Supporting Information

Corannulene-Based Acenes

Qi Xu,[1,2] Chu Wang,[1] Xuebo Chen,[1] Ying Wang,[1] Zhenyao Shen[2] and Hua Jiang*[1]

[1] College of Chemistry, Beijing Normal University, Beijing 100875, P. R. China
[2] School of Environment, Beijing Normal University, Beijing 100875, P. R. China

*E-mail: jiangh@bnu.edu.cn

CONTENTS

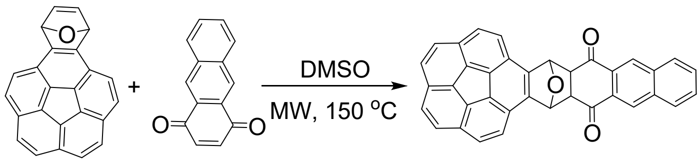
1. General Procedures and Materials 3
2. Synthesis 3
3 X-ray Crystallography....................7
4 Photophysical Study....................13
5 CV and DPV Experiments 14
6 Diels-Alder reactions between **CORA-monPA/bisPA** and **C_{60}** 14
7 Computational Method....................16
8 NMR and Mass Spectra 59
9 Reference....................65

1. General Procedures and Materials

Unless otherwise noted, all materials including dry solvent were obtained from commercial suppliers and used without further purification. All reactions were performed with dry solvents under Argon in dried glassware with standard vacuum-line techniques. Work-up and purification procedures were carried out with reagent-grade solvents under air.

Analytical TLC was carried out using tapered silica plates with a preadsorbent zone. NMR spectra were recorded on JOEL 400 MHz and JOEL 600 MHz. Chemical shifts were reported relative to the standard solvent signals on literature. The chemical shift references were as follows: (^{1}H) dichloromethane-d, 5.32 ppm; (^{13}C) dichloromethane-d, 53.84; (^{1}H) chloroform-d, 7.26 ppm; (^{13}C) chloroform-d, 77.16 ppm. Mass spectra (ESI, MALDI-TOF) were acquired on GCT and FT-ICR spectrometer (Bruker Daltonics Inc. APEXII, BIFLEX III), respectively. Emission spectrum were measured on FS5 and FLS980, and UV-Vis spectrum were recorded on Shimadzu UV- 3600.

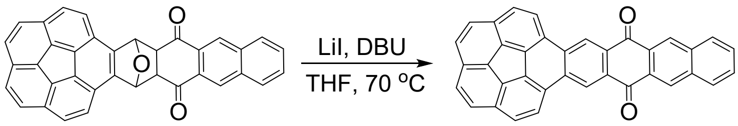
2. Synthesis



1 **2** 3

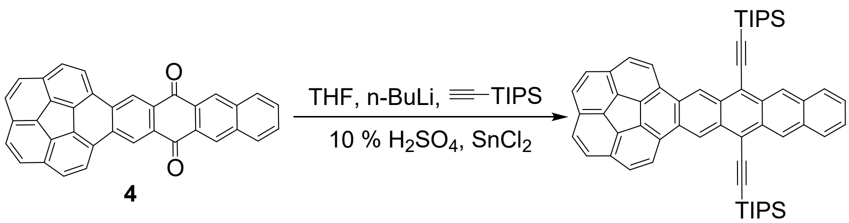
Into to an oven-dried (10-20 mL) glass reaction vial equipped with a Teflon coated magnetic stirring bar was placed **1** (150 mg, 0.47 mmol), **2** (200 mg, 0.96 mmol) and 3,6-di-(2-pyridyl)-1,2,4,5-tetrazine (225 mg, 0.95 mmol). The vial was then sealed with a PTFE-Silicon septum in an Intellivent Cap and purged repeatedly with argon. Anhydrous DMSO (10 mL) was added to this solid mixture, and the vial was then irradiated with microwaves in a CEM Discover Microwave Unit, at 150 °C for 1 hour under argon atmosphere. The reaction mixture was cooled and then washed with excess methylene chloride, washed well with water. Removal of the solvent under reduced pressure and purified by column chromatography on SiO_2 (DCM/EA = 10/1, v/v, R_f = 0.30.) to give **3** (156 mg, 66 %) as a yellow solid. m.p. > 300 °C. ^{1}H NMR (600 MHz, Chloroform-*d,* 298 K) δ: 7.84-7.82 (d, J = 8.7 Hz, 2 H), 7.70-7.68 (d, J = 8.7 Hz, 2 H), 7.50-7.49 (d, J = 8.5 Hz, 2 H), 7.23-7.22 (d, J = 8.6 Hz, 2 H), 7.12-7.11 (dd, J_1 = 6.3 Hz, J_2 = 3.1 Hz, 2 H), 6.73-6.71 (dd, J_1 = 6.1 Hz, J_2 = 3.3 Hz, 2 H), 6.53-

6.52 (dd, J_1 = 3.6, J_1 = 1.9 Hz, 2 H), 6.51 (s, 2 H), 3.88-3.87 (dd, J_1 = 3.8 Hz, J_2 = 1.8 Hz, 2 H). ^{13}C (100 MHz, $CDCl_3$, 298 K) δ: 193.5, 141.8, 140.1, 136.9, 135.7, 134.3, 132.9, 131.9, 130.3, 129.7, 129.6, 129.5, 129.0, 127.9, 127.6, 127.5, 127.3, 127.1, 126.8, 126.3, 126.1, 125.0, 124.6, 83.0, 53.5, 50.8. HR-MS (ESI): Exact mass calculated for $[C_{36}H_{19}O_3]^+$: m/z = 499.1256, found: m/z (%) = 499.1707 (100).



3 4

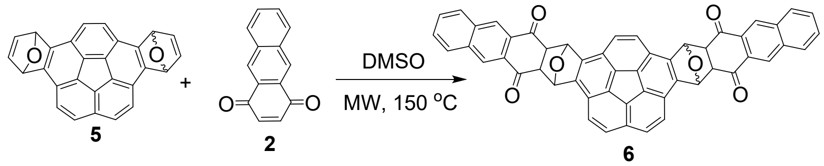
A suspension of **3** (50 mg, 0.1 mmol), DBU (0.15 mL, 1 mmol) and LiI (15 mg, 0.11 mmol) in dry THF (20 mL) was refluxed for 3 h. After cooling the reaction mixture to room temperature, the resulting yellow crude mixture was filtered and the residue washed with 100 mL THF, 50 mL H_2O and 50 mL methanol. After drying in vacuum 41 mg of yellow solid **4** (Yield: 82 %) could be isolated. m.p. > 300 °C. Very low solubility of 4 in common deuterated solvents prevented its characterization by NMR.



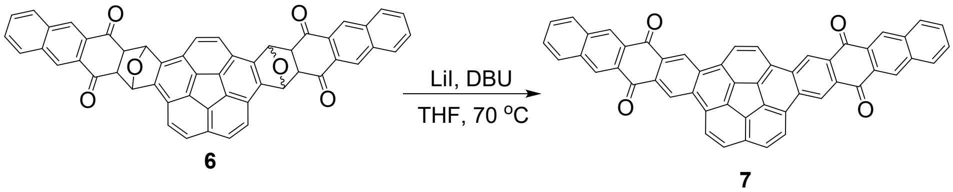
4

CORA-monPA

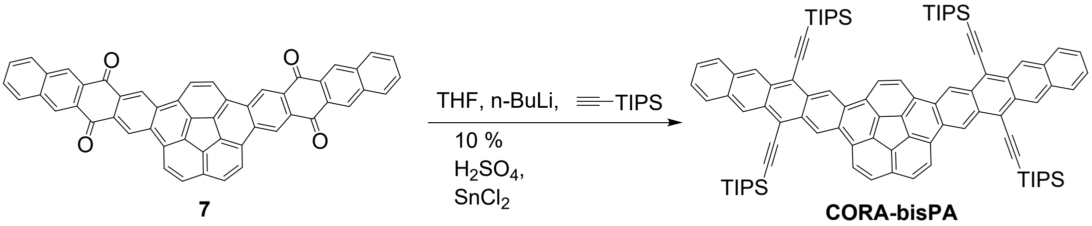
To a solution of 0.285 mL (0.127 mmol) of triisopropylsilyl acetylene in 3 mL dry hexane cooled to -10 °C was added 0.75 mL n-BuLi (1.6 M in hexane, 1.2 mmol) drop wise. After stirring for 1 h at -10 °C, the solution was diluted with 8 mL of dry hexane and 2 mL of dry THF and 40 mg (0.083 mmol) **4** was added in portions. The resulting suspension was stirred for at last 2 h at -10 °C and then at RT for 20 h. 2.5 mL of a degassed 10 % H_2SO_4 was added and the mixture was stirred for 5 min at RT and then 150 mg $SnCl_2$ (0.79 mmol) was added. The resulting red mixture was stirred for 1 h in the dark at RT, excess with 200 ml DCM and subjected to H_2O workup (3 x 200 mL). The organic fractions were separated and solvent was removed on a rotary evaporator. The crude product was purified by column chromatography on SiO_2 (PE/DCM = 5/1, v/v, R_f = 0.25.) to give **CORA-monPA** (20 mg, 30 %) as a black solid. m.p. > 300 °C. ^{1}H NMR (400 MHz, Chloroform-*d,* 298 K) δ: 9.85 (s, 2 H), 9.42 (s, 2 H), 8.29-8.27 (d, J = 8.6 Hz, 2 H), 8.09-8.06 (dd, J_1 = 6.5 Hz, J_2 = 3.3 Hz, 2 H), 7.97-7.95 (d, J = 8.6 Hz, 2 H), 7.85-7.78 (m, 4 H), 7.52-7.50 (dd, J_1 = 6.7 Hz, J_1 = 3.1 Hz, 2 H), 1.46-4.45 (42 H). ^{13}C (100 MHz, $CDCl_3$, 298 K) δ: 135.7, 132.8, 132.4, 131.0, 130.8, 130.7, 129.2, 128.8, 127.9, 127.2, 126.5, 126.3, 124.1, 123.8, 118.9, 107.0, 104.4, 19.2, 11.9. HR-MS (MALDI-TOF): Exact mass calculated for [$C_{58}H_{58}Si_2$]: m/z = 810.4077, found: m/z (%) = 810.3805 (100).



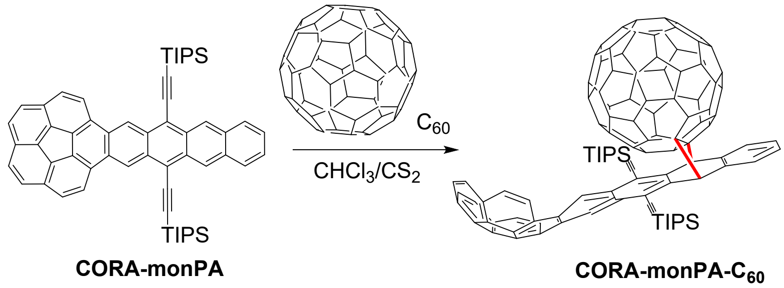
Into to an oven-dried (10-20 mL) glass reaction vial equipped with a Teflon coated magnetic stirring bar was placed **5** (147 mg, 0.39 mmol), **2** (300 mg, 1.44 mmol) and 3,6-di-(2-pyridyl)-1,2,4,5-tetrazine (250 mg, 1.06 mmol). The vial was then sealed with a PTFE-Silicon septum in an Intellivent Cap and purged repeatedly with argon. Anhydrous DMSO (20 mL) was added to this solid mixture, and the vial was then irradiated with microwaves in a CEM Discover Microwave Unit, at 150 °C for 1 hour under argon atmosphere. The reaction mixture was cooled and then washed with excess methylene chloride, washed well with water. Removal of the solvent under reduced pressure and purified by column chromatography on SiO_2 (DCM/EA = 8/1, v/v, R_f = 0.30.) to give **6** (134 mg, 46 %) as a yellow solid. m.p. > 300 °C. ^1H NMR (600 MHz, CD_2Cl_2, 298 K) δ: 8.57 (s, 1 H), 8.24 (d, J = 1.3 Hz, 2 H), 8.02 (d, J = 1.3 Hz, 4 H), 7.84-7.82 (d, J = 8.7 Hz, 3 H), 7.77-7.76 (d, J = 8.5 Hz, 3H), 7.66-7.65 (d, J = 3.4 Hz, 4H), 7.64 (s, 1 H), 7.61-7.58 (dd, J_1 = 8.5 Hz, J_1 = 4.5 Hz, 6 H), 7.28-7.27 (m, 4 H), 7.04 (s 1 H), 6.97-6.94 (2 H), .68 (m, 2 H), 6.56-6.53 (m, 5 H), 6.46-6.43 (m, 8 H), 6.33 (d, J = 0.8 Hz, 2H), 3.81 (dt, J_1 = 4.0 Hz, J_2= 1.4 Hz, 4H). ^{13}C (100 MHz, $CDCl_3$, 298 K) δ: 193.8, 193.7, 184.7, 171.2, 141.8, 141.7, 140.1, 137.7, 136.7, 135.2, 135.0, 134.9, 133.9, 133.7, 131.9, 131.7, 130.3, 129.6, 128.9, 128.7, 128.4, 127.9, 127.8, 127.5, 127.4, 127.1, 126.9, 126.6, 126.0, 125.6, 125.3, 124.9, 124.5, 124.2, 123.2, 123.1, 123.0, 83.2, 83.0, 60.5, 51.0, 50.8, 21.1, 14.3. HR-MS (ESI): Exact mass calculated for [$C_{52}H_{27}O_6$]$^+$: m/z = 747.1729, found: m/z (%) = 747.3087 (100).



A suspension of **6** (110 mg, 0.15 mmol), DBU (0.45 mL, 3 mmol) and LiI (45 mg, 0.33 mmol) in dry THF (30 mL) was refluxed for 3 h. After cooling the reaction mixture to room temperature, the resulting yellow crude mixture was filtered and the residue washed with 100 mL THF, 50 mL H_2O and 50 mL methanol. After drying in vacuum 53 mg of yellow solid **7** (Yield: 50 %) could be isolated. m.p. > 300 °C. Very low solubility of 4 in common deuterated solvents prevented its characterization by NMR.



To a solution of 0.285 mL (0.127 mmol) of triisopropylsilyl acetylene in 3 mL dry hexane cooled to -10 °C was added 0.75 mL n-BuLi (1.6 M in hexane, 1.2 mmol) drop wise. After stirring for 1 h at -10 °C, the solution was diluted with 8 mL of dry hexane and 2 mL of dry THF and 46 mg (0.06 mmol) **7** was added in portions. The resulting suspension was stirred for at last 2 h at -10 °C and then at RT for 20 h. 2.5 mL of a degassed 10 % H_2SO_4 was added and the mixture was stirred for 5 min at RT and then 150 mg $SnCl_2$ (0.79 mmol) was added. The resulting red mixture was stirred for 1 h in the dark at RT, excess with 200 ml DCM and subjected to H_2O workup (3 x 200 mL). The organic fractions were separated and solvent was removed on a rotary evaporator. The crude product was purified by column chromatography on SiO_2 (PE/DCM = 4/1, v/v, R_f = 0.25.) to give **CORA-bisPA** (21 mg, 24 %) as a black solid. m.p. > 300 °C. ^{1}H NMR (600 MHz, Chloroform-*d,* 298 K) δ: 9.94 (s, 2H), 9.85 (s, 2H), 9.42 (d, *J* = 7.0 Hz, 4H), 8.44 (s, 2H), 8.36 (d, *J* = 8.6 Hz, 2H), 8.08 (t, *J* = 5.5 Hz, 4H), 8.05 (d, *J* = 8.5 Hz, 2H), 7.53–7.50 (m, 4H), 1.49 (d, *J* = 5.7 Hz, 42H), 1.46 (d, *J* = 5.9 Hz, 42H). ^{13}C (100 MHz, $CDCl_3$, 298 K) δ: 137.4, 136.0, 135.3, 133.0, 132.8, 132.4, 131.7, 131.2, 131.1, 130.8, 130.7, 130.1, 130.0, 129.8, 129.6, 129.3, 128.8, 128.1, 126.6, 126.5, 126.3, 124.9, 124.1, 124.0, 119.0, 118.9, 107.1, 107.0, 104.4, 19.2, 11.9. HR-MS (MALDI-TOF): Exact mass calculated for [$C_{96}H_{106}Si_4$]: m/z = 1371.7405, found: m/z (%) = 1371.7425 (100).



To a solution of **CORA-monPA** (10 mg, 0.012 mmol) in $CHCl_3$ (4 mL), C_{60} (10 mg, 0.014 mmol) in CS_2 (2 mL) was added. The reaction mixture was stirred at 24 h at room temperature. Then the solvent was removed on a rotary evaporator. The crude product was purified by column chromatography on SiO_2 (PE/DCM = 5/1, v/v, R_f = 0.23.) to give **CORA-monPA-C_{60}** (11 mg, 58 %) as a black solid. m.p. > 300 °C. ^{1}H NMR (400 MHz, Chloroform-*d,* 298 K) δ: δ 9.80 (s, 2H), 8.34 (d, J = 8.8 Hz, 2H), 7.99 (d, J = 8.7 Hz, 2H), 7.88–7.80 (m, 6H), 7.56 (dd, J_1 = 5.5 Hz, J_2 = 3.2 Hz, 2H), 6.68 (s, 2H), 1.33 (q, J = 3.2, 2.4 Hz, 42H). ^{13}C (100 MHz, $CDCl_3$, 298 K) δ: 155.0, 154.7, 147.1, 146.3, 146.2, 146.0, 145.7, 145.4, 145.3, 145.2, 145.1, 144.5, 144.4, 142.8, 142.6, 142.4, 142.2, 141.9, 141.8, 141.5, 140.9, 140.0, 139.8, 136.9, 136.7, 135.5, 135.4, 132.9, 130.7, 129.1, 128.1, 128.0, 127.3, 126.5, 124.4, 123.7, 118.2, 103.4, 102.7, 72.0, 57.0, 29.8, 19.2, 11.7.

3 X-ray Crystallography

Crystals suitable for X-ray analysis were obtained by slow diffusion of acetonitrile into chloroform solution of chlorbenzene or 1,2-dichlorobenzene solutions of **CORA-monPA** and **CORA-bisPA**. The single crystal of **CORA-monPA-C_{60}** was obtained by slow diffusion of acetonitrile into toluene/CS_2 solution. Single-crystal X-ray diffraction data were collected on a Super Nova, Dual, Cu at zero, Atlas S2 diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2[S1], the structure was solved with the ShelXT[S2] structure solution program using Direct Methods and refined with the ShelXL[S3] refinement package using Least Squares minimization. The disordered solvent molecules were removed with the SQUEEZE routine in PLATON[S4] and the solvent-free model was employed for the final refinement. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were positioned by geometric idealization. Additional crystal and refinement information is summarized in **Table S1-3**.

Crystal Structure Data of **CORA-monPA** (CCDC number: 1976762)

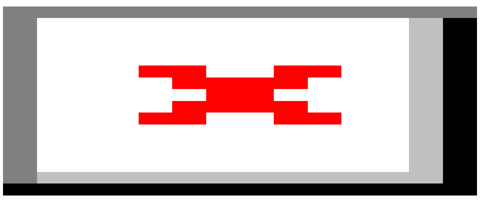


Figure S1. Crystal structure of **CORA-monPA** was obtained by slow diffusion of acetonitrile into chlorbenzene or 1,2-dichlorobenzene solutions. The thermal ellipsoids are set at a 50 % probability level. Hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for compound **CORA-monPA**.

Identification code	**CORA-monPA**
Empirical formula	$C_{116}H_{116}Si_4$
Formula weight	1622.44
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	15.8079(2)
b/Å	17.6450(2)
c/Å	17.2287(3)
α/°	90
β/°	107.979(2)
γ/°	90
Volume/Å^3	4570.95(12)
Z	2
ρ_{calc}g/cm^3	1.179
μ/mm^{-1}	0.979
F(000)	1736.0
Crystal size/mm^3	0.05 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.392 to 151.158
Index ranges	$-19 \leq h \leq 19$, $-22 \leq k \leq 21$, $-20 \leq l \leq 21$
Reflections collected	31565
Independent reflections	15965 [R_{int} = 0.0457, R_{sigma} = 0.0402]
Data/restraints/parameters	15965/1/1105
Goodness-of-fit on F^2	0.909
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.1314
Final R indexes [all data]	R_1 = 0.0509, wR_2 = 0.1350
Largest diff. peak/hole / e Å^{-3}	0.84/-0.41

Crystal Structure Data of **CORA-bisPA** (CCDC number: 2172312)

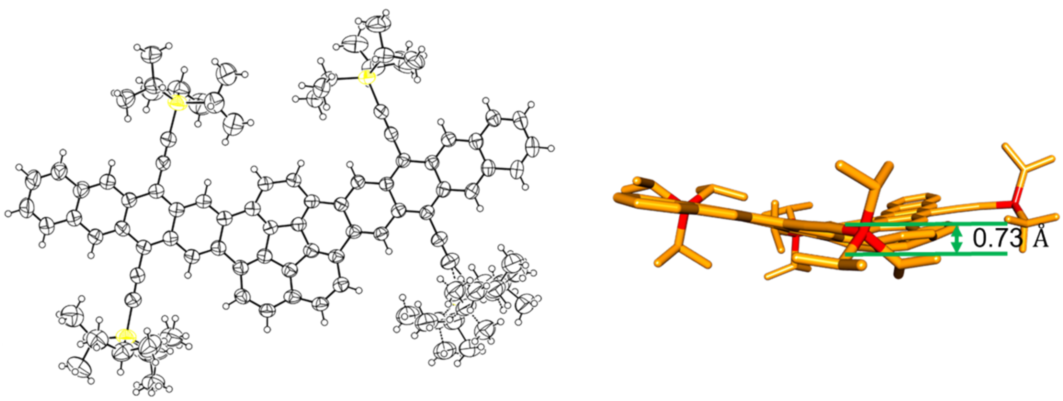


Figure S2. Crystal structure of **CORA-bisPA** was obtained by slow diffusion of acetonitrile into chlorbenzene or 1,2-dichlorobenzene solutions. The thermal ellipsoids are set at a 50% probability level. Hydrogen atoms are omitted for clarity.

Table S2. Crystal data and structure refinement for compound **CORA-bisPA**.

Identification code	**CORA-bisPA**
Empirical formula	$C_{96}H_{106}Si_4$
Formula weight	1372.16
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.74760(10)
b/Å	16.0057(3)
c/Å	57.0011(11)
α/°	90
β/°	92.5220(10)
γ/°	90
Volume/Å^3	7973.1(2)
Z	4
ρ_{calc}g/cm^3	1.143
μ/mm^{-1}	1.032
F(000)	2952.0
Crystal size/mm^3	0.35 × 0.31 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.224 to 134.158
Index ranges	$-8 \leq h \leq 10$, $-19 \leq k \leq 19$, $-68 \leq l \leq 65$
Reflections collected	51982
Independent reflections	14177 [R_{int} = 0.0425, R_{sigma} = 0.0340]
Data/restraints/parameters	14177/368/1030
Goodness-of-fit on F^2	1.943
Final R indexes [I>=2σ (I)]	R_1 = 0.1390, wR_2 = 0.4377
Final R indexes [all data]	R_1 = 0.1536, wR_2 = 0.4519
Largest diff. peak/hole / e Å^{-3}	1.31/-0.69

Crystal Structure Data of **CORA-monPA-C$_{60}$** (CCDC number: 2172313)

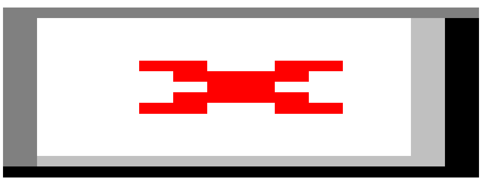


Figure S3. Crystal structure of **CORA-monPA-C$_{60}$** was obtained by slow diffusion of acetonitrile into toluene/CS_2 solution. The thermal ellipsoids are set at a 50% probability level. Hydrogen atoms are omitted for clarity.

Table S3. Crystal data and structure refinement for compound **CORA-monPA-C_{60}**.

Identification code	**CORA-monPA-C60**
Empirical formula	$C_{236}H_{116}Si_4$
Formula weight	3063.64
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	15.8622(3)
b/Å	16.2342(4)
c/Å	32.4713(5)
α/°	101.559(2)
β/°	91.737(2)
γ/°	118.326(2)
Volume/Å^3	7134.6(3)
Z	2
ρ_{calc}g/cm^3	1.426
μ/mm^{-1}	0.930
F(000)	3176.0
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.28 to 144.448
Index ranges	$-17 \leq h \leq 19$, $-20 \leq k \leq 18$, $-32 \leq l \leq 39$
Reflections collected	53863
Independent reflections	27273 [R_{int} = 0.0341, R_{sigma} = 0.0454]
Data/restraints/parameters	27273/0/2161
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0986, wR_2 = 0.2744
Final R indexes [all data]	R_1 = 0.1204, wR_2 = 0.2983
Largest diff. peak/hole / e Å^{-3}	1.87/-1.12

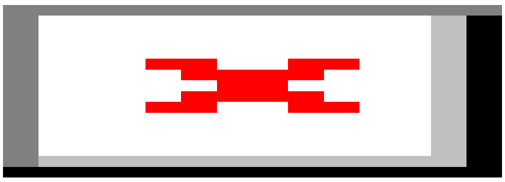


Figure S4. Crystal packing of **CORA-monPA** from top (a) and side (b) view, hydrogen atoms are omitted for clarity.

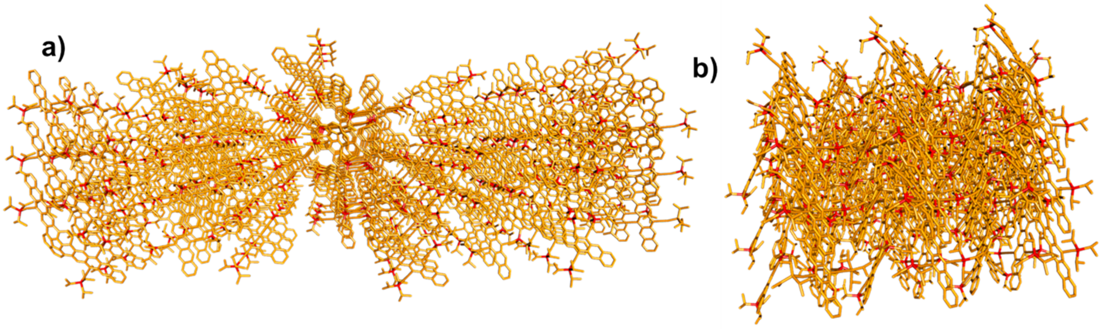


Figure S5. Crystal packing of **CORA-bisPA** from top (a) and side (b) view, hydrogen atoms are omitted for clarity.

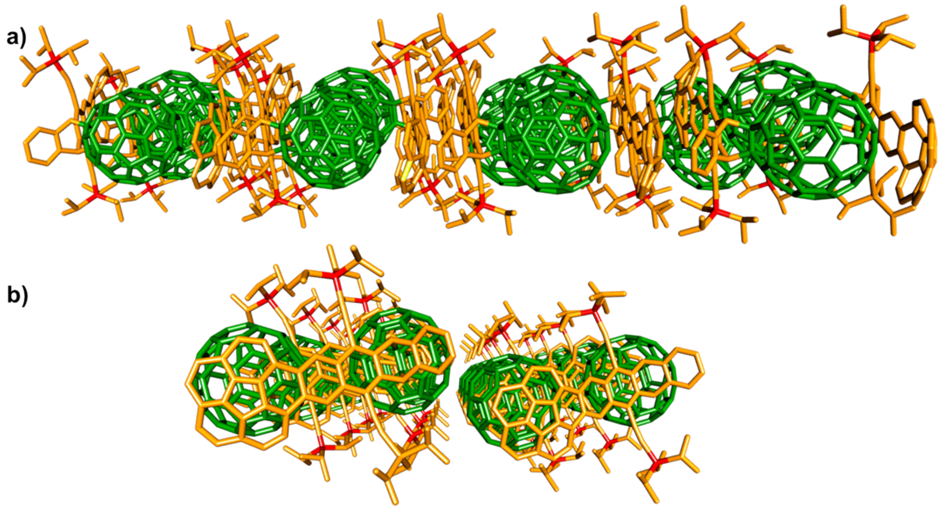


Figure S6. Crystal packing of **CORA-monPA-C$_{60}$** from top view, hydrogen atoms are omitted for clarity.

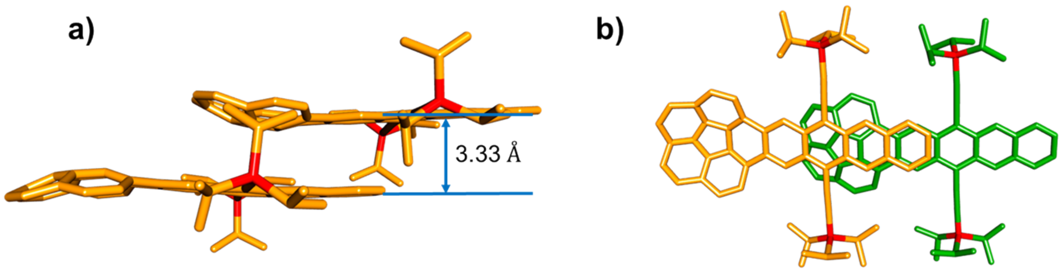


Figure S7. The distances of **CORA-monPA** in the solid phase. Hydrogen atoms are omitted for clarity.

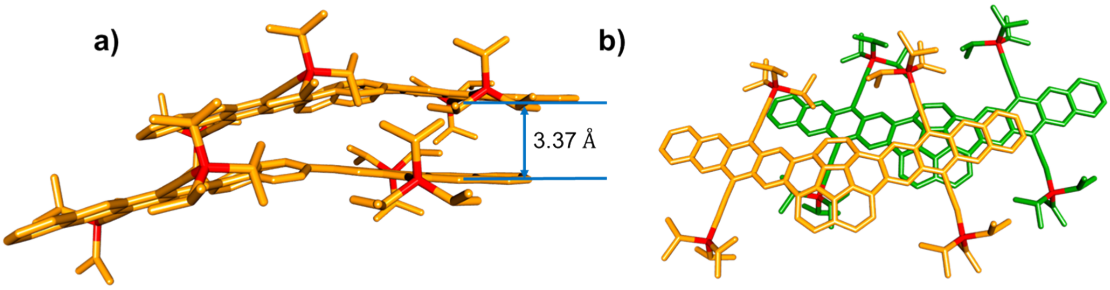


Figure S8. The distances of **CORA-bisPA** in the solid phase. Hydrogen atoms are omitted for clarity.

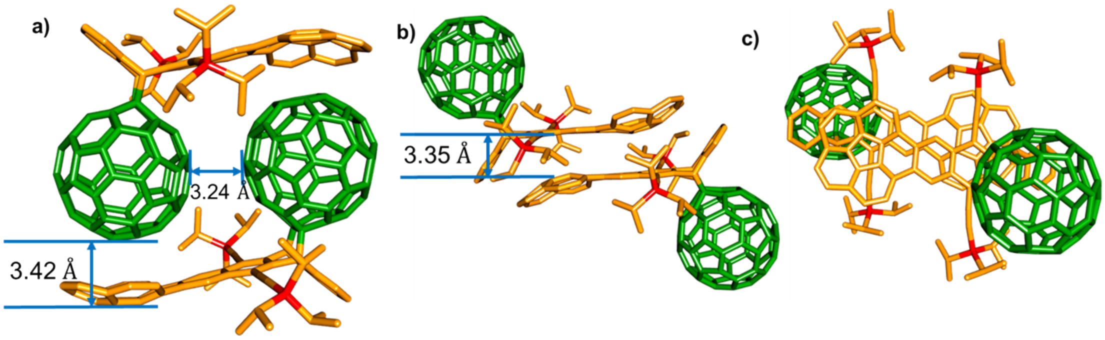


Figure S9. The distances of **CORA-monPA-C_{60}** in the solid phase. Hydrogen atoms are omitted for clarity. Furthermore, the crystal packings reveal that the surface–to–surface distance between corannulene unit and C_{60} and the C_{60}–C_{60} in the dimer formed by the adduct CORA-monPA-C_{60}, as shown in Figure S9, are close to the distance of aromatic π-π stacks, suggesting that the intermolecular repulsion of CORA-monPA-C_{60} is smaller than that of CORA-monPA-C_{60}-3 and consequently leading to the formation of the stable adduct of CORA-monPA-C_{60}.

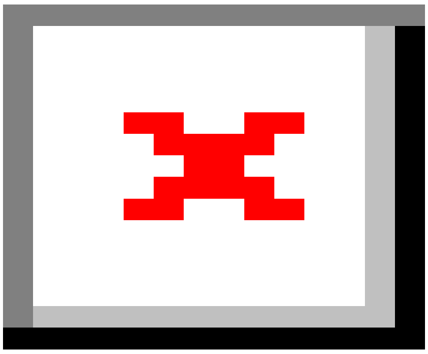


Figure S10. Bond lengths for **CORA-monPA** are listed, *t*-Bu groups and hydrogen atoms are omitted for clarity.

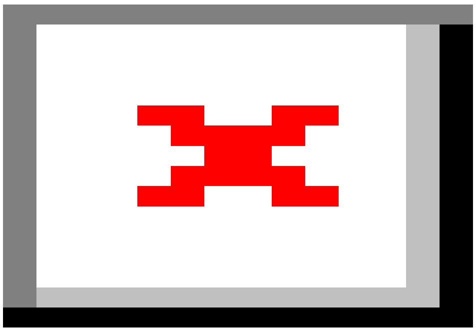


Figure S11. Bond lengths for **CORA-bisPA** are listed, *t*-Bu groups and hydrogen atoms are omitted for clarity.

4 Photophysical Study

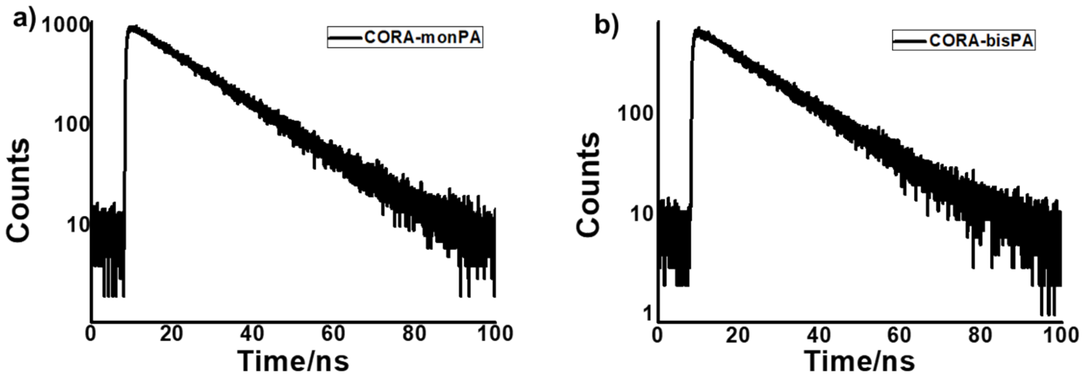


Figure S12. Fluorescence lifetimes measured at 603 nm, 607 nm for **CORA-monPA** and **CORA-bisPA** in $CHCl_3$, respectively.

Table S4. Absorption and emission data for bis(TIPS-ethynyl)-substituted tetracene (**TIPS-Tc**) and bis(TIPS-ethynyl)-substituted pentacene (**TIPS-Pc**).

Compounds	**λ_{abs}[nm]** [S5]	**λ_{em}[nm]** [S5]	**Φ_F** [S5]
TIPS-Tc	534	546	64 %
TIPS-Pc	643	652	21 %

5 CV and DPV Experiments

CV and DPV experiments were carried out with an electrochemical workstation from Chenhua Instruments Co. (Shanghai, China), employing a glass carbon electrode with 4 mm in diameter as the working electrode, a platinum wire as counter electrode and an Ag/AgCl electrode as reference electrode. 0.1 M of tetrabutylammonium perchlorate (TBAP) in DCM was used as electrolyte.

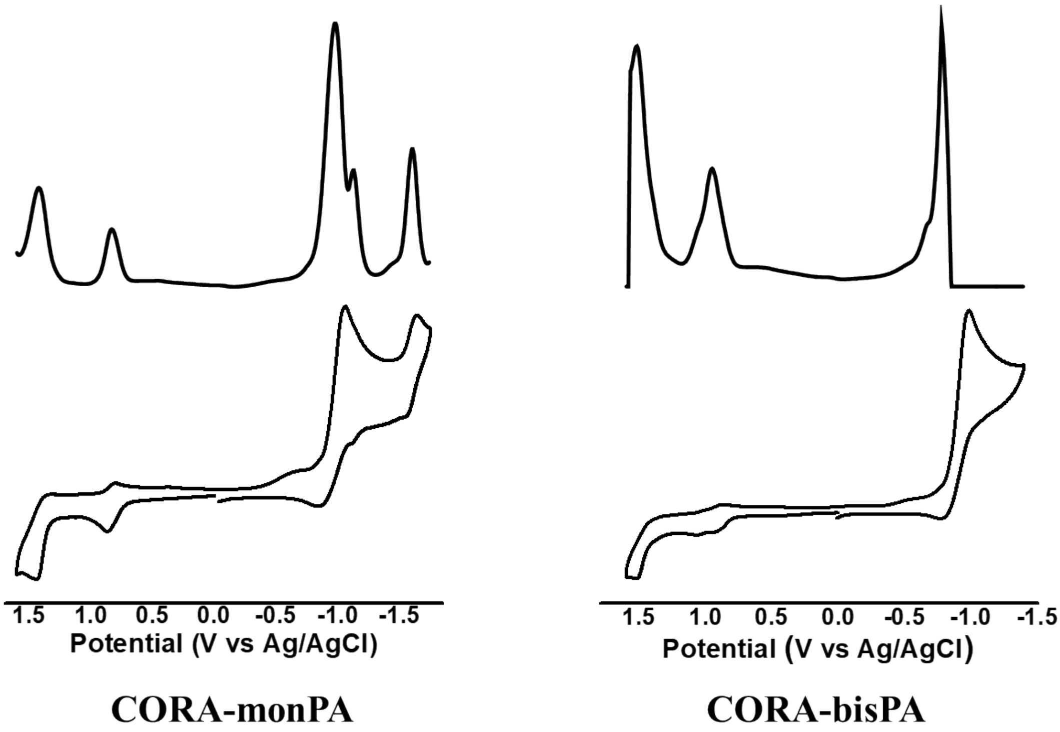


Figure S13. DPV (Top) and CV (Bottom) experiments of **CORA-monPA** (a) and **CORA-bisPA** (b) at 298 K.

6 Diels-Alder reactions between CORA-monPA/bisPA and C_{60}

Using the second-order rate law, $1/\mathbf{c}_{\text{CORA-monPA}} = kt + 1/\mathbf{c}_0$, the association rate constant (k) was determined at the early stage of the Diels-Alder reaction from the slope of the straight line in the plot of $1/[\mathbf{c}_{\text{CORA-monPA}}]$ against t (hours or mins) at T K, k = slope, the half-life of the Diels-Alder reaction was given by $t_{1/2} = 1/(kc_0)$. $[\mathbf{c}_{\text{CORA-monPA}}]$ was determined based on $[\mathbf{c}_0]$ - $[\mathbf{c}_{\text{CORA-monPA-C60}}]$, where $[\mathbf{c}_{\text{CORA-monPA-C60}}]$ is the concentration of the adduct from over a period of time determined from the integration of characteristics signal.

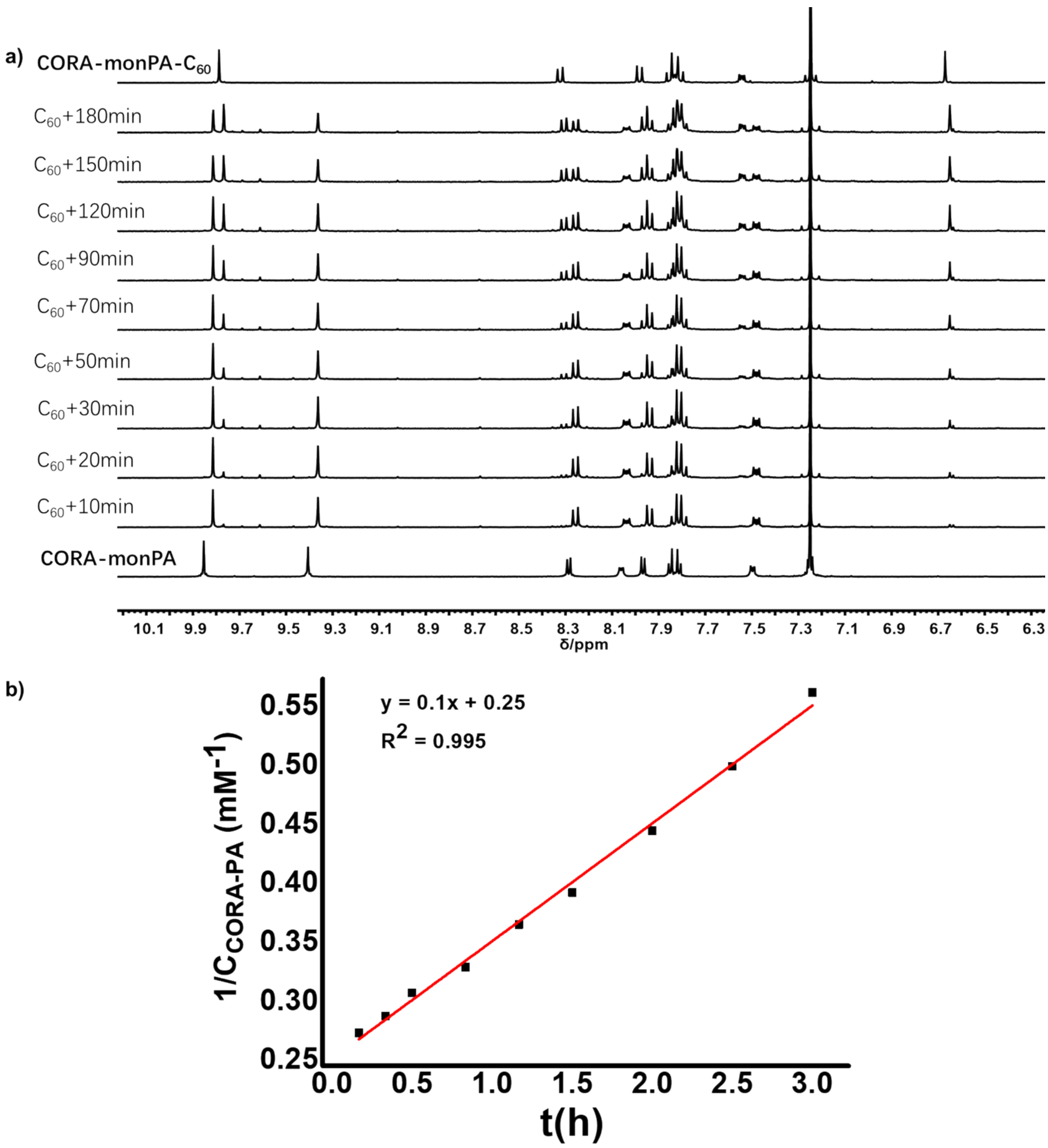


Figure S14. (a) Partial ^{1}H NMR (400 MHz, 298 K) spectra at various time intervals of **CORA-monPA** (4.0 mM, $CDCl_3$, C_0 = 4.0 mM) mixed with 1.0 equiv C_{60} at 298 K. (b) The linear plot of 1/$\mathbf{c}_{\text{CORA-monPA}}$ VS t at 298 K. The [$\mathbf{c}_{\text{CORA-monPA}}$] and [$\mathbf{c}_{\text{CORA-monPA-C60}}$] of the reaction of **CORA-monPA** added equimolar C_{60} with time at 298 K. [$\mathbf{c}_{\text{CORA-monPA}}$] and [$\mathbf{c}_{\text{CORA-monPA-C60}}$] were determined based on the integration values of the signals at δ 9.81 ppm and 9.76 ppm, respectively. k($\mathbf{c}_{\text{CORA-monPA-C60}}$) = slope = 0.1 $mM^{-1}h^{-1}$ = 0.028 $M^{-1}S^{-1}$, $t_{1/2(\mathbf{c}_{\text{CORA-monPA-C60}})}$ = 2.5 h.

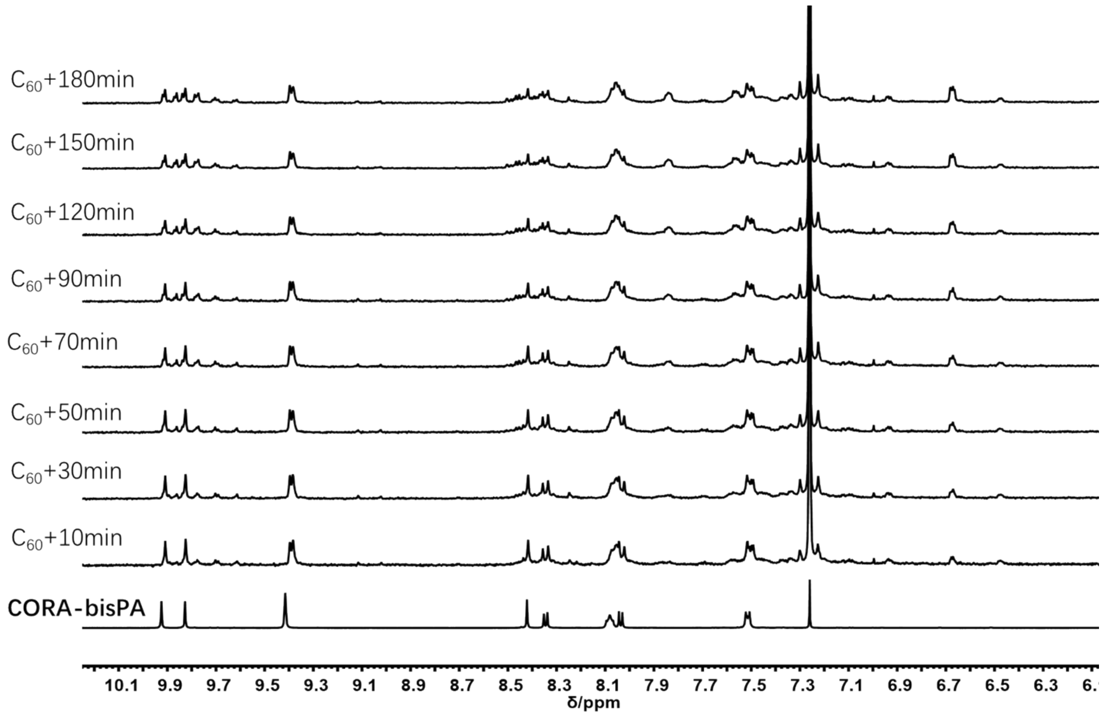


Figure S15. Partial ^{1}H NMR (400 MHz, 298 K) spectra at various time intervals of **CORA-bisPA** (4.0 mM, $CDCl_3$) mixed with 2.0 equiv C_{60} at 298 K.

7 Computational Method

All calculations were performed using the Gaussian 09[S6] program package. The geometries of molecule **CORA-monPA/bisPA** were first optimized at the B3LYP level of density functional theory (DFT) with the 6-31G(d) basis set and polarizable continuum solvation model (PCM). All structures are ground-state minima according to the analysis of their harmonic vibrational analytical frequencies computed at the same level, which show no imaginary frequencies. The first sixty vertical transition energies for **CORA-monPA/bisPA** were calculated by time-dependent density functional theory (TD-DFT) at the B3LYP/6-31G(d)/PCM level. All bright states (oscillator strength f > 0.1) and corresponding main single electron transition are listed in Table **S4-5**. UV-vis spectra of **CORA-monPA/bisPA** were simulated according to TD-DFT results. Nucleus independent chemical shifts (NICS) calculations of **CORA-monPA/bisPA** are at the GIAO-B3LYP/6-311+G(2d,p)/PCM level and were all carried out according to published procedures.[S7] The ACID plots were generated with Gaussian 09 using the CSGT method and ACID 2.0.0.[S8] The geometries involved in the DA reaction of C_{60} with **CORA-monPA** were optimized at the M06-2X level of density functional theory (DFT) with the 6-31G(d) basis set and polarizable continuum solvation model (PCM).[S9] Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary frequency) and to evaluate zero-point energy and Gibbs free energy at 298 K and 1 atm. Transition states were also verified by IRC calculations.

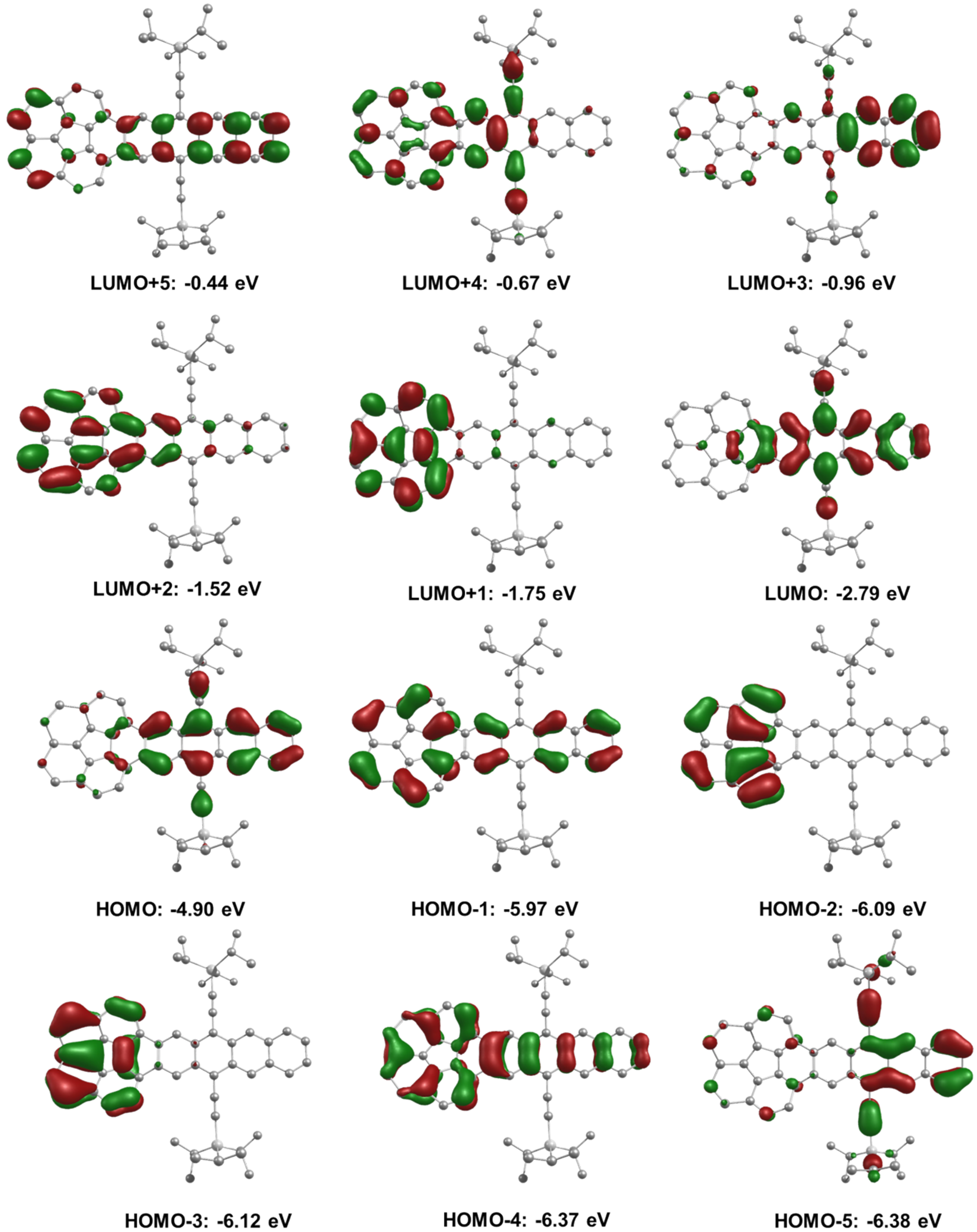


Figure S16. Kohn-Sham frontier orbitals and frontier orbital energies for **CORA-monPA** at the optimized S0 geometry at B3LYP/6-31G(d) level of theory in chloroform solution.

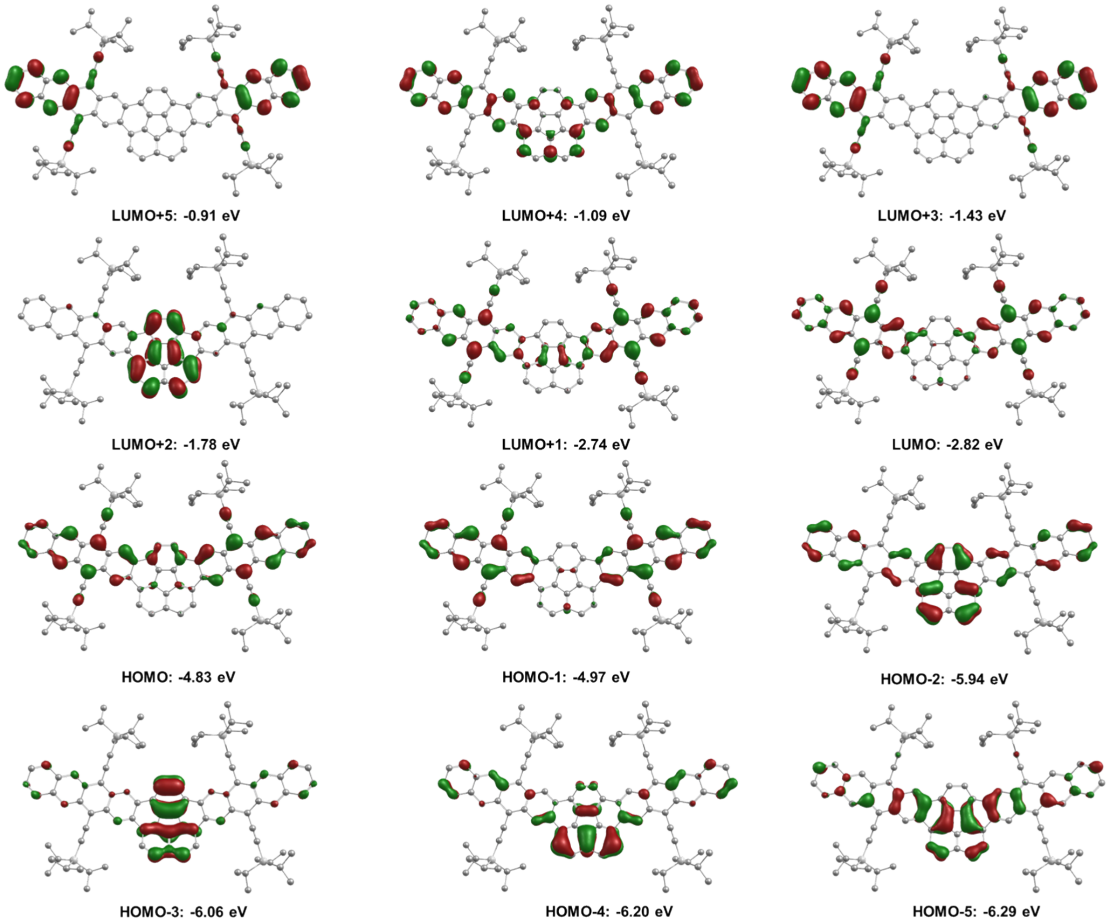


Figure S17. Kohn-Sham frontier orbitals and frontier orbital energies for **CORA-bisPA** at the optimized S0 geometry at B3LYP/6-31G(d) level of theory in chloroform solution.

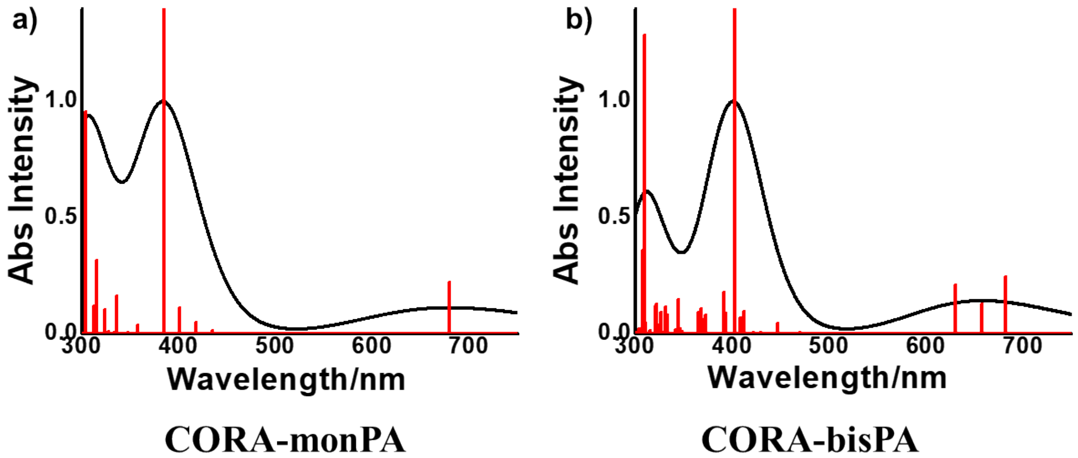


Figure S18. Simulated UV-vis spectra of **CORA-monPA** (a) and **CORA-bisPA** (b) at the B3LYP/6-31G(d)/PCM level of theory.

Table S5. TD-DFT singlet excitation energies E, excitation wavelengths λ, oscillator strengths $f > 0.1$, and orbital contributions for **CORA-monPA** at the optimized S0 ground state geometry in chloroform.

Energy (eV)	Wavelength (nm)	Osc. Strength	Major contributions
1.83	679	0.2213	H→L (100%)
3.09	401	0.1110	H-5→L (90%)
3.22	385	1.7884	H-4→L (62%)
			H→L+2 (33%)
3.69	336	0.1648	H-3→L+2 (20%)
			H-1→L+1 (37%)
			H→L+4 (33%)
3.94	315	0.3162	H-10→L (28%)
			H-1→L+2 (22%)
			H→L+5 (29%)
3.96	313	0.1208	H-3→L+2 (64%)
			H-1→L+1 (22%)
4.07	304	0.9566	H-10→L (22%)
			H-4→L+1 (18%)
			H-2→L+2 (12%)
			H-1→L+2 (15%)
			H→L+5 (22%)
4.16	298	0.1225	H-4→L+1 (17%)
			H-3→L+1 (14%)
			H-2→L+2 (53%)
4.38	283	0.1556	H-5→L+1 (14%)
			H-4→L+2 (62%)
4.95	251	0.2186	H-5→L+3 (75%)
4.98	249	0.1106	H-2→L+3 (16%)
			H-2→L+4 (60%)

Table S6. TD-DFT singlet excitation energies E, excitation wavelengths λ, oscillator strengths $f > 0.1$, and orbital contributions for **CORA-bisPA** at the optimized S0 ground state geometry in chloroform.

Energy (eV)	Wavelength (nm)	Osc. Strength	Major contributions
1.82	681	0.2464	H→L+1 (98%)
1.89	657	0.1301	H-1→L (98%)
1.97	630	0.2122	H-1→L+1 (99%)
3.08	402	3.4074	H-5→L (44%)
			H-4→L+1 (11%)
			H→L+3 (37%)
3.17	391	0.1782	H-7→L+1 (25%)
			H-6→L (38%)
			H-4→L (11%)
3.37	368	0.1102	H-7→L (27%)

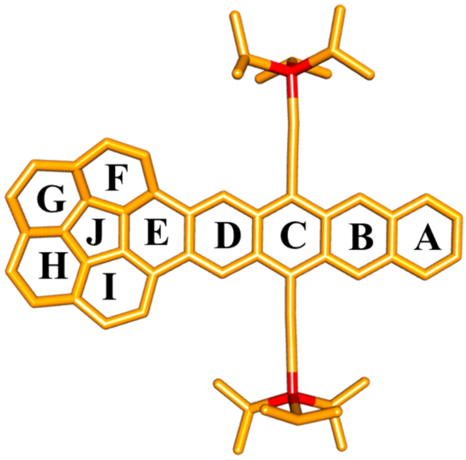
3.60	345	0.1466	H-6→L+1 (51%) H-1→L+4 (11%) H-1→L+5 (14%)
3.60	344	0.1431	H→L+5 (26%) H→L+6 (24%) H-1→L+4 (10%) H-1→L+5 (14%) H→L+5 (24%) H→L+6 (31%)
3.74	331	0.1158	H-2→L+2 (81%)
3.86	321	0.1272	H-1→L+6 (53%) H→L+5 (12%)
3.86	321	0.1195	H-4→L+2 (30%) H-3→L+2 (12%) H-2→L+3 (11%) H-1→L+6 (14%)
4.01	310	1.2887	H-2→L+3 (36%) H-1→L+7 (40%)
4.03	307	0.3601	H-15→L+1 (20%) H→L+7 (55%)
4.20	295	0.1706	H-17→L (11%) H-16→L+1 (11%) H-6→L+2 (11%) H-5→L+3 (10%) H-1→L+7 (24%)

Table S7. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree)[a]

optimized structure	**imaginary frequencies**	**E(H)**	**E+ZPE(H)**	**G(H)**
C_{60}	0	-2285.45657206	-2285.075284	-2285.118236
CORA-monPA	0	-2823.08273276	-2822.086046	-2822.183005
TS1	1	-5108.53832256	-5107.158129	-5107.267146
CORA-monPA-C_{60}	0	-5108.59424510	-5107.210099	-5107.319379
TS2	1	-5108.54321690	-5107.164384	-5107.274929
CORA-monPA-C_{60}-3	0	-5108.58161974	-5107.199995	-5107.309726

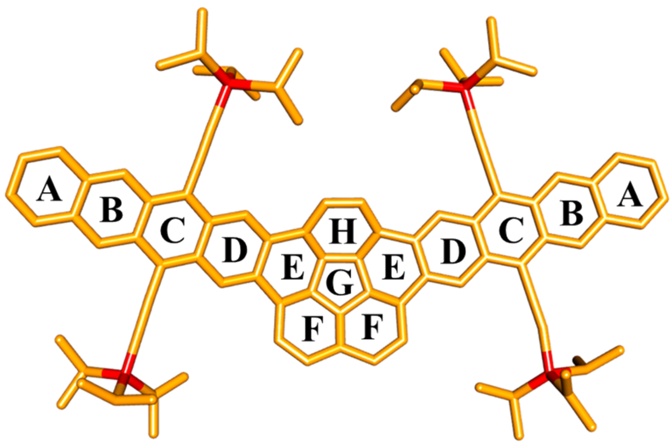
a) *E*: electronic energy; *ZPE*: zero-point energy; *G*: sum of electronic and thermal free energies.

Table S8. NICS(1)$_{ZZ}$ and NICS(-1)$_{ZZ}$ for **CORA-monPA** at the optimized S0 geometry at B3LYP/6-311+G(2d,p) level of theory in chloroform solution. The position 1 Å above the ring center is defined as "1" and the position 1 Å under the ring center is defined as "-1".



	NICS(1)$_{ZZ}$	NICS(-1)$_{ZZ}$	Average value
A	-22.4	-22.6	-22.5
B	-32.7	-32.6	-32.6
C	-26.1	-26.0	-26.0
D	-21.5	-21.6	-21.6
E	-2.7	2.3	-0.2
F	-22.4	-14.8	-18.6
G	-21.0	-14.8	-17.9
H	-24.1	-15.1	-19.6
I	-24.5	-14.3	-19.4
J	12.4	12.1	12.3

Table S9. NICS(1)$_{ZZ}$ and NICS(-1)$_{ZZ}$ for **CORA-bisPA** at the optimized S0 geometry at B3LYP/6-311+G(2d,p) level of theory in chloroform solution. The position 1 Å above the ring center is defined as "1" and the position 1 Å under the ring center is defined as "-1".



	$NICS(1)_{ZZ}$	$NICS(-1)_{ZZ}$	Average value
A	-22.4	-21.8	-22.1
B	-32.3	-31.7	-32.2
C	-25.8	-25.7	-25.8
D	-20.9	-22.0	-21.5
E	-0.1	5.1	2.5
F	-21.0	-13.5	-17.2
G	12.6	10.2	11.4
H	-13.3	-17.0	-15.1

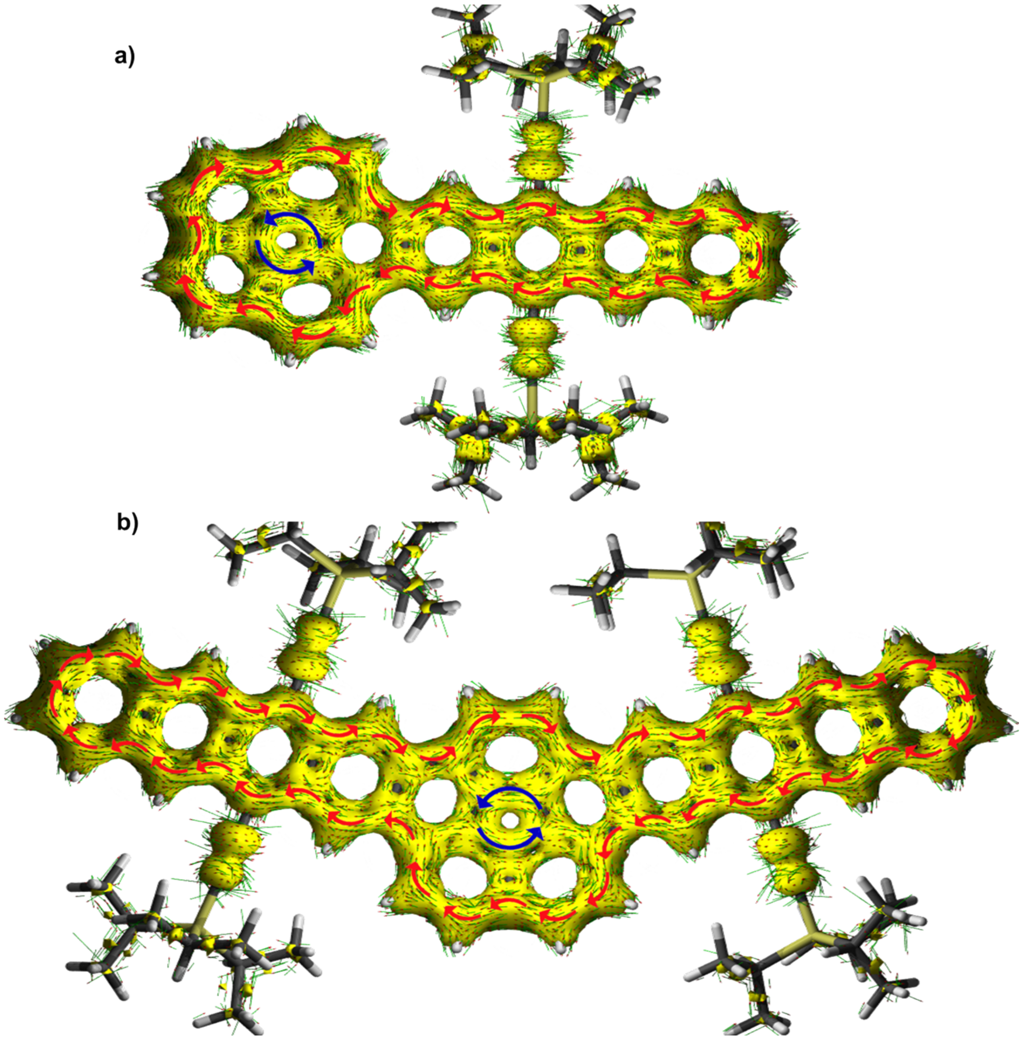


Figure S19. ACID plots of **CORA-monPA** (a) and **CORA-bisPA** (b) (Iso value: 0.05 a.u.). The direction of external magnetic vector is orthogonal with respect to the central ring plane and points upward.

Table S10. Cartesian coordinates of optimized species.

Optimized S0 geometry of **CORA-monPA** (at the B3LYP/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	14	0	9.177416	3.025107	6.379628
2	14	0	10.403508	14.637295	8.445127
3	6	0	10.774180	9.571226	6.753837
4	6	0	9.935769	10.225932	7.709995
5	6	0	11.454255	7.525127	5.574287
6	1	0	11.339490	6.460089	5.400873
7	6	0	10.092183	11.619046	7.946285
8	6	0	7.141761	9.438851	10.090373
9	6	0	6.981643	7.981779	9.852266
10	6	0	7.802828	7.377086	8.924984
11	1	0	7.696416	6.313983	8.737339
12	6	0	12.429436	8.227083	4.867539
13	6	0	9.308152	4.838767	6.726702
14	6	0	4.549076	9.705754	12.750300
15	6	0	9.611986	7.420143	7.229829
16	6	0	4.305371	7.452699	12.388510
17	6	0	8.794641	8.076756	8.183242
18	6	0	5.251362	9.381975	11.570899
19	6	0	10.232390	12.818747	8.149400
20	6	0	12.585278	9.646825	5.102593
21	6	0	5.098573	7.971277	11.344013
22	6	0	8.955989	9.491157	8.422475
23	6	0	9.478642	15.536508	7.027741
24	1	0	9.635604	16.611958	7.204231
25	6	0	10.612789	8.151387	6.513429
26	6	0	13.589210	10.359223	4.368457
27	1	0	13.703996	11.425383	4.547384
28	6	0	11.758957	10.274025	6.033318
29	1	0	11.874458	11.338595	6.211571
30	6	0	4.854896	10.798924	13.549517
31	6	0	8.108537	10.114975	9.378767
32	1	0	8.234845	11.180518	9.538376
33	6	0	13.286747	7.590510	3.911636
34	1	0	13.167365	6.524135	3.737513
35	6	0	9.442826	6.031491	6.972618

36	6	0	3.966407	8.518758	13.256523
37	6	0	4.348427	6.127296	12.798968
38	6	0	6.305287	10.127028	11.098516
39	6	0	10.410823	2.135436	7.547677
40	1	0	10.337798	1.066352	7.294095
41	6	0	5.920012	5.794367	10.911169
42	1	0	6.560023	5.103527	10.369492
43	6	0	5.134867	5.277376	11.942866
44	1	0	5.197701	4.211970	12.151458
45	6	0	12.272837	15.080038	8.510227
46	1	0	12.571623	14.867795	9.548237
47	6	0	5.987305	7.205944	10.627063
48	6	0	12.535667	16.578895	8.254963
49	1	0	12.279650	16.863548	7.227169
50	1	0	13.598940	16.813238	8.400176
51	1	0	11.963485	17.227037	8.928086
52	6	0	5.831571	11.687163	12.973932
53	1	0	6.110090	12.596673	13.501011
54	6	0	4.338567	10.706363	14.900292
55	1	0	4.474105	11.543030	15.581701
56	6	0	11.867677	2.577609	7.307020
57	1	0	12.195863	2.392305	6.278619
58	1	0	12.551596	2.034129	7.973168
59	1	0	11.995540	3.648112	7.508841
60	6	0	14.385914	9.712197	3.463710
61	1	0	15.144066	10.261619	2.912636
62	6	0	14.232746	8.308543	3.232274
63	1	0	14.876893	7.816210	2.509089
64	6	0	6.526202	11.362108	11.807940
65	1	0	7.316457	12.035487	11.486522
66	6	0	13.162807	14.212168	7.599900
67	1	0	13.043379	13.144655	7.812191
68	1	0	14.222259	14.466423	7.740877
69	1	0	12.931153	14.367478	6.538971
70	6	0	3.486140	6.951340	14.978438

71	1	0	3.173862	6.713816	15.992749
72	6	0	3.818228	5.902855	14.128745
73	1	0	3.753584	4.887490	14.512956
74	6	0	7.189931	0.963106	6.813512
75	1	0	7.601252	0.415633	5.958263
76	1	0	6.127908	0.693968	6.891909
77	1	0	7.686458	0.587060	7.716161
78	6	0	3.647784	8.338999	14.590866
79	6	0	7.352071	2.490259	6.669635
80	1	0	6.838518	2.786956	5.741548
81	6	0	10.045418	15.203140	5.633931
82	1	0	11.103321	15.471876	5.538124
83	1	0	9.496743	15.746869	4.852791
84	1	0	9.953370	14.132594	5.413505
85	6	0	3.766473	9.539992	15.394199
86	1	0	3.476792	9.511476	16.442073
87	6	0	10.050795	2.290599	9.038071
88	1	0	10.045483	3.345351	9.339512
89	1	0	10.788158	1.774597	9.668193
90	1	0	9.067381	1.871152	9.276041
91	6	0	7.961075	15.271232	7.065791
92	1	0	7.740438	14.204098	6.939092
93	1	0	7.453767	15.808725	6.253147
94	1	0	7.505085	15.595445	8.007950
95	6	0	10.589049	3.740900	3.917221
96	1	0	10.243652	4.773044	4.034454
97	1	0	10.721935	3.552596	2.842957
98	1	0	11.579105	3.665698	4.383521
99	6	0	9.592826	2.733160	4.521440
100	1	0	8.630884	2.886807	4.007788
101	6	0	10.044440	1.288241	4.222909
102	1	0	11.007232	1.059869	4.696064
103	1	0	10.172661	1.142101	3.141862
104	1	0	9.322392	0.540006	4.568174
105	6	0	9.549545	14.987576	10.127013

106	1	0	8.521157	14.616396	9.998446
107	6	0	9.461535	16.486983	10.472237
108	1	0	10.455531	16.916922	10.645557
109	1	0	8.880877	16.639386	11.392133
110	1	0	8.980008	17.072021	9.679946
111	6	0	6.644024	3.220991	7.825435
112	1	0	7.106143	2.995585	8.794000
113	1	0	5.591168	2.913973	7.888689
114	1	0	6.665656	4.307216	7.689649
115	6	0	10.179067	14.197925	11.290464
116	1	0	10.208999	13.121284	11.087845
117	1	0	9.607837	14.348211	12.216831
118	1	0	11.206989	14.525652	11.490808

Optimized S0 geometry of **CORA-bisPA** (at the B3LYP/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.979681	7.275793	36.222879
2	14	0	3.121610	9.232469	42.292247
3	14	0	11.087809	16.161344	36.887205
4	6	0	4.360448	12.153445	32.602375
5	6	0	-3.679984	10.155182	30.123559
6	6	0	-3.974004	9.475396	31.369024
7	6	0	4.711004	13.264225	31.843355
8	6	0	2.195651	11.799273	31.515289
9	6	0	-2.975005	9.407994	32.391930
10	6	0	-1.410553	10.674187	30.946759
11	6	0	-2.393580	10.750480	29.929418
12	6	0	-6.222644	8.945261	30.545970
13	6	0	-1.702751	9.997251	32.187636
14	6	0	2.862667	10.778865	33.677126
15	6	0	3.145934	11.455384	32.444130
16	6	0	-0.119120	11.245414	30.778235
17	1	0	0.087079	11.744135	29.837269

18	6	0	0.573094	10.475085	33.009054
19	6	0	4.841486	11.918954	33.906629
20	6	0	0.871356	11.175219	31.733258
21	6	0	-4.674555	10.207774	29.128331
22	1	0	-4.451279	10.716114	28.195463
23	6	0	1.599163	10.393660	34.073427
24	6	0	-0.682739	9.933228	33.177175
25	1	0	-0.915528	9.414467	34.101245
26	6	0	-5.928974	9.625610	29.302462
27	6	0	-5.243879	8.890919	31.537013
28	1	0	-5.462399	8.378255	32.468583
29	6	0	-3.540501	8.163956	34.658656
30	6	0	5.713195	12.761695	34.550393
31	6	0	3.903836	11.062891	34.574593
32	6	0	-3.268590	8.741602	33.613309
33	6	0	2.608115	12.837081	30.601171
34	1	0	1.936840	13.155439	29.808148
35	6	0	-2.101773	11.411182	28.704768
36	6	0	7.149614	12.530503	40.983121
37	6	0	6.103539	11.900791	40.237212
38	6	0	3.807293	13.532731	30.752724
39	1	0	4.014300	14.354891	30.071892
40	6	0	5.162740	11.068970	40.905651
41	6	0	-7.514331	8.347407	30.713809
42	1	0	-7.732111	7.836955	31.648596
43	6	0	3.770617	10.985543	35.944944
44	6	0	-6.941905	9.674584	28.289704
45	1	0	-6.718456	10.186757	27.357184
46	6	0	5.752277	14.067084	32.433836
47	1	0	6.129312	14.936780	31.901186
48	6	0	8.959576	14.384630	38.220379
49	6	0	5.828596	12.528437	36.007814
50	6	0	7.999390	13.574734	38.888096
51	6	0	6.814340	13.134602	36.756236
52	1	0	7.532625	13.780183	36.262246

53	6	0	-1.853056	11.975524	27.646493
54	6	0	7.280695	12.341699	42.371944
55	1	0	6.571251	11.694954	42.877783
56	6	0	4.858296	11.644415	36.703199
57	6	0	1.474424	10.168433	35.481733
58	1	0	0.523950	9.850509	35.901214
59	6	0	-8.452350	8.416751	29.720162
60	1	0	-9.428314	7.959714	29.857826
61	6	0	2.514997	10.451894	36.378537
62	1	0	2.308366	10.337344	37.438954
63	6	0	6.954954	12.952951	38.160062
64	6	0	6.002934	12.105508	38.838444
65	6	0	6.224225	13.828947	33.724465
66	1	0	6.945604	14.529565	34.134927
67	6	0	-8.162259	9.089657	28.491301
68	1	0	-8.922854	9.132141	27.716704
69	6	0	8.105241	13.381000	40.302467
70	6	0	9.807379	15.073492	37.665471
71	6	0	4.351182	10.356411	41.484239
72	6	0	9.239595	13.810331	42.434291
73	6	0	4.984177	11.482435	38.065789
74	1	0	4.287005	10.835857	38.587982
75	6	0	8.291684	12.951911	43.112121
76	6	0	9.120605	13.997742	41.058122
77	1	0	9.829720	14.642261	40.548910
78	6	0	8.426039	12.760798	44.526199
79	1	0	7.713525	12.114449	45.032467
80	6	0	11.771463	16.894850	34.162719
81	6	0	10.272345	14.437631	43.204986
82	1	0	10.982560	15.082143	42.693123
83	6	0	3.321466	9.338164	44.206257
84	1	0	2.632190	10.143615	44.504062
85	6	0	9.427946	13.378492	45.223765
86	1	0	9.520564	13.227147	46.295615
87	6	0	-5.570741	8.106303	36.901017

88	1	0	-5.238081	9.130450	37.130486
89	6	0	10.542102	18.363729	38.678748
90	1	0	9.854226	17.732164	39.254499
91	1	0	10.213721	19.404431	38.805679
92	1	0	11.534511	18.276468	39.133760
93	6	0	10.363648	14.228901	44.554141
94	1	0	11.150906	14.708733	45.128869
95	6	0	-2.354138	9.020697	37.847391
96	1	0	-2.113969	9.630943	36.967456
97	1	0	-1.527411	9.135151	38.561848
98	1	0	-3.248443	9.450887	38.311872
99	6	0	12.782748	15.731806	37.689616
100	1	0	13.089318	14.810502	37.169676
101	6	0	2.862825	8.055547	44.931803
102	1	0	1.846247	7.752970	44.656574
103	1	0	2.875704	8.205423	46.019808
104	1	0	3.526923	7.210725	44.714433
105	6	0	-6.719818	8.230431	35.882847
106	1	0	-6.393954	8.719392	34.958238
107	1	0	-7.541914	8.827024	36.301374
108	1	0	-7.134432	7.251467	35.615796
109	6	0	10.544135	17.975145	37.187643
110	1	0	11.295709	18.599108	36.679406
111	6	0	-4.100292	5.413846	35.773443
112	1	0	-3.132980	5.208441	35.288850
113	6	0	-2.546163	7.540038	37.467530
114	1	0	-2.839321	6.997810	38.380099
115	6	0	4.726567	9.748412	44.684902
116	1	0	5.489705	9.018700	44.388798
117	1	0	4.753686	9.822186	45.780845
118	1	0	5.022632	10.720952	44.278738
119	6	0	-4.203112	4.483829	36.998898
120	1	0	-3.394944	4.652181	37.719738
121	1	0	-4.151262	3.431709	36.687584
122	1	0	-5.153142	4.616522	37.529514

123	6	0	1.372688	9.902214	41.858706
124	1	0	1.276450	10.792616	42.500353
125	6	0	-1.220029	6.932124	36.971937
126	1	0	-1.300795	5.856263	36.780494
127	1	0	-0.424230	7.074485	37.715896
128	1	0	-0.885704	7.407610	36.041246
129	6	0	9.892753	15.215363	34.393601
130	6	0	-6.072945	7.483489	38.219329
131	1	0	-6.472818	6.474801	38.060819
132	1	0	-6.883971	8.088280	38.646949
133	1	0	-5.283489	7.412072	38.976796
134	6	0	3.465716	7.461642	41.643407
135	1	0	2.781869	6.803308	42.201013
136	6	0	13.863069	16.796763	37.409697
137	1	0	14.000565	16.982989	36.338874
138	1	0	14.833661	16.475760	37.811462
139	1	0	13.618102	17.755352	37.883368
140	6	0	12.728231	15.400105	39.192764
141	1	0	12.429976	16.267926	39.793253
142	1	0	13.717436	15.083784	39.551381
143	1	0	12.023169	14.589672	39.404293
144	6	0	4.907999	7.007545	41.947731
145	1	0	5.070636	5.979142	41.597311
146	1	0	5.139018	7.029135	43.018417
147	1	0	5.638486	7.647610	41.438596
148	6	0	-5.197354	5.082340	34.744407
149	1	0	-6.199644	5.203363	35.172139
150	1	0	-5.112409	4.038654	34.412238
151	1	0	-5.132871	5.718659	33.854421
152	6	0	9.171212	18.284848	36.558617
153	1	0	9.158128	18.114068	35.476598
154	1	0	8.896096	19.334794	36.728590
155	1	0	8.383524	17.663824	37.002162
156	6	0	3.164624	7.283770	40.142911
157	1	0	3.771842	7.960635	39.529132

158	1	0	2.111949	7.468651	39.903637
159	1	0	3.397564	6.258875	39.823032
160	6	0	1.194190	10.379229	40.405385
161	1	0	1.956542	11.112286	40.120910
162	1	0	0.211079	10.851894	40.274454
163	1	0	1.248742	9.546301	39.694084
164	6	0	0.243122	8.929436	42.254511
165	1	0	0.290426	7.997554	41.677189
166	1	0	-0.739775	9.380371	42.061493
167	1	0	0.274844	8.663184	43.316925
168	14	0	-1.439844	12.789977	26.036458
169	6	0	-2.838893	14.033633	25.601348
170	1	0	-2.584450	14.944236	26.165019
171	6	0	0.231847	13.687907	26.314997
172	1	0	0.911663	12.897561	26.668535
173	6	0	-2.518235	10.565776	24.537110
174	6	0	-0.038456	10.491235	25.037318
175	6	0	-4.242733	13.596144	26.062360
176	6	0	0.839932	14.280179	25.028475
177	6	0	-1.240098	11.404801	24.727118
178	1	0	-1.033771	11.920587	23.776464
179	6	0	0.154820	14.756779	27.421403
180	6	0	11.202409	15.738619	35.011558
181	1	0	11.930183	14.913418	34.967176
182	1	0	0.905366	11.046122	25.083548
183	1	0	-0.168557	9.976107	25.997148
184	1	0	0.071476	9.718928	24.263888
185	1	0	-2.804167	10.060742	25.467877
186	1	0	-3.370364	11.173601	24.213398
187	1	0	-2.361976	9.787878	23.777216
188	1	0	1.836490	14.697331	25.227360
189	1	0	0.950386	13.532516	24.234330
190	1	0	0.223686	15.096712	24.632942
191	1	0	1.150825	15.167455	27.636915
192	1	0	-0.481600	15.599528	27.123545

193	1	0	-0.249615	14.352478	28.356490
194	6	0	-2.854388	14.409570	24.104756
195	1	0	-3.118918	13.550662	23.475850
196	1	0	-3.600306	15.192682	23.912779
197	1	0	-1.887033	14.787461	23.755472
198	1	0	-4.271808	13.384478	27.136129
199	1	0	-4.979272	14.384252	25.854066
200	1	0	-4.578351	12.693270	25.537616
201	1	0	9.524313	14.328593	34.919290
202	1	0	9.100022	15.973229	34.420184
203	1	0	10.044821	14.940536	33.340875
204	1	0	11.912631	16.573030	33.122095
205	1	0	11.092115	17.755407	34.145496
206	1	0	12.741690	17.249578	34.527623

Optimized S0 geometry of $\mathbf{C_{60}}$ (at the M06-2X/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.361719	-2.395828	2.221062
2	6	0	-1.807699	-2.896849	0.933725
3	6	0	-0.888494	-3.426295	0.039349
4	6	0	0.519058	-3.479471	0.391053
5	6	0	0.945273	-3.000823	1.621404
6	6	0	-0.016607	-2.446087	2.556525
7	6	0	-2.144744	-1.216439	2.539654
8	6	0	-3.075257	-0.988250	1.449484
9	6	0	-2.867059	-2.026428	0.456343
10	6	0	-2.960473	-1.722995	-0.894341
11	6	0	-0.986390	-3.108944	-1.373294
12	6	0	1.291044	-3.195936	-0.804974
13	6	0	2.455551	-2.446757	-0.718553
14	6	0	2.901565	-1.946257	0.568650
15	6	0	2.163576	-2.217295	1.712205
16	6	0	1.955420	-1.179475	2.705075

17	6	0	0.607975	-1.320619	3.226673
18	6	0	-0.140283	-0.192801	3.531291
19	6	0	-1.547400	-0.139541	3.179573
20	6	0	-3.367532	0.307425	1.048027
21	6	0	-2.743013	1.433865	1.717737
22	6	0	-1.853023	1.215347	2.759327
23	6	0	-0.635188	1.999592	2.850066
24	6	0	0.423509	1.128946	3.327205
25	6	0	1.710978	1.264048	2.828544
26	6	0	2.494349	0.084035	2.510366
27	6	0	3.266679	0.367538	1.314263
28	6	0	3.465065	-0.624539	0.364895
29	6	0	0.360188	-2.967778	-1.895205
30	6	0	2.144743	1.216440	-2.539654
31	6	0	1.547399	0.139542	-3.179573
32	6	0	0.140284	0.192802	-3.531291
33	6	0	-0.607974	1.320620	-3.226673
34	6	0	0.016606	2.446086	-2.556526
35	6	0	1.807698	2.896849	-0.933725
36	6	0	2.867059	2.026427	-0.456344
37	6	0	3.075257	0.988251	-1.449482
38	6	0	3.367532	-0.307424	-1.048026
39	6	0	2.743013	-1.433867	-1.717737
40	6	0	1.853023	-1.215348	-2.759327
41	6	0	-0.423509	-1.128946	-3.327204
42	6	0	-1.710977	-1.264048	-2.828543
43	6	0	-2.494349	-0.084034	-2.510365
44	6	0	-1.955421	1.179477	-2.705076
45	6	0	-2.163576	2.217296	-1.712206
46	6	0	-0.945274	3.000823	-1.621405
47	6	0	-0.519058	3.479471	-0.391053
48	6	0	0.888494	3.426295	-0.039349
49	6	0	2.960474	1.722995	0.894342
50	6	0	1.998823	2.276700	1.829614
51	6	0	0.986389	3.108943	1.373294

52	6	0	-0.360187	2.967776	1.895205
53	6	0	-1.291045	3.195935	0.804973
54	6	0	-2.455550	2.446757	0.718553
55	6	0	-2.901566	1.946257	-0.568650
56	6	0	-3.465065	0.624540	-0.364896
57	6	0	-3.266679	-0.367537	-1.314263
58	6	0	0.635189	-1.999592	-2.850066
59	6	0	-1.998823	-2.276699	-1.829613
60	6	0	1.361719	2.395827	-2.221063

Optimized S0 geometry of **CORA-monPA** (at the M06-2X/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-6.070585	-0.983656	-0.248994
2	14	0	5.701855	-2.063803	-0.062985
3	6	0	0.386220	-2.889190	0.075497
4	6	0	1.220421	-1.740979	-0.026119
5	6	0	-1.860975	-3.869590	0.144619
6	1	0	-2.940747	-3.745455	0.130871
7	6	0	2.638004	-1.893625	-0.023391
8	6	0	0.965290	1.969827	-0.351378
9	6	0	-0.505710	2.139096	-0.357888
10	6	0	-1.296347	1.025263	-0.256198
11	1	0	-2.377448	1.132830	-0.257453
12	6	0	-1.320266	-5.142453	0.259487
13	6	0	-4.226746	-1.136844	-0.182060
14	6	0	1.795947	5.588074	-0.523802
15	6	0	-1.598431	-1.420963	-0.069633
16	6	0	-0.484875	5.852084	-0.532415
17	6	0	-0.763990	-0.292058	-0.150955
18	6	0	1.219258	4.322054	-0.745659
19	6	0	3.852660	-2.000664	-0.025708
20	6	0	0.112070	-5.303273	0.288852
21	6	0	-0.211668	4.487529	-0.750674

22	6	0	0.663019	-0.454622	-0.134909
23	6	0	6.192969	-2.716350	-1.773548
24	1	0	7.284661	-2.852828	-1.763751
25	6	0	-1.044820	-2.727470	0.050542
26	6	0	0.654356	-6.626758	0.413613
27	1	0	1.734867	-6.740961	0.437972
28	6	0	0.925392	-4.183049	0.196108
29	1	0	2.005870	-4.301705	0.216953
30	6	0	3.045203	5.766363	0.040127
31	6	0	1.481210	0.706701	-0.238039
32	1	0	2.558478	0.565693	-0.237760
33	6	0	-2.147100	-6.312783	0.350252
34	1	0	-3.226109	-6.184233	0.322824
35	6	0	-3.015123	-1.263083	-0.120913
36	6	0	0.749235	6.533283	-0.391655
37	6	0	-1.663638	6.311547	0.023985
38	6	0	1.851245	3.153052	-0.421599
39	6	0	-6.681460	-1.099309	1.543653
40	1	0	-7.772701	-0.962016	1.512810
41	6	0	-2.395213	3.953736	-0.021153
42	1	0	-3.169866	3.231596	0.222546
43	6	0	-2.670208	5.298970	0.189542
44	1	0	-3.647031	5.571074	0.580912
45	6	0	6.316198	-3.195670	1.336984
46	1	0	6.472182	-2.542408	2.208039
47	6	0	-1.096429	3.494348	-0.430847
48	6	0	7.665961	-3.839945	0.986114
49	1	0	7.566216	-4.527390	0.137818
50	1	0	8.047925	-4.420530	1.834348
51	1	0	8.427871	-3.098544	0.720757
52	6	0	3.792572	4.550278	0.209835
53	1	0	4.803314	4.591627	0.607509
54	6	0	3.263806	7.086534	0.594727
55	1	0	4.239839	7.336845	1.002277
56	6	0	-6.380611	-2.471509	2.160313

57	1	0	-6.905038	-3.281818	1.644351
58	1	0	-6.684613	-2.496820	3.213941
59	1	0	-5.305892	-2.689820	2.122207
60	6	0	-0.166116	-7.708497	0.498989
61	1	0	0.252647	-8.705442	0.593437
62	6	0	-1.590888	-7.549016	0.464787
63	1	0	-2.223325	-8.428802	0.530189
64	6	0	3.218786	3.303661	-0.004865
65	1	0	3.808354	2.424020	0.240581
66	6	0	5.291809	-4.266989	1.732559
67	1	0	4.349702	-3.822690	2.067688
68	1	0	5.681678	-4.895017	2.542999
69	1	0	5.060867	-4.928050	0.888316
70	6	0	-0.372921	8.307873	0.716140
71	1	0	-0.363917	9.270416	1.220867
72	6	0	-1.578468	7.646686	0.579339
73	1	0	-2.474171	8.112374	0.981893
74	6	0	-7.876383	1.211122	-0.576122
75	1	0	-8.676162	0.484529	-0.755221
76	1	0	-8.140465	2.131108	-1.110900
77	1	0	-7.878042	1.444294	0.494819
78	6	0	0.882899	7.708999	0.311090
79	6	0	-6.502254	0.697981	-1.033593
80	1	0	-6.558952	0.510176	-2.115613
81	6	0	5.537901	-4.072774	-2.067400
82	1	0	5.839624	-4.843501	-1.349920
83	1	0	5.811047	-4.427296	-3.068681
84	1	0	4.444535	-3.992533	-2.030614
85	6	0	2.239960	8.005748	0.723481
86	1	0	2.448285	8.946168	1.226887
87	6	0	-6.075157	0.010897	2.412337
88	1	0	-4.980875	-0.061070	2.425044
89	1	0	-6.425036	-0.073861	3.448372
90	1	0	-6.339096	1.011135	2.054236
91	6	0	5.841914	-1.702795	-2.869818

92	1	0	4.768599	-1.476297	-2.863239
93	1	0	6.087674	-2.102678	-3.861063
94	1	0	6.383966	-0.759130	-2.747605
95	6	0	-5.914094	-3.694789	-1.226076
96	1	0	-4.863252	-3.533463	-1.486288
97	1	0	-6.317029	-4.460195	-1.900558
98	1	0	-5.946177	-4.104546	-0.209821
99	6	0	-6.725470	-2.397667	-1.339789
100	1	0	-6.618439	-2.032113	-2.371682
101	6	0	-8.217553	-2.657404	-1.087708
102	1	0	-8.393201	-3.008205	-0.063944
103	1	0	-8.597053	-3.429152	-1.767989
104	1	0	-8.825106	-1.758497	-1.238635
105	6	0	6.276651	-0.273172	0.173236
106	1	0	5.849392	0.288641	-0.670997
107	6	0	7.805211	-0.159381	0.109754
108	1	0	8.270136	-0.691381	0.948981
109	1	0	8.124184	0.887884	0.173892
110	1	0	8.214452	-0.575962	-0.818138
111	6	0	-5.423108	1.764937	-0.804605
112	1	0	-5.252335	1.937727	0.265368
113	1	0	-5.720674	2.722841	-1.249505
114	1	0	-4.468102	1.469167	-1.251163
115	6	0	5.737325	0.340272	1.470564
116	1	0	4.644533	0.278282	1.528946
117	1	0	6.022479	1.396971	1.551054
118	1	0	6.144868	-0.172021	2.350488

Optimized S0 geometry of **TS1** (at the M06-2X/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.256993	5.813017	1.476853
2	14	0	-1.017854	-5.831150	1.824477
3	6	0	-2.933336	0.583058	1.684737

4	6	0	-4.886546	-1.092953	0.469013
5	6	0	-3.795473	-1.633817	1.107729
6	1	0	-3.676712	-2.713133	1.142426
7	6	0	-7.007878	-1.306329	-0.628161
8	6	0	-7.146936	0.125770	-0.660984
9	6	0	-5.027143	0.371861	0.431871
10	6	0	0.870062	1.478327	0.452397
11	6	0	-7.885681	-1.843885	-1.591197
12	6	0	-1.669511	-1.421112	2.359936
13	6	0	-5.874364	-1.952922	-0.216621
14	6	0	0.230059	0.667637	-0.464397
15	6	0	-2.802002	-0.839278	1.730577
16	6	0	-0.708013	-0.603627	2.974666
17	6	0	-0.827477	0.817778	2.908103
18	6	0	-4.057846	1.141553	1.029633
19	1	0	-4.141316	2.223946	1.000583
20	6	0	1.114713	-1.331291	0.663020
21	6	0	-7.680554	-3.063417	-2.208131
22	6	0	-8.108092	0.440847	-1.642515
23	6	0	-8.565017	-0.770300	-2.218073
24	6	0	-9.078452	-0.848768	-3.493072
25	6	0	1.571889	0.932177	1.626953
26	6	0	-6.600887	-3.832367	-1.650808
27	1	0	-6.387915	-4.823592	-2.043332
28	6	0	-5.736029	-3.297922	-0.705247
29	1	0	-4.879774	-3.895649	-0.404629
30	6	0	2.795517	1.743588	1.754075
31	6	0	0.355461	-0.790191	-0.353530
32	6	0	-2.005478	2.820268	2.110254
33	6	0	-6.159711	0.995396	-0.284841
34	6	0	1.693874	-0.505099	1.735899
35	6	0	-1.470667	-2.833061	2.299106
36	6	0	3.035703	-1.069714	1.968077
37	6	0	5.227207	1.686198	1.476124
38	6	0	0.516849	-1.122721	3.511826

39	1	0	0.656923	-2.202358	3.494030
40	6	0	4.014095	1.185866	2.085264
41	6	0	3.178129	-2.286106	1.203608
42	6	0	-8.397012	-3.228972	-3.455938
43	1	0	-8.342817	-4.181155	-3.977177
44	6	0	2.742273	2.835487	0.810203
45	6	0	-6.283353	2.320146	-0.830533
46	1	0	-5.560402	3.085561	-0.559097
47	6	0	1.267945	-0.358810	4.449348
48	6	0	1.985936	-2.447627	0.396428
49	6	0	-1.922465	1.402742	2.253464
50	6	0	-9.058708	-2.179818	-4.064465
51	1	0	-9.502747	-2.343506	-5.042841
52	6	0	-8.141951	1.649463	-2.311749
53	6	0	1.550396	2.668522	0.003161
54	6	0	1.158577	1.052672	4.368883
55	6	0	0.294383	1.581704	3.370177
56	1	0	0.261868	2.660875	3.231513
57	6	0	4.137902	-0.272061	2.196202
58	6	0	0.260605	1.006106	-1.870788
59	6	0	6.099857	0.556063	1.211740
60	6	0	-9.316199	0.434910	-4.120978
61	1	0	-9.780749	0.468393	-5.103030
62	6	0	-7.233440	2.635968	-1.792526
63	1	0	-7.217060	3.632412	-2.226325
64	6	0	5.425179	-0.650436	1.655564
65	6	0	5.991076	2.719045	-0.623592
66	6	0	0.459383	-1.331139	-1.691050
67	6	0	1.291900	-2.415503	-1.951169
68	6	0	-1.282375	-4.033862	2.196696
69	6	0	6.882704	0.533788	0.065791
70	6	0	2.070566	-2.991717	-0.878209
71	6	0	6.825511	1.638842	-0.873821
72	6	0	-2.100492	4.025419	1.947884
73	6	0	2.105293	-2.435245	-3.151131

74	6	0	2.000190	1.861892	5.170390
75	1	0	1.926850	2.942904	5.089049
76	6	0	1.563915	3.012961	-1.341491
77	6	0	5.178892	2.747362	0.577459
78	6	0	3.904318	3.338971	0.239240
79	6	0	2.046105	-1.377463	-4.047716
80	6	0	-8.874098	1.618065	-3.560990
81	1	0	-9.005988	2.539426	-4.122279
82	6	0	0.399076	-0.224824	-2.628706
83	6	0	6.924453	1.091963	-2.212918
84	6	0	4.414763	-2.671031	0.703084
85	6	0	6.183467	1.647165	-3.246766
86	6	0	2.781254	3.528286	-1.942871
87	6	0	5.528175	0.785400	-4.213467
88	6	0	5.567751	-1.830000	0.931199
89	6	0	3.387085	-3.033180	-2.818304
90	6	0	1.172963	-0.248458	-3.780964
91	6	0	3.923652	3.686514	-1.172005
92	6	0	3.366677	-3.379743	-1.409678
93	6	0	5.217066	3.302027	-1.705574
94	6	0	7.023625	-0.695742	-0.693129
95	6	0	0.904902	2.160688	-2.304198
96	6	0	7.046564	-0.351292	-2.101266
97	6	0	5.726725	-2.712090	-1.240477
98	6	0	1.848785	0.956498	-4.227859
99	6	0	5.310016	2.776222	-2.986964
100	6	0	4.509600	-3.222581	-0.638440
101	6	0	2.877588	2.980127	-3.282560
102	6	0	5.645499	-0.593091	-4.107345
103	6	0	1.717898	2.133452	-3.504370
104	6	0	4.248654	1.381267	-4.550429
105	6	0	6.422687	-1.174399	-3.028212
106	6	0	3.263189	-0.869751	-4.650542
107	6	0	5.747380	-2.380872	-2.588105
108	6	0	2.213624	-0.935337	5.330340

109	1	0	2.305773	-2.017300	5.371466
110	6	0	3.140830	0.572976	-4.762194
111	6	0	4.488135	-1.439790	-4.333051
112	6	0	6.379129	-1.849794	-0.270368
113	6	0	2.987698	-0.129927	6.131595
114	1	0	3.695436	-0.572544	6.825157
115	6	0	4.551427	-2.544648	-3.394767
116	6	0	2.880560	1.278771	6.050294
117	1	0	3.507478	1.899887	6.681978
118	6	0	4.114051	2.611922	-3.793183
119	6	0	-0.869629	6.115088	0.218281
120	1	0	-0.925690	7.169109	-0.091741
121	6	0	0.557253	-5.945659	0.773522
122	1	0	0.448478	-5.197195	-0.024542
123	6	0	1.812827	-5.599078	1.581844
124	1	0	1.716481	-4.638182	2.100289
125	1	0	2.694250	-5.535154	0.929368
126	1	0	2.015582	-6.369251	2.336700
127	6	0	-2.029471	-7.461951	3.993198
128	1	0	-2.773642	-6.713466	4.289673
129	1	0	-1.793335	-8.056690	4.883887
130	1	0	-2.494378	-8.128766	3.259201
131	6	0	-2.460494	-5.626492	-0.578696
132	1	0	-2.441278	-4.535945	-0.446956
133	1	0	-3.341729	-5.871503	-1.185363
134	1	0	-1.573138	-5.901514	-1.157434
135	6	0	-1.624754	8.328419	2.677152
136	1	0	-0.733603	8.400002	2.044593
137	1	0	-1.430737	8.904141	3.590276
138	1	0	-2.446706	8.824066	2.148551
139	6	0	-0.764341	-6.790648	3.447444
140	1	0	-0.046503	-7.586066	3.192647
141	6	0	-2.526215	-6.336974	0.782413
142	1	0	-2.464984	-7.422455	0.614667
143	6	0	0.700935	-7.331890	0.130830

144	1	0	0.789009	-8.113403	0.895871
145	1	0	1.605091	-7.380899	-0.487841
146	1	0	-0.152880	-7.586927	-0.506027
147	6	0	-1.977297	6.874373	3.023048
148	1	0	-1.103645	6.423475	3.517084
149	6	0	-3.154308	6.822264	4.004515
150	1	0	-4.029977	7.334643	3.588917
151	1	0	-2.899018	7.326169	4.944324
152	1	0	-3.449257	5.794275	4.242998
153	6	0	-0.128525	-5.908934	4.532355
154	1	0	0.801971	-5.439487	4.197083
155	1	0	0.097975	-6.502191	5.426530
156	1	0	-0.814447	-5.106808	4.827420
157	6	0	-3.867093	-6.022357	1.458182
158	1	0	-4.025043	-6.598368	2.373115
159	1	0	-4.700695	-6.242548	0.778885
160	1	0	-3.931412	-4.959653	1.724280
161	6	0	-3.963174	5.979515	0.661828
162	1	0	-3.865176	5.399689	-0.269120
163	6	0	-5.116070	5.363081	1.464238
164	1	0	-4.904828	4.329616	1.760879
165	1	0	-6.040083	5.361507	0.872484
166	1	0	-5.316416	5.931199	2.378334
167	6	0	0.495527	5.871486	0.875626
168	1	0	0.695684	6.582279	1.685123
169	1	0	1.307767	5.957456	0.141640
170	1	0	0.547038	4.860215	1.297670
171	6	0	-1.043060	5.234629	-1.024606
172	1	0	-1.073591	4.171935	-0.751602
173	1	0	-0.202135	5.367478	-1.717148
174	1	0	-1.963236	5.470833	-1.569396
175	6	0	-4.279768	7.432265	0.280966
176	1	0	-4.447502	8.043256	1.176262
177	1	0	-5.193256	7.486417	-0.323171
178	1	0	-3.471373	7.897691	-0.294805

Optimized S0 geometry of **TS2** (at the M06-2X/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.680106	5.825320	1.512182
2	14	0	-2.198940	-5.041512	2.691323
3	6	0	-1.763092	1.577012	1.902277
4	6	0	-4.242131	0.648037	0.908406
5	6	0	-3.379362	-0.206711	1.578592
6	1	0	-3.654243	-1.249317	1.712810
7	6	0	-6.352852	1.116821	-0.121907
8	6	0	-5.964799	2.486579	-0.306857
9	6	0	-3.844026	2.038789	0.717101
10	6	0	0.132894	1.333983	-0.508691
11	6	0	-7.414484	0.845673	-1.009946
12	6	0	-1.201919	-0.660028	2.723230
13	6	0	-5.507054	0.145222	0.340773
14	6	0	-0.713298	0.696068	-1.392498
15	6	0	-2.160640	0.234252	2.109582
16	6	0	-0.243017	-0.100941	3.661882
17	6	0	0.171018	1.246995	3.434554
18	6	0	-2.607612	2.445189	1.197724
19	1	0	-2.278789	3.469218	1.042294
20	6	0	-0.614643	-1.352626	-0.035681
21	6	0	-7.694746	-0.417914	-1.492725
22	6	0	-6.796237	3.035931	-1.305404
23	6	0	-7.689871	2.027071	-1.741224
24	6	0	-8.258756	2.017992	-2.994937
25	6	0	0.560336	0.713898	0.761386
26	6	0	-6.935972	-1.470172	-0.869158
27	1	0	-7.115372	-2.503871	-1.154203
28	6	0	-5.888666	-1.199660	-0.000210
29	1	0	-5.291113	-2.036712	0.351449
30	6	0	1.984877	1.065385	0.890365

31	6	0	-1.102289	-0.698332	-1.146442
32	6	0	0.084841	3.244169	1.995139
33	6	0	-4.709808	2.965159	-0.039096
34	6	0	0.173381	-0.665990	1.003268
35	6	0	-1.531952	-2.045729	2.827082
36	6	0	1.232642	-1.624848	1.368665
37	6	0	4.254961	0.159621	0.788463
38	6	0	0.349517	-0.845444	4.671282
39	1	0	0.043812	-1.877514	4.826179
40	6	0	2.924303	0.166062	1.352265
41	6	0	0.973212	-2.889451	0.725183
42	6	0	-8.484590	-0.430684	-2.706418
43	1	0	-8.806520	-1.382495	-3.120674
44	6	0	2.341392	2.004284	-0.145071
45	6	0	-4.374589	4.186819	-0.722883
46	1	0	-3.414411	4.662056	-0.542040
47	6	0	1.333485	-0.281969	5.499957
48	6	0	-0.174066	-2.720340	-0.144423
49	6	0	-0.422777	1.944662	2.299996
50	6	0	-8.750634	0.723230	-3.418474
51	1	0	-9.271278	0.638009	-4.368684
52	6	0	-6.420684	4.099091	-2.102954
53	6	0	1.191345	2.174078	-1.010430
54	6	0	1.760389	1.063479	5.262510
55	6	0	1.178301	1.795103	4.214687
56	1	0	1.511107	2.811666	4.022628
57	6	0	2.534524	-1.228251	1.599778
58	6	0	-0.524237	0.854459	-2.815584
59	6	0	4.692606	-1.220952	0.683505
60	6	0	-8.042801	3.230310	-3.758014
61	1	0	-8.509700	3.334769	-4.733929
62	6	0	-5.191711	4.731576	-1.703033
63	1	0	-4.839675	5.607392	-2.241573
64	6	0	3.630010	-2.074750	1.184211
65	6	0	5.398858	0.646083	-1.338881

66	6	0	-1.150163	-1.378915	-2.420119
67	6	0	-0.733703	-2.703072	-2.527294
68	6	0	-1.779690	-3.238950	2.833748
69	6	0	5.458176	-1.626494	-0.400258
70	6	0	-0.238469	-3.392096	-1.359010
71	6	0	5.817595	-0.673234	-1.436045
72	6	0	0.645534	4.299216	1.751631
73	6	0	0.064277	-3.121333	-3.664141
74	6	0	2.770690	1.625106	6.098854
75	1	0	3.092634	2.646036	5.909491
76	6	0	1.367007	2.350930	-2.377661
77	6	0	4.603823	1.071747	-0.202682
78	6	0	3.623827	2.019087	-0.678301
79	6	0	0.403582	-2.206695	-4.650967
80	6	0	-7.172501	4.216670	-3.334967
81	1	0	-6.983362	5.059779	-3.994153
82	6	0	-0.792059	-0.422824	-3.453534
83	6	0	5.766172	-1.358989	-2.712466
84	6	0	2.019479	-3.719847	0.342750
85	6	0	5.298669	-0.697416	-3.839171
86	6	0	2.708936	2.354527	-2.938860
87	6	0	4.419950	-1.381745	-4.769603
88	6	0	3.381845	-3.301058	0.573623
89	6	0	1.049197	-4.080131	-3.194240
90	6	0	-0.036225	-0.826821	-4.544518
91	6	0	3.808834	2.191753	-2.109454
92	6	0	0.863270	-4.249314	-1.765429
93	6	0	4.908534	1.339112	-2.517712
94	6	0	5.193032	-2.902866	-1.039893
95	6	0	0.490139	1.673089	-3.303078
96	6	0	5.381135	-2.737628	-2.467228
97	6	0	3.301854	-4.407116	-1.497061
98	6	0	1.027129	0.025158	-5.047550
99	6	0	4.858799	0.681935	-3.739419
100	6	0	1.963402	-4.410164	-0.935427

101	6	0	2.655972	1.667902	-4.215061
102	6	0	4.052148	-2.699334	-4.535785
103	6	0	1.284521	1.245934	-4.438973
104	6	0	3.435715	-0.425726	-5.242701
105	6	0	4.544562	-3.393423	-3.360096
106	6	0	1.739878	-2.207307	-5.212434
107	6	0	3.480830	-4.245904	-2.863837
108	6	0	1.929706	-1.015340	6.569254
109	1	0	1.599475	-2.035411	6.746624
110	6	0	2.124783	-0.828125	-5.458320
111	6	0	2.682518	-3.122129	-4.763541
112	6	0	4.177699	-3.720382	-0.563798
113	6	0	2.893055	-0.444617	7.352629
114	1	0	3.340949	-1.009240	8.164320
115	6	0	2.329294	-4.078164	-3.731136
116	6	0	3.320424	0.893374	7.113327
117	1	0	4.088815	1.328254	7.744785
118	6	0	3.707145	0.849614	-4.606798
119	6	0	0.997483	6.778759	0.029653
120	1	0	1.581773	7.707512	-0.050188
121	6	0	-0.773146	-5.879806	1.764427
122	1	0	-0.588506	-5.286111	0.858046
123	6	0	0.511772	-5.895371	2.600299
124	1	0	0.772703	-4.896079	2.968061
125	1	0	1.358497	-6.262305	2.006824
126	1	0	0.405334	-6.558970	3.467922
127	6	0	-3.736358	-5.943366	4.986880
128	1	0	-4.195614	-4.964597	5.168583
129	1	0	-3.719063	-6.476182	5.945369
130	1	0	-4.387905	-6.502446	4.306844
131	6	0	-3.446858	-4.568659	0.222941
132	1	0	-3.107836	-3.523707	0.263245
133	1	0	-4.334881	-4.604731	-0.420774
134	1	0	-2.655638	-5.146911	-0.267374
135	6	0	4.435391	6.332923	1.014161

136	1	0	4.107646	7.087283	0.289727
137	1	0	5.410927	5.956766	0.683565
138	1	0	4.590395	6.836012	1.976016
139	6	0	-2.313225	-5.793109	4.436703
140	1	0	-1.891300	-6.804502	4.331861
141	6	0	-3.776039	-5.085923	1.632319
142	1	0	-4.089586	-6.137643	1.553606
143	6	0	-1.166444	-7.300296	1.337258
144	1	0	-1.453648	-7.912184	2.201985
145	1	0	-0.325345	-7.806093	0.848001
146	1	0	-2.008484	-7.299600	0.636600
147	6	0	3.429720	5.181859	1.155950
148	1	0	3.332861	4.690381	0.175646
149	6	0	3.944702	4.122627	2.139101
150	1	0	4.152463	4.554586	3.123436
151	1	0	4.879709	3.682906	1.769762
152	1	0	3.224108	3.308280	2.274130
153	6	0	-1.441353	-5.021969	5.439500
154	1	0	-0.406545	-4.914098	5.098105
155	1	0	-1.424348	-5.534919	6.408751
156	1	0	-1.841967	-4.014588	5.600459
157	6	0	-4.935802	-4.273039	2.220294
158	1	0	-5.302914	-4.683945	3.163594
159	1	0	-5.780044	-4.244723	1.519298
160	1	0	-4.631621	-3.235811	2.411441
161	6	0	1.486920	6.873388	3.082009
162	1	0	0.409742	6.844682	3.303408
163	6	0	2.231768	6.286651	4.284551
164	1	0	1.946877	5.245676	4.479007
165	1	0	2.024940	6.866409	5.192110
166	1	0	3.314976	6.313700	4.118489
167	6	0	1.151015	5.993859	-1.278266
168	1	0	2.195994	5.748401	-1.496019
169	1	0	0.760484	6.568792	-2.126515
170	1	0	0.593272	5.050158	-1.233725

171	6	0	-0.467664	7.163746	0.272142
172	1	0	-1.090729	6.267975	0.376410
173	1	0	-0.864501	7.749558	-0.565485
174	1	0	-0.590871	7.757965	1.184989
175	6	0	1.885841	8.340017	2.867843
176	1	0	2.956630	8.437209	2.652557
177	1	0	1.681709	8.927006	3.771549
178	1	0	1.335884	8.801530	2.040724

Optimized S0 geometry of **CORA-monPA-C_{60}** (at the M06-2X/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.191662	5.890207	1.557020
2	14	0	-2.105629	-5.968908	1.640890
3	6	0	-3.222016	0.667927	0.887403
4	6	0	-5.466859	-0.794180	-0.100389
5	6	0	-4.342634	-1.444994	0.390216
6	1	0	-4.320752	-2.529752	0.395486
7	6	0	-7.724545	-0.785346	-0.918801
8	6	0	-7.733256	0.648298	-0.913396
9	6	0	-5.475926	0.676383	-0.096542
10	6	0	1.315475	1.427850	0.011942
11	6	0	-8.775462	-1.218410	-1.756099
12	6	0	-2.058168	-1.474329	1.388649
13	6	0	-6.609562	-1.547631	-0.659072
14	6	0	0.944821	0.734801	-1.118324
15	6	0	-3.213418	-0.763668	0.887529
16	6	0	-0.967587	-0.741616	1.839566
17	6	0	-0.977889	0.675528	1.840370
18	6	0	-4.359256	1.338137	0.394692
19	1	0	-4.351051	2.423028	0.407218
20	6	0	1.340921	-1.438975	0.003011
21	6	0	-8.783369	-2.446442	-2.401861
22	6	0	-8.789177	1.075669	-1.747172

23	6	0	-9.431552	-0.073217	-2.268563
24	6	0	-10.138795	-0.072715	-3.458097
25	6	0	1.484102	0.797722	1.401923
26	6	0	-7.718693	-3.327529	-1.993073
27	1	0	-7.662612	-4.332329	-2.405092
28	6	0	-6.681339	-2.895844	-1.166621
29	1	0	-5.866482	-3.589160	-0.977594
30	6	0	2.817224	1.437019	1.817659
31	6	0	0.958306	-0.745201	-1.123046
32	6	0	-2.086366	2.818200	1.418504
33	6	0	-6.626981	1.421091	-0.648768
34	6	0	1.498040	-0.814845	1.397353
35	6	0	-2.054177	-2.899654	1.437134
36	6	0	2.843311	-1.431691	1.808506
37	6	0	5.226696	1.199874	2.189759
38	6	0	0.331730	-1.315823	2.367300
39	1	0	0.320200	-2.406723	2.378202
40	6	0	3.866191	0.750821	2.387649
41	6	0	3.141333	-2.568968	0.980369
42	6	0	-9.687248	-2.515168	-3.532376
43	1	0	-9.806788	-3.456592	-4.063580
44	6	0	3.093957	2.585051	0.997044
45	6	0	-6.713404	2.772321	-1.146076
46	1	0	-5.904686	3.472221	-0.953455
47	6	0	0.582856	-0.723994	3.738327
48	6	0	2.212659	-2.573512	-0.134659
49	6	0	-2.075877	1.392995	1.385869
50	6	0	-10.329643	-1.389282	-4.033638
51	1	0	-10.926437	-1.495414	-4.936586
52	6	0	-8.811042	2.308434	-2.383582
53	6	0	2.165288	2.579792	-0.117879
54	6	0	0.568956	0.678830	3.741284
55	6	0	0.308764	1.271381	2.372795
56	1	0	0.275860	2.361843	2.388660
57	6	0	3.879678	-0.729864	2.382765

58	6	0	1.380893	1.179261	-2.423427
59	6	0	6.079579	0.031892	2.063279
60	6	0	-10.345491	1.246057	-4.023071
61	1	0	-10.944258	1.352300	-4.924699
62	6	0	-7.755995	3.198434	-1.968851
63	1	0	-7.711481	4.206622	-2.373983
64	6	0	5.248264	-1.152354	2.181948
65	6	0	6.613755	2.352838	0.502252
66	6	0	1.402468	-1.172915	-2.431026
67	6	0	2.215907	-2.302634	-2.572117
68	6	0	-2.065514	-4.121900	1.503494
69	6	0	7.163644	0.044707	1.185555
70	6	0	2.631188	-3.021750	-1.393015
71	6	0	7.431660	1.227192	0.382285
72	6	0	-2.112457	4.041058	1.460452
73	6	0	3.326923	-2.286777	-3.505801
74	6	0	0.788081	1.383871	4.922112
75	1	0	0.778082	2.470938	4.922953
76	6	0	2.575279	3.043922	-1.373267
77	6	0	5.495846	2.342630	1.427932
78	6	0	4.400323	3.053495	0.816146
79	6	0	3.575841	-1.148194	-4.275510
80	6	0	-9.716061	2.375447	-3.513302
81	1	0	-9.846863	3.319533	-4.037087
82	6	0	1.662922	0.008308	-3.233793
83	6	0	7.873736	0.786096	-0.926132
84	6	0	4.456164	-3.011759	0.796255
85	6	0	7.479039	1.484170	-2.069708
86	6	0	3.939021	3.511649	-1.564434
87	6	0	7.076439	0.756260	-3.261192
88	6	0	5.538411	-2.284918	1.412756
89	6	0	4.434561	-3.005626	-2.896466
90	6	0	2.721108	0.021011	-4.142333
91	6	0	4.831562	3.516333	-0.493596
92	6	0	4.003217	-3.462953	-1.587100

93	6	0	6.203540	3.080841	-0.688070
94	6	0	7.453276	-1.127347	0.374558
95	6	0	2.173201	2.324760	-2.557059
96	6	0	7.887193	-0.669727	-0.930893
97	6	0	6.259474	-2.996291	-0.707848
98	6	0	3.554105	1.206586	-4.267763
99	6	0	6.627074	2.653678	-1.948213
100	6	0	4.895744	-3.458227	-0.516263
101	6	0	4.378533	3.070571	-2.876577
102	6	0	7.089331	-0.639520	-3.265760
103	6	0	3.284309	2.335329	-3.490619
104	6	0	5.973723	1.476012	-3.875570
105	6	0	7.505384	-1.367561	-2.078967
106	6	0	4.935962	-0.685492	-4.469689
107	6	0	6.675215	-2.553475	-1.965176
108	6	0	0.818088	-1.428714	4.916338
109	1	0	0.832336	-2.515656	4.912967
110	6	0	4.922543	0.770391	-4.464988
111	6	0	6.000006	-1.375413	-3.884786
112	6	0	6.656335	-2.268658	0.487170
113	6	0	1.030156	-0.720998	6.104799
114	1	0	1.206524	-1.262678	7.029959
115	6	0	5.744050	-2.558314	-3.082063
116	6	0	1.014840	0.676158	6.107831
117	1	0	1.179020	1.217635	7.035344
118	6	0	5.696060	2.648836	-3.065198
119	6	0	-1.331618	6.601217	-0.000904
120	1	0	-1.413649	7.695735	0.088657
121	6	0	-0.998173	-6.688862	0.249578
122	1	0	-1.460132	-6.337850	-0.685120
123	6	0	0.452185	-6.172728	0.263604
124	1	0	0.500920	-5.078514	0.261811
125	1	0	0.998283	-6.529689	-0.620309
126	1	0	0.998433	-6.532207	1.144256
127	6	0	-2.476271	-6.633894	4.474279

128	1	0	-2.936419	-5.669677	4.722375
129	1	0	-2.011709	-7.015365	5.393846
130	1	0	-3.278015	-7.327663	4.199375
131	6	0	-4.311780	-6.537233	-0.131068
132	1	0	-4.226175	-5.536355	-0.574332
133	1	0	-5.355200	-6.858074	-0.253211
134	1	0	-3.688975	-7.213967	-0.724998
135	6	0	-1.111718	7.921869	3.324498
136	1	0	-0.746493	8.440610	2.430449
137	1	0	-0.423521	8.160866	4.146494
138	1	0	-2.085484	8.353830	3.583927
139	6	0	-1.419850	-6.487203	3.363012
140	1	0	-0.995330	-7.488593	3.188603
141	6	0	-3.922609	-6.526501	1.361172
142	1	0	-3.971780	-7.564705	1.726203
143	6	0	-1.018823	-8.231109	0.231943
144	1	0	-0.554643	-8.648747	1.134254
145	1	0	-0.452964	-8.615359	-0.627423
146	1	0	-2.034041	-8.639046	0.164124
147	6	0	-1.205092	6.396290	3.122885
148	1	0	-0.188115	6.034618	2.903885
149	6	0	-1.656079	5.698578	4.419943
150	1	0	-2.646169	6.041406	4.741376
151	1	0	-0.956713	5.918369	5.238243
152	1	0	-1.703778	4.610116	4.304357
153	6	0	-0.273167	-5.578367	3.850817
154	1	0	0.537675	-5.491068	3.119958
155	1	0	0.160689	-5.971764	4.780344
156	1	0	-0.639938	-4.566232	4.059703
157	6	0	-4.950236	-5.698308	2.158045
158	1	0	-4.759110	-5.710004	3.234872
159	1	0	-5.964636	-6.088011	1.997441
160	1	0	-4.947273	-4.650304	1.836044
161	6	0	-4.055754	6.345724	1.522580
162	1	0	-4.414558	5.871915	0.594994

163	6	0	-4.875892	5.744865	2.680100
164	1	0	-4.709519	4.667059	2.786487
165	1	0	-5.950368	5.901615	2.514100
166	1	0	-4.625397	6.216702	3.637360
167	6	0	0.167509	6.252358	-0.067287
168	1	0	0.719922	6.621492	0.804302
169	1	0	0.629187	6.696066	-0.959847
170	1	0	0.323622	5.168371	-0.126068
171	6	0	-2.041158	6.184991	-1.303902
172	1	0	-2.019803	5.096296	-1.437491
173	1	0	-1.544564	6.631377	-2.175993
174	1	0	-3.089989	6.502071	-1.325487
175	6	0	-4.320351	7.859059	1.393894
176	1	0	-4.000046	8.400714	2.291532
177	1	0	-5.393935	8.052673	1.265513
178	1	0	-3.802729	8.303814	0.536194

Optimized S0 geometry of **CORA-monPA-C_{60}-3** (at the M06-2X/6-31G(d)/PCM level)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.356657	-5.534566	-1.423335
2	14	0	0.202984	5.816267	-1.704952
3	6	0	-2.278620	-0.364805	-1.169384
4	6	0	-4.126470	1.412839	-0.020755
5	6	0	-2.951734	1.887468	-0.627965
6	1	0	-2.751389	2.955375	-0.653499
7	6	0	-6.259892	1.787137	0.998168
8	6	0	-6.504055	0.377223	1.014017
9	6	0	-4.368770	-0.009151	0.003529
10	6	0	-0.015555	-1.409118	0.518118
11	6	0	-7.126474	2.385460	1.938655
12	6	0	-0.735391	1.407658	-1.858436
13	6	0	-5.064060	2.344146	0.627932

14	6	0	-0.204943	-0.648319	1.641321
15	6	0	-2.051528	1.018058	-1.207808
16	6	0	-0.639074	0.732566	-3.215876
17	6	0	-0.864394	-0.668881	-3.171182
18	6	0	-3.412671	-0.867059	-0.565597
19	1	0	-3.570754	-1.942035	-0.537764
20	6	0	0.440752	1.401463	0.426761
21	6	0	-6.845393	3.578659	2.573164
22	6	0	-7.519657	0.125861	1.962480
23	6	0	-7.905341	1.363134	2.533609
24	6	0	-8.446876	1.470798	3.795466
25	6	0	0.151459	-0.850458	-0.895625
26	6	0	-5.690848	4.266577	2.053952
27	1	0	-5.416785	5.236874	2.460164
28	6	0	-4.840605	3.675554	1.131427
29	1	0	-3.934117	4.210667	0.861535
30	6	0	1.334280	-1.690741	-1.377922
31	6	0	0.031772	0.812942	1.593773
32	6	0	-1.451214	-2.620479	-1.741925
33	6	0	-5.564642	-0.557060	0.664835
34	6	0	0.408729	0.728193	-0.946197
35	6	0	-0.529328	2.850381	-1.920596
36	6	0	1.791096	1.120593	-1.467802
37	6	0	3.707382	-1.840282	-1.920724
38	6	0	-0.316734	1.350905	-4.392091
39	1	0	-0.133228	2.422512	-4.417854
40	6	0	2.422502	-1.194837	-2.045855
41	6	0	2.313855	2.216445	-0.703942
42	6	0	-7.583181	3.790675	3.801044
43	1	0	-7.470799	4.732009	4.332556
44	6	0	1.491254	-2.845406	-0.541297
45	6	0	-5.803495	-1.875953	1.194315
46	1	0	-5.131415	-2.691083	0.938132
47	6	0	-0.218994	0.592066	-5.590352
48	6	0	1.478577	2.391709	0.466727

49	6	0	-1.154104	-1.191548	-1.774500
50	6	0	-8.341670	2.791364	4.380261
51	1	0	-8.799372	2.981109	5.347594
52	6	0	-7.655849	-1.078720	2.622657
53	6	0	0.658116	-2.670247	0.631428
54	6	0	-0.443931	-0.813262	-5.545408
55	6	0	-0.763267	-1.427875	-4.303793
56	1	0	-0.926487	-2.502074	-4.262715
57	6	0	2.659419	0.265832	-2.093717
58	6	0	0.252501	-1.121999	2.925360
59	6	0	4.732568	-0.814298	-1.891784
60	6	0	-8.792908	0.204633	4.407157
61	1	0	-9.285901	0.199684	5.375868
62	6	0	-6.802560	-2.126479	2.122851
63	1	0	-6.874263	-3.123794	2.548692
64	6	0	4.083678	0.478916	-1.996624
65	6	0	5.018056	-3.143477	-0.293269
66	6	0	0.629030	1.198621	2.850047
67	6	0	1.607692	2.187457	2.896026
68	6	0	-0.303128	4.044220	-1.929166
69	6	0	5.853754	-0.970322	-1.091051
70	6	0	2.041664	2.803994	1.669783
71	6	0	5.996271	-2.158894	-0.267690
72	6	0	-1.751891	-3.796621	-1.678885
73	6	0	2.767538	2.022892	3.751170
74	6	0	-0.339502	-1.565802	-6.744239
75	1	0	-0.512694	-2.638048	-6.703713
76	6	0	1.074672	-3.162005	1.863629
77	6	0	3.853031	-2.984757	-1.142369
78	6	0	2.711823	-3.503576	-0.435461
79	6	0	2.894618	0.884787	4.535669
80	6	0	-8.418910	-1.003862	3.851083
81	1	0	-8.630770	-1.916362	4.402159
82	6	0	0.765360	0.011097	3.672341
83	6	0	6.590880	-1.759118	0.990643

84	6	0	3.680408	2.459955	-0.627231
85	6	0	6.181436	-2.357931	2.174499
86	6	0	2.360568	-3.829376	1.978113
87	6	0	5.979107	-1.548708	3.362263
88	6	0	4.591839	1.565265	-1.290144
89	6	0	3.923313	2.549592	3.046546
90	6	0	1.866714	-0.141074	4.501027
91	6	0	3.158837	-3.995598	0.857371
92	6	0	3.474441	3.035278	1.755773
93	6	0	4.588790	-3.770073	0.944534
94	6	0	6.372928	0.161674	-0.343226
95	6	0	0.869880	-2.364281	3.043475
96	6	0	6.823508	-0.324991	0.944036
97	6	0	5.559834	2.208974	0.750239
98	6	0	2.518399	-1.434863	4.611496
99	6	0	5.157787	-3.385291	2.151476
100	6	0	4.273458	2.869274	0.635047
101	6	0	2.952717	-3.429666	3.240604
102	6	0	6.201917	-0.180025	3.318246
103	6	0	2.030110	-2.521429	3.899055
104	6	0	4.828774	-2.075864	4.072246
105	6	0	6.636679	0.446064	2.083175
106	6	0	4.178411	0.225128	4.655000
107	6	0	5.990362	1.740833	1.984716
108	6	0	0.102210	1.199426	-6.832208
109	1	0	0.272023	2.272771	-6.858760
110	6	0	3.946016	-1.208654	4.702338
111	6	0	5.283628	0.727574	3.981261
112	6	0	5.755661	1.401380	-0.440997
113	6	0	0.197237	0.446206	-7.975189
114	1	0	0.443440	0.919811	-8.920432
115	6	0	5.153533	1.914501	3.158385
116	6	0	-0.025917	-0.951733	-7.930631
117	1	0	0.051309	-1.535985	-8.842278
118	6	0	4.321078	-3.210342	3.325165

119	6	0	-1.681374	-6.068980	0.266506
120	1	0	-2.109858	-7.056995	0.493436
121	6	0	2.034179	5.780984	-1.206511
122	1	0	2.122007	5.053499	-0.386062
123	6	0	2.931101	5.312379	-2.357971
124	1	0	2.615877	4.338694	-2.750678
125	1	0	3.972159	5.215069	-2.024880
126	1	0	2.915974	6.032988	-3.185476
127	6	0	-1.246361	7.589936	-3.490886
128	1	0	-2.140548	6.956363	-3.499701
129	1	0	-1.235122	8.149752	-4.433919
130	1	0	-1.352400	8.312553	-2.674872
131	6	0	-0.486610	5.657974	1.011233
132	1	0	-0.711373	4.590571	0.880127
133	1	0	-1.068967	6.015280	1.869070
134	1	0	0.574971	5.741175	1.268832
135	6	0	-1.747997	-8.114990	-2.510129
136	1	0	-1.318760	-8.386151	-1.539481
137	1	0	-1.225640	-8.697000	-3.278876
138	1	0	-2.794199	-8.439092	-2.512085
139	6	0	0.025015	6.745160	-3.356612
140	1	0	0.885811	7.431073	-3.382462
141	6	0	-0.851959	6.446388	-0.257028
142	1	0	-0.600457	7.505081	-0.095566
143	6	0	2.487368	7.151340	-0.685022
144	1	0	2.372754	7.926843	-1.453018
145	1	0	3.546901	7.128851	-0.403075
146	1	0	1.915617	7.467192	0.194681
147	6	0	-1.627603	-6.612072	-2.799909
148	1	0	-0.557470	-6.355384	-2.808513
149	6	0	-2.205152	-6.276470	-4.180034
150	1	0	-3.260695	-6.566619	-4.241399
151	1	0	-1.671570	-6.819321	-4.969311
152	1	0	-2.140076	-5.205530	-4.404879
153	6	0	0.147322	5.786980	-4.550936

154	1	0	1.056153	5.177454	-4.507925
155	1	0	0.159950	6.345913	-5.494460
156	1	0	-0.707911	5.101810	-4.578917
157	6	0	-2.360877	6.336367	-0.511585
158	1	0	-2.708019	7.015557	-1.293230
159	1	0	-2.922881	6.568479	0.402418
160	1	0	-2.631699	5.317375	-0.816406
161	6	0	-4.251876	-5.416658	-1.389727
162	1	0	-4.474395	-4.956110	-0.414864
163	6	0	-4.845817	-4.506275	-2.472101
164	1	0	-4.400439	-3.506239	-2.453645
165	1	0	-5.928155	-4.398244	-2.331037
166	1	0	-4.686798	-4.921718	-3.473185
167	6	0	-0.153082	-6.205257	0.212877
168	1	0	0.166765	-6.995967	-0.474180
169	1	0	0.254880	-6.437015	1.204688
170	1	0	0.312301	-5.270473	-0.121858
171	6	0	-2.107323	-5.093557	1.372227
172	1	0	-1.805738	-4.066464	1.131540
173	1	0	-1.636246	-5.357701	2.327234
174	1	0	-3.191825	-5.097352	1.525258
175	6	0	-4.915094	-6.800336	-1.416571
176	1	0	-4.783536	-7.275902	-2.395779
177	1	0	-5.993945	-6.717046	-1.239354
178	1	0	-4.503957	-7.476790	-0.658205

----

8 NMR and Mass Spectra

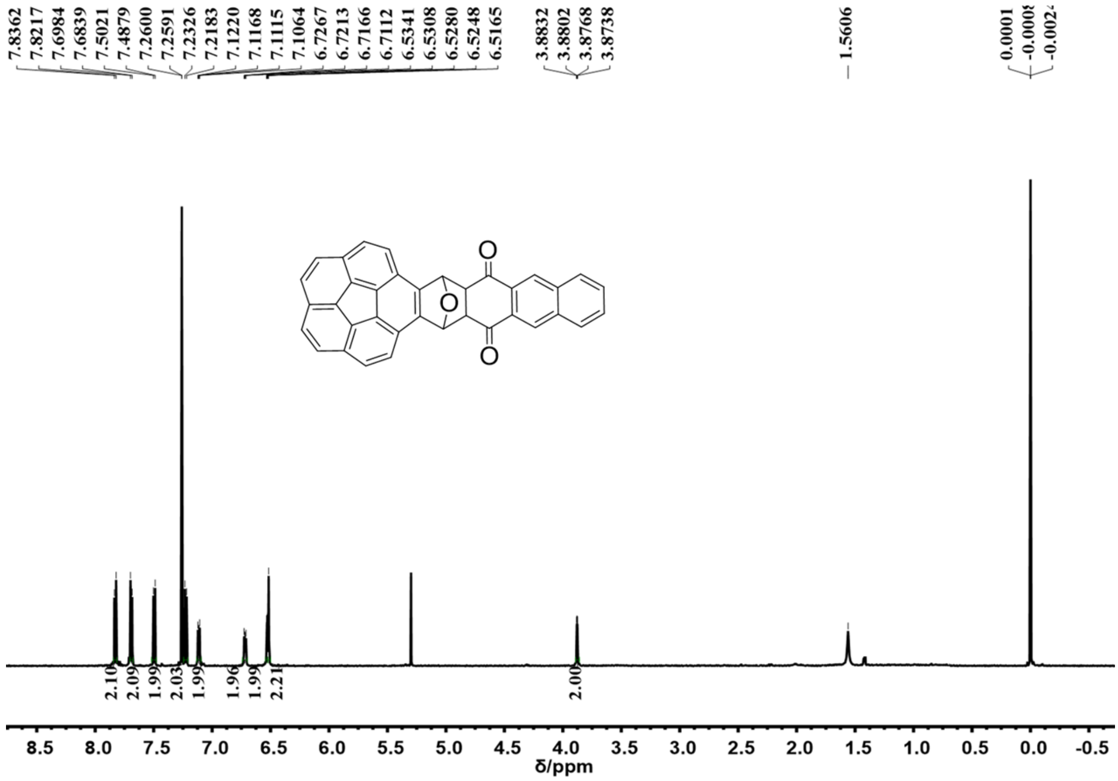


Figure S20. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of **3**.

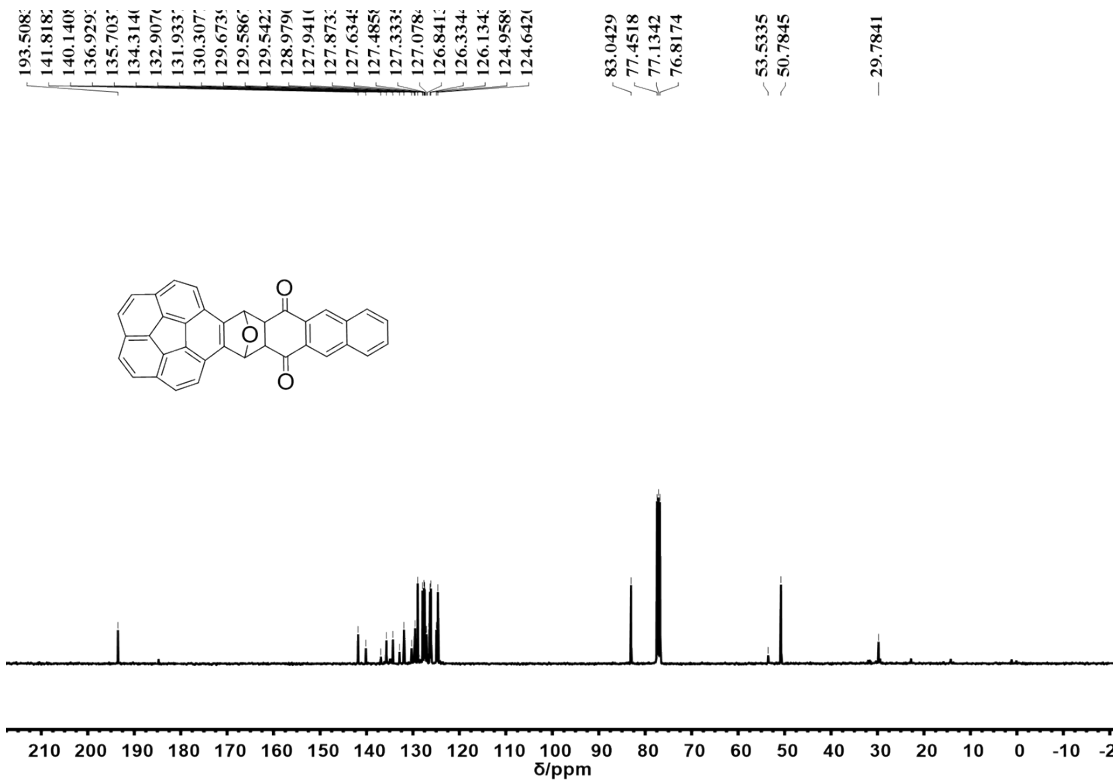


Figure S21. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **3**.

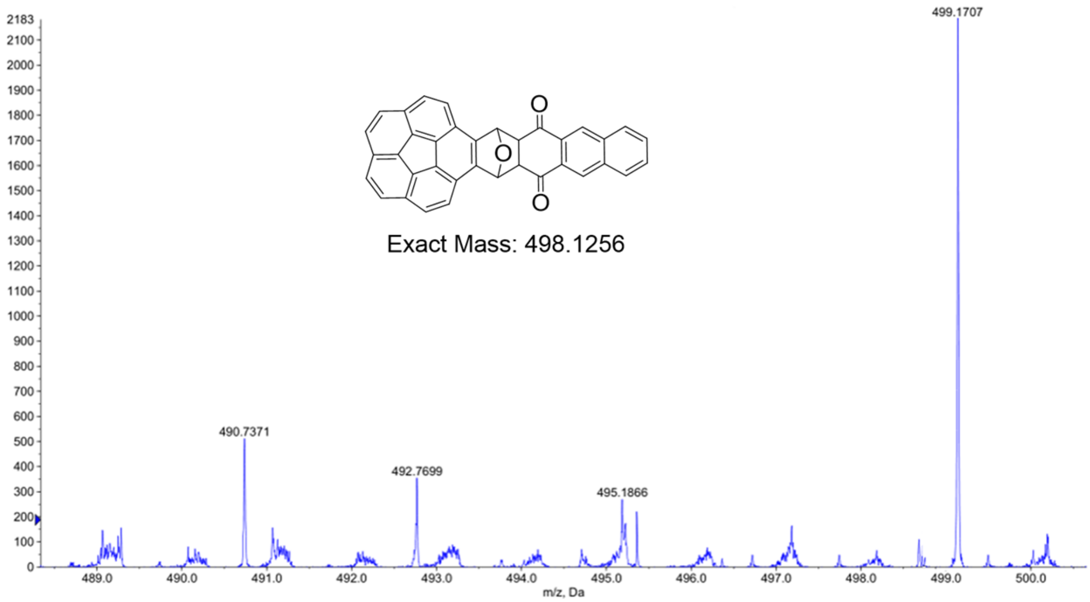


Figure S22. High-resolution mass spectrum (ESI) of **3**.

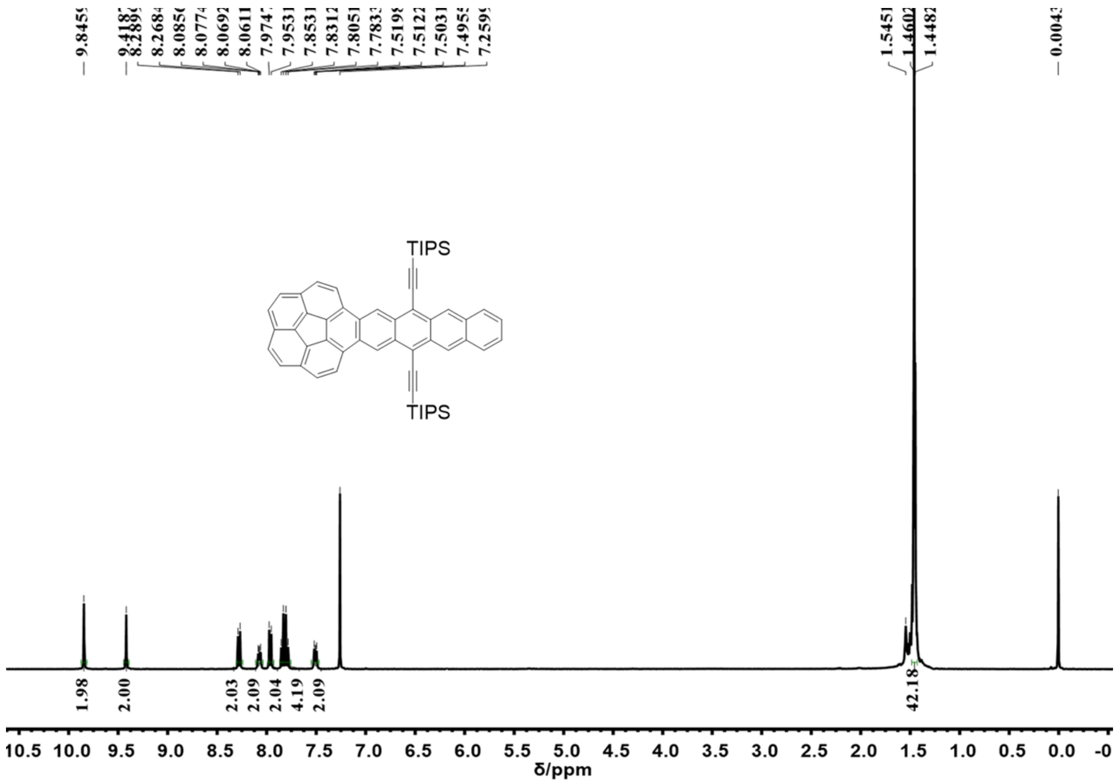


Figure S23. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **CORA-monPA**.

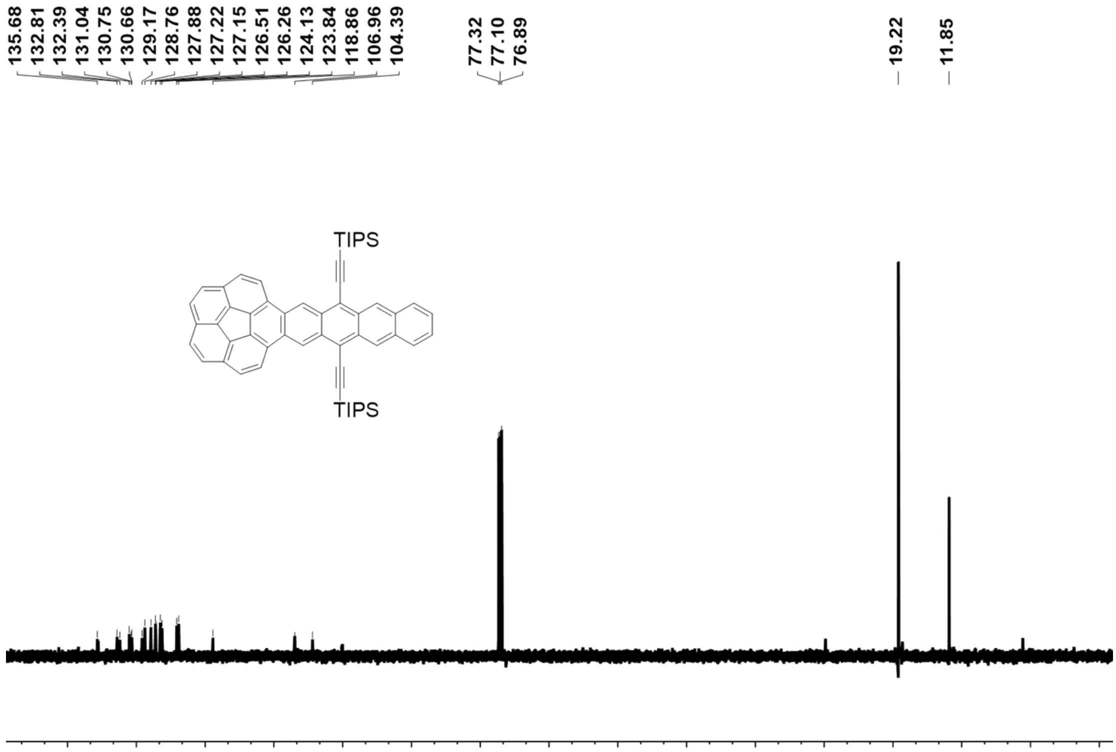


Figure S24. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **CORA-monPA**.

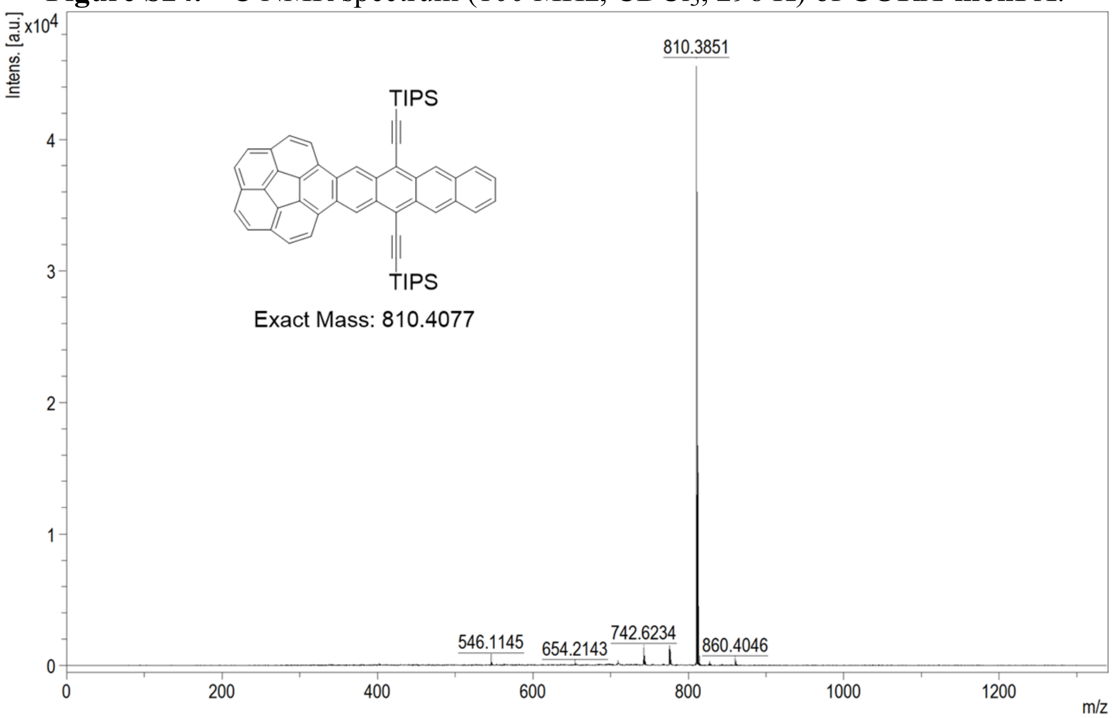


Figure S25. High-resolution mass spectrum (MALDT-TOF) of **CORA-monPA**.

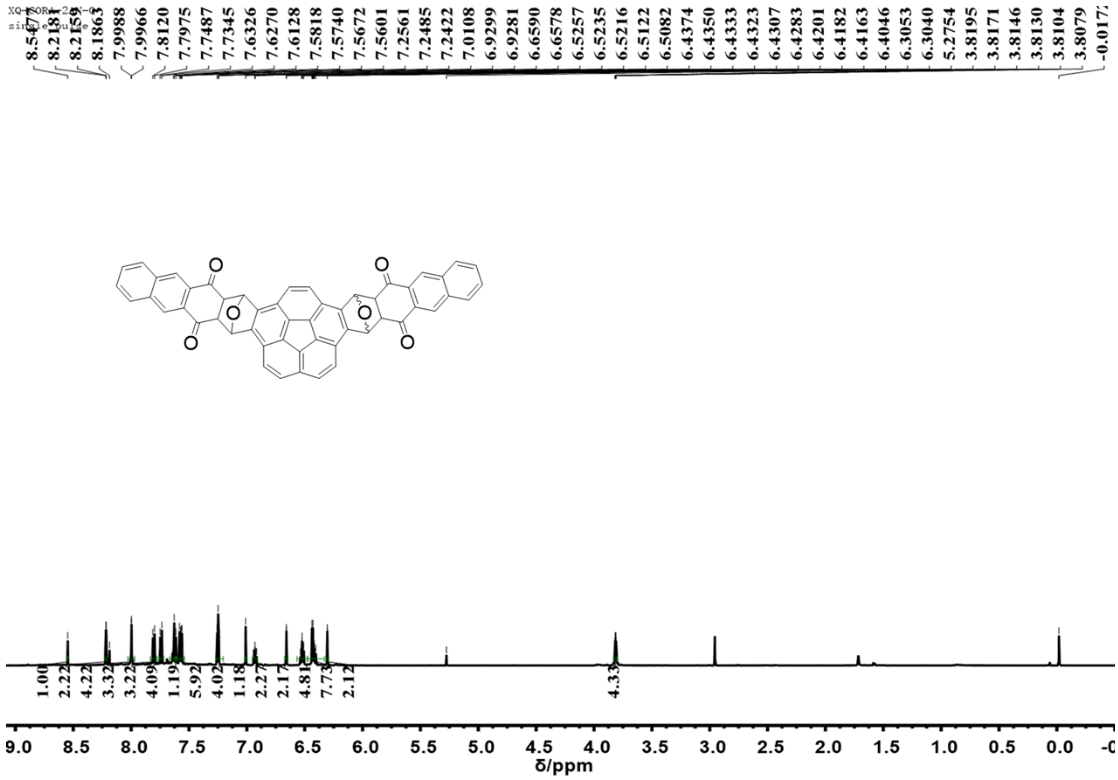


Figure S26. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of **6**.

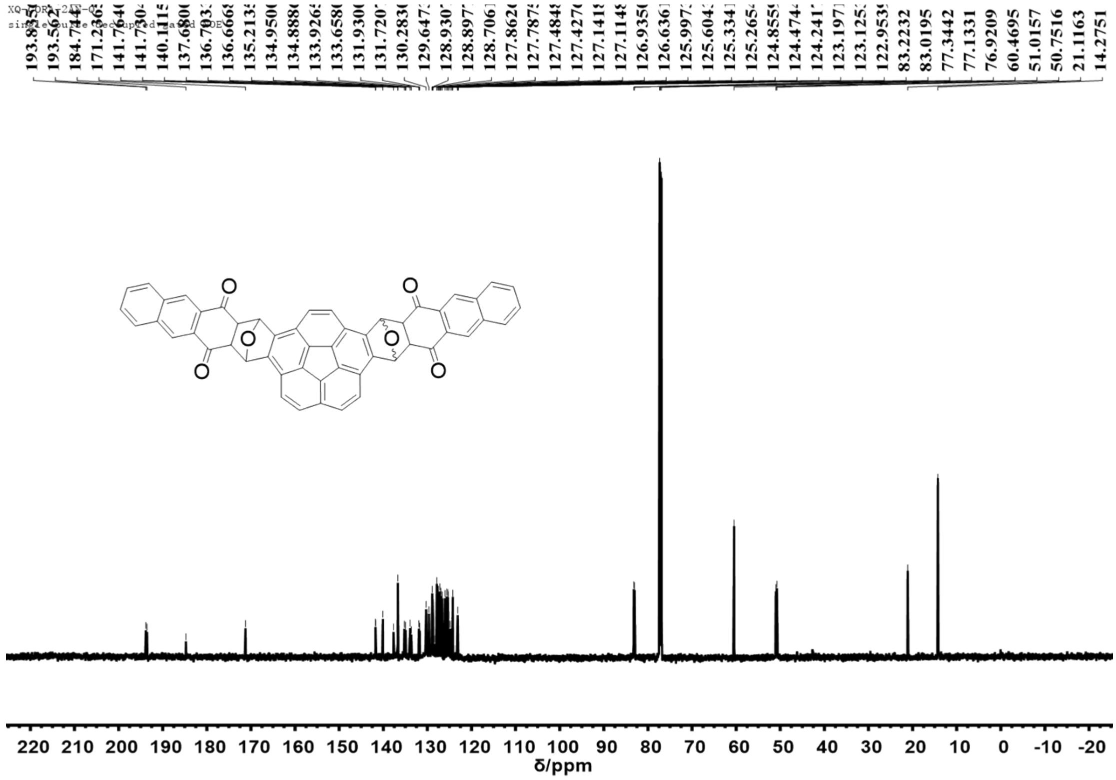


Figure S27. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **6**.

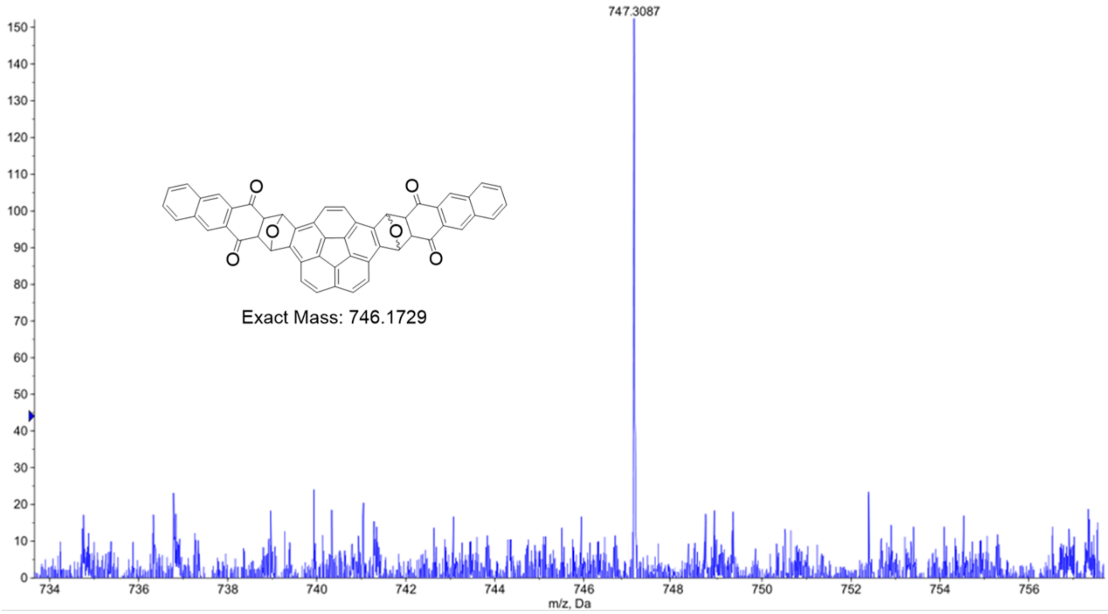


Figure S28. High-resolution mass spectrum (ESI) of **6**.

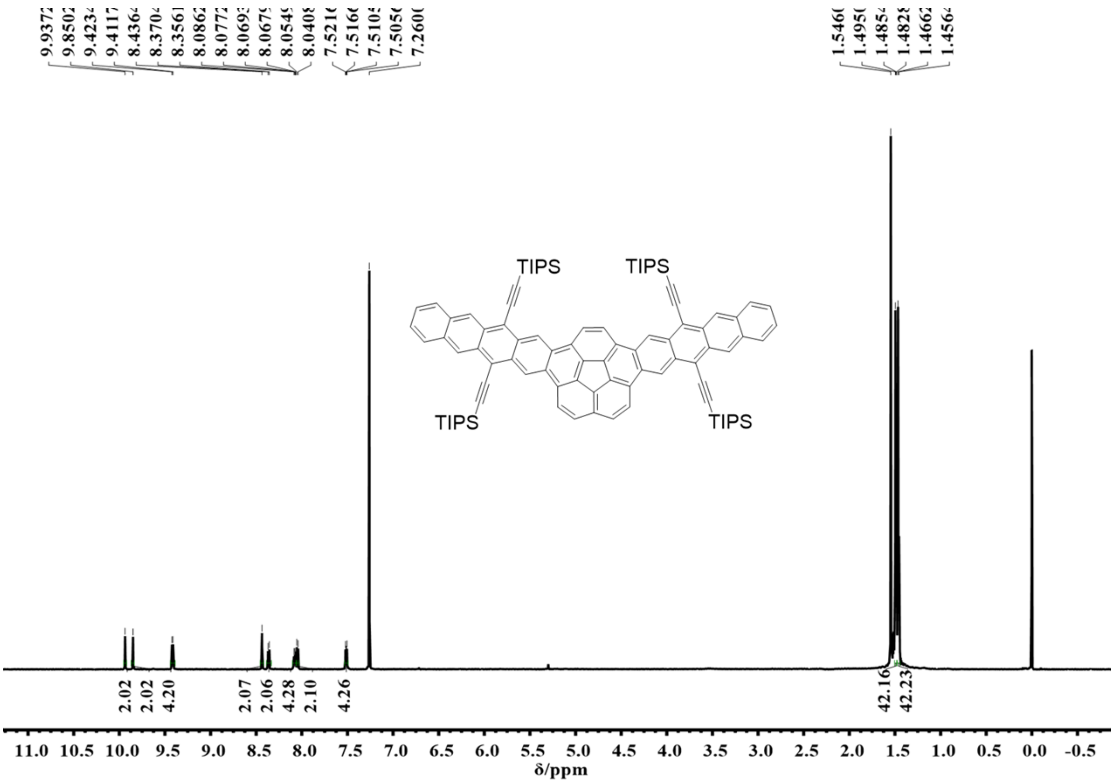


Figure S29. ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of **CORA-bisPA**.

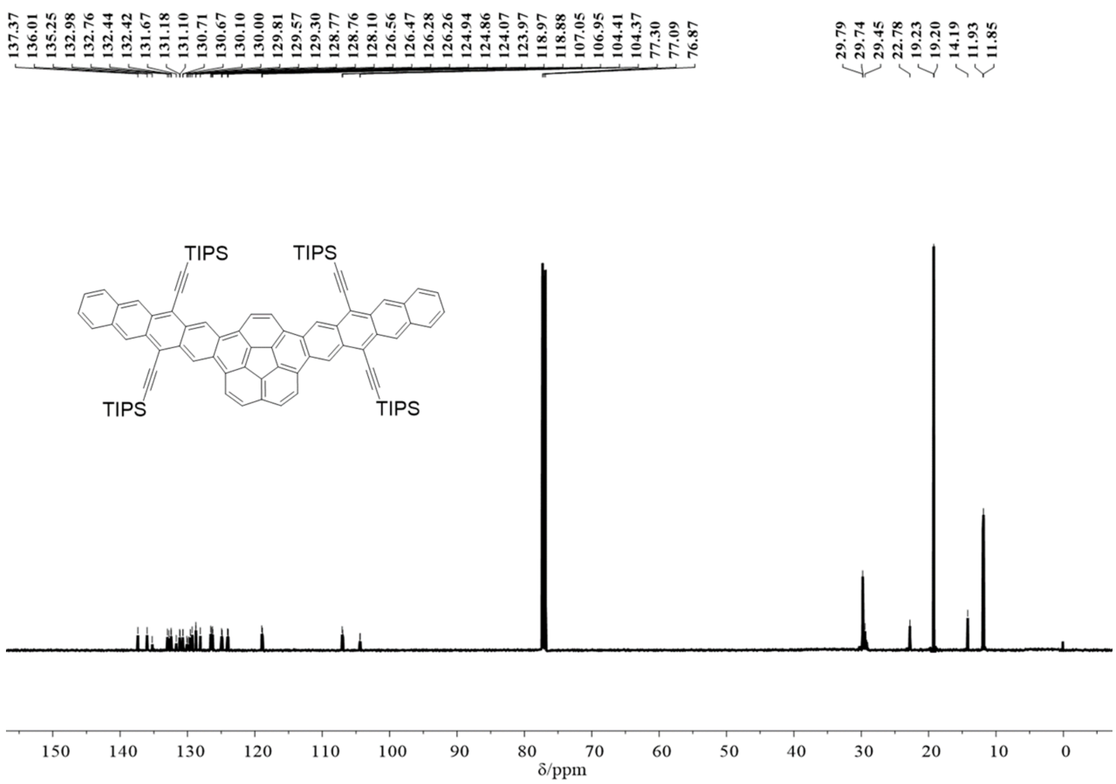


Figure S30. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **CORA-bisPA**.

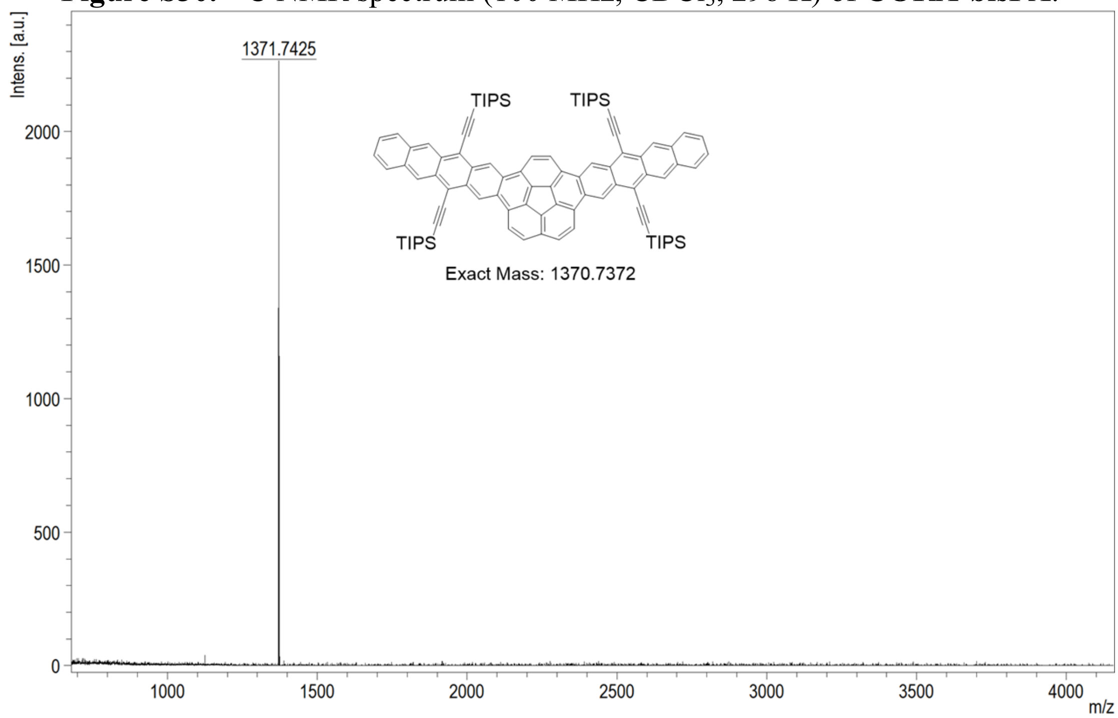


Figure S31. High-resolution mass spectrum (MALDI-TOF) of **CORA-bisPA**.

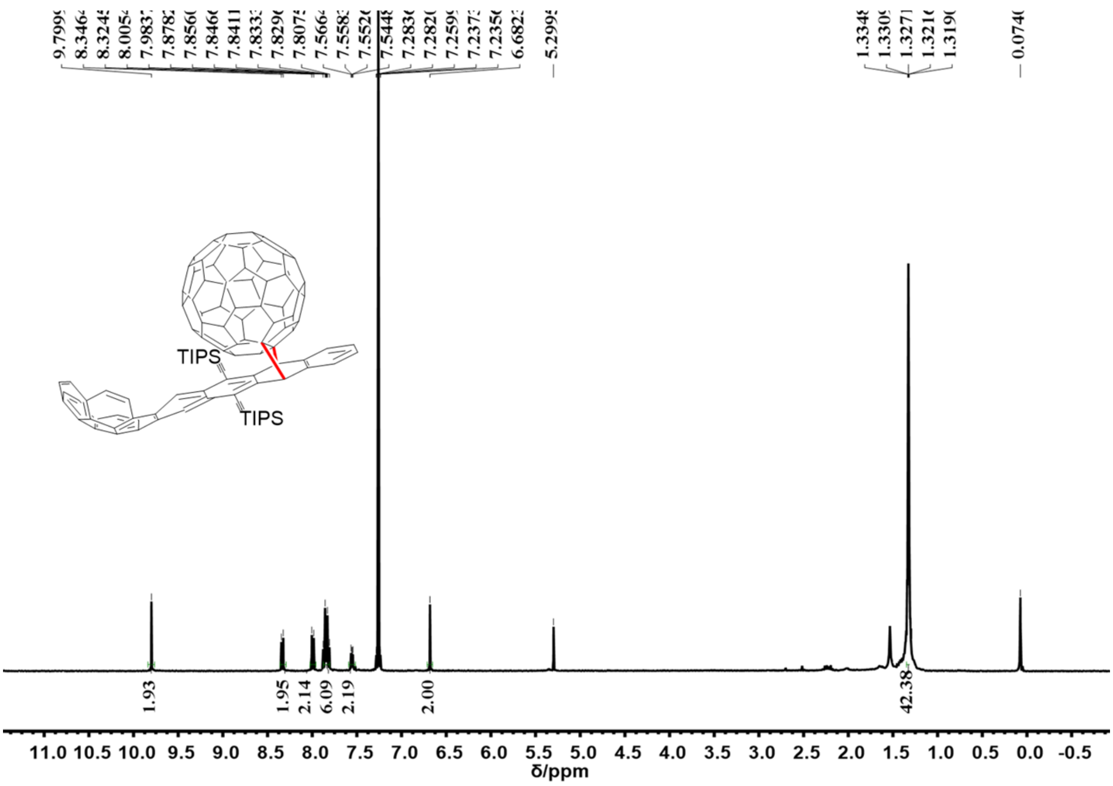


Figure S32. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **CORA-monPA-C_{60}**.

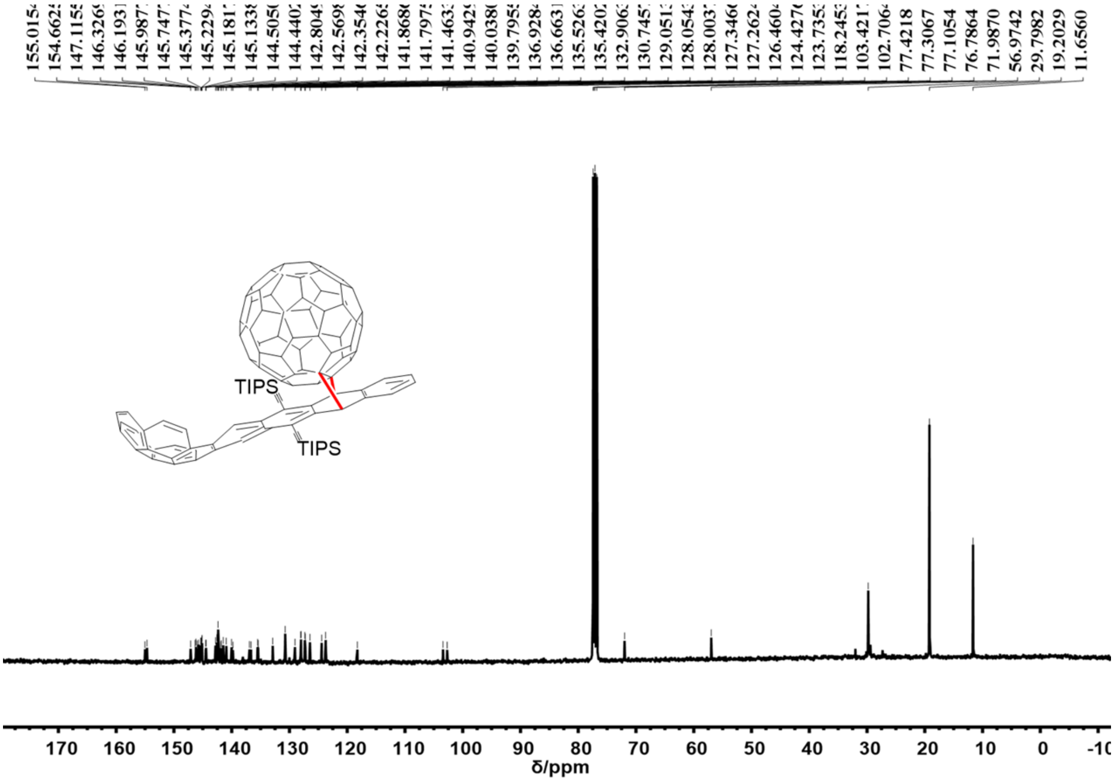


Figure S33. ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **CORA-monPA-C_{60}**.

9 Reference

(S1) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J; Howard, J. A. K.; Puschmann, H.

J. *Appl. Cryst.* **2009**, 42, 339-341.
(S2) Sheldrick, G. M. *Acta Cryst.* **2015**, A71, 3-8.
(S3) Sheldrick, G. M. *Acta Cryst.* **2015**, C71, 3-8.
(S4) Spek, A. L. *Acta Cryst.* **2015**, C71, 9-18.
(S5) Yamakado, T.; Takahashi, S.; Watanabe, K.; Matsumoto, Y.; Osuka, A.; Saito, S. *Angew. Chem. Int. Ed.* **2018**, 57, 5438-5443.
(S6) Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.
(S7) (a) Poater, J.; Bofill, J. M.; Alemany, P.; Solà, M. *J. Org. Chem.* **2006**, 71, 1700-1702. (b) Fallah-Bagher-Shaidaei, H.; Wannere, C. S.; Corminboeuf, C.; Puchta, R.; Schleyer, P. v. R. *Org. Lett.* **2006**, 8, 863-866. (c) Chen, W.; Li, X.; Long, G.; Li, Y.; Ganguly, R.; Zhang, M.; Aratani, N.; Yamada, H.; Liu, M.; Zhang, Q. *Angew. Chem. Int. Ed.* **2018**, 57, 13555-13559.
(S8) (a) Herges, R.; Geuenich, D. *J. Phy. Chem. A.* **2001**, 105, 3214-3220. (b) Geuenich, D.; Hess, K.; Kohler, F.; Herges, R. *Chem. Rev.* **2005**, 105, 3758-3772.
(S9) Cao, Y.; Liang, Y.; Zhang, L.; Osuna, S.; Hoyt, A.-L. M.; Briseno, A. L.; Houk, K. N. *J. Am. Chem. Soc.* **2014**, 136, 10743-10751.