Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

C2-insertion into a fullerene orifice

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1. General

The ^{1}H and ^{13}C 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 $CDCl_3$ (δ 7.26 ppm in ^{1}H NMR, δ 77.00 ppm in ^{13}C NMR), CD_2Cl_2 (δ 5.32 ppm in ^{1}H NMR, δ 53.80 ppm in ^{13}C NMR), and acetone-d_6 (δ 2.05 ppm in ^{1}H NMR, δ 29.92 ppm in ^{13}C NMR). APCI (atmospheric pressure chemical ionization) mass spectra were measured on a Bruker micrOTOF-Q II. The high-performance liquid chromatography (HPLC) was performed with the use of a Cosmosil Buckyprep column (250 mm in length, 4.6 mm in inner diameter) for analytical purpose and the same columns (250 mm in length, 20 mm in inner diameter) for preparative purpose. 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. Toluene was purchased from Kanto Chemical Co., Inc. Carbon disulfide, triisopropyl phosphite, carbon tetrachloride, acetonitrile, and acetone were purchased from FUJIFILM Wako Pure Chemical Corporation. Toluene, hexane, and ethyl acetate were purchased from Nacalai Tesque, Inc. 1-Chloronaphthalene and *o*-dichlorobenzene (ODCB) were purchased from Sigma-Aldroch Co. LLC. *N*-Phenylmaleimide was purchased from Tokyo Chemical Industry Co. Ltd.

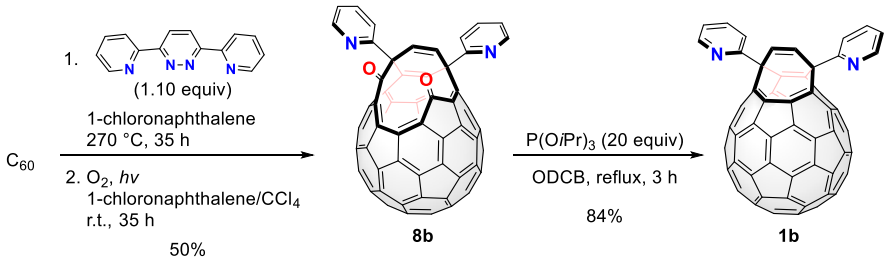
All reactions were carried out under Ar atmosphere. Triisopropyl phosphite and 1-chloronapthahelene were distilled prior to use. Unless otherwise noted, materials purchased from commercial suppliers were used without further purification. Compound H_2O@**1a**[1] was synthesized according to literature procedures.

2. Computational Methods

All calculations were conducted using the Gaussian 09 program. All structures at the stationary and transition states were optimized at the B3LYP/6-31G(d) and B3LYP-D3/6-31G(d) levels of theory without any symmetry assumptions and confirmed by the frequency analyses at the same level of theory. The electrostatic potential maps were drawn at the B3LYP/6-31G(d) level of theory.

3. Synthesis

3.1. Synthesis of 1b



Powdery C_{60} (3.00 g, 4.16 mmol), 3,6-di(pyridine-2-yl)pyridazine (1.08 g, 4.59 mmol, 1.10 equiv), and 1-chloronaphthalene (120 mL) were placed into a 200-mL two-neck flask and degassed through three vacuum-Ar cycles. The resulting solution was heated at 270 °C for 35 h (sand bath). After cooled down to room temperature, the crude mixture was transferred into a 1-L two-neck flask and diluted with CCl_4 (360 mL), bubbled with O_2 for 5 min, and then irradiated by six white LED lamps at room temperature for 35 h. The chromatographic purification using silica gel (toluene to toluene/EtOAc (10:1)) gave recovered C_{60} (1.22 g, 1.69 mmol, 41%) followed by **8b** (1.91 g, 1.99 mmol, 50%) as black powders.

Powdery **8b** (100 mg, 104 μmol) was placed into a 20-mL Schlenk tube and degassed through three vacuum-Ar cycles. P(O*i*Pr)$_3$ (0.480 mL, ρ = 0.9035 g/mL, 2.08 mmol, 20.0 equiv) and ODCB (4.48 mL) were added and heated at 180 °C for 3 h (aluminum block heater). The solvent and residual phosphite were removed under a reduced pressure. The crude mixture was purified by column chromatography using silica gel (CS_2/acetone (20:1)) to give **1b** (80.8 mg, 87.2 μmol, 84%) as a black powder.

8b: ^{1}H NMR (500 MHz, CS_2/$CDCl_3$ (1:1)) δ 8.65 (dt, J = 4.0, 1.2 Hz, 1H), 8.54 (dt, J = 4.0, 1.2 Hz, 1H), 7.79 (td, J = 8.0, 1.7 Hz, 1H), 7.78 (td, J = 8.0, 1.7 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.30–7.22 (m, 2H), 7.12 (d, J = 12.3 Hz, 1H), 7.09 (d, J = 12.3 Hz, 1H); ^{13}C NMR (126 MHz, CS_2/$CDCl_3$ (1:1)) δ 198.63, 190.67, 166.38, 153.18, 149.69, 149.08, 149.00, 148.43, 147.55, 147.53, 147.40, 147.06, 146.50, 146.17, 146.09, 146.02, 145.79, 145.72, 145.69, 145.60, 145.48, 145.44, 145.28, 145.07, 144.76, 144.40, 144.36, 144.02, 143.90, 143.67, 142.72, 142.37, 142.21, 141.97, 141.77, 141.70, 141.31, 140.94, 140.24, 140.07, 139.83, 139.81, 139.77, 139.57, 139.53, 139.36, 138.81, 138.69, 138.67, 137.11, 136.98, 136.95, 136.92, 136.21, 135.63, 135.46, 134.82,

134.55, 133.01, 131.72, 131.69, 131.54, 130.98, 130.01, 128.72, 123.13, 122.87, 122.38, 121.83, 60.49, 54.18 (The sum of carbon signals must be 74 in theory. Observed 71. The three sp^2 carbon signals are overlapped.); HRMS (APCI) *m*/*z*: $[M]^{\bullet-}$ Calcd for $C_{74}H_{10}N_2O_2$ (**8b**) 958.0748; Found 958.0728.

1b: ^{1}H NMR (800 MHz, CS_2/acetone-d_6 (5:1)) δ 8.70 (ddd, J = 1.0, 1.8, 4.8 Hz, 2H), 7.95 (dt, J = 1.0, 7.9 Hz, 2H), 7.89 (td, J = 1.8, 7.9 Hz, 2H), 7.36 (ddd, J = 1.0, 4.8, 7.9 Hz, 2H), 6.41 (s, 2H); ^{13}C NMR (201 MHz, CS_2/acetone-d_6 (5:1)) δ 166.72, 152.03, 150.23, 150.10, 147.65, 146.22, 146.15, 145.79, 145.07, 145.00, 144.91, 144.85, 144.76, 144.64, 144.55, 144.35, 144.33, 144.22, 144.16, 144.09, 143.80, 143.20, 141.25, 141.13, 141.10, 141.05, 140.60, 138.76, 137.65, 137.56, 137.09, 136.93, 136.02, 135.77, 131.04, 127.83, 124.11, 122.85, 57.81 (The sum of carbon signals must be 39 in theory. Observed 39.); HRMS (APCI) *m*/*z*: $[M]^+$ Calcd for $C_{74}H_{11}N_2$ (**1b**+H) 927.0917; Found 927.0878.

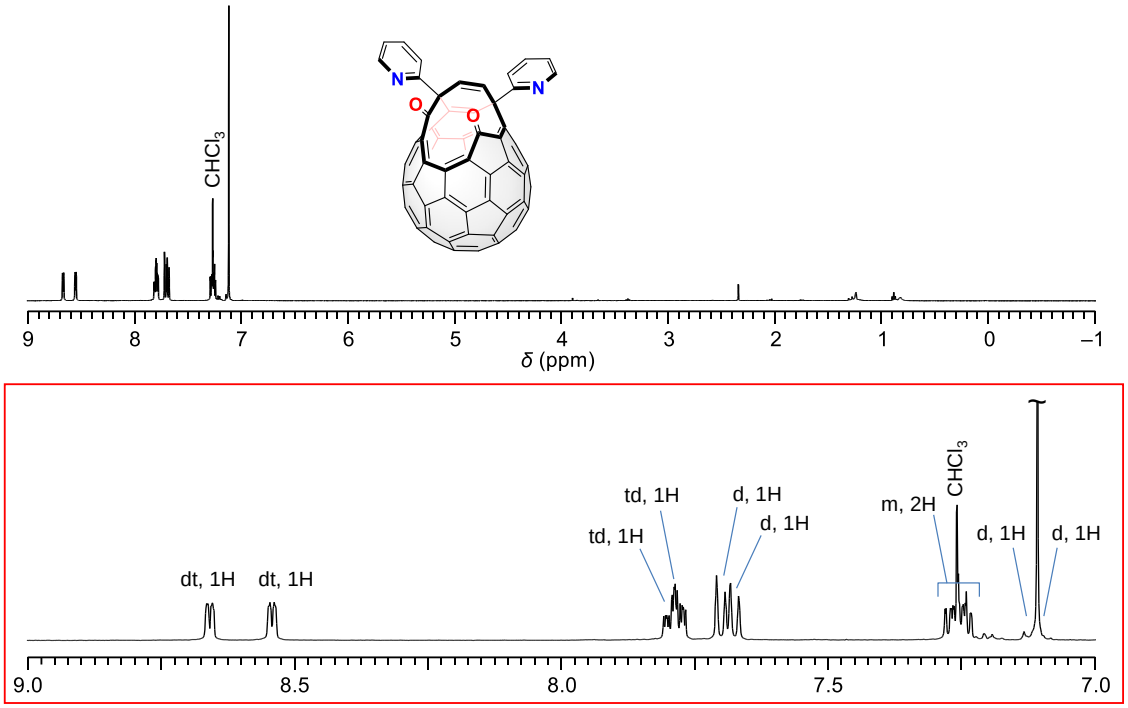


Figure S1. ^{1}H NMR spectra (500 MHz, CS_2/$CDCl_3$ (1:1)) of **8b**.

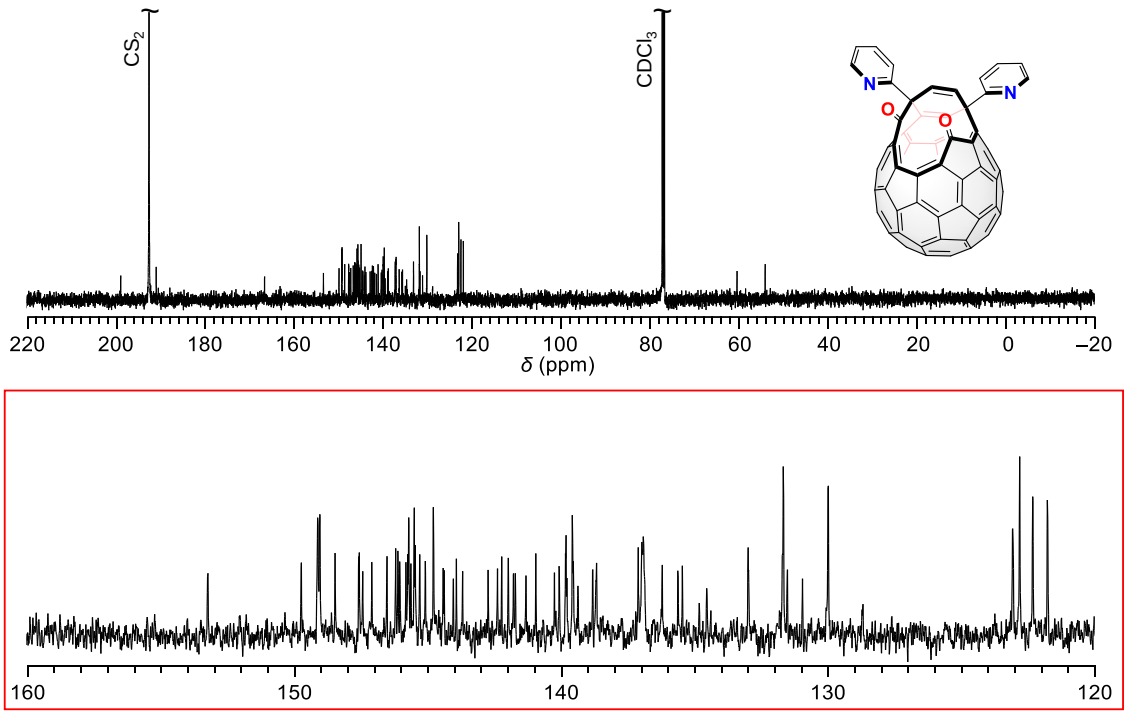


Figure S2. ^{13}C NMR spectra (126 MHz, CS_2/$CDCl_3$ (1:1)) of **8b**.

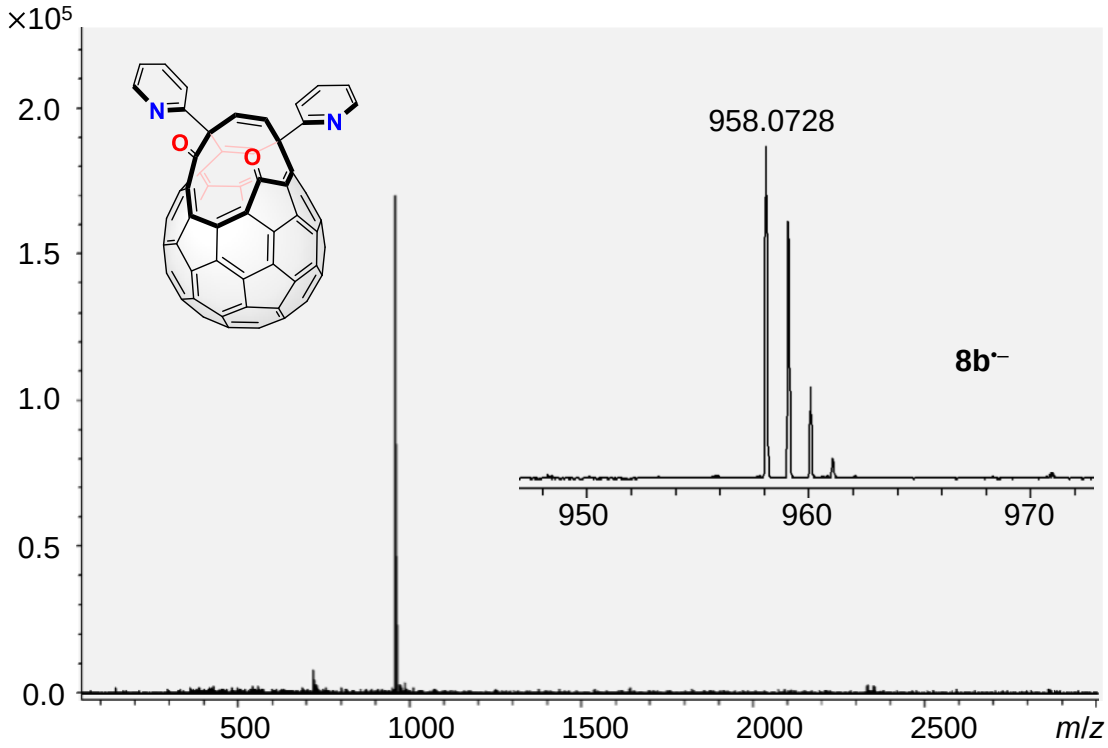


Figure S3. APCI mass spectrum (negative ion mode) of **8b**.

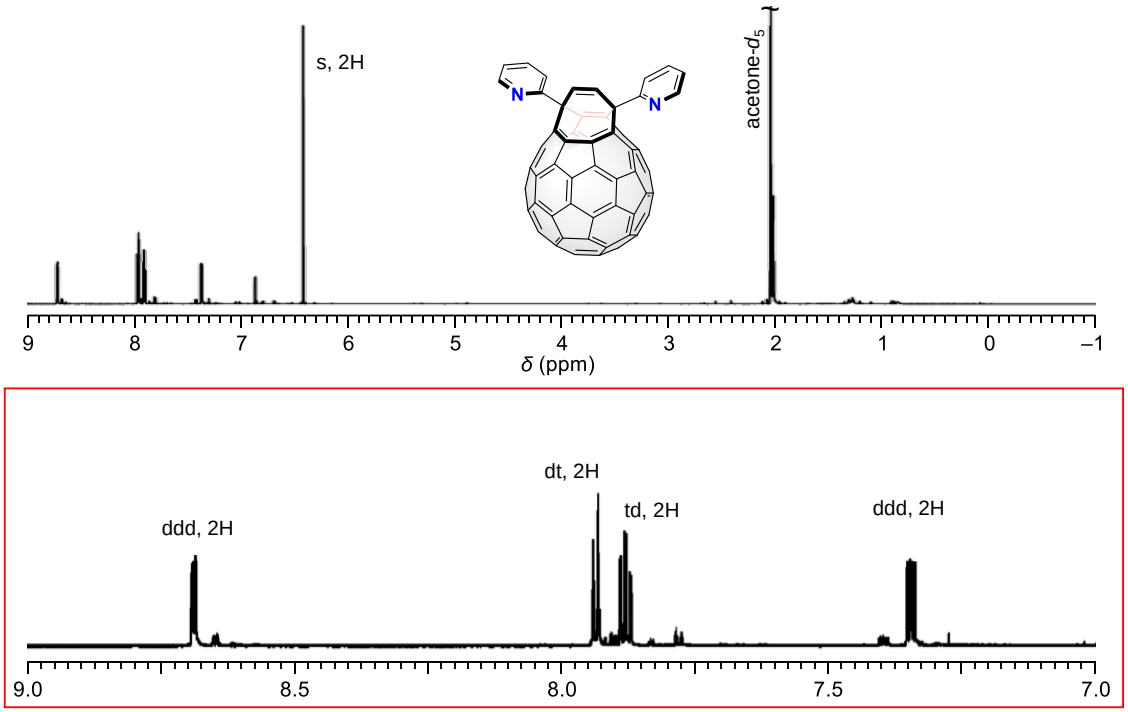


Figure S4. ^{1}H NMR spectra (800 MHz, CS_2/acetone-d_6 (5:1)) of **1b**.

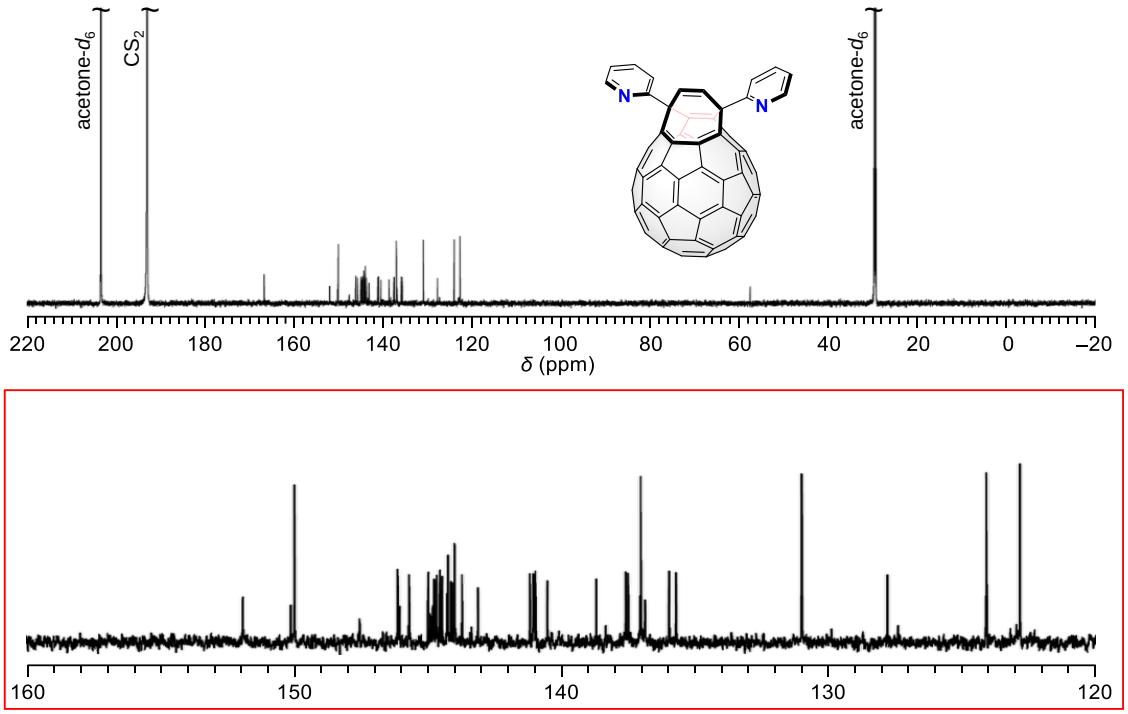


Figure S5. ^{13}C NMR spectra (201 MHz, CS_2/acetone-d_6 (5:1)) of **1b**.

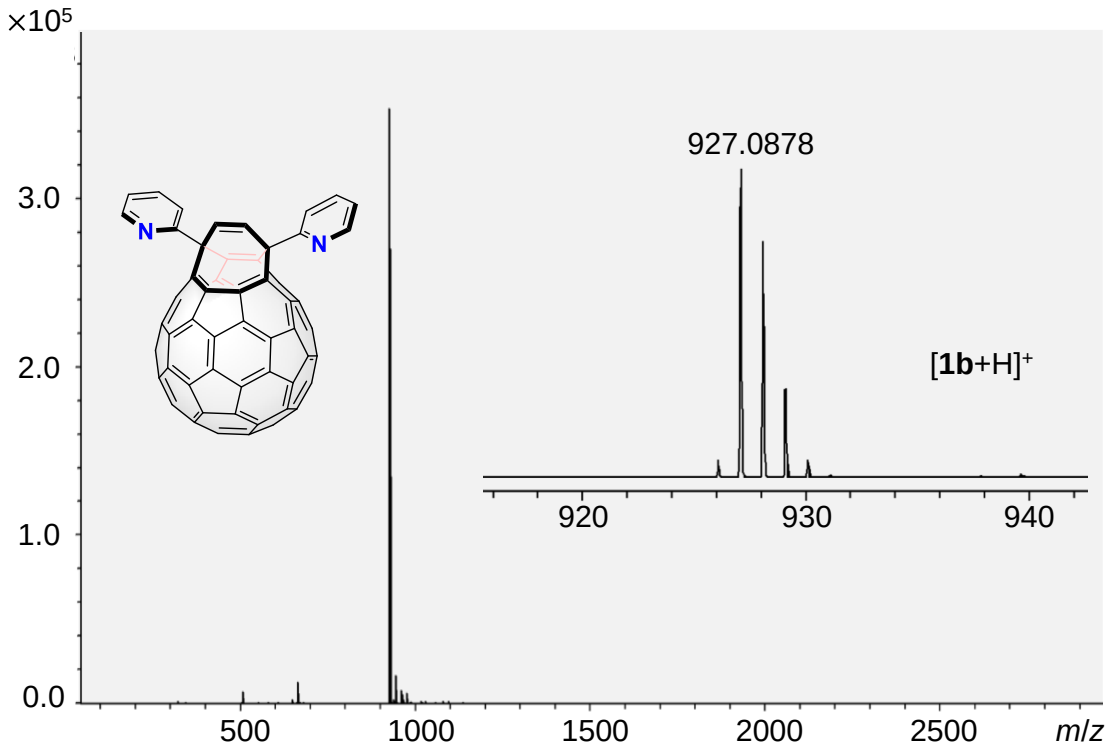
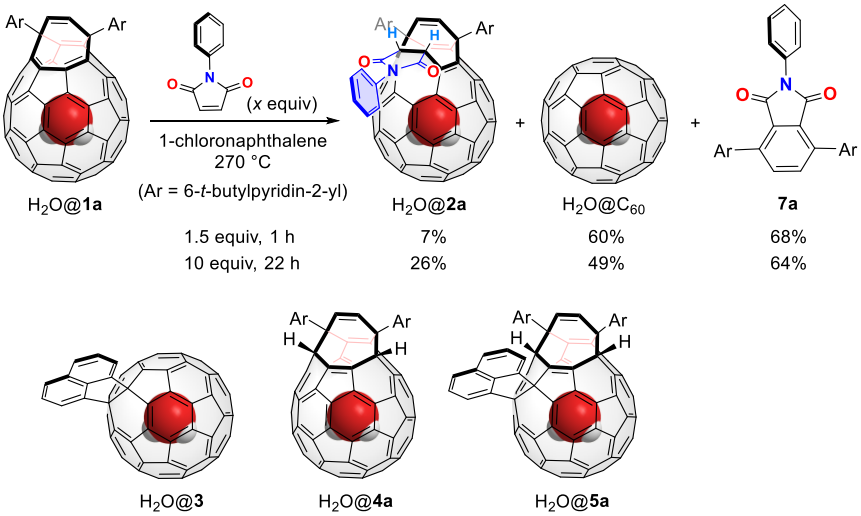


Figure S6. APCI mass spectrum (positive ion mode) of **1b**.

3.2. Synthesis of H_2O@2a



[1.5 equiv, 1 h]

Powdery H_2O@**1a** (H_2O: 60%, 20.0 mg, 19.0 μmol) and *N*-phenylmaleimide (4.95 mg, 28.6 μmol, 1.50 equiv) were placed into a 20-mL Schlenk tube and degassed through five vacuum-Ar cycles. 1-Chloronaphthalene (0.952 mL) was added and the resulting solution was heated at 270 °C for 1 h (sand bath). The crude mixture was precipitated by addition of CH_3CN and filtrated. The filtrate was evaporated to give a 1-chloronaphthalene solution. The filtered black powder was purified by column chromatography using silica gel (CS_2/hexane (1:2)) to give H_2O@C_{60} (8.37 mg, 11.4 μmol, 60%) followed by a mixture of H_2O@**3**, H_2O@**4a**, and H_2O@**5a** and then unreacted H_2O@**1a** (4.21 mg, 4.01 μmol, 21%) as black powders. To the column, the 1-chloronaphthalene solution was added and the purification was continued with the use of CS_2/acetone (100:1) as an eluent, giving **7a** (6.31 mg, 12.9 μmol, 68%) as a colorless crystalline powder and H_2O@**2a** (1.74 mg, 1.42 μmol, 7%) as a reddish brown powder. The mixture of H_2O@**3**, H_2O@**4a**, and H_2O@**5a** was separable by a careful chromatography using silica gel (CS_2/hexane).

[10 equiv, 22 h]

Powdery H_2O@**1a** (H_2O: 60%, 20.0 mg, 19.0 μmol) and *N*-phenylmaleimide (33.0 mg, 191 μmol, 10.0 equiv) were placed into a 20-mL Schlenk tube and degassed through five vacuum-Ar cycles. 1-Chloronaphthalene (0.952 mL) was added and the resulting solution was heated at 270 °C for 22 h (sand bath). The crude mixture was precipitated by addition of CH_3CN and filtrated. The filtrate was evaporated to give a 1-chloronaphthalene solution. The filtered black powder was purified by column chromatography using silica gel (CS_2/hexane (1:2)) to give H_2O@C_{60} (6.80 mg, 9.30 μmol, 49%) followed by a mixture of H_2O@**3**, H_2O@**4a**, and H_2O@**5a** as a black powder. To the column, the 1-

chloronaphthalene solution was added and the purification was continued with the use of CS_2/acetone (100:1) as an eluent, giving **7a** (5.94 mg, 12.1 μmol, 64%) as a colorless crystalline powder and H_2O@**2a** (6.08 mg, 4.97 μmol, 26%) as a reddish brown powder.

$H_2O@C_{60}$: ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ (1:1)) δ –4.64 (s, 2H); HRMS (APCI) *m*/*z*: $[M]^{\bullet-}$ Calcd for $C_{60}H_2O$ ($H_2O@C_{60}$) 738.0113; Found 738.0140. (These data matched well the reported ones.[2])

H_2O@**2a**: ^{1}H NMR (500 MHz, CS_2/CD_2Cl_2 (1:1) δ 7.78 (t, J = 7.6 Hz, 2H), 7.65 (d, J = 7.6 Hz, 2H), 7.51–7.42 (m, 3H), 7.34 (d, J = 7.6 Hz, 2H), 7.27 (d, J = 7.6 Hz, 2H), 7.03 (s, 2H), 5.60 (s, 2H), 1.34 (s, 19H), –8.28 (s, 2H); ^{13}C NMR (126 MHz, CS_2/CD_2Cl_2 (1:1)) δ 175.97, 169.28, 164.62, 147.91, 147.84, 147.37, 147.34, 147.20, 146.49, 146.23, 145.84, 145.70, 145.67, 145.58, 145.33, 145.28, 145.22, 142.88, 142.60, 141.35, 141.33, 140.13, 139.91, 138.96, 138.43, 137.93, 137.70, 137.58, 137.29, 135.58, 135.00, 132.47, 132.35, 131.71, 131.22, 130.17, 129.60, 129.47, 127.09, 120.63, 117.68, 58.24, 38.03, 30.07 (The sum of carbon signals must be 47 in theory. Observed 44. One sp^3 and two sp^2 carbon signals are overlapped.); HRMS (APCI) *m*/*z*: $[M]^{\bullet-}$ Calcd for $C_{92}H_{35}N_3O_3$ (H_2O@**2a**) 1229.2684; Found 1229.2653.

H_2O@**3**: ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ (1:1)) δ 8.17 (d, 2H, J = 7.5 Hz), 8.03 (d, 2H, J = 8.0 Hz), 7.87 (dd, 2H, J = 7.5, 8.0 Hz), –7.50 (s, 2H); HRMS (APCI) *m*/*z*: $[M]^{\bullet-}$ Calcd for $C_{70}H_8O$ (H_2O@**3**) 864.0581; Found 864.0569. (These data matched well the reported ones.[2])

H_2O@**4a**: ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ (1:1)) δ 7.68 (t, 2H, J = 7.5 Hz), 7.51 (d, 2H, J = 7.5 Hz), 7.27 (d, 2H, J = 7.5 Hz), 7.05 (s, 2H), 6.70 (s, 2H), 1.41 (s, 18H), –8.22 (s, 2H); HRMS (APCI) *m*/*z*: $[M]^{\bullet-}$ Calcd for $C_{82}H_{30}N_2O$ (H_2O@**4a**) 1058.2365; Found 1058.2373. (These data matched well the reported ones.[2])

H_2O@**5a**: ^{1}H NMR (500 MHz, $CDCl_3/CS_2$ (1:1)) δ 7.94 (t, 2H, J = 8.0 Hz), 7.89 (d, 1H, J = 6.9 Hz), 7.80 (t, 1H, J = 8.0 Hz), 7.73 (d, 1H, J = 6.9 Hz), 7.68 (t, 1H, J = 8.0 Hz), 7.58 (t, 1H, J = 8.0 Hz), 7.53 (t, 1H, J = 8.0 Hz), 7.34 (d, 1H, J = 7.5 Hz), 7.29 (d, 1H, J = 7.5 Hz), 7.19 (d, 1H, J = 8.0 Hz), 7.06 (d, 1H, J = 8.0 Hz), 6.48 (d, 1H, J = 3.4 Hz), 6.48 (d, 1H, J = 9.7 Hz), 6.24 (d, 1H, J = 9.7 Hz), 5.75 (d, 1H, J = 3.4 Hz), 1.35 (s, 9H), 0.87 (s, 9H), –10.2 (s, 2H); HRMS (APCI) *m*/*z*: $[M]^{\bullet-}$ Calcd for $C_{94}H_{34}N_2O$ (H_2O@**5a**)

1185.2867; Found 1184.2846. (These data matched well the reported ones.[2])

7a: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (s, 2H), 7.76 (d, J = 7.7 Hz, 2H), 7.72 (t, J = 7.7 Hz, 2H), 7.50–7.35 (m, 7H), 1.46 (s, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.05, 166.50, 151.96, 140.26, 136.95, 135.58, 131.62, 128.88, 127.97, 127.76, 126.86, 122.63, 118.50, 37.62, 30.18 (The sum of carbon signals must be 15 in theory. Observed 15.); HRMS (APCI) m/z: $[M]^{\bullet-}$ Calcd for $C_{32}H_{31}N_3O_2$ (**7a**) 489.2422; Found 489.2431.

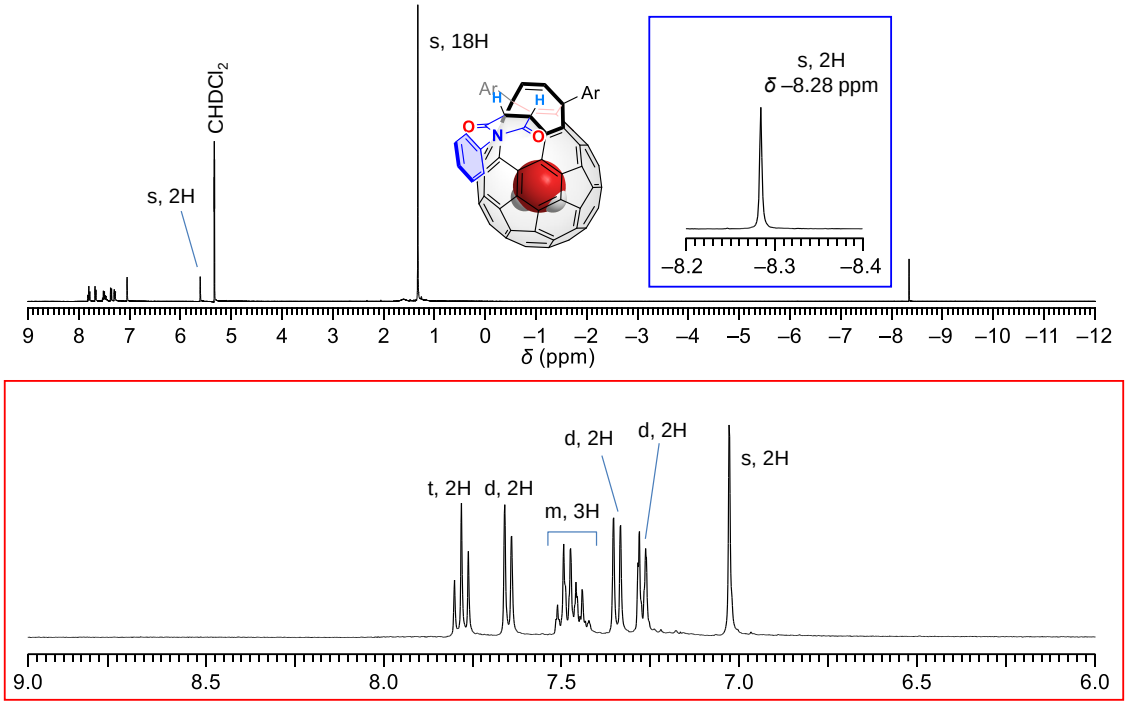


Figure S7. ^{1}H NMR spectra (500 MHz, CS_2/CD_2Cl_2 (1:1)) of H_2O@**2a**.

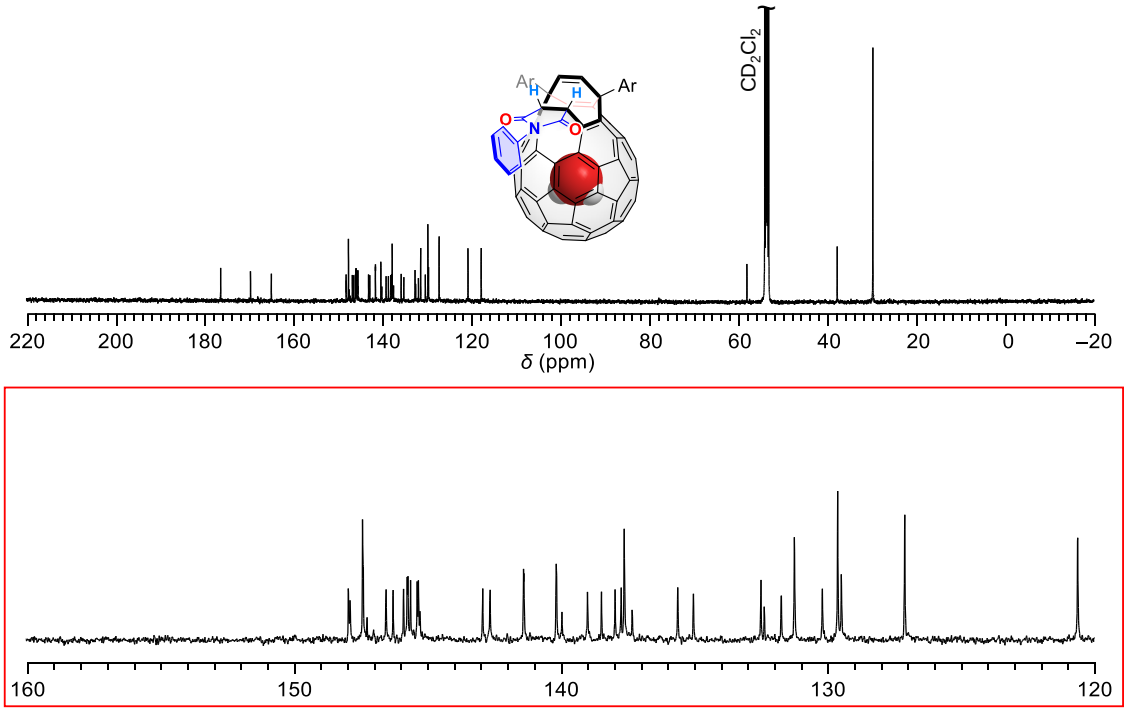


Figure S8. ^{13}C NMR spectra (126 MHz, CS_2/CD_2Cl_2 (1:1)) of H_2O@**2a**.

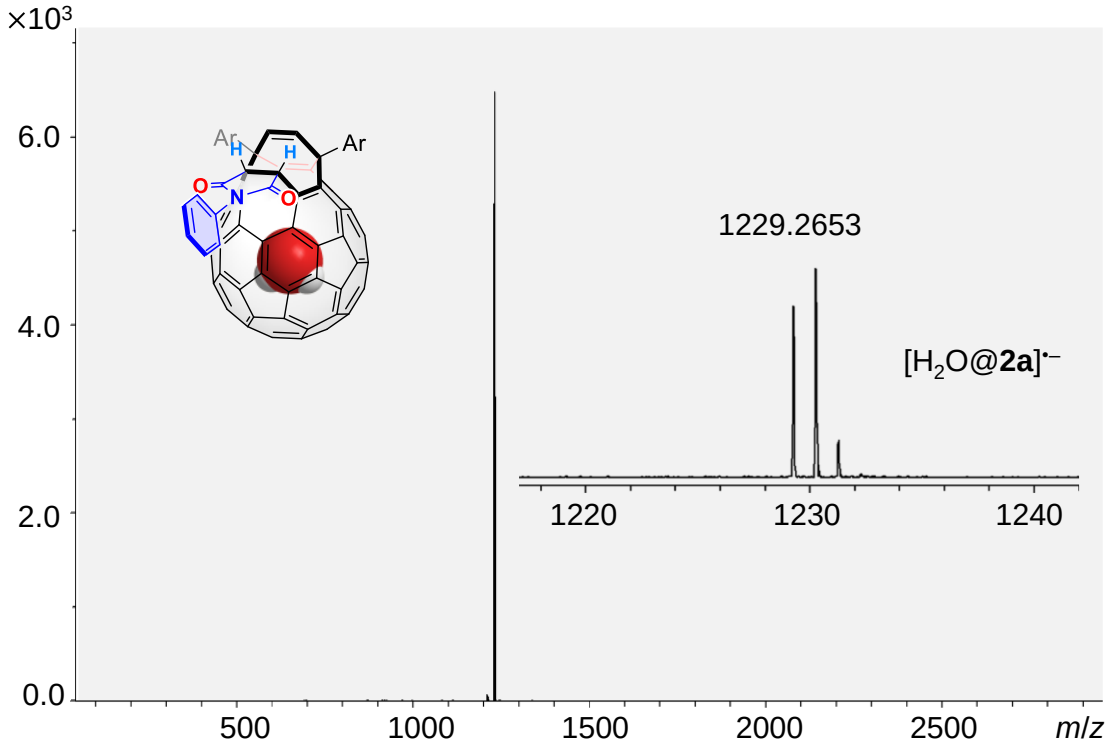


Figure S9. APCI mass spectrum (negative ion mode) of H_2O@**2a**.

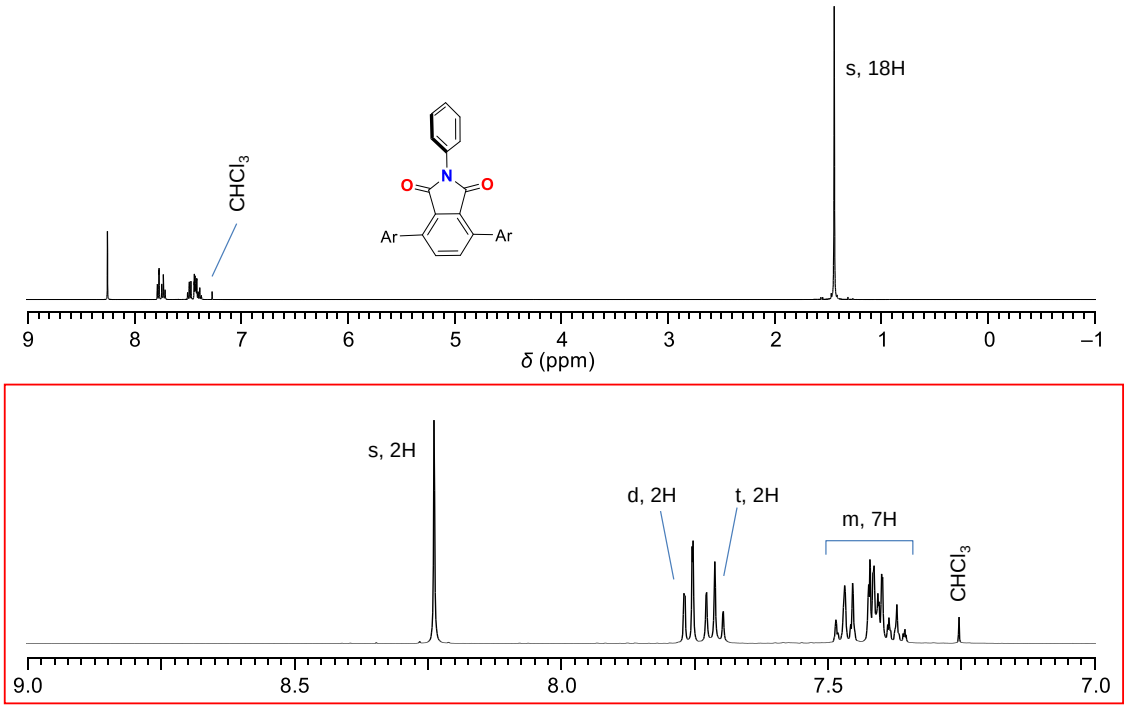


Figure S10. ^{1}H NMR spectra (500 MHz, $CDCl_3$) of **7a**.

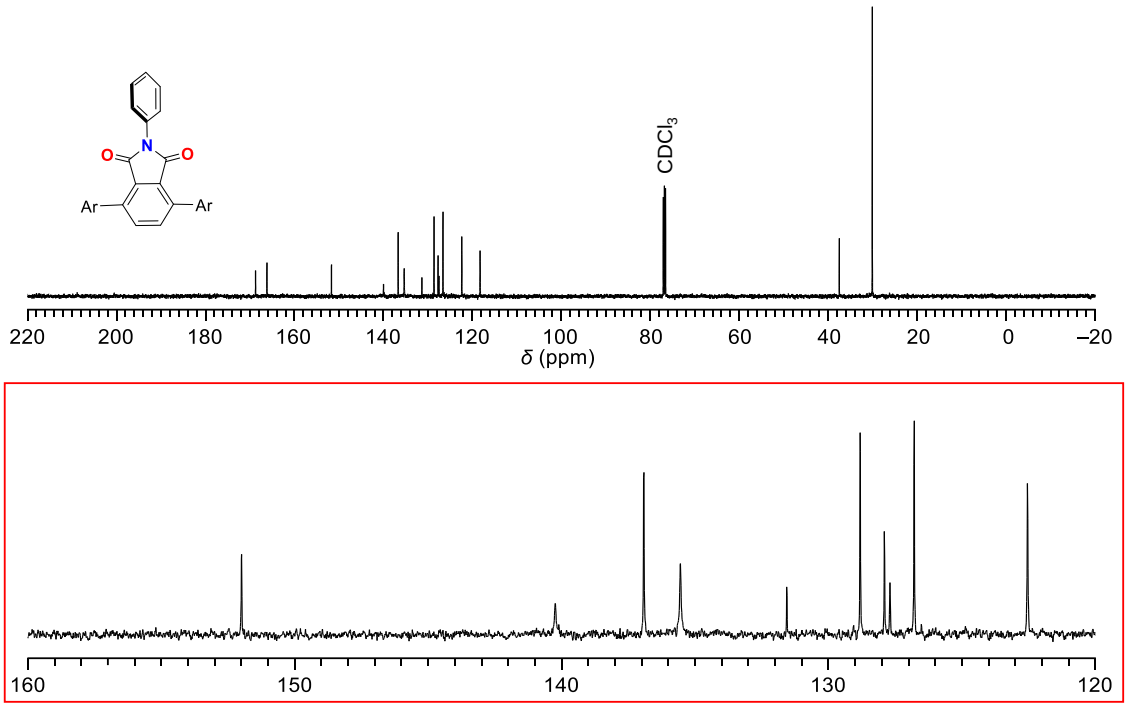


Figure S11. ^{13}C NMR spectra (126 MHz, $CDCl_3$) of **7a**.

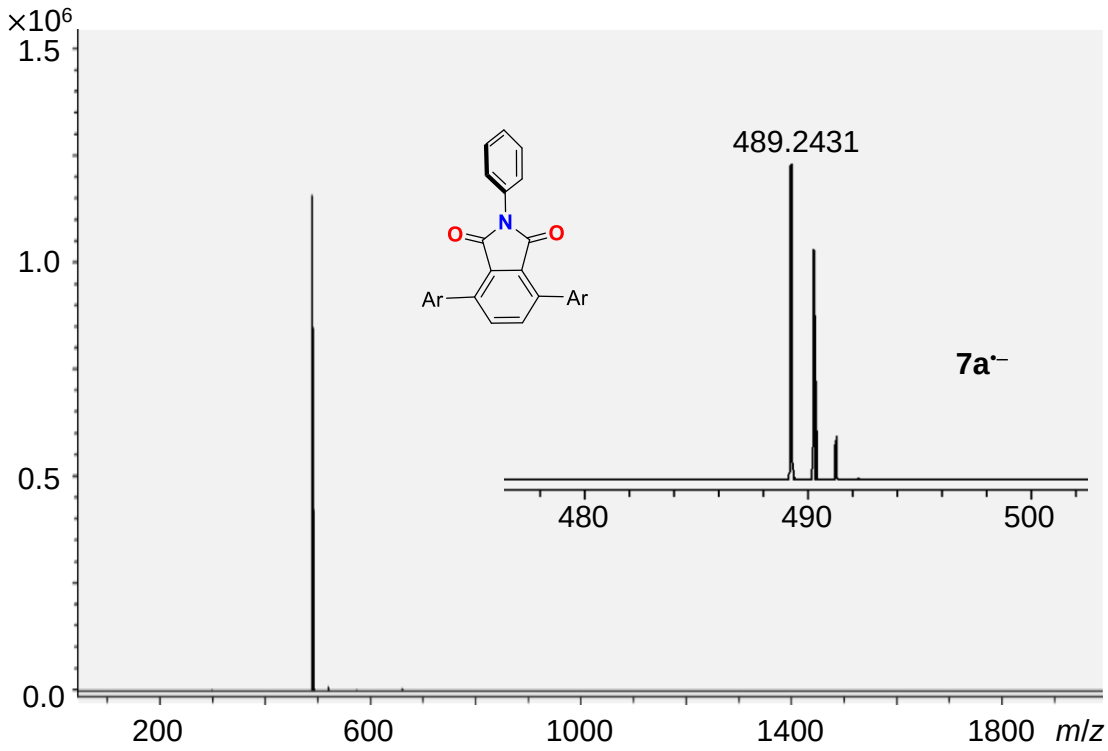
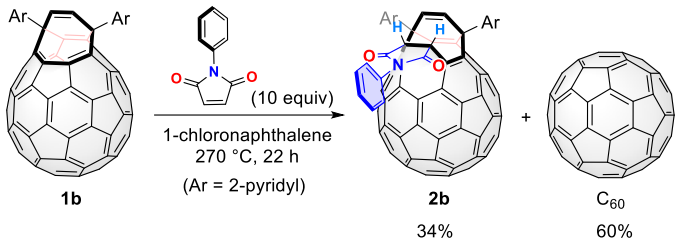


Figure S12. APCI mass spectrum (negative ion mode) of **7a**.

3.3. Synthesis of 2b



Powdery **1b** (20.0 mg, 21.6 μmol) and *N*-phenylmaleimide (37.4 mg, 216 μmol, 10.0 equiv) were placed into a 20-mL Schlenk tube and degassed through five vacuum-Ar cycles. 1-Chloronaphthalene (1.08 mL) was added and the resulting solution was heated at 270 °C for 22 h (sand bath). The crude mixture was purified by column chromatography using silica gel (CS_2 to CS_2/acetone (5:1)) to give $H_2O@C_{60}$ (9.33 mg, 12.9 μmol, 60%) followed by **2b** (8.12 mg, 7.38 μmol, 34%) as black powders.

2b: ^{1}H NMR (800 MHz, CS_2/CD_2Cl_2 (1:1)) δ 8.77 (dt, J = 1.4, 5.2 Hz, 2H), 7.90–7.86 (m, 4H), 7.52–7.44 (m, 3H), 7.39–7.35 (m, 2H), 7.28-7.24 (m, 2H), 6.96 (s, 2H), 5.52 (s, 2H); ^{13}C NMR (201 MHz, CS_2/CD_2Cl_2 (1:1)) δ 175.44, 166.41, 150.18, 147.60, 147.52, 147.29, 147.06, 147.03, 146.17, 145.93, 145.68, 145.66, 145.52, 145.44, 145.20, 145.19, 145.02, 142.92, 142.59, 141.23, 141.19, 140.50, 140.09, 139.82, 139.34, 138.29, 138.00, 137.77, 137.32, 137.08, 135.50, 134.39, 132.65, 132.25, 131.48, 131.00, 130.44, 129.57, 129.47, 127.06, 126.90, 124.00, 122.85, 79.44, 58.02 (The sum of carbon signals must be 45 in theory. Observed 45.); HRMS (APCI) *m*/*z*: $[M]^+$ Calcd for $C_{84}H_{18}N_3O_2$ (**2b**+H) 1100.1394; Found 1100.1446.

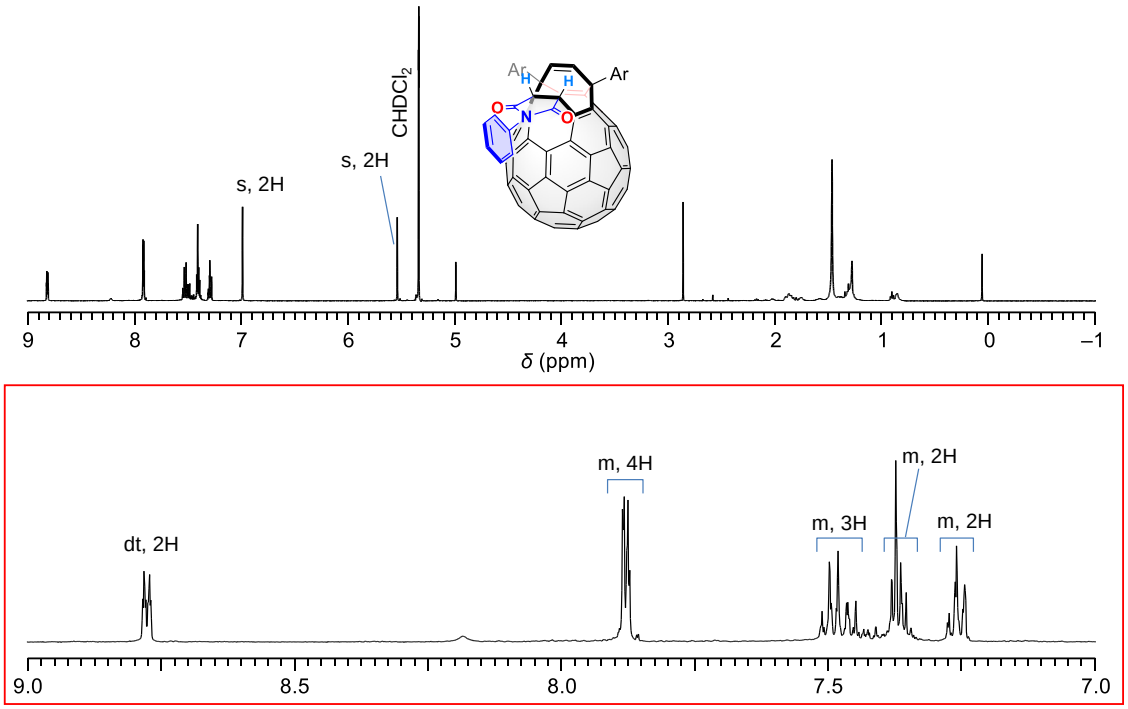


Figure S13. ^{1}H NMR spectra (800 MHz, CS_2/CD_2Cl_2 (1:1)) of **2b**.

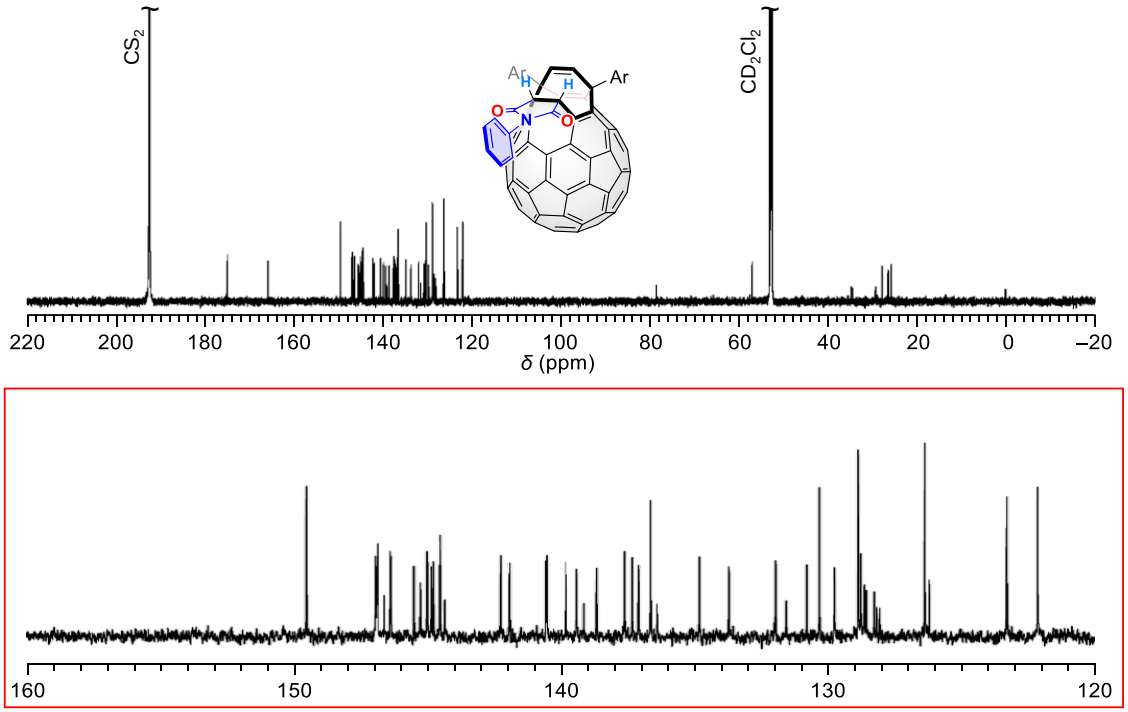


Figure S14. ^{13}C NMR spectra (201 MHz, CS_2/CD_2Cl_2 (1:1)) of **2b**.

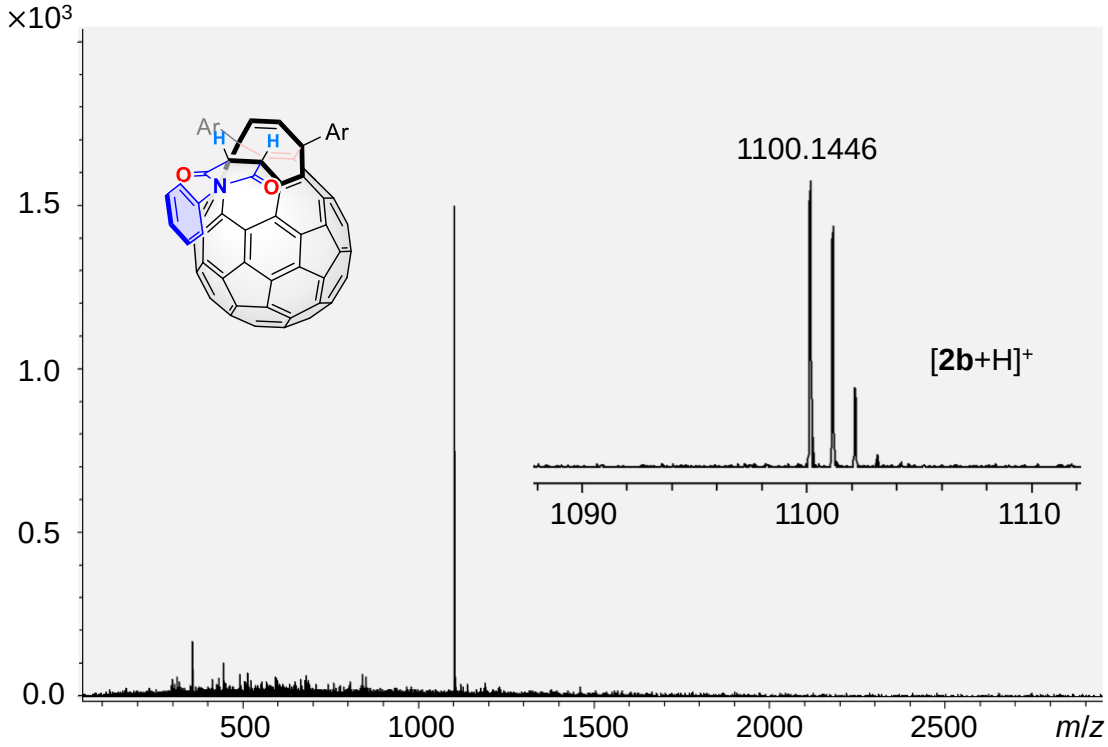


Figure S15. APCI mass spectrum (positive ion mode) of **2b**.

4. Single Crystal X-Ray-Structures

4.1. Crystal Structure of $[(H_2O)_{0.645(8)}@\mathbf{1a}]_{0.5}$•(toluene)

Single crystals of $H_2O@\mathbf{1a}$ were obtained from a toluene 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 monochromater. A total of 13832 reflections were measured at the maximum 2θ angle of 50.00°, of which 5149 were independent reflections (R_{int} = 0.0257). The structure was solved by direct methods (SHELXT-2014/5[3]) and refined by the full-matrix least-squares on F^2 (SHELXL-2018/3[3]). All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed using AFIX instructions except for the encapsulated H_2O molecule. The two toluene molecules are disordered on a special position. Thus, (C44 to C50) and (C51 to C57) were placed and their occupancies were refined to be 0.50. The *t*-butyl group (C41 to C43) was refined using the SIMU instruction. The occupancy of the encapsulated H_2O molecule was refined to be 0.645(8). The crystal data are as follows: $C_{48}H_{21.65}NO_{0.32}$; FW = 617.47, crystal size 0.33 × 0.24 × 0.13 mm^3, monoclinic, $P2_1/n$, a = 11.7831(12) Å, b = 16.8231(17) Å, c = 14.2431(14) Å, β = 94.160(2)°, V = 2815.9(5) Å^3, Z = 4, D_c = 1.456 g cm^{-3}. The refinement converged to R_1 = 0.0426, wR_2 = 0.1135 ($I > 2\sigma(I)$), GOF = 1.070. The data was deposited at the Cambridge Crystallographic Data Centre (CCDC 2190896).

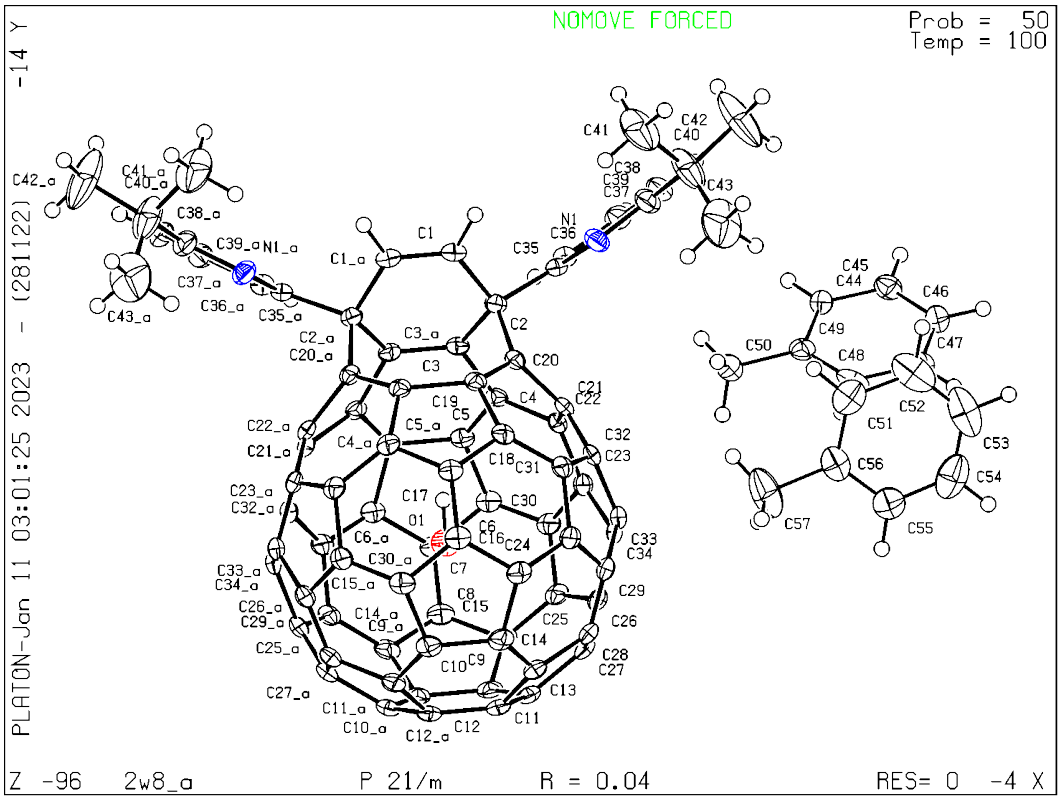


Figure S16. Single crystal X-ray structure of $[(H_2O)_{0.645(8)}@\mathbf{1a}]_{0.5}$•(toluene). Thermal ellipsoids are shown at 50% probability.

4.2. Crystal Structure of $(7a)_2$

Single crystals of **7a** were obtained from a CS_2/hexane 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 monochromater. A total of 26065 reflections were measured at the maximum 2θ angle of 49.98°, of which 9562 were independent reflections (R_{int} = 0.0484). The structure was solved by direct methods (SHELXT-2014/5[3]) and refined by the full-matrix least-squares on F^2 (SHELXL-2018/3[3]). All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed using AFIX instructions. The crystal data are as follows: $C_{32}H_{31}N_3O_2$; FW = 489.60, crystal size 0.48 × 0.15 × 0.08 mm^3, monoclinic, $P2_2/c$, a = 23.689(3) Å, b = 19.477(3) Å, c = 11.8763(15) Å, β = 98.836(2)°, V = 5414.5(12) Å^3, Z = 8, D_c = 1.201 g cm^{-3}. The refinement converged to R_1 = 0.0503, wR_2 = 0.1396 ($I > 2\sigma(I)$), GOF = 1.021. The data was deposited at the Cambridge Crystallographic Data Centre (CCDC 2190897).

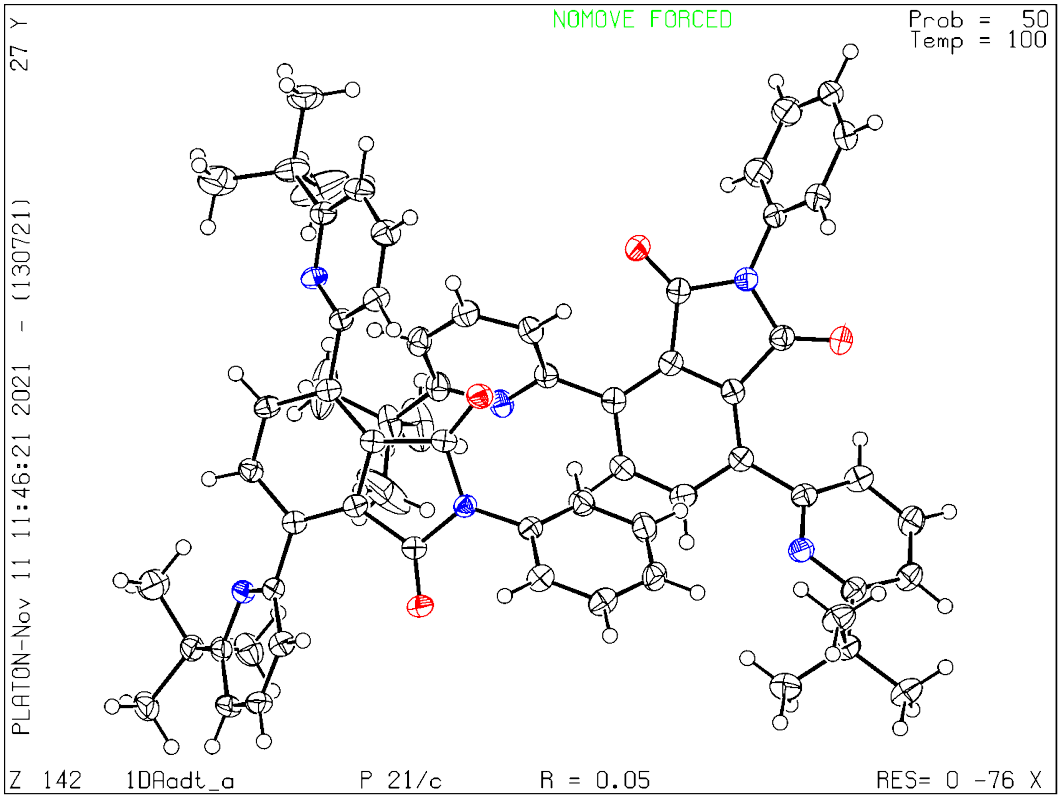


Figure S17. Single crystal X-ray structure of $(\mathbf{7a})_2$. Thermal ellipsoids are shown at 50% probability.

5. DFT Calculations

5.1. Reaction Mechanism

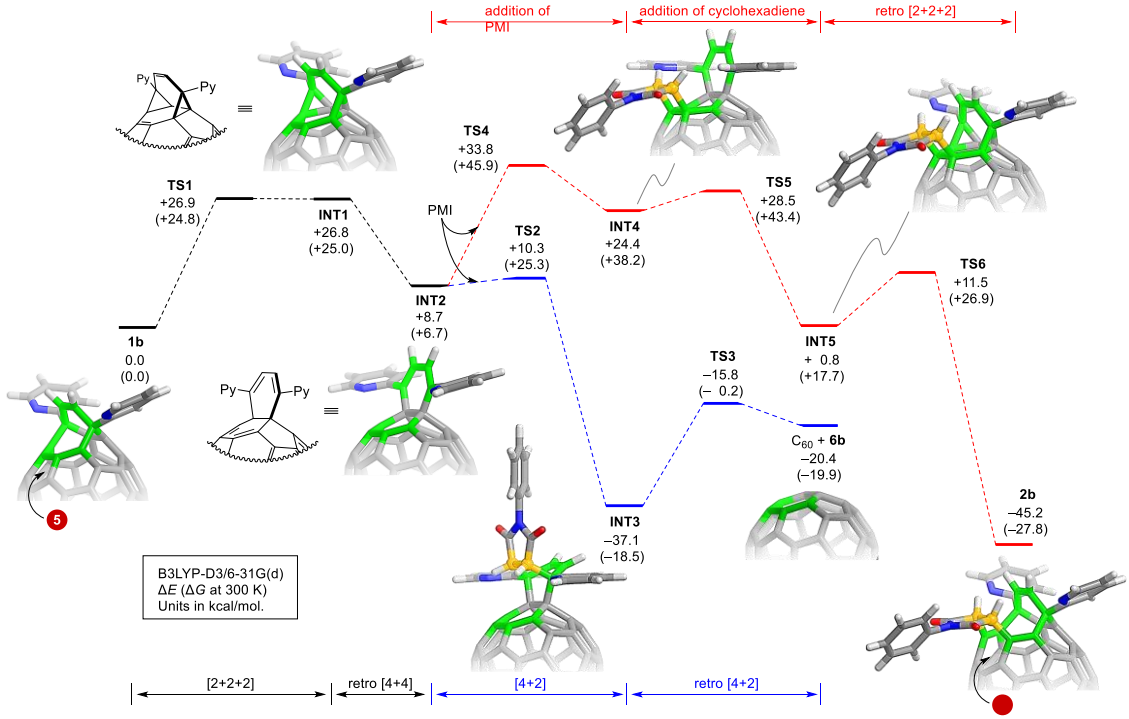
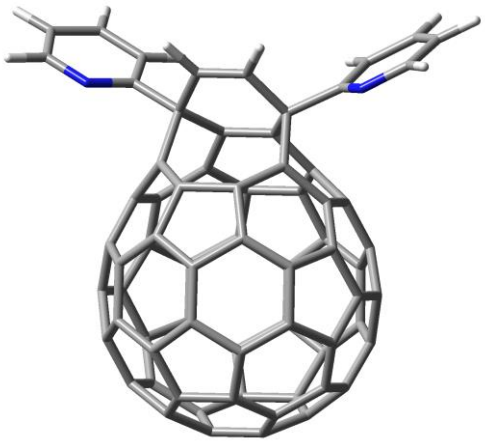


Figure S18. Plausible reaction profile on a conversion of **1b** into C_{60} (blue line) and **2b** (red line), calculated at the B3LYP-D3/6-31G(d) level of theory. Relative energies ΔE were given in kcal/mol. The values in parentheses represent ΔG (kcal/mol) at 298 K. The values in red circles indicate the ring size.

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



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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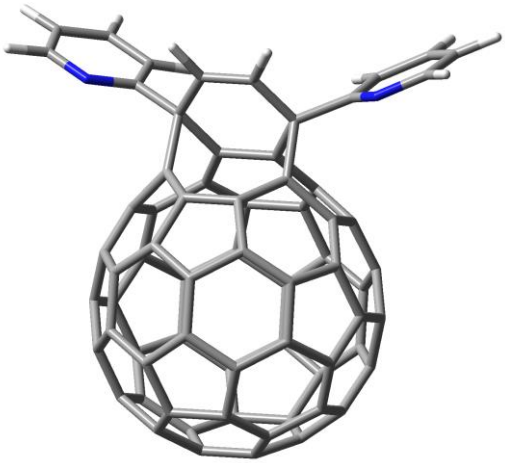
2	6	0	4.279398	0.662935	-1.254046
3	6	0	3.265124	1.446186	-0.460872
4	6	0	1.969066	1.646545	-1.249622
5	6	0	1.465536	0.759460	-2.211025
6	6	0	1.465536	-0.759460	-2.211025
7	6	0	0.243270	-1.153731	-2.893688
8	6	0	-0.473319	-2.291918	-2.536191
9	6	0	-0.093380	-2.989429	-1.329975
10	6	0	1.036439	-2.577650	-0.618833
11	6	0	1.969066	-1.646546	-1.249622
12	6	0	3.265124	-1.446185	-0.460871
13	6	0	2.668582	-0.691899	0.711954
14	6	0	2.668582	0.691900	0.711954
15	6	0	1.689879	1.417138	1.488123
16	6	0	0.956944	2.521024	0.853825
17	6	0	1.036439	2.577650	-0.618834
18	6	0	-0.093380	2.989429	-1.329975
19	6	0	-0.473320	2.291917	-2.536191
20	6	0	0.243269	1.153730	-2.893688
21	6	0	-0.464956	-0.000000	-3.379465
22	6	0	-1.853021	-0.000001	-3.503909
23	6	0	-2.603746	-1.176859	-3.106334
24	6	0	-1.923895	-2.299682	-2.631259
25	6	0	-2.439143	-3.019876	-1.481146
26	6	0	-1.300608	-3.438681	-0.682087
27	6	0	-1.368773	-3.433392	0.703031
28	6	0	-0.233792	-2.956889	1.472412
29	6	0	0.956944	-2.521023	0.853826
30	6	0	1.689880	-1.417137	1.488123
31	6	0	1.096935	-0.725838	2.548522
32	6	0	1.096935	0.725839	2.548522
33	6	0	-0.132833	1.166254	3.157194
34	6	0	-0.777940	2.281598	2.642333
35	6	0	-0.233792	2.956889	1.472411
36	6	0	-1.368773	3.433392	0.703030
37	6	0	-1.300609	3.438680	-0.682088
38	6	0	-2.439143	3.019875	-1.481147
39	6	0	-1.923895	2.299681	-2.631260
40	6	0	-2.603746	1.176857	-3.106335
41	6	0	-3.818003	0.727638	-2.448523
42	6	0	-3.818003	-0.727639	-2.448523
43	6	0	-4.314006	-1.425214	-1.344475
44	6	0	-3.610443	-2.598483	-0.853030
45	6	0	-3.689907	-2.597007	0.599253
46	6	0	-2.596495	-3.015517	1.360240
47	6	0	-2.229053	-2.296429	2.562193
48	6	0	-0.777939	-2.281597	2.642334
49	6	0	-0.132833	-1.166253	3.157195
50	6	0	-0.893006	0.000000	3.565333
51	6	0	-2.280601	0.000000	3.467710
52	6	0	-2.966255	1.177384	2.961342
53	6	0	-2.229053	2.296429	2.562192
54	6	0	-2.596495	3.015517	1.360239
55	6	0	-3.689908	2.597007	0.599252
56	6	0	-4.447125	1.425273	1.004841
57	6	0	-4.091354	0.728156	2.160501
58	6	0	-4.091354	-0.728156	2.160501
59	6	0	-2.966255	-1.177384	2.961342
60	6	0	-4.447125	-1.425273	1.004842
61	6	0	-4.827020	-0.697985	-0.196379
62	6	0	-4.827020	0.697984	-0.196379
63	6	0	-4.314007	1.425214	-1.344476
64	6	0	-3.610443	2.598483	-0.853031
65	6	0	3.908443	-2.788038	-0.089491
66	6	0	4.480399	-3.011269	1.166010
67	6	0	5.107405	-4.232683	1.407647
68	6	0	5.145982	-5.183543	0.388940
69	6	0	4.561058	-4.857780	-0.835936
70	6	0	3.908443	2.788038	-0.089491
71	6	0	4.480400	3.011268	1.166010
72	6	0	5.107406	4.232682	1.407647
73	6	0	5.145982	5.183543	0.388941
74	6	0	4.561056	4.857781	-0.835935
75	7	0	3.958458	3.689356	-1.079780
76	7	0	3.958460	-3.689354	-1.079780
77	1	0	4.964725	-1.240793	-1.866035
78	1	0	4.964725	1.240793	-1.866036
79	1	0	4.425468	-2.248294	1.935213
80	1	0	5.555616	-4.437174	2.376185
81	1	0	5.618662	-6.150161	0.533723
82	1	0	4.576856	-5.566375	-1.662319
83	1	0	4.425470	2.248292	1.935211
84	1	0	5.555618	4.437173	2.376184
85	1	0	5.618662	6.150161	0.533724
86	1	0	4.576853	5.566378	-1.662317

The total electronic energy was calculated to be –2935.3108853 Hartree.

Table S2. Optimized structure of **TS1** (B3LYP-D3/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	6	0	1.004324	2.600605	-0.601046
5	6	0	2.428327	0.735778	0.301590
6	6	0	1.392672	-0.698510	-2.175454
7	6	0	-0.495749	-2.283596	-2.545502
8	6	0	1.634468	1.430988	1.348555
9	6	0	-2.444428	-3.016285	-1.461603
10	6	0	-0.097586	-3.008222	-1.331175
11	6	0	0.209084	-1.154225	-2.919577
12	6	0	1.936005	1.551044	-1.120660
13	6	0	3.976232	2.799171	-0.127180
14	6	0	1.133577	0.736618	2.431109
15	6	0	-1.893472	-0.000002	-3.504002
16	6	0	-0.498770	-0.000001	-3.416415
17	6	0	3.360704	1.502783	-0.596277
18	6	0	0.918263	2.576542	0.840019
19	6	0	-0.244879	3.024785	1.491588
20	6	0	3.360706	-1.502780	-0.596275
21	6	0	1.392671	0.698510	-2.175454
22	6	0	1.133578	-0.736615	2.431110
23	6	0	1.936006	-1.551042	-1.120658
24	6	0	0.209083	1.154224	-2.919577
25	6	0	4.313263	0.667518	-1.394473
26	6	0	-1.304408	3.455340	-0.674557
27	6	0	4.448053	2.950487	1.179610
28	6	0	-1.378806	3.478495	0.719353
29	6	0	-0.076348	-1.174271	3.093824
30	6	0	3.976236	-2.799167	-0.127179
31	6	0	1.004327	-2.600604	-0.601044
32	6	0	-0.244876	-3.024785	1.491589
33	6	0	-3.843046	-0.728394	-2.416580
34	6	0	-0.750716	-2.309626	2.645136
35	6	0	0.918265	-2.576541	0.840020
36	6	0	-4.321964	-1.425029	-1.307838
37	6	0	-1.944329	2.293412	-2.617425
38	6	0	-0.076349	1.174272	3.093823
39	6	0	-1.304404	-3.455342	-0.674555
40	6	0	-3.682894	2.599860	0.630335
41	6	0	-2.919281	1.177852	2.977106
42	6	0	-0.821457	0.000001	3.509442
43	6	0	-3.611509	2.597151	-0.822748
44	6	0	-2.635901	1.174041	-3.092047
45	6	0	-3.611507	-2.597155	-0.822746
46	6	0	-3.843047	0.728389	-2.416581
47	6	0	-2.592746	-3.034946	1.384468
48	6	0	-4.430986	-1.424375	1.042279
49	6	0	-4.056467	0.725771	2.194252
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54	6	0	-4.823215	0.698126	-0.150806
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56	6	0	-4.056467	-0.725773	2.194253
57	6	0	5.156135	-5.162211	0.578237
58	6	0	-4.823214	-0.698131	-0.150806
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63	6	0	-1.944326	-2.293415	-2.617423
64	6	0	-0.750718	2.309627	2.645135
65	6	0	-2.635900	-1.174045	-3.092047
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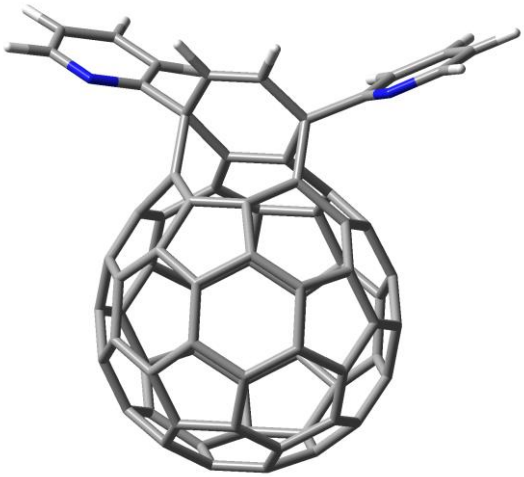
67	6	0	-2.202457	2.308410	2.582288
68	6	0	-2.444431	3.016282	-1.461604
69	6	0	-3.682891	-2.599863	0.630336
70	6	0	-2.919280	-1.177853	2.977107
71	6	0	5.047042	4.157065	1.538097
72	6	0	-2.592748	3.034944	1.384466
73	6	0	4.448045	-2.950490	1.179614
74	6	0	-2.214589	-0.000000	3.457568
75	6	0	-1.378803	-3.478496	0.719355
76	6	0	-2.202455	-2.308410	2.582290
77	1	0	5.013684	-1.223528	-2.010878
78	1	0	5.013683	1.223532	-2.010879
79	1	0	4.333815	2.142688	1.895132
80	1	0	4.733370	-5.665363	-1.482100
81	1	0	5.610938	6.120085	0.811591
82	1	0	4.733340	5.665379	-1.482090
83	1	0	5.610948	-6.120080	0.811587
84	1	0	5.418724	-4.308964	2.547756
85	1	0	5.418739	4.308958	2.547751
86	1	0	4.333797	-2.142695	1.895140

The total electronic energy was calculated to be –2935.2680429 Hartree.

The imaginary frequency was found at –294.67 cm^{-1}.

Table S3. Optimized structure of **INT1** (B3LYP-D3/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	7	0	-4.104856	-3.756847	-1.061037
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5	6	0	-2.398857	-0.744132	0.262988
6	6	0	-1.386501	0.693503	-2.174541
7	6	0	0.494127	2.282334	-2.547299
8	6	0	-1.631012	-1.432318	1.343513
9	6	0	2.441630	3.015831	-1.461608
10	6	0	0.095388	3.009938	-1.330867
11	6	0	-0.211247	1.155790	-2.928571
12	6	0	-1.929033	-1.532452	-1.095544
13	6	0	-3.982142	-2.801409	-0.128553
14	6	0	-1.137230	-0.737787	2.427681
15	6	0	1.892359	-0.000001	-3.507445
16	6	0	0.496831	-0.000001	-3.425711
17	6	0	-3.373722	-1.506716	-0.603530
18	6	0	-0.914144	-2.579019	0.842664
19	6	0	0.246802	-3.029783	1.495335
20	6	0	-3.373723	1.506717	-0.603530
21	6	0	-1.386501	-0.693503	-2.174541
22	6	0	-1.137230	0.737788	2.427680
23	6	0	-1.929032	1.532451	-1.095544
24	6	0	-0.211247	-1.155791	-2.928571
25	6	0	-4.320007	-0.668190	-1.401037
26	6	0	1.302429	-3.456933	-0.674513
27	6	0	-4.432561	-2.956376	1.185609
28	6	0	1.379033	-3.481713	0.720547
29	6	0	0.072718	1.175153	3.091883
30	6	0	-3.982141	2.801410	-0.128554
31	6	0	-1.001034	2.600360	-0.595935
32	6	0	0.246803	3.029783	1.495334
33	6	0	3.840890	0.728436	-2.417199
34	6	0	0.749990	2.311813	2.647125
35	6	0	-0.914144	2.579019	0.842663
36	6	0	4.319230	1.424799	-1.308219
37	6	0	1.941886	-2.292856	-2.617862
38	6	0	0.072718	-1.175153	3.091883
39	6	0	1.302430	3.456932	-0.674513
40	6	0	3.681296	-2.599926	0.630175
41	6	0	2.917004	-1.177660	2.976695
42	6	0	0.817406	0.000000	3.506450
43	6	0	3.608829	-2.596808	-0.822893
44	6	0	2.634064	-1.173560	-3.093204
45	6	0	3.608830	2.596806	-0.822893
46	6	0	3.840890	-0.728438	-2.417199
47	6	0	2.592059	3.036296	1.384899
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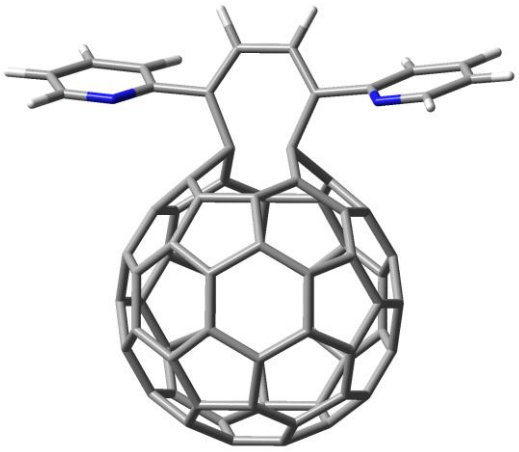
49	6	0	4.053983	-0.725584	2.194041
50	6	0	-4.676013	4.910104	-0.697354
51	6	0	-5.147239	-5.167918	0.591929
52	6	0	4.319230	-1.424801	-1.308219
53	6	0	4.428857	-1.424343	1.041765
54	6	0	4.820776	-0.698156	-0.151055
55	6	0	-4.676016	-4.910102	-0.697352
56	6	0	4.053983	0.725583	2.194041
57	6	0	-5.147234	5.167921	0.591928
58	6	0	4.820776	0.698155	-0.151055
59	6	0	-5.023517	4.164620	1.551830
60	6	0	0.494127	-2.282335	-2.547298
61	6	0	-2.398857	0.744133	0.262987
62	6	0	-1.631012	1.432318	1.343513
63	6	0	1.941887	2.292855	-2.617862
64	6	0	0.749990	-2.311813	2.647126
65	6	0	2.634064	1.173558	-3.093204
66	6	0	0.095387	-3.009938	-1.330867
67	6	0	2.201193	-2.309203	2.583267
68	6	0	2.441629	-3.015832	-1.461608
69	6	0	3.681296	2.599926	0.630174
70	6	0	2.917004	1.177659	2.976694
71	6	0	-5.023524	-4.164615	1.551829
72	6	0	2.592058	-3.036297	1.384900
73	6	0	-4.432556	2.956380	1.185609
74	6	0	2.211099	-0.000000	3.455723
75	6	0	1.379034	3.481712	0.720546
76	6	0	2.201193	2.309202	2.583267
77	1	0	-5.024765	1.221367	-2.015241
78	1	0	-5.024765	-1.221367	-2.015241
79	1	0	-4.308349	-2.149731	1.900680
80	1	0	-4.758339	5.666336	-1.476161
81	1	0	-5.596916	-6.126861	0.830789
82	1	0	-4.758340	-5.666336	-1.476159
83	1	0	-5.596909	6.126865	0.830788
84	1	0	-5.378276	4.318889	2.567202
85	1	0	-5.378286	-4.318883	2.567201
86	1	0	-4.308343	2.149735	1.900682

The total electronic energy was calculated to be –2935.2682462 Hartree.

Table S4. Optimized structure of **INT2** (B3LYP-D3/6-31G(d))

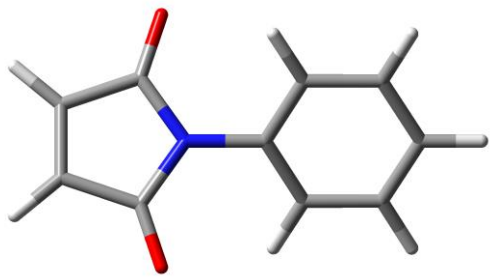


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.060827	-0.724088	0.118146
2	7	0	3.720475	-3.567679	-1.198266
3	7	0	3.721988	3.566939	-1.198383
4	6	0	0.958698	2.562446	-0.767302
5	6	0	2.535768	0.817173	-0.084489
6	6	0	1.249085	-0.740081	-2.334393
7	6	0	-0.646489	-2.312274	-2.597381
8	6	0	1.756420	1.427474	1.113415
9	6	0	-2.521280	-3.037172	-1.378359
10	6	0	-0.174754	-3.028636	-1.437618
11	6	0	0.049301	-1.175179	-3.020485
12	6	0	1.709536	1.432557	-1.241788
13	6	0	4.065669	2.938465	-0.061407
14	6	0	1.361991	0.740484	2.235657
15	6	0	-2.083412	0.000150	-3.434665
16	6	0	-0.687420	0.000012	-3.446267
17	6	0	3.944044	1.450460	-0.031632
18	6	0	0.996510	2.565784	0.679920
19	6	0	-0.102842	3.029562	1.410827
20	6	0	3.943655	-1.451299	-0.031589
21	6	0	1.249237	0.739770	-2.334425
22	6	0	1.361837	-0.740625	2.235686
23	6	0	1.709236	-1.432911	-1.241724
24	6	0	0.049535	1.175075	-3.020533
25	6	0	5.061015	0.722941	0.118140
26	6	0	-1.328264	3.484423	-0.679714
27	6	0	4.549770	3.625578	1.061116
28	6	0	-1.293793	3.488172	0.714015
29	6	0	0.201795	-1.176117	2.983793
30	6	0	4.064791	-2.939339	-0.061409
31	6	0	0.958195	-2.562646	-0.767198
32	6	0	-0.103445	-3.029454	1.410953
33	6	0	-3.957641	-0.727653	-2.220434
34	6	0	-0.514743	-2.313045	2.592831
35	6	0	0.995997	-2.565924	0.680026
36	6	0	-4.364593	-1.425623	-1.081364
37	6	0	-2.096884	2.310078	-2.565304
38	6	0	0.202030	1.176235	2.983744
39	6	0	-1.328954	-3.484161	-0.679570
40	6	0	-3.594237	2.604772	0.802467
41	6	0	-2.648249	1.177875	3.079824
42	6	0	-0.511873	0.000139	3.447058
43	6	0	-3.631099	2.604325	-0.651503
44	6	0	-2.802958	1.177086	-2.974950
45	6	0	-3.631615	-2.603606	-0.651396
46	6	0	-3.957497	0.728372	-2.220464
47	6	0	-2.449277	-3.039107	1.471868
48	6	0	-4.303939	-1.425306	1.269109
49	6	0	-3.839601	0.728326	2.386205
50	6	0	3.851049	-4.896979	-1.244328
51	6	0	4.326687	5.666129	-0.179990
52	6	0	-4.364311	1.426470	-1.081423
53	6	0	-4.303657	1.426240	1.269050
54	6	0	-4.780832	0.698420	0.105210
55	6	0	3.853136	4.896184	-1.244427
56	6	0	-3.839746	-0.727437	2.386235
57	6	0	4.324599	-5.667109	-0.180023
58	6	0	-4.780970	-0.697441	0.105239
59	6	0	4.681458	-5.012639	0.997768
60	6	0	-0.646031	2.312324	-2.597477
61	6	0	2.535574	-0.817643	-0.084453
62	6	0	1.756113	-1.427735	1.113469
63	6	0	-2.097341	-2.309741	-2.565208
64	6	0	-0.514283	2.313287	2.592736
65	6	0	-2.803191	-1.176626	-2.974901
66	6	0	-0.174156	3.028635	-1.437741
67	6	0	-1.965152	2.311617	2.635339
68	6	0	-2.520679	3.037642	-1.378484
69	6	0	-3.594753	-2.603999	0.802575
70	6	0	-2.648483	-1.177192	3.079873
71	6	0	4.682947	5.011519	0.997904
72	6	0	-2.448675	3.039682	1.471742
73	6	0	4.548874	-3.626642	1.061006
74	6	0	-1.905932	0.000277	3.502415
75	6	0	-1.294484	-3.487857	0.714159
76	6	0	-1.965611	-2.311088	2.635434
77	1	0	6.016838	-1.236173	0.190174
78	1	0	6.017163	1.234770	0.190169
79	1	0	4.798790	3.075274	1.962593
80	1	0	3.561681	-5.369244	-2.181590
81	1	0	4.407890	6.744646	-0.275357
82	1	0	3.564239	5.368557	-2.181780
83	1	0	4.405325	-6.745661	-0.275402
84	1	0	5.048790	-5.570162	1.855129
85	1	0	5.050280	5.568895	1.855360
86	1	0	4.798346	-3.076435	1.962417

The total electronic energy was calculated to be –2935.2970318 Hartree.

Table S5. Optimized structure of *N*-phenylmaleimide (B3LYP-D3/6-31G(d))

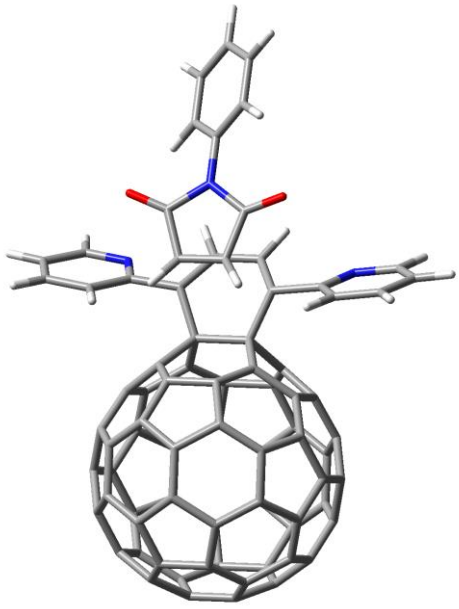


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.754769	-1.072578	-0.552401
2	6	0	1.360721	-1.075316	-0.563740
3	6	0	0.665046	0.000006	-0.000001
4	6	0	1.360729	1.075323	0.563736
5	6	0	2.754777	1.072577	0.552393
6	6	0	3.456806	-0.000003	-0.000005
7	7	0	-0.761691	0.000004	0.000005
8	6	0	-1.574406	1.129334	-0.236045
9	6	0	-2.993133	0.652875	-0.137841
10	6	0	-2.993127	-0.652895	0.137818
11	6	0	-1.574397	-1.129323	0.236108
12	8	0	-1.192636	2.255793	-0.468216
13	8	0	-1.192614	-2.255792	0.468210
14	1	0	3.291538	-1.912489	-0.984492
15	1	0	0.815145	-1.907554	-0.990692
16	1	0	0.815160	1.907566	0.990690
17	1	0	3.291552	1.912485	0.984481
18	1	0	4.543175	-0.000006	-0.000007
19	1	0	-3.824725	1.330425	-0.282379
20	1	0	-3.824714	-1.330464	0.282300

The total electronic energy was calculated to be –590.4952533 Hartree.

Table S6. Optimized structure of **TS2** (B3LYP-D3/6-31G(d))

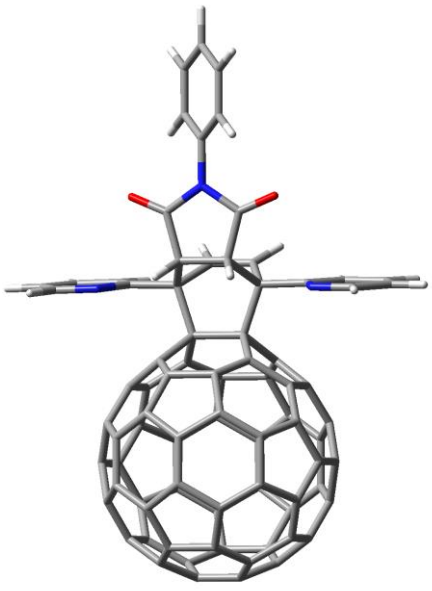


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.549385	-0.657762	1.263859
2	7	0	3.358625	-3.395977	1.509965
3	7	0	3.202440	3.449381	1.612717
4	6	0	-0.259573	2.578609	-0.593560
5	6	0	1.271930	0.834813	0.183477
6	6	0	0.171388	-0.708646	-2.165836
7	6	0	-1.680813	-2.291821	-2.585111
8	6	0	0.403560	1.428391	1.328464
9	6	0	-3.634983	-3.046900	-1.519730
10	6	0	-1.291390	-3.016109	-1.400086
11	6	0	-0.965435	-1.146712	-2.948961
12	6	0	0.531222	1.455213	-1.018612
13	6	0	2.835038	2.932835	0.425987
14	6	0	-0.069413	0.726928	2.409996
15	6	0	-3.069576	0.015457	-3.509469
16	6	0	-1.677228	0.026936	-3.420074
17	6	0	2.690593	1.434710	0.415174
18	6	0	-0.329213	2.566741	0.853221
19	6	0	-1.485915	3.012709	1.500856
20	6	0	2.717087	-1.370392	0.392793
21	6	0	0.159470	0.772089	-2.153299
22	6	0	-0.056343	-0.752759	2.396865
23	6	0	0.555143	-1.405938	-1.043759
24	6	0	-0.985577	1.204194	-2.928071
25	6	0	3.536730	0.725503	1.276435
26	6	0	-2.556263	3.480183	-0.672985
27	6	0	2.619377	3.748819	-0.693822
28	6	0	-2.625530	3.466672	0.718912
29	6	0	-1.264158	-1.205802	3.051559
30	6	0	2.911775	-2.861095	0.358456

31	6	0	-0.215601	-2.550591	-0.639933	71	6	0	2.772928	5.126293	-0.571622
32	6	0	-1.432660	-3.046104	1.445423	72	6	0	-3.830654	3.002663	1.383580
33	6	0	-5.023371	-0.739492	-2.447009	73	6	0	2.681038	-3.653715	-0.775402
34	6	0	-1.938907	-2.345559	2.598850	74	6	0	-3.415218	-0.051540	3.420733
35	6	0	-0.283803	-2.567932	0.806642	75	6	0	-2.564483	-3.505254	0.654954
36	6	0	-5.508462	-1.451753	-1.348168	76	6	0	-3.388774	-2.354294	2.530661
37	6	0	-3.170417	2.317617	-2.621673	77	1	0	4.329012	-1.198193	1.788022
38	6	0	-1.284694	1.146534	3.072713	78	1	0	4.308766	1.272560	1.805512
39	6	0	-2.495377	-3.491357	-0.736941	79	1	0	2.344822	3.323733	-1.649684
40	6	0	-4.918461	2.565361	0.625439	80	1	0	3.923466	-5.095681	2.521998
41	6	0	-4.134040	1.123825	2.954153	81	1	0	3.275165	6.727405	0.801724
42	6	0	-2.021290	-0.039830	3.470515	82	1	0	3.649794	5.139026	2.697827
43	6	0	-4.846054	2.579375	-0.827018	83	1	0	3.519158	-6.644653	0.599592
44	6	0	-3.832093	1.182334	-3.093695	84	1	0	2.722628	-5.650974	-1.573725
45	6	0	-4.800488	-2.628673	-0.874995	85	1	0	2.612975	5.769911	-1.431878
46	6	0	-5.036099	0.716185	-2.433744	86	1	0	2.355289	-3.212327	-1.707199
47	6	0	-3.777474	-3.074546	1.327779	87	8	0	5.441671	2.351434	-1.180025
48	6	0	-5.626164	-1.474912	0.999860	88	8	0	5.420990	-2.245726	-1.339620
49	6	0	-5.265662	0.671798	2.168146	89	7	0	5.738673	0.038886	-0.930134
50	6	0	3.564053	-4.713989	1.567841	90	6	0	3.629871	0.766830	-1.554408
51	6	0	3.143603	5.659035	0.660865	91	6	0	3.621899	-0.624853	-1.594834
52	6	0	-5.533389	1.399272	-1.321980	92	6	0	4.990794	-1.110496	-1.296051
53	6	0	-5.651185	1.377232	1.026175	93	6	0	8.009407	0.951248	-0.761571
54	6	0	-6.032277	0.656588	-0.176680	94	6	0	7.384735	-1.013538	0.522524
55	6	0	3.351855	4.772213	1.717123	95	6	0	9.622039	-0.106077	0.707787
56	6	0	-5.252924	-0.784037	2.154719	96	6	0	9.285665	0.897858	-0.201240
57	6	0	3.339629	-5.578955	0.496794	97	6	0	8.667724	-1.061765	1.063036
58	6	0	-6.019904	-0.739048	-0.189525	98	6	0	7.056111	-0.005416	-0.393823
59	6	0	2.893557	-5.026644	-0.701514	99	6	0	5.007604	1.216568	-1.217514
60	6	0	-1.721141	2.329510	-2.542857	100	1	0	2.967836	1.399137	-2.124857
61	6	0	1.286873	-0.795918	0.169105	101	1	0	2.941179	-1.220438	-2.182514
62	6	0	0.429351	-1.426116	1.303135	102	1	0	7.744902	1.732660	-1.461439
63	6	0	-3.130033	-2.304105	-2.664262	103	1	0	6.645669	-1.758493	0.791900
64	6	0	-1.979402	2.282440	2.641288	104	1	0	10.619914	-0.144425	1.135906
65	6	0	-3.811556	-1.172026	-3.115161	105	1	0	10.020981	1.646024	-0.484550
66	6	0	-1.344066	3.038669	-1.344862	106	1	0	8.918606	-1.848550	1.769173
67	6	0	-3.429243	2.267255	2.573217	---					
68	6	0	-3.688223	3.030107	-1.463714	The total electronic energy was calculated to be –3525.7897535 Hartree.					
69	6	0	-4.872929	-2.642647	0.577547	The imaginary frequency was found at –381.22 cm^{-1}.					
70	6	0	-4.113436	-1.230564	2.932499						

Table S7. Optimized structure of **INT3** (B3LYP-D3/6-31G(d))

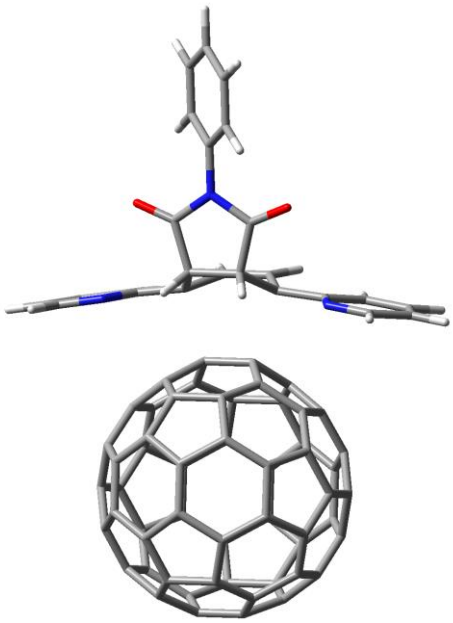


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.322832	0.708092	-1.727404
2	7	0	2.781586	3.441029	0.753527
3	7	0	2.794456	-3.448095	0.631221
4	6	0	-0.177353	-2.576765	0.512519
5	6	0	1.267769	-0.796468	-0.321490
6	6	0	0.293756	0.699370	2.100576
7	6	0	-1.553644	2.257614	2.627591
8	6	0	0.380036	-1.396279	-1.426773
9	6	0	-3.566247	2.999367	1.665810
10	6	0	-1.230161	3.000299	1.433441
11	6	0	-0.809004	1.116173	2.941991
12	6	0	0.616089	-1.445410	0.909723
13	6	0	2.813434	-2.838191	-0.562817
14	6	0	-0.156002	-0.687960	-2.476414
15	6	0	-2.871303	-0.077193	3.590322
16	6	0	-1.484535	-0.071257	3.432777
17	6	0	2.785498	-1.312218	-0.519296
18	6	0	-0.320026	-2.548624	-0.928610

19	6	0	-1.500841	-3.001136	-1.525451	64	6	0	-2.057652	-2.261579	-2.631798
20	6	0	2.780247	1.345986	-0.470167	65	6	0	-3.644312	1.105794	3.246644
21	6	0	0.296369	-0.779797	2.070340	66	6	0	-1.218915	-3.057540	1.309666
22	6	0	-0.158940	0.791565	-2.446379	67	6	0	-3.502531	-2.265064	-2.493574
23	6	0	0.612008	1.413643	0.968537	68	6	0	-3.554911	-3.075233	1.541337
24	6	0	-0.804645	-1.234944	2.893855	69	6	0	-4.900672	2.604558	-0.373103
25	6	0	3.326300	-0.627049	-1.751920	70	6	0	-4.242108	1.227875	-2.778563
26	6	0	-2.457659	-3.503683	0.691804	71	6	0	2.757776	-4.951491	-1.712813
27	6	0	2.778963	-3.558032	-1.761398	72	6	0	-3.836612	-3.018403	-1.294623
28	6	0	-2.595616	-3.477099	-0.695236	73	6	0	2.763098	3.633387	-1.633832
29	6	0	-1.402361	1.238297	-3.038694	74	6	0	-3.556087	0.062908	-3.315058
30	6	0	2.801809	2.872665	-0.460724	75	6	0	-2.608805	3.496572	-0.552515
31	6	0	-0.186338	2.556890	0.617589	76	6	0	-3.511270	2.355524	-2.399069
32	6	0	-1.512238	3.059044	-1.401206	77	8	0	5.534933	-2.288616	0.482200
33	6	0	-4.882354	0.666683	2.632498	78	8	0	5.525702	2.295553	0.553629
34	6	0	-2.066357	2.363275	-2.536967	79	7	0	5.854856	0.002658	0.582073
35	6	0	-0.329794	2.586649	-0.823379	80	6	0	3.609169	-0.771390	0.693377
36	6	0	-5.429058	1.385330	1.567243	81	6	0	3.607539	0.765126	0.721787
37	6	0	-2.988690	-2.369761	2.680968	82	6	0	5.078464	1.171475	0.616713
38	6	0	-1.397851	-1.114522	-3.086526	83	6	0	8.026101	-0.889690	1.258643
39	6	0	-2.470735	3.466394	0.834422	84	6	0	7.919350	0.874060	-0.406543
40	6	0	-4.891076	-2.602122	-0.479686	85	6	0	10.062210	-0.026059	0.274242
41	6	0	-4.237633	-1.125730	-2.826858	86	6	0	9.415647	-0.900756	1.149492
42	6	0	-2.165878	0.067981	-3.433991	87	6	0	9.310453	0.860147	-0.499357
43	6	0	-4.747758	-2.631507	0.967324	88	6	0	7.280995	-0.001315	0.477340
44	6	0	-3.639878	-1.248145	3.198665	89	6	0	5.081296	-1.169741	0.576722
45	6	0	-4.757533	2.575291	1.074014	90	1	0	3.733492	1.305873	-2.532807
46	6	0	-4.879528	-0.788820	2.602751	91	1	0	3.740853	-1.193552	-2.577701
47	6	0	-3.848113	3.058004	-1.170396	92	1	0	2.742527	-3.048965	-2.717645
48	6	0	-5.660583	1.433003	-0.772079	93	1	0	2.745621	5.184594	1.844956
49	6	0	-5.335138	-0.695874	-1.982314	94	1	0	2.750490	-6.665704	-0.386444
50	6	0	2.757669	4.771731	0.837967	95	1	0	2.763643	-5.228605	1.661651
51	6	0	2.763574	-5.583607	-0.472427	96	1	0	2.725185	6.691675	-0.152492
52	6	0	-5.423618	-1.465371	1.508938	97	1	0	2.706420	5.633783	-2.436073
53	6	0	-5.655589	-1.418240	-0.830632	98	1	0	2.731454	-5.529758	-2.632230
54	6	0	-5.985797	-0.715819	0.398033	99	1	0	2.725844	3.157651	-2.607086
55	6	0	2.775189	-4.780992	0.669555	100	1	0	3.210961	-1.219177	1.606122
56	6	0	-5.337901	0.759738	-1.952399	101	1	0	3.209700	1.178478	1.650661
57	6	0	2.742054	5.613236	-0.275698	102	1	0	7.519001	-1.571613	1.930320
58	6	0	-5.988043	0.679626	0.426594	103	1	0	7.332156	1.564492	-0.998719
59	6	0	2.736731	5.024232	-1.537173	104	1	0	11.145824	-0.034964	0.195598
60	6	0	-1.545005	-2.365578	2.533187	105	1	0	9.992648	-1.595008	1.753908
61	6	0	1.264945	0.817477	-0.289120	106	1	0	9.805862	1.544785	-1.182167
62	6	0	0.374106	1.458255	-1.368474	---					
63	6	0	-2.997283	2.250017	2.775576	The total electronic energy was calculated to be –3525.8652006 Hartree.					

Table S8. Optimized structure of **TS3** (B3LYP-D3/6-31G(d))

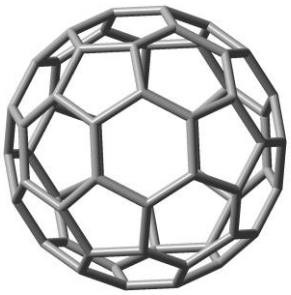


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.339849	0.729113	-1.971284
2	7	0	2.882330	3.430236	0.535681
3	7	0	2.890488	-3.438863	0.407117
4	6	0	-0.167692	-2.588346	0.424182
5	6	0	1.056125	-0.727103	-0.450124
6	6	0	0.378764	0.688196	2.008595
7	6	0	-1.433348	2.249957	2.625285
8	6	0	0.270951	-1.383857	-1.531986
9	6	0	-3.492390	2.994301	1.767504
10	6	0	-1.170087	2.999124	1.414794
11	6	0	-0.674349	1.110687	2.910463
12	6	0	0.627677	-1.436047	0.781015
13	6	0	2.919984	-2.852809	-0.804530
14	6	0	-0.312737	-0.677302	-2.567739
15	6	0	-2.703347	-0.084948	3.651668
16	6	0	-1.324741	-0.079272	3.433627
17	6	0	3.080840	-1.373825	-0.798544
18	6	0	-0.385216	-2.557254	-1.008961
19	6	0	-1.598352	-2.999346	-1.544997
20	6	0	3.075100	1.410476	-0.744835
21	6	0	0.379354	-0.778750	1.974976
22	6	0	-0.313586	0.795354	-2.533909
23	6	0	0.627447	1.400496	0.846488
24	6	0	-0.673148	-1.243259	2.856505
25	6	0	3.342673	-0.645167	-1.997672
26	6	0	-2.438197	-3.503306	0.721273
27	6	0	2.721074	-3.590654	-1.982350
28	6	0	-2.648870	-3.473599	-0.657289
29	6	0	-1.583250	1.249152	-3.061090
30	6	0	2.912443	2.888841	-0.696411
31	6	0	-0.169793	2.566563	0.542785
32	6	0	-1.601250	3.066815	-1.405181
33	6	0	-4.761448	0.661750	2.797718
34	6	0	-2.216419	2.371692	-2.513727
35	6	0	-0.387869	2.601187	-0.890116
36	6	0	-5.360272	1.382743	1.763264
37	6	0	-2.866185	-2.372919	2.738720
38	6	0	-1.582130	-1.107265	-3.115175
39	6	0	-2.441349	3.464805	0.881628
40	6	0	-4.929539	-2.597102	-0.318852
41	6	0	-4.401952	-1.116750	-2.694856
42	6	0	-2.367686	0.078190	-3.418471
43	6	0	-4.710784	-2.630060	1.118037
44	6	0	-3.490607	-1.254090	3.294187
45	6	0	-4.713186	2.572588	1.237889
46	6	0	-4.760770	-0.793273	2.764241
47	6	0	-3.922588	3.060846	-1.049171
48	6	0	-5.714065	1.436356	-0.560789
49	6	0	-5.453369	-0.688358	-1.791335
50	6	0	2.690618	4.743188	0.654814
51	6	0	2.523760	-5.572311	-0.640429
52	6	0	-5.359120	-1.466531	1.697772
53	6	0	-5.713088	-1.413199	-0.626512
54	6	0	-5.979574	-0.714500	0.619486
55	6	0	2.700854	-4.755508	0.478257
56	6	0	-5.453955	0.766269	-1.757750
57	6	0	2.511339	5.599804	-0.433323
58	6	0	-5.979906	0.680632	0.651585
59	6	0	2.517201	5.040821	-1.709323
60	6	0	-1.431147	-2.369146	2.519488
61	6	0	1.057085	0.749480	-0.416849
62	6	0	0.269300	1.454051	-1.466857
63	6	0	-2.868208	2.242301	2.844831
64	6	0	-2.214304	-2.254199	-2.620091
65	6	0	-3.491592	1.098711	3.348245
66	6	0	-1.167400	-3.061384	1.275560
67	6	0	-3.649555	-2.255691	-2.401999
68	6	0	-3.489637	-3.074850	1.627644
69	6	0	-4.931811	2.605728	-0.199092
70	6	0	-4.403130	1.236672	-2.640724
71	6	0	2.529183	-4.967239	-1.895240
72	6	0	-3.919709	-3.011584	-1.188693
73	6	0	2.711776	3.668728	-1.846564
74	6	0	-3.748385	0.072963	-3.217471
75	6	0	-2.652130	3.498992	-0.496812
76	6	0	-3.651848	2.361925	-2.296173
77	1	0	3.381212	1.273074	-2.908503
78	1	0	3.387073	-1.153007	-2.954787
79	1	0	2.703679	-3.105943	-2.951547
80	1	0	2.674054	5.130135	1.672020
81	1	0	2.376469	-6.641637	-0.525930
82	1	0	2.683992	-5.179251	1.480729
83	1	0	2.362044	6.663967	-0.279957
84	1	0	2.365340	5.660416	-2.588742
85	1	0	2.379450	-5.554752	-2.796725
86	1	0	2.693408	3.219519	-2.832698
87	8	0	5.651534	-2.296536	0.475640
88	8	0	5.648703	2.289270	0.536211
89	7	0	5.967751	-0.004752	0.574460
90	6	0	3.712269	-0.775943	0.454585

91	6	0	3.711982	0.767969	0.483552	101	1	0	3.243491	1.172030	1.383115
92	6	0	5.197924	1.166471	0.538403	102	1	0	7.483322	-1.575469	2.097936
93	6	0	8.057143	-0.893832	1.482123	103	1	0	7.602051	1.552807	-0.843870
94	6	0	8.124279	0.865250	-0.190402	104	1	0	11.270411	-0.034899	0.752276
95	6	0	10.184561	-0.027996	0.715888	105	1	0	9.961773	-1.592807	2.184693
96	6	0	9.450651	-0.901596	1.520482	106	1	0	10.080653	1.538120	-0.764449
97	6	0	9.517300	0.854334	-0.135638						
98	6	0	7.398009	-0.009272	0.623479	The total electronic energy was calculated to be –3525.8312491 Hartree.					
99	6	0	5.198510	-1.175285	0.502347	The imaginary frequency was found at –414.47 cm^{-1}.					
100	1	0	3.239962	-1.213303	1.336532						

Table S9. Optimized structure of C_{60} (B3LYP-D3/6-31G(d))

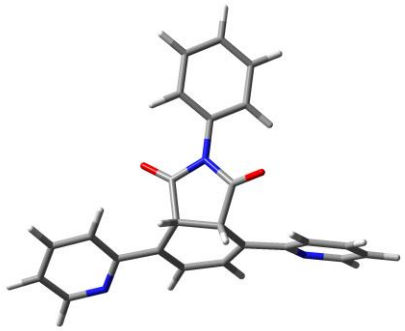


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.407680	-0.728179	-0.679370
2	6	0	2.790905	-0.954231	-1.976325
3	6	0	1.937872	-2.042302	-2.162857
4	6	0	1.665687	-2.949649	-1.060103
5	6	0	2.257844	-2.733147	0.184234
6	6	0	3.146518	-1.599405	0.378594
7	6	0	2.452230	0.340379	-2.544381
8	6	0	0.710425	-1.881642	-2.925261
9	6	0	0.270799	-3.350135	-1.141506
10	6	0	1.480034	-2.908081	1.400018
11	6	0	2.917504	-1.072669	1.713985
12	6	0	3.450101	0.706106	-0.446173
13	6	0	0.141035	-3.291933	1.321732
14	6	0	-0.475958	-3.518146	0.024928
15	6	0	-0.846390	-2.666099	2.185797
16	6	0	-1.844387	-3.031553	0.087692
17	6	0	1.274553	0.494540	-3.275986
18	6	0	-0.319859	-2.689986	-2.294028
19	6	0	-2.073715	-2.505391	1.423320
20	6	0	-1.633457	-2.223925	-2.234081
21	6	0	0.385814	-0.639352	-3.470610
22	6	0	1.887635	-1.881298	2.345064
23	6	0	2.958829	0.303656	1.937891
24	6	0	0.455066	1.681231	-3.093060
25	6	0	3.230481	1.211428	0.835463
26	6	0	2.860205	1.366533	-1.598956
27	6	0	1.971575	0.929258	2.802391
28	6	0	2.411518	2.398406	1.018544
29	6	0	2.073715	2.505391	-1.423320
30	6	0	-2.411518	-2.398406	-1.018544
31	6	0	0.940040	-1.280893	3.174404
32	6	0	-0.982777	-0.153355	-3.407458
33	6	0	1.633457	2.223925	2.234081
34	6	0	1.844387	3.031553	-0.087692
35	6	0	0.846390	2.666099	-2.185797
36	6	0	-0.141035	3.291933	-1.321732
37	6	0	-0.940040	1.280893	-3.174404
38	6	0	-1.971575	-0.929258	-2.802391
39	6	0	-2.958829	-0.303656	-1.937891
40	6	0	0.475958	3.518146	-0.024928
41	6	0	-0.270799	3.350135	1.141506
42	6	0	-1.665687	2.949649	1.060103
43	6	0	0.319859	2.689986	2.294028
44	6	0	-0.455066	-1.681231	3.093060
45	6	0	-2.917504	1.072669	-1.713985
46	6	0	0.982777	0.153355	3.407458
47	6	0	-0.385814	0.639352	3.470610
48	6	0	-1.887635	1.881298	-2.345064
49	6	0	-3.230481	-1.211428	-0.835463
50	6	0	-3.450101	-0.706106	0.446173
51	6	0	-1.480034	2.908081	-1.400018
52	6	0	-2.257844	2.733147	-0.184234
53	6	0	-0.710425	1.881642	2.925261
54	6	0	-1.937872	2.042302	2.162857
55	6	0	-3.146518	1.599405	-0.378594
56	6	0	-1.274553	-0.494540	3.275986
57	6	0	-2.860205	-1.366533	1.598956
58	6	0	-3.407680	0.728179	0.679370
59	6	0	-2.452230	-0.340379	2.544381
60	6	0	-2.790905	0.954231	1.976325

The total electronic energy was calculated to be –2286.2863809 Hartree.

Table S10. Optimized structure of **6b** (B3LYP-D3/6-31G(d))

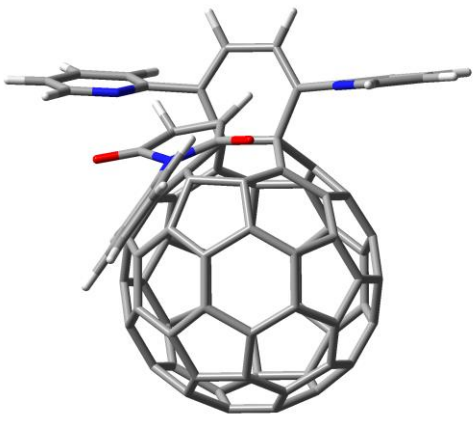


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.109968	-2.268717	-0.967416
2	7	0	2.580163	-2.957734	-1.148616
3	7	0	-4.287724	-1.746374	-0.612551
4	6	0	-3.505969	-0.810071	-0.029150
5	6	0	-2.049920	-1.031532	-0.115412
6	6	0	0.778250	-1.803613	-0.053807
7	6	0	-1.519024	-1.958788	-0.945907
8	6	0	-4.062867	0.304287	0.624275
9	6	0	2.155284	-2.349381	-0.018613
10	6	0	3.788364	-3.516376	-1.157766
11	6	0	-6.248820	-0.538686	0.094932
12	6	0	-5.609181	-1.601602	-0.551121
13	6	0	4.655171	-3.516869	-0.060741
14	6	0	4.221040	-2.894067	1.106550
15	6	0	-5.448137	0.433922	0.688300
16	6	0	2.961088	-2.300624	1.133014
17	8	0	-1.591076	1.875461	-0.512593
18	8	0	2.311986	0.547491	1.484757
19	7	0	0.541257	1.468765	0.310457
20	6	0	-1.098806	-0.202474	0.715194
21	6	0	0.306723	-0.802798	0.997498
22	6	0	1.208742	0.443649	0.996670
23	6	0	2.452301	2.708352	-0.565098
24	6	0	0.468249	3.913707	0.148782
25	6	0	2.375594	5.122518	-0.725787
26	6	0	3.057722	3.917050	-0.903267
27	6	0	1.081605	5.115622	-0.202461
28	6	0	1.157883	2.712265	-0.036559
29	6	0	-0.801695	1.159580	0.062536
30	1	0	0.248526	-2.988599	-1.695560
31	1	0	-2.186060	-2.529778	-1.582664
32	1	0	-3.429098	1.080908	1.033062
33	1	0	4.085672	-3.988608	-2.093367
34	1	0	-7.332499	-0.478570	0.119942
35	1	0	-6.195235	-2.378994	-1.039972
36	1	0	5.631766	-3.986454	-0.127778
37	1	0	4.853390	-2.864002	1.989687
38	1	0	-5.892021	1.291717	1.186362
39	1	0	2.624071	-1.791034	2.025163
40	1	0	-1.563112	0.039924	1.680458
41	1	0	0.372369	-1.253390	1.995329
42	1	0	2.978747	1.770426	-0.696909
43	1	0	-0.539500	3.903602	0.545089
44	1	0	2.849882	6.062071	-0.995135
45	1	0	4.064916	3.913521	-1.310127
46	1	0	0.543256	6.048923	-0.063796

The total electronic energy was calculated to be –1239.552198 Hartree.

Table S11. Optimized structure of **TS4** (B3LYP-D3/6-31G(d))

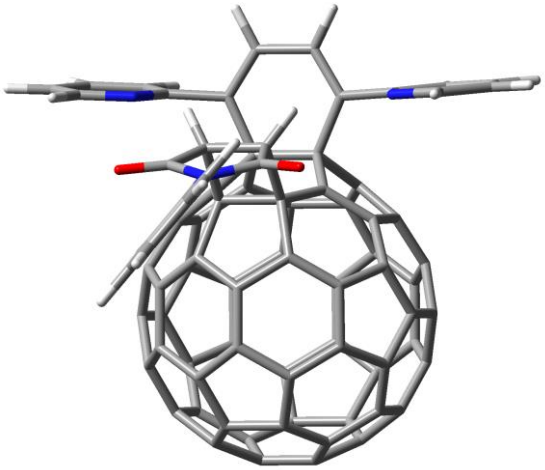


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.806290	4.616902	0.821301
2	7	0	2.482612	2.578184	3.329753
3	7	0	2.612179	2.788508	-3.162950
4	6	0	0.113413	0.883057	-2.512624
5	6	0	0.453061	2.513169	-0.752730
6	6	0	1.824997	0.157908	0.749322
7	6	0	0.740899	-1.627370	2.231412
8	6	0	-0.968617	2.610522	-1.367972
9	6	0	-1.326108	-2.477283	2.937986
10	6	0	0.055310	-0.590289	2.976501
11	6	0	1.478152	-1.275588	1.108771
12	6	0	0.898164	1.176653	-1.378871

13	6	0	1.586812	3.593874	-2.830231	62	6	0	-0.957573	2.533482	1.474684
14	6	0	-2.116675	2.914404	-0.672911	63	6	0	-0.119603	-2.799141	2.203336
15	6	0	0.587221	-3.236815	-0.114995	64	6	0	-3.479035	1.608341	-2.274888
16	6	0	1.374357	-2.071893	-0.080868	65	6	0	-0.193946	-3.586764	1.050955
17	6	0	1.290121	3.658240	-1.367976	66	6	0	0.023542	-0.416973	-3.048028
18	6	0	-1.049397	1.756816	-2.515170	67	6	0	-4.333266	0.435331	-2.298961
19	6	0	-2.273720	1.286625	-2.997096	68	6	0	-1.356636	-2.306580	-3.107918
20	6	0	1.287256	3.593438	1.515947	69	6	0	-3.730643	-2.092699	2.532349
21	6	0	1.696098	0.178794	-0.775611	70	6	0	-5.070267	0.030771	1.177265
22	6	0	-2.111214	2.874432	0.806045	71	6	0	1.191584	4.180074	-5.125736
23	6	0	0.913240	1.104010	1.400377	72	6	0	-3.650149	-0.606187	-3.057948
24	6	0	1.449667	-1.199946	-1.225185	73	6	0	0.891175	4.283815	3.917627
25	6	0	1.814312	4.646234	-0.628589	74	6	0	-5.003513	0.915740	0.025243
26	6	0	-1.245617	-0.908700	-3.507596	75	6	0	-2.346640	-0.274311	3.447529
27	6	0	0.851539	4.310409	-3.778220	76	6	0	-4.311446	0.307311	2.312684
28	6	0	-2.380197	-0.080623	-3.485774	77	1	0	2.353015	5.392399	1.351756
29	6	0	-3.382459	2.330568	1.233990	78	1	0	2.375943	5.435986	-1.120812
30	6	0	1.554352	3.487712	2.979377	79	1	0	0.026175	4.939353	-3.460723
31	6	0	0.136287	0.740535	2.497550	80	1	0	3.516014	1.675789	4.862497
32	6	0	-2.246580	1.119151	3.035831	81	1	0	2.537160	3.199584	-6.512429
33	6	0	-1.479828	-4.087095	0.596960	82	1	0	3.751684	1.995420	-4.680649
34	6	0	-3.458851	1.481100	2.345871	83	1	0	2.420060	3.014884	6.675424
35	6	0	-1.029257	1.614185	2.567128	84	1	0	0.698519	4.726234	6.021970
36	6	0	-2.640502	-3.777696	1.307313	85	1	0	0.636304	4.720803	-5.887217
37	6	0	-0.143495	-2.667425	-2.402191	86	1	0	0.141787	4.996377	3.588532
38	6	0	-3.392032	2.394139	-1.118726	87	8	0	4.419240	-1.073121	2.361042
39	6	0	-1.208297	-1.102237	3.412131	88	8	0	4.874175	-0.705829	-2.215249
40	6	0	-3.756724	-1.947458	-2.658356	89	7	0	4.675861	-1.296390	0.049755
41	6	0	-5.081499	0.096251	-1.173075	90	6	0	3.469899	0.565735	0.818439
42	6	0	-4.173501	2.037861	0.052205	91	6	0	3.704225	0.701512	-0.627950
43	6	0	-2.590774	-2.810692	-2.689713	92	6	0	4.474673	-0.456920	-1.093240
44	6	0	-0.205720	-3.517420	-1.294086	93	6	0	6.348000	-2.859306	-0.827420
45	6	0	-2.564258	-2.956090	2.504219	94	6	0	4.713875	-3.611896	0.804534
46	6	0	-1.486606	-4.044692	-0.858575	95	6	0	6.356063	-5.161132	-0.068900
47	6	0	-3.619086	-0.775031	3.005164	96	6	0	6.887312	-4.145139	-0.864703
48	6	0	-4.525387	-2.373337	1.357572	97	6	0	5.270433	-4.888079	0.766434
49	6	0	-5.188125	-1.292918	-0.759522	98	6	0	5.257569	-2.595840	0.008409
50	6	0	2.767954	2.429888	4.626706	99	6	0	4.245728	-0.668312	1.231553
51	6	0	2.245367	3.337996	-5.475934	100	1	0	3.584804	1.406124	1.501027
52	6	0	-2.654631	-3.697539	-1.540019	101	1	0	3.705022	1.618985	-1.204773
53	6	0	-4.540267	-2.293901	-1.492637	102	1	0	6.751599	-2.070549	-1.448684
54	6	0	-3.861217	-3.376951	-0.797701	103	1	0	3.870202	-3.396093	1.448937
55	6	0	2.924623	2.666000	-4.456501	104	1	0	6.783726	-6.159500	-0.099679
56	6	0	-5.181282	-1.333360	0.688041	105	1	0	7.730667	-4.348883	-1.518818
57	6	0	2.154993	3.177294	5.635300	106	1	0	4.847812	-5.672620	1.388056
58	6	0	-3.854118	-3.415893	0.596296	---					
59	6	0	1.201177	4.125234	5.269194	The total electronic energy was calculated to be –3525.7522948 Hartree.					
60	6	0	0.711219	-1.492234	-2.368411	The imaginary frequency was found at –495.82 cm^{-1}.					
61	6	0	0.459068	2.468440	0.846230						

Table S12. Optimized structure of **INT4** (B3LYP-D3/6-31G(d))



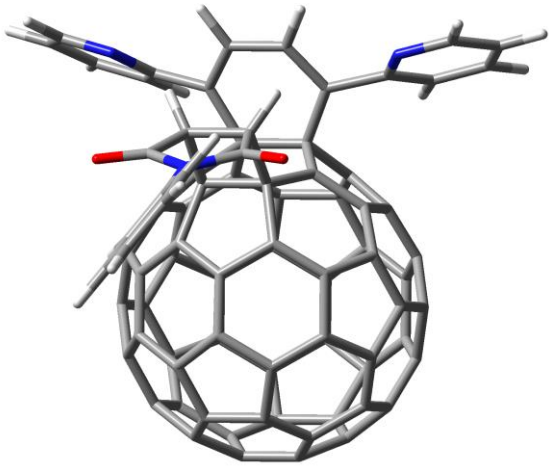
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.840031	4.543067	0.858607
2	7	0	2.474405	2.650755	3.395368
3	7	0	2.551420	2.821955	-3.200501
4	6	0	0.118888	0.857521	-2.455151
5	6	0	0.411378	2.498522	-0.728455
6	6	0	1.824140	0.150706	0.801447
7	6	0	0.701726	-1.643879	2.253240
8	6	0	-0.999230	2.594133	-1.362566
9	6	0	-1.361073	-2.507745	2.936918
10	6	0	-0.004715	-0.607642	2.989335
11	6	0	1.458945	-1.293029	1.148063
12	6	0	0.879312	1.165814	-1.345763
13	6	0	1.524533	3.600282	-2.811851
14	6	0	-2.163018	2.891317	-0.685586
15	6	0	0.601447	-3.269628	-0.079268
16	6	0	1.380393	-2.088804	-0.041278
17	6	0	1.271624	3.632886	-1.339719
18	6	0	-1.056741	1.725739	-2.493406
19	6	0	-2.263556	1.246118	-2.999787
20	6	0	1.242093	3.560271	1.547947
21	6	0	1.840833	0.190772	-0.758186
22	6	0	-2.177741	2.853155	0.791203
23	6	0	0.851305	1.094358	1.419833
24	6	0	1.483138	-1.232851	-1.186037
25	6	0	1.855773	4.579012	-0.590098
26	6	0	-1.191196	-0.945652	-3.482943
27	6	0	0.743902	4.325240	-3.716622
28	6	0	-2.346116	-0.125891	-3.482420
29	6	0	-3.448984	2.294464	1.202211
30	6	0	1.463196	3.456429	3.021759
31	6	0	0.069329	0.728852	2.496495
32	6	0	-2.323091	1.090171	3.014703
33	6	0	-1.468996	-4.133803	0.605935
34	6	0	-3.530366	1.442409	2.312237
35	6	0	-1.106882	1.594515	2.556991
36	6	0	-2.641460	-3.827134	1.297267
37	6	0	-0.098967	-2.705873	-2.369666
38	6	0	-3.425515	2.355171	-1.149950
39	6	0	-1.259291	-1.124315	3.404562
40	6	0	-3.712063	-2.009004	-2.681299
41	6	0	-5.080005	0.031101	-1.223713
42	6	0	-4.219351	1.990902	0.009714
43	6	0	-2.538048	-2.862747	-2.694439
44	6	0	-0.169207	-3.559948	-1.264607
45	6	0	-2.589377	-2.997234	2.491056
46	6	0	-1.454470	-4.096110	-0.849407
47	6	0	-3.669369	-0.818203	2.972459
48	6	0	-4.535161	-2.432828	1.318513
49	6	0	-5.177367	-1.360936	-0.807548
50	6	0	2.715017	2.505910	4.702343
51	6	0	2.092594	3.420984	-5.485817
52	6	0	-2.613395	-3.753591	-1.547053
53	6	0	-4.507175	-2.358987	-1.533208
54	6	0	-3.832433	-3.438055	-0.824683
55	6	0	2.819419	2.738299	-4.507481
56	6	0	-5.191692	-1.398352	0.632735
57	6	0	1.975196	3.152124	5.695611
58	6	0	-3.846362	-3.474270	0.568494
59	6	0	0.935326	3.993120	5.304015
60	6	0	0.747164	-1.525263	-2.321822
61	6	0	0.395742	2.457599	0.863726
62	6	0	-1.027318	2.521174	1.474832
63	6	0	-0.144331	-2.825199	2.223566
64	6	0	-3.484653	1.562169	-2.304242
65	6	0	-0.192571	-3.620088	1.073784
66	6	0	0.054933	-0.452070	-3.017310
67	6	0	-4.320259	0.376046	-2.337301
68	6	0	-1.301456	-2.351225	-3.089438
69	6	0	-3.763206	-2.143344	2.498826
70	6	0	-5.103586	-0.029816	1.122843
71	6	0	1.036682	4.233855	-5.078171
72	6	0	-3.609242	-0.661108	-3.082882
73	6	0	0.670834	4.147965	3.942428
74	6	0	-5.032490	0.855684	-0.027616
75	6	0	-2.414551	-0.305075	3.423977
76	6	0	-4.365963	0.256573	2.267570
77	1	0	2.417154	5.290913	1.396278
78	1	0	2.444878	5.351764	-1.077212
79	1	0	-0.079417	4.932229	-3.354570
80	1	0	3.533781	1.837535	4.960977
81	1	0	2.350144	3.312952	-6.534938
82	1	0	3.649822	2.089709	-4.779128
83	1	0	2.210728	2.995221	6.743740
84	1	0	0.334091	4.514836	6.043525
85	1	0	0.444726	4.782395	-5.805646
86	1	0	-0.139363	4.778830	3.591691
87	8	0	4.557151	-0.926341	2.329226
88	8	0	4.634243	-0.784084	-2.279727
89	7	0	4.732325	-1.177003	0.017323
90	6	0	3.377854	0.581332	0.814720
91	6	0	3.394383	0.622060	-0.715384
92	6	0	4.320879	-0.491569	-1.147060
93	6	0	6.596461	-2.507280	-0.851841
94	6	0	5.108991	-3.447614	0.822938
95	6	0	6.942359	-4.765859	-0.048760

96	6	0	7.314025	-3.703031	-0.873700	103	1	0	4.252409	-3.337401	1.477152
97	6	0	5.840719	-4.633078	0.799428	104	1	0	7.507205	-5.693816	-0.067309
98	6	0	5.493420	-2.385706	-0.002436	105	1	0	8.168098	-3.800249	-1.538091
99	6	0	4.286860	-0.559503	1.207316	106	1	0	5.543687	-5.456359	1.442992
100	1	0	3.555393	1.479059	1.405793						
101	1	0	3.581445	1.551028	-1.252960						
102	1	0	6.874187	-1.682071	-1.495702						

The total electronic energy was calculated to be –3525.7672077 Hartree.

Table S13. Optimized structure of **TS5** (B3LYP-D3/6-31G(d))

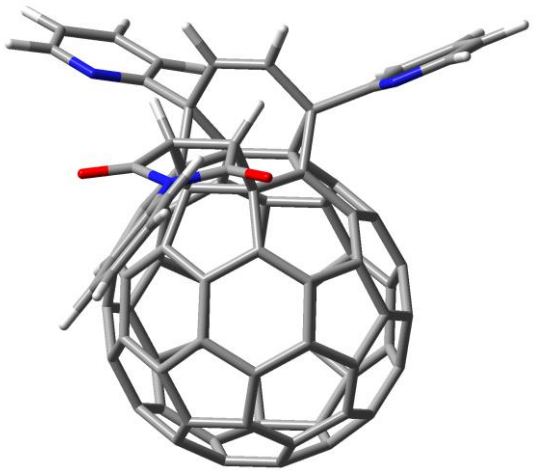


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.531732	-1.069149	2.340384
2	8	0	4.610402	-0.976800	-2.268724
3	6	0	2.558158	3.602036	0.782554
4	7	0	4.700735	-1.342261	0.031882
5	7	0	2.578564	3.311931	3.630555
6	7	0	2.658932	3.422868	-3.464998
7	6	0	0.144857	0.849829	-2.513971
8	6	0	0.352794	2.450794	-0.741408
9	6	0	1.875278	0.197732	0.813296
10	6	0	0.744000	-1.590604	2.271046
11	6	0	-1.023086	2.539154	-1.391958
12	6	0	-1.304915	-2.483973	2.962827
13	6	0	0.024744	-0.553735	3.016771
14	6	0	3.450847	0.501551	0.813514
15	6	0	3.468790	0.527126	-0.717744
16	6	0	1.488726	-1.239730	1.164816
17	6	0	0.950445	1.203831	-1.398082
18	6	0	1.496700	3.653690	-2.820795
19	6	0	-2.192195	2.818532	-0.716878
20	6	0	0.673033	-3.238745	-0.043768
21	6	0	1.426299	-2.046778	-0.016604
22	6	0	1.480799	3.239631	-1.391766
23	6	0	-1.055382	1.665865	-2.524287
24	6	0	-2.261278	1.162098	-3.024253
25	6	0	1.448196	3.195063	1.526127
26	6	0	1.893922	0.222557	-0.764316
27	6	0	-2.208774	2.795133	0.757486
28	6	0	0.917975	1.158494	1.456818
29	6	0	1.516000	-1.202842	-1.169924
30	6	0	2.573802	3.623205	-0.611324
31	6	0	-1.154112	-0.991435	-3.486563
32	6	0	0.416347	4.297292	-3.441786
33	6	0	-2.321579	-0.202532	-3.502069
34	6	0	-3.473167	2.225726	1.174022
35	6	0	1.431447	3.563725	2.967462
36	6	0	0.087956	0.769217	2.542538
37	6	0	-2.329037	1.065966	3.008938
38	6	0	-1.374391	-4.141402	0.647385
39	6	0	-3.540789	1.388112	2.292881
40	6	0	-1.112519	1.584748	2.551844
41	6	0	-2.553942	-3.851493	1.334295
42	6	0	-0.029030	-2.708613	-2.336499
43	6	0	-3.446709	2.263073	-1.179571
44	6	0	-1.231765	-1.101663	3.427350
45	6	0	-3.656212	-2.099462	-2.672237
46	6	0	-5.066798	-0.081683	-1.234105
47	6	0	-4.238490	1.899916	-0.016992
48	6	0	4.321374	-0.651604	-1.139136
49	6	0	-2.461092	-2.926015	-2.670197
50	6	0	-0.085004	-3.560426	-1.228653
51	6	0	-2.519514	-3.008641	2.520334
52	6	0	6.479572	-2.789493	-0.827885
53	6	0	-1.357896	-4.118205	-0.809238
54	6	0	-3.650798	-0.859748	2.981756
55	6	0	-4.478762	-2.502131	1.336468
56	6	0	-5.139462	-1.468089	-0.804468
57	6	0	2.646023	3.637777	4.921854
58	6	0	4.938434	-3.625759	0.854084
59	6	0	1.720967	4.403521	-5.455506
60	6	0	-2.521929	-3.806263	-1.512988
61	6	0	-4.446799	-2.456785	-1.515317
62	6	0	-3.748462	-3.510504	-0.796331
63	6	0	6.686506	-5.059673	-0.010474
64	6	0	7.122270	-4.027194	-0.842597
65	6	0	5.595903	-4.854087	0.837449
66	6	0	2.755994	3.789855	-4.743296
67	6	0	-5.155821	-1.491195	0.642229
68	6	0	1.594667	4.228994	5.629161
69	6	0	-3.764331	-3.532855	0.600166
70	6	0	0.422398	4.517389	4.936007
71	6	0	0.795576	-1.517791	-2.302404
72	6	0	0.335334	2.426143	0.827134
73	6	0	-1.054962	2.494216	1.449516
74	6	0	-0.080581	-2.781816	2.248927
75	6	0	5.387405	-2.595096	0.021725
76	6	0	-3.488941	1.461694	-2.325861
77	6	0	4.286434	-0.694841	1.215737
78	6	0	-0.111473	-3.597399	1.112953
79	6	0	0.092704	-0.457528	-3.030773
80	6	0	-4.310366	0.265982	-2.351730
81	6	0	-1.237080	-2.387634	-3.067708
82	6	0	-3.714706	-2.182246	2.521870
83	6	0	-5.093491	-0.119195	1.117651
84	6	0	0.532885	4.669945	-4.780706
85	6	0	-3.582476	-0.763082	-3.087882
86	6	0	0.336818	4.187657	3.583537
87	6	0	-5.034032	0.753976	-0.044052

88	6	0	-2.399676	-0.313259	3.441738	99	1	0	7.193106	-6.020755	-0.023311
89	6	0	-4.362276	0.192489	2.262415	100	1	0	7.967868	-4.181124	-1.507048
90	1	0	3.401223	4.014894	1.327060	101	1	0	5.249505	-5.653530	1.486342
91	1	0	3.718493	1.392584	1.378608	102	1	0	3.708423	3.578333	-5.226238
92	1	0	3.746734	1.438063	-1.244913	103	1	0	1.702923	4.461989	6.683852
93	1	0	3.428682	4.052167	-1.123981	104	1	0	-0.415252	4.998044	5.433708
94	1	0	-0.487021	4.513570	-2.885150	105	1	0	-0.293299	5.166412	-5.282027
95	1	0	6.806306	-1.987046	-1.477494	106	1	0	-0.553609	4.421832	3.013437
96	1	0	3.587087	3.410409	5.419613	---					
97	1	0	4.091058	-3.458948	1.508204	The total electronic energy was calculated to be –3525.7607413 Hartree.					
98	1	0	1.853429	4.669971	-6.499459	The imaginary frequency was found at –284.57 cm^{-1}.					

Table S14. Optimized structure of **INT5** (B3LYP-D3/6-31G(d))

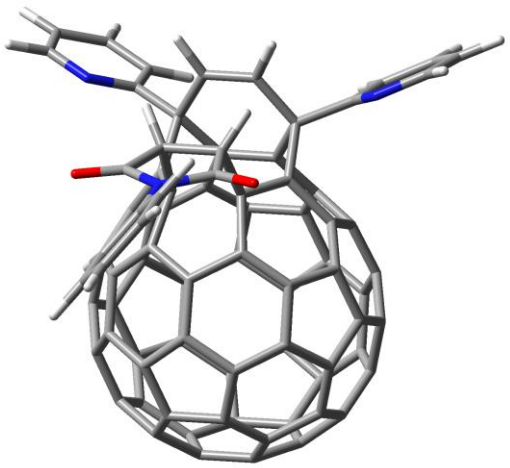


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.563925	-0.924345	2.352859
2	8	0	4.645381	-0.857816	-2.256597
3	6	0	2.425199	3.443975	0.736391
4	7	0	4.758598	-1.191019	0.046701
5	7	0	2.059646	3.241389	3.828631
6	7	0	2.154712	3.315360	-3.708589
7	6	0	0.127594	0.891535	-2.592050
8	6	0	0.142557	2.421779	-0.723895
9	6	0	1.916745	0.368829	0.837972
10	6	0	0.865605	-1.470889	2.282964
11	6	0	-1.182851	2.424649	-1.410659
12	6	0	-1.115238	-2.513043	2.980488
13	6	0	0.069010	-0.477977	3.026813
14	6	0	3.478399	0.640231	0.818217
15	6	0	3.497601	0.657540	-0.716468
16	6	0	1.576880	-1.071873	1.177113
17	6	0	1.045884	1.404380	-1.505447
18	6	0	1.257927	3.674956	-2.779064
19	6	0	-2.368060	2.624226	-0.738839
20	6	0	0.914910	-3.129315	-0.018999
21	6	0	1.574893	-1.888506	0.001440
22	6	0	1.362061	2.920615	-1.478815
23	6	0	-1.137289	1.585275	-2.570657
24	6	0	-2.316974	0.990178	-3.052072
25	6	0	1.324714	2.890401	1.571710
26	6	0	1.937446	0.385078	-0.781005
27	6	0	-2.386159	2.609514	0.735243
28	6	0	1.008237	1.373887	1.560852
29	6	0	1.606826	-1.048735	-1.157141
30	6	0	2.441604	3.457208	-0.605948
31	6	0	-1.067305	-1.065770	-3.489428
32	6	0	0.337508	4.709686	-2.966751
33	6	0	-2.281458	-0.374129	-3.519952
34	6	0	-3.612066	1.971239	1.154497
35	6	0	1.187736	3.619679	2.883089
36	6	0	0.063724	0.839660	2.614461
37	6	0	-2.391586	0.929405	3.015754
38	6	0	-1.049556	-4.191620	0.675259
39	6	0	-3.620575	1.148127	2.284181
40	6	0	-1.200544	1.533896	2.575665
41	6	0	-2.248753	-3.990511	1.359422
42	6	0	0.186734	-2.668764	-2.312020
43	6	0	-3.583033	1.994656	-1.200757
44	6	0	-1.152651	-1.135195	3.442806
45	6	0	-3.474154	-2.358501	-2.668451
46	6	0	-5.035695	-0.449433	-1.244007
47	6	0	-4.351726	1.588207	-0.036397
48	6	0	4.357631	-0.522939	-1.129785
49	6	0	-2.217284	-3.089336	-2.656657
50	6	0	0.192541	-3.521748	-1.203370
51	6	0	-2.281395	-3.141271	2.541263
52	6	0	6.571479	-2.601142	-0.801687
53	6	0	-1.031474	-4.177007	-0.782317
54	6	0	-3.579942	-1.091474	2.988322
55	6	0	-4.273870	-2.798600	1.346127
56	6	0	-5.005171	-1.833348	-0.804846
57	6	0	2.018695	3.878943	5.003643
58	6	0	5.038666	-3.469665	0.871393
59	6	0	1.250682	5.008078	-5.165626
60	6	0	-2.213530	-3.961785	-1.491550
61	6	0	-4.238856	-2.770127	-1.504498
62	6	0	-3.461081	-3.757844	-0.778817
63	6	0	6.820215	-4.867057	0.015228
64	6	0	7.239532	-3.825318	-0.813848
65	6	0	5.721083	-4.684427	0.857330
66	6	0	2.142261	3.973653	-4.872725
67	6	0	-5.023099	-1.847938	0.646787
68	6	0	1.121795	4.910019	5.292082
69	6	0	-3.478460	-3.771976	0.620274
70	6	0	0.228835	5.305442	4.297345
71	6	0	0.922054	-1.425182	-2.287134
72	6	0	0.124099	2.406741	0.777687
73	6	0	-1.217806	2.396254	1.431880
74	6	0	0.130185	-2.714494	2.264667
75	6	0	5.471322	-2.429575	0.042314
76	6	0	-3.563451	1.194249	-2.346489
77	6	0	4.321305	-0.553302	1.226690
78	6	0	0.163524	-3.544885	1.139273
79	6	0	0.143548	-0.417538	-3.030319

80	6	0	-4.302879	-0.054661	-2.364785	95	1	0	6.884976	-1.791747	-1.449383
81	6	0	-1.040827	-2.452454	-3.053723	96	1	0	2.737227	3.546097	5.750440
82	6	0	-3.538428	-2.410667	2.536797	97	1	0	4.184745	-3.320606	1.521142
83	6	0	-5.064641	-0.473042	1.112781	98	1	0	1.281298	5.502067	-6.131965
84	6	0	0.331954	5.384244	-4.187035	99	1	0	7.346283	-5.817651	0.004456
85	6	0	-3.505075	-1.030650	-3.094407	100	1	0	8.091499	-3.961625	-1.473981
86	6	0	0.264387	4.652719	3.065766	101	1	0	5.387579	-5.491298	1.503776
87	6	0	-5.067064	0.391732	-0.057204	102	1	0	2.880266	3.655424	-5.606812
88	6	0	-2.367355	-0.443987	3.457024	103	1	0	1.128754	5.386851	6.267455
89	6	0	-4.359808	-0.100899	2.258982	104	1	0	-0.483265	6.106562	4.475359
90	1	0	3.244561	3.902365	1.283717	105	1	0	-0.377138	6.187163	-4.368883
91	1	0	3.785965	1.527127	1.368493	106	1	0	-0.415283	4.923319	2.264467
92	1	0	3.816156	1.558279	-1.237299	---					
93	1	0	3.273789	3.926470	-1.123928	The total electronic energy was calculated to be –3525.804876 Hartree.					
94	1	0	-0.363076	4.964684	-2.178447						

Table S15. Optimized structure of **TS6** (B3LYP-D3/6-31G(d))



Standard orientation:

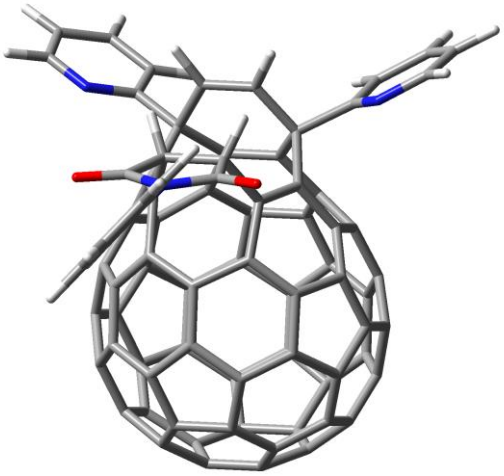
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.562508	-1.003533	2.348916
2	8	0	4.642311	-0.936990	-2.259965
3	6	0	2.451602	3.356051	0.730160
4	7	0	4.762355	-1.266580	0.043070
5	7	0	2.134850	3.206593	3.790071
6	7	0	2.221261	3.273721	-3.676726
7	6	0	0.120816	0.883932	-2.567159
8	6	0	0.093069	2.618703	-0.694774
9	6	0	1.942546	0.339967	0.927352
10	6	0	0.823175	-1.486662	2.278921
11	6	0	-1.185518	2.476812	-1.405095
12	6	0	-1.171582	-2.503784	2.979824
13	6	0	0.035171	-0.484780	3.006028
14	6	0	3.493174	0.574842	0.811626
15	6	0	3.511127	0.591616	-0.715211
16	6	0	1.566308	-1.096676	1.187637
17	6	0	1.153747	1.350413	-1.611691
18	6	0	1.307119	3.645119	-2.770434
19	6	0	-2.380725	2.659965	-0.735346
20	6	0	0.856482	-3.132844	-0.017724
21	6	0	1.549042	-1.906028	0.001809
22	6	0	1.352019	2.855776	-1.474739
23	6	0	-1.131588	1.609937	-2.552621
24	6	0	-2.316556	1.018588	-3.029489
25	6	0	1.316064	2.827584	1.562021
26	6	0	1.964439	0.356806	-0.871929
27	6	0	-2.398067	2.646270	0.731114
28	6	0	1.114904	1.319814	1.666497
29	6	0	1.595422	-1.075028	-1.167895
30	6	0	2.467335	3.368539	-0.606526
31	6	0	-1.108607	-1.058631	-3.474927
32	6	0	0.428055	4.712614	-2.965946
33	6	0	-2.306164	-0.346531	-3.503118
34	6	0	-3.624248	2.012591	1.151185
35	6	0	1.240894	3.593460	2.870260
36	6	0	0.059702	0.835860	2.588422
37	6	0	-2.388031	0.962243	2.995002
38	6	0	-1.124529	-4.180198	0.676777
39	6	0	-3.625794	1.189773	2.276653
40	6	0	-1.192221	1.562216	2.557561
41	6	0	-2.321544	-3.966895	1.362280
42	6	0	0.125518	-2.676227	-2.307914
43	6	0	-3.596354	2.034392	-1.196084
44	6	0	-1.190649	-1.123187	3.430500
45	6	0	-3.529487	-2.320467	-2.665013
46	6	0	-5.070466	-0.394050	-1.241115
47	6	0	-4.372204	1.636543	-0.035133
48	6	0	4.360566	-0.599007	-1.132842
49	6	0	-2.282898	-3.069456	-2.654171
50	6	0	0.125371	-3.523670	-1.198819
51	6	0	-2.344764	-3.117930	2.544327
52	6	0	6.579634	-2.670084	-0.805943
53	6	0	-1.107110	-4.166620	-0.778383
54	6	0	-3.613160	-1.047293	2.983745
55	6	0	-4.333734	-2.750498	1.349443
56	6	0	-5.055562	-1.779317	-0.801492
57	6	0	2.156838	3.865302	4.953513
58	6	0	5.051396	-3.544217	0.868438
59	6	0	1.421578	5.020930	-5.129159
60	6	0	-2.287572	-3.940121	-1.487953
61	6	0	-4.299932	-2.723937	-1.500390
62	6	0	-3.532791	-3.720683	-0.774967
63	6	0	6.839460	-4.933900	0.013053
64	6	0	7.253536	-3.890976	-0.817231
65	6	0	5.739676	-4.755765	0.855211
66	6	0	2.268461	3.951792	-4.828222
67	6	0	-5.072869	-1.792934	0.650613
68	6	0	1.303451	4.929486	5.253655
69	6	0	-3.549579	-3.733879	0.624033
70	6	0	0.388343	5.334469	4.283196
71	6	0	0.877555	-1.444117	-2.282835

72	6	0	0.075953	2.605221	0.748319
73	6	0	-1.219072	2.450365	1.425460
74	6	0	0.071039	-2.718794	2.263026
75	6	0	5.478954	-2.502977	0.038354
76	6	0	-3.570914	1.232679	-2.336404
77	6	0	4.325351	-0.629287	1.222909
78	6	0	0.097443	-3.545167	1.138250
79	6	0	0.106635	-0.428734	-3.009532
80	6	0	-4.328036	-0.007600	-2.358703
81	6	0	-1.099850	-2.447270	-3.049495
82	6	0	-3.591518	-2.369154	2.539622
83	6	0	-5.098460	-0.416075	1.115660
84	6	0	0.485562	5.409936	-4.172176
85	6	0	-3.541092	-0.990688	-3.084843
86	6	0	0.357366	4.657524	3.064443
87	6	0	-5.097770	0.447538	-0.054850
88	6	0	-2.388703	-0.411447	3.443280
89	6	0	-4.382898	-0.050660	2.257609
90	1	0	3.286864	3.773682	1.285106
91	1	0	3.838850	1.456180	1.349028
92	1	0	3.865791	1.486575	-1.223424
93	1	0	3.315047	3.796831	-1.133796
94	1	0	-0.289135	4.976831	-2.195883
95	1	0	6.889157	-1.859779	-1.454470
96	1	0	2.892081	3.523854	5.679910
97	1	0	4.197015	-3.398427	1.518288
98	1	0	1.499103	5.531027	-6.084411
99	1	0	7.370179	-5.881911	0.003140
100	1	0	8.105963	-4.023805	-1.477481
101	1	0	5.410324	-5.563599	1.502577
102	1	0	3.019385	3.622376	-5.544073
103	1	0	1.360234	5.423765	6.218631
104	1	0	-0.291485	6.161136	4.470447
105	1	0	-0.190227	6.239679	-4.360422
106	1	0	-0.342652	4.935097	2.283372

The total electronic energy was calculated to be –3525.787778 Hartree.

The imaginary frequency was found at –563.53 cm^{-1}.

Table S16. Optimized structure of **2b** (B3LYP-D3/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.656918	-1.112462	2.319673
2	8	0	4.719566	-1.021633	-2.278034
3	6	0	2.496947	3.119253	0.731593
4	7	0	4.885415	-1.343830	0.018079
5	7	0	2.157479	3.056211	3.788164
6	7	0	2.213543	3.159686	-3.666154
7	6	0	0.092825	0.824707	-2.604478
8	6	0	0.043592	2.795050	-0.649816
9	6	0	2.060937	0.145661	1.372329
10	6	0	0.686941	-1.598787	2.301659
11	6	0	-1.178675	2.543617	-1.379594
12	6	0	-1.349930	-2.544303	2.985310
13	6	0	-0.057223	-0.584601	3.025388
14	6	0	3.440193	0.379703	0.801603
15	6	0	3.452917	0.403538	-0.735229
16	6	0	1.542103	-1.218160	1.268239
17	6	0	1.288674	1.182948	-1.860963
18	6	0	1.365101	3.570491	-2.714530
19	6	0	-2.388473	2.721476	-0.703914
20	6	0	0.664988	-3.124145	-0.038369
21	6	0	1.469997	-1.951584	-0.015419
22	6	0	1.344341	2.684855	-1.457322
23	6	0	-1.129978	1.619792	-2.509901
24	6	0	-2.340543	1.063681	-2.970809
25	6	0	1.320076	2.642228	1.555194
26	6	0	2.083747	0.183469	-1.334629
27	6	0	-2.400113	2.701011	0.743324
28	6	0	1.257912	1.129692	1.914732
29	6	0	1.563325	-1.182316	-1.276393
30	6	0	2.507571	3.138336	-0.601817
31	6	0	-1.252744	-1.069173	-3.488565
32	6	0	0.629385	4.754740	-2.817719
33	6	0	-2.404822	-0.295176	-3.473692
34	6	0	-3.638332	2.095308	1.167431
35	6	0	1.321383	3.492388	2.836894
36	6	0	0.050465	0.750590	2.628977
37	6	0	-2.388442	0.979402	2.962723
38	6	0	-1.352716	-4.163045	0.653804
39	6	0	-3.637797	1.258180	2.274738
40	6	0	-1.170764	1.548236	2.537360
41	6	0	-2.544948	-3.934428	1.348354
42	6	0	-0.081934	-2.719674	-2.336938
43	6	0	-3.619498	2.128263	-1.164903
44	6	0	-1.308682	-1.167505	3.437404
45	6	0	-3.713214	-2.226881	-2.663786
46	6	0	-5.173729	-0.249630	-1.222088
47	6	0	-4.412315	1.752313	-0.010163
48	6	0	4.410450	-0.722090	-1.148127
49	6	0	-2.501364	-3.029523	-2.668729
50	6	0	-0.093145	-3.525507	-1.210818
51	6	0	-2.543468	-3.103329	2.542016
52	6	0	6.872955	-2.492993	-0.833353
53	6	0	-1.340962	-4.142573	-0.792346
54	6	0	-3.714700	-0.974616	2.981658
55	6	0	-4.514336	-2.645048	1.352181
56	6	0	-5.208135	-1.636424	-0.792537
57	6	0	2.259948	3.771633	4.913238
58	6	0	5.475989	-3.564321	0.841327
59	6	0	1.623649	5.090561	-4.978143
60	6	0	-2.521871	-3.893976	-1.499319
61	6	0	-4.491336	-2.604603	-1.498401
62	6	0	-3.755302	-3.635834	-0.779680
63	6	0	7.437991	-4.698594	-0.009201

64	6	0	7.706915	-3.610508	-0.841408	87	6	0	-5.173590	0.586110	-0.032774
65	6	0	6.323289	-4.670780	0.831442	88	6	0	-2.460596	-0.393165	3.425759
66	6	0	2.331721	3.905772	-4.769565	89	6	0	-4.446950	0.051906	2.266183
67	6	0	-5.219980	-1.657148	0.662681	90	1	0	3.351454	3.492815	1.289247
68	6	0	1.547566	4.949573	5.144827	91	1	0	3.862784	1.289066	1.227923
69	6	0	-3.766730	-3.655768	0.616497	92	1	0	3.877461	1.328052	-1.125309
70	6	0	0.695588	5.408711	4.141459	93	1	0	3.370556	3.528062	-1.134859
71	6	0	0.724366	-1.533056	-2.333315	94	1	0	-0.034613	5.060397	-2.016541
72	6	0	0.032422	2.775419	0.730366	95	1	0	7.070068	-1.649519	-1.483631
73	6	0	-1.201334	2.503807	1.433069	96	1	0	2.945138	3.381497	5.663742
74	6	0	-0.118952	-2.784940	2.258758	97	1	0	4.609292	-3.534726	1.490593
75	6	0	5.759164	-2.476530	0.010111	98	1	0	1.752018	5.654464	-5.896933
76	6	0	-3.600868	1.322923	-2.295399	99	1	0	8.093138	-5.565284	-0.016841
77	6	0	4.383551	-0.763898	1.194660	100	1	0	8.570090	-3.627176	-1.500795
78	6	0	-0.112012	-3.558176	1.109784	101	1	0	6.106648	-5.514559	1.480405
79	6	0	-0.008111	-0.498759	-3.040100	102	1	0	3.026425	3.535506	-5.521404
80	6	0	-4.409748	0.117114	-2.334107	103	1	0	1.663107	5.488217	6.080325
81	6	0	-1.300985	-2.458132	-3.076159	104	1	0	0.126013	6.324837	4.271982
82	6	0	-3.755351	-2.300720	2.540365	105	1	0	0.192320	6.443451	-4.086486
83	6	0	-5.192920	-0.283054	1.132099	106	1	0	-0.071377	4.999212	2.161816
84	6	0	0.759072	5.523221	-3.973757	---					
85	6	0	-3.665745	-0.888876	-3.066406	The total electronic energy was calculated to be –3525.878158 Hartree.					
86	6	0	0.582402	4.672337	2.962987						

5.2. Electrostatic Potential Maps

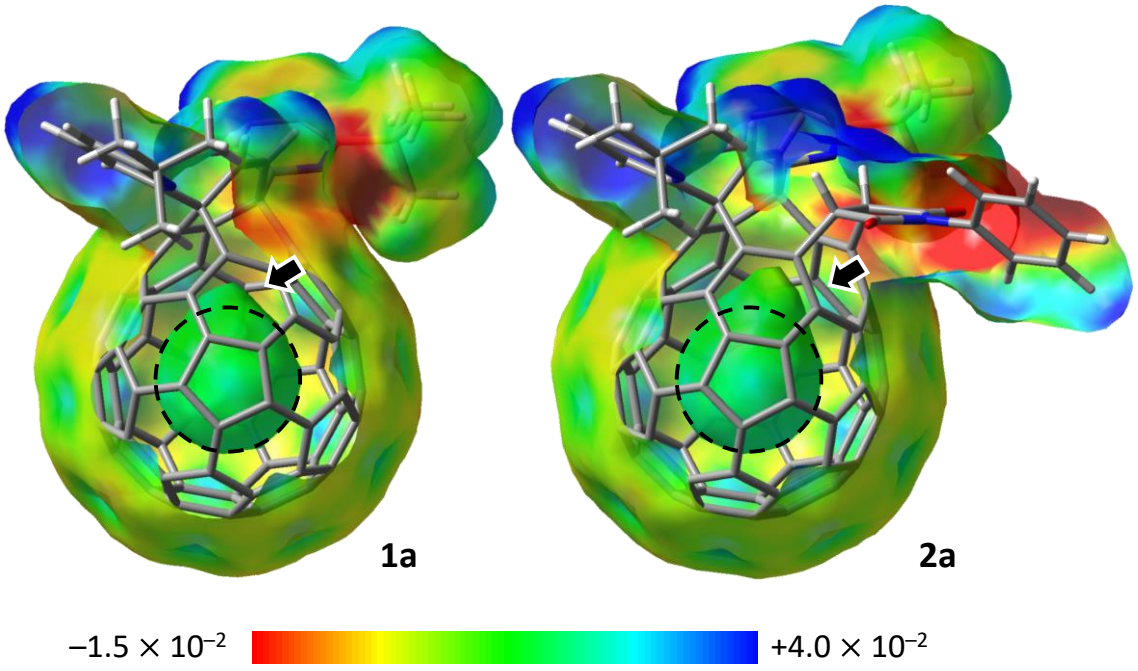
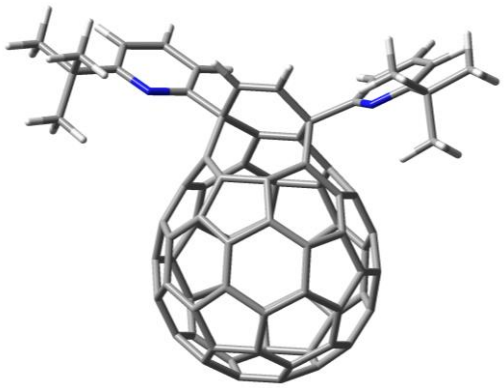


Figure S19. Electrostatic potential maps of **1a** and **2a** (B3LYP/6-31G(d)). The dot circles represent a spherical potential surface originated from pristine C_{60}.

Table S17. Optimized structure of **1a** (B3LYP/6-31G(d))



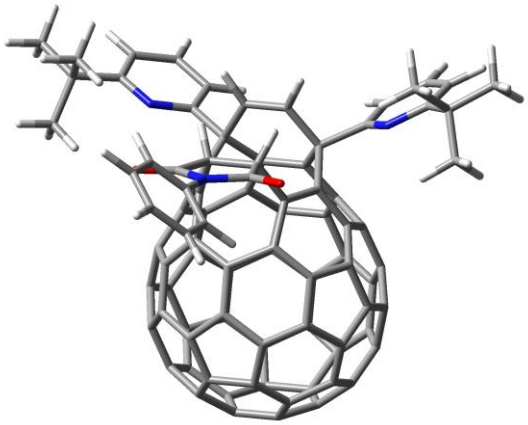
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.845560	0.663256	-0.361390
2	6	0	-3.845593	-0.663070	-0.361389
3	6	0	-2.720255	-1.450227	0.260811
4	6	0	-1.565205	-1.649235	-0.722719
5	6	0	-1.219825	-0.760050	-1.752293
6	6	0	-1.219789	0.760107	-1.752296
7	6	0	-0.120482	1.153102	-2.620229
8	6	0	0.643896	2.291822	-2.383044
9	6	0	0.461227	2.990266	-1.132262
10	6	0	-0.541215	2.579013	-0.249632
11	6	0	-1.565126	1.649311	-0.722721
12	6	0	-2.720183	1.450352	0.260812
13	6	0	-1.941195	0.692769	1.319411
14	6	0	-1.941231	-0.692681	1.319415
15	6	0	-0.851369	-1.417743	1.932820
16	6	0	-0.227698	-2.522274	1.191337
17	6	0	-0.541336	-2.578988	-0.249630
18	6	0	0.461086	-2.990289	-1.132258
19	6	0	0.643789	-2.291855	-2.383042
20	6	0	-0.120537	-1.153100	-2.620229
21	6	0	0.501155	-0.000014	-3.212440
22	6	0	1.851271	-0.000047	-3.558272
23	6	0	2.655854	1.176499	-3.286825
24	6	0	2.060165	2.299441	-2.708783
25	6	0	2.752266	3.019321	-1.656168
26	6	0	1.756492	3.438973	-0.685703
27	6	0	2.044953	3.433698	0.670802
28	6	0	1.047409	2.957608	1.611742
29	6	0	-0.227579	2.522284	1.191334
30	6	0	-0.851299	1.417778	1.932817
31	6	0	-0.096278	0.725737	2.884371
32	6	0	-0.096314	-0.725735	2.884374
33	6	0	1.215232	-1.165522	3.288005
34	6	0	1.770867	-2.281777	2.678834
35	6	0	1.047270	-2.957657	1.611745
36	6	0	2.044793	-3.433794	0.670806
37	6	0	1.756331	-3.439058	-0.685699
38	6	0	2.752125	-3.019456	-1.656164
39	6	0	2.060056	-2.299543	-2.708780
40	6	0	2.655799	-1.176630	-3.286823
41	6	0	3.960084	-0.727936	-2.832667
42	6	0	3.960120	0.727745	-2.832670
43	6	0	4.625027	1.424980	-1.820704
44	6	0	4.008698	2.596987	-1.222916
45	6	0	4.319222	2.595851	0.197546
46	6	0	3.361648	3.015748	1.123384
47	6	0	3.190496	2.296664	2.368430
48	6	0	1.770975	2.281693	2.678830
49	6	0	1.215288	1.165464	3.288002
50	6	0	2.030601	-0.000048	3.569376
51	6	0	3.385197	-0.000079	3.252877
52	6	0	3.981981	-1.177751	2.645303
53	6	0	3.190389	-2.296812	2.368432
54	6	0	3.361507	-3.015906	1.123387
55	6	0	4.319101	-2.596057	0.197549
56	6	0	5.131321	-1.424858	0.477222
57	6	0	4.964425	-0.728238	1.675142
58	6	0	4.964459	0.728005	1.675142
59	6	0	3.982038	1.177565	2.645303
60	6	0	5.131385	1.424616	0.477220
61	6	0	5.315208	0.697823	-0.769432
62	6	0	5.315177	-0.698075	-0.769432
63	6	0	4.624959	-1.425200	-1.820700
64	6	0	4.008578	-2.597180	-1.222913
65	6	0	-3.309907	2.786038	0.741737
66	6	0	-3.746292	2.962397	2.058143
67	6	0	-4.353429	4.170303	2.386863
68	6	0	-4.507008	5.150491	1.406972
69	6	0	-4.053539	4.890922	0.107111
70	6	0	-3.310050	-2.785883	0.741732
71	6	0	-3.746517	-2.962184	2.058121
72	6	0	-4.353741	-4.170045	2.386839
73	6	0	-4.507330	-5.150246	1.406962
74	6	0	-4.053779	-4.890735	0.107119
75	7	0	-3.472550	-3.717232	-0.200717
76	7	0	-3.472393	3.717379	-0.200725
77	6	0	-4.163138	5.892915	-1.051617
78	6	0	-4.163412	-5.892735	-1.051600
79	6	0	-4.936704	5.226694	-2.211987
80	6	0	-2.733394	6.243316	-1.525772
81	6	0	-4.888390	7.186578	-0.641644
82	6	0	-4.936918	-5.226474	-2.211991
83	6	0	-4.888753	-7.186347	-0.641634
84	6	0	-2.733679	-6.243219	-1.525727
85	1	0	-4.625809	1.237902	-0.851222
86	1	0	-4.625876	-1.237674	-0.851220
87	1	0	-3.610359	2.180170	2.797347
88	1	0	-4.704616	4.349986	3.399741
89	1	0	-4.974730	6.095532	1.655549
90	1	0	-3.610582	-2.179940	2.797308
91	1	0	-4.704993	-4.349683	3.399703
92	1	0	-4.975127	-6.095251	1.655535
93	1	0	-4.981961	5.902807	-3.074005
94	1	0	-5.965448	4.987922	-1.915530
95	1	0	-4.445960	4.299905	-2.520259
96	1	0	-2.774589	6.912987	-2.393204
97	1	0	-2.186466	5.339286	-1.807016
98	1	0	-2.168686	6.749955	-0.733832
99	1	0	-4.949408	7.862231	-1.501983

100	1	0	-4.357712	7.719547	0.156059	107	1	0	-4.358141	-7.719331	0.156104
101	1	0	-5.912735	6.991492	-0.302574	108	1	0	-2.774891	-6.912907	-2.393144
102	1	0	-4.982175	-5.902582	-3.074013	109	1	0	-2.169011	-6.749868	-0.733764
103	1	0	-4.446125	-4.299704	-2.520243	110	1	0	-2.186700	-5.339223	-1.806978
104	1	0	-5.965660	-4.987661	-1.915565						
105	1	0	-4.949777	-7.862014	-1.501962						
106	1	0	-5.913099	-6.991189	-0.302609						

The total electronic energy was calculated to be –3249.6746378 Hartree.

Table S18. Optimized structure of **2a** (B3LYP/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.779575	0.700551	-2.144749
2	6	0	-1.515548	1.524376	-2.013205
3	6	0	-1.052277	1.911570	-0.577047
4	6	0	-1.568349	1.393268	0.598312
5	6	0	-2.963539	0.826531	0.740435
6	6	0	-2.990085	-0.710496	0.750871
7	6	0	-1.615881	-1.327548	0.619523
8	6	0	-1.118070	-1.880709	-0.547803
9	6	0	-1.568257	-1.499553	-1.989622
10	6	0	-0.338469	-0.703751	-2.456311
11	6	0	-0.314344	0.679061	-2.466847
12	6	0	0.951785	1.372683	-2.546576
13	6	0	1.184332	2.494260	-1.638174
14	6	0	0.219742	2.614127	-0.545851
15	6	0	0.682503	3.029601	0.705735
16	6	0	0.231357	2.329755	1.893970
17	6	0	-0.704090	1.301345	1.775544
18	6	0	-0.445560	0.027379	2.486770
19	6	0	-0.748772	-1.247439	1.795278
20	6	0	0.150780	-2.305385	1.929157
21	6	0	0.576734	-3.039036	0.752219
22	6	0	0.128333	-2.627072	-0.505767
23	6	0	1.096355	-2.557237	-1.599451
24	6	0	0.902618	-1.442472	-2.525086
25	6	0	2.026696	-0.781290	-3.027752
26	6	0	2.051919	0.665147	-3.038874
27	6	0	3.408980	1.085853	-2.793156
28	6	0	3.638874	2.207836	-2.008498
29	6	0	2.512944	2.912734	-1.420165
30	6	0	2.951009	3.398453	-0.125999
31	6	0	4.311987	2.951561	0.109108
32	6	0	4.739685	2.210559	-1.060954
33	6	0	5.541510	1.074469	-0.914655
34	6	0	5.283499	-0.104498	-1.724148
35	6	0	4.239148	-0.093397	-2.645465
36	6	0	3.368345	-1.245105	-2.775322
37	6	0	3.559306	-2.362431	-1.973669
38	6	0	2.409627	-3.018488	-1.374830
39	6	0	2.830859	-3.499037	-0.073112
40	6	0	1.926206	-3.488797	0.979559
41	6	0	2.344917	-3.052699	2.296072
42	6	0	1.243886	-2.296964	2.857696
43	6	0	1.475614	-1.157437	3.609552
44	6	0	0.644816	0.015476	3.400625
45	6	0	1.516053	1.161771	3.591655
46	6	0	1.323777	2.297601	2.822946
47	6	0	2.450419	3.005421	2.249659
48	6	0	2.046805	3.435336	0.926465
49	6	0	4.702329	2.532832	1.385153
50	6	0	3.747506	2.560517	2.480510
51	6	0	3.962844	1.381222	3.303608
52	6	0	2.869931	0.703151	3.853321
53	6	0	2.844719	-0.742315	3.864581
54	6	0	3.913325	-1.466292	3.325588
55	6	0	3.656844	-2.649912	2.520612
56	6	0	4.611685	-2.672037	1.425034
57	6	0	4.206611	-3.096325	0.155458
58	6	0	4.659612	-2.388832	-1.025799
59	6	0	5.500666	-1.279281	-0.896729
60	6	0	5.905963	-0.826732	0.422322
61	6	0	5.931238	0.628352	0.411219
62	6	0	5.518318	1.342538	1.537985
63	6	0	5.061881	0.631856	2.724560
64	6	0	5.037564	-0.764446	2.735271
65	6	0	5.468653	-1.508677	1.559834
66	6	0	-1.837583	-2.766914	-2.825319
67	6	0	-1.547548	-2.839063	-4.191296
68	6	0	-1.913031	-3.995935	-4.872703
69	6	0	-2.552384	-5.026783	-4.184544
70	6	0	-2.819729	-4.870780	-2.818193
71	6	0	-3.507918	-5.935811	-1.952511
72	6	0	-1.740047	2.786939	-2.869366
73	6	0	-1.439492	2.828992	-4.234314
74	6	0	-1.760278	3.987718	-4.934727
75	6	0	-2.367950	5.049813	-4.265755
76	6	0	-2.650495	4.922531	-2.899458
77	6	0	-3.313021	6.020585	-2.055454
78	6	0	-3.669491	-1.094019	2.073464
79	6	0	-3.624596	1.250512	2.059707
80	6	0	-4.683612	0.110330	4.018937
81	6	0	-4.234123	0.972543	5.023927
82	6	0	-4.888397	0.990923	6.254734
83	6	0	-5.977148	0.149686	6.489261
84	6	0	-6.415336	-0.711781	5.482429
85	6	0	-5.776110	-0.732805	4.243518
86	8	0	-3.905090	-2.216428	2.458073
87	6	0	-2.802785	-0.633978	-2.134732
88	7	0	-2.336617	3.796664	-2.233057
89	7	0	-4.014551	0.089199	2.751443

90	7	0	-2.462857	-3.746945	-2.170412	112	1	0	-3.743226	-1.159022	-2.282027
91	6	0	-4.591314	5.443966	-1.404848	113	1	0	-5.061910	6.198796	-0.763995
92	6	0	-3.687779	7.256129	-2.892134	114	1	0	-4.354051	4.570468	-0.791943
93	6	0	-2.323618	6.441419	-0.943691	115	1	0	-5.321822	5.144744	-2.166675
94	6	0	-2.508307	-6.392721	-0.864190	116	1	0	-4.161885	8.005631	-2.248986
95	6	0	-3.955404	-7.157685	-2.773282	117	1	0	-4.398798	7.010595	-3.690062
96	6	0	-4.743699	-5.303953	-1.271842	118	1	0	-2.807893	7.725506	-3.347808
97	8	0	-3.810215	2.385151	2.435554	119	1	0	-2.787251	7.187354	-0.287305
98	1	0	-3.701213	1.255823	-2.299909	120	1	0	-1.414782	6.883160	-1.369948
99	1	0	-3.596800	1.229381	-0.050816	121	1	0	-2.032528	5.578390	-0.338788
100	1	0	-3.634654	-1.101070	-0.037453	122	1	0	-2.984703	-7.116819	-0.192658
101	1	0	-1.049989	-2.019814	-4.699176	123	1	0	-2.167312	-5.539849	-0.270931
102	1	0	-1.701709	-4.096662	-5.934187	124	1	0	-1.629274	-6.872509	-1.311396
103	1	0	-2.836852	-5.931344	-4.708417	125	1	0	-4.449093	-7.881850	-2.115977
104	1	0	-0.967061	1.985993	-4.727045	126	1	0	-3.107751	-7.669279	-3.244349
105	1	0	-1.538515	4.065761	-5.995990	127	1	0	-4.671151	-6.883783	-3.557676
106	1	0	-2.616690	5.956175	-4.804392	128	1	0	-5.227584	-6.036226	-0.614928
107	1	0	-3.390239	1.625730	4.839223	129	1	0	-5.481224	-4.978485	-2.015903
108	1	0	-4.540169	1.664225	7.032919	130	1	0	-4.454462	-4.438497	-0.670131
109	1	0	-6.480706	0.164716	7.451875	---					
110	1	0	-7.260437	-1.371679	5.657207	The total electronic energy was calculated to be –3840.204568 Hartree.					
111	1	0	-6.110248	-1.405928	3.463595						

6. References

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(3) G. M. Sheldrick, *Acta Crystallogr. A*, 2015, **71**, 3–8.