Electronic Supplementary Information

A calix[3]carbazole-based cavitand: synthesis, structure and its complexation with fullerenes

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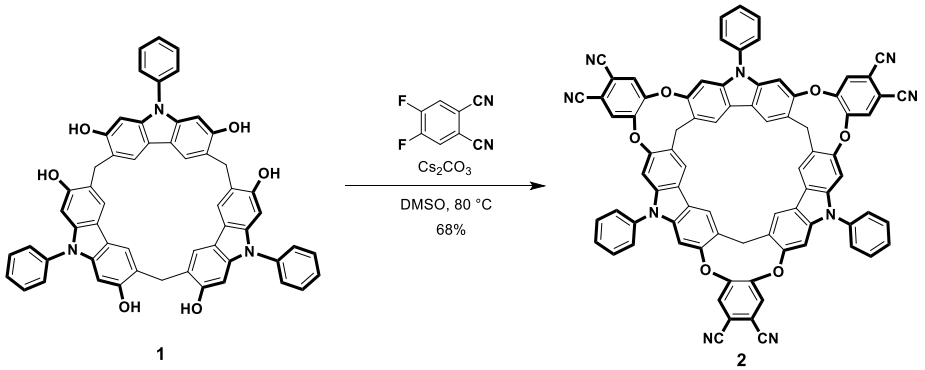
1. General information

All the reagents and solvents were commercially available and used without further purification. Unless otherwise stated, the reactions were carried out under inert and anhydrous conditions. Thin layer chromatography (TLC) was performed by silica gel GF_{254}. The melting point was determined by WRR melting point apparatus without correction. ^{1}H, ^{13}C NMR spectra were recorded on Bruker® AVIII 300 MHz NMR, Bruker® AVIII 500 MHz NMR and Bruker 700 MHz NMR spectrometers and reported in parts per million (ppm) from internal standard TMS. Matrix-Assisted Laser Desorption/Ionization Time-of-Flight (MALDI-TOF) mass spectrometry were recorded on the Autoflex III. Single crystal data were collected on a Bruker Smart APEXII CCD diffractometer using graphite monochromated CuKα radiation. Ultraviolet-visible spectra were recorded on PerkinElmer® UV/Vis/NIR spectrometer (Lambda 950), and fluorescence spectra and transient photoluminance decay characteristics were measured using the Edinburgh Instruments FLS1000 spectrometer. Based on density functional theory (DFT), the structures were optimized by using the B3LYP functional and 6-31G(d) basis set carried out by Gaussian 16 program.[S1]

2. Synthesis and characterization

The synthetic procedures of calix[3]carbazole **1** were described in the literatures.[S2, S3]



1 2

Calix[3]carbazole-based deep cavitand (**2**): To a solution of **1** (172 mg, 0.2 mmol) and Cs_2CO_3 (1.303 g, 4 mmol) in anhydrous dimethyl sulfoxide (20 mL) was added 4,5-difluorophthalonitrile (148 mg, 0.9 mmol) under argon. The mixture was stirred and heated at 80 °C for 24 hours. Then the reaction was quenched by the addition of water (50 mL), and extracted with dichloromethane (3 × 100 mL). The combined organic layer was dried with anhydrous $MgSO_4$, and concentrated under a reduced pressure

to give a crude solid. The solid was purified by column chromatography with CH_2Cl_2 as the eluent to give **2** as light yellow solid (167 mg, 68 %). M.p.: > 280 °C. ^{1}H NMR (300 MHz, $CDCl_3$, 298K): δ 7.99 (s, 6H), 7.62 (s, 6H), 7.57 (t, *J* = 7.2 Hz, 6H), 7.47 (t, *J* = 7.4 Hz, 3H), 7.39 (d, *J* = 8.2 Hz, 6H), 7.09 (s, 6H), 4.67 (d, *J* = 13.1 Hz, 3H), 3.89 (d, *J* = 13.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$, 298 K): δ 153.7, 141.6, 136.8, 130.5, 128.6, 126.6, 122.3, 120.9, 114.7, 112.4, 102.4, 29.9. MALDI-TOF MS: *m/z* calcd for [M] $C_{81}H_{39}N_9O_6$: 1233.3023; found: 1233.3021.

3. NMR and mass spectra of 2

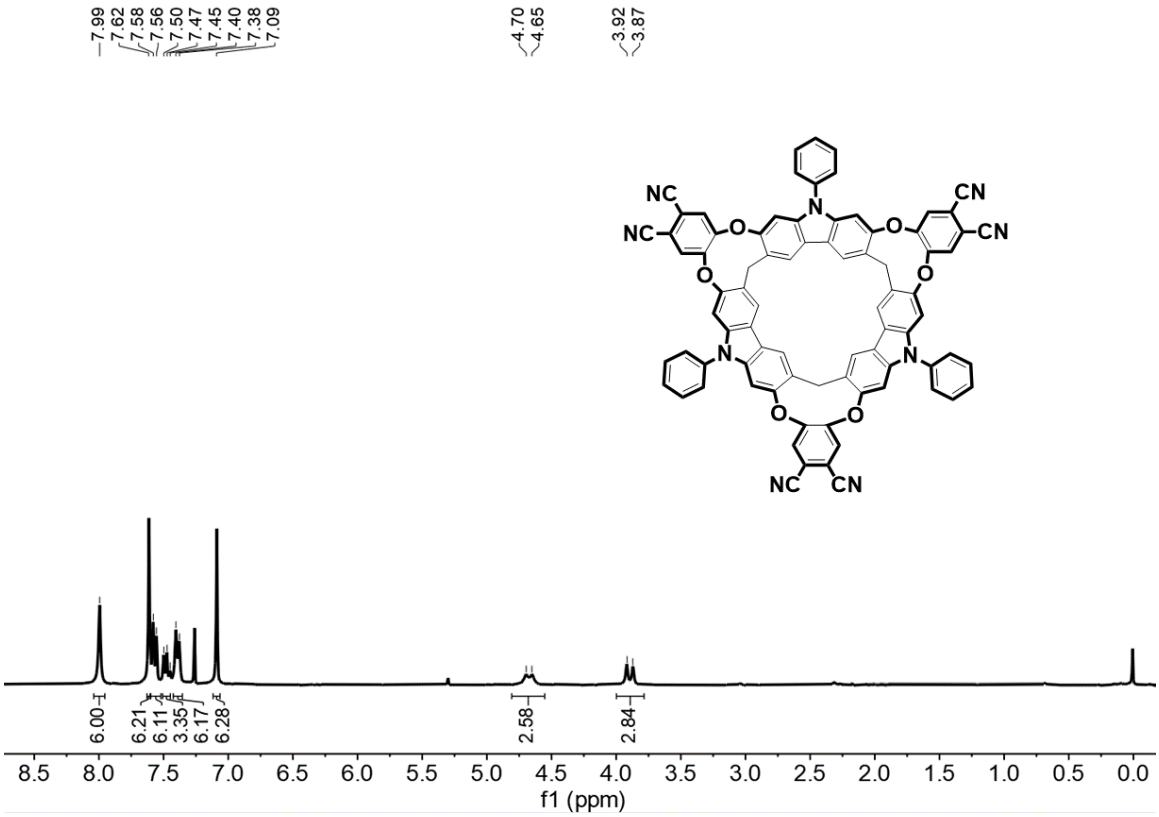


Fig. S1 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298K) of **2**.

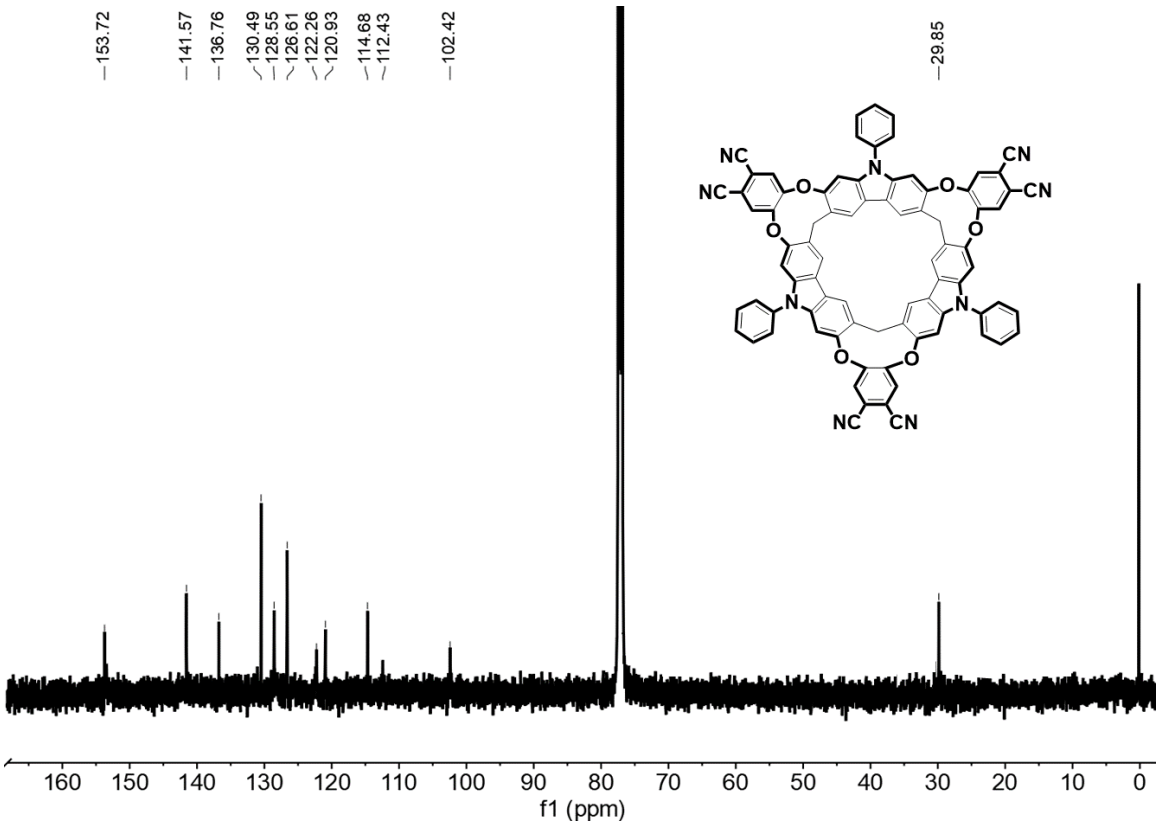


Fig. S2 ^{13}C NMR spectrum (126 MHz, $CDCl_3$, 298K) of **2**.

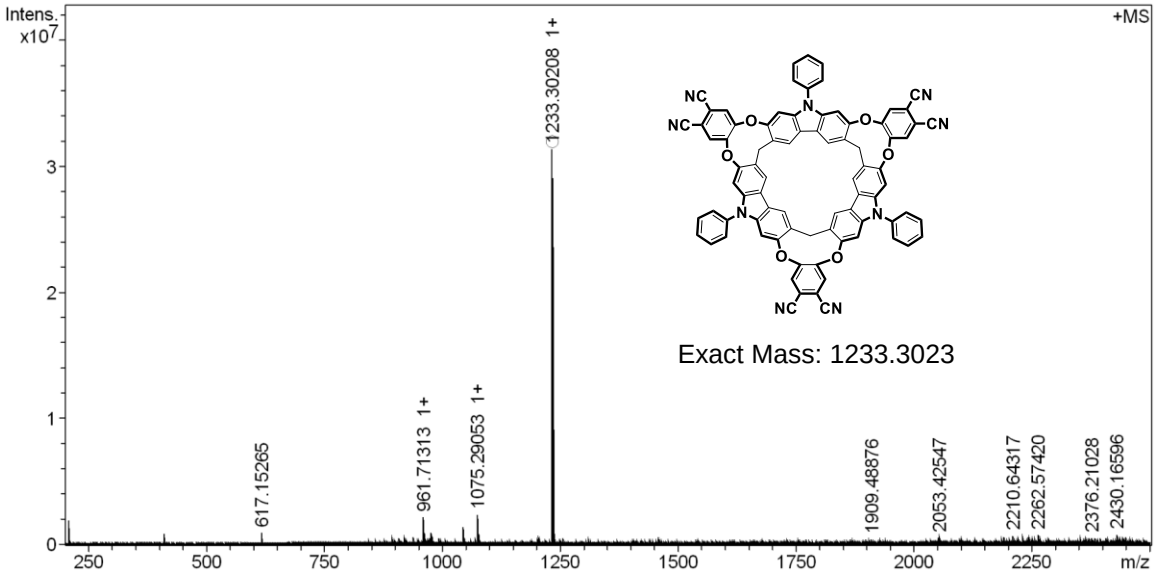


Fig. S3 MALDI-TOF mass spectrum of **2**.

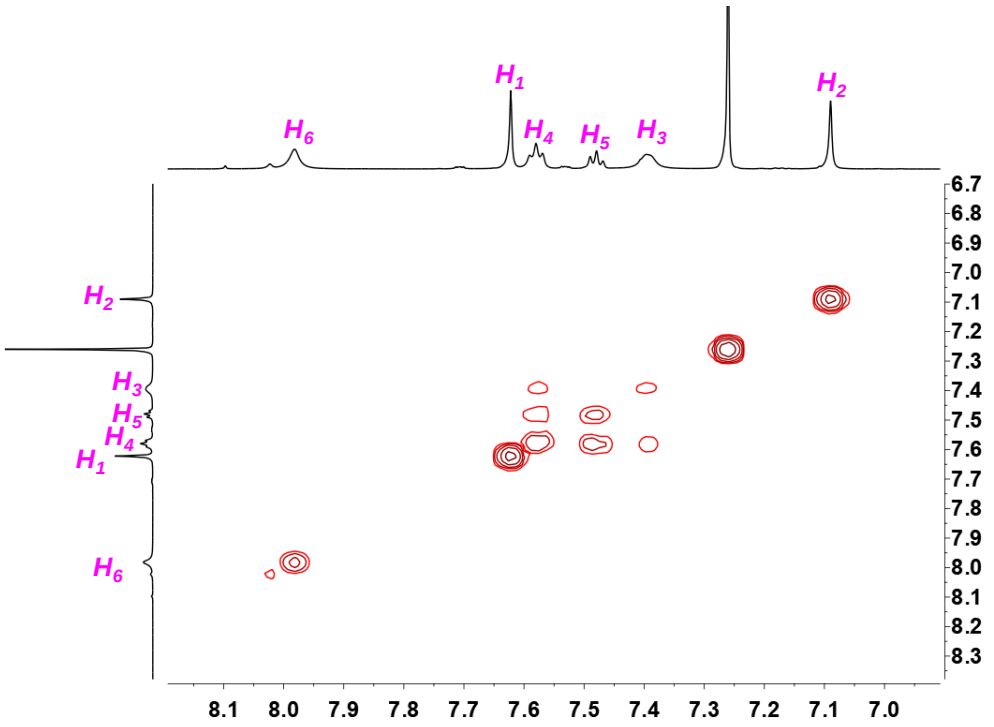


Fig. S4 ^{1}H-^{1}H COSY spectrum (700 MHz, $CDCl_3$, 298 K) of **2**.

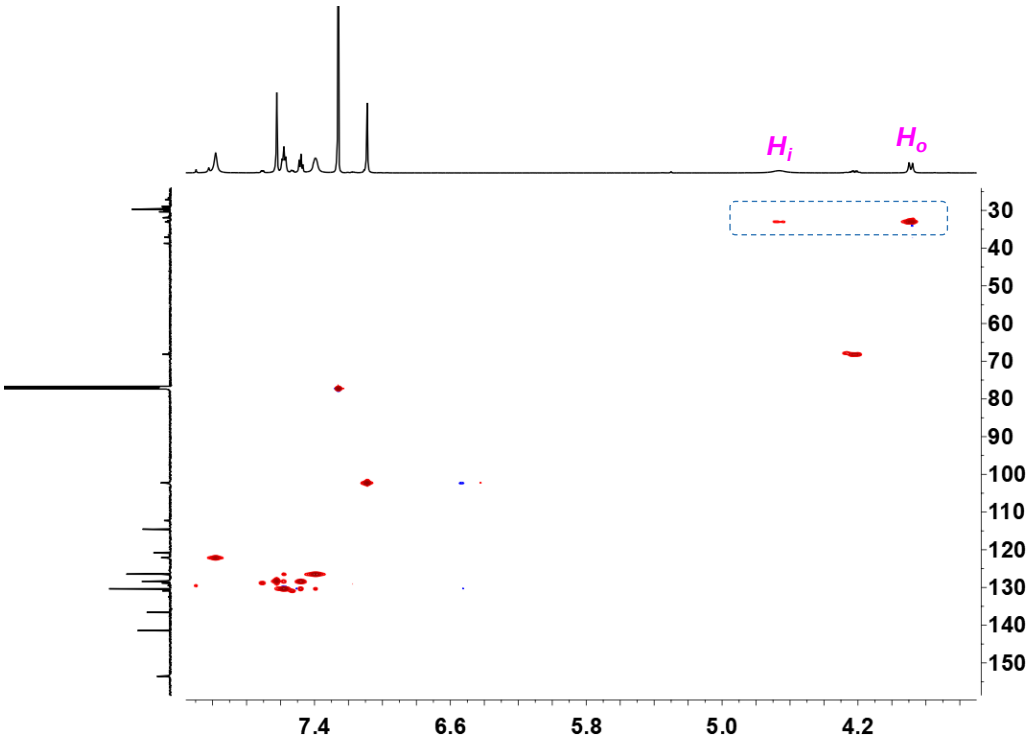


Fig. S5 ^{1}H-^{13}C HSQC spectrum (700 MHz, $CDCl_3$, 298 K) of **2**.

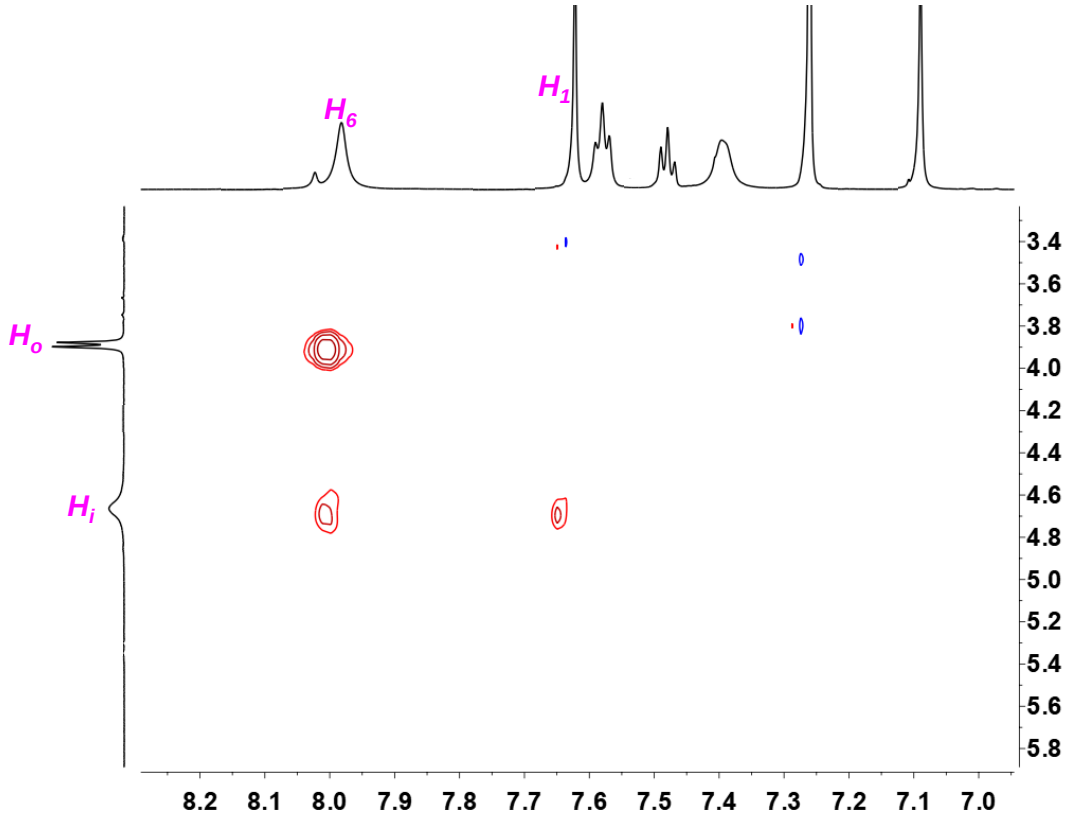


Fig. S6 2D NOESY spectrum (700 MHz, $CDCl_3$, 298 K) of **2**.

4. X-ray crystal structures and crystallographic data

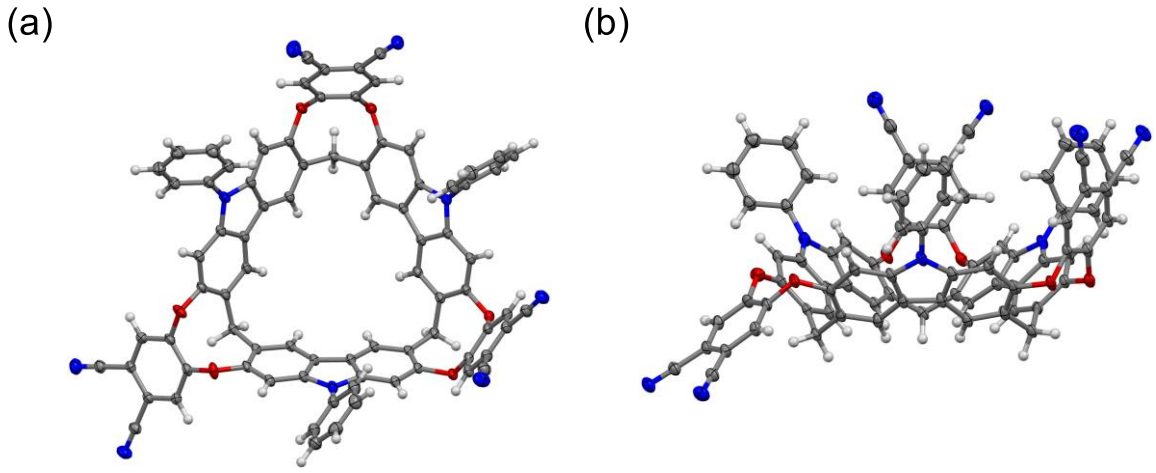


Fig. S7 ORTEP drawing of **2-c1** from (a) top view and (b) side view (the thermal ellipsoids are displayed at a 30 % probability).

Table S1. X-ray crystallographic and the refinement data of **2-c1**.

CCDC	2305712
Empirical formula	$C_{81}H_{39}N_9O_6$
Formula weight	1233.30
Temperature/K	169.99(10)
Crystal system	monoclinic
Space group	$P2_1/m$
a/Å	12.7611(3)
b/Å	18.5038(3)
c/Å	14.1018(3)
α/°	90
β/°	100.643(2)
γ/°	90
Volume/Å^3	3272.56(12)
Z	4
ρcalcg/cm^3	1.394
μ/mm^{-1}	0.959
F(000)	1415.0
Crystal size/mm^3	0.33 × 0.26 × 0.14
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.378 to 151.102
Index ranges	-16 ≤ h ≤ 15, -19 ≤ k ≤ 23, -17 ≤ l ≤ 17
Reflections collected	25286
Independent reflections	6729 [R_{int} = 0.0449, R_{sigma} = 0.0362]
Data/restraints/parameters	6729/0/445
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0457, wR_2 = 0.1254
Final R indexes [all data]	R_1 = 0.0602, wR_2 = 0.1341
Largest diff. peak/hole / e Å^{-3}	0.26/-0.27

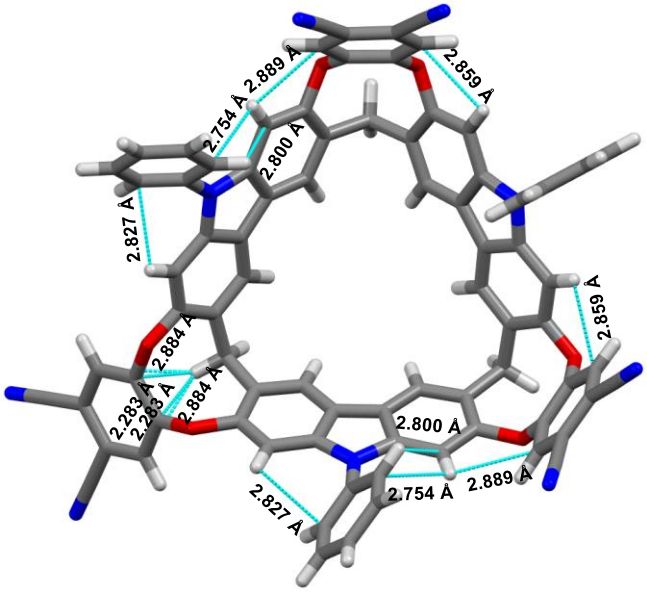


Fig. S8 The multiple intramolecular C-H···π interactions of **2-c1**.

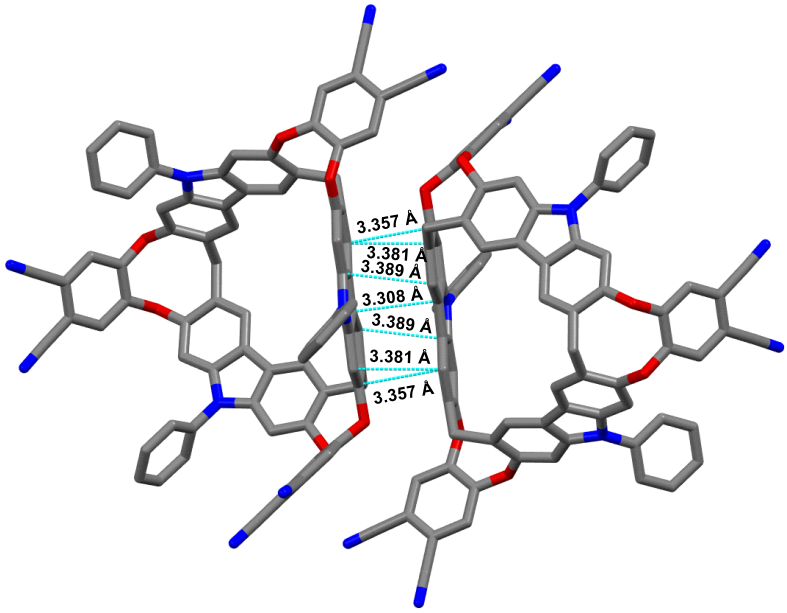


Fig. S9 The multiple intermolecular π···π interactions of two **2-c1** molecules.

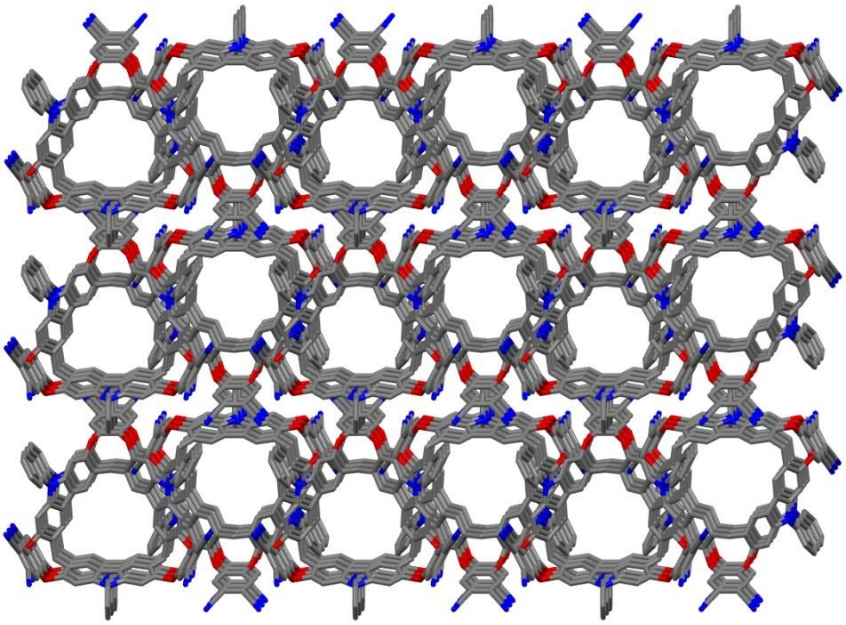


Fig. S10 The packing mode of **2-c1** viewed along *a* axis.

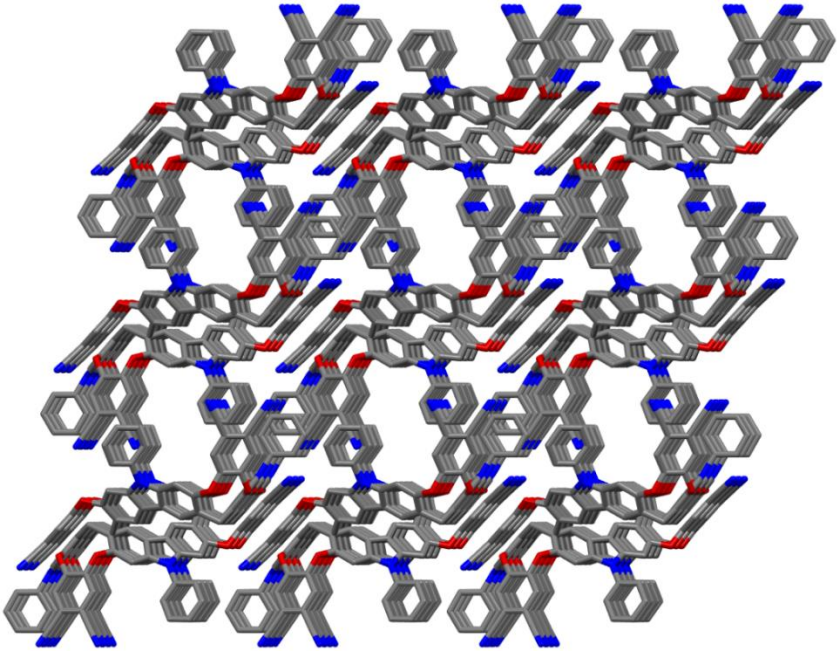


Fig. S11 The packing mode of **2-c1** viewed along *b* axis.

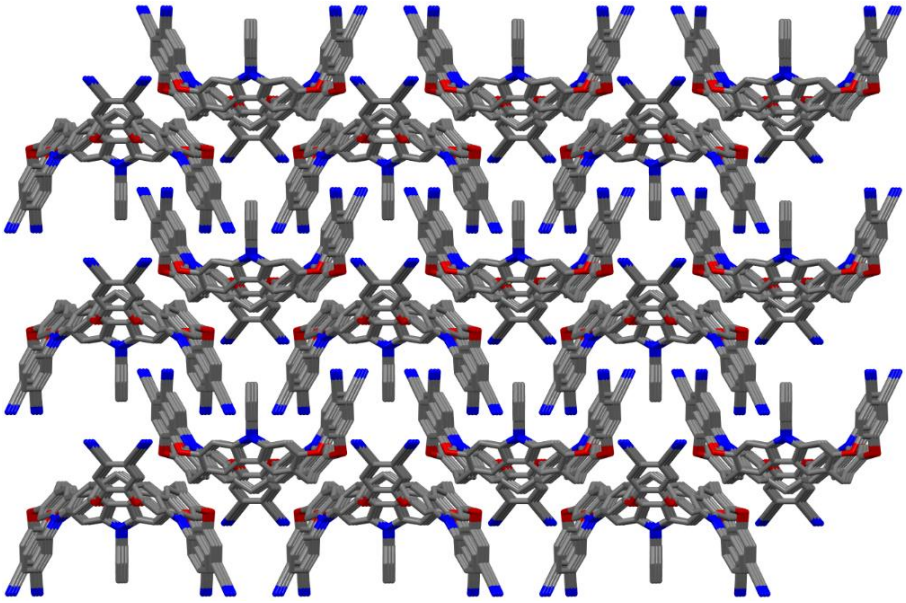


Fig. S12 The packing mode of **2-c1** viewed along *c* axis.

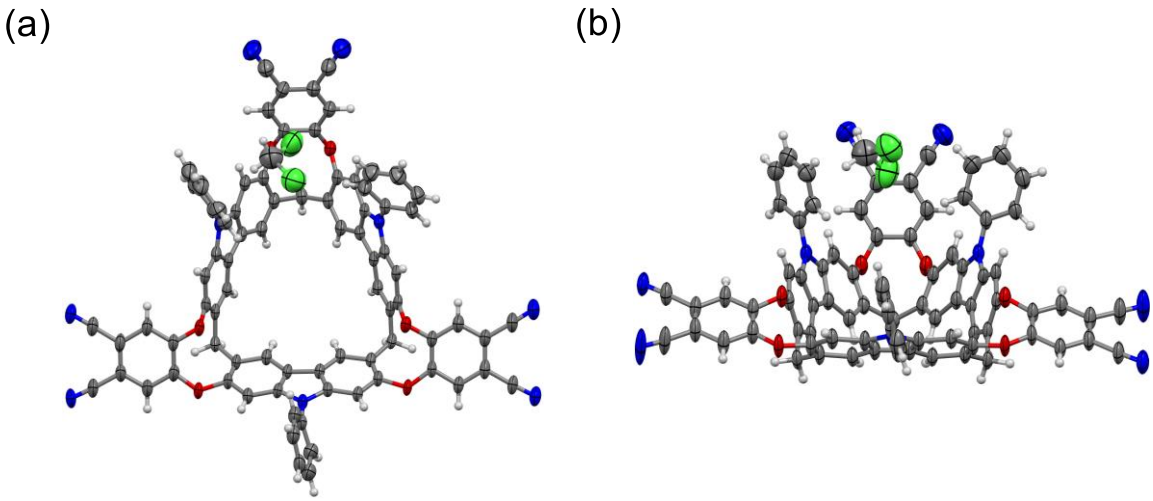


Fig. S13 ORTEP drawing of **2-c2** from (a) top view and (b) side view (the thermal ellipsoids are displayed at a 30 % probability).

Table S2. X-ray crystallographic and the refinement data of **2-c2**.

CCDC	2305713
Empirical formula	$C_{82}H_{41}Cl_2N_9O_6$
Formula weight	1317.26
Temperature/K	169.98(10)
Crystal system	monoclinic
Space group	*I2/a*
a/Å	30.8326(16)
b/Å	13.5754(7)
c/Å	31.1005(15)
α/°	90
β/°	106.960(6)
γ/°	90
Volume/Å^3	12451.4(12)
Z	8
ρcalcg/cm^3	1.359
μ/mm^{-1}	1.059
F(000)	5243.0
Crystal size/mm^3	0.3 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.942 to 152.224
Index ranges	-38 ≤ h ≤ 38, -16 ≤ k ≤ 16, -39 ≤ l ≤ 38
Reflections collected	80263
Independent reflections	12769 [R_{int} = 0.0935, R_{sigma} = 0.0458]
Data/restraints/parameters	12769/282/975
Goodness-of-fit on F^2	1.532
Final R indexes [I>=2σ (I)]	R_1 = 0.1210, wR_2 = 0.2740
Final R indexes [all data]	R_1 = 0.1954, wR_2 = 0.3023
Largest diff. peak/hole / e Å^{-3}	0.54/-0.46

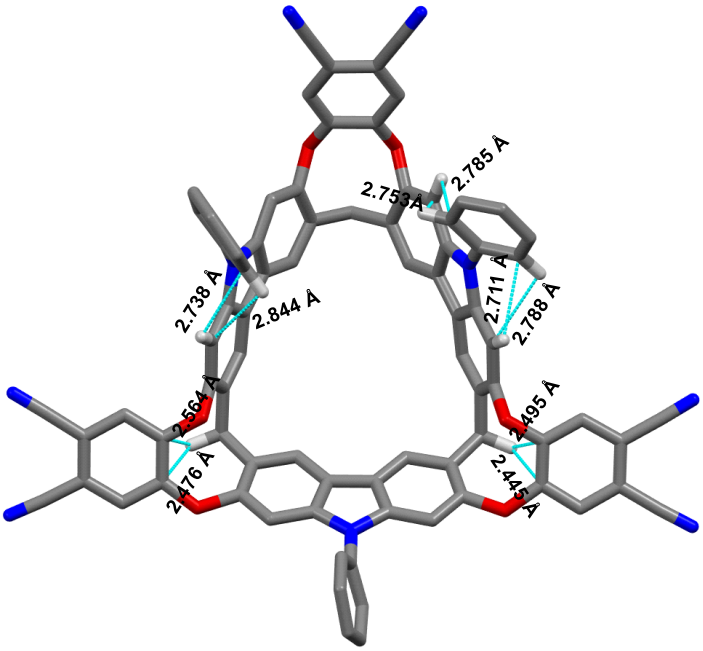


Fig. S14 The multiple intramolecular C-H···π interactions of **2-c2**.

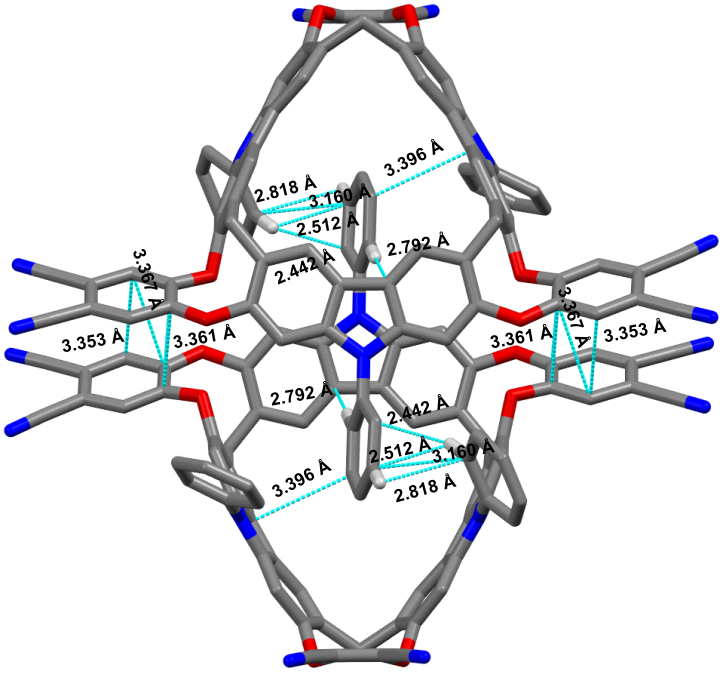


Fig. S15 The multiple intermolecular π···π and C-H···π interactions of two **2-c2** molecules.

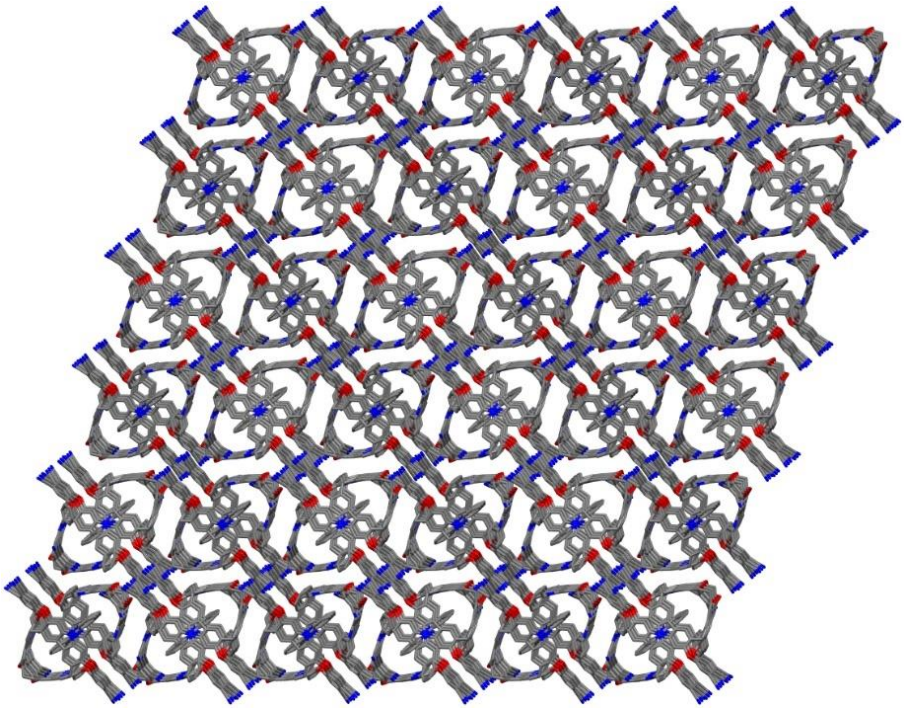


Fig. S16 The packing mode of **2-c2** viewed along *b* axis.

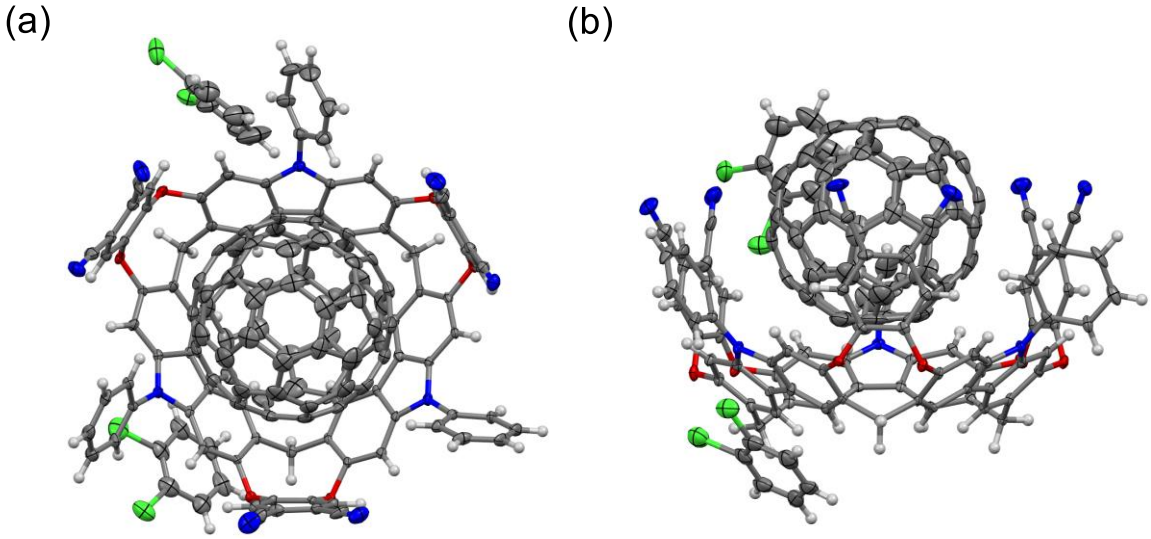


Fig. S17 ORTEP drawing of **C_{60}@2** from (a) top view and (b) side view (the thermal ellipsoids are displayed at a 30 % probability).

Table S3. X-ray crystallographic and the refinement data of **C_{60}@2**

CCDC	2305715
Empirical formula	$C_{153}H_{47}Cl_4N_9O_6$
Formula weight	2248.79
Temperature/K	169.98(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.0791(4)
b/Å	32.0488(9)
c/Å	27.0224(9)
α/°	90
β/°	94.916(3)
γ/°	90
Volume/Å^3	11285.3(6)
Z	4
ρcalcg/cm^3	1.324
μ/mm^{-1}	1.493
F(000)	4576.0
Crystal size/mm^3	0.45 × 0.35 × 0.31
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.286 to 152.546
Index ranges	-16 ≤ h ≤ 16, -39 ≤ k ≤ 23, -33 ≤ l ≤ 33
Reflections collected	80169
Independent reflections	22551 [R_{int} = 0.0963, R_{sigma} = 0.0906]
Data/restraints/parameters	22551/633/1550
Goodness-of-fit on F^2	1.512
Final R indexes [I>=2σ (I)]	R_1 = 0.1425, wR_2 = 0.4056
Final R indexes [all data]	R_1 = 0.1961, wR_2 = 0.4366
Largest diff. peak/hole / e Å^{-3}	2.07/-1.08

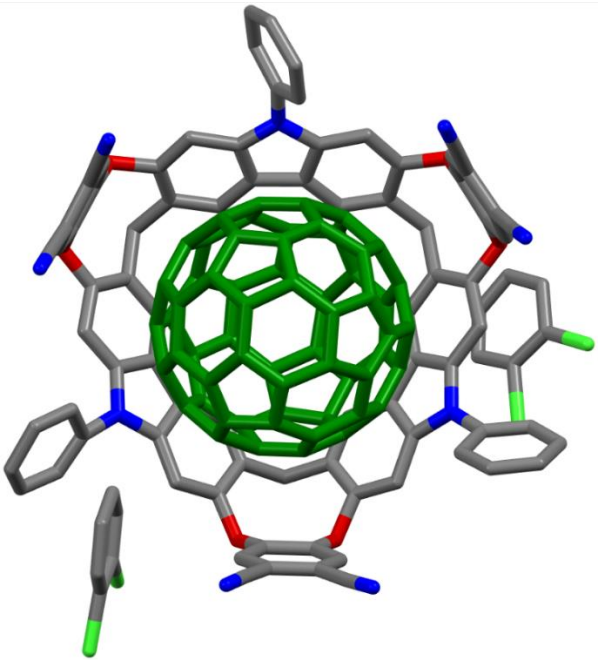


Fig. S18 Crystal structure of complex **C_{60}@2** with two *o*-DCBs around from top view.

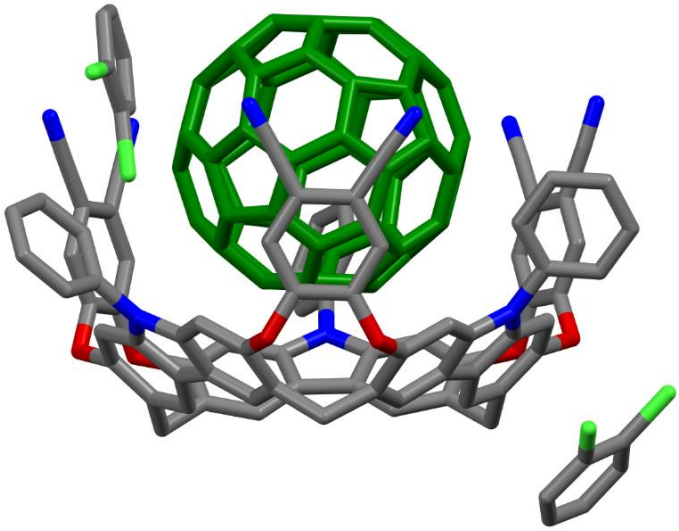


Fig. S19 Crystal structure of complex **C_{60}@2** with two *o*-DCBs around from side view.

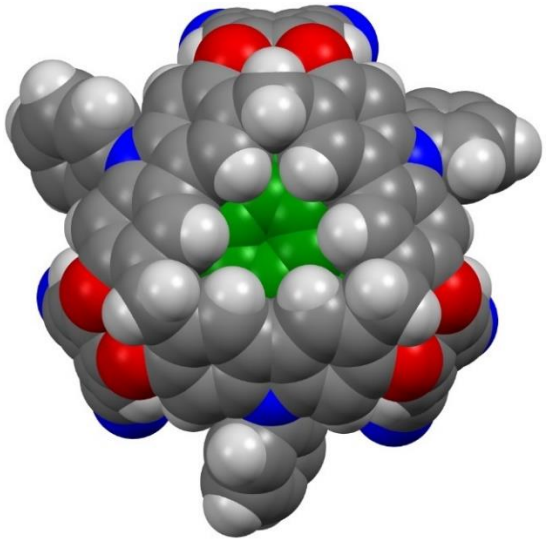


Fig. S20 Space-filling model of the 1:1 complexation between **2** and C_{60} from top view.

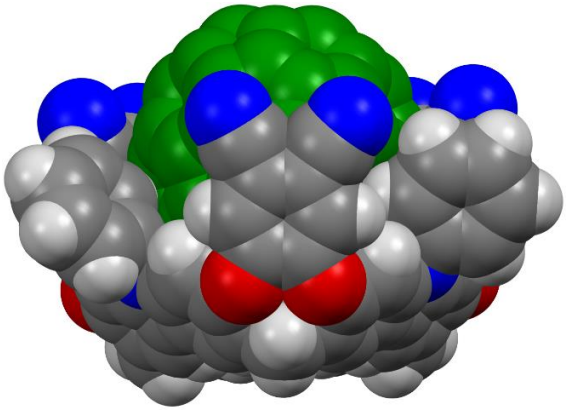


Fig. S21 Space-filling model of the 1:1 complexation between **2** and C_{60} from side view.

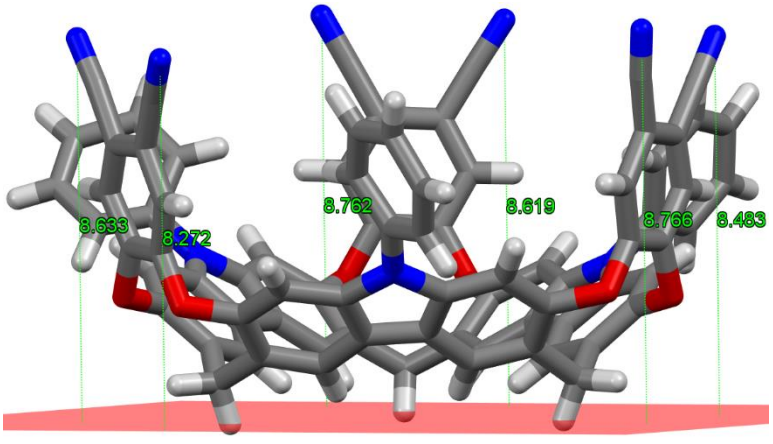


Fig. S22 Side view of **2** showing the cavity depth.

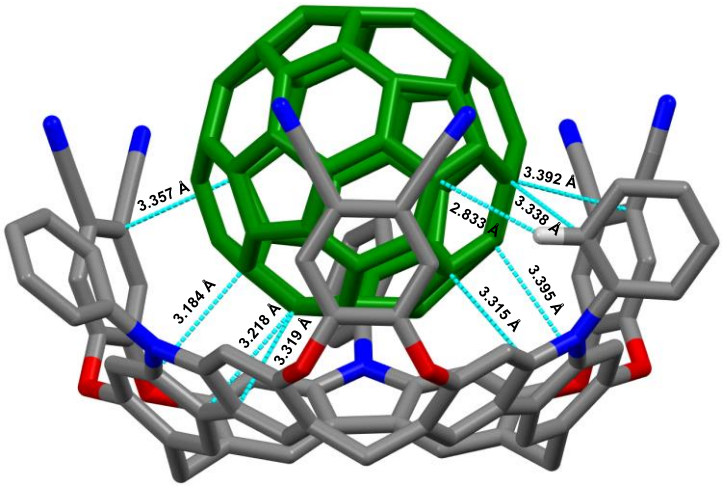


Fig. S23 The multiple intermolecular interactions between **2** and encapsulated C_{60} molecule.

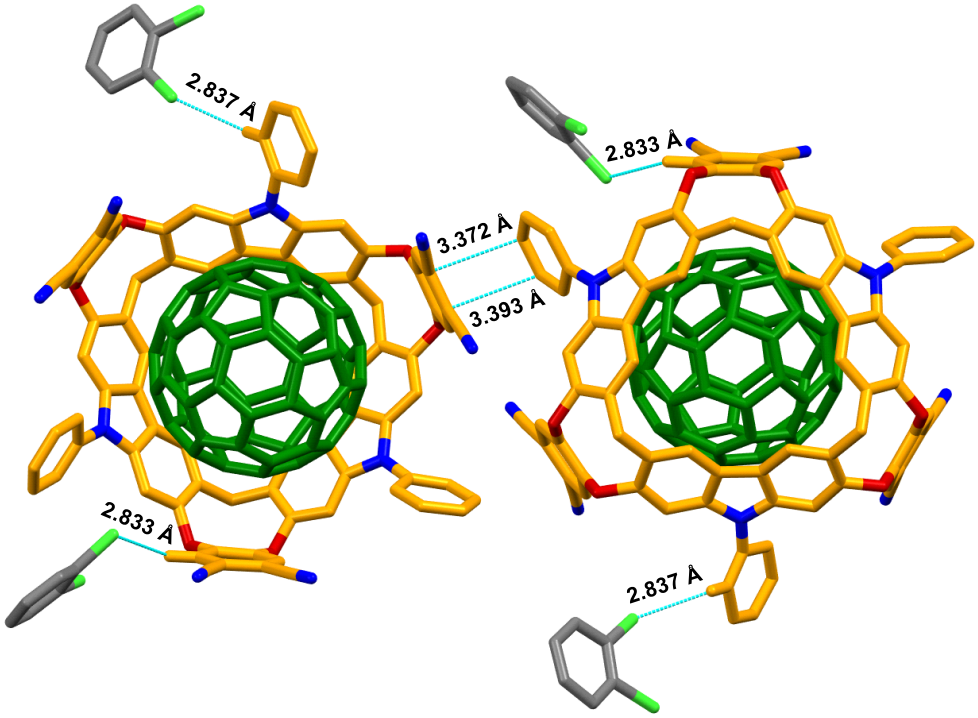


Fig. S24 Intermolecular interactions between the adjacent complexes **C_{60}@2** and four *o*-DCBs.

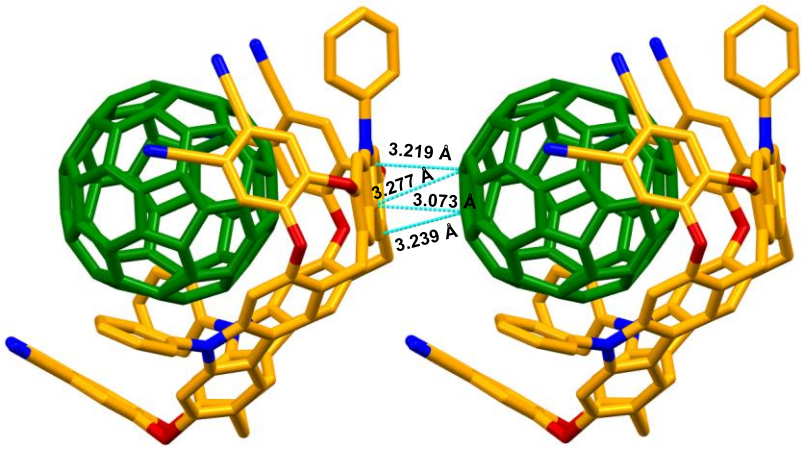


Fig. S25 The multiple intermolecular π···π interactions of two adjacent complexes **C_{60}@2**.

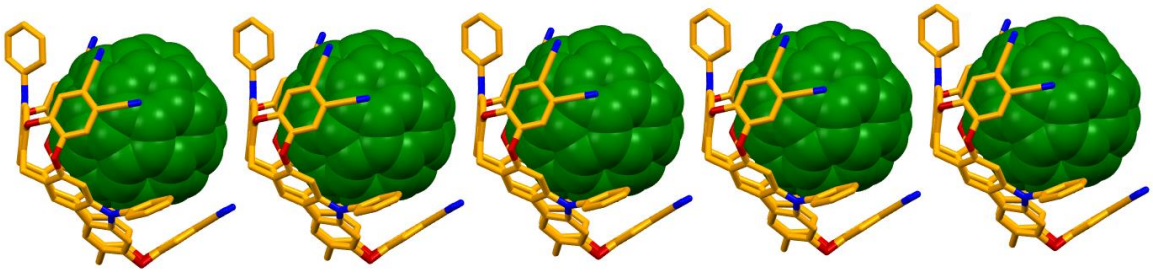


Fig. S26 The ordered packing mode of complexes **C_{60}@2**.

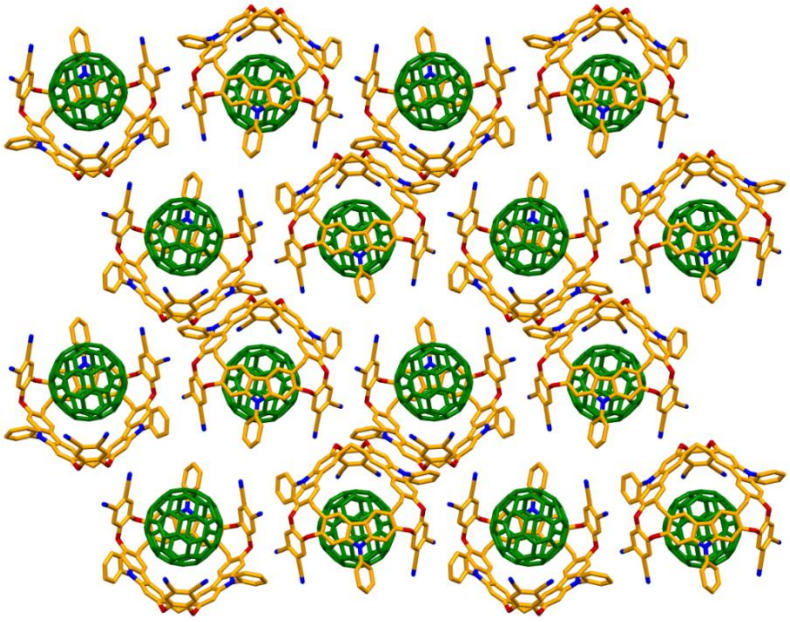


Fig. S27 The packing mode of complexes **C_{60}@2** viewed along *a* axis.

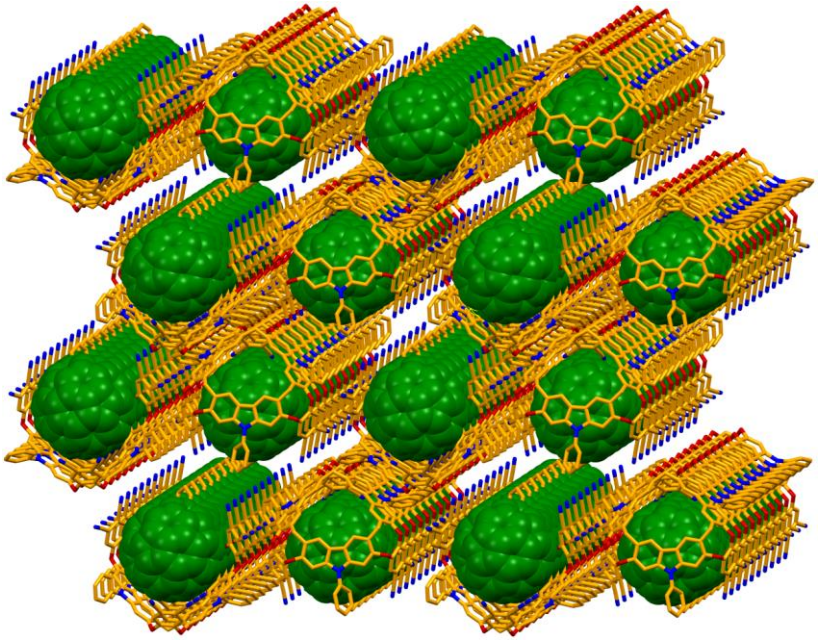


Fig. S28 The tubular packing structure of complexes **C_{60}@2**.

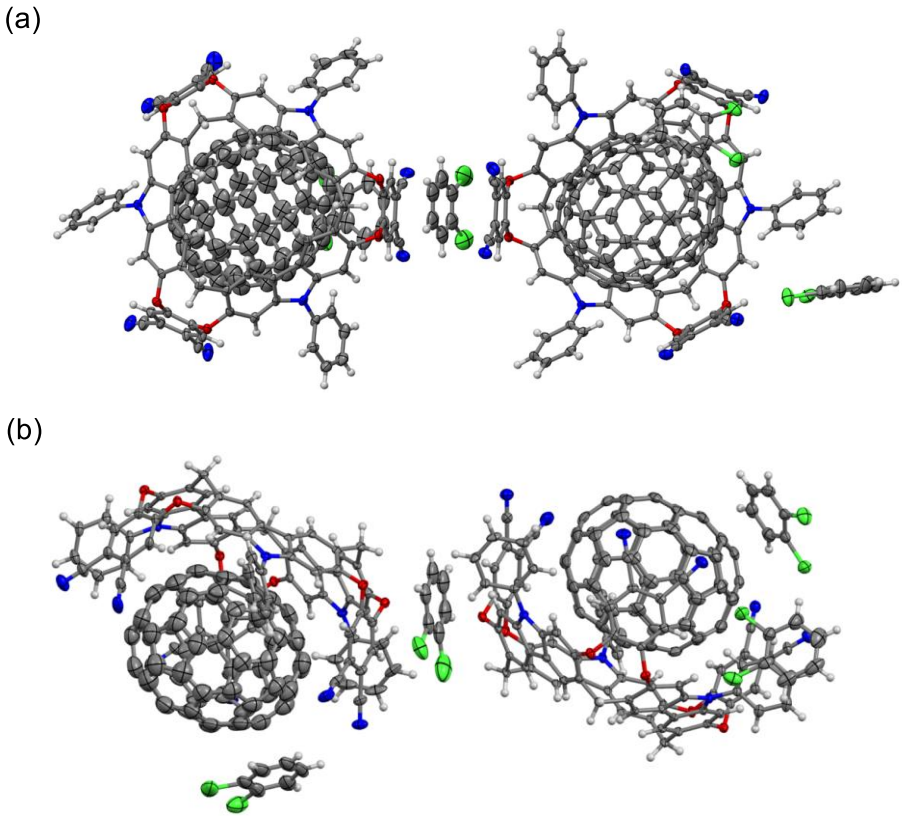


Fig. S29 ORTEP drawing of **C_{70}@2** from (a) top view and (b) side view (the thermal ellipsoids are displayed at a 30 % probability).

Table S4. X-ray crystallographic and the refinement data of **C_{70}@2**

CCDC	2305716
Empirical formula	$C_{163}H_{47}Cl_4N_9O_6$
Formula weight	2368.89
Temperature/K	169.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	26.5926(7)
b/Å	32.9430(7)
c/Å	30.1206(12)
α/°	90
β/°	113.007(4)
γ/°	90
Volume/Å^3	24288.0(14)
Z	8
ρcalcg/cm^3	1.296
μ/mm^{-1}	1.417
F(000)	9632.0
Crystal size/mm^3	0.42 × 0.39 × 0.37
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.498 to 152.092
Index ranges	$-32 \le h \le 32$, $-30 \le k \le 41$, $-37 \le l \le 37$
Reflections collected	175708
Independent reflections	48649 [R_{int} = 0.1184, R_{sigma} = 0.1032]
Data/restraints/parameters	48649/1187/3277
Goodness-of-fit on F^2	1.395
Final R indexes [I>=2σ (I)]	R_1 = 0.1108, wR_2 = 0.2615
Final R indexes [all data]	R_1 = 0.2002, wR_2 = 0.2962
Largest diff. peak/hole / e Å^{-3}	0.96/-0.63

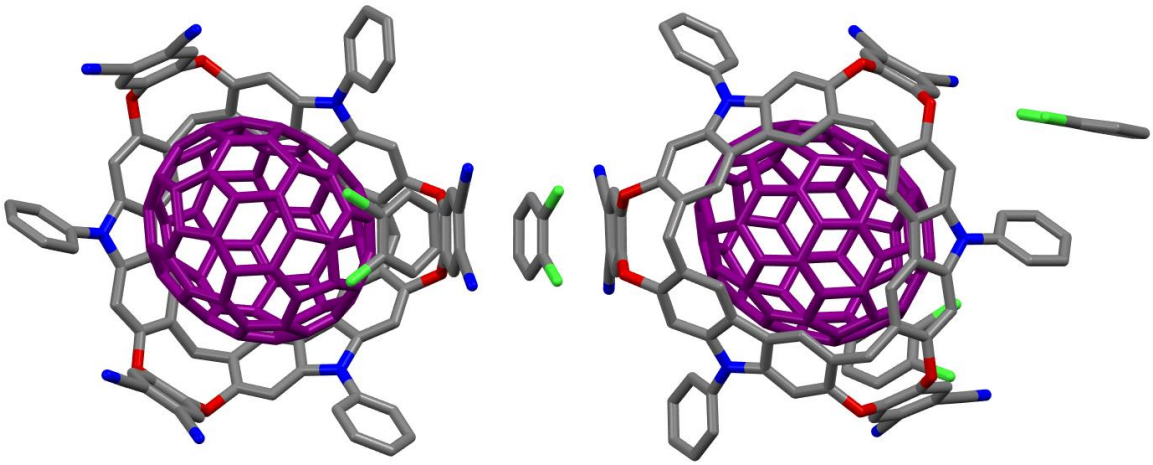


Fig. S30 Crystal structure of complexes **C_{70}@2** with four *o*-DCBs around from top view.

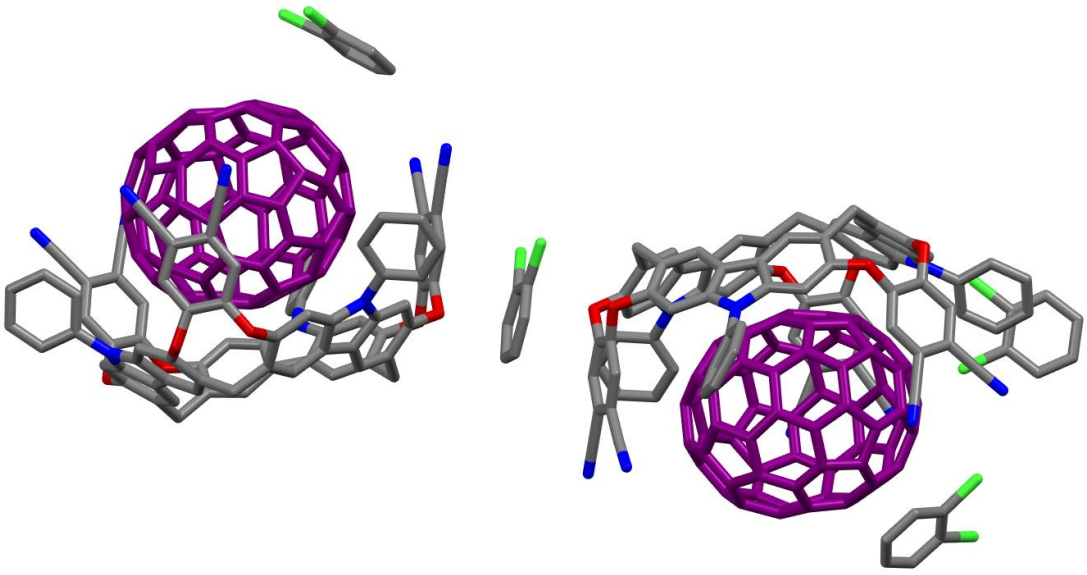


Fig. S31 Crystal structure of complexes **C_{70}@2** with four *o*-DCBs around from side view.

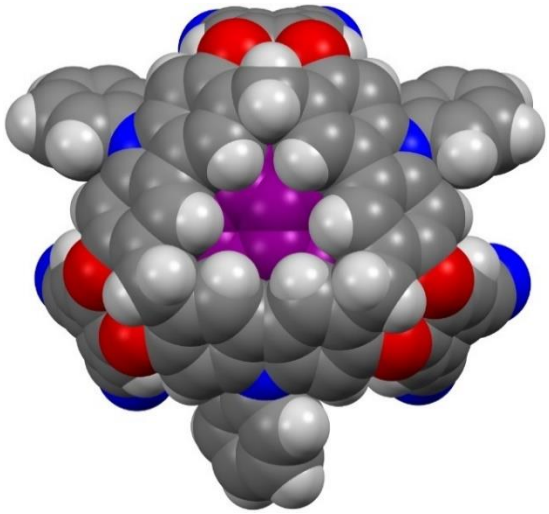


Fig. S32 Space-filling model of the 1:1 complexation between **2** and C_{70} from top view.

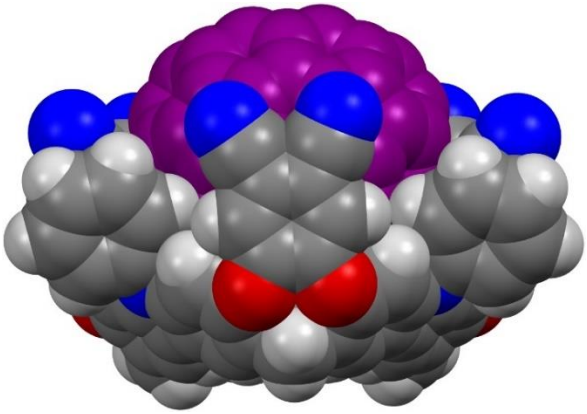


Fig. S33 Space-filling model of the 1:1 complexation between **2** and C_{70} from side view.

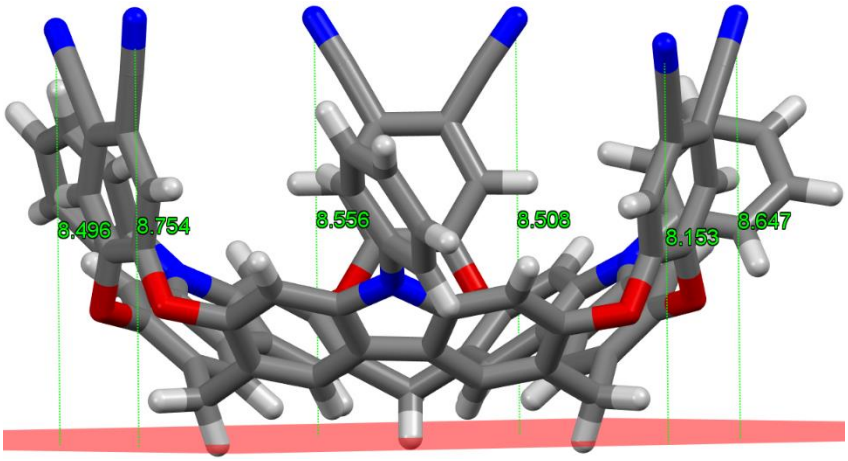


Fig. S34 Side view of **2** showing the cavity depth.

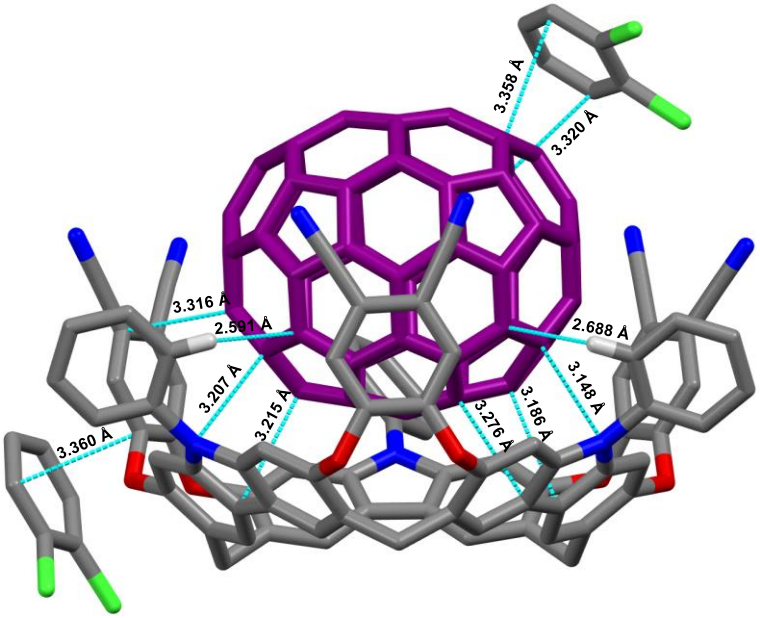


Fig. S35 The multiple intermolecular interactions between **2** and encapsulated C_{70} molecule and *o*-DCBs.

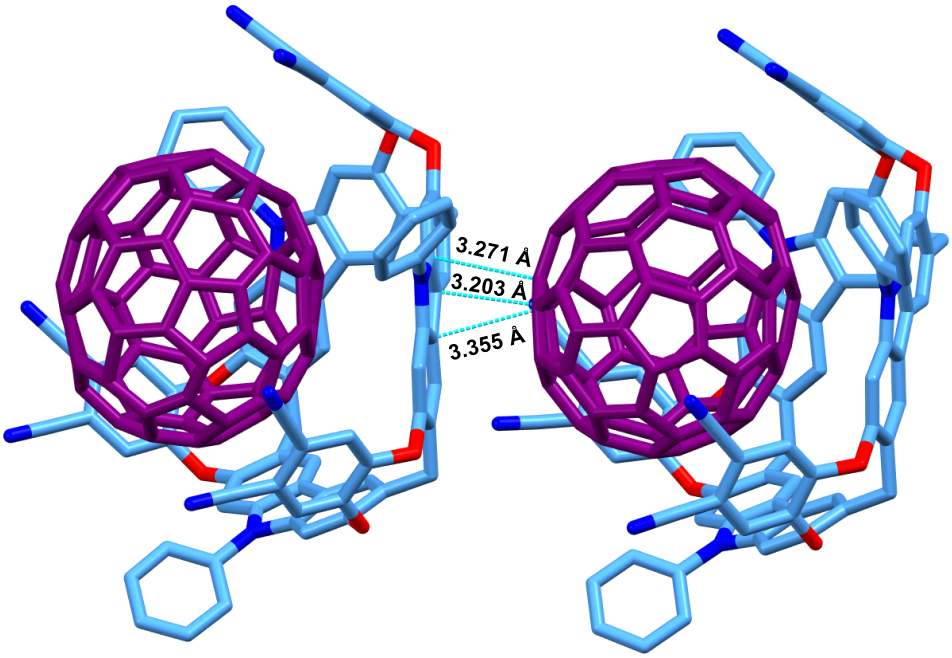


Fig. S36 The multiple intermolecular π···π interactions of two adjacent complexes **C_{70}@2**.

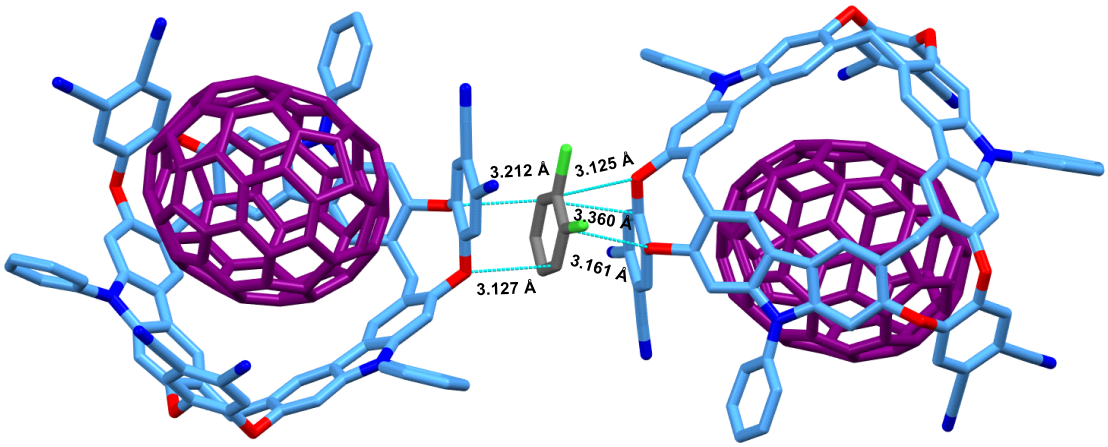


Fig. S37 The multiple intermolecular interactions between two adjacent complexes **C_{70}@2** and *o*-DCB.

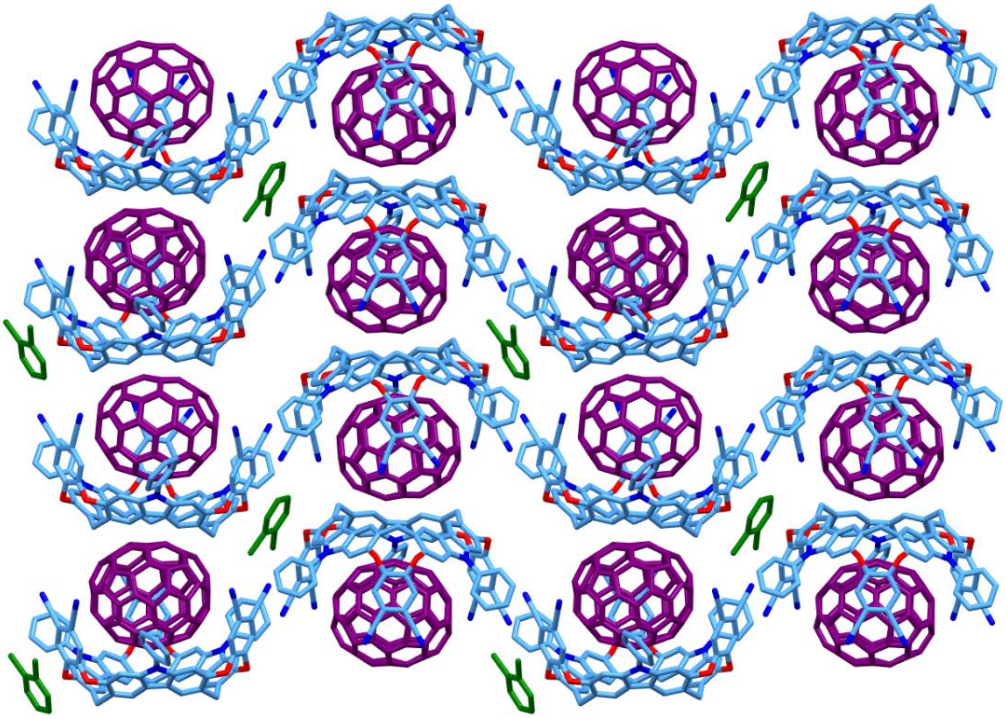


Fig. S38 The packing mode of complexes **C_{70}@2** containing *o*-DCBs viewed along *c* axis.

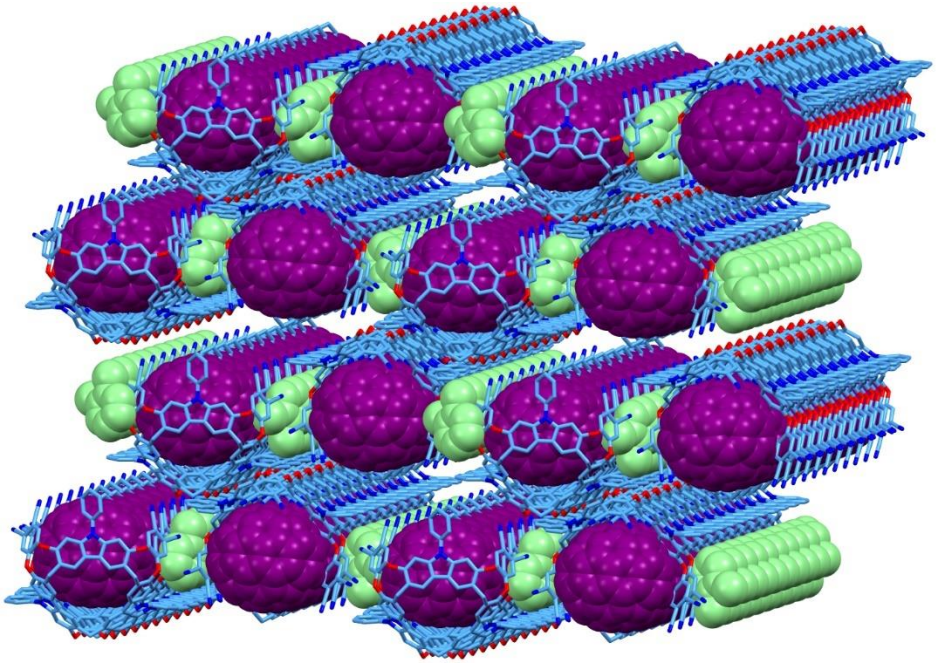


Fig. S39 The tubular packing structure of complexes **C_{70}@2** containing *o*-DCBs.

5. Photophysical properties

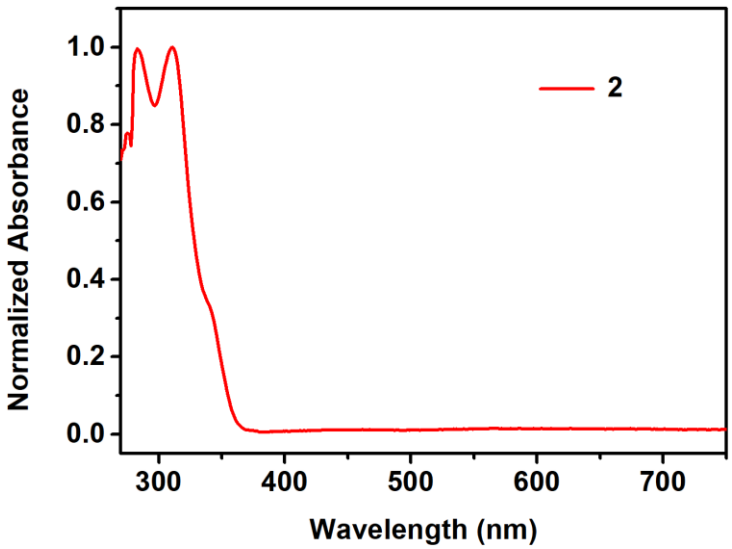


Fig. S40 UV-vis absorption spectrum of **2** (c = 1.0 ×10^{-5} M) in toluene at 298 K.

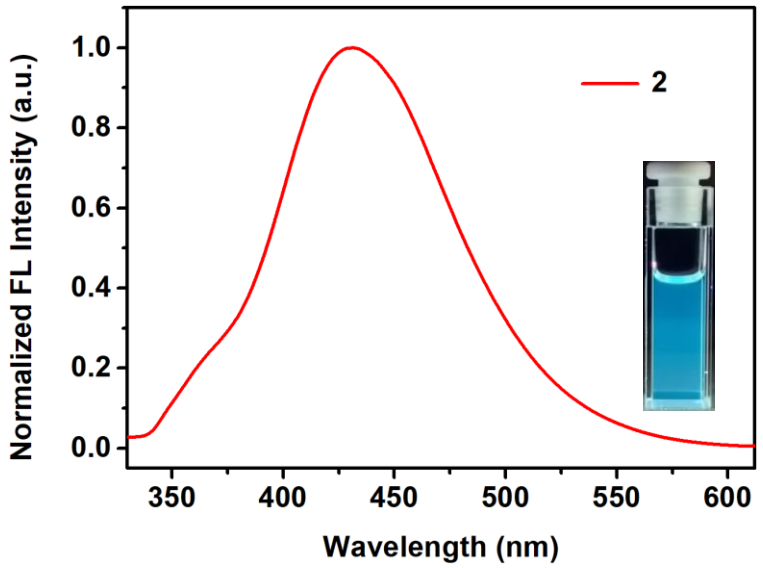


Fig. S41 Fluorescence spectrum of **2** (c = 1.0 ×10^{-5} M, excited at 311 nm) in toluene at 298 K.

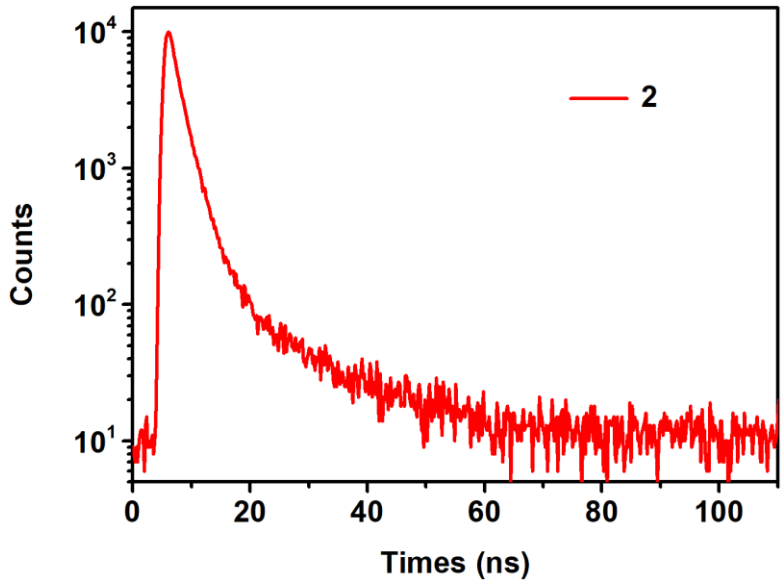


Fig. S42 Transient decay spectrum of **2** (c = 1.0×10^{-5} mol/L) in toluene at 298 K.

6. Electrochemical measurements

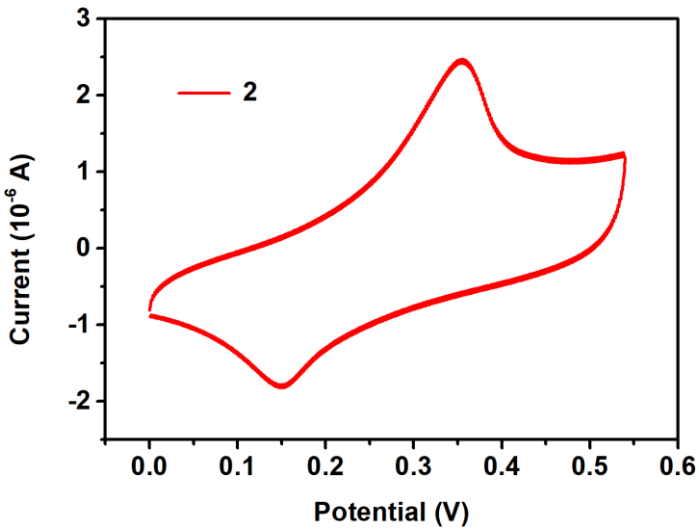


Fig. S43 Cyclic voltammogram of **2** in CH_2Cl_2 containing 0.1 M *n*-Bu_4NPF_6 at room temperature at a scan rate of 0.1 V/s.

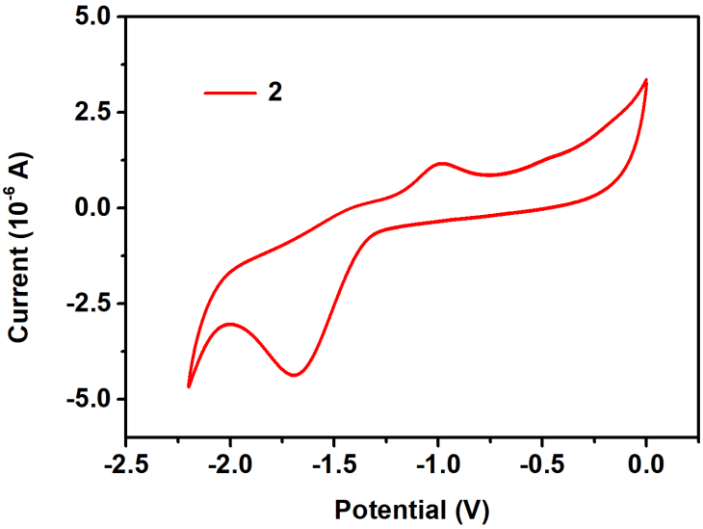


Fig. S44 Cyclic voltammogram of **2** in THF containing 0.1 M *n*-Bu_4NPF_6 at room temperature at a scan rate of 0.1 V/s.

7. UV-vis absorption spectra studies of complexations

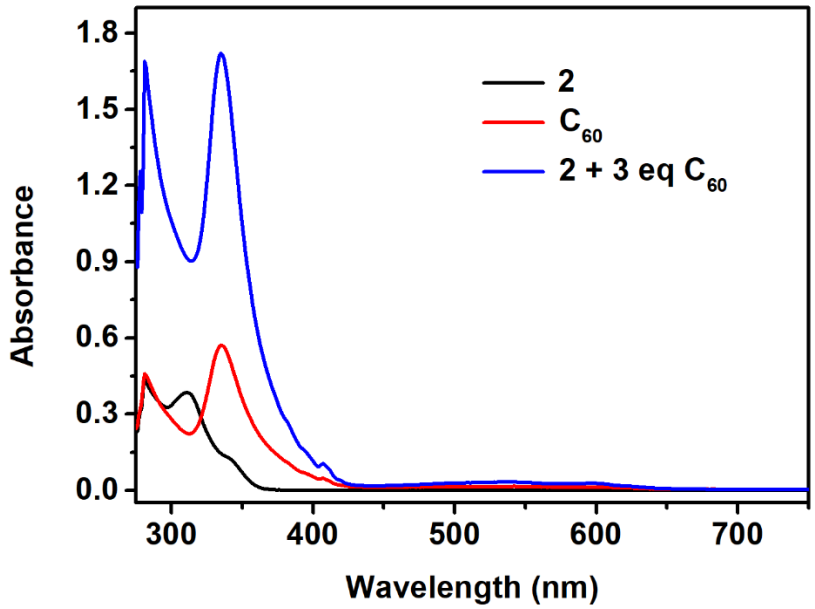


Fig. S45 UV-vis absorption spectra of C_{60} and **2** (1.0×10^{-5} M) in the absence and presence of C_{60} (3 equiv.) in toluene.

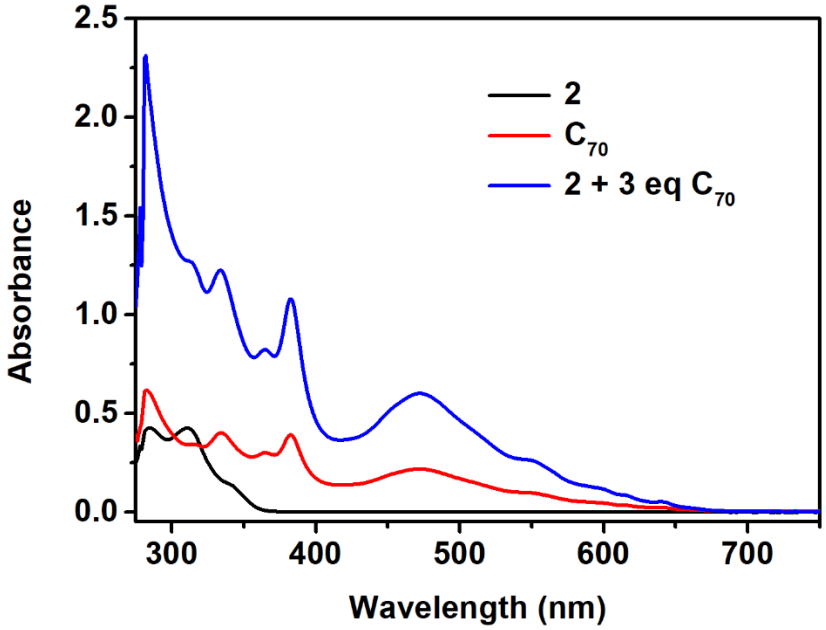


Fig. S46 UV-vis absorption spectra of C_{70} and **2** (1.0×10^{-5} M) in the absence and presence of C_{70} (3 equiv.) in toluene.

8. MALDI-TOF mass spectra studies of complexations

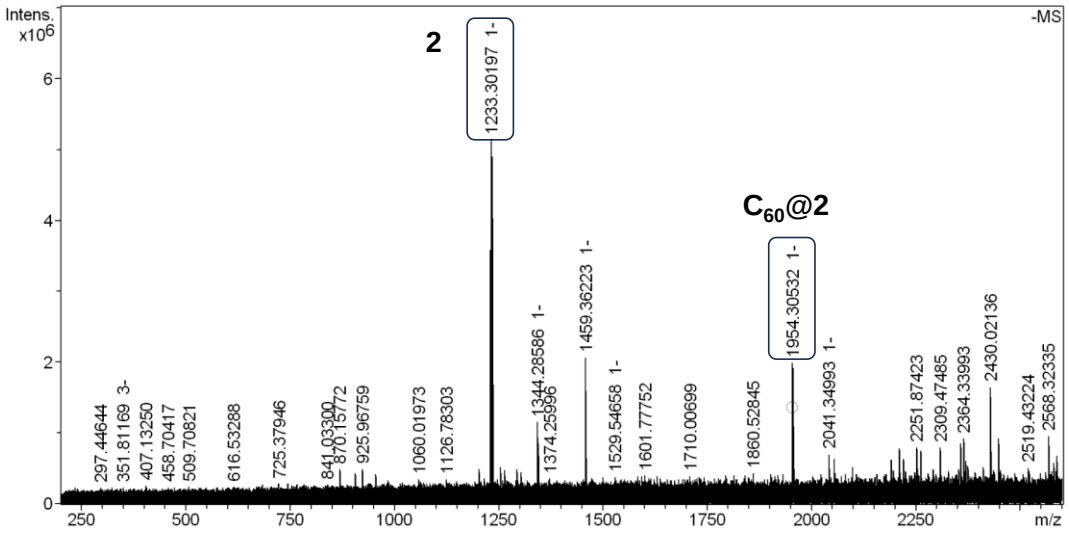


Fig. S47 MALDI-TOF mass spectrum of complex **C_{60}@2**.

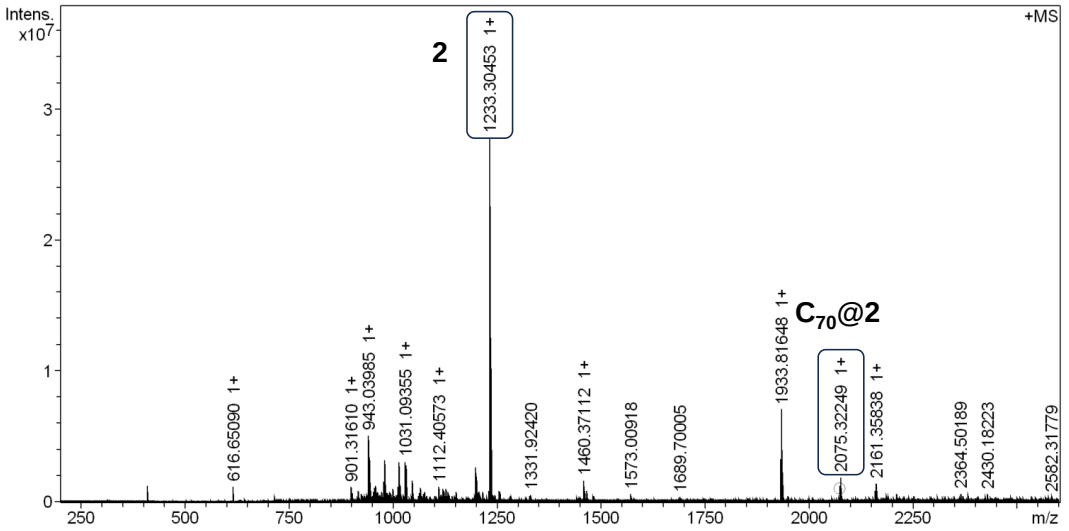


Fig. S48 MALDI-TOF mass spectrum of complex **C_{70}@2**.

9. Color changes of complexations

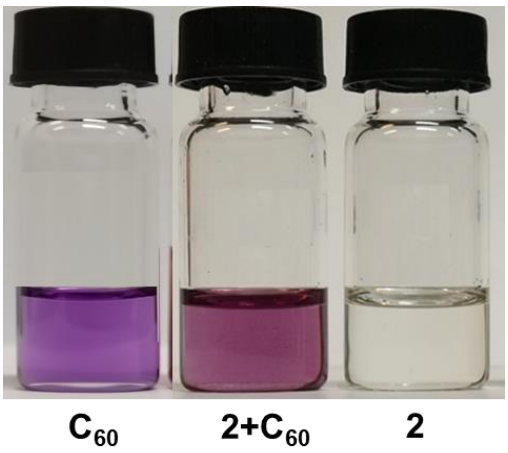


Fig. S49 Solution of C_{60} (left), C_{60} mixed with one equivalent of **2** (mid) and **2** (right), 1.0×10^{-3} M in toluene.

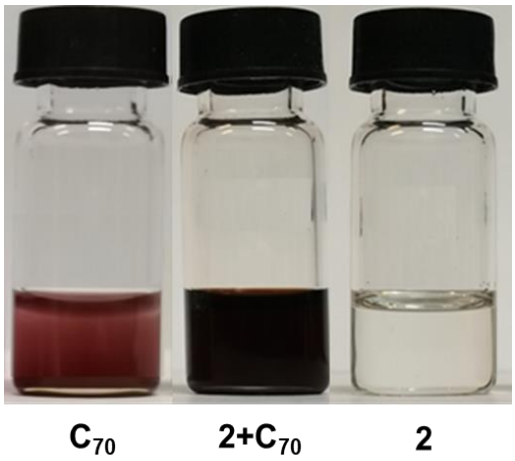


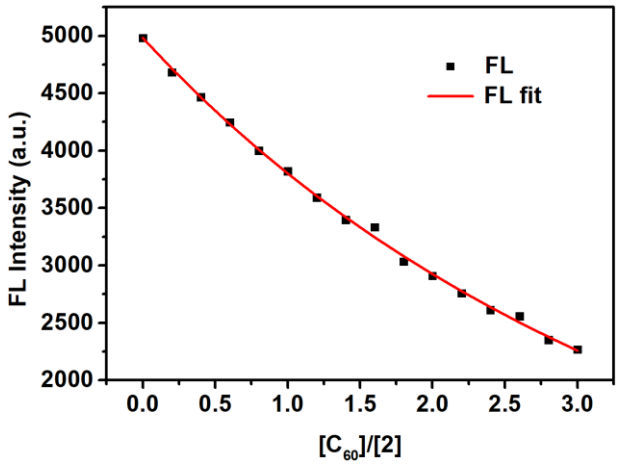
Fig. S50 Solution of C_{70} (left), C_{70} mixed with one equivalent of **2** (mid) and **2** (right), 1.0×10^{-3} M in toluene.

10. Determination of the association constants

Fluorescence titration experiments were performed at 298 K. A stock solution of the cavitand **2** (1.0×10^{-4} M in toluene) was mixed with a stock solution of fullerenes C_{60} and C_{70} (1.0×10^{-3} M in toluene) to give samples with a concentration of [H] = 1.0×10^{-5} M (for **2**) and [G] = (0-3) $\times 10^{-5}$ M (for the corresponding fullerene). The emission spectra (excited at 311 nm) were measured for each sample, and the emission at 431 nm was monitored and fitted to a binding isotherm using Bindfit.[S4-6] The

resulting fits were used to calculate K_a values in addition to an error margin for 95% confidence of fit.

Titration of fullerence C_{60} with cavitand 2



Fitter: UV 1:1 | Fit | Summary | Save

Details

Time to fit	0.2136 s
SSR	17080.5037
Fitted datapoints	16
Fitted params	2

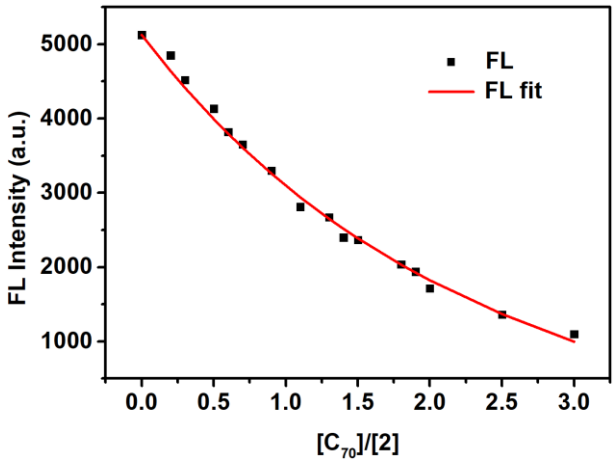
Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	24334.06 M^{-1}	± 1.7960 %	100.00 M^{-1}

Back Next

Fig. S51 Nonlinear fitting curve (left) and association constant (right) for host **2** and guest C_{60}.

Titration of fullerence C_{70} with cavitand 2



Fitter: UV 1:1 | Fit | Summary | Save

Details

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Fitted datapoints	16
Fitted params	2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	53046.18 M^{-1}	± 4.5115 %	100.00 M^{-1}

Back Next

Fig. S52 Nonlinear fitting curve (left) and association constant (right) for host **2** and guest C_{70}.

11. Theoretical calculations

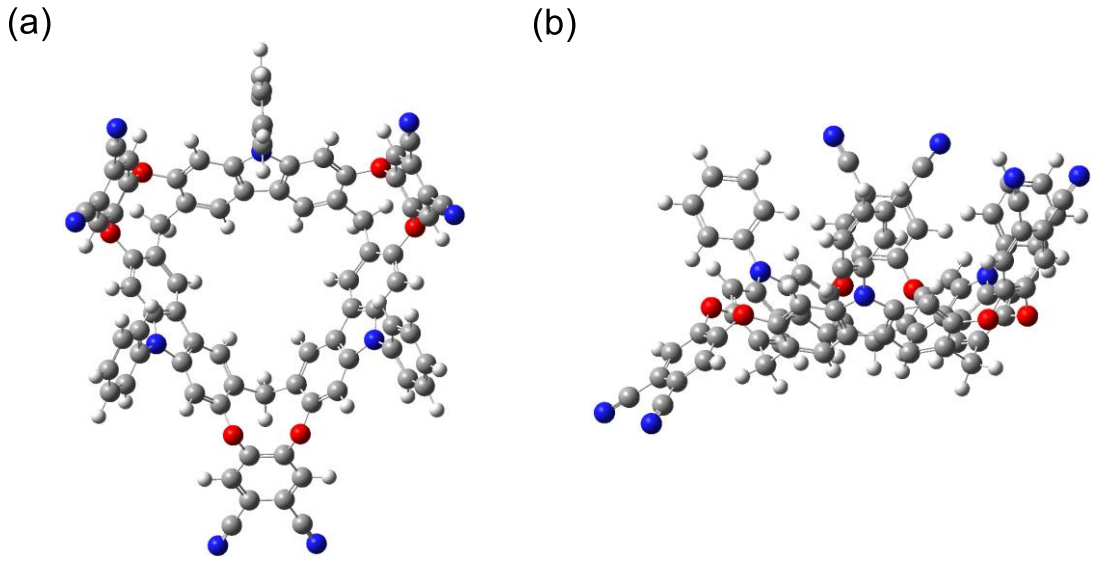

Fig. S53 Optimized structure of **2-c1** from (a) top view and (b) side view at the B3LYP/6-31G(d) level of theory.

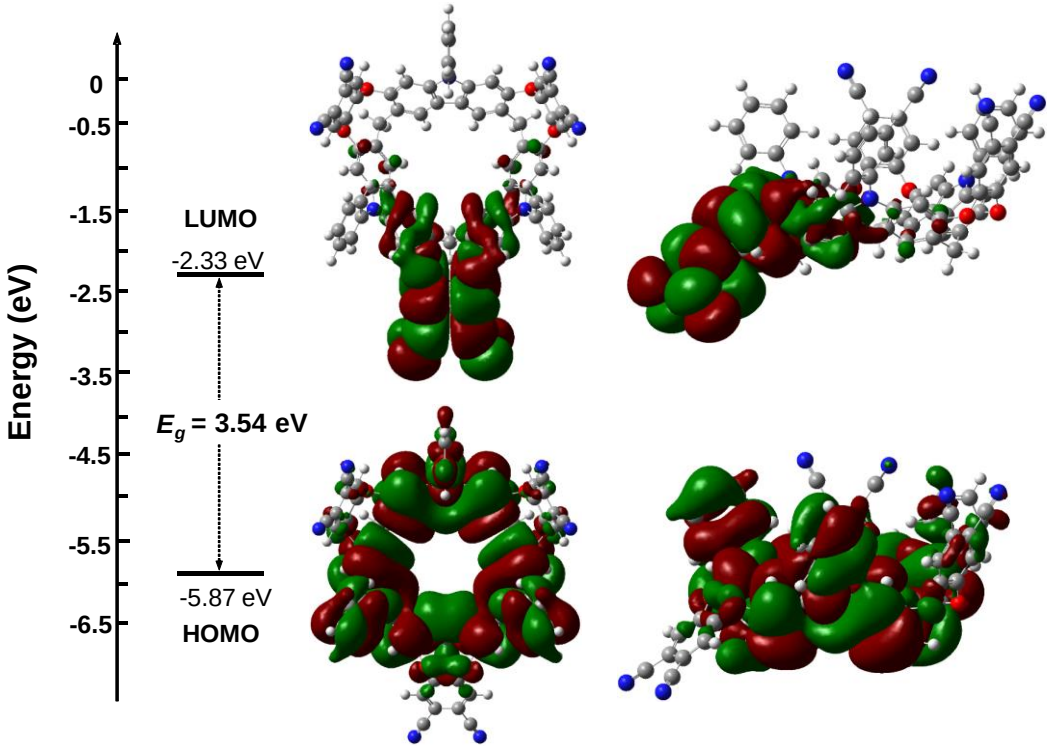

Fig. S54 Frontier molecular orbitals and HOMO-LUMO energy gap of **2-c1** calculated at the B3LYP/6-31G(d) level of theory.

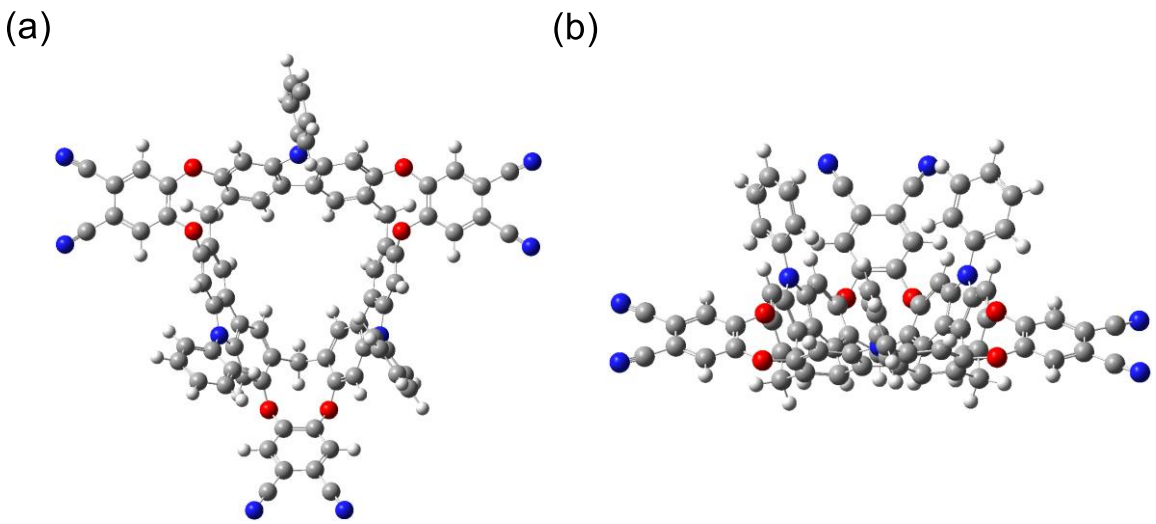

Fig. S55 Optimized structure of **2-c2** from (a) top view and (b) side view at the B3LYP/6-31G(d) level of theory.

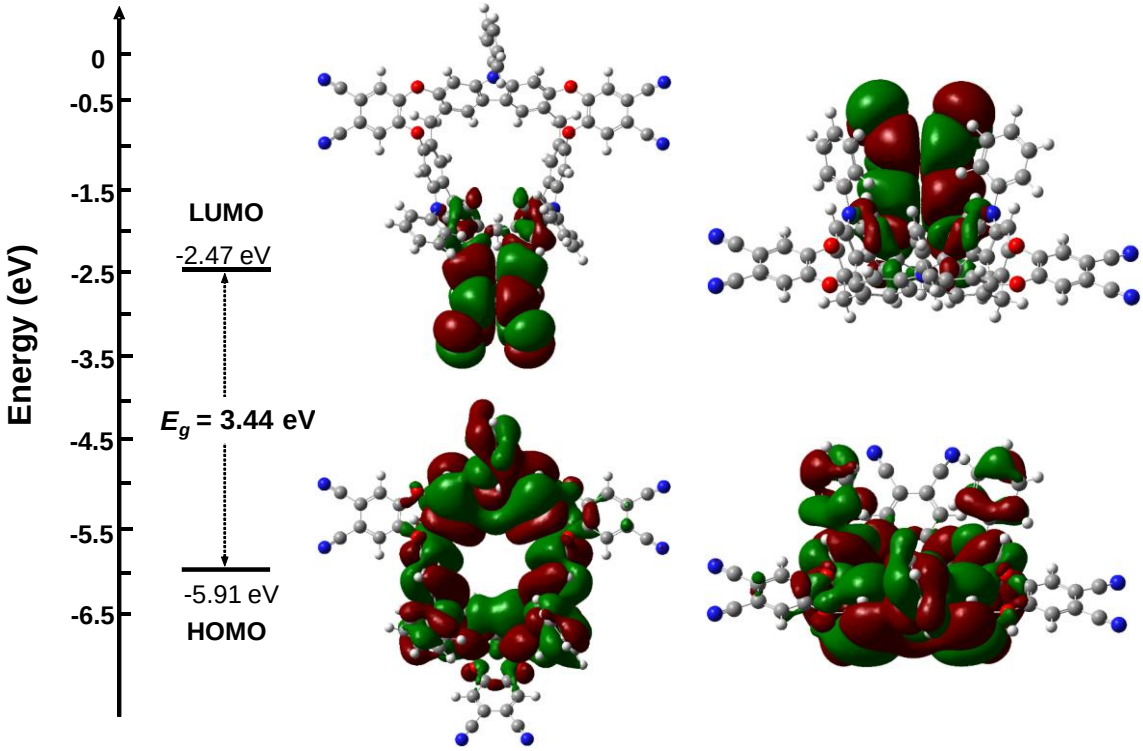

Fig. S56 Frontier molecular orbitals and HOMO-LUMO energy gap of **2-c2** calculated at the B3LYP/6-31G(d) level of theory.

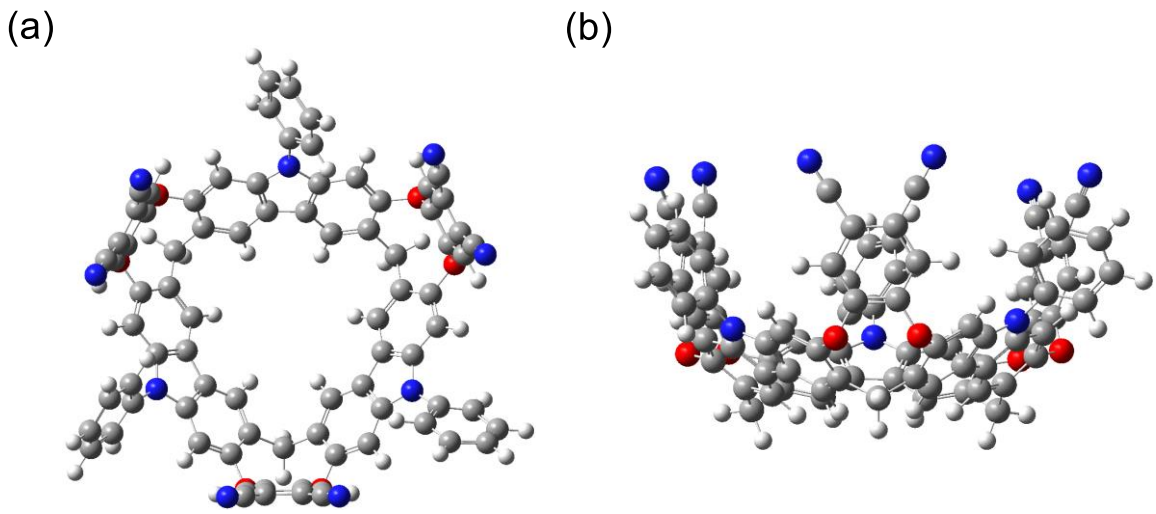

Fig. S57 Optimized structure of **2-c3** from (a) top view and (b) side view at the B3LYP/6-31G(d) level of theory.

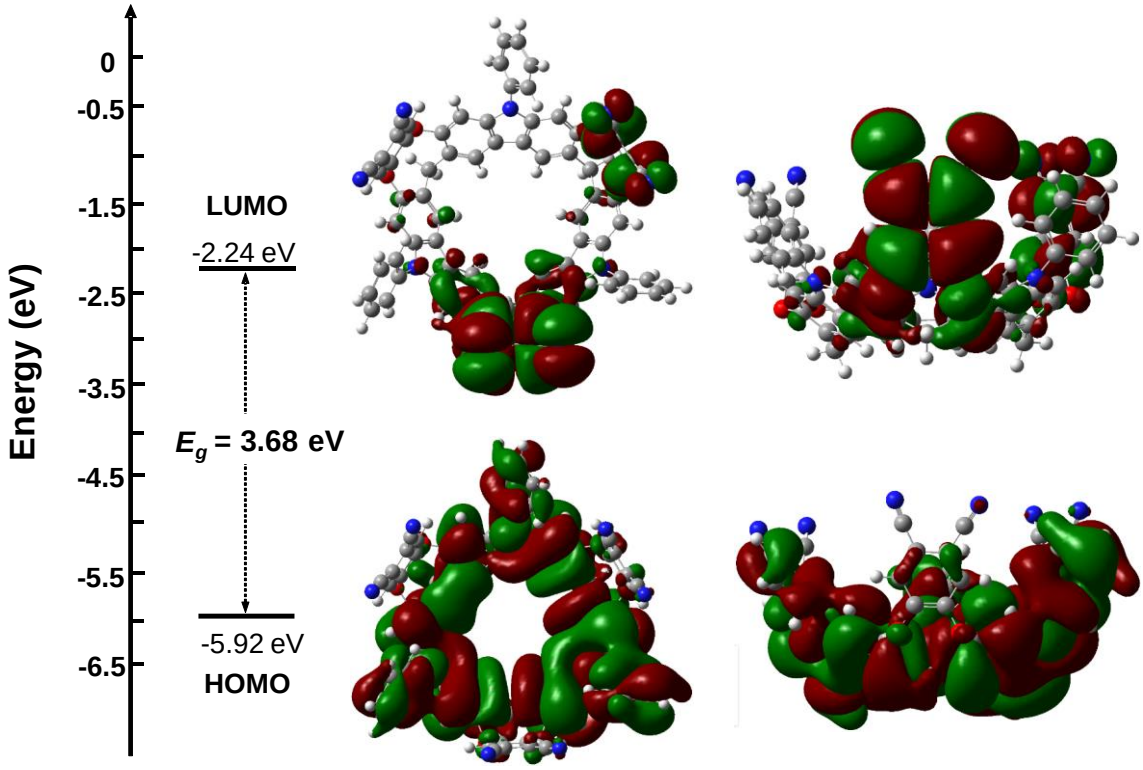

Fig. S58 Frontier molecular orbitals and HOMO-LUMO energy gap of **2-c3** calculated at the B3LYP/6-31G(d) level of theory.

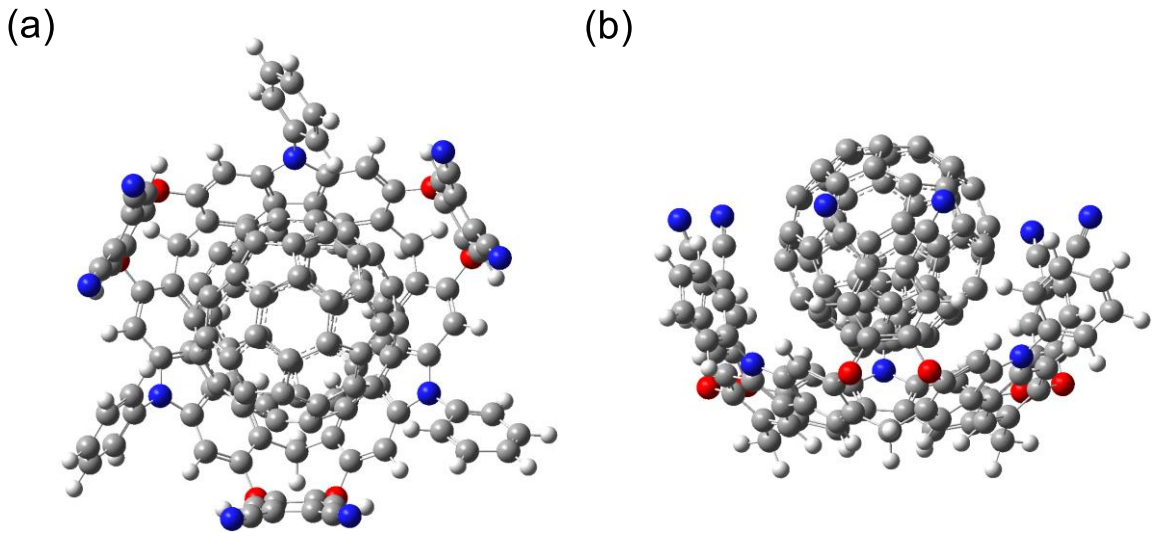

Fig. S59 Optimized structure of **C_{60}@2** from (a) top view and (b) side view at the B3LYP/6-31G(d) level of theory.

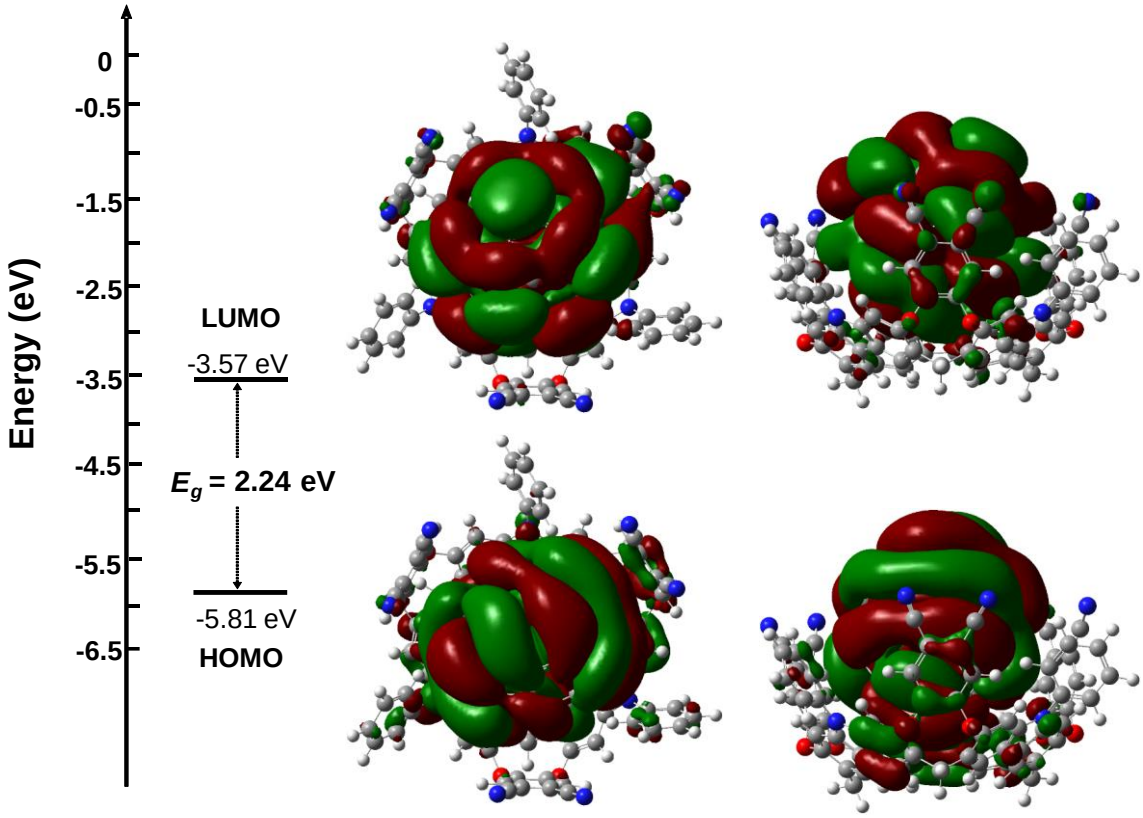

Fig. S60 Frontier molecular orbitals and HOMO-LUMO energy gap of **C_{60}@2** calculated at the B3LYP/6-31G(d) level of theory.

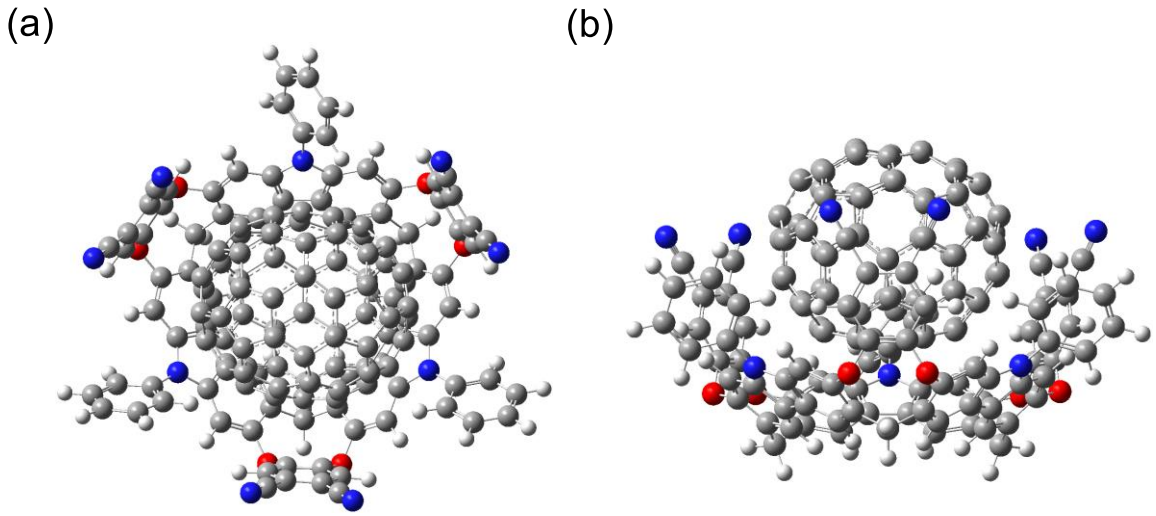

Fig. S61 Optimized structure of **C_{70}@2** from (a) top view and (b) side view at the B3LYP/6-31G(d) level of theory.

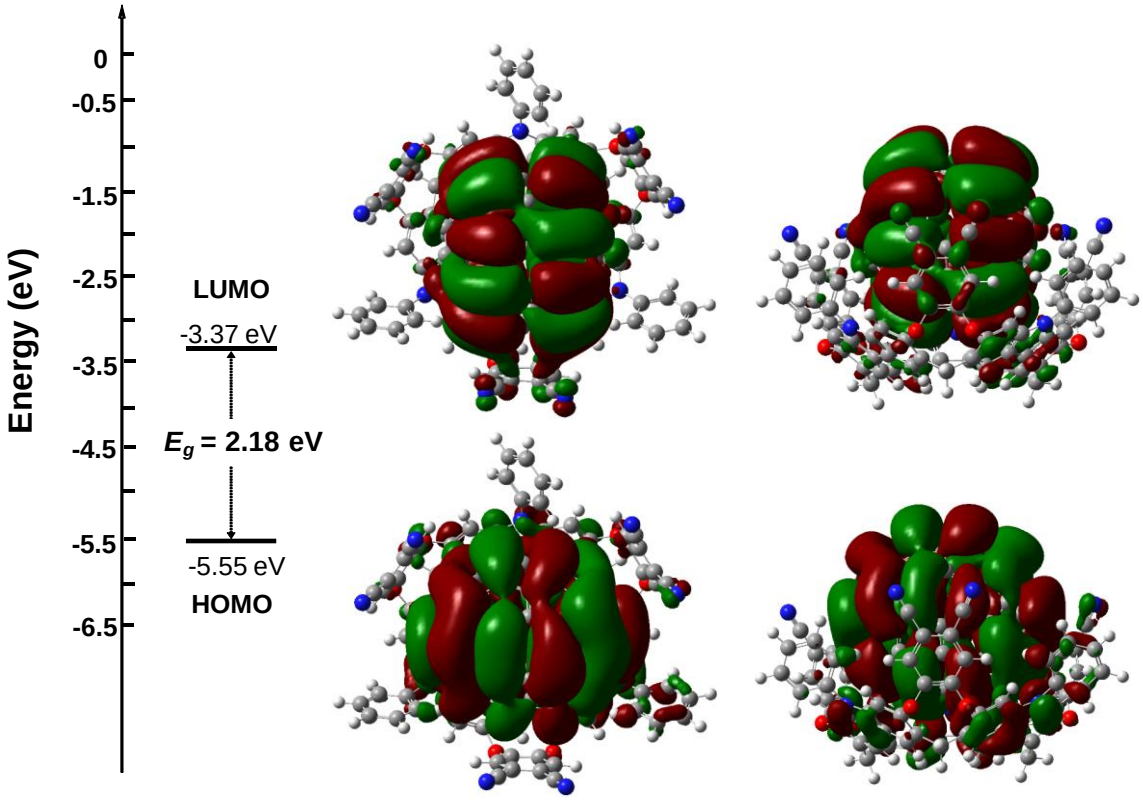

Fig. S62 Frontier molecular orbitals and HOMO-LUMO energy gap of **C_{70}@2** calculated at the B3LYP/6-31G(d) level of theory.

Electrostatic potential (ESP) calculations

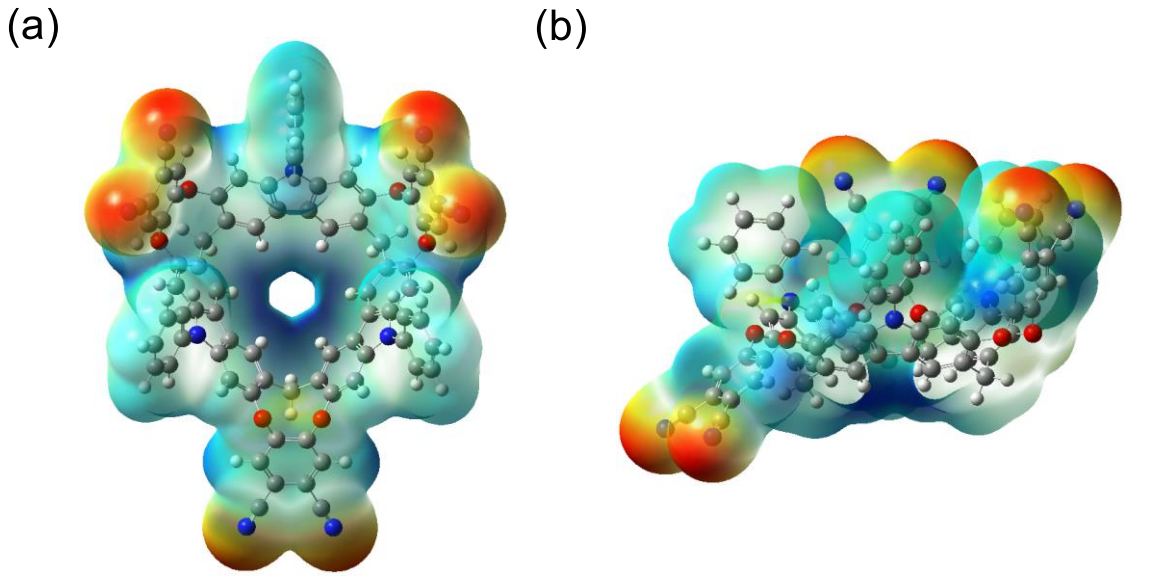

Fig. S63 Electrostatic potential (ESP) map of **2-c1** from (a) top view and (b) side view.

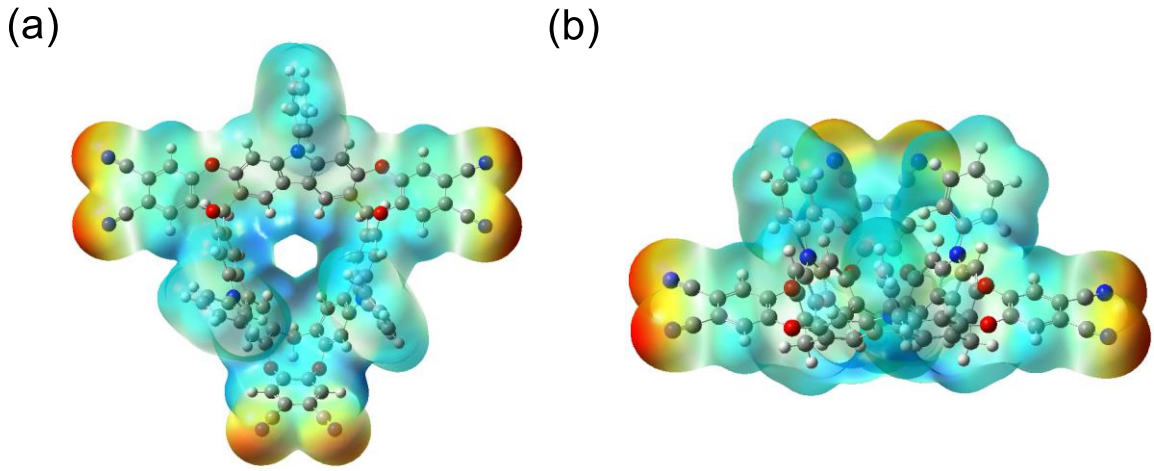

Fig. S64 Electrostatic potential (ESP) map of **2-c2** from (a) top view and (b) side view.

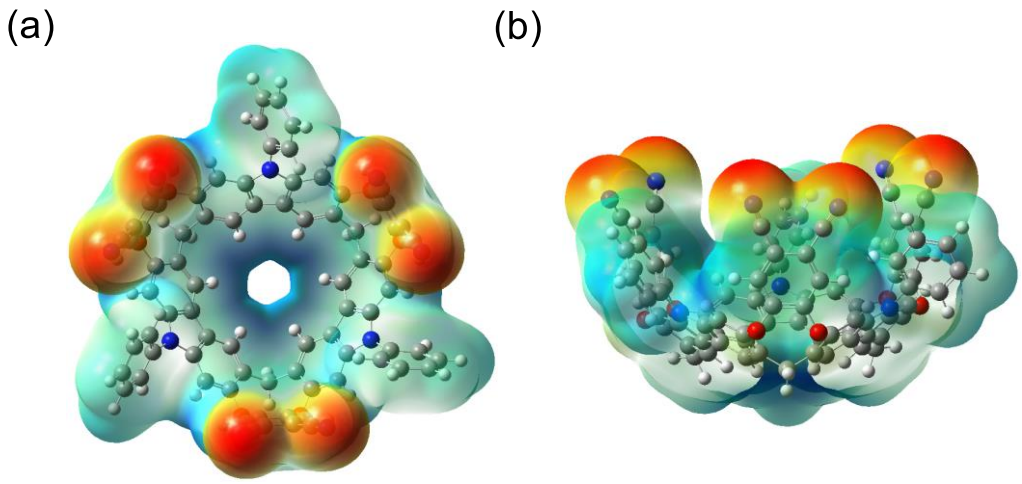

Fig. S65 Electrostatic potential (ESP) map of **2-c3** from (a) top view and (b) side view.

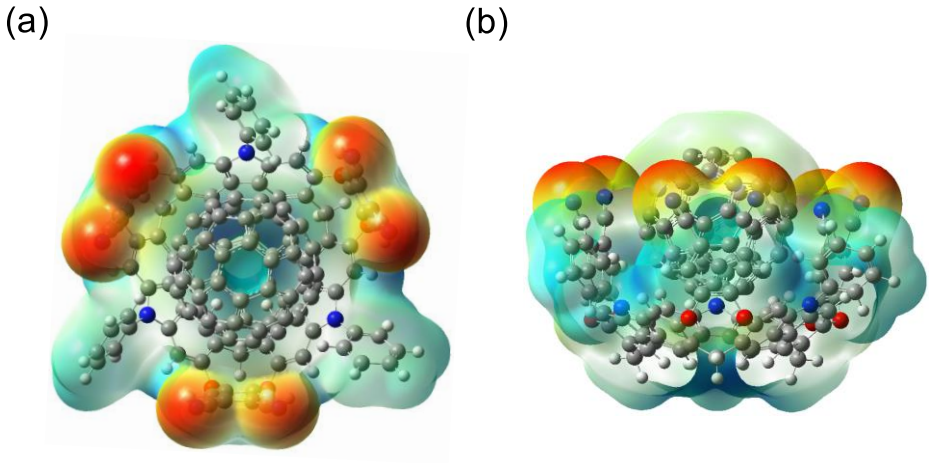

Fig. S66 Electrostatic potential (ESP) map of **C_{60}@2** from (a) top view and (b) side view.

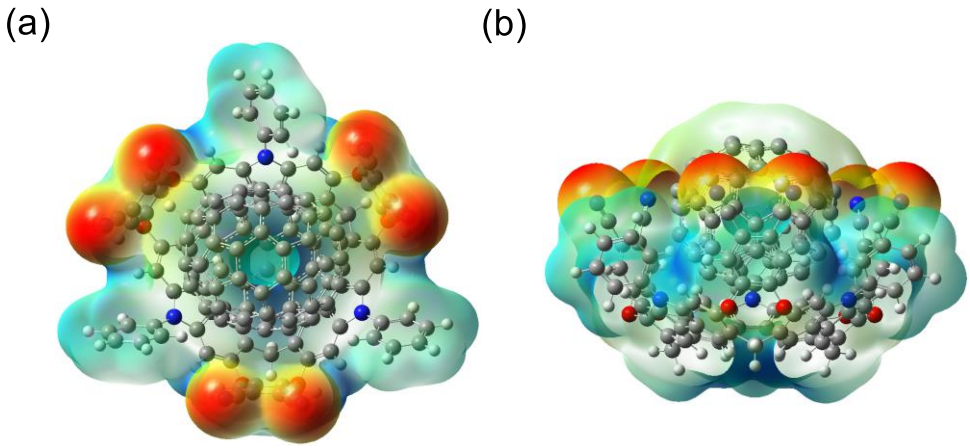

Fig. S67 Electrostatic potential (ESP) map of **C_{70}@2** from (a) top view and (b) side view.

Independent gradient model (IGM) analysis

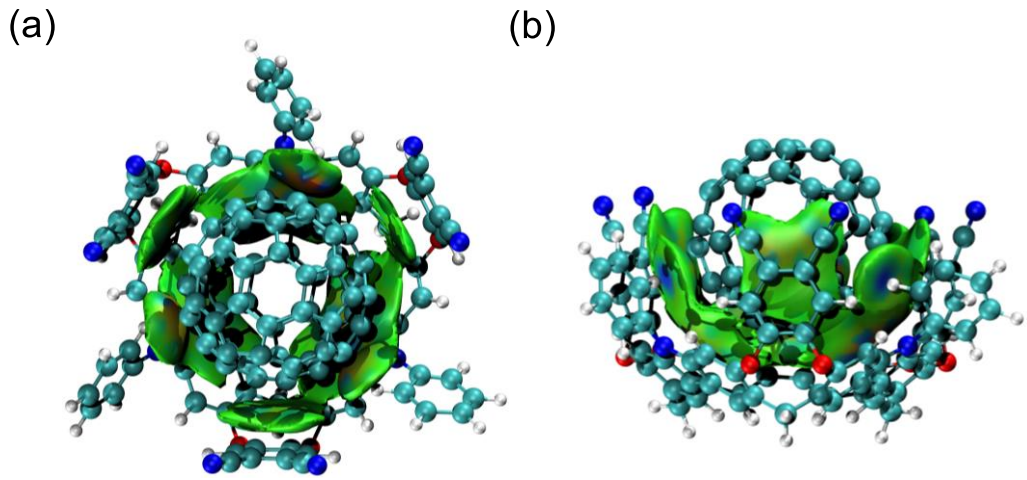

Fig. S68 Independent gradient model (IGM) analysis of **C_{60}@2** from (a) top view and (b) side view.

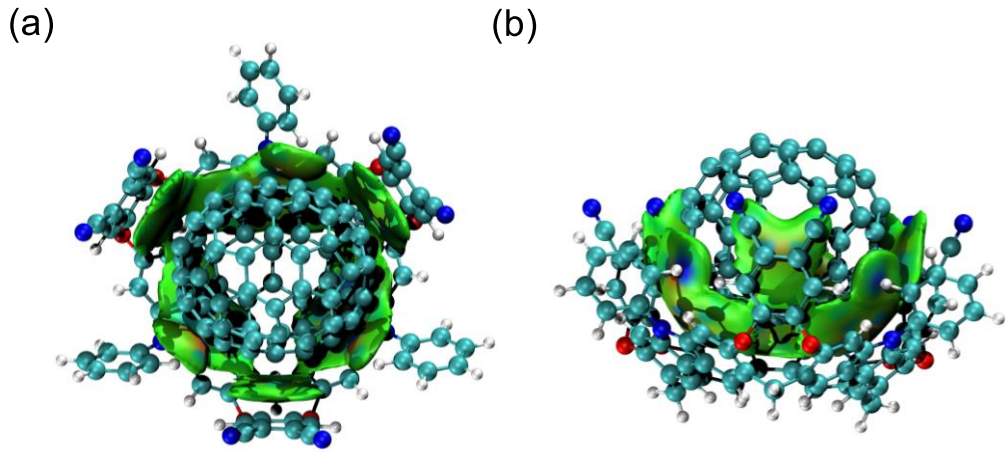

Fig. S69 Independent gradient model (IGM) analysis of **C_{70}@2** from (a) top view and (b) side view.

12. Cartesian coordinates of the optimized structure

2-c1

O	8.2653	9.1036	1.2926	C	4.8822	12.6237	9.2806
O	7.7543	7.7748	3.6502	C	4.014	13.8778	9.4098
O	5.679	12.5317	11.5993	H	3.3215	13.8778	8.7023
N	9.418	13.8778	0.8561	H	3.5576	13.8778	10.2883
N	7.5009	9.5121	8.2539	C	8.7198	12.7609	1.2571
C	8.0725	10.4908	1.5241	C	7.3024	8.6699	4.6399
N	0.7379	11.902	14.7376	C	6.8773	10.8527	2.1835
C	6.6797	10.5338	8.7886	C	10.7694	13.8778	0.3751

N	13.9952	8.0245	1.116
C	6.251	10.344	6.5372
C	4.6109	13.18	12.1445
C	5.659	12.0437	10.2866
C	5.9639	9.8161	2.8008
H	5.025	10.1257	2.7488
H	6.037	8.966	2.2987
C	8.9826	11.3921	1.0346
H	9.7578	11.1071	0.5653
C	5.8951	11.0354	7.7555
C	7.2458	9.4246	6.8845
C	6.6361	12.1994	2.3812
H	5.8493	12.4697	2.8399
C	7.5239	13.1657	1.921
C	5.0145	12.0945	8.0024
H	4.5017	12.4554	7.2888
C	6.3437	9.5895	4.2386
C	9.293	8.518	2.0022
C	2.571	13.1756	13.4047
C	7.776	8.5442	5.931
H	8.4287	7.8936	6.1616
C	6.5764	11.0198	10.086
H	7.1031	10.6718	10.7958
C	10.5825	8.5259	1.4678
H	10.7468	8.9412	0.6293
C	5.793	10.4456	5.2325
H	5.1211	11.0777	5.0055
C	13.389	13.8778	-0.5165
H	14.2862	13.8778	-0.8288
C	11.6252	7.9265	2.1623
C	9.0462	7.8879	3.2113
C	3.6078	12.4696	12.7948
H	3.6283	11.5203	12.8231
C	10.0976	7.2605	3.8939
H	9.9229	6.8049	4.7089
C	11.0253	13.8778	-0.9808
H	10.3095	13.8778	-1.6054
C	8.5643	8.8302	8.9446
C	11.391	7.2975	3.3922
C	1.5465	12.4631	14.1432
C	12.9516	7.9897	1.5874
N	13.2951	6.2886	4.8082
C	11.8087	13.8778	1.2757
H	11.6224	13.8778	2.2073
C	8.3308	8.2217	10.1587
H	7.4682	8.2394	10.5562
C	12.4621	6.7301	4.1486
C	9.8328	8.8046	8.3611
H	9.9947	9.2499	7.5377
C	12.3392	13.8778	-1.4197
H	12.5224	13.8778	-2.3518
C	9.4	7.5777	10.7887
H	9.2582	7.1707	11.6353
C	10.8534	8.1172	9.0047
H	11.7106	8.0604	8.5991
C	10.6351	7.516	10.2272
H	11.342	7.0633	10.672
C	13.1276	13.8778	0.8398
H	13.8412	13.8778	1.467
O	8.2653	18.652	1.2926
O	7.7543	19.981	3.6502
O	5.679	15.224	11.5993
N	7.5009	18.2436	8.2539
C	8.0725	17.2649	1.5241
N	0.7379	15.8537	14.7376
C	6.6797	17.2219	8.7886
C	4.8822	15.132	9.2806
C	8.7198	14.9948	1.2571
C	7.3024	19.0857	4.6399
C	6.8773	16.903	2.1835
N	13.995	19.7312	1.116
C	6.251	17.4117	6.5372
C	4.6109	14.5757	12.1445
C	5.659	15.712	10.2866
C	5.9639	17.9396	2.8008
H	5.025	17.63	2.7488
H	6.037	18.7897	2.2987
C	8.9826	16.3636	1.0346
H	9.7578	16.6486	0.5653
C	5.8951	16.7203	7.7555
C	7.2458	18.3311	6.8845
C	6.6361	15.5563	2.3812

H	5.8493	15.286	2.8399	C	10.0976	20.4952	3.8939
C	7.5239	14.59	1.921	H	9.9229	20.9507	4.7089
C	5.0145	15.6612	8.0024	C	8.5643	18.9255	8.9446
H	4.5017	15.3003	7.2888	C	11.391	20.4582	3.3922
C	6.3437	18.1662	4.2386	C	1.5465	15.2926	14.1432
C	9.293	19.2377	2.0022	C	12.9516	19.7659	1.5874
C	2.571	14.5801	13.4047	N	13.2951	21.4672	4.8082
C	7.776	19.2114	5.931	C	8.3308	19.5339	10.1587
H	8.4287	19.8622	6.1616	H	7.4682	19.5163	10.5562
C	6.5764	16.7359	10.086	C	12.4621	21.0255	4.1486
H	7.1031	17.0839	10.7958	C	9.8328	18.9512	8.3611
C	10.5825	19.2297	1.4678	H	9.9947	18.5058	7.5377
H	10.7468	18.8145	0.6293	C	9.4	20.178	10.7887
C	5.793	17.3101	5.2325	H	9.2582	20.5849	11.6353
H	5.1211	16.678	5.0055	C	10.8534	19.6385	9.0047
C	11.6252	19.8292	2.1623	H	11.7106	19.6953	8.5991
C	9.0462	19.8677	3.2113	C	10.6351	20.2396	10.2272
C	3.6078	15.2861	12.7948	H	11.342	20.6924	10.672
H	3.6283	16.2354	12.8231				

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O	17.4524	12.245	4.0573	C	15.724	9.3358	2.5429
O	17.0422	9.4091	4.5038	H	15.5461	8.4161	2.6974
O	13.1847	3.6138	10.852	C	16.4722	10.0689	3.4409
O	14.5932	3.6816	13.1459	C	14.9797	11.9328	0.0059
O	21.9603	9.6005	12.412	C	14.4698	9.1919	0.4346
O	22.4736	12.4133	12.047	C	16.1628	8.8145	5.4007
N	14.5828	12.3265	-0.9371	C	16.1333	7.4325	5.451
N	13.8456	8.5959	-0.315	H	16.5839	6.8977	4.8084
N	15.2719	5.5184	6.8367	C	15.4062	6.8719	6.4955
N	14.2685	-1.963	9.5164	C	14.6043	5.4695	8.0685
N	16.2968	-1.8395	13.0058	C	14.2612	4.3794	8.8235
N	19.1116	5.6487	12.9115	H	14.3724	3.4935	8.4985
N	24.1629	9.4851	17.816	C	13.74	4.6319	10.0938
N	25.2952	13.1559	17.0494	C	13.6544	5.927	10.6423
N	20.8671	12.5029	7.4849	C	13.873	6.9981	9.7912
C	16.7197	11.4278	3.2571	H	13.7227	7.8839	10.0994
C	16.2255	12.0468	2.1186	C	14.3086	6.7863	8.4951
H	16.3767	12.9744	1.9787	C	14.7682	7.6633	7.4745
C	15.5085	11.3124	1.184	C	14.7647	9.0426	7.3311
C	15.225	9.9861	1.3836	H	14.2936	9.5809	7.9559

C	15.4447	9.6412	6.2813
C	15.5385	11.1427	6.1498
H	15.2429	11.4135	5.2447
H	14.9359	11.5697	6.8094
C	15.8852	4.4269	6.1602
C	13.9256	2.5264	11.1674
C	13.8394	1.3765	10.4582
H	13.3207	1.3527	9.6636
C	14.4909	0.2539	10.8699
C	15.2124	0.2593	12.0628
C	15.2917	1.4254	12.8005
H	15.7808	1.4415	13.6148
C	14.6665	2.5495	12.3543
C	14.3923	-0.9598	10.1113
C	15.8486	-0.8973	12.5447
C	15.4978	4.7242	12.9195
C	16.8668	4.4812	13.0266
H	17.2027	3.599	13.1355
C	17.7368	5.5931	12.9671
C	19.4613	7.0022	12.9124
C	20.7336	7.5914	12.741
H	21.5235	7.0749	12.6303
C	20.7473	8.9951	12.7458
C	19.6385	9.7851	12.9763
C	18.3973	9.1607	13.0894
H	17.6141	9.6819	13.2203
C	18.3032	7.7855	13.0117
C	17.1891	6.8854	12.9856
C	15.8034	7.066	12.8059
H	15.449	7.9458	12.76
C	14.9594	5.9935	12.6961
C	13.5399	6.1307	12.149
H	12.9455	5.4473	12.5486
H	13.1737	7.0281	12.3522
C	20.0048	4.5586	12.7508
C	19.7038	3.5011	11.914
H	18.8869	3.5054	11.4311
C	20.5644	2.4463	11.7712
H	20.3523	1.7478	11.1639
C	21.7262	2.3866	12.4911
H	24.8382	14.2001	4.7511
H	22.2917	1.6233	12.4413
C	22.0596	3.4536	13.2884
H	22.8952	3.4633	13.7371
C	21.1897	4.5097	13.4413
H	21.4156	5.2176	14.0344
C	22.533	10.3635	13.4074
C	22.8961	9.796	14.5988
H	22.6727	8.889	14.7693
C	23.5827	10.5196	15.5632
C	23.9062	11.8568	15.2922
C	23.526	12.4527	14.1053
H	23.7521	13.3564	13.9214
C	22.7978	11.6911	13.1759
C	23.9291	9.9548	16.8135
C	24.6778	12.6102	16.256
C	21.4287	12.1038	11.1382
C	21.7845	12.4066	9.8442
H	22.6643	12.6874	9.6223
C	20.7847	12.2803	8.8681
C	19.6056	12.2409	6.9524
C	19.1612	12.3251	5.6334
H	19.7384	12.6044	4.9326
C	17.8496	11.9844	5.3906
C	16.9505	11.6192	6.3794
C	17.4083	11.554	7.7092
H	16.8225	11.291	8.4095
C	18.7447	11.8825	7.982
C	19.5109	11.9111	9.2224
C	19.1753	11.6165	10.5361
H	18.2912	11.3499	10.7586
C	20.1632	11.7196	11.5359
C	19.7329	11.3015	12.9115
H	18.8521	11.701	13.1226
H	20.3878	11.6249	13.5799
C	21.9519	12.955	6.7685
C	22.3841	14.28	6.9164
H	21.9532	14.8656	7.5273
C	23.4569	14.7184	6.1489
H	23.7302	15.6259	6.2097
C	24.1365	13.8646	5.2951
C	23.8001	12.5301	5.2356

H	24.2975	11.9136	4.7108	C	22.7078	12.1337	5.9764
H	22.4577	11.2187	5.9313	H	17.6216	1.8011	4.3228
C	17.2648	4.5043	5.9496	C	15.8165	2.3146	5.0571
H	17.744	5.2471	6.2986	H	15.3611	1.517	4.8107
C	17.9457	3.5323	5.2535	C	15.1544	3.3626	5.661
H	18.8793	3.5884	5.084	H	14.2078	3.355	5.7341
C	17.1831	2.4789	4.8221				

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O	2.5817	26.5896	12.5308	C	0.0449	27.9972	12.4788
O	-3.8368	33.449	20.4305	H	0.6223	27.9462	11.6765
O	-4.0857	23.9212	21.0282	H	-0.8973	27.9572	12.1781
O	2.4798	29.3679	12.2408	C	-3.0395	24.1299	17.6076
O	-2.4144	34.6867	18.4296	C	1.8478	22.6611	16.213
O	-2.7798	22.3457	19.181	C	-1.1922	31.9357	15.5642
N	-4.0267	28.7853	21.9533	C	-4.1587	29.3445	19.748
N	1.8408	21.0561	22.3919	C	-4.059	29.8272	21.0672
N	0.8159	32.9321	15.163	C	1.9235	33.8115	15.303
N	0.0081	23.4725	25.1784	C	-4.0774	27.5844	21.2046
N	7.3321	30.5521	15.2519	C	-4.2624	26.8838	18.8999
N	7.7371	26.7351	15.4403	H	-4.3395	27.0991	17.9772
N	0.7289	23.5177	15.9007	C	-0.4971	23.5498	16.5603
N	0.3902	33.7442	24.4918	C	-2.2436	23.0848	18.0869
N	2.4728	35.6062	21.5222	C	1.3815	35.2441	21.3607
C	-3.9778	32.0655	20.2138	C	-4.1647	31.6261	18.9053
C	-2.4527	31.8065	16.1376	C	-4.3815	24.4856	18.2323
H	-3.0267	31.0922	15.8881	H	-5.0014	24.7943	17.5253
C	-0.4453	31.1072	14.6353	H	-4.7738	23.6775	18.6503
C	-1.2652	24.6157	16.0326	C	5.5504	29.0074	14.2073
C	-0.6829	26.3489	14.2046	C	-4.239	25.5717	19.2822
H	-1.529	26.781	14.2128	C	1.7827	35.1473	14.9934
C	-4.2514	30.2422	18.6657	H	0.9649	35.4601	14.6257
H	-4.3693	29.9159	17.7807	C	-1.8254	34.4893	19.6565
C	-1.9798	33.7615	17.4219	C	-2.2073	22.5829	20.3861
C	3.4903	28.7926	12.9769	C	-2.859	23.4245	21.3176
C	-2.537	33.8544	20.6769	C	2.4847	21.9791	15.225
C	1.8129	25.0205	14.1857	H	2.1737	22.0382	14.3287
H	2.653	24.5778	14.1708	C	-0.428	22.2066	21.9611
C	3.5403	27.3988	13.0953	C	-2.2788	23.6104	22.5857
C	0.7928	31.7523	14.428	H	-2.7276	24.1341	23.2377

C	-4.025	28.9208	23.3638	C	0.0389	34.7697	21.1561
C	6.7844	27.0556	14.9288	C	-1.007	21.9759	20.7253
C	-1.0735	23.0399	22.8819	H	-0.5806	21.3962	20.1044
C	6.5508	29.8406	14.7861	C	-4.1101	25.2833	20.658
C	2.8105	36.0325	15.2088	C	3.1396	33.3372	15.7769
H	2.6985	36.9521	15.0008	H	3.2514	32.4119	15.9548
C	0.8155	21.5656	22.2384	C	0.3306	26.8117	13.37
C	3.383	21.8156	17.8284	C	-0.6938	29.8942	13.9811
H	3.6972	21.7585	18.7245	H	-1.5345	29.4648	14.0861
C	-0.088	33.9204	23.4526	C	-0.3726	33.0115	15.8738
C	4.0122	35.5774	15.7284	C	-2.5339	24.8776	16.5496
H	4.7161	36.1907	15.9062	H	-3.0588	25.5742	16.1734
C	4.1894	34.2121	15.995	C	-0.659	34.1192	22.1684
H	5.0224	33.8922	16.3188	C	2.2437	22.5752	17.5403
C	-0.4378	23.3027	24.1742	H	1.7583	23.0152	18.2272
C	3.5954	21.2003	15.5265	C	-4.1771	27.9145	19.8396
H	4.036	20.7077	14.8461	C	-0.5513	34.9559	19.9122
C	4.0494	21.1522	16.8323	H	-0.073	35.4106	19.2291
H	4.8304	20.6531	17.04	C	-2.9801	30.0105	25.3265
C	-0.7617	33.9679	16.8242	H	-2.3279	30.5723	25.7305
H	-0.2151	34.7135	17.0421	C	-1.016	22.7412	17.5753
C	-2.9626	29.7669	23.9669	H	-0.5398	21.9853	17.8991
H	-2.2768	30.1357	23.421	C	-0.451	25.2429	15.0365
C	-4.9348	28.4497	24.1634	C	4.4717	29.5522	13.5342
H	-5.6313	27.9081	23.8099	H	4.4124	30.4987	13.4597
C	-3.9953	29.4016	26.1045	C	-2.8605	32.7507	17.0934
H	-3.9885	29.5026	27.0502	C	0.2845	29.3134	13.1761
C	-4.9107	28.7285	25.5553	C	-3.9598	31.2056	21.3284
H	-5.6148	28.3936	26.0971	H	-3.8848	31.5402	22.2144
C	0.7629	24.5683	15.0042	C	1.5706	26.1451	13.3996
C	5.6439	27.6068	14.2907	C	-4.2095	32.5907	17.753
C	-1.9664	33.6929	21.9342	H	-4.5199	33.4729	18.0771
H	-2.4666	33.2907	22.633	H	-4.8631	32.2666	17.0824
C	4.6503	26.8088	13.7388	C	1.7788	31.2175	13.6096
H	4.7183	25.8636	13.7948	H	2.6024	31.6655	13.4571
C	-4.0532	26.2672	21.638	C	1.4935	29.9967	13.0334
H	-3.9997	26.0473	22.561				

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O	2.5729	26.5925	12.5421	O	-3.8352	33.4545	20.4265

O	-4.0843	23.9296	21.0269
O	2.4843	29.3628	12.2346
O	-2.3965	34.6851	18.435
O	-2.7603	22.3585	19.1816
N	-4.0203	28.7955	21.9557
N	1.8308	21.0272	22.3865
N	0.8231	32.9215	15.1711
N	0.0032	23.4629	25.2053
N	7.3815	30.4912	15.2707
N	7.7576	26.7287	15.4
N	0.7508	23.5094	15.89
N	0.4002	33.7346	24.4972
N	2.4849	35.5966	21.533
C	-3.9966	32.0808	20.1896
C	-2.4422	31.8245	16.1376
H	-3.0122	31.1055	15.8881
C	-0.43	31.1139	14.6246
C	-1.266	24.6218	16.0273
C	-0.7159	26.3515	14.2234
H	-1.5658	26.7759	14.2272
C	-4.2711	30.2477	18.6819
H	-4.4228	29.9294	17.7987
C	-1.9916	33.7762	17.438
C	3.5001	28.7798	12.985
C	-2.5283	33.8352	20.6822
C	1.7914	25.0343	14.2073
H	2.6363	24.6008	14.2131
C	3.5481	27.3915	13.0953
C	0.7868	31.7338	14.4523
C	0.0356	27.985	12.4815
H	-0.9103	27.9295	12.196
H	0.5998	27.9325	11.6683
C	-3.0414	24.1327	17.5996
C	1.8278	22.6617	16.2023
C	-1.1935	31.927	15.5642
C	-4.154	29.3388	19.7534
C	-4.0617	29.8438	21.0834
C	1.9035	33.8179	15.2923
C	-4.0684	27.61	21.1911
C	-4.2655	26.8761	18.8757
H	-4.3473	27.1001	17.957
C	-0.5021	23.5591	16.5576
C	-2.2349	23.0623	18.1219
C	1.3712	35.2377	21.3742
C	-4.1594	31.6386	18.9349
C	-4.3672	24.4853	18.2484
H	-5.0062	24.7655	17.5467
H	-4.735	23.6792	18.6902
C	5.5223	29.0426	14.1992
C	-4.2348	25.5878	19.2634
C	1.7962	35.1351	15.0338
H	0.9664	35.4675	14.7119
C	-1.8276	34.4941	19.6511
C	-2.2022	22.5976	20.3726
C	-2.8547	23.4277	21.3446
C	2.495	21.9743	15.2573
H	2.2008	22.0367	14.3572
C	-0.4236	22.2162	21.9557
C	-2.3044	23.5879	22.5642
H	-2.7518	24.1035	23.2253
C	-4.0199	28.9176	23.3799
C	6.7899	27.0556	14.9261
C	-1.1147	23.0142	22.8442
C	6.5524	29.831	14.7834
C	2.8403	36.0293	15.2115
H	2.7396	36.9418	14.9724
C	0.8341	21.6009	22.2357
C	3.3708	21.8156	17.8176
H	3.672	21.7476	18.7148
C	-0.0876	33.9365	23.4472
C	4.0468	35.5646	15.7526
H	4.7543	36.1673	15.9491
C	4.182	34.2281	15.9896
H	5.0177	33.9008	16.3008
C	-0.4508	23.277	24.158
C	3.5835	21.1843	15.5426
H	4.0047	20.6674	14.8659
C	4.0488	21.165	16.8538
H	4.8457	20.6946	17.0681
C	-0.747	33.9704	16.8053
H	-0.2008	34.7202	17.0103
C	-2.935	29.7445	23.9803

H	-2.2468	30.1041	23.4358
C	-4.8973	28.4786	24.1688
H	-5.5937	27.946	23.8036
C	-4.0546	29.3631	26.1099
H	-4.0899	29.4752	27.0523
C	-4.917	28.7189	25.5526
H	-5.6317	28.3677	26.0701
C	0.7604	24.5875	14.988
C	5.6504	27.6389	14.3069
C	-1.9822	33.7121	21.9207
H	-2.4909	33.3276	22.624
C	4.6557	26.8216	13.7065
H	4.7494	25.878	13.7257
C	-4.0564	26.2544	21.6299
H	-4.0084	26.0252	22.551
C	0.029	34.7697	21.1346
C	-1.0132	21.9791	20.7361
H	-0.5982	21.3796	20.1275
C	-4.1171	25.2961	20.6472
C	3.1288	33.3147	15.7957
H	3.2361	32.3921	15.9923
C	0.351	26.8088	13.3753
C	-0.6891	29.9054	14.0026
H	-1.5197	29.4669	14.1485
C	-0.355	33.0372	15.8819
C	-2.5435	24.8731	16.5549
H	-3.073	25.57	16.1848
C	-0.6697	34.1512	22.1711
C	2.2463	22.5784	17.5403
H	1.7746	23.0263	18.2335
C	-4.176	27.8793	19.8422
C	-0.5531	34.946	19.9338
H	-0.0686	35.3993	19.2552
C	-2.9433	29.9784	25.3399
H	-2.2742	30.5042	25.762
C	-1.0368	22.729	17.5592
H	-0.5713	21.9513	17.8403
C	-0.4374	25.2288	15.0607
C	4.4885	29.5554	13.5369
H	4.4333	30.4995	13.4397
C	-2.8783	32.7503	17.0719
C	0.2704	29.3243	13.1573
C	-3.966	31.2091	21.3392
H	-3.8844	31.55	22.2213
C	1.5564	26.1557	13.3969
C	-4.2105	32.6161	17.7342
H	-4.8718	32.2904	17.0743
H	-4.5086	33.5063	18.0509
C	1.7518	31.2219	13.6042
H	2.5519	31.6997	13.4143
C	1.4943	29.972	13.0388
C	1.5866	31.3918	22.093
C	1.7019	31.8693	20.8438
C	1.0195	31.6033	19.6538
C	-0.1116	30.8245	19.8638
C	-0.3823	30.3791	21.1561
C	0.4315	30.4688	22.3542
C	0.7536	29.4176	23.2022
C	0.1648	28.1805	22.9465
C	-0.721	27.9401	21.7188
C	-0.9938	29.0619	20.9057
C	-0.9922	28.7478	19.4734
C	-0.3511	29.924	18.7869
C	0.3885	29.5746	17.6534
C	0.6176	28.1068	17.2253
C	0.0735	27.1005	18.0465
C	-0.7103	27.3857	19.1611
C	-0.2922	26.2992	19.9876
C	-0.3086	26.6422	21.3338
C	0.7247	26.0236	22.093
C	1.8888	25.2705	21.6057
C	1.9487	24.9884	20.2703
C	0.77	25.466	19.5596
C	0.9206	26.014	18.2188
C	2.1674	26.107	17.6669
C	3.3126	25.6198	18.3426
C	3.1662	25.1038	19.7103
C	3.913	25.2897	20.8815
C	3.1974	25.5237	22.0688
C	3.3741	26.5396	23.0111
C	4.5128	27.3248	22.8495
C	5.3264	27.0428	21.7538

C	5.0221	26.123	20.6984
C	5.2979	26.6326	19.3926
C	5.8259	27.9113	19.6565
C	5.565	29.0106	18.8273
C	4.7911	28.7894	17.6211
C	4.1382	27.5427	17.3357
C	4.5031	26.421	18.2026
C	2.7596	27.2415	17.0476
C	1.9542	28.3728	16.8619
C	2.5678	29.6387	16.9507
C	1.5158	30.4175	17.473
C	1.7473	31.4046	18.4611
C	3.0562	31.6258	18.9215
C	3.1074	31.927	20.3026
C	4.2269	31.4623	21.0026
C	3.9557	30.9175	22.2707
C	2.6768	30.7636	22.9061
C	2.1193	29.6131	23.5334
C	2.9294	28.5074	23.7865
C	2.2733	27.2928	23.5684
C	0.9468	27.03	23.1295
C	4.2291	28.6709	23.2884
C	4.7927	29.7733	22.5292
C	5.8606	28.2126	21.0322
C	5.5796	29.533	21.3796
C	5.2604	30.6098	20.5584
C	5.2108	30.3438	19.2042
C	4.1731	30.9399	18.4503
C	3.8989	29.9656	17.4111

C_{70}@2

O	7.5901	35.3571	4.9156
O	9.0614	33.8904	6.7945
O	9.6687	24.362	6.675
O	8.1946	22.9138	4.8446
O	2.5248	27.4633	-1.3136
O	2.4224	30.2713	-1.2515
N	9.4129	29.093	7.98
N	4.6303	24.1716	1.7004
N	4.1822	33.733	1.7625
N	3.2324	36.7842	8.5642
N	5.1332	34.2113	11.0705
N	6.123	23.5931	11.2257
N	3.9374	21.352	8.5947
N	-2.5221	26.7464	1.6247
N	-2.4871	30.637	1.8991
C	9.3486	33.2523	4.0758
H	9.9753	32.9949	3.354
H	9.6608	34.1098	4.46
C	7.0946	35.136	6.1882
C	5.9143	35.7609	6.5818
H	5.4594	36.3259	5.9673
C	5.4005	35.5784	7.8295
C	6.0642	34.7647	8.7527
C	7.2785	34.1612	8.3729
H	7.7447	33.6058	8.9863
C	7.7935	34.3783	7.0975
C	4.183	36.2439	8.2481
C	5.5617	34.4814	10.0613
C	9.1806	32.5124	6.4987
C	9.36	32.1873	5.1513
C	9.5121	30.8419	4.828
H	9.6331	30.5797	3.9229
C	9.4867	29.8862	5.833
C	9.5536	28.4229	5.802
C	9.6617	27.5067	4.7714
H	9.7209	27.8085	3.8725
C	9.6834	26.1386	5.0514
C	9.6282	25.7489	6.3878
C	9.583	26.6344	7.4524
H	9.6015	26.332	8.3524
C	9.5091	27.9917	7.1391
C	9.377	30.2621	7.1835
C	9.2199	31.5834	7.5467
H	9.1425	31.8492	8.4553
C	9.4615	29.0491	9.407
C	8.6418	28.1159	10.0724

H	8.0393	27.5633	9.5888
C	8.7333	28.0246	11.4475
H	8.1832	27.4084	11.9132
C	9.6218	28.8218	12.1545
H	9.6952	28.7425	13.0991
C	10.3747	29.6981	11.4836
H	10.9659	30.26	11.9734
C	10.3316	29.8282	10.0946
H	10.8951	30.4453	9.6432
C	9.7673	25.1388	3.9397
H	10.1848	24.3078	4.2785
H	10.3408	25.4983	3.2188
C	8.468	23.7931	7.0559
C	7.7221	23.0614	6.1133
C	6.5835	22.4062	6.5403
H	6.0986	21.872	5.9212
C	6.1371	22.507	7.8295
C	6.8741	23.2752	8.7555
C	8.0577	23.8843	8.3479
H	8.582	24.3664	8.9779
C	4.9217	21.8827	8.262
C	6.4311	23.4528	10.1306
C	7.6169	23.7391	3.8371
C	8.4001	24.8163	3.3769
C	7.8348	25.6185	2.3816
H	8.3238	26.3613	2.0471
C	6.5822	25.35	1.877
C	5.7142	26.049	0.9826
C	5.8408	27.234	0.2423
H	6.6616	27.7121	0.2548
C	4.7857	27.7093	-0.5013
C	3.6087	26.9727	-0.5232
C	3.4501	25.7634	0.1164
H	2.6487	25.2576	0.0369
C	4.5128	25.3239	0.883
C	5.8812	24.226	2.3316
C	6.3902	23.408	3.3381
H	5.9081	22.6566	3.6624
C	3.6997	23.1075	1.8021
C	2.336	23.3764	1.9574
H	2.0235	24.2734	1.9962
C	1.4557	22.3222	2.0516
H	0.5276	22.4951	2.159
C	1.8964	21.0143	1.9906
H	1.2755	20.2989	2.0328
C	3.2235	20.7607	1.8714
H	3.5308	19.8621	1.8799
C	4.1519	21.8102	1.7328
H	5.0742	21.6262	1.5926
C	4.9219	29.0057	-1.2892
H	5.8333	29.0515	-1.6761
H	4.2774	28.9937	-2.041
C	1.5378	28.1274	-0.603
C	1.5137	29.5153	-0.5462
C	0.4712	30.1603	0.1303
H	0.4619	31.1083	0.1899
C	-0.538	29.424	0.7098
C	-0.5382	28.0233	0.6099
C	0.5028	27.3858	-0.0444
H	0.51	26.4385	-0.1144
C	-1.6234	30.0967	1.3557
C	-1.6311	27.3097	1.1672
C	3.4337	30.8913	-0.4963
C	4.6817	30.2407	-0.458
C	5.6692	30.7935	0.3202
H	6.5277	30.3867	0.3512
C	5.4226	31.9547	1.0707
C	6.2181	32.7206	1.9898
C	7.4945	32.5678	2.5279
H	8.0506	31.858	2.2293
C	7.9554	33.4395	3.4908
C	7.1034	34.4607	3.9255
C	5.8557	34.6821	3.4068
H	5.3177	35.4073	3.7017
C	5.4115	33.8005	2.4315
C	4.1671	32.5958	0.9482
C	3.1686	32.0703	0.1719
H	2.3269	32.5013	0.0933
C	3.102	34.6425	2.0073
C	3.3373	36.013	1.8853
H	4.1711	36.3334	1.5631
C	2.3424	36.8925	2.2429

H	2.4975	37.8267	2.1658
C	1.138	36.4514	2.7059
H	0.4752	37.0759	2.9718
C	0.8831	35.0876	2.7863
H	0.0373	34.7814	3.0876
C	1.8673	34.1738	2.4287
H	1.6946	33.2405	2.47
C	6.2074	27.7347	7.2944
C	1.0047	28.7494	3.5709
C	4.5628	27.6556	3.5959
C	3.8336	25.6428	8.883
C	-0.4081	29.5861	5.4202
C	5.6208	26.5158	5.4756
C	5.4222	31.2893	7.9099
C	3.7331	25.6231	4.4415
C	6.041	28.9009	5.1124
C	1.1235	30.9401	4.1365
C	0.5561	27.4679	4.045
C	2.351	28.7362	3.0996
C	2.9343	32.5411	5.4146
C	5.3627	31.3848	5.5449
C	2.5151	30.9895	3.6902
C	-0.3995	29.7212	8.0679
C	-0.6911	28.5813	7.3831
C	1.0551	25.5012	5.2622
C	0.4031	29.7838	4.2613
C	2.1448	24.76	7.3554
C	0.7637	31.6418	5.2095
C	-0.1504	30.9203	5.9719
C	-0.2238	30.9401	7.3221
C	-0.6636	28.3903	5.9969
C	3.4087	31.8756	4.2973
C	1.3521	26.3445	4.0617
C	-0.2135	27.3196	5.1873
C	4.6762	31.2168	4.3999
C	1.0343	25.3859	7.86
C	1.6531	32.6235	7.336
C	6.0792	30.1758	7.3082
C	2.6459	26.4302	3.6513
C	5.215	28.9174	4.0201
C	3.053	32.6531	7.8406
C	4.2538	24.9807	6.6345
C	3.8338	32.6366	6.5153
C	0.0432	26.2095	7.2445
C	-0.3327	27.4152	8.0984
C	1.6442	32.462	5.9165
C	3.14	27.6326	3.1828
C	3.0904	29.8595	3.1994
C	6.182	27.6853	5.8638
C	4.5536	30.0045	3.7179
C	0.0032	26.1534	5.9359
C	4.8803	26.5257	4.3639
C	3.3997	24.8687	5.6337
C	0.6536	31.8131	8.0928
C	5.0473	32.0404	6.726
C	3.3425	25.0004	7.9792
C	2.0991	24.9477	5.6531
C	6.1689	30.0572	5.9885
C	6.0704	29.0623	8.018
C	2.4921	28.6209	10.2886
C	3.2444	27.458	10.089
C	2.7196	26.2655	9.5401
C	1.3457	26.2391	9.2185
C	0.5574	27.4481	9.2711
C	1.1025	28.5748	9.8977
C	0.3827	29.7969	9.382
C	1.0848	31.0587	9.2129
C	2.3781	31.1377	9.7868
C	2.9974	29.9287	10.2637
C	3.3161	32.0107	8.9994
C	4.5832	31.2333	9.0466
C	4.4287	29.9452	9.7924
C	5.2268	28.9075	9.2906
C	4.6208	27.682	9.6343
C	4.9201	26.5949	8.8858
C	5.6465	26.5949	7.7574
C	5.2624	25.7417	6.6955

13. References

S1. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

S2. P. Yang, Y. Jian, X. Zhou, G. Li, T. Deng, H. Shen, Z. Yang, Z. Tian, *J. Org. Chem.*, 2016, **81**, 2974-2980.

S3. F. Zhang, X. -S. Du, D. -W. Zhang, Y. -F. Wang, H. -Y. Lu, C. -F. Chen, *Angew. Chem. Int. Ed.*, 2021, **60**, 15291-15295.

S4. P. Thordarson, *Chem. Soc. Rev.*, 2011, **40**, 1305-1323.

S5. D. B. Hibbert and P. Thordarson, *Chem. Commun.*, 2016, **52**, 12792-12805.

S6. http://app.supramolecular.org/bindfit/