Supporting Information

Bilateral π-Extension of an Open-[60]Fullerene in a Helical Manner

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1. General

The ^{1}H, ^{13}C, and ^{19}F NMR measurements were carried out at room temperature unless otherwise noted with a JEOL JNM ECA500 and Bruker Avance III 800US Plus instruments. The NMR chemical shifts were reported in ppm with reference to residual protons and carbons of acetone-d_6 (δ 2.05 ppm in ^{1}H NMR, δ 29.92 ppm in ^{13}C NMR). The ^{19}F NMR chemical shift was calibrated with a signal of trifluoroacetic acid in acetone-d_6/CS$_2$ (1:5) (δ –76.55 ppm). APCI (atmospheric pressure chemical ionization) mass spectra were measured on a Bruker micrOTOF-Q II. UV-vis-NIR absorption spectra were measured with a Shimadzu UV-3150 spectrometer. Thin layer chromatography (TLC) was performed on glass plates coated with 0.25 mm thick silica gel 60F-254 (Merck). Column chromatography was performed using PSQ 60B (Fuji Silysia).

Fullerene C$_{60}$ was purchased from SES Research Co. o-Dichlorobenzene (ODCB) was purchased from Sigma-Aldrich Co. LLC. 4,5-Dimethyl-1,2-phenylenediamine and p-tolyl isocyanate were purchased from Tokyo Chemical Industry Co. Ltd. Benzene and toluene were purchased from Nakalai Tesque, Inc. Pyridine (dehydrated), carbon disulfide, acetone, ethyl acetate, and trifluoroacetic acid were purchased from FUJIFILM Wako Pure Chemical Corporation.

All reactions were carried out under Ar atmosphere except for cases showing specific notation. Unless otherwise noted, materials purchased from commercial suppliers were used without further purification. Compounds **1**, **2**, and **6** were synthesized according to literature procedures.[1]

2. Computational Methods

All calculations were conducted using the Gaussian 09 program. All structures at the stationary states were optimized at the B3LYP/6-31G(d) or B3LYP-D3/6-31G(d) level of theory without any symmetry assumptions and confirmed by the frequency analyses at the same level of theory. Using the geometries optimized at the B3LYP-D3/6-31G(d) level of theory, natural population analysis was performed at the same level of theory. Using the geometries optimized at the B3LYP/6-31G(d) level of theory, TD-DFT calculations were conducted at the CAM-B3LYP/6-31G(d) level of theory.

3. Synthesis

3.1. Synthesis of 3
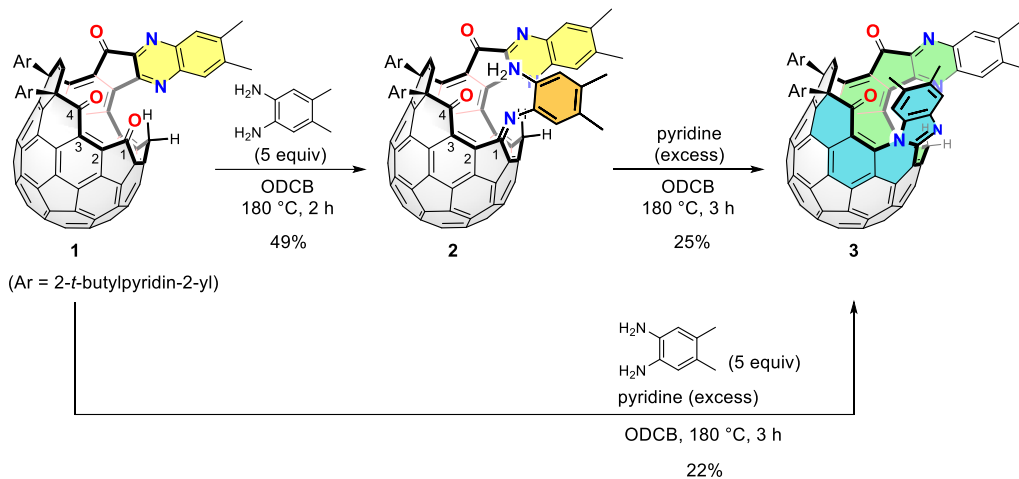
[Stepwise synthesis]

Powdery **1** (5.05 mg, 4.14 µmol) and 4,5-dimethyl-1,2-phenylenediamine (2.81 mg, 20.6 µmol, 4.99 equiv) were placed into a Schlenk tube and degassed through three vacuum-Ar cycles. ODCB (0.250 mL) was added and the resulting solution was heated at 180 °C for 2 h (aluminum block heater). The crude mixture was purified by column chromatography using silica gel (toluene/ethyl acetate (50:1) to (30:1)) to give unreacted **1** (2.54 mg, 2.08 µmol, 50%) followed by **2** (2.70 mg, 2.02 µmol, 49%) as brown powders. Subsequently, **2** (8.04 mg, 6.00 µmol) was placed into a Schlenk tube and degassed through three vacuum-Ar cycles. ODCB (0.400 mL) and pyridine (24.0 µL, $\rho = 0.982$ g/mL, 298 µmol, 50 equiv) were added and the resulting solution was heated at 180 °C for 3 h (aluminum block heater). The junk material produced during the reaction was firstly removed by column chromatography using silica gel (toluene/ethyl acetate (100:1)) to give a mixture containing **3** (4.85 mg). The mixture was then purified by column chromatography using silica gel (CS$_2$/acetone (150:1)) to give **3** (1.98 mg, 1.48 µmol, 25%) as a brown powder.

[One-pot synthesis]

Powdery **1** (25.0 mg, 20.5 µmol) and 4,5-dimethyl-1,2-phenylenediamine (13.9 mg, 102 µmol, 4.98 equiv) were placed into a Schlenk tube and degassed through three vacuum-Ar cycles. ODCB (1.25 mL) and pyridine (68.4 µL, $\rho = 0.982$ g/mL, 849 µmol, 41 equiv) were added and the resulting solution was heated at 180 °C for 3 h (aluminum block heater). The junk material produced during the reaction was firstly removed by column chromatography using silica gel (toluene/ethyl acetate (100:1)) to give a mixture

containing **3** (10.8 mg). The mixture was then purified by column chromatography using silica gel (CS$_2$/acetone (200:1)) to give **3** (5.90 mg, 4.41 μmol, 22%) as a brown powder.

2: ^{1}H NMR (500 MHz, acetone-d_6/CS$_2$ (1:5)) δ 8.11 (s, 1H), 8.04 (s, 1H), 7.67 (t, 1H, $J = 7.5$ Hz), 7.65 (d, 1H, $J = 10.3$ Hz), 7.56 (t, 1H, $J = 7.5$ Hz), 7.47 (d, 1H, $J = 7.5$ Hz), 7.28 (d, 1H, $J = 7.5$ Hz), 7.25 (d, 1H, $J = 7.5$ Hz), 7.14 (d, 1H, $J = 7.5$ Hz), 6.55 (d, 1H, $J = 10.3$ Hz), 4.69 (d, 1H, $J = 20.9$ Hz), 3.26 (d, 1H, $J = 20.9$ Hz), 2.68 (s, 3H), 2.67 (s, 3H), 1.21 (s, 9H), 1.11 (s, 9H), −10.73 (br s, trace); HRMS (APCI) m/z: [M]$^{\bullet-}$ Calcd for C$_{90}$H$_{36}$N$_4$O$_3$ (**2**) 1220.2793; Found 1220.2768. (These data matched well with the reported ones.[1])

3: ^{1}H NMR (500 MHz, acetone-d_6/CS$_2$ (1:5), room temperature) δ 8.12 (s, 1H), 8.00 (s, 1H), 7.62 (t, 2H, $J = 7.5$ Hz), 7.35 (d, 1H, $J = 7.5$ Hz), 7.31 (br d, 1H, $J = 9.2$ Hz), 7.25 (d, 1H, $J = 7.5$ Hz), 7.21 (d, 1H, $J = 7.5$ Hz), 7.16 (s, 1H), 7.15 (d, 1H, $J = 7.5$ Hz), 7.14 (s, 1H), 6.09 (br d, 1H, $J = 9.2$ Hz), 5.13 (br s, 1H), 2.74 (s, 3H), 2.72 (s, 3H), 2.38 (s, 3H), 2.37 (s, 3H), 1.35 (s, 9H), 1.21 (s, 9H) (One of the proton signals, which was assigned as methylene protons, was not observed due to severe broadening at room temperature while it appeared at δ 3.12 ppm (d, 1H, $J = 20.2$ Hz) at –30 °C and the coupling partner was observed as a doublet signal at δ 5.15 ppm (d, 1H, $J = 20.2$ Hz).); ^{13}C NMR (201 MHz, acetone-d_6/CS$_2$ (1:5), –30 °C) δ 192.00, 187.42, 168.12, 167.60, 163.80, 163.71, 154.23, 153.91, 153.32, 152.56, 151.97, 151.31, 151.25, 150.78, 150.53, 149.95, 149.66, 149.56, 149.45, 149.28, 148.53, 148.33, 147.83, 147.77, 147.42, 147.25, 147.21, 146.51, 146.39, 145.93, 145.70, 144.77, 144.45, 144.26, 144.06, 143.60, 143.27, 143.15, 143.03, 142.34, 142.23, 142.13, 141.87, 141.40, 140.88, 139.97, 139.06, 137.78, 137.67, 137.51, 137.43, 136.84, 136.37, 135.62, 135.42, 135.23, 135.17, 135.06, 134.40, 134.03, 133.25, 132.67, 132.47, 132.24, 131.29, 130.55, 130.38, 130.29, 130.27, 129.92, 129.42, 127.24, 124.92, 124.81, 124.61, 121.67, 121.39, 120.92, 120.57, 117.88, 117.71, 114.99, 58.69, 52.83, 44.82, 37.82, 37.72, 30.63, 30.32, 21.54, 21.53, 21.06, 21.02 (The sum of carbon signals must be 94 in theory. Observed 93. One sp^2 carbon signal is overlapped.); HRMS (APCI) m/z: [M]$^{\bullet-}$ Calcd for C$_{98}$H$_{44}$N$_6$O$_2$ (**3**) 1336.3531; Found 1336.3477.
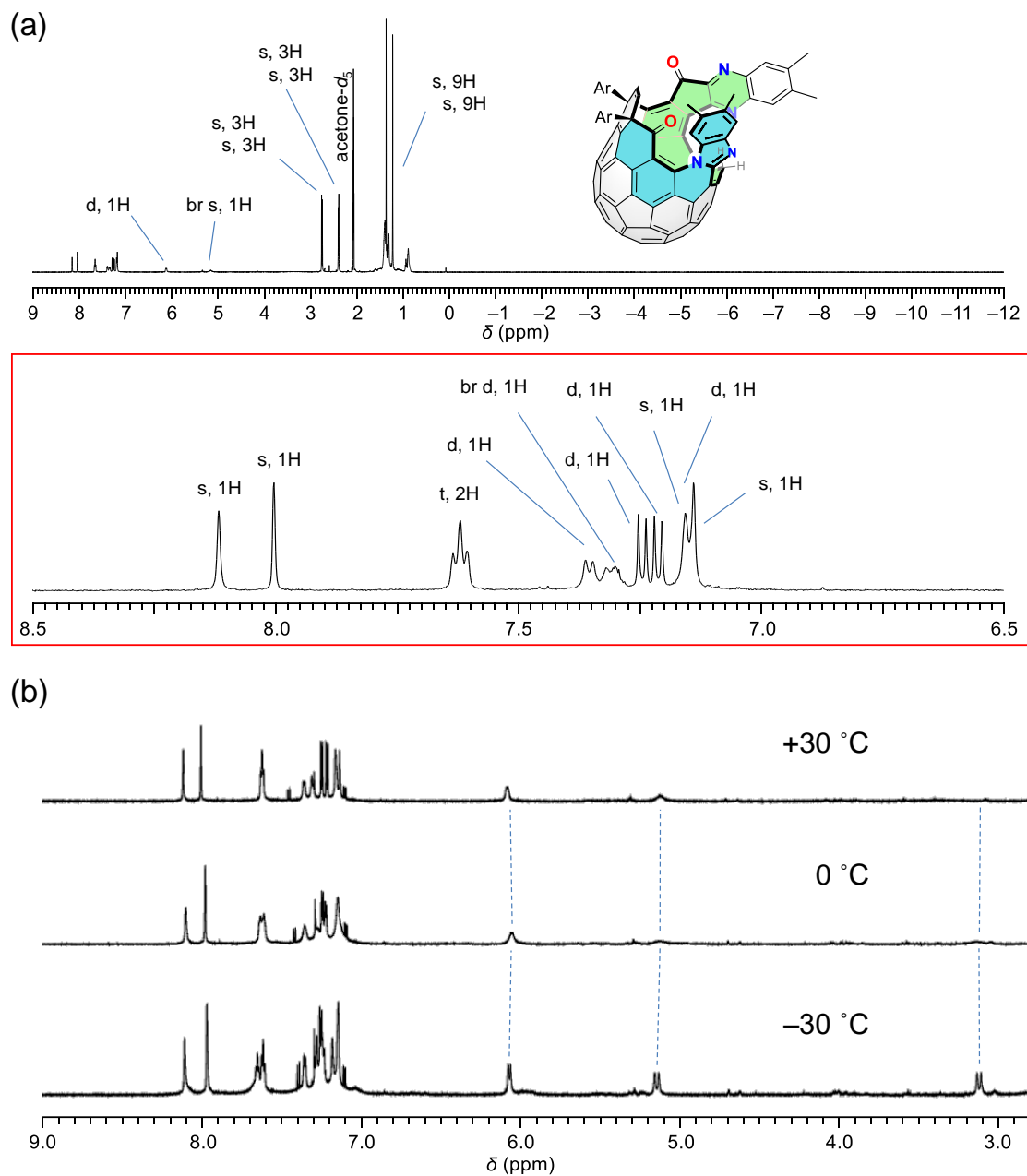
Figure S1. ^{1}H NMR spectra (acetone-d_6/CS$_2$ (1:5)) of **3** at (a) room temperature (500 MHz) and (b) variable temperatures at +30, 0, and –30 °C (800 MHz). The signal broadening might be caused by the insertion/escape dynamics of the guest molecules such as H$_2$O, N$_2$, and Ar.
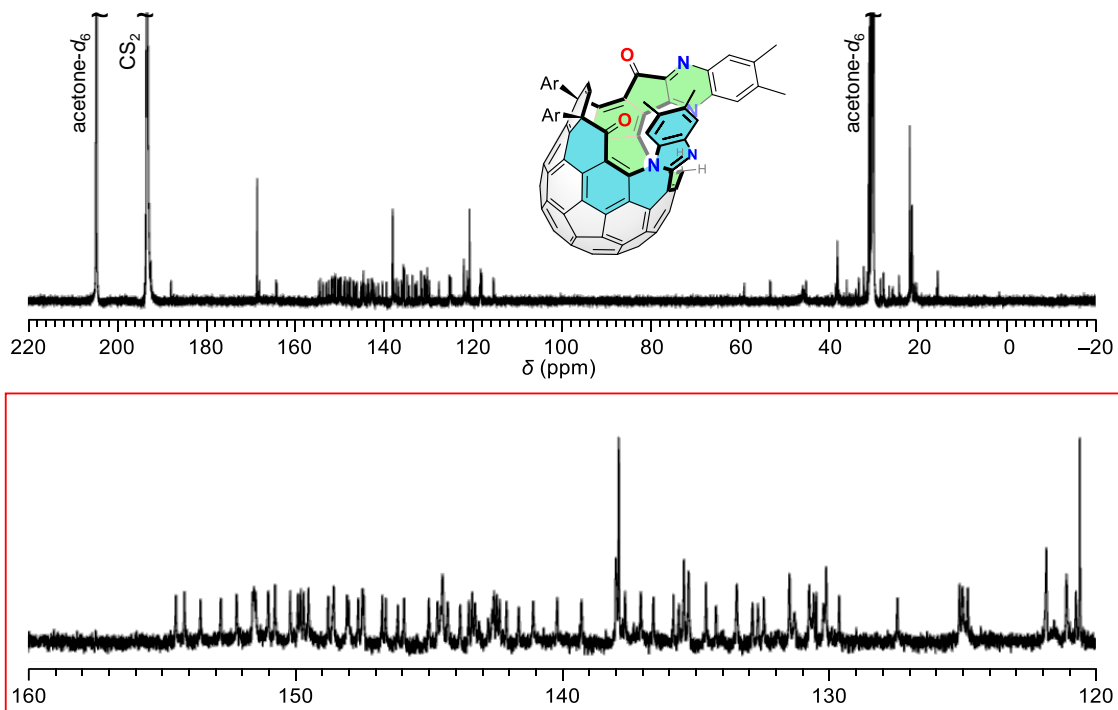
Figure S2. ^{13}C NMR spectra (201 MHz, acetone-d_6/CS$_2$ (1:5), –30 °C) of **3**.
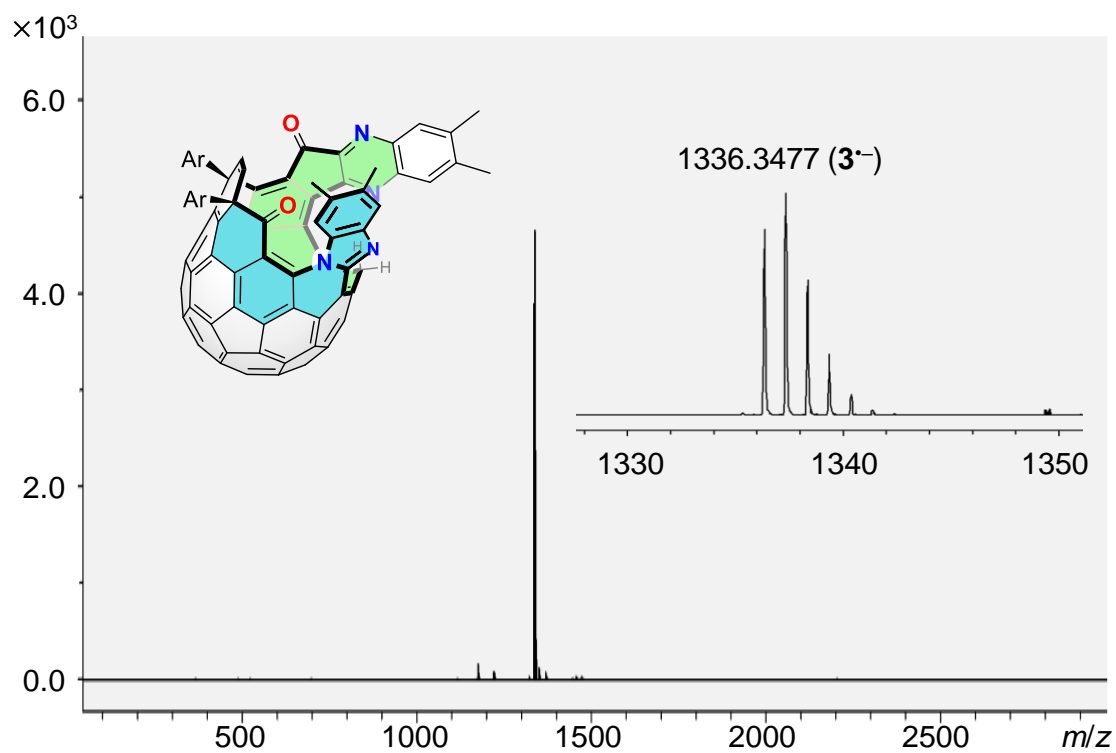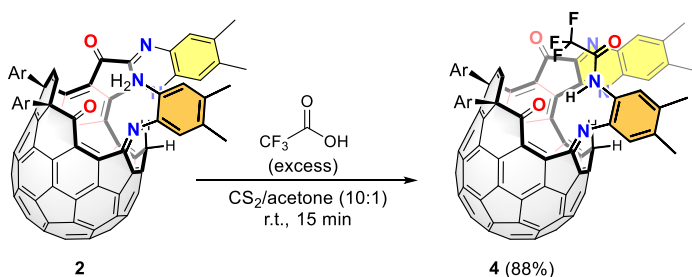

Figure S3. APCI mass spectra (negative ion mode) of **3**.

3.2. Synthesis of 4

Powdery **1** (10.0 mg, 7.47 μmol) was placed into a 5-mL glass vial. CS_2 (0.500 mL), acetone (super dehydrated, 50 μL), and trifluoroacetic acid (50 μL, ρ = 1.49 g/mL, 653 μmol, 88 equiv) were added and the resulting solution was stirred at room temperature for 15 min under air. After removal of the solvent, the crude mixture was purified by column chromatography using silica gel (toluene/ethyl acetate (50:1)) to give **4** (9.39 mg, 6.54 μmol, 88%) as a brown powder.

4: ^{1}H NMR (500 MHz, acetone-d_6/CS_2 (1:5)) δ 9.96 (s, 0.82H), 9.94 (s, 0.18H), 8.15 (s, 1H), 7.68 (t, 1H, J = 8.0 Hz), 7.61 (s, 1H), 7.603 (t, 0.82H, J = 8.0 Hz), 7.600 (t, 0.16H, J = 8.0 Hz), 7.461 (d, 1H, J = 10.9 Hz), 7.459 (d, 1H, J = 8.0 Hz), 7.42 (s, 1H), 7.25 (d, 1H, J = 8.0 Hz), 7.23 (s, 1H), 7.184 (d, 1H, J = 8.0 Hz), 7.175 (d, 1H, J = 8.0 Hz), 6.46 (d, 1H, J = 10.9 Hz), 3.93 (d, 0.82H, J = 20.6 Hz), 3.90 (d, 0.18H, J = 20.6 Hz), 2.79 (s, 0.54H), 2.78 (s, 2.56H), 2.68 (s, 0.54H), 2.65 (s, 2.56H), 2.43 (d, 0.82H, J = 20.6 Hz), 2.31 (d, 0.82H, J = 20.6 Hz), 2.14 (s, 3H), 1.23 (s, 1.62H), 1.22 (s, 7.38H), 1.16 (s, 1.62H), 1.15 (t, 7.38H), −10.97 (br s, 0.76H) (A part of signals corresponding to the empty and encapsulated ones was separately observed.); ^{13}C NMR (201 MHz, acetone-d_6/CS_2 (1:5)) δ 193.12 (confirmed by HMBC), 187.71, 187.64, 168.55, 168.53, 168.52, 168.51, 163.86, 163.71, 163.52, 163.40, 158.83, 158.65, 154.87 (q, ${}^{2}J_{CF}$ = 38.2 Hz), 154.21, 154.20, 153.33, 153.08, 153.04, 153.00, 152.44, 152.35, 151.10, 150.98, 150.95, 150.91, 150.86, 150.79, 150.72, 149.95, 149.81, 149.80, 149.62, 149.58, 149.52, 149.28, 149.26, 149.22, 149.10, 149.01, 148.99, 148.82, 148.79, 148.37, 148.36, 147.34, 147.08, 147.00, 146.92, 146.86, 146.77, 146.72, 146.65, 146.64, 146.34, 146.31, 146.20, 146.13, 145.78, 145.74, 145.08, 145.05, 144.93, 144.84, 144.77, 144.69, 144.59, 144.59, 144.53, 144.26, 144.05, 143.99, 143.98, 143.97, 143.95, 143.85, 143.71, 143.55, 143.49, 143.35, 142.99, 142.01, 141.97, 141.92, 141.64, 141.63, 141.62, 141.52, 141.33, 141.28, 140.24, 139.76, 139.56, 139.35, 138.41, 138.40, 138.06, 138.03, 137.97, 137.86, 137.80, 137.69, 137.46, 137.40, 137.33, 137.11, 136.99, 136.85, 136.74, 136.43, 136.37, 136.23, 136.07, 135.77, 135.18, 135.01, 134.98, 134.87, 134.25, 133.47, 133.37, 133.22, 133.17, 133.06, 132.92, 132.89,

132.64, 132.47, 132.45, 132.43, 131.79, 131.69, 130.42, 130.00, 129.87, 129.36, 128.79, 127.94, 127.70, 125.66, 120.80, 120.79, 120.77, 120.69, 120.63, 120.02, 120.00, 117.89, 117.86, 117.86, 116.33 (q, $^1J_{CF} = 289$ Hz), 60.41, 60.27, 53.46, 43.35, 43.19, 38.00, 37.99, 37.98, 37.96, 30.55, 30.54, 30.38, 30.36, 21.54, 21.15, 20.96, 19.90 (The carbon signals of the empty and encapsulated ones were separately observed. The sum of carbon signals must be 96 in theory. Observed 168 (for two components). The 16 sp^2, 6 sp^3, and 2 carbonyl carbon signals are overlapped.); ^{19}F NMR (471 MHz, acetone-d_6/CS$_2$ (1:5)) δ – 73.0; HRMS (APCI) m/z: [M]$^{\bullet-}$ Calcd for C$_{100}$H$_{45}$F$_3$N$_6$O$_3$ (**4**) 1434.3511; Found 1434.3468.

Figure S4. ^{1}H NMR spectra (500 MHz, acetone-d_6/CS$_2$ (1:5)) of **4**.
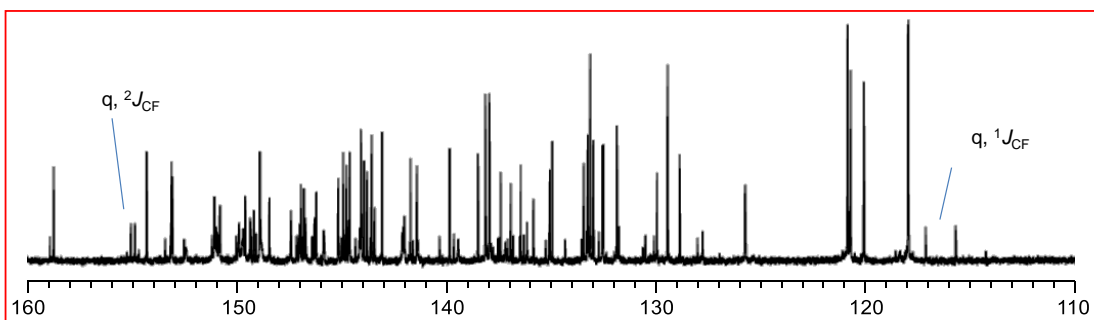
Figure S5. ^{13}C NMR spectra (201 MHz, acetone-d_6/CS$_2$ (1:5)) of **4**.

Figure S6. HMBC spectrum (800 MHz, acetone-d_6/CS$_2$ (1:5)) of **4**.
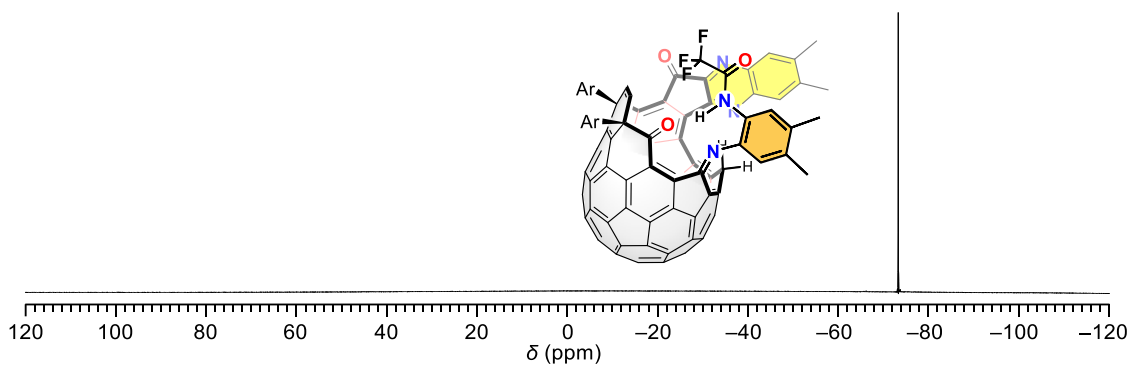
Figure S7. ^{19}F NMR spectrum (471 MHz, acetone-d_6/CS$_2$ (1:5)) of **4**.

S11
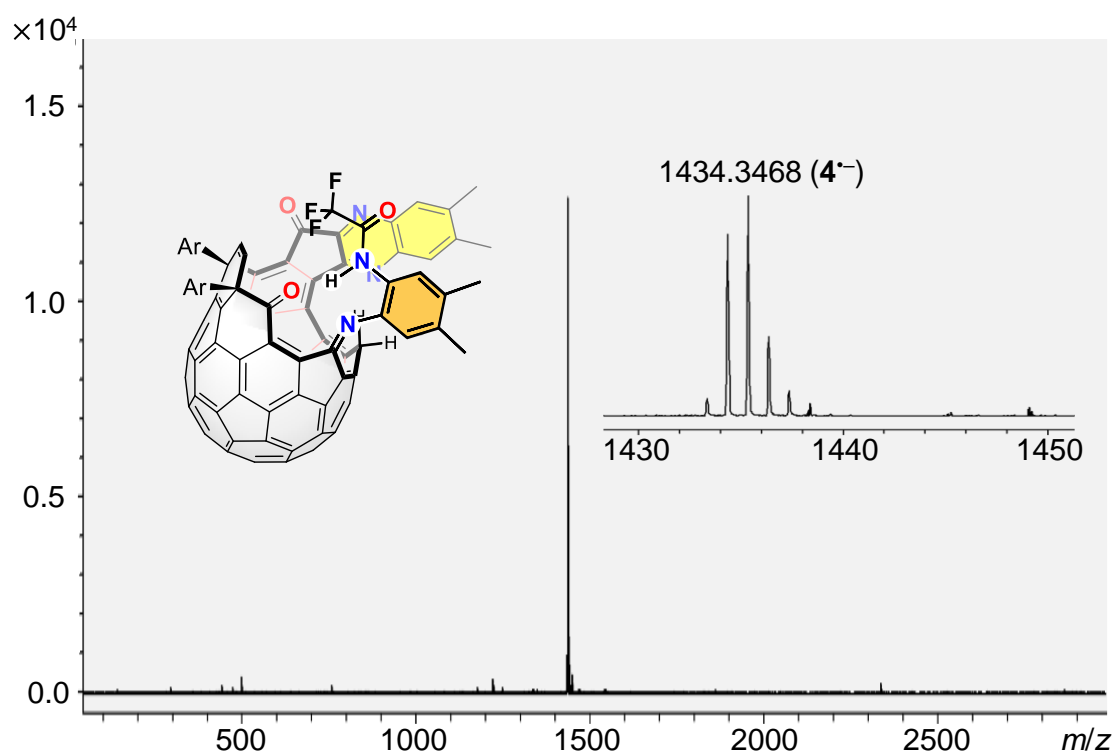
Figure S8. APCI mass spectra (negative ion mode) of **4**.

3.3. Synthesis of 5
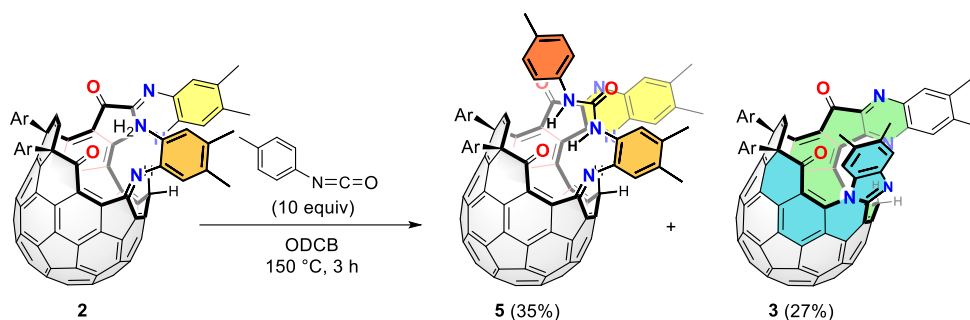
Powdery **2** (10.0 mg, 7.47 µmol) was placed into a 5-mL glass vial and degassed through three vacuum-Ar cycles. ODCB (0.500 mL) and *p*-tolyl isocyanate (9.21 µL, ρ = 1.06 g/mL, 73.3 µmol, 10 equiv) were added and the resulting solution was heated at 150 °C for 3 h (aluminum block heater). The crude mixture was purified by column chromatography using silica gel (toluene/ethyl acetate (50:1) to (20:1)) to give **3** (2.69 mg, 2.01 µmol, 27%) followed by **5** (3.90 mg, 2.65 µmol, 35%) as brown powders.

5: ^{1}H NMR (500 MHz, acetone-d_6/CS$_2$ (1:5)) δ 8.93 (s, 0.84H), 8.88 (s, 0.16H), 8.22 (s, 1H), 7.64 (t, 1H, *J* = 8.0 Hz), 7.610 (s, 1H), 7.605 (t, 0.84H, *J* = 8.0 Hz), 7.60 (t, 0.16H, *J* = 8.0 Hz), 7.56 (d, 0.84H, *J* = 10.3 Hz), 7.54 (d, 0.16H, *J* = 10.3 Hz), 7.49 (d, 1.68H, *J* = 8.0 Hz), 7.48 (d, 0.32H, *J* = 8.0 Hz), 7.41 (d, 1H, *J* = 8.0 Hz), 7.33 (s, 0.84H), 7.32 (s, 0.16H), 7.24 (d, 1H, *J* = 8.0 Hz), 7.22 (s, 1H), 7.204 (d, 1H, *J* = 8.0 Hz), 7.199 (d, 1H, *J* = 8.0 Hz), 7.10 (d, 2H, *J* = 8.0 Hz), 7.03 (s, 0.84H), 7.02 (s, 0.16H), 6.45 (d, 0.84H, *J* = 10.3 Hz), 6.43 (d, 0.16H, *J* = 10.3 Hz), 4.05 (d, 0.84H, *J* = 20.6 Hz), 4.02 (d, 0.84H, *J* = 20.6 Hz), 2.76 (s, 3H), 2.64 (s, 3H), 2.47 (d, 0.84H, *J* = 20.6 Hz), 2.38 (s, 3H), 2.37 (d, 0.16H, *J* = 20.6 Hz), 1.86(s, 2.52H), 1.85 (s, 0.48H), 1.23 (s 1.62H), 1.219 (s, 7.56H), 1.215 (s 1.44H), 1.19 (s, 7.56H), 1.18 (s 1.44H), –10.97 (br s, 0.62H) (A part of signals corresponding to the empty and encapsulated ones was separately observed.); ^{13}C NMR (126 MHz, acetone-d_6/CS$_2$ (1:5)) δ 195.82, 187.73, 168.55, 163.63, 163.46, 155.19, 154.98, 154.13, 152.94, 152.35, 152.17, 151.42, 151.03, 150.92, 150.54, 149.73, 149.64, 149.57, 149.47, 149.29, 149.13, 148.96, 148.85, 148.53, 148.14, 147.31, 147.05, 146.86, 146.76, 146.61, 145.79, 144.93, 144.86, 144.67, 144.63, 144.15, 144.11, 144.00, 143.76, 143.65, 143.59, 143.36, 142.75, 142.03, 141.94, 141.84, 141.68, 141.65, 141.55, 141.39, 139.69, 138.81, 138.03, 137.88, 137.36, 137.27, 136.88, 136.72, 136.53, 136.50, 135.84, 135.64, 135.43, 134.45, 134.26, 133.33, 133.00, 132.85, 132.80, 132.16, 131.26, 129.94, 129.78, 129.30, 128.24, 126.95, 124.20, 121.35, 120.71, 120.67, 118.99, 118.57, 118.07, 117.94, 59.94, 53.38, 43.67, 43.54, 37.94, 37.91, 30.52, 30.40, 21.72, 21.51, 21.12, 21.01,

19.85 (The sum of carbon signals must be 100 in theory. Observed 97. The 3 sp^2 carbon signals are overlapped.); HRMS (APCI) m/z: $[M+H]^+$ Calcd for $C_{106}H_{54}N_7O_3$ (**5**) 1472.4283; Found 1472.4227.
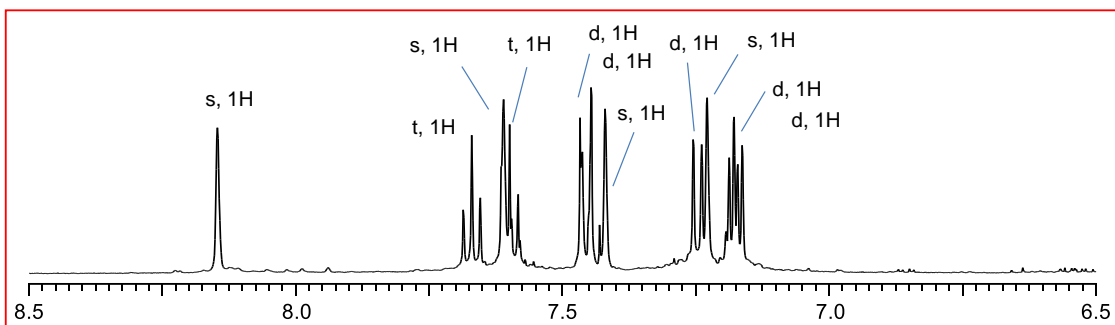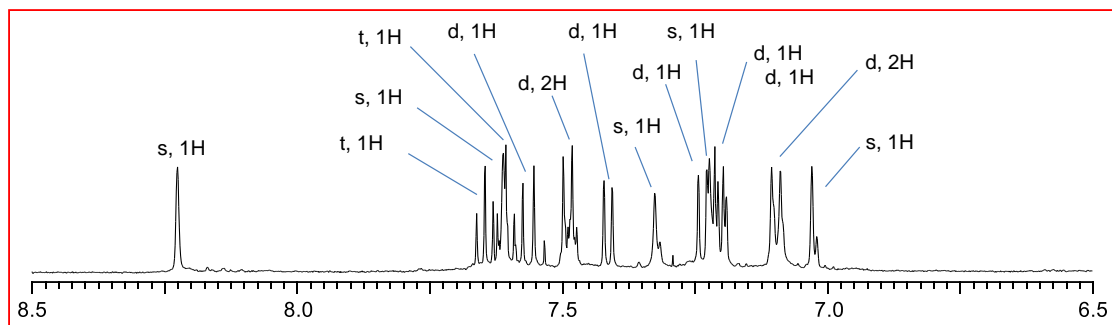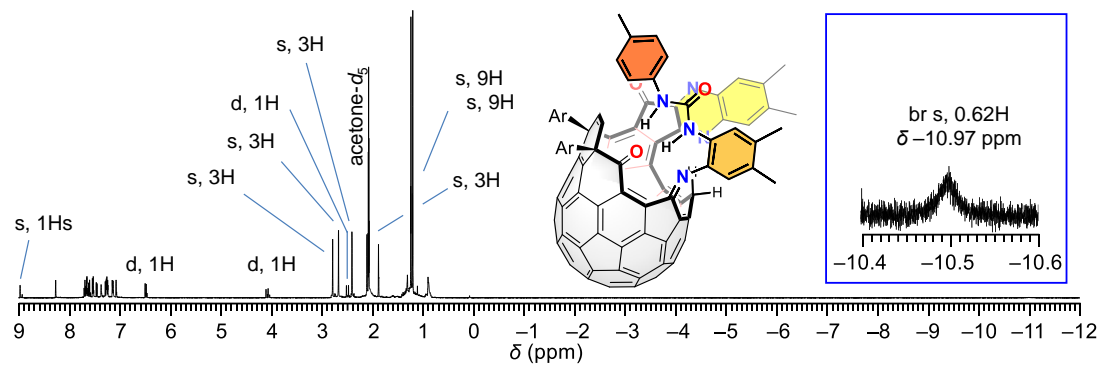
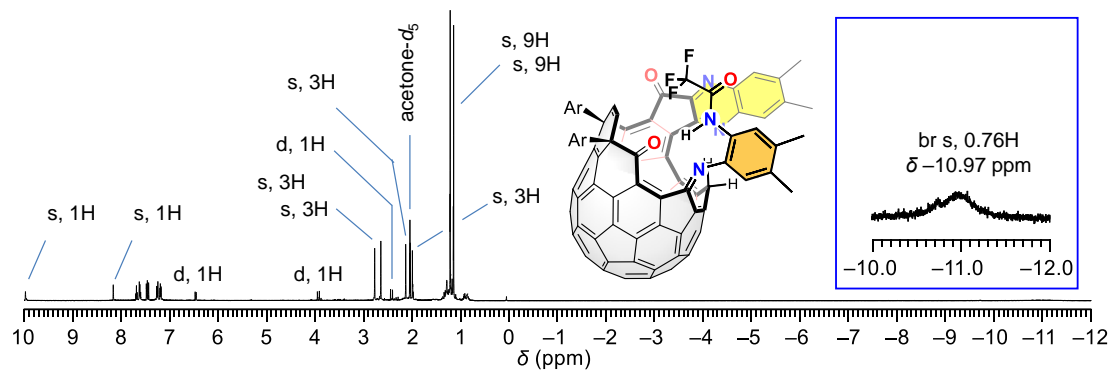**Figure S9.** ^{1}H NMR spectra (500 MHz, acetone-d_6/CS$_2$ (1:5)) of **5**.
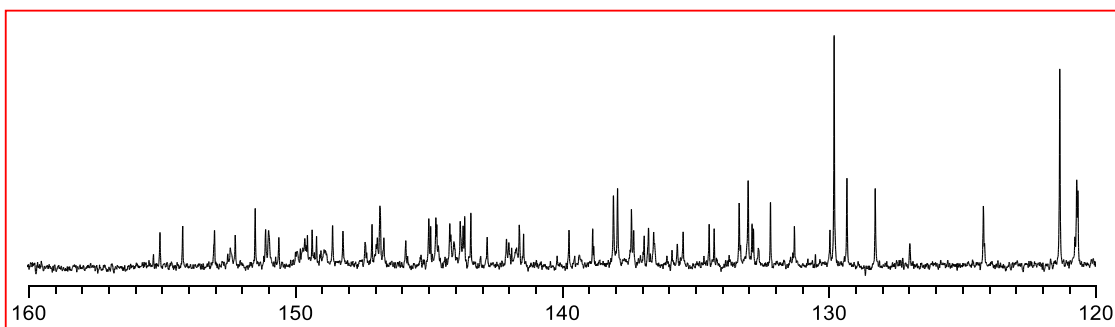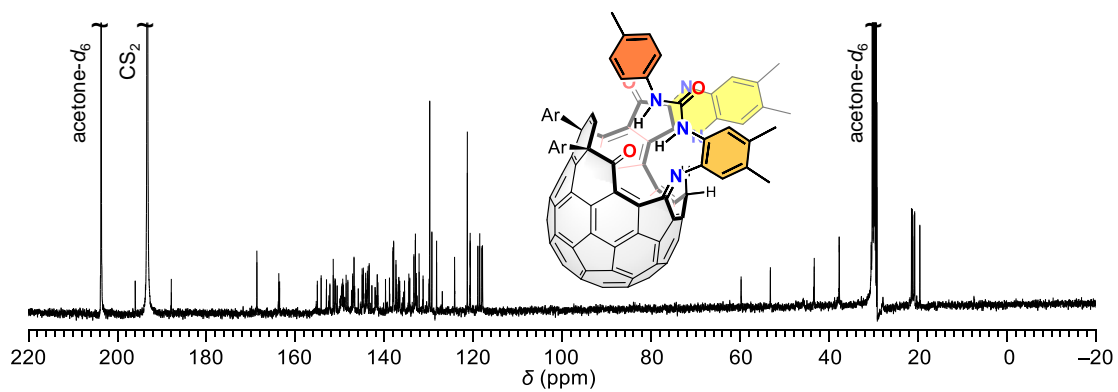
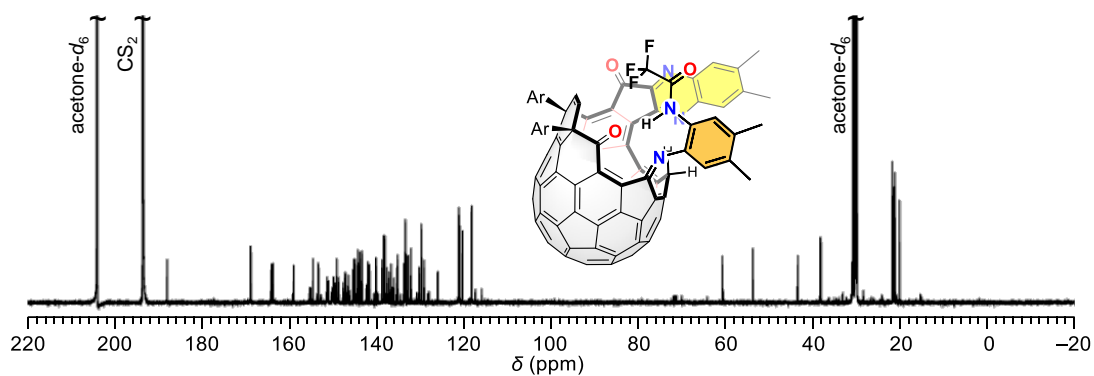**Figure S10.** ^{13}C NMR spectra (126 MHz, acetone-d_6/CS$_2$ (1:5)) of **5**.
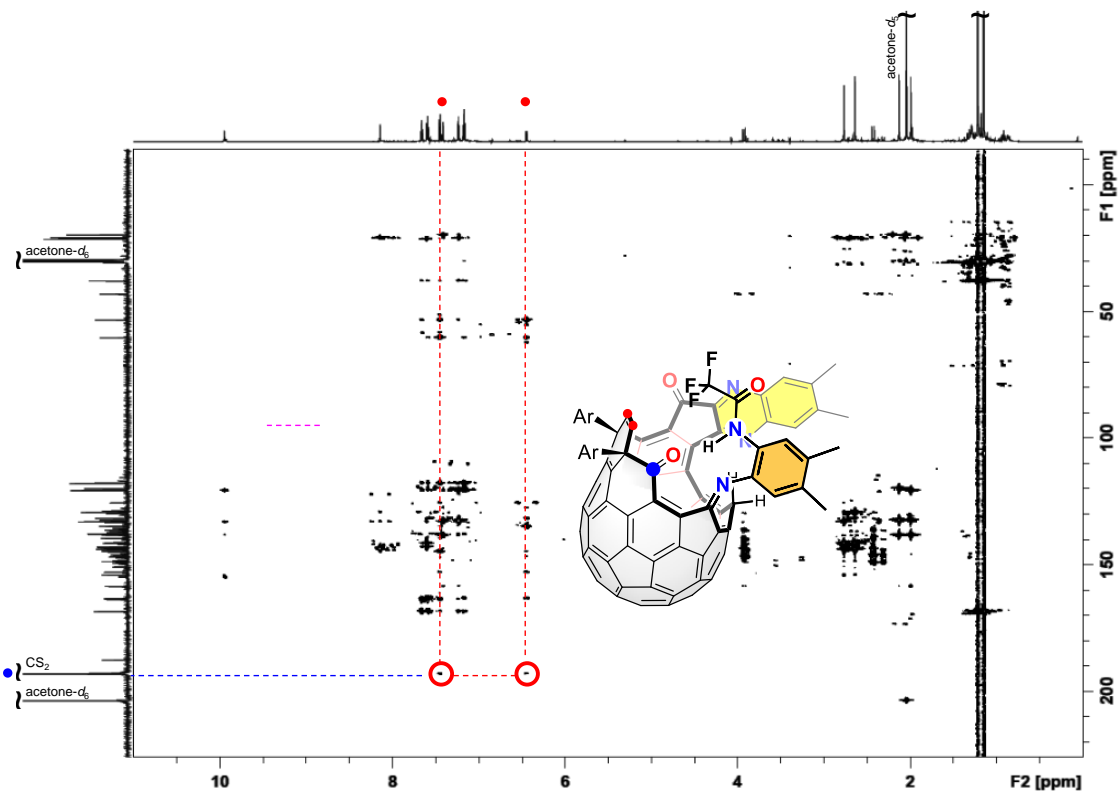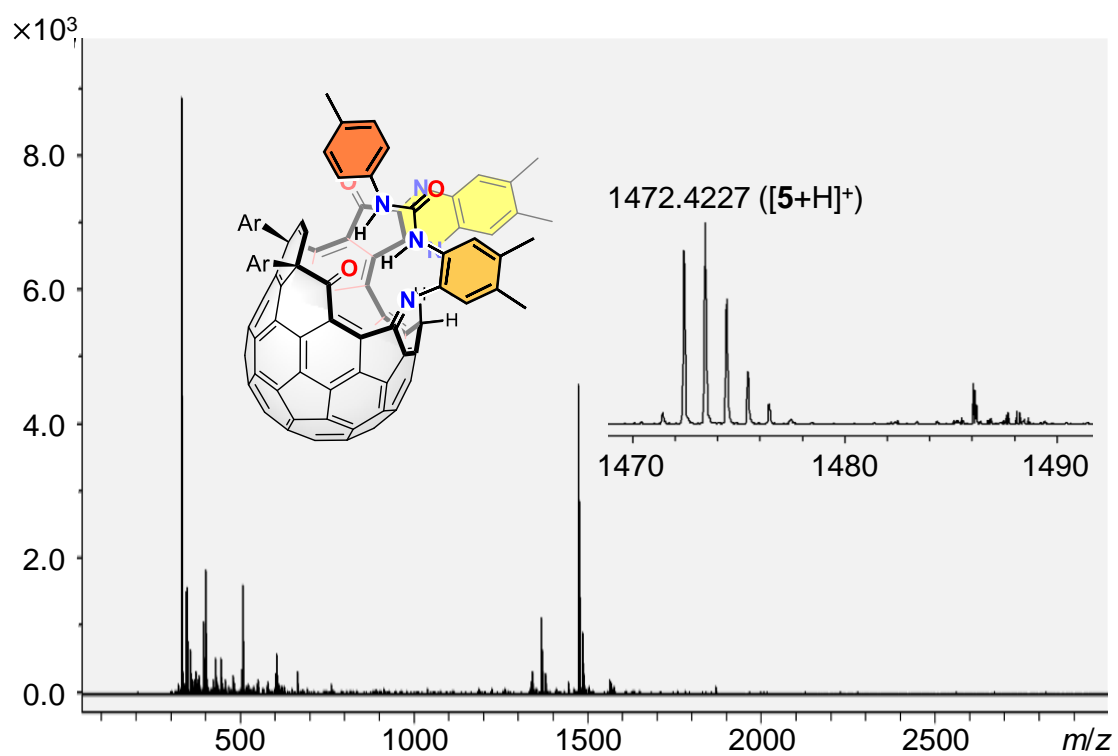
Figure S11. APCI mass spectra (positive ion mode) of **5**.

4. UV-Vis-NIR Absorption
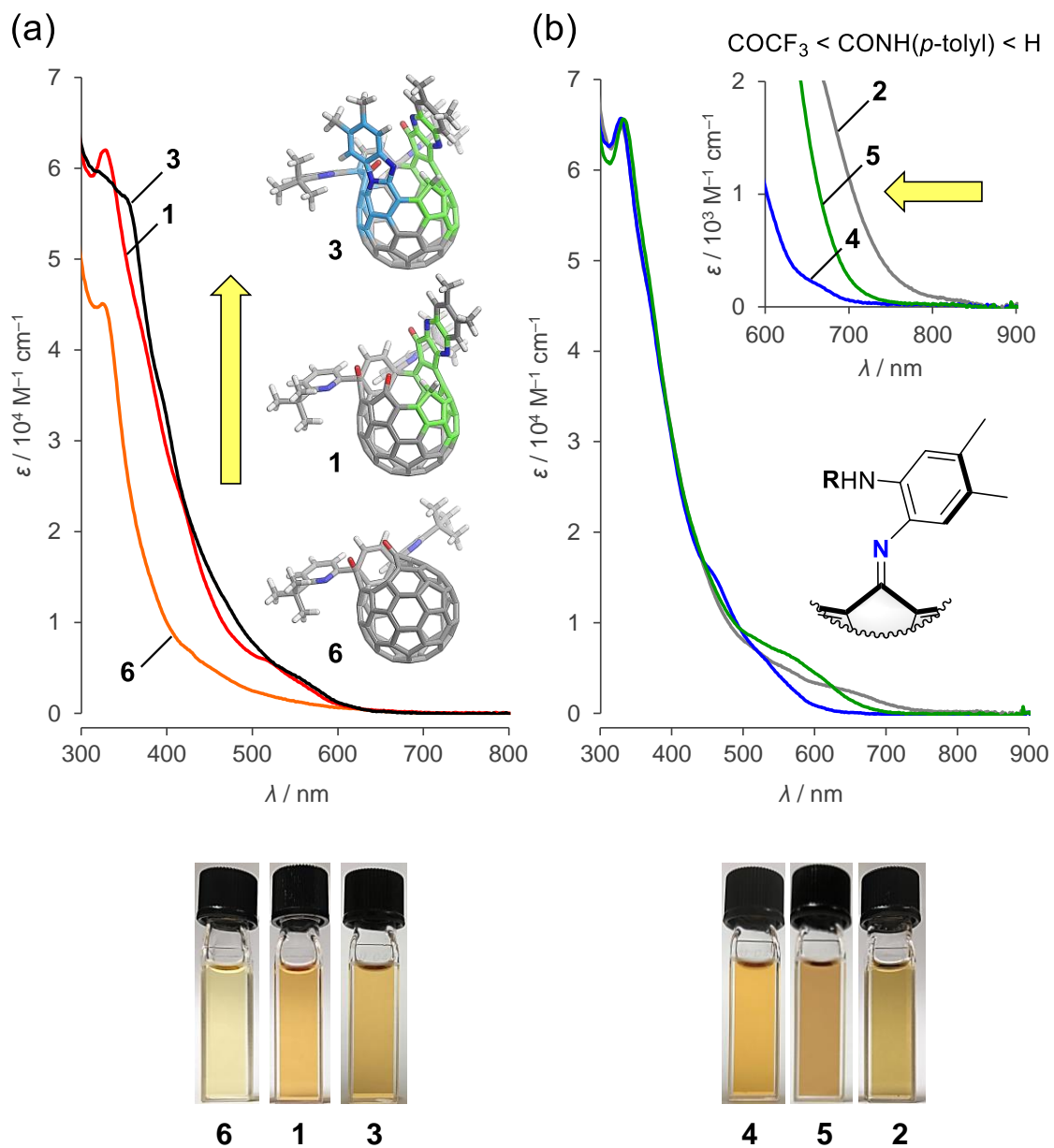
Figure S12. UV-vis-NIR absorption spectra of (a) **1**, **3**, and **6** and (b) **2**, **4**, and **5** (50 μM in benzene).

5. Single Crystal X-Ray-Structure of [{(H$_2$O)$_{0.448(16)}$(N$_2$)$_{0.340(11)}$}@3] •(acetone)$_{2.22}$•(CS$_2$)$_{0.22}$

Single crystals of **3** were obtained from a CS$_2$/acetone solution by slow evaporation at room temperature. Intensity data were collected at 100 K on a Bruker Single Crystal CCD X-ray Diffractometer (SMART APEX II) with Mo Kα radiation (λ = 0.71073 Å) and graphite monochromator. A total of 35704 reflections were measured at the maximum 2θ angle of 49.8°, of which 13071 were independent reflections (R_{int} = 0.0458). The structure was solved by direct methods (SHELXT-2014/5[2]) and refined by the full-matrix least-squares on F^2 (SHELXL-2018/3[2]). This crystal contains acetone molecules, one of which was disordered with a CS$_2$ molecule at the same site. Thus, (O6–C105–C106–C107) and (S1–C108–S2) were placed and their occupancies were refined to be 0.779(4) and 0.221(4), respectively. The occupancies of other two acetone molecules, i.e., (O5–C102–C103–C104) and (O4–C99–C100–C101), were refined to be 0.883(5) and 0.548(5), respectively. The encapsulated H$_2$O molecule is disordered with N$_2$ at the same site and their occupancies were refined to be 0.448(16) and 0.340(11), respectively. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed using AFIX instructions except for the encapsulated H$_2$O molecule. The CS$_2$ molecule disordered with one of the acetone molecules were refined using SIMU and DFIX instructions. The encapsulated H$_2$O and N$_2$ molecules were refined using SIMU and DFIX instructions. The crystal data are as follows: C$_{104.85}$H$_{58.16}$N$_{6.68}$O$_{4.66}$S$_{0.44}$; FW = 1500.15, crystal size 0.13 × 0.09 × 0.08 mm^3, monoclinic, $P2_1/n$, a = 15.004(4) Å, b = 17.383(5) Å, c = 28.473(8) Å, β = 91.101(4)°, V = 7425(4) Å^3, Z = 4, D_c = 1.342 g cm^{-3}. The refinement converged to R_1 = 0.0519, wR_2 = 0.1236 ($I > 2\sigma(I)$), GOF = 1.017. The data was deposited at the Cambridge Crystallographic Data Centre (CCDC 2236614).
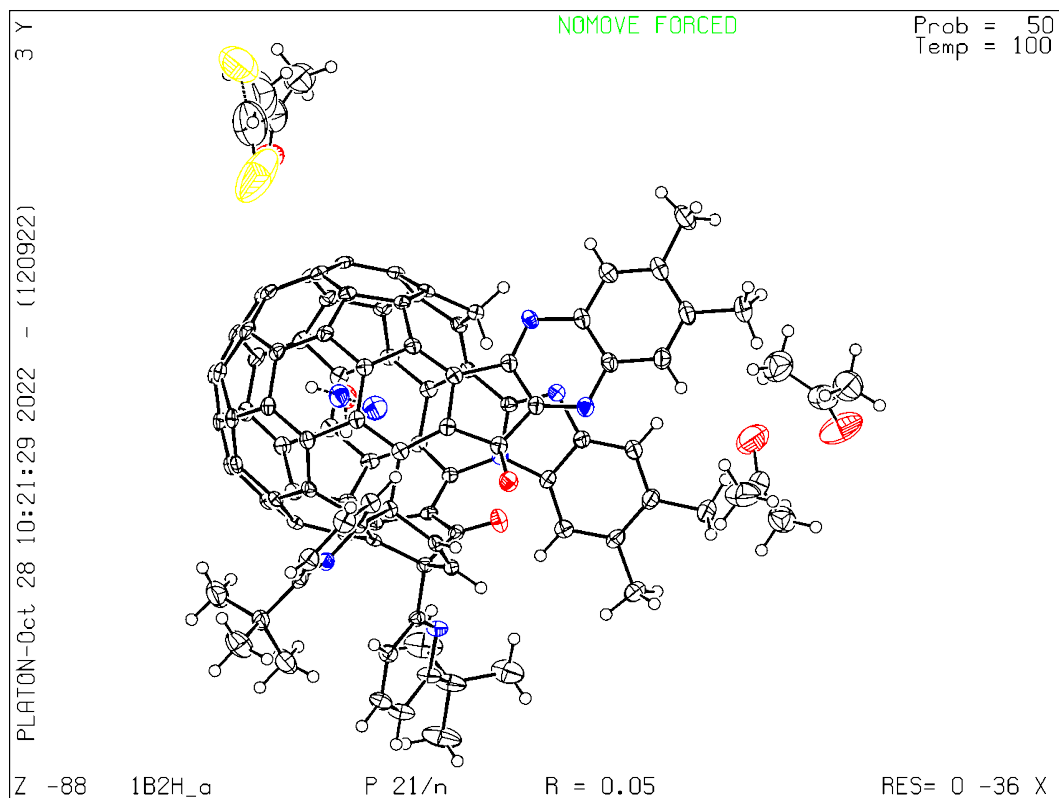
Figure S13. Single crystal X-ray structure of [{(H$_2$O)$_{0.448(16)}$(N$_2$)$_{0.340(11)}$}@**3**]•(acetone)$_{2.22}$•(CS$_2$)$_{0.22}$. Thermal ellipsoids are shown at 50% probability.

6. DFT Calculations

6.1. Optimized Structures of 1 and 2

(a)

(b)

1

2

	q_{NPA}
C(1)	+0.261
C(2)	+0.016
C(3)	−0.079
C(4)	+0.613
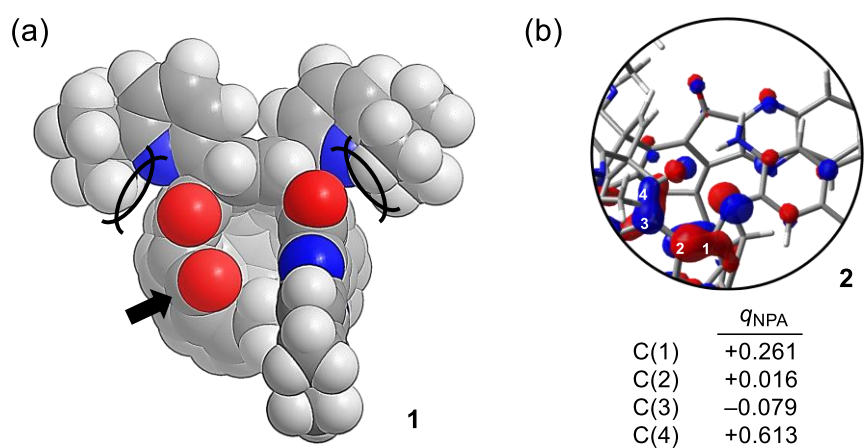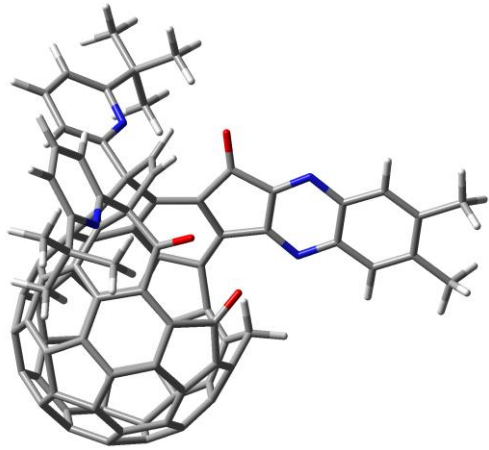
Figure S14. (a) Space-filling model of **1** and (b) the LUMO+1 of **2** and natural charges q_{NPA} of selected carbon atoms. The calculations were performed at the B3LYP-D3/6-31G(d) level of theory.

Table S1. Optimized structure of **1** (B3LYP-D3/6-31G(d))
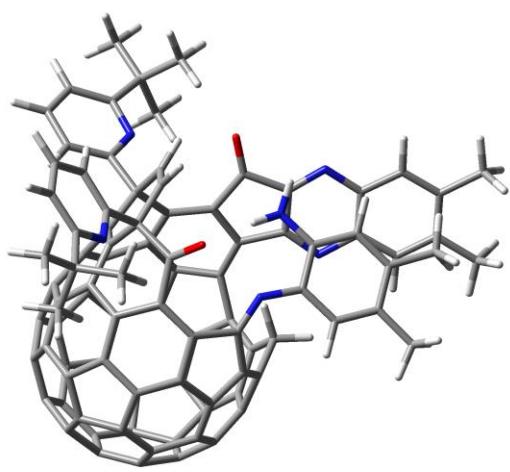
Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.005463	3.220738	1.589752
2	6	0	0.735428	3.366164	0.486717
3	6	0	0.424358	2.728688	-0.849704
4	6	0	1.387370	1.562405	-1.203653
5	6	0	2.527633	1.177372	-0.486190
6	6	0	3.454352	1.949221	0.425930
7	6	0	4.347269	0.916495	1.058107
8	6	0	4.077738	-0.351174	0.464931
9	6	0	2.087911	-3.052891	1.039027
10	6	0	0.794411	-3.680269	1.541832
11	6	0	-0.150078	-3.118999	2.384538
12	6	0	-0.118962	-1.698194	2.915263
13	6	0	-1.570091	-1.209578	2.780559
14	6	0	-1.975591	0.055656	2.356222
15	6	0	-1.184045	1.286412	2.660550
16	6	0	-1.297624	2.475086	1.649218
17	7	0	-3.320913	2.854721	2.967564
18	8	0	3.590053	3.151468	0.548965
19	8	0	-0.507677	1.387619	3.661375
20	7	0	1.776047	3.966450	-2.431764
21	6	0	-1.723692	1.952163	0.296303
22	6	0	-1.388482	1.435190	-2.063075
23	7	0	5.260364	1.121222	1.972655
24	6	0	-2.892746	1.098199	0.297399
25	6	0	0.961369	0.699148	-2.262729
26	8	0	0.879811	-1.061676	3.174204
27	6	0	-0.777798	-0.202127	-3.789346
28	6	0	2.030715	4.948249	-3.313146
29	6	0	0.030824	-1.384839	-4.038657
30	6	0	0.557641	3.834719	-1.912501
31	6	0	-0.370390	0.789356	-2.875218
32	6	0	-2.709253	0.977992	-2.146246
33	6	0	-0.974055	2.103643	-0.849320
34	6	0	1.204566	-1.544329	-3.330194
35	6	0	-3.112310	-0.045327	-3.076674
36	6	0	2.500776	-1.073961	-1.452153
37	6	0	-2.157441	-0.621661	-3.903779
38	6	0	-3.475694	0.796062	-0.932105
39	6	0	-3.069441	0.159239	1.405204
40	6	0	1.657493	-0.511233	-2.455061
41	6	0	-2.476143	4.749330	1.765760
42	6	0	-2.413043	3.411221	2.167217
43	6	0	0.767424	-3.908846	-2.968781
44	6	0	-3.902837	-0.955819	1.199491
45	6	0	-4.340890	-0.345106	-1.123257
46	6	0	-3.533376	5.516670	2.244123
47	6	0	3.020363	-0.179366	-0.536073
48	6	0	-2.198043	-2.053882	-4.163862
49	6	0	1.023648	5.837133	-3.708483
50	6	0	0.524969	-4.792395	-1.860571
51	6	0	-3.173749	-2.850877	-3.558407
52	6	0	2.310368	-2.551418	-1.521687
53	6	0	-4.479317	4.936467	3.091447
54	6	0	3.480801	5.000753	-3.804613
55	6	0	-0.501607	4.687835	-2.238988
56	6	0	2.047205	-3.394461	-0.450290
57	6	0	-4.346109	3.586577	3.437964
58	6	0	-4.132849	-0.867589	-2.456781
59	6	0	-0.861505	-5.221550	-1.918965
60	6	0	-0.954745	-5.130398	0.533710
61	6	0	1.604314	-2.811549	-2.773676
62	6	0	-3.561131	-2.236374	1.763890
63	6	0	-0.831999	-2.524062	-4.253252
64	6	0	-2.804859	-4.137293	-2.992389
65	6	0	1.126202	-4.497498	-0.632105
66	6	0	-0.253597	5.700503	-3.160574
67	6	0	-2.360757	-2.352004	2.454568
68	6	0	0.367309	-4.675126	0.589387
69	6	0	-1.481169	-4.583949	-3.067626
70	6	0	-0.472195	-3.763659	-3.713743
71	6	0	-1.523115	-3.520209	2.261804
72	6	0	-4.162480	-2.244173	-2.683639
73	6	0	-4.404508	-3.153253	-1.576514
74	6	0	-4.566875	-1.208742	-0.061261
75	6	0	-2.967395	-4.939337	-0.662217
76	6	0	-4.607265	-2.642909	-0.288733
77	6	0	3.835650	3.632326	-4.429042
78	6	0	-3.986782	-3.282536	0.850991
79	6	0	-1.934536	-4.534998	1.405148
80	6	0	-1.588545	-5.394845	-0.742512
81	6	0	-3.182780	-4.409357	0.669541
82	6	0	-3.565981	-4.321848	-1.766452
83	6	0	4.389264	5.254389	-2.578611
84	6	0	3.709018	6.107859	-4.846086
85	6	0	-5.323714	2.824056	4.338636
86	6	0	-6.405885	3.739832	4.933931
87	6	0	-4.526987	2.165570	5.487252
88	6	0	-6.000215	1.723005	3.489433
89	6	0	5.943443	-0.006522	2.345080
90	7	0	4.731376	-1.450052	0.771360
91	6	0	5.683504	-1.284622	1.742882
92	6	0	6.437634	-2.400597	2.169299
93	6	0	6.937659	0.087893	3.345584
94	6	0	7.661594	-1.014752	3.754361
95	6	0	7.405474	-2.290109	3.149455
96	6	0	8.190506	-3.502150	3.584970
97	6	0	8.714227	-0.884275	4.826988

98	1	0	0.322852	3.681625	2.519747
99	1	0	1.644444	3.950421	0.510423
100	1	0	2.980930	-3.461122	1.528570
101	1	0	2.104504	-1.979773	1.230642
102	1	0	-1.718558	5.163443	1.108904
103	1	0	-3.622667	6.562546	1.961906
104	1	0	1.223577	6.623897	-4.425949
105	1	0	-5.301828	5.530874	3.470372
106	1	0	-1.480387	4.554108	-1.789680
107	1	0	-1.048149	6.382426	-3.452551
108	1	0	4.886202	3.621799	-4.742839
109	1	0	3.214729	3.429000	-5.310088
110	1	0	3.676751	2.827492	-3.706335
111	1	0	5.443868	5.229460	-2.878771
112	1	0	4.222845	4.498420	-1.805964
113	1	0	4.185375	6.238290	-2.138968
114	1	0	4.756596	6.102688	-5.166553
115	1	0	3.495503	7.102206	-4.436339
116	1	0	3.088514	5.961741	-5.738535

117	1	0	-7.031468	4.193804	4.156325
118	1	0	-5.968398	4.543565	5.537960
119	1	0	-7.064879	3.156351	5.586063
120	1	0	-5.198269	1.569435	6.116877
121	1	0	-4.050472	2.924051	6.119459
122	1	0	-3.742994	1.514404	5.092022
123	1	0	-6.687964	1.136191	4.110094
124	1	0	-5.254056	1.046727	3.063386
125	1	0	-6.575312	2.159995	2.664066
126	1	0	6.228767	-3.356531	1.696917
127	1	0	7.110815	1.066253	3.784524
128	1	0	8.050421	-3.706397	4.654120
129	1	0	9.267515	-3.358533	3.430823
130	1	0	7.886336	-4.393370	3.029030
131	1	0	8.493015	-1.529310	5.686854
132	1	0	8.784935	0.145293	5.188478
133	1	0	9.703996	-1.180625	4.456803

The total electronic energy was calculated to be –3896.03493370 Hartree.

Table S2. Optimized structure of 2 (B3LYP-D3/6-31G(d))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.685981	2.971190	1.908816
2	6	0	-0.166826	3.386538	0.756190
3	6	0	-0.621677	2.932388	-0.613471
4	6	0	0.420420	2.029477	-1.327262
5	6	0	1.731670	1.756891	-0.901065
6	6	0	2.720420	2.539799	-0.060372
7	6	0	3.944236	1.665269	0.042931
8	6	0	3.707227	0.449663	-0.659770
9	6	0	2.192400	-2.607263	-0.157242
10	6	0	1.134096	-3.535097	0.435726
11	6	0	0.302851	-3.299261	1.525503
12	6	0	0.188809	-2.037398	2.353027
13	6	0	-1.295460	-1.773278	2.448052
14	6	0	-1.984969	-0.555897	2.375706
15	6	0	-1.400417	0.746478	2.800133
16	6	0	-1.849132	2.027002	2.022279
17	7	0	-3.660893	1.880551	3.653614
18	8	0	2.662313	3.682983	0.352596
19	8	0	-0.626661	0.853531	3.732431
20	7	0	0.261591	4.656931	-2.063464
21	6	0	-2.409902	1.640106	0.676056

22	6	0	-2.423515	1.556653	-1.757956
23	7	0	5.077806	1.965692	0.622033
24	6	0	-3.415575	0.599863	0.703112
25	6	0	-0.067708	1.293975	-2.455747
26	6	0	-1.908546	0.353453	-3.836099
27	6	0	0.221927	5.802998	-2.762978
28	6	0	-0.995167	-0.608092	-4.434100
29	6	0	-0.831542	4.210515	-1.448148
30	6	0	-1.489654	1.240852	-2.824065
31	6	0	-3.656227	0.891454	-1.719717
32	6	0	-1.898418	2.089596	-0.521171
33	6	0	0.302764	-0.661587	-3.970843
34	6	0	-4.067233	-0.026296	-2.751062
35	6	0	1.847162	-0.268503	-2.278155
36	6	0	-3.206730	-0.283786	-3.809827
37	6	0	-4.156533	0.389312	-0.458082
38	6	0	-3.236660	-0.514963	1.635863
39	6	0	0.750165	0.282046	-2.996595
40	6	0	-3.314141	4.032632	2.655374
41	6	0	-2.987289	2.684381	2.833217
42	6	0	0.303278	-3.092994	-3.987461
43	6	0	-3.912872	-1.717291	1.355118
44	6	0	-4.861526	-0.844371	-0.721299
45	6	0	-4.387519	4.536439	3.382900
46	6	0	2.403441	0.548639	-1.313929
47	6	0	-3.081131	-1.640152	-4.326207
48	6	0	-0.964346	6.540411	-2.865520
49	6	0	0.410153	-4.162857	-3.031297
50	6	0	-3.792966	-2.685114	-3.730354
51	6	0	1.877144	-1.721440	-2.593893
52	6	0	-5.090351	3.695604	4.248295
53	6	0	1.557150	6.209934	-3.394725
54	6	0	-2.052345	4.891907	-1.484394
55	6	0	1.941997	-2.744769	-1.657371
56	6	0	-4.699647	2.356133	4.362712
57	6	0	-4.822005	-1.106073	-2.143944
58	6	0	-0.881832	-4.822150	-2.945630
59	6	0	-0.525726	-5.120257	-0.531367
60	6	0	0.990879	-1.906475	-3.738230
61	6	0	-3.271074	-2.980157	1.601899
62	6	0	-1.701625	-1.836428	-4.717842
63	6	0	-3.133903	-3.955502	-3.478174
64	6	0	1.176465	-3.950491	-1.878869
65	6	0	-2.109040	6.074652	-2.215695

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66	6	0	-1.955882	-2.976830	2.053153	111	1	0	-2.743230	4.652403	1.971832
67	6	0	0.692851	-4.433454	-0.600453	112	1	0	-4.678818	5.578519	3.279010
68	6	0	-1.795901	-4.138120	-3.843795	113	1	0	-1.003484	7.460324	-3.436871
69	6	0	-1.062731	-3.059800	-4.482621	114	1	0	-5.925914	4.083504	4.818315
70	6	0	-0.997588	-3.924432	1.529954	115	1	0	-2.921448	4.502004	-0.964675
71	6	0	-4.683282	-2.412502	-2.614947	116	1	0	-3.038942	6.633751	-2.281497
72	6	0	-4.573662	-3.511181	-1.671186	117	1	0	3.034351	5.290354	-4.709561
73	6	0	-4.748433	-1.888294	0.184828	118	1	0	1.358676	4.858767	-5.109068
74	6	0	-2.731778	-5.122163	-1.339973	119	1	0	2.144113	4.128219	-3.696512
75	6	0	-4.609371	-3.252515	-0.295663	120	1	0	3.558589	6.686151	-2.667807
76	6	0	2.054358	5.046760	-4.282314	121	1	0	2.659515	5.564994	-1.615009
77	6	0	-3.693208	-3.934179	0.593108	122	1	0	2.258984	7.291588	-1.621900
78	6	0	-1.401658	-4.851818	0.573826	123	1	0	2.413154	7.726615	-4.685089
79	6	0	-1.338714	-5.297828	-1.719005	124	1	0	1.120584	8.345976	-3.651632
80	6	0	-2.770296	-4.847687	0.082272	125	1	0	0.728029	7.353317	-5.073687
81	6	0	-3.614686	-4.462514	-2.202750	126	1	0	-7.323698	2.351778	5.454132
82	6	0	2.571550	6.449854	-2.251906	127	1	0	-6.166919	2.742440	6.746656
83	6	0	1.438432	7.482783	-4.248274	128	1	0	-6.981807	1.172904	6.725782
84	6	0	-5.391785	1.325662	5.261150	129	1	0	-4.793939	-0.065842	6.829359
85	6	0	-6.529956	1.942550	6.090426	130	1	0	-3.928981	1.483780	6.885817
86	6	0	-4.337479	0.718959	6.214571	131	1	0	-3.507989	0.286328	5.649060
87	6	0	-5.967371	0.208539	4.360407	132	1	0	-6.441955	-0.565098	4.975829
88	6	0	6.035562	0.988219	0.521490	133	1	0	-5.177357	-0.257129	3.765217
89	7	0	4.585289	-0.523762	-0.753839	134	1	0	-6.722507	0.607406	3.672324
90	6	0	5.780060	-0.259962	-0.138517	135	1	0	6.581200	-2.175662	-0.662922
91	6	0	6.801579	-1.235242	-0.165550	136	1	0	7.475708	2.162571	1.586335
92	6	0	7.307104	1.206961	1.097508	137	1	0	9.394929	-2.376767	1.393550
93	6	0	8.298315	0.246020	1.053784	138	1	0	10.012387	-1.723446	-0.120012
94	6	0	8.036395	-1.008382	0.410848	139	1	0	8.752221	-2.968739	-0.148068
95	6	0	9.101196	-2.076440	0.379159	140	1	0	9.836523	-0.225620	2.499586
96	6	0	9.638057	0.498407	1.698441	141	1	0	9.686362	1.501013	2.132549
97	6	0	3.168914	-0.133865	2.923321	142	1	0	10.459178	0.403310	0.976852
98	6	0	4.549689	-0.193040	3.167115	143	1	0	5.104121	0.738190	3.242346
99	6	0	5.220167	-1.403668	3.327657	144	1	0	2.565055	-3.495410	2.962209
100	6	0	4.505327	-2.622215	3.220076	145	1	0	1.517963	1.041947	2.901379
101	6	0	3.135020	-2.571618	2.991967	146	1	0	2.986109	1.900605	2.992573
102	6	0	2.440638	-1.355208	2.852121	147	1	0	5.693185	-4.039713	4.362832
103	7	0	2.512097	1.059855	2.688744	148	1	0	4.510475	-4.782860	3.275731
104	7	0	1.066516	-1.214795	2.788733	149	1	0	5.999989	-4.078981	2.629137
105	6	0	5.210040	-3.947780	3.380979	150	1	0	7.106243	-0.407343	3.682199
106	6	0	6.692179	-1.418404	3.656340	151	1	0	6.874424	-1.888331	4.631931
107	1	0	-0.288885	3.336711	2.851008	152	1	0	7.261483	-1.991227	2.914865
108	1	0	0.656201	4.087298	0.750895						
109	1	0	3.215973	-2.878424	0.130432						
110	1	0	2.051502	-1.578848	0.180418						

The total electronic energy was calculated to be –4241.2453416 Hartree.

6.2. Molecular Orbitals of 1 and 3
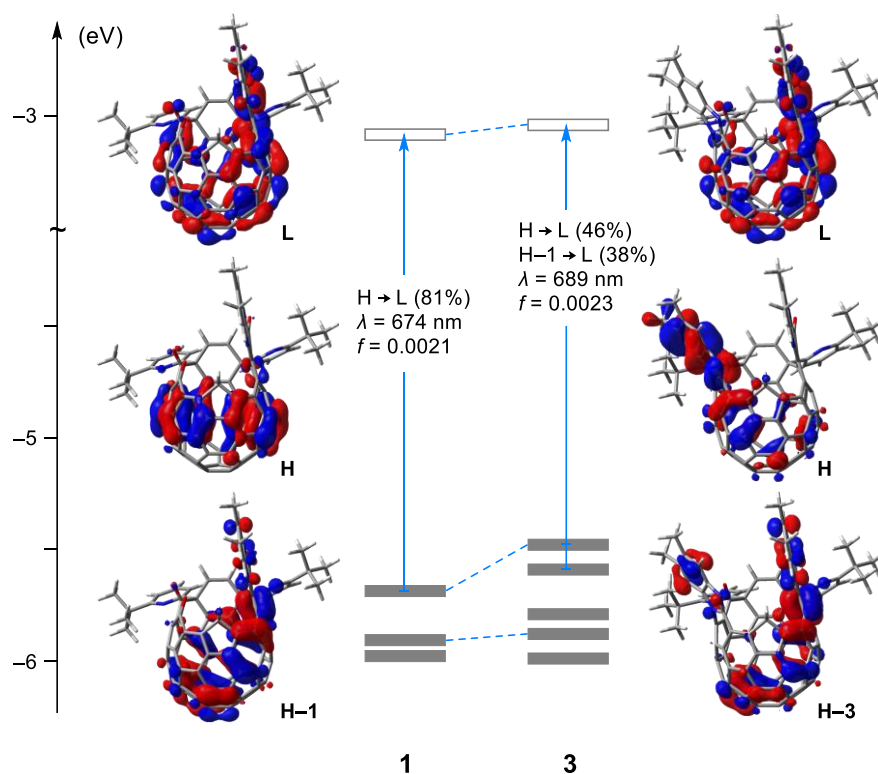
Figure S15. Kohn–Sham HOMO and LUMO levels of **1** and **3** with optical transitions (TD CAM-B3LYP/6-31G(d)//B3LYP/6-31G(d)). The transition energies were calibrated with a factor of 0.72.

L
−3.08

H
−5.69

H−1
−5.91

H−2
−5.98

H−3
−6.16
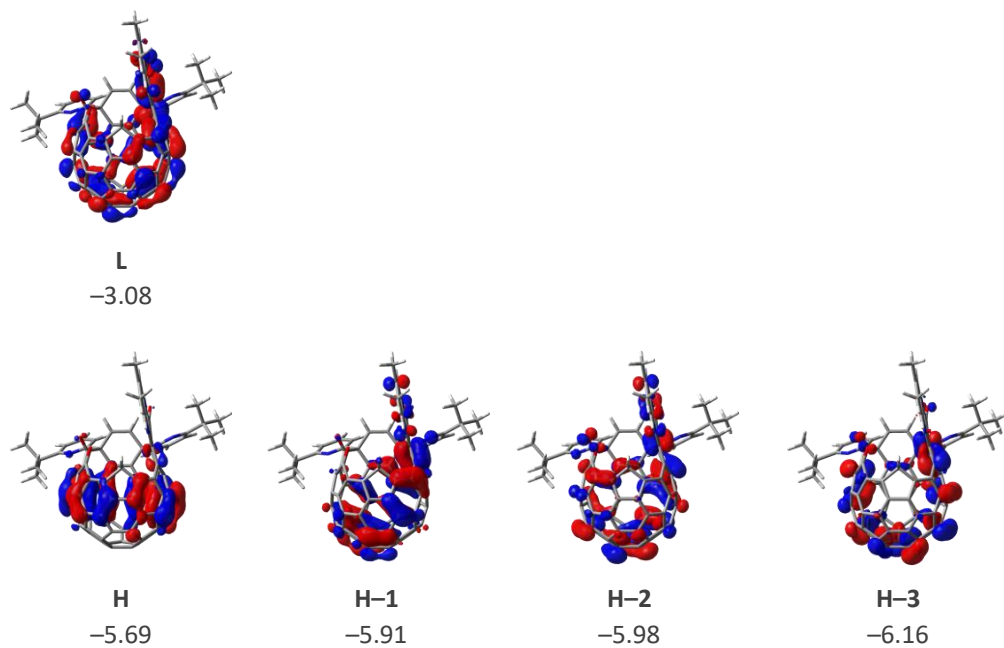
Figure S16. Molecular orbitals of **1** (B3LYP/6-31G(d)).

L
−3.04

H
−5.48

H−1
−5.59

H−2
−5.79

H−3
−5.88

H−4
−5.99
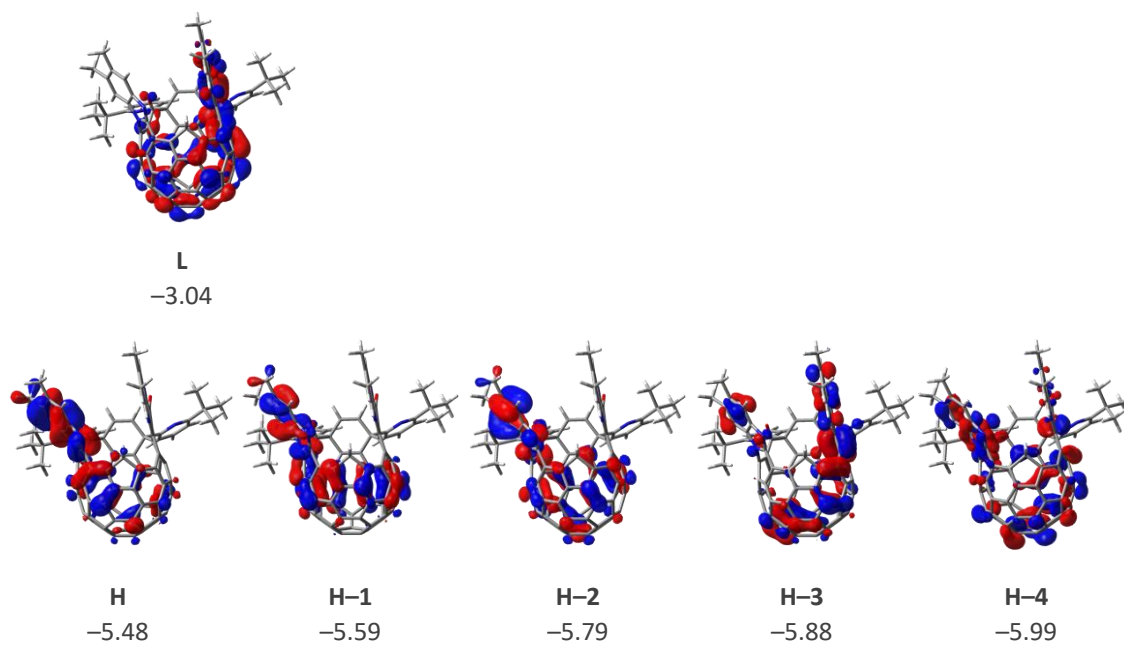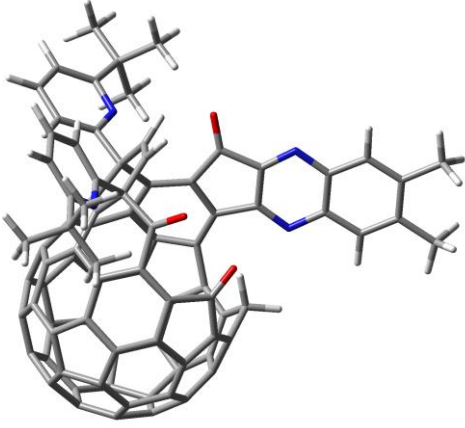
Figure S17. Molecular orbitals of **3** (B3LYP/6-31G(d)).

Table S3. Optimized structure of **1** (B3LYP/6-31G(d))

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.116698	3.234480	1.486122
2	6	0	0.646435	3.346853	0.399679
3	6	0	0.381895	2.669674	-0.929199
4	6	0	1.383241	1.513811	-1.225209
5	6	0	2.526871	1.183880	-0.478607
6	6	0	3.433542	2.021187	0.396500
7	6	0	4.371232	1.047319	1.055224
8	6	0	4.121593	-0.257348	0.540920
9	6	0	2.107237	-3.028323	1.239444
10	6	0	0.800770	-3.647815	1.727515
11	6	0	-0.178649	-3.075256	2.523847
12	6	0	-0.194646	-1.643012	3.030712
13	6	0	-1.646034	-1.178378	2.811533
14	6	0	-2.063634	0.064480	2.327922
15	6	0	-1.310559	1.327711	2.606158
16	6	0	-1.416950	2.478405	1.544788
17	7	0	-3.446213	2.934403	2.861446
18	8	0	3.520479	3.231137	0.484223
19	8	0	-0.659343	1.479098	3.617509
20	7	0	1.696086	3.909340	-2.574553
21	6	0	-1.788819	1.892010	0.198735
22	6	0	-1.374954	1.283638	-2.128916
23	7	0	5.302937	1.327721	1.930381
24	6	0	-2.938589	1.009903	0.200947
25	6	0	0.994248	0.593232	-2.248662
26	8	0	0.777766	-0.994262	3.349263
27	6	0	-0.690062	-0.404369	-3.777755
28	6	0	1.904355	4.879696	-3.483772
29	6	0	0.146647	-1.579609	-3.959601
30	6	0	0.491836	3.757448	-2.024033
31	6	0	-0.325418	0.629012	-2.892651
32	6	0	-2.683929	0.796680	-2.229646
33	6	0	-1.005474	2.009515	-0.932425
34	6	0	1.301970	-1.688447	-3.212760
35	6	0	-3.043641	-0.266841	-3.131722
36	6	0	2.547440	-1.115885	-1.328903
37	6	0	-2.057125	-0.855054	-3.911950
38	6	0	-3.479757	0.646304	-1.031578
39	6	0	-3.129685	0.109050	1.339700
40	6	0	1.714491	-0.613109	-2.370400
41	6	0	-2.620568	4.741148	1.516027
42	6	0	-2.548151	3.435441	2.004476
43	6	0	0.900156	-4.044187	-2.772560
44	6	0	-3.934177	-1.030707	1.151084
45	6	0	-4.318132	-0.517121	-1.202944
46	6	0	-3.675244	5.542781	1.949875
47	6	0	3.047693	-0.164324	-0.457156
48	6	0	-2.064267	-2.296166	-4.118351
49	6	0	0.866514	5.734520	-3.873766
50	6	0	0.643940	-4.889921	-1.639160
51	6	0	-3.041231	-3.089002	-3.509309
52	6	0	2.378769	-2.600900	-1.338365
53	6	0	-4.603722	5.022857	2.845161
54	6	0	3.339151	4.971305	-4.021653
55	6	0	-0.593954	4.579665	-2.348692
56	6	0	2.102640	-3.410694	-0.242872
57	6	0	-4.460845	3.698989	3.291037
58	6	0	-4.065199	-1.084517	-2.509366
59	6	0	-0.731336	-5.349524	-1.719114
60	6	0	-0.894061	-5.167189	0.724599
61	6	0	1.709405	-2.923306	-2.595830
62	6	0	-3.585235	-2.281767	1.771984
63	6	0	-0.688095	-2.742393	-4.153711
64	6	0	-2.664344	-4.345805	-2.885293
65	6	0	1.205240	-4.536282	-0.407609
66	6	0	-0.393463	5.578374	-3.295096
67	6	0	-2.403632	-2.347133	2.500039
68	6	0	0.416556	-4.682861	0.799106
69	6	0	-1.330574	-4.768424	-2.907515
70	6	0	-0.319910	-3.952989	-3.556522
71	6	0	-1.539727	-3.505735	2.373882
72	6	0	-4.064177	-2.469094	-2.685071
73	6	0	-4.320073	-3.340490	-1.551406
74	6	0	-4.558139	-1.344207	-0.115785
75	6	0	-2.876128	-5.062710	-0.531350
76	6	0	-4.566781	-2.785898	-0.289706
77	6	0	3.731377	3.602368	-4.622479
78	6	0	-3.966283	-3.369583	0.889133
79	6	0	-1.908246	-4.559042	1.545136
80	6	0	-1.487152	-5.492358	-0.556943
81	6	0	-3.137235	-4.486535	0.772336
82	6	0	-3.455498	-4.498857	-1.674276
83	6	0	4.277042	5.297916	-2.835638
84	6	0	3.493286	6.056198	-5.101679
85	6	0	-5.455932	3.082492	4.285629
86	6	0	-6.870609	3.085125	3.659201
87	6	0	-5.468202	3.924435	5.583581
88	6	0	-5.067642	1.635572	4.636018
89	6	0	6.030995	0.243511	2.342443
90	7	0	4.810964	-1.319824	0.895555
91	6	0	5.787769	-1.073111	1.825023
92	6	0	6.589914	-2.140333	2.288773
93	6	0	7.056956	0.424282	3.298439
94	6	0	7.829382	-0.630472	3.743631
95	6	0	7.589411	-1.946550	3.223662
96	6	0	8.423426	-3.112631	3.694039
97	6	0	8.915138	-0.400061	4.765947

98	1	0	0.177115	3.731950	2.405426		117	1	0	-6.893222	2.495308	2.735699
99	1	0	1.549966	3.940072	0.437278		118	1	0	-7.213283	4.098126	3.420176
100	1	0	2.984559	-3.435374	1.759365		119	1	0	-7.592647	2.646391	4.358143
101	1	0	2.129186	-1.950879	1.406985		120	1	0	-6.170541	3.491396	6.305670
102	1	0	-1.870454	5.116994	0.828563		121	1	0	-5.777310	4.959599	5.400647
103	1	0	-3.767813	6.565945	1.594734		122	1	0	-4.475813	3.945250	6.047583
104	1	0	1.030578	6.510029	-4.612253		123	1	0	-5.786518	1.229263	5.357363
105	1	0	-5.426532	5.637455	3.195631		124	1	0	-4.067708	1.584330	5.076356
106	1	0	-1.561597	4.434151	-1.879845		125	1	0	-5.068800	0.994358	3.749937
107	1	0	-1.211923	6.233372	-3.583019		126	1	0	6.394190	-3.128138	1.880883
108	1	0	4.773344	3.623978	-4.963529		127	1	0	7.215961	1.431580	3.672533
109	1	0	3.098757	3.351912	-5.482895		128	1	0	8.332627	-3.262054	4.777523
110	1	0	3.623464	2.809398	-3.878134		129	1	0	9.489608	-2.955584	3.486402
111	1	0	5.322258	5.297638	-3.168144		130	1	0	8.118165	-4.039410	3.200473
112	1	0	4.162632	4.564084	-2.033257		131	1	0	8.745171	-0.989297	5.676201
113	1	0	4.055343	6.288963	-2.421409		132	1	0	8.964812	0.653648	5.053738
114	1	0	4.529836	6.077190	-5.456064		133	1	0	9.901325	-0.690540	4.381638
115	1	0	3.259965	7.055632	-4.715862							
116	1	0	2.851830	5.864318	-5.970299							

The total electronic energy was calculated to be –3895.8110862 Hartree.

Table S4. Optimized structure of 3 (B3LYP/6-31G(d))
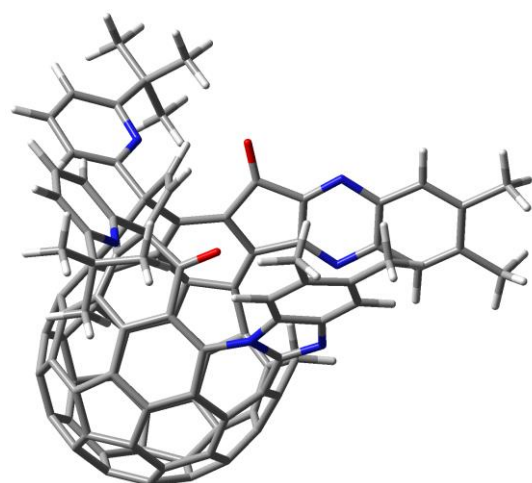
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.274942	1.388035	3.115837
2	6	0	-0.319794	0.233521	3.414853
3	6	0	0.097779	-1.127591	2.896646
4	6	0	-0.897285	-1.735319	1.861639
5	6	0	-2.159875	-1.234656	1.502156
6	6	0	-3.147637	-0.373121	2.257409
7	6	0	-4.242678	-0.057111	1.275564
8	6	0	-3.988534	-0.751150	0.057913
9	6	0	-2.393493	-0.266080	-3.062681
10	6	0	-1.210477	0.317313	-3.839945
11	6	0	-0.413287	1.401782	-3.485437
12	6	0	-0.828960	2.500456	-2.630047
13	6	0	1.362855	2.451021	-1.553355
14	6	0	1.893421	2.124279	-0.287163
15	6	0	1.134137	2.374168	0.976180
16	6	0	1.497639	1.523208	2.243687
17	7	0	3.205297	3.291910	2.426172
18	8	0	-3.173724	-0.079078	3.437330
19	8	0	0.199264	3.146781	1.056633
20	7	0	-0.936202	-2.668497	4.481022
21	6	0	2.024071	0.175871	1.814289
22	6	0	1.953417	-2.248641	1.578981
23	7	0	-5.296314	0.688908	1.491462
24	6	0	3.093930	0.221448	0.844616
25	6	0	-0.395418	-2.827645	1.084540
26	6	0	1.462775	-4.232031	0.218713
27	6	0	-0.975829	-3.435628	5.585503
28	6	0	0.608888	-4.733954	-0.844230
29	6	0	0.196264	-2.058845	4.129928
30	6	0	1.009279	-3.255768	1.126138
31	6	0	3.234559	-2.222389	1.013619
32	6	0	1.435546	-1.027157	2.150958
33	6	0	-0.656559	-4.199646	-0.981077
34	6	0	3.682799	-3.217247	0.074102
35	6	0	-2.168981	-2.462133	-0.626003
36	6	0	2.809501	-4.226772	-0.309091
37	6	0	3.808050	-0.954753	0.621402
38	6	0	3.035379	1.229680	-0.215519
39	6	0	-1.145684	-3.256648	-0.029614
40	6	0	2.938096	1.856313	4.329023
41	6	0	2.601905	2.269587	3.033631
42	6	0	-0.464174	-4.132956	-3.399414
43	6	0	3.764228	0.973000	-1.386924
44	6	0	4.596315	-1.175643	-0.565570
45	6	0	3.946479	2.545256	4.990787
46	6	0	-2.752129	-1.528674	0.214488
47	6	0	2.775984	-4.667768	-1.696044
48	6	0	0.165497	-3.617216	6.376371
49	6	0	-0.455872	-3.146223	-4.441462
50	6	0	3.590876	-4.047082	-2.648283
51	6	0	-2.094823	-2.715675	-2.100997
52	6	0	4.579823	3.614263	4.354528
53	6	0	-2.343273	-4.059564	5.897740
54	6	0	1.376429	-2.179067	4.873205
55	6	0	-2.087778	-1.770442	-3.123810
56	6	0	4.182006	3.970144	3.061793
57	6	0	4.538712	-2.581263	-0.907854
58	6	0	0.891936	-3.067762	-4.982486
59	6	0	0.626607	-0.632735	-5.176407
60	6	0	-1.230804	-3.882993	-2.261069
61	6	0	3.188591	1.285617	-2.668582
62	6	0	1.404207	-4.992531	-2.022131
63	6	0	3.047453	-3.711107	-3.953062
64	6	0	-1.220392	-1.991947	-4.262916
65	6	0	1.350651	-2.978984	6.010773

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66	6	0	1.913283	1.852261	-2.752713	110	1	0	2.414028	1.029576	4.796548
67	6	0	-0.665417	-0.713867	-4.655981	111	1	0	4.239087	2.257522	5.997358
68	6	0	1.717915	-4.022390	-4.264258	112	1	0	0.137138	-4.241746	7.261017
69	6	0	0.877075	-4.679441	-3.279495	113	1	0	5.365658	4.158107	4.864736
70	6	0	1.005225	1.371545	-3.795281	114	1	0	2.284103	-1.671420	4.564431
71	6	0	4.489913	-2.978752	-2.244829	115	1	0	2.247796	-3.106604	6.611346
72	6	0	4.491674	-1.973374	-3.293373	116	1	0	-3.801045	-5.299252	4.849988
73	6	0	4.580043	-0.211214	-1.560861	117	1	0	-2.116888	-5.729279	4.493327
74	6	0	2.796714	-1.504681	-5.024890	118	1	0	-2.824932	-4.269548	3.776945
75	6	0	4.529389	-0.617156	-2.950322	119	1	0	-4.356923	-3.321221	6.304148
76	6	0	-2.798734	-4.889820	4.676342	120	1	0	-3.383355	-2.229929	5.288594
77	6	0	3.672043	0.323100	-3.632751	121	1	0	-3.077901	-2.330491	7.030727
78	6	0	1.482416	0.423299	-4.714580	122	1	0	-3.298182	-5.394846	7.313389
79	6	0	1.422012	-1.832462	-5.349227	123	1	0	-2.017223	-4.421876	8.041910
80	6	0	2.826271	-0.106860	-4.643466	124	1	0	-1.606810	-5.807928	7.007749
81	6	0	3.601852	-2.425687	-4.347679	125	1	0	6.743107	5.182683	3.287242
82	6	0	-3.352073	-2.912397	6.142241	126	1	0	5.538989	6.284783	3.991127
83	6	0	-2.303435	-4.970809	7.136952	127	1	0	6.307904	6.676590	2.449750
84	6	0	4.794615	5.135484	2.271581	128	1	0	4.062512	6.962252	1.326482
85	6	0	5.908465	5.854003	3.053131	129	1	0	3.264794	6.590819	2.867901
86	6	0	3.672368	6.149284	1.950544	130	1	0	2.852561	5.658629	1.418533
87	6	0	5.381649	4.585065	0.951946	131	1	0	5.782643	5.405610	0.344954
88	6	0	-6.155056	0.770065	0.427650	132	1	0	4.615356	4.064510	0.371890
89	7	0	-4.798344	-0.715851	-0.977986	133	1	0	6.197858	3.879553	1.148375
90	6	0	-5.908374	0.067675	-0.799771	134	1	0	-6.644992	-0.354582	-2.767518
91	6	0	-6.848220	0.187749	-1.848366	135	1	0	-7.483089	2.077998	1.481852
92	6	0	-7.323726	1.558003	0.541519	136	1	0	-9.085486	2.102984	-3.199205
93	6	0	-8.230628	1.666583	-0.494406	137	1	0	-9.961795	0.708975	-2.575240
94	6	0	-7.985917	0.961858	-1.720606	138	1	0	-8.631890	0.472335	-3.721039
95	6	0	-8.964571	1.064839	-2.864371	139	1	0	-9.503578	3.318331	-1.087792
96	6	0	-9.467182	2.517270	-0.338369	140	1	0	-9.500970	2.981939	0.650860
97	6	0	-1.756647	4.278717	-1.887687	141	1	0	-10.383457	1.926218	-0.464197
98	6	0	-2.612976	5.363875	-1.660923	142	1	0	-3.614478	5.353188	-2.081438
99	6	0	-2.159600	6.450497	-0.921037	143	1	0	1.029394	5.383269	-0.211788
100	6	0	-0.827915	6.459297	-0.404985	144	1	0	-3.365803	-0.040124	-3.518625
101	6	0	0.022923	5.376068	-0.614966	145	1	0	-0.931798	7.819781	1.283210
102	6	0	-0.457085	4.286811	-1.339780	146	1	0	0.707606	7.505859	0.698270
103	7	0	-1.964915	3.153811	-2.670300	147	1	0	-0.375037	8.575775	-0.206769
104	7	0	0.128426	3.099081	-1.784858	148	1	0	-4.054588	7.462106	-1.136894
105	6	0	-0.329564	7.649542	0.381159	149	1	0	-3.239362	7.799934	0.396774
106	6	0	-3.076388	7.626690	-0.675112	150	1	0	-2.667142	8.559245	-1.085666
107	1	0	-0.114362	2.313421	3.528004						
108	1	0	-1.180603	0.228972	4.069408						
109	1	0	-2.436560	0.120455	-2.043873						

The total electronic energy was calculated to be –4239.8124923 Hartree.

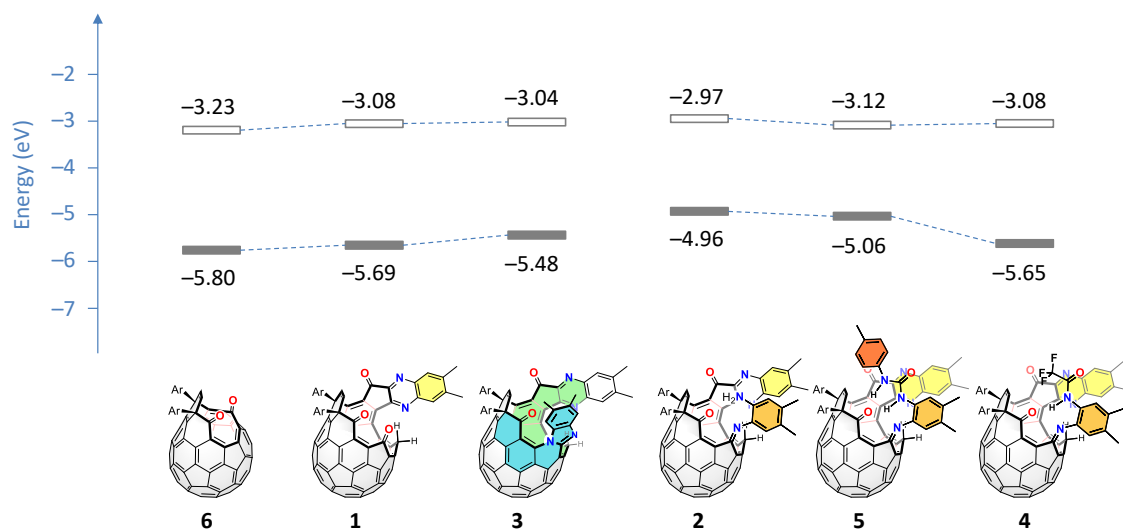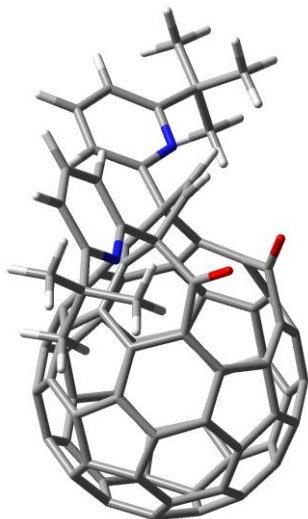## 6.3. Orbital Energy Levels of 1–6

Figure S18. Orbital energy levels of **1**–**6** (B3LYP/6-31G(d)).

Table S5. Optimized structure of **6** (B3LYP/6-31G(d))

Standard orientation:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-3.612146	0.691073	1.357564
2	6	0	-3.058414	1.881440	1.142633
3	6	0	-1.967315	2.144450	0.131789
4	6	0	-0.572352	2.349622	0.762941
5	6	0	-0.192273	1.951591	2.037491
6	6	0	-0.767972	0.897452	2.999073
7	6	0	0.429751	-0.031757	3.245382
8	6	0	0.653408	-1.393655	3.044970
9	6	0	-0.064629	-2.366076	2.112693
10	6	0	-1.194585	-2.165762	1.305074
11	6	0	-2.450023	-1.480133	1.734306
12	6	0	-3.173107	-0.574873	0.668448
13	6	0	-2.207101	-0.304227	-0.466658
14	6	0	-1.729426	0.950838	-0.784440
15	6	0	-0.687362	1.109764	-1.773121
16	6	0	0.378630	2.093095	-1.554356
17	6	0	0.490788	2.656439	-0.197085
18	6	0	1.777458	2.958263	0.284263
19	6	0	2.136053	2.653041	1.650450
20	6	0	1.185228	2.024727	2.432702
21	6	0	1.552672	0.876835	3.241682
22	6	0	2.873865	0.459096	3.273755
23	6	0	3.132026	-0.952812	3.222252
24	6	0	2.051840	-1.833855	3.082578
25	6	0	2.221237	-2.992663	2.244439
26	6	0	0.946689	-3.276229	1.635670
27	6	0	0.901429	-3.832052	0.356061
28	6	0	-0.118102	-3.390635	-0.553084
29	6	0	-1.115169	-2.510913	-0.109757
30	6	0	-1.572271	-1.468458	-1.034894
31	6	0	-0.877603	-1.300814	-2.232424
32	6	0	-0.451306	0.025517	-2.629006
33	6	0	0.771397	-0.108944	-3.376271
34	6	0	1.751259	0.863392	-3.248926
35	6	0	1.550276	1.974447	-2.333845
36	6	0	2.857294	2.320300	-1.808553
37	6	0	2.968904	2.793285	-0.510828
38	6	0	4.051318	2.336091	0.346383
39	6	0	3.520631	2.224388	1.687688
40	6	0	3.889943	1.148169	2.496805
41	6	0	4.810768	0.147801	1.996397
42	6	0	4.354525	-1.153938	2.463772
43	6	0	4.492146	-2.271994	1.643652
44	6	0	3.410166	-3.234113	1.558591
45	6	0	3.359987	-3.741802	0.197699
46	6	0	2.131355	-4.046775	-0.385891
47	6	0	1.875887	-3.688561	-1.768959
48	6	0	0.484382	-3.292390	-1.868407
49	6	0	0.120756	-2.237439	-2.693337
50	6	0	1.132511	-1.512652	-3.433620
51	6	0	2.470385	-1.893570	-3.355256
52	6	0	3.502500	-0.876656	-3.255086
53	6	0	3.148769	0.475732	-3.218629
54	6	0	3.837810	1.384293	-2.324435
55	6	0	4.860622	0.914880	-1.495605
56	6	0	5.202375	-0.496851	-1.504541
57	6	0	4.536335	-1.373317	-2.363158
58	6	0	4.127585	-2.687040	-1.892287
59	6	0	2.852716	-3.011114	-2.505668
60	6	0	4.383083	-3.059243	-0.568871
61	6	0	5.081480	-2.147230	0.324639
62	6	0	5.492857	-0.893706	-0.136472
63	6	0	5.354504	0.274953	0.713705
64	6	0	4.964866	1.394737	-0.129184
65	6	0	-4.399879	-1.341005	0.120640
66	6	0	-5.470071	-0.644613	-0.451805
67	6	0	-6.538331	-1.385771	-0.944597
68	6	0	-6.510483	-2.776948	-0.849050
69	6	0	-5.399555	-3.399094	-0.266181
70	6	0	-2.389668	3.420766	-0.628466
71	6	0	-3.143838	3.361074	-1.804778
72	6	0	-3.551612	4.561424	-2.377317
73	6	0	-3.204663	5.766929	-1.767619
74	6	0	-2.456695	5.740843	-0.583672
75	7	0	-2.069597	4.573645	-0.037344
76	8	0	-1.816225	0.864584	3.591145
77	8	0	-2.920978	-1.651716	2.838261
78	7	0	-4.366168	-2.671581	0.198049
79	6	0	-5.263679	-4.919164	-0.098754
80	6	0	-2.011416	6.999834	0.174290
81	6	0	-5.079178	-5.230098	1.404654
82	6	0	-4.015074	-5.392761	-0.877330
83	6	0	-6.496622	-5.677293	-0.621455
84	6	0	-2.547996	6.922042	1.621814
85	6	0	-2.524856	8.292988	-0.482725
86	6	0	-0.465607	7.027881	0.204339
87	1	0	-4.364915	0.568882	2.129692
88	1	0	-3.368151	2.743083	1.727043
89	1	0	-5.461053	0.439297	-0.499612
90	1	0	-7.391174	-0.885652	-1.396489
91	1	0	-7.342985	-3.361401	-1.221860
92	1	0	-3.396628	2.407246	-2.255463
93	1	0	-4.135335	4.561097	-3.294300
94	1	0	-3.515806	6.705670	-2.209879
95	1	0	-4.917559	-6.304780	1.551269

96	1	0	-5.967338	-4.939683	1.978407
97	1	0	-4.222325	-4.687155	1.811701
98	1	0	-3.870616	-6.471006	-0.739509
99	1	0	-3.117954	-4.875535	-0.527194
100	1	0	-4.122709	-5.200766	-1.951858
101	1	0	-6.355494	-6.753763	-0.474483
102	1	0	-6.657592	-5.511162	-1.693350
103	1	0	-7.410185	-5.390019	-0.087672
104	1	0	-2.197129	7.783598	2.202259
105	1	0	-2.204215	6.007667	2.112304

106	1	0	-3.644632	6.927754	1.637644
107	1	0	-2.187764	9.158925	0.097764
108	1	0	-3.620225	8.327372	-0.518018
109	1	0	-2.143526	8.414971	-1.503428
110	1	0	-0.113406	7.887511	0.787047
111	1	0	-0.052883	7.113421	-0.808126
112	1	0	-0.070945	6.114063	0.656623

The total electronic energy was calculated to be –3400.1159847 Hartree.

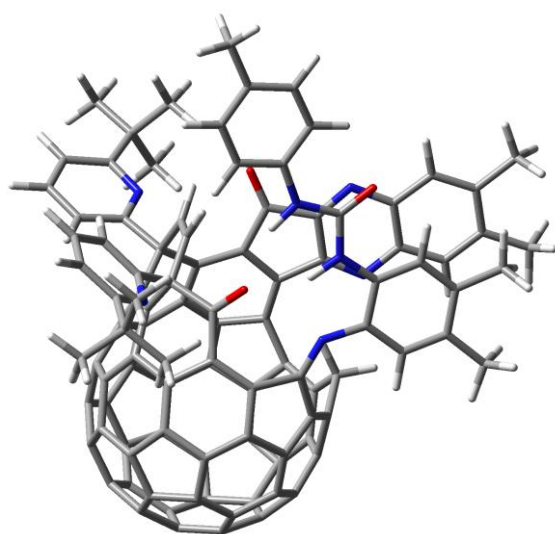## Table S6. Optimized structure of 4 (B3LYP/6-31G(d))
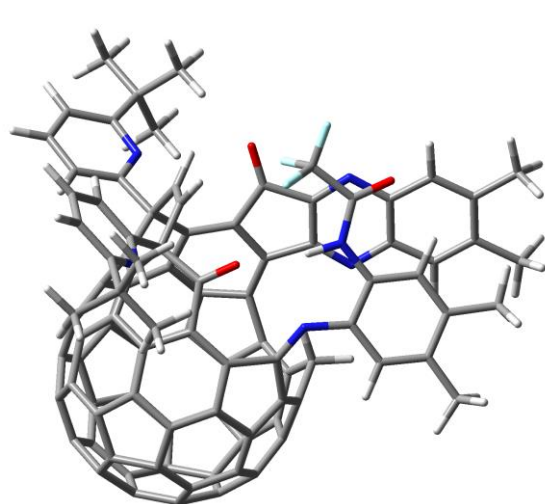
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.292295	3.097899	1.337802
2	6	0	-0.213912	3.428633	0.049343
3	6	0	-1.083161	2.859947	-1.053147
4	6	0	-0.324337	1.852974	-1.966493
5	6	0	1.049077	1.565686	-1.933131
6	6	0	2.235959	2.396661	-1.499851
7	6	0	3.410694	1.458454	-1.514779
8	6	0	2.994675	0.202734	-2.044066
9	6	0	1.723697	-2.855520	-0.864036
10	6	0	0.878814	-3.680438	0.107657
11	6	0	0.449630	-3.344913	1.384861
12	6	0	0.679010	-2.069335	2.177284
13	6	0	-0.721093	-1.638066	2.580303
14	6	0	-1.357505	-0.387539	2.540627
15	6	0	-0.604742	0.902104	2.522793
16	6	0	-1.318426	2.160200	1.917682
17	7	0	-2.223482	2.193890	4.207306
18	8	0	2.308504	3.595569	-1.312737
19	8	0	0.528827	1.010384	2.950418
20	7	0	-0.818533	4.410572	-2.918545
21	6	0	-2.316325	1.705637	0.876141
22	6	0	-3.142695	1.420037	-1.399709
23	7	0	4.638203	1.735523	-1.155925
24	6	0	-3.254230	0.698862	1.322296
25	6	0	-1.140569	1.007947	-2.782575
26	6	0	-3.327176	0.000923	-3.395283
27	6	0	-1.134891	5.488222	-3.659931
28	6	0	-2.652042	-1.051570	-4.137363

29	6	0	-1.591727	4.054945	-1.892612
30	6	0	-2.605093	0.970258	-2.672843
31	6	0	-4.293546	0.801139	-0.897944
32	6	0	-2.242375	2.049253	-0.458532
33	6	0	-1.274200	-1.115782	-4.084295
34	6	0	-5.024195	-0.189655	-1.645471
35	6	0	0.728393	-0.618204	-3.000622
36	6	0	-4.553105	-0.578574	-2.893097
37	6	0	-4.347217	0.427142	0.498661
38	6	0	-2.787771	-0.340082	2.244247
39	6	0	-0.533941	-0.098115	-3.412245
40	6	0	-2.547939	4.178437	2.898004
41	6	0	-2.065757	2.879518	3.068986
42	6	0	-1.307351	-3.534353	-3.858578
43	6	0	-3.552163	-1.519198	2.328187
44	6	0	-5.116435	-0.789138	0.599865
45	6	0	-3.217078	4.771433	3.966667
46	6	0	1.562514	0.284408	-2.363127
47	6	0	-4.609652	-1.981091	-3.280709
48	6	0	-2.279472	6.243934	-3.377938
49	6	0	-0.922850	-4.524676	-2.891896
50	6	0	-5.108882	-2.936355	-2.390333
51	6	0	0.634098	-2.104026	-3.140491
52	6	0	-3.376530	4.059692	5.151340
53	6	0	-0.150673	5.811251	-4.792763
54	6	0	-2.744918	4.764448	-1.537453
55	6	0	0.980190	-3.057876	-2.188925
56	6	0	-2.862334	2.756792	5.244364
57	6	0	-5.550827	-1.177007	-0.724643
58	6	0	-2.131417	-5.122980	-2.351405
59	6	0	-1.038818	-5.247741	-0.155029
60	6	0	-0.563770	-2.358332	-3.936646
61	6	0	-2.904814	-2.790969	2.497671
62	6	0	-3.424659	-2.269644	-4.060080
63	6	0	-4.423173	-4.207551	-2.235094
64	6	0	0.167925	-4.249355	-2.060294
65	6	0	-3.088485	5.872792	-2.303750
66	6	0	-1.518138	-2.828651	2.528858
67	6	0	0.105590	-4.621332	-0.661903
68	6	0	-3.270442	-4.479260	-2.981058
69	6	0	-2.759101	-3.491485	-3.913968
70	6	0	-0.806871	-3.882095	1.838671
71	6	0	-5.590904	-2.525011	-1.083061
72	6	0	-5.202019	-3.539162	-0.118882
73	6	0	-4.730869	-1.750911	1.520108
74	6	0	-3.386405	-5.208204	-0.229172
75	6	0	-4.786703	-3.157451	1.162873
76	6	0	-0.024544	4.571642	-5.707068
77	6	0	-3.652939	-3.807077	1.780496
78	6	0	-1.516126	-4.853421	1.140904
79	6	0	-2.188275	-5.481175	-1.006762
80	6	0	-2.967350	-4.815319	1.101119
81	6	0	-4.483196	-4.579947	-0.830392

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82	6	0	1.225715	6.125033	-4.159737
83	6	0	-0.603904	7.013964	-5.638271
84	6	0	-2.996707	1.936836	6.536528
85	6	0	-4.489766	1.818210	6.922379
86	6	0	-2.229275	2.657963	7.670498
87	6	0	-2.414476	0.523529	6.360965
88	6	0	5.521348	0.703520	-1.327006
89	7	0	3.816131	-0.804869	-2.246706
90	6	0	5.114553	-0.555235	-1.885004
91	6	0	6.092648	-1.557947	-2.072707
92	6	0	6.874185	0.887051	-0.959462
93	6	0	7.816415	-0.104865	-1.148052
94	6	0	7.415843	-1.355600	-1.727870
95	6	0	8.434090	-2.444210	-1.962993
96	6	0	9.254119	0.127408	-0.751894
97	6	0	4.067048	-0.896297	2.350431
98	6	0	5.413486	-1.265747	2.237836
99	6	0	5.794063	-2.606174	2.151377
100	6	0	4.809799	-3.619594	2.176931
101	6	0	3.471063	-3.246786	2.254059
102	6	0	3.064580	-1.901933	2.318331
103	7	0	3.639020	0.434983	2.509042
104	7	0	1.755341	-1.461675	2.506872
105	6	0	5.191066	-5.080558	2.135211
106	6	0	7.259229	-2.957425	2.061830
107	6	0	4.424141	1.549301	2.510024
108	8	0	5.631036	1.605272	2.342219
109	6	0	3.625518	2.863100	2.710885
110	9	0	4.452425	3.865833	3.011445
111	9	0	2.718288	2.750281	3.705342
112	9	0	2.957528	3.185081	1.582899
113	1	0	0.405931	3.530308	2.046033
114	1	0	0.537864	4.134388	-0.276957
115	1	0	2.763680	-3.202582	-0.922413
116	1	0	1.768672	-1.804746	-0.570553
117	1	0	-2.391357	4.708155	1.964276
118	1	0	-3.606464	5.782271	3.876708
119	1	0	-2.540460	7.107097	-3.978615
120	1	0	-3.889744	4.511963	5.993659

121	1	0	-3.353658	4.451559	-0.695601
122	1	0	-3.980861	6.447137	-2.067958
123	1	0	0.715197	4.756349	-6.495237
124	1	0	-0.981556	4.337872	-6.189564
125	1	0	0.288775	3.697438	-5.130887
126	1	0	1.974277	6.289824	-4.944240
127	1	0	1.560147	5.302929	-3.521191
128	1	0	1.177264	7.031922	-3.544798
129	1	0	0.126368	7.199908	-6.433589
130	1	0	-0.677471	7.930633	-5.041283
131	1	0	-1.574454	6.835939	-6.116905
132	1	0	-5.063102	1.321187	6.131536
133	1	0	-4.948212	2.795846	7.107468
134	1	0	-4.594190	1.225217	7.838672
135	1	0	-2.313003	2.088234	8.603727
136	1	0	-2.623320	3.663294	7.857405
137	1	0	-1.165429	2.752508	7.425746
138	1	0	-2.511197	-0.029883	7.302533
139	1	0	-1.357553	0.556274	6.083082
140	1	0	-2.942049	-0.032015	5.579722
141	1	0	5.768678	-2.498634	-2.509319
142	1	0	7.142525	1.840853	-0.515848
143	1	0	8.923556	-2.749535	-1.029360
144	1	0	9.230849	-2.109909	-2.639741
145	1	0	7.968832	-3.329764	-2.405037
146	1	0	9.594316	-0.608022	-0.011395
147	1	0	9.383715	1.122548	-0.318328
148	1	0	9.930112	0.043302	-1.612671
149	1	0	6.165621	-0.490000	2.239146
150	1	0	2.713969	-4.021214	2.302375
151	1	0	2.639462	0.532544	2.704127
152	1	0	5.842327	-5.354902	2.975208
153	1	0	4.305161	-5.721237	2.179111
154	1	0	5.739128	-5.332844	1.217850
155	1	0	7.879275	-2.056690	2.048254
156	1	0	7.580178	-3.572756	2.912725
157	1	0	7.480722	-3.536081	1.155499

The total electronic energy was calculated to be –4691.3524818 Hartree.

Table S7. Optimized structure of **5** (B3LYP/6-31G(d))

Standard orientation:

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
Number	Number	Type	X	Y	Z
1	6	0	-1.361951	2.544752	0.774693
2	6	0	-1.182449	2.030041	1.990865
3	6	0	0.148521	1.607273	2.576214
4	6	0	0.298530	0.061182	2.685013
5	6	0	-0.701419	-0.897660	2.449507
6	6	0	-2.207475	-0.832055	2.577069
7	6	0	-2.715204	-2.144908	2.046582
8	6	0	-1.605107	-2.967499	1.699732
9	6	0	0.508392	-3.565407	-1.057802
10	6	0	1.277296	-3.115473	-2.301832
11	6	0	1.059370	-1.995721	-3.096935
12	6	0	0.024434	-0.895991	-2.959291
13	6	0	0.839469	0.383008	-3.001011
14	6	0	0.782678	1.552130	-2.218715
15	6	0	-0.434700	2.032240	-1.511894
16	6	0	-0.252010	2.862440	-0.195633
17	7	0	-0.164963	4.661248	-1.874307
18	8	0	-2.902118	0.015659	3.104175
19	8	0	-1.566090	1.832334	-1.930030
20	7	0	-0.254421	1.522037	4.981858
21	6	0	1.107716	2.575431	0.402668

22	6	0	2.636766	1.686441	2.081003	94	6	0	-4.567614	-6.428190	0.550450
23	7	0	-3.965610	-2.519598	1.954168	95	6	0	-4.799897	-7.841974	0.075936
24	6	0	2.217370	2.693696	-0.517063	96	6	0	-7.093091	-6.109444	0.771897
25	6	0	1.630528	-0.427079	2.866862	97	6	0	-3.508410	-1.554878	-2.594621
26	6	0	4.097341	-0.136583	2.839806	98	6	0	-4.534912	-2.510165	-2.662952
27	6	0	-0.283564	2.023582	6.230264	99	6	0	-4.278091	-3.813369	-3.082184
28	6	0	4.283668	-1.577409	2.782111	100	6	0	-2.963624	-4.201445	-3.450633
29	6	0	0.246608	2.247340	3.981878	101	6	0	-1.943099	-3.264578	-3.357850
30	6	0	2.813492	0.441908	2.810165	102	6	0	-2.170330	-1.944178	-2.918973
31	6	0	3.719023	2.203732	1.358935	103	7	0	-3.686025	-0.230464	-2.235793
32	6	0	1.300724	2.057247	1.667249	104	7	0	-1.251951	-0.911573	-2.849899
33	6	0	3.169377	-2.381293	2.654423	105	6	0	-2.672832	-5.600801	-3.939655
34	6	0	5.026816	1.601078	1.392798	106	6	0	-5.414982	-4.802615	-3.159641
35	6	0	0.946885	-2.659884	2.015898	107	6	0	-4.866147	0.437490	-1.926324
36	6	0	5.219766	0.445599	2.138487	108	8	0	-5.971874	-0.090966	-1.894123
37	6	0	3.503473	2.713009	0.022197	109	7	0	-4.616678	1.771799	-1.660312
38	6	0	2.035660	2.232874	-1.894943	110	6	0	-5.539162	2.780734	-1.331935
39	6	0	1.863845	-1.807262	2.696108	111	6	0	-6.915952	2.564874	-1.160507
40	6	0	-0.539139	5.338455	0.397610	112	6	0	-7.744010	3.636804	-0.833462
41	6	0	-0.329057	4.364137	-0.579667	113	6	0	-7.255025	4.937925	-0.661548
42	6	0	4.273781	-3.805144	1.025029	114	6	0	-8.170871	6.076140	-0.275365
43	6	0	3.195317	1.943764	-2.637779	115	6	0	-5.880833	5.135472	-0.840149
44	6	0	4.681338	2.418495	-0.757451	116	6	0	-5.034229	4.081356	-1.170256
45	6	0	-0.576749	6.671058	-0.009426	117	1	0	-2.365747	2.807816	0.454814
46	6	0	-0.371111	-2.237280	2.019302	118	1	0	-2.036736	1.872024	2.635260
47	6	0	6.057680	-0.622461	1.612182	119	1	0	-0.166589	-4.408359	-1.255650
48	6	0	0.216223	3.303074	6.502672	120	1	0	-0.116418	-2.765423	-0.655554
49	6	0	4.118183	-4.168603	-0.356347	121	1	0	-0.678481	5.059839	1.436610
50	6	0	6.638374	-0.499747	0.346388	122	1	0	-0.739093	7.461672	0.718571
51	6	0	1.774970	-3.635075	1.244805	123	1	0	0.200105	3.705464	7.508476
52	6	0	-0.410582	6.978799	-1.355771	124	1	0	-0.443697	8.011884	-1.686192
53	6	0	-0.906574	1.103822	7.289723	125	1	0	1.154508	4.106123	3.335128
54	6	0	0.754222	3.538490	4.168521	126	1	0	1.130534	5.059155	5.647243
55	6	0	1.638857	-3.954811	-0.101765	127	1	0	-0.604688	-0.936849	7.998974
56	6	0	-0.204964	5.940038	-2.278086	128	1	0	0.904208	-0.099243	7.587099
57	6	0	5.638615	1.736038	0.085825	129	1	0	-0.156773	-0.691582	6.295151
58	6	0	5.220288	-3.588514	-1.104220	130	1	0	-2.840457	0.140346	7.600489
59	6	0	3.677036	-3.167905	-2.969691	131	1	0	-2.462213	0.453908	5.889549
60	6	0	3.131919	-3.516337	1.770116	132	1	0	-2.962921	1.784261	6.946750
61	6	0	3.207382	0.834353	-3.550923	133	1	0	-1.297681	1.017835	9.419956
62	6	0	5.472088	-1.881534	2.019450	134	1	0	-1.410885	2.653412	8.764352
63	6	0	6.629171	-1.631143	-0.564953	135	1	0	0.180002	1.904058	9.025340
64	6	0	2.826523	-4.190080	-0.893914	136	1	0	2.112433	6.675759	-3.612107
65	6	0	0.738604	4.063288	5.456424	137	1	0	1.080377	8.108738	-3.463024
66	6	0	2.074730	0.036886	-3.638841	138	1	0	1.331518	7.363892	-5.047619
67	6	0	2.603200	-3.676366	-2.230168	139	1	0	-1.187453	7.141427	-5.381993
68	6	0	6.050090	-2.843768	-0.173622	140	1	0	-1.487232	7.881749	-3.803269
69	6	0	5.460168	-2.974830	1.146180	141	1	0	-2.183038	6.296802	-4.182701
70	6	0	2.203182	-1.398794	-3.740438	142	1	0	0.299717	5.161212	-5.633714
71	6	0	6.424274	0.706518	-0.434029	143	1	0	-0.648981	4.236028	-4.449419
72	6	0	6.279666	0.322819	-1.827180	144	1	0	1.093634	4.402819	-4.237503
73	6	0	4.529026	2.048327	-2.084495	145	1	0	-2.423967	-6.556967	0.414575
74	6	0	5.610581	-1.844140	-2.804409	146	1	0	-6.269727	-3.646139	1.608111
75	6	0	5.352079	0.987437	-2.638504	147	1	0	-5.422605	-7.869411	-0.827450
76	6	0	-0.142397	-0.239672	7.290054	148	1	0	-5.321733	-8.439811	0.834180
77	6	0	4.529323	0.237165	-3.560690	149	1	0	-3.854130	-8.341717	-0.151667
78	6	0	3.467081	-1.979254	-3.747107	150	1	0	-7.328496	-6.404134	-0.258874
79	6	0	5.004122	-3.099088	-2.390069	151	1	0	-7.817553	-5.349132	1.075885
80	6	0	4.654994	-1.150203	-3.643624	152	1	0	-7.252973	-6.996571	1.398092
81	6	0	6.407120	-1.121031	-1.908791	153	1	0	-5.539253	-2.203728	-2.403722
82	6	0	-2.383726	0.853912	6.903934	154	1	0	-0.942284	-3.547353	-3.664329
83	6	0	-0.850242	1.713311	8.701296	155	1	0	-2.820071	0.304938	-2.300557
84	6	0	-0.028022	6.226226	-3.776596	156	1	0	-3.265828	-5.857171	-4.827332
85	6	0	1.195799	7.150046	-3.980853	157	1	0	-1.616838	-5.713015	-4.204711
86	6	0	-1.297942	6.929878	-4.311879	158	1	0	-2.906128	-6.356088	-3.177158
87	6	0	0.191509	4.925556	-4.568536	159	1	0	-6.358580	-4.342640	-2.853946
88	6	0	-4.137671	-3.790463	1.475030	160	1	0	-5.542983	-5.191590	-4.178355
89	7	0	-1.727404	-4.195858	1.245015	161	1	0	-5.234025	-5.670090	-2.511395
90	6	0	-3.023497	-4.625222	1.124632	162	1	0	-3.645802	2.066414	-1.699053
91	6	0	-3.280421	-5.936797	0.664381	163	1	0	-7.317293	1.569408	-1.286979
92	6	0	-5.448171	-4.304002	1.340078	164	1	0	-8.808582	3.448662	-0.707729
93	6	0	-5.681432	-5.589849	0.893516	165	1	0	-7.734489	7.046860	-0.535123

166	1	0	-8.369340	6.087411	0.805263
167	1	0	-9.141574	6.000020	-0.778747
168	1	0	-5.461526	6.132661	-0.723363

| 169 | 1 | 0 | -3.971590 | 4.266742 | -1.315682 |

The total electronic energy was calculated to be –4680.0658406 Hartree.

Table S8. Optimized structure of 2 (B3LYP/6-31G(d))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.685981	2.971190	1.908816
2	6	0	-0.166826	3.386538	0.756190
3	6	0	-0.621677	2.932388	-0.613471
4	6	0	0.420420	2.029477	-1.327262
5	6	0	1.731670	1.756891	-0.901065
6	6	0	2.720420	2.539799	-0.060372
7	6	0	3.944236	1.665269	0.042931
8	6	0	3.707227	0.449663	-0.659770
9	6	0	2.192400	-2.607263	-0.157242
10	6	0	1.134096	-3.535097	0.435726
11	6	0	0.302851	-3.299261	1.525503
12	6	0	0.188809	-2.037398	2.353027
13	6	0	-1.295460	-1.773278	2.448052
14	6	0	-1.984969	-0.555897	2.375706
15	6	0	-1.400417	0.746478	2.800133
16	6	0	-1.849132	2.027002	2.022279
17	7	0	-3.660893	1.880551	3.653614
18	8	0	2.662313	3.682983	0.352596
19	8	0	-0.626661	0.853531	3.732431
20	7	0	0.261591	4.656931	-2.063464
21	6	0	-2.409902	1.640106	0.676056
22	6	0	-2.423515	1.556653	-1.757956
23	7	0	5.077806	1.965692	0.622033
24	6	0	-3.415575	0.599863	0.703112
25	6	0	-0.067708	1.293975	-2.455747
26	6	0	-1.908546	0.353453	-3.836099
27	6	0	0.221927	5.802998	-2.762978
28	6	0	-0.995167	-0.608092	-4.434100
29	6	0	-0.831542	4.210515	-1.448148
30	6	0	-1.489654	1.240852	-2.824065
31	6	0	-3.656227	0.891454	-1.719717
32	6	0	-1.898418	2.089596	-0.521171
33	6	0	0.302764	-0.661587	-3.970843
34	6	0	-4.067233	-0.026296	-2.751062
35	6	0	1.847162	-0.268503	-2.278155
36	6	0	-3.206730	-0.283786	-3.809827
37	6	0	-4.156533	0.389312	-0.458082
38	6	0	-3.236660	-0.514963	1.635863
39	6	0	0.750165	0.282046	-2.996595
40	6	0	-3.314141	4.032632	2.655374
41	6	0	-2.987289	2.684381	2.833217
42	6	0	0.303278	-3.092994	-3.987461
43	6	0	-3.912872	-1.717291	1.355118
44	6	0	-4.861526	-0.844371	-0.721299
45	6	0	-4.387519	4.536439	3.382900
46	6	0	2.403441	0.548639	-1.313929
47	6	0	-3.081131	-1.640152	-4.326207
48	6	0	-0.964346	6.540411	-2.865520
49	6	0	0.410153	-4.162857	-3.031297
50	6	0	-3.792966	-2.685114	-3.730354
51	6	0	1.877144	-1.721440	-2.593893
52	6	0	-5.090351	3.695604	4.248295
53	6	0	1.557150	6.209934	-3.394725
54	6	0	-2.052345	4.891907	-1.484394
55	6	0	1.941997	-2.744769	-1.657371
56	6	0	-4.699647	2.356133	4.362712
57	6	0	-4.822005	-1.106073	-2.143944
58	6	0	-0.881832	-4.822150	-2.945630
59	6	0	-0.525726	-5.120257	-0.531367
60	6	0	0.990879	-1.906475	-3.738230
61	6	0	-3.271074	-2.980157	1.601899
62	6	0	-1.701625	-1.836428	-4.717842
63	6	0	-3.133903	-3.955502	-3.478174
64	6	0	1.176465	-3.950491	-1.878869
65	6	0	-2.109040	6.074652	-2.215695
66	6	0	-1.955882	-2.976830	2.053153
67	6	0	0.692851	-4.433454	-0.600453
68	6	0	-1.795901	-4.138120	-3.843795
69	6	0	-1.062731	-3.059800	-4.482621
70	6	0	-0.997588	-3.924432	1.529954
71	6	0	-4.683282	-2.412502	-2.614947
72	6	0	-4.573662	-3.511181	-1.671186
73	6	0	-4.748433	-1.888294	0.184828
74	6	0	-2.731778	-5.122163	-1.339973
75	6	0	-4.609371	-3.252515	-0.295663
76	6	0	2.054358	5.046760	-4.282314
77	6	0	-3.693208	-3.934179	0.593108
78	6	0	-1.401658	-4.851818	0.573826
79	6	0	-1.338714	-5.297828	-1.719005
80	6	0	-2.770296	-4.847687	0.082272
81	6	0	-3.614686	-4.462514	-2.202750
82	6	0	2.571550	6.449854	-2.251906
83	6	0	1.438432	7.482783	-4.248274
84	6	0	-5.391785	1.325662	5.261150
85	6	0	-6.529956	1.942550	6.090426
86	6	0	-4.337479	0.718959	6.214571
87	6	0	-5.967371	0.208539	4.360407
88	6	0	6.035562	0.988219	0.521490
89	7	0	4.585289	-0.523762	-0.753839
90	6	0	5.780060	-0.259962	-0.138517
91	6	0	6.801579	-1.235242	-0.165550
92	6	0	7.307104	1.206961	1.097508
93	6	0	8.298315	0.246020	1.053784
94	6	0	8.036395	-1.008382	0.410848
95	6	0	9.101196	-2.076440	0.379159

96	6	0	9.638057	0.498407	1.698441	126	1	0	-7.323698	2.351778	5.454132
97	6	0	3.168914	-0.133865	2.923321	127	1	0	-6.166919	2.742440	6.746656
98	6	0	4.549689	-0.193040	3.167115	128	1	0	-6.981807	1.172904	6.725782
99	6	0	5.220167	-1.403668	3.327657	129	1	0	-4.793939	-0.065842	6.829359
100	6	0	4.505327	-2.622215	3.220076	130	1	0	-3.928981	1.483780	6.885817
101	6	0	3.135020	-2.571618	2.991967	131	1	0	-3.507989	0.286328	5.649060
102	6	0	2.440638	-1.355208	2.852121	132	1	0	-6.441955	-0.565098	4.975829
103	7	0	2.512097	1.059855	2.688744	133	1	0	-5.177357	-0.257129	3.765217
104	7	0	1.066516	-1.214795	2.788733	134	1	0	-6.722507	0.607406	3.672324
105	6	0	5.210040	-3.947780	3.380979	135	1	0	6.581200	-2.175662	-0.662922
106	6	0	6.692179	-1.418404	3.656340	136	1	0	7.475708	2.162571	1.586335
107	1	0	-0.288885	3.336711	2.851008	137	1	0	9.394929	-2.376767	1.393550
108	1	0	0.656201	4.087298	0.750895	138	1	0	10.012387	-1.723446	-0.120012
109	1	0	3.215973	-2.878424	0.130432	139	1	0	8.752221	-2.968739	-0.148068
110	1	0	2.051502	-1.578848	0.180418	140	1	0	9.836523	-0.225620	2.499586
111	1	0	-2.743230	4.652403	1.971832	141	1	0	9.686362	1.501013	2.132549
112	1	0	-4.678818	5.578519	3.279010	142	1	0	10.459178	0.403310	0.976852
113	1	0	-1.003484	7.460324	-3.436871	143	1	0	5.104121	0.738190	3.242346
114	1	0	-5.925914	4.083504	4.818315	144	1	0	2.565055	-3.495410	2.962209
115	1	0	-2.921448	4.502004	-0.964675	145	1	0	1.517963	1.041947	2.901379
116	1	0	-3.038942	6.633751	-2.281497	146	1	0	2.986109	1.900605	2.992573
117	1	0	3.034351	5.290354	-4.709561	147	1	0	5.693185	-4.039713	4.362832
118	1	0	1.358676	4.858767	-5.109068	148	1	0	4.510475	-4.782860	3.275731
119	1	0	2.144113	4.128219	-3.696512	149	1	0	5.999989	-4.078981	2.629137
120	1	0	3.558589	6.686151	-2.667807	150	1	0	7.106243	-0.407343	3.682199
121	1	0	2.659515	5.564994	-1.615009	151	1	0	6.874424	-1.888331	4.631931
122	1	0	2.258984	7.291588	-1.621900	152	1	0	7.261483	-1.991227	2.914865
123	1	0	2.413154	7.726615	-4.685089						
124	1	0	1.120584	8.345976	-3.651632						
125	1	0	0.728029	7.353317	-5.073687						

The total electronic energy was calculated to be -4241.2453416 Hartree.

7. References

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