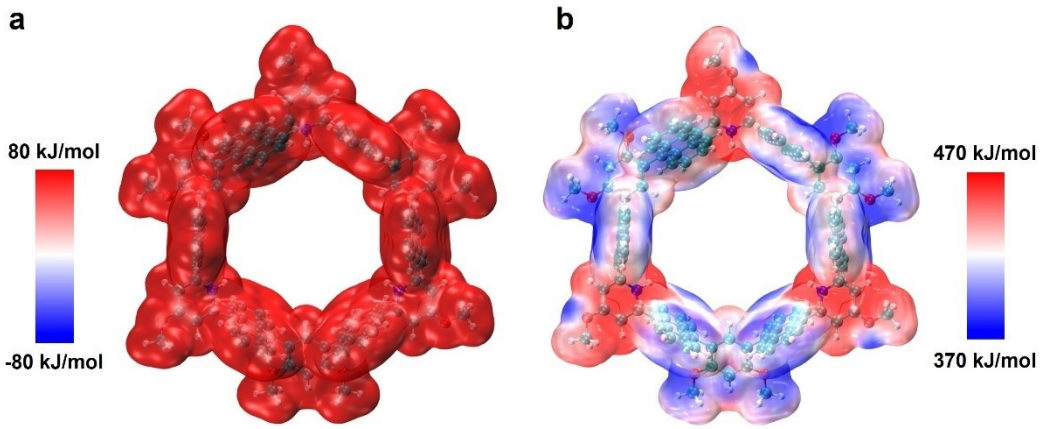


Figure S25. Electrostatic potential surface (EPS) of (**1**+3H)$^{3+}$ with different scalebars: a) share the same scalebar with **1** and b) scalebar from 370 kJ/mol to 470 kJ/mol

9. Atomic Coordinaes Information

For nanotube **1**:

H	4.93130800	-5.08010100	4.56563600
C	4.32761700	-5.48580700	3.75960100
H	5.75746400	-5.01766000	2.25863000
C	4.78718100	-5.45033600	2.47731000
C	2.28899300	-6.57740600	3.05337400
C	4.01106700	-5.97686200	1.39225500
C	3.05350200	-6.05154400	4.05130200
C	2.73825500	-6.57259900	1.69114500
C	4.46919700	-5.92831900	0.06396200
H	2.69370100	-6.06295300	5.07563800
H	1.31989300	-7.00736800	3.28409200
C	3.68274300	-6.46152200	-0.97279200
C	4.11072300	-6.41389600	-2.33943700
C	2.42137600	-7.07572700	-0.67329400
H	0.71425100	-8.11565100	-1.53137900
C	1.96750600	-7.12333300	0.65519600
C	3.35177100	-6.94795700	-3.33764200
H	5.05713700	-5.93592700	-2.56974500
H	3.69294500	-6.89946400	-4.36721500
C	2.10852000	-7.57450100	-3.03791900
H	1.51627100	-8.00321300	-3.84059900
C	1.66100500	-7.63520800	-1.75209300
C	-0.73805500	7.67359400	0.83733800
C	1.76264400	8.82323400	1.38271200
C	-0.64971500	8.96439100	1.37927600
C	0.44602600	6.98765600	0.58314500
C	1.70144000	7.53044700	0.84166600
C	0.59368900	9.53770400	1.65464200
H	0.65132000	10.53408100	2.07009100
C	6.92226300	-6.08770600	-0.48334800

C	7.13887100	-3.29213500	-0.56481000
C	8.15410500	-5.49299500	-0.76594000
C	5.78516800	-5.30099700	-0.24563200
C	5.92532200	-3.91675400	-0.29337200
C	8.25971700	-4.10089500	-0.80307600
H	9.02446500	-6.10814500	-0.94742200
H	2.68919400	7.81922500	-3.93656200
C	3.21058400	7.29963200	-3.13846800
H	1.86806300	7.96436300	-1.63081400
C	2.75340600	7.38018700	-1.85743500
C	5.04574900	5.88433100	-2.44818000
C	3.42079900	6.70327000	-0.78365300
C	4.37144600	6.53155200	-3.43986600
C	4.60872700	5.95289300	-1.08350600
C	2.94354400	6.76505400	0.53705400
H	4.71814300	6.46413400	-4.46652400
H	5.92898000	5.30150400	-2.68735400
C	3.62774100	6.09440500	1.56622700
C	3.16136800	6.12608500	2.92069500
C	4.82494900	5.36034300	1.27226300
H	6.42046900	4.16267000	2.14011000
C	5.29964200	5.30150600	-0.04899900
C	3.83786800	5.48779200	3.91690600
H	2.24823100	6.66881400	3.14178800
H	3.46700800	5.52234400	4.93673200
C	5.03517300	4.77302900	3.62807600
H	5.56865000	4.27327700	4.43087700
C	5.51008200	4.71216900	2.35200000
H	6.74385700	-1.63717700	-5.15319900
C	6.88986900	-1.10257800	-4.21958000
H	6.89222700	-2.87018200	-3.03624800
C	6.97460800	-1.78827000	-3.04476500
C	7.16817700	1.00680900	-3.06950100
C	7.16478600	-1.10673000	-1.79865900

C	6.98681900	0.31849300	-4.23176300
C	7.26809500	0.32492600	-1.81205100
C	7.24955900	-1.80585300	-0.58241600
H	6.91193300	0.85244100	-5.17413900
H	7.23591300	2.08982200	-3.08599900
C	7.42925300	-1.10543400	0.62329700
C	7.52513600	-1.78433800	1.88236500
C	7.53277700	0.32623600	0.61137500
H	7.81216200	2.09038600	1.85396500
C	7.45447900	1.01908900	-0.60662300
C	7.70250700	-1.09645500	3.04549800
H	7.45508100	-2.86683600	1.89440400
H	7.77143900	-1.63005000	3.98851100
C	7.80380400	0.32419600	3.03288400
H	7.94779700	0.85999600	3.96611300
C	7.72459700	1.00904500	1.85738700
C	6.55141700	4.54177800	-0.34882300
C	8.80985700	3.09801600	-0.87113600
N	6.45552800	3.20022800	-0.35916000
C	7.73550300	5.22306700	-0.58607600
C	8.89561300	4.49042600	-0.85756400
C	7.57111800	2.50995300	-0.61472400
H	-4.92454900	4.79822000	4.39272400
C	-4.34374500	5.25235900	3.59556000
H	-5.79910500	4.83312200	2.10883500
C	-4.83199000	5.27380900	2.32336600
C	-2.33359400	6.39913700	2.89898800
C	-4.08571200	5.86375700	1.25051900
C	-3.07127500	5.82070600	3.88819600
C	-2.80995300	6.44932000	1.54848000
C	-4.57494400	5.89344400	-0.06652000
H	-2.69202300	5.79131600	4.90508500
H	-1.36338400	6.83047200	3.12232700
C	-3.82055000	6.48402600	-1.09354200

C	-4.27243600	6.49871800	-2.45508200
C	-2.55069600	7.08295500	-0.78953900
H	-0.86506100	8.16943100	-1.62420600
C	-2.06059200	7.05999500	0.52762500
C	-3.53399100	7.08515800	-3.43890300
H	-5.21902100	6.02825600	-2.69927700
H	-3.89360600	7.08212800	-4.46332200
C	-2.28831200	7.70374200	-3.13265700
H	-1.71476600	8.17577100	-3.92448500
C	-1.81555700	7.70028500	-1.85474900
C	0.65484200	-7.76942500	0.96189200
C	-1.77261700	-8.90776800	1.47620400
C	0.62091300	-9.05368300	1.48308400
N	-0.44922600	-7.04962800	0.69480900
C	-1.62943800	-7.62232000	0.95273300
C	-0.61917400	-9.64253200	1.75103400
C	-6.99801500	6.15054000	-0.60237800
C	-7.20160700	3.42996700	-0.64554200
C	-8.24027400	5.57857800	-0.87681600
C	-5.91424700	5.30249000	-0.37005400
N	-5.99684700	3.96805800	-0.38758800
C	-8.33775800	4.18327800	-0.89596900
H	-2.47448100	-7.72258100	-3.85885800
C	-3.01642300	-7.22940900	-3.05763600
H	-1.70984200	-7.94397900	-1.54471400
C	-2.58978700	-7.35141200	-1.76914300
C	-4.86815800	-5.83785500	-2.36601200
C	-3.28476100	-6.70932300	-0.69214700
C	-4.17167400	-6.45428500	-3.36221900
C	-4.46050400	-5.94553200	-0.99652700
C	-2.85124500	-6.81932700	0.63928700
H	-4.49620900	-6.35883400	-4.39386100
H	-5.74777400	-5.24720400	-2.59980700
C	-3.55965800	-6.18809000	1.67384600

C	-3.12680400	-6.25761700	3.03965400
C	-4.74861900	-5.44114000	1.36975300
H	-6.37470400	-4.28499900	2.22987100
C	-5.18529800	-5.32775200	0.03816700
C	-3.83217300	-5.65176000	4.03588300
H	-2.21832400	-6.80219100	3.27512700
H	-3.48614900	-5.71464000	5.06303500
C	-5.02612000	-4.93444000	3.73855500
H	-5.58419800	-4.46556000	4.54322100
C	-5.46581400	-4.83342800	2.45276200
H	-6.68143300	1.70147100	-5.19767300
C	-6.83902400	1.18154600	-4.25765900
H	-6.88527100	2.97063700	-3.11294700
C	-6.95319400	1.88765100	-3.09750500
C	-7.11201700	-0.90961700	-3.07439900
C	-7.15995800	1.22437600	-1.84321300
C	-6.92129000	-0.24047500	-4.24632700
C	-7.23672700	-0.20899400	-1.83054200
C	-7.27919400	1.93703400	-0.64010300
H	-6.82769800	-0.78956400	-5.17826900
H	-7.16693800	-1.99328200	-3.06640300
C	-7.46505700	1.25969400	0.57504700
C	-7.58931000	1.96150000	1.81914900
C	-7.54032500	-0.17374700	0.58647600
H	-7.80420900	-1.91789000	1.85407900
C	-7.42868900	-0.89164600	-0.61712800
C	-7.77096300	1.29216800	2.99226100
H	-7.54343600	3.04551300	1.81595400
H	-7.86179000	1.84203800	3.92401000
C	-7.84761500	-0.13004100	3.00418800
H	-7.99659900	-0.65057100	3.94524800
C	-7.73933800	-0.83505000	1.84278100
C	-6.41177000	-4.54203900	-0.27713200
C	-8.71399800	-3.04352100	-0.84959300

C	-6.37892400	-3.15097800	-0.32183100
C	-7.63576800	-5.18132800	-0.52478300
C	-8.78216700	-4.43804400	-0.81477800
C	-7.50353100	-2.38026500	-0.60060800
H	-9.72071400	-4.94007000	-1.00443500
O	-9.77894800	-2.25115600	-1.11572300
O	-7.62079300	-6.53366900	-0.46262600
O	3.00435800	9.31096600	1.61267900
O	-1.82700300	9.59312900	1.60632600
C	-11.02953100	-2.86212800	-1.37929300
H	-10.97963100	-3.50709300	-2.26404200
H	-11.72594800	-2.04507200	-1.56679000
H	-11.37741800	-3.44553800	-0.51912400
C	-8.81993600	-7.23858900	-0.73006300
H	-9.60267100	-6.98391700	-0.00639600
H	-8.57088400	-8.29536800	-0.63513900
H	-9.18054800	-7.04025700	-1.74586800
C	3.13172300	10.60375500	2.17755000
H	4.20252500	10.77815000	2.28195600
H	2.65732700	10.65611700	3.16415800
H	2.70159100	11.36975100	1.52220200
C	-1.80450000	10.89339700	2.16800500
H	-1.32942100	10.89273000	3.15573100
H	-2.84789700	11.19145400	2.26919800
H	-1.28649800	11.60251000	1.51211500
H	5.05219600	-3.29798600	-0.10341800
H	-5.43717600	-2.64555300	-0.12400300
H	0.38807700	5.98890600	0.15831100
O	9.41698000	-3.44730500	-1.06115400
O	6.73963300	-7.42759400	-0.41909000
C	10.58321900	-4.20957400	-1.31723000
H	11.37705800	-3.48568400	-1.50087300
H	10.45843400	-4.84414300	-2.20208800
H	10.85086300	-4.83079300	-0.45484500

C	7.84427800	-8.27616300	-0.67608300
H	8.23401300	-8.12702300	-1.68953400
H	7.46572800	-9.29369600	-0.58080000
H	8.64723000	-8.11805800	0.05299300
H	1.53524400	-9.60096000	1.68376300
H	-2.76598200	-9.30027700	1.65477300
H	-9.29086700	3.70865400	-1.10102200
H	-6.84965400	7.22265200	-0.56724100
H	7.77178900	6.30662100	-0.56601200
H	9.66645900	2.46601800	-1.06978400
O	10.01472100	5.19641400	-1.08167800
O	-9.36728600	6.26460100	-1.12256600
O	-0.59908800	-10.88674100	2.25374900
C	11.21448700	4.48431800	-1.35798500
H	11.98181400	5.24326900	-1.50484200
H	11.11444200	3.88336200	-2.26789500
H	11.49187600	3.84040700	-0.51686000
C	-9.30398900	7.68545200	-1.11604800
H	-8.99938700	8.06104200	-0.13361300
H	-10.31345300	8.02757000	-1.34030300
H	-8.61370000	8.05161900	-1.88323300
C	-1.84212600	-11.51532800	2.54089900
H	-2.40389100	-10.95043900	3.29225900
H	-1.59195900	-12.49899100	2.93608200
H	-2.44500200	-11.62716900	1.63366300

For C_{60}:

C	-0.11214170	4.19728824	-0.18922765
C	0.28169987	3.50667625	-1.46022228
C	-0.75412343	2.46615466	-1.76530072
C	-1.59406271	3.39918256	1.61933389
C	-0.54289164	3.81509356	2.60512719
C	0.61294396	4.37306927	2.16959114
C	0.83892643	4.57266864	0.70111415

C	1.58859872	3.25916834	-1.71936640
C	2.64057942	3.67459267	-0.73485784
C	2.28475208	4.29796471	0.41473910
C	-0.38223331	1.27625795	-2.29772948
C	1.06355520	1.00187159	-2.58390231
C	-2.21658577	2.12780310	2.11285320
C	-1.94138313	0.04538481	-0.82603336
C	-1.00594340	0.00445854	-1.80566083
C	-0.51472418	2.79944024	3.70773719
C	-1.54915015	1.75711806	3.40322010
C	2.95263037	3.92753304	1.70573994
C	1.91942031	3.97427693	2.79071751
C	-1.91112560	-0.96897102	0.27772230
C	-2.30331262	-0.27891501	1.54957656
C	1.33438391	-0.43860944	-2.26771742
C	0.05531455	-1.05558795	-1.78673724
C	1.94452488	3.05614104	3.78769177
C	0.66561872	2.43923248	4.26890491
C	-1.70047572	-0.61433467	2.71599005
C	-1.30409571	0.45515353	3.68916137
C	0.08036594	-1.97414012	-0.79029879
C	-0.95299736	-1.92798808	0.29456955
C	3.54973601	0.24288429	-1.40318803
C	2.51492401	-0.79916984	-1.70732246
C	4.30523711	2.28000204	0.45029161
C	3.91207317	2.96979925	1.72261572
C	0.93646906	0.99815294	4.58421469
C	0.00112341	0.05654493	4.30941398
C	4.57624702	0.83894342	0.76684902
C	4.21796160	-0.12819028	-0.11315444
C	2.54290781	-1.81466559	-0.60506459
C	1.38691664	-2.37252094	-0.16955229
C	-0.28515961	-2.29847439	1.58537884
C	-0.64058760	-1.67467922	2.73494808

C	1.16091564	-2.57383352	1.29867244
C	3.59610973	-1.40061101	0.38012048
C	-2.57616076	1.16128337	1.23288912
C	-2.35184134	1.36250350	-0.23553503
C	-1.78853035	2.51200709	-0.68170575
C	-1.39163556	3.58247590	0.29207617
C	1.99901839	1.94337182	-2.30909483
C	3.30447053	1.54490012	-1.68889547
C	3.70119473	2.61474519	-0.71593502
C	0.41130038	-1.25956085	3.71961080
C	2.11195047	-2.19795608	2.18879427
C	1.71801728	-1.50725814	3.46010338
C	2.38218246	0.72360652	4.29779696
C	3.00574715	1.99558739	3.80617455
C	2.75320206	-0.46609970	3.76445813
C	3.94044159	1.95466779	2.82591591
C	4.34983824	0.63776647	2.23471809
C	3.39145479	-1.58270514	1.70726575
C	3.78640800	-0.51150126	2.68040432

For C_{70}:

C	2.41701857	-0.24953628	2.92455252
C	2.88979621	-1.44476163	2.22282348
C	1.77578258	-2.39536649	2.20721868
C	0.63480288	-1.78841103	2.91648151
C	1.02564425	-0.48144652	3.35252176
C	2.80277867	0.99844401	2.49687522
C	3.72438551	-1.32402889	1.12106449
C	1.55334399	-3.17693509	1.09783821
C	-0.70262165	-2.07986783	2.54593054
C	0.09501414	0.58451691	3.43632984
C	0.17517556	-3.40108240	0.62469290
C	2.43010591	-3.05776945	-0.06899646
C	-1.66068913	-1.09160170	2.88711307

C	0.19104611	-3.40848903	-0.80754570
C	3.48628772	-2.15740262	-0.06345756
C	4.13622978	0.00949423	0.66355895
C	-0.94157101	-2.91866463	1.35343543
C	-1.59326549	-1.12918567	-3.14219709
C	1.57901882	-3.18999576	-1.25341987
C	3.74988958	-1.33861725	-1.25353703
C	4.15243027	-0.00035132	-0.80478123
C	3.68795780	1.13605349	1.33759027
C	1.82120822	2.09879820	2.46910130
C	3.22838636	2.31071691	0.59178220
C	2.07966262	2.89750854	1.30860723
C	2.94119419	-1.47451981	-2.37330038
C	-2.92942243	-0.96691526	2.14675483
C	-1.26903123	0.21503456	3.32394873
C	-2.28644048	1.17787781	2.86480931
C	3.71722691	1.11755022	-1.50258472
C	0.50880260	1.92557420	2.97624176
C	2.85939778	0.96435008	-2.67991075
C	-3.32668378	0.44252622	2.14246162
C	-1.90176990	2.42629563	2.43601952
C	-2.53162412	3.02333308	1.25650450
C	-0.47439343	2.79447091	2.43882871
C	1.82625032	-2.42387993	-2.36801855
C	-0.21697601	3.59224530	1.27817997
C	2.48445691	-0.28975074	-3.10159829
C	1.87691481	2.06251775	-2.68621701
C	0.70184641	-1.82640326	-3.11078248
C	3.24352167	2.30192633	-0.78323207
C	-2.87764196	-0.99438507	-2.43001024
C	1.10245894	-0.52639790	-3.55738257
C	-1.47948576	3.73655866	0.53058587
C	1.03376474	3.55301850	0.61114141
C	1.04927249	3.54102227	-0.86515315

C	-3.92599485	0.99871262	1.02096003
C	-1.19323199	0.17117254	-3.58996603
C	-0.18574005	3.57177402	-1.56081354
C	-3.27771129	0.41476008	-2.45587192
C	-1.46406078	3.72680756	-0.84448598
C	-3.51462373	2.33165481	0.56249213
C	-3.90080739	0.98413067	-1.35500645
C	-3.50003468	2.32333573	-0.90515319
C	-4.16395644	0.16594030	-0.16400129
C	-3.78601429	-1.16899646	-0.15055109
C	-3.12364556	-1.75981773	-1.31521745
C	-2.22180968	1.14099103	-3.16651596
C	-2.50046765	3.00434874	-1.58567365
C	2.11025266	2.87549038	-1.53003495
C	-0.41890348	2.75930279	-2.71733089
C	-1.84635752	2.39511042	-2.74564753
C	0.17346520	0.53835996	-3.67621441
C	0.57632636	1.88411041	-3.22172110
C	-3.15140657	-1.74688390	1.03619652
C	-2.12002313	-2.70321435	0.59458001
C	-0.64324929	-2.11117465	-2.76427320
C	-2.10304807	-2.71020049	-0.83742061
C	-0.90818532	-2.93382048	-1.56655939

For complex **1**⊃C_{60}:

H	2.95243641	1.78376098	-7.32726588
C	1.91146834	2.00845864	-7.11403359
H	2.37686476	3.90917704	-6.29562847
C	1.56450205	3.22121183	-6.52041163
C	-0.40641661	1.40526930	-7.13148753
C	0.22265614	3.56187113	-6.20117852
C	0.92172842	1.09402355	-7.41651895
C	-0.79143611	2.63221807	-6.52808987
C	-0.12959012	4.79143800	-5.56214340

H	1.17342857	0.13799243	-7.86622046
H	-1.15303731	0.64901530	-7.36835801
C	-1.48535811	5.07449097	-5.21061044
C	-1.86645624	6.25786297	-4.52232178
C	-2.49882883	4.14960628	-5.54971984
H	-4.64409392	3.76744600	-5.40752824
C	-2.15245213	2.94778382	-6.23907606
C	-3.18758193	6.53267516	-4.17272072
H	-1.11873068	6.99592351	-4.23942038
H	-3.43225344	7.44790879	-3.64175887
C	-4.17727090	5.62841000	-4.50310409
H	-5.21163026	5.82024371	-4.23336094
C	-3.83556603	4.45954533	-5.18094848
C	3.85458082	-2.75267490	6.46635382
C	6.13100636	-1.18821021	7.04791451
C	4.76112682	-3.16546378	7.46211990
C	4.10738259	-1.55990232	5.77581238
C	5.23178912	-0.76936292	6.04880578
C	5.88871222	-2.38052419	7.74560811
H	6.57874391	-2.69653220	8.51628488
C	1.25860019	6.86227640	-6.04515246
C	2.65744189	6.47685836	-3.62539600
C	2.26457712	7.75788249	-5.65306839
C	0.93323223	5.77005476	-5.21747096
C	1.63853088	5.59878304	-4.01874274
C	2.96525193	7.57439195	-4.45199096
H	2.50437482	8.60068100	-6.28718747
H	2.73447684	2.92204572	8.17052542
C	3.34914308	2.91999697	7.27513110
H	3.83992139	0.86707911	7.48537227
C	3.98822079	1.75023251	6.86732018
C	4.29118139	4.04031163	5.37931974
C	4.79417212	1.68436363	5.69898543
C	3.49665029	4.06935788	6.52412037

C	4.96292778	2.86653809	4.94277761
C	5.42352720	0.47684042	5.26555327
H	2.99556438	4.98726106	6.81743246
H	4.36406344	4.96353018	4.80698299
C	6.18931556	0.43761610	4.06002937
C	6.77920390	-0.75772549	3.56723427
C	6.36894664	1.62351113	3.31245692
H	7.27376278	2.43094615	1.49769915
C	5.78493410	2.84212807	3.77563180
C	7.51282125	-0.80168385	2.38294621
H	6.66404472	-1.69381265	4.10969974
H	7.93692491	-1.74006390	2.03810777
C	7.68688236	0.35631068	1.65169678
H	8.24617679	0.34206930	0.72091578
C	7.12756162	1.54633533	2.11377972
H	0.15164921	8.32018078	0.21596927
C	1.09349814	7.77974546	0.19127594
H	1.07001929	7.61794509	-1.92439482
C	1.63223415	7.36802777	-1.02684778
C	2.96643501	6.78528114	1.30577753
C	2.84999236	6.64269495	-1.11847605
C	1.76095861	7.48226014	1.36342699
C	3.54217577	6.35573325	0.08046678
C	3.38572177	6.19139434	-2.36377040
H	1.34852165	7.78026609	2.32304247
H	3.44841403	6.55190331	2.25388221
C	4.58812752	5.41933073	-2.41128823
C	5.12033409	4.90281733	-3.62387895
C	5.28410555	5.14380670	-1.21332834
H	7.02480171	4.11125935	-0.39249419
C	4.77799892	5.64520730	0.02399276
C	6.28618617	4.14006846	-3.67012733
H	4.61641071	5.08801010	-4.57026839
H	6.65156547	3.75906105	-4.61927004

C	6.96396809	3.86851602	-2.49847916
H	7.86845984	3.26743064	-2.51139477
C	6.47005931	4.36503512	-1.29360340
C	6.06386411	4.10012962	3.05817263
C	6.51942018	6.40291614	1.64568706
N	5.32987741	4.32459898	1.94588645
C	7.03619501	4.98966824	3.50610190
C	7.26346233	6.16096113	2.79228144
C	5.56892778	5.46074723	1.25424445
H	2.83956804	-7.24787801	2.27916070
C	2.81721292	-6.50134237	3.06773295
H	0.75944840	-6.83034323	3.46946814
C	1.63556599	-6.25512912	3.76445044
C	3.89173244	-4.81246276	4.38450996
C	1.54179502	-5.27567812	4.78900911
C	3.95139934	-5.77820719	3.38091971
C	2.70077288	-4.53020748	5.10560688
C	0.32867138	-5.02039958	5.49590575
H	4.88028404	-5.95187448	2.84558584
H	4.80689949	-4.26248056	4.59417596
C	0.24449765	-3.96812667	6.45752828
C	-0.97122167	-3.62479675	7.10871878
C	1.40405385	-3.22821080	6.78160178
H	2.15706604	-1.61410326	8.04572644
C	2.63578856	-3.52735145	6.12161623
C	-1.05417823	-2.60630356	8.05647203
H	-1.89559859	-4.14457241	6.86240030
H	-2.00620801	-2.37137959	8.52360969
C	0.08259180	-1.89566892	8.38734659
H	0.03891813	-1.09721089	9.12236183
C	1.28846808	-2.20377150	7.75948868
C	-3.22236136	2.04020908	-6.69229167
C	-5.25103209	0.35255808	-7.42113427
C	-3.82125197	2.19891410	-7.93858042

N	-3.59247095	1.07332257	-5.82255063
C	-4.59701136	0.24747272	-6.19307902
C	-4.85022985	1.34130080	-8.30908792
C	-1.12177159	-6.94976301	6.13350501
C	-2.70712420	-6.34926854	3.98324665
C	-2.25112196	-7.72121015	5.89783341
C	-0.84227386	-5.88896775	5.27147785
N	-1.61407174	-5.58480662	4.20409809
C	-3.05792077	-7.41397457	4.80865996
H	-7.32345218	2.29723552	-2.62674018
C	-7.06351095	1.25666393	-2.79749345
H	-5.87439479	1.71984914	-4.49116742
C	-6.23901284	0.90777308	-3.86552780
C	-7.17052763	-1.05663033	-2.18741171
C	-5.84577222	-0.43240344	-4.12564317
C	-7.53242979	0.26913985	-1.95443442
C	-6.32588343	-1.44394879	-3.26268301
C	-4.98878939	-0.78406555	-5.21249102
H	-8.17126347	0.52074125	-1.11300112
H	-7.55940727	-1.80105184	-1.49572171
C	-4.54777095	-2.12995318	-5.39434561
C	-3.61632291	-2.49766830	-6.40255736
C	-5.04117773	-3.14518799	-4.54282736
H	-4.96501908	-5.29138409	-4.14612884
C	-5.94584494	-2.80282127	-3.49150572
C	-3.19473557	-3.81262976	-6.59154648
H	-3.17845846	-1.74185504	-7.05259810
H	-2.47373509	-4.04841287	-7.36898702
C	-3.69539361	-4.80811825	-5.77573728
H	-3.37848317	-5.83880350	-5.90625316
C	-4.60249958	-4.47701334	-4.77034619
H	-5.59827924	-2.49682326	5.05108714
C	-5.54235408	-3.10118974	4.15047450
H	-3.95819528	-4.28772032	4.91502194

C	-4.61261274	-4.13537262	4.05859071
C	-6.27674525	-3.62756780	1.93190489
C	-4.47921704	-4.94488528	2.89848211
C	-6.38034552	-2.84760845	3.08268287
C	-5.33211914	-4.68116817	1.80219377
C	-3.51896997	-5.99703951	2.80367268
H	-7.10877343	-2.04369970	3.13323741
H	-6.95435889	-3.39052739	1.11431792
C	-3.35847624	-6.74056762	1.59474568
C	-2.35711107	-7.73696115	1.43790552
C	-4.21513610	-6.48255619	0.50046529
H	-4.67882665	-7.09046209	-1.54518980
C	-5.21250170	-5.46583932	0.61332380
C	-2.20304877	-8.46938622	0.26204616
H	-1.65539073	-7.94626678	2.24341946
H	-1.41991854	-9.21789653	0.18403011
C	-3.05028771	-8.22842536	-0.80136462
H	-2.94623510	-8.78774041	-1.72648946
C	-4.03722245	-7.25135284	-0.68119942
C	-6.45320344	-3.86369218	-2.58447788
C	-7.32877110	-5.82298277	-0.74948943
C	-5.67834959	-4.21174956	-1.47061696
C	-7.68226053	-4.51988009	-2.78512668
C	-8.10788165	-5.49456437	-1.86942502
C	-6.09550037	-5.17683530	-0.54484516
H	-9.04967106	-6.00183419	-2.03004745
O	-7.67518245	-6.75802923	0.19280579
O	-8.38565413	-4.14028854	-3.90064952
O	7.20559701	-0.36345834	7.26622522
O	4.45128216	-4.34035423	8.10047606
C	-8.94271481	-7.38661807	0.07333211
H	-9.75440533	-6.65294213	0.11653384
H	-9.06167592	-8.06399650	0.92443785
H	-8.99919903	-7.98767770	-0.83998540

C	-9.66688880	-4.71658378	-4.10731259
H	-9.59087831	-5.79638298	-4.27124543
H	-10.09106954	-4.27248670	-5.01298425
H	-10.34294717	-4.48751182	-3.27698482
C	8.16955266	-0.76408487	8.22863259
H	8.95797216	-0.00553622	8.24810064
H	8.63221519	-1.71719849	7.95218843
H	7.72987564	-0.81195230	9.23016201
C	5.36218033	-4.82988860	9.07359203
H	6.34490688	-5.02653490	8.63256349
H	4.97092837	-5.78012268	9.44959689
H	5.43812821	-4.14289879	9.92267164
H	1.39546904	4.75587879	-3.37719370
H	-4.72462855	-3.71572144	-1.31687227
H	3.40979936	-1.23266347	5.00917495
O	3.96428459	8.39964924	-3.99998999
O	0.53469060	6.96637761	-7.20632591
C	4.33158027	9.50646271	-4.81014733
H	5.14107139	10.03893231	-4.30162772
H	3.49632833	10.20473726	-4.92634293
H	4.71107588	9.17570739	-5.78248204
C	0.84437575	8.03102596	-8.09317177
H	0.64973538	9.00202844	-7.62631026
H	0.18689436	7.94336096	-8.96346410
H	1.87754833	7.96151449	-8.44899234
H	-3.49441458	2.98735504	-8.60962500
H	-6.05218373	-0.34112101	-7.64688259
H	-3.94689085	-8.00162718	4.60060863
H	-0.45400381	-7.13552889	6.96625488
H	7.60893493	4.77298004	4.40266713
H	6.65535895	7.29062968	1.03973350
O	8.23203077	6.97442024	3.31117595
O	-2.67098037	-8.78582219	6.64558138
O	-5.37887456	1.57476839	-9.54801160

C	8.49293976	8.18807781	2.61581487
H	9.28040523	8.72089366	3.15741765
H	7.60662408	8.83092637	2.59800320
H	8.85939894	7.99090144	1.60295458
C	-1.87708538	-9.13163128	7.77458196
H	-0.86768912	-9.42800193	7.47078027
H	-2.34517519	-9.99273581	8.26108385
H	-1.84751616	-8.31314897	8.50141522
C	-6.42475986	0.70943392	-9.97450021
H	-6.07861121	-0.32768035	-10.03573328
H	-6.72656955	1.01998391	-10.97939099
H	-7.29934304	0.79698726	-9.32147369
C	-0.43557971	3.15662722	-1.47254344
C	0.01025456	2.31172999	-2.62653318
C	-1.11413025	1.39440289	-2.99476262
C	-2.22403594	2.71801831	0.17517534
C	-1.25111165	3.07662327	1.25927921
C	0.01517920	3.44207193	0.94220499
C	0.44347634	3.48304311	-0.49362480
C	1.29228870	1.87891003	-2.69581291
C	2.26540561	2.24121742	-1.61440308
C	1.86115888	3.00079456	-0.56750067
C	-0.84900596	0.12701773	-3.39498742
C	0.57002215	-0.35403784	-3.46912101
C	-3.07267534	1.58515515	0.67041520
C	-2.72481773	-0.75783844	-2.05246830
C	-1.69677435	-1.00531971	-2.89990707
C	-1.49901227	2.16533362	2.42376507
C	-2.62414295	1.24315011	2.06019224
C	2.30980364	2.66263931	0.82218857
C	1.16881952	2.93500453	1.75629235
C	-2.96509874	-1.66329217	-0.88560789
C	-3.42109407	-0.82866549	0.26975493
C	0.59810807	-1.78421190	-3.01889238

C	-0.80282574	-2.18751949	-2.66776134
C	0.94415695	2.11113370	2.80928792
C	-0.45747757	1.70699852	3.15993295
C	-3.01902997	-1.13882784	1.52645432
C	-2.60021499	-0.04962356	2.46754423
C	-1.02496997	-3.00925111	-1.61262300
C	-2.16030901	-2.73267875	-0.67692641
C	2.76476576	-1.32036278	-1.91786987
C	1.63968374	-2.24239595	-2.28207513
C	3.56675078	0.75480482	-0.12712409
C	3.11809804	1.59498158	1.03132851
C	-0.43079675	0.27630638	3.60916970
C	-1.44803919	-0.55814357	3.28193812
C	3.59314351	-0.67627904	0.32214528
C	3.21259847	-1.66117251	-0.52806804
C	1.39247539	-3.15422285	-1.11737400
C	0.12669591	-3.52028227	-0.79962676
C	-1.71957447	-3.08015919	0.71138077
C	-2.12485487	-2.32066545	1.75821630
C	-0.30330961	-3.56575266	0.63733794
C	2.36402150	-2.79503834	-0.03334306
C	-3.45331481	0.60109001	-0.18032328
C	-3.02399304	0.64471064	-1.61719467
C	-2.25799412	1.66887990	-2.06556719
C	-1.83760203	2.75806615	-1.12343305
C	1.58695836	0.47903953	-3.13810231
C	2.74075392	-0.02786804	-2.32486689
C	3.16166183	1.06229229	-1.38389487
C	-1.15528301	-1.96269373	2.84359107
C	0.57454087	-3.23914743	1.61684809
C	0.12671924	-2.39601303	2.77279499
C	0.98585744	-0.20422606	3.53161324
C	1.83637696	0.92867296	3.03949056
C	1.24867187	-1.47178018	3.13167786

C	2.86766968	0.68359124	2.19505810
C	3.16093870	-0.71969858	1.75676561
C	1.97526447	-2.83489780	1.26433098
C	2.39176989	-1.74314035	2.20178588

For complex **1**⊃C_{70}:

H	2.93334861	1.62842249	-7.28959282
C	1.90209767	1.92312770	-7.10552561
H	2.38270057	3.84188721	-6.29569687
C	1.59711933	3.13271952	-6.55926286
C	-0.44802728	1.32465623	-7.23929077
C	0.22600758	3.51660439	-6.30706244
C	0.85747453	0.99835622	-7.44822180
C	-0.81532821	2.59943078	-6.66288392
C	-0.10400286	4.75670777	-5.72095805
H	1.13893771	0.03588753	-7.87238308
H	-1.24562398	0.62456319	-7.48894379
C	-1.45067614	5.09400646	-5.46645771
C	-1.81765649	6.34099095	-4.83342593
C	-2.49257502	4.18350324	-5.83484980
H	-4.65106267	3.85486713	-5.84339352
C	-2.15944064	2.95720408	-6.44347184
C	-3.12131046	6.65376032	-4.59292382
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