

Electronic Supplementary Information

Assembly and Optical Properties of 1D Helical Bundles Induced by Triphenylamine, Side Chains and Solvents in Crystals

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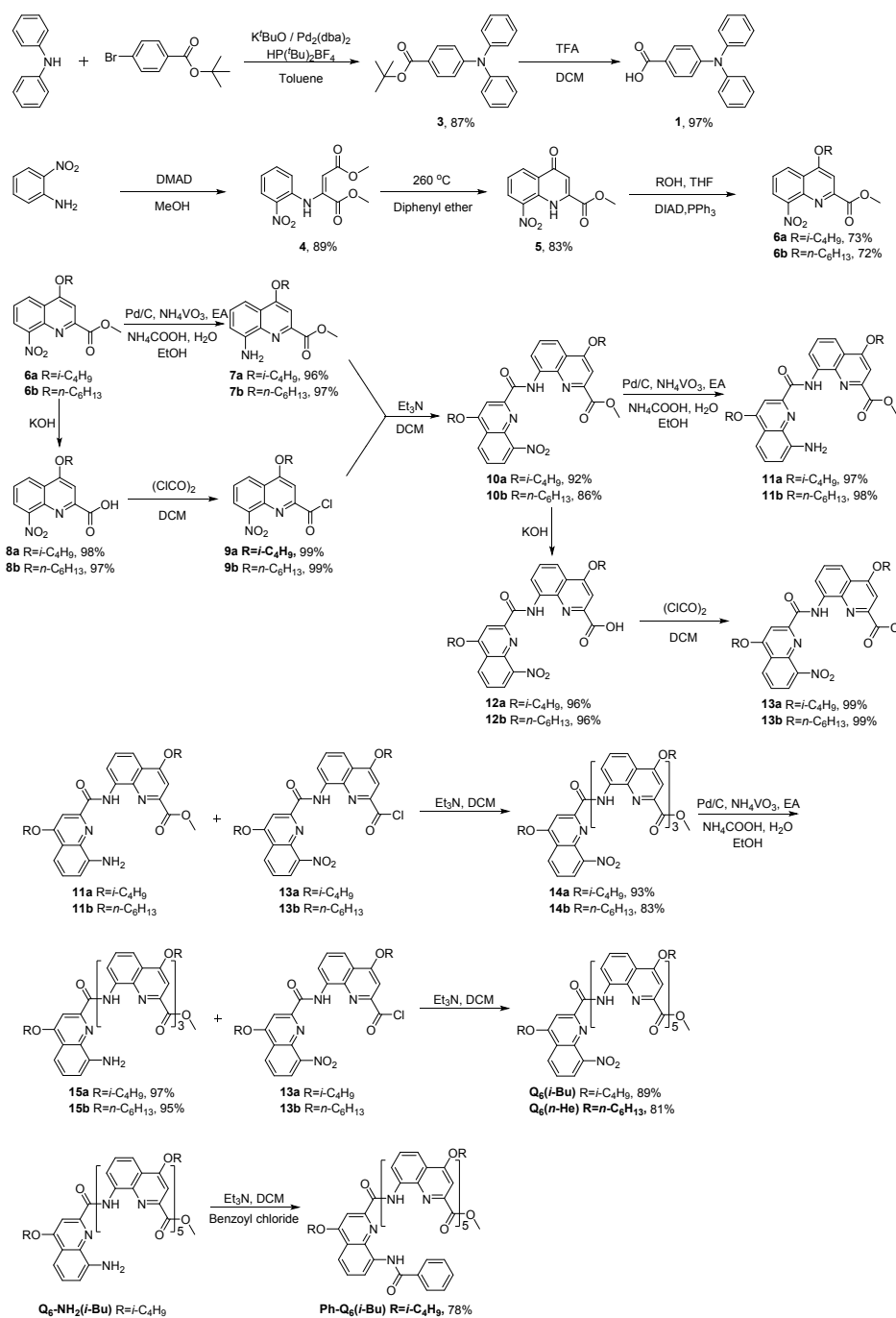
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1. Synthetic procedures



Scheme S1 Synthesis of quinoline amide hexamer derivatives.

Compound 3: An oven dried 250 mL 2-neck round bottom flask containing a stir bar was charged with potassium *tert*-butoxide (4.18 g, 37.2 mmol), diphenylamine (3.00 g, 17.7 mmol), and *tert*-butyl-4-bromobenzoate (4.92 g, 19.2 mmol). The flask was fitted with septa, purged with argon, toluene (88 mL) was added at once *via* syringe, and the system was purged with argon once more. Next, Pd₂(dba)₃ (811 mg, 886 μmol) and HP(*t*Bu)₃BF₄ (514 mg, 1.77 mmol) were added together at once and the system was purged with argon. The solution was allowed to stir (24 h), after which it was poured into water (100 mL) and the organic layer was separated.

The aqueous layer was extracted with methylene chloride (75 mL), the organic extracts were combined, dried over MgSO₄, filtered, and concentrated in vacuo. The crude solid was purified via column chromatography using an eluent of methylene chloride–hexanes yielding a white solid (5.35 g, 87.00%). ¹H NMR (400 MHz, CDCl₃): δ = 7.82 (d, 2H, *J* = 8.88 Hz), 7.31–7.27 (m, 4H), 7.13–6.98 (m, 6H), 6.97 (d, 2H, *J* = 8.84 Hz), 1.57 (s, 9H). ¹³C NMR (101 MHz, CDCl₃): δ = 165.76, 151.73, 146.97, 130.77, 129.62, 125.69, 124.45, 124.28, 120.54, 80.52, 28.39.

Compound 1: A 25 mL vial containing a stir bar was charged with **1** (1.73 g, 5 mmol), methylene chloride (10 mL), and trifluoroacetic acid (3.71 mL, 50 mmol) was allowed to stir (room temperature, 6 h), solvent was removed in vacuo yielding as white solids, (1.41 g, 97.13%). ¹H NMR (400 MHz, CDCl₃): δ = 7.93–7.89 (m, 2H), 7.35–7.30 (m, 4H), 7.18–7.11 (m, 6H), 7.01–6.97 (m, 2H). ¹³C NMR (101 MHz, CDCl₃): δ = 172.30, 152.81, 146.53, 131.70, 129.75, 126.17, 124.82, 120.90, 119.57.

Compound 6b: Add **5** (4.00 g, 16.13 mmol) and triphenylphosphine (4.65 g, 17.75 mmol) into the reaction flask under a nitrogen atmosphere. Add *n*-hexanol (2.23 mL, 17.75 mmol) into the flask using a syringe through the septum and cool it down to 0 °C by placing it in an ice bath. 120 mL of dry THF was added to the reaction vial through the septum using a syringe. By using a dry syringe, deliver diisopropyl azodicarboxylate (3.98 mL, 17.75 mmol) to the solution and stir the reaction mixture further at 0 °C for 30 min. Remove the ice bath. Let the reaction mixture warm up to room temperature and stir it for 12 h. Remove the solvents using a rotary evaporator. The crude mixture was dissolved in 80 mL of cold methanol (–18 °C) and the solution was left at –18 °C for 12 h. After the addition of cold methanol, the product was crystallized and isolated by cold filtration yielding a yellow solid (3.80 g, 71.00%). ¹H NMR (400 MHz, CDCl₃): δ = 8.47 (dd, *J* = 8.5, 1.3 Hz, 1H), 8.10 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.67–7.63 (m, 2H), 4.32 (t, *J* = 6.5 Hz, 2H), 4.03 (s, 3H), 1.98 (dq, *J* = 13.2, 6.5 Hz, 2H), 1.60 – 1.53 (m, 2H), 1.42 – 1.35 (m, 4H), 0.93 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ = 165.87, 162.92, 151.42, 148.46, 140.17, 126.61, 126.06, 125.27, 123.45, 102.31, 69.82, 53.55, 31.58, 28.82, 25.81, 22.69, 14.15. MS: Calcd for C₁₇H₂₁N₂O₅ (M⁺) 333.14505, Found: 333.14449.

Compound 7b: 6b (0.33 g, 1 mmol) was dissolved in 10 mL ethyl acetate and 2 mL ethanol, and Palladium 10% on carbon (31 mg) and ammonium vanadate (15.10 mg) was added into **6b** solution. Ammonium formate (1.26 g, 20 mmol) was dissolved in 2 mL H₂O, which was added into solution drop by drop. After reflux at 90 °C for 6 h. After cooling to room temperature, the Palladium 10% on carbon was washed off with diatomaceous earth, and the filtrate was collected and extracted with ethyl acetate and water. The organic phase was dried with anhydrous MgSO₄, filtered, and evaporated under vacuum. The product was dried and a yellow solid was gained (0.29 g, 96.68%). ¹H NMR (400 MHz, CDCl₃): δ = 7.51 – 7.49 (m, 2H), 7.38 – 7.34 (m, 1H), 6.93 (dd, *J* = 7.5, 1.2 Hz, 1H), 5.11 (s, 2H), 4.23 (t, *J* = 6.5 Hz, 2H), 4.07 – 3.98 (m, 3H), 1.94 (dt, *J* = 14.4, 6.5 Hz, 2H), 1.60–1.51 (m, 2H), 1.43–1.35 (m, 4H), 0.92 (dd, *J* = 8.1, 5.9 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃): δ = 166.54, 162.72, 145.93, 144.97, 138.47, 128.70, 123.09, 110.96, 109.76, 100.89, 68.94, 52.95, 31.64, 28.97, 25.88, 22.72, 14.17. MS: Calcd for C₁₇H₂₃N₂O₃ (M⁺) 303.17087, Found: 303.17031.

Compound 8b: 6b (0.33 g, 1 mmol) was dissolved in 10 mL 1,4-dioxane, and potassium hydroxide powder (0.56 g, 10 mmol) was added into **6b** solution and reacted for 12 h. After that diluted aqueous citric acid solution was added into it to make pH of the solution to 5~6

after which was washed by dichloromethane and water. The organic phase was dried with anhydrous MgSO_4 , filtered, and evaporated under vacuum. The product was dried and a yellow solid was gained (0.31 g, 96.39%). ^1H NMR (400 MHz, CDCl_3): δ = 8.54 (dd, J = 8.5, 1.4 Hz, 1H), 8.23 (dd, J = 7.5, 1.4 Hz, 1H), 7.75 – 7.71 (m, 2H), 4.37 (t, J = 6.5 Hz, 2H), 2.00 (dt, J = 14.4, 6.5 Hz, 2H), 1.62 – 1.51 (m, 2H), 1.47 – 1.33 (m, 4H), 1.25 (s, 1H), 0.95 – 0.91 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3): δ = 164.42, 163.78, 149.41, 147.22, 138.47, 127.36, 126.63, 126.37, 123.82, 100.36, 70.46, 31.55, 28.74, 25.76, 22.69, 14.15. MS: Calcd for $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_5$ (M^+) 319.12940, Found: 319.12884.

Compound 10b: Oxalyl chloride (0.34 mL, 4 mmol) was added dropwise to a solution of **8b** (0.35 g, 1.1 mmol) in anhydrous DCM at 0 °C under nitrogen with stirring, and the reaction mixture was then warmed to room temperature. After 2 h, excess oxalyl chloride was distilled off under reduced pressure. The freshly obtained **9b** was dissolved in DCM, transferred to a double-necked flask containing a solution of **7b** (0.30 g, 1 mmol) and triethylamine (2.5 mmol) in anhydrous DCM, and stirred for 12 hours. The resulting solution was diluted with DCM (30 mL) and washed successively with 0.5 M HCl (40 mL), water (20 mL) and sat. aq. Na_2CO_3 (25 mL). The organic phase was dried with anhydrous MgSO_4 , filtered, and evaporated under vacuum. The crude mixture was dissolved in 80 mL of cold methanol (–18 °C) and the solution is left at –18 °C for 12 h. After the addition of cold methanol, the product was crystallized and isolated by cold filtration yielding a yellow solid (0.52 g, 86.16%). ^1H NMR (400 MHz, CDCl_3): δ = 11.87 (1H, s), 9.09 (1H, dd, J = 1.3, 6.7 Hz), 8.52 (1H, dd, J = 1.3, 6.7 Hz), 8.19 (1H, dd, J = 1.3, 6.7 Hz), 8.00 (1H, m), 7.96 (1H, s), 7.66 (3H, m), 4.39 (2H, d, J = 6.7 Hz), 4.30 (2H, d, J = 6.7 Hz), 4.23 (3H, s), 2.00–1.95 (4H, m), 1.60–1.55 (6H, m), 1.43–1.38 (6H, m), 0.96–0.92 (6H, m). ^{13}C NMR (101 MHz, CDCl_3): δ = 167.08, 163.37, 162.90, 162.66, 154.11, 148.46, 147.95, 139.89, 139.53, 134.99, 127.95, 126.95, 125.59, 125.50, 123.57, 122.42, 118.90, 116.91, 101.62, 100.36, 69.89, 69.29, 53.82, 31.65, 31.62, 28.97, 28.87, 25.89, 25.84, 22.73, 14.18. MS: Calcd for $\text{C}_{33}\text{H}_{39}\text{N}_4\text{O}_7$ (M^+) 603.28187, Found: 603.28132.

Compound 11b: This compound was prepared from **10b** according to the procedure for **7b**. The product was dried and a yellow solid was gained (0.56 g, 97.86%). ^1H NMR (400 MHz, CDCl_3): δ = 9.03 (d, J = 7.7 Hz, 1H), 7.92 (d, J = 8.5 Hz, 1H), 7.75 (s, 1H), 7.64 (t, J = 8.2 Hz, 1H), 7.53 (d, J = 7.9 Hz, 2H), 7.37 (t, J = 7.9 Hz, 1H), 7.00 (d, J = 7.5 Hz, 1H), 5.53 (s, 2H), 4.33–4.26 (m, 4H), 4.09 (s, 3H), 1.98 (dd, J = 12.9, 6.3 Hz, 4H), 1.58 (s, 6H), 1.43–1.37 (m, 6H), 0.94 (td, J = 7.0, 1.7 Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3): δ = 165.52, 163.27, 148.38, 146.91, 144.86, 137.49, 135.34, 128.58, 128.25, 123.13, 122.31, 117.30, 115.80, 111.01, 109.68, 101.44, 98.33, 69.23, 69.06, 53.11, 31.69, 29.85, 29.05, 28.99, 25.92, 22.76, 14.20. MS: Calcd for $\text{C}_{33}\text{H}_{41}\text{N}_4\text{O}_5$ (M^+) 573.30770, Found: 573.30714.

Compound 12b: **10b** (0.60 g, 1 mmol) was dissolved in 10 mL THF, and potassium hydroxide powder (0.56 g, 10 mmol) was added into **10b** solution and reacted for 12 h. After that diluted aqueous citric acid solution was added into it to make pH of the solution to 5~6 after which was washed by dichloromethane and water. The organic phase was dried with anhydrous MgSO_4 , filtered, and evaporated under vacuum. The product was dried and a yellow solid was gained (0.56 g, 95.58%). ^1H NMR (400 MHz, CDCl_3): δ = 11.62 (s, 1H), 9.09 (d, J = 7.7 Hz, 1H), 8.48 (d, J = 8.3 Hz, 1H), 8.23 (dd, J = 7.5, 1.2 Hz, 1H), 8.01 (d, J = 8.3 Hz, 1H), 7.86 (s, 1H), 7.75 (s, 1H), 7.64 (td, J = 7.9, 3.3 Hz, 2H), 4.34 (dt, J = 13.0, 6.4 Hz, 4H), 2.09–

1.87 (m, 4H), 1.62–1.52 (m, 6H), 1.39 (dt, $J = 12.6, 6.3$ Hz, 6H), 1.24 (s, 1H), 0.94 (t, $J = 7.0$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3): $\delta = 164.83, 163.93, 163.56, 162.20, 153.40, 147.30, 146.79, 139.25, 138.56, 134.14, 128.42, 127.39, 126.05, 125.65, 123.44, 122.93, 119.48, 117.24, 100.27, 100.05, 70.02, 69.73, 31.61, 28.88, 28.83, 25.83, 22.71, 14.17$. MS: Calcd for $\text{C}_{32}\text{H}_{37}\text{N}_4\text{O}_7(\text{M}^+)$ 589.26622, Found: 589.26567.

Compound 14b: Oxalyl chloride (4 mmol) was added dropwise to a solution of **12b** (0.65 g, 1.1 mmol) in anhydrous DCM at 0 °C under nitrogen with stirring, and the reaction mixture was then warmed to room temperature. After 2 h, excess oxalyl chloride was distilled off under reduced pressure. The freshly obtained **13b** was dissolved in DCM, transferred to a double-necked flask containing a solution of **11b** (1 mmol) and triethylamine (2.5 mmol) in anhydrous DCM, and stirred for 12 hours. The resulting solution was diluted with DCM (30 mL) and washed successively with 0.5 M HCl (40 mL), water (20 mL) and sat. aq. Na_2CO_3 (25 mL). The organic phase was dried with anhydrous MgSO_4 , filtered, and evaporated under vacuum. The crude mixture was dissolved in 80 mL of cold methanol (−18 °C) and the solution was left at −18 °C for 12 h. After the addition of cold methanol, the product was crystallized and isolated by cold filtration yielding a yellow solid (0.94 g, 82.56%). ^1H NMR (400 MHz, CDCl_3): $\delta = 12.31$ (s, 1H), 11.90 (s, 1H), 11.67 (s, 1H), 9.13 (dd, $J = 7.5, 1.1$ Hz, 1H), 8.54 (dd, $J = 8.2, 1.4$ Hz, 1H), 8.35–8.37 (m, 1H), 8.14 (dd, $J = 7.5, 1.1$ Hz, 1H), 7.96–8.00 (m, 2H), 7.85–7.90 (m, 2H), 7.74 (t, $J = 8.0$ Hz, 1H), 7.57–7.61 (m, 2H), 7.47 (s, 1H), 7.37 (t, $J = 8.0$ Hz, 1H), 7.25–7.29 (m, 2H), 6.85 (s, 1H), 6.68 (s, 1H), 4.37–4.48 (m, 4H), 4.05–4.12 (m, 4H), 3.45 (s, 3H), 1.92–2.17 (m, 8H), 1.57–1.72 (m, 9H), 1.40–1.52 (m, 15H), 0.91–1.00 (m, 12H). ^{13}C NMR (101 MHz, CDCl_3): $\delta = 164.16, 163.60, 163.26, 163.14, 162.46, 161.71, 160.78, 153.71, 151.15, 149.15, 145.71, 145.30, 139.32, 139.19, 138.32, 135.30, 134.12, 133.89, 128.13, 127.46, 126.85, 126.08, 124.34, 123.92, 122.17, 122.08, 121.99, 117.82, 117.06, 116.90, 116.68, 116.34, 116.12, 100.61, 100.27, 98.89, 97.67, 69.86, 69.58, 69.21, 69.06, 52.54, 31.72, 29.04, 28.93, 25.97, 25.93, 25.88, 22.79, 14.24$. MS: Calcd for $\text{C}_{65}\text{H}_{76}\text{N}_8\text{O}_{11}(\text{M}^+)$ 1144.56336, Found: 1144.55498.

Compound 15b: This compound was prepared from **14b** according to the procedure for **7b**. The product was dried and then a yellow solid was gained (1.06 g, 94.36%). ^1H NMR (400 MHz, CDCl_3): $\delta = 12.45$ (s, 1H), 11.94 (s, 1H), 11.81 (s, 1H), 9.03 (d, $J = 7.5$ Hz, 1H), 8.43 (d, $J = 7.6$ Hz, 1H), 8.06 – 7.95 (m, 3H), 7.83 (d, $J = 8.3$ Hz, 1H), 7.72 (dd, $J = 13.5, 5.4$ Hz, 2H), 7.63 (t, $J = 8.0$ Hz, 1H), 7.51 (d, $J = 8.2$ Hz, 1H), 7.32 (s, 1H), 7.02 (t, $J = 7.9$ Hz, 1H), 6.91 (s, 1H), 6.68 (s, 1H), 5.96 (d, $J = 7.4$ Hz, 1H), 4.42 (t, $J = 6.4$ Hz, 4H), 4.19 – 4.00 (m, 5H), 3.79 (s, 2H), 3.52 (s, 3H), 2.17 – 2.03 (m, 5H), 1.99 (dd, $J = 13.9, 6.8$ Hz, 6H), 1.63 (dd, $J = 15.0, 6.9$ Hz, 15H), 1.55 – 1.37 (m, 22H), 1.33 – 1.17 (m, 10H), 1.05 – 0.93 (m, 16H). ^{13}C NMR (101 MHz, CDCl_3): $\delta = 163.09, 162.42, 160.90, 160.79, 149.75, 143.26, 142.19, 138.02, 135.74, 134.76, 133.87, 127.54, 121.96, 117.25, 116.49, 109.78, 100.39, 98.56, 68.96, 52.43, 31.75, 31.67, 29.08, 28.99, 28.92, 25.93, 25.86, 22.75, 14.23$. MS: Calcd for $\text{C}_{65}\text{H}_{77}\text{N}_8\text{O}_9(\text{M}^+)$ 1113.58135, Found: 1113.58080.

Compound $\text{Q}_6(n\text{-He})$: This compound was prepared from **15b** according to the procedure for **14b**. The product was dried and a yellow solid was gained (0.35 g, 80.38%). ^1H NMR (400 MHz, CDCl_3): $\delta = 11.82$ (s, 1H), 11.61 (s, 1H), 11.54 (s, 1H), 11.36 (d, $J = 8.2$ Hz, 2H), 8.51 (d, $J = 7.8$ Hz, 1H), 8.36 (d, $J = 8.2$ Hz, 1H), 8.26–8.29 (m, 1H), 8.21 (d, $J = 6.4$ Hz, 1H), 8.11 (d, $J = 7.8$ Hz, 1H), 8.02–8.07 (m, 2H), 7.93–8.00 (m, 2H), 7.76 (d, $J = 8.2$ Hz, 1H),

7.64 (t, $J = 8.0$ Hz, 1H), 7.38-7.48 (m, 5H), 7.32 (t, $J = 8.0$ Hz, 1H), 7.22-7.26 (m, 2H), 7.14 (q, $J = 8.1$ Hz, 2H), 6.81 (s, 1H), 6.73 (s, 1H), 6.54 (s, 1H), 6.47 (s, 1H), 4.24-4.62 (m, 5H), 4.07-4.21 (m, 6H), 3.94 (s, 2H), 3.14 (s, 3H), 1.85-2.20 (m, 14H), 1.38-1.72 (m, 43H), 1.20-1.27 (m, 2H), 0.83-1.05 (m, 23H). ^{13}C NMR (101 MHz, CDCl_3): $\delta = 163.94, 163.31, 163.21, 163.09, 162.69, 162.09, 161.38, 161.24, 160.86, 160.22, 160.19, 153.09, 150.59, 149.46, 148.92, 148.81, 145.31, 144.85, 138.88, 138.45, 138.34, 138.10, 137.72, 134.22, 133.90, 133.77, 133.63, 132.77, 128.13, 127.48, 127.08, 127.00, 126.53, 126.03, 125.87, 124.01, 123.68, 122.72, 122.39, 121.93, 121.74, 121.53, 117.12, 117.04, 116.77, 116.67, 116.42, 116.06, 116.00, 115.73, 100.17, 99.96, 99.71, 98.05, 97.76, 97.66, 77.45, 77.35, 77.14, 76.82, 69.68, 69.50, 69.43, 69.37, 69.19, 69.14, 68.76, 52.20, 31.76, 31.63, 29.79, 29.14, 29.01, 28.89, 28.80, 25.94, 25.89, 25.77, 22.80, 22.75, 22.72, 14.30, 14.26, 14.22, 14.19, 1.12$. MS: Calcd for $\text{C}_{97}\text{H}_{111}\text{N}_{12}\text{O}_{15}$ (M^+) 1683.82919, Found: 1683.82863.

Compound $\text{Q}_6\text{-NH}_2(n\text{-He})$: This compound was prepared from $\text{Q}_6(n\text{-He})$ according to the procedure for **7b**. The product was dried and a yellow solid was gained (0.58 g, 95.35%). ^1H NMR (400 MHz, CDCl_3): $\delta = 11.86$ (s, 1H), 11.68 (d, $J = 21.5$ Hz, 2H), 11.43 (s, 1H), 11.38 (s, 1H), 8.60 (d, $J = 7.3$ Hz, 1H), 8.20 (d, $J = 6.9$ Hz, 1H), 8.10-8.15 (m, 1H), 8.05 (d, $J = 8.7$ Hz, 1H), 7.90-7.99 (m, 5H), 7.78 (d, $J = 7.8$ Hz, 1H), 7.65 (q, $J = 8.4$ Hz, 1H), 7.54 (d, $J = 7.3$ Hz, 1H), 7.29-7.46 (m, 5H), 6.97 (s, 1H), 6.88 (t, $J = 7.8$ Hz, 1H), 6.80 (s, 1H), 6.73 (s, 1H), 6.54 (s, 1H), 6.47 (s, 1H), 5.78 (d, $J = 7.3$ Hz, 1H), 4.60 (dd, $J = 14.6, 6.4$ Hz, 1H), 4.43 (q, $J = 7.6$ Hz, 2H), 4.04-4.34 (m, 13H), 3.94 (s, 3H), 3.36 (s, 2H), 3.15 (d, $J = 5.0$ Hz, 5H), 1.87-2.18 (m, 22H), 1.42-1.71 (m, 71H), 1.20-1.32 (m, 9H), 0.93-1.05 (m, 33H). ^{13}C NMR (101 MHz, CDCl_3): $\delta = 163.93, 163.60, 163.23, 163.08, 162.95, 162.69, 162.16, 161.87, 161.63, 161.26, 160.79, 159.25, 150.58, 150.20, 149.65, 149.12, 148.09, 145.30, 143.07, 138.92, 138.40, 138.12, 137.72, 136.10, 133.79, 133.73, 133.51, 132.90, 127.57, 126.99, 126.78, 126.51, 126.37, 122.85, 122.58, 122.00, 121.92, 121.63, 117.10, 116.92, 116.77, 116.68, 116.42, 116.31, 115.98, 115.73, 115.42, 109.96, 109.50, 100.13, 99.62, 98.66, 98.22, 98.05, 97.77, 97.47, 77.44, 77.33, 77.13, 76.81, 69.48, 69.30, 69.17, 68.76, 52.16, 32.02, 31.78, 31.68, 31.64, 31.52, 30.27, 29.80, 29.41, 29.14, 29.06, 28.98, 28.90, 25.94, 25.89, 25.81, 22.80, 14.30, 14.25, 14.20, 1.12$. MS: Calcd for $\text{C}_{97}\text{H}_{113}\text{N}_{12}\text{O}_{13}$ (M^+) 1653.85501, Found: 1653.85445.

Compound Ph- $\text{Q}_6(i\text{-Bu})$: This compound was prepared from $\text{Q}_6\text{-NH}_2(i\text{-Bu})$ and benzoyl chloride according to the procedure for **TPA- $\text{Q}_6(i\text{-Bu})$** . The crude product was purified by column chromatography eluting with petroleum ether/ethyl acetate = 4/1 to get the compound as a yellow solid (78.24%). ^1H NMR (400 MHz, CDCl_3): $\delta = 11.77$ (s, 1H), 11.58 (s, 1H), 11.39 (s, 1H), 11.31 (s, 1H), 11.26 (s, 1H), 9.63 (s, 1H), 8.52 (d, $J = 7.4$ Hz, 1H), 8.18 (d, $J = 7.4$ Hz, 1H), 8.14 – 8.03 (m, 4H), 8.02 – 7.94 (m, 3H), 7.86 – 7.78 (m, 2H), 7.57 (t, $J = 9.1$ Hz, 2H), 7.45 (dd, $J = 15.3, 7.6$ Hz, 2H), 7.39 – 7.34 (m, 1H), 7.29 (d, $J = 7.7$ Hz, 2H), 7.25 – 7.13 (m, 4H), 7.04 (s, 1H), 6.81 (s, 1H), 6.72 (t, $J = 7.2$ Hz, 2H), 6.65 (s, 1H), 6.46 (s, 2H), 4.42 – 4.36 (m, 1H), 4.23 – 4.16 (m, 1H), 4.10 (dd, $J = 15.0, 8.9$ Hz, 2H), 3.99 (d, $J = 6.5$ Hz, 1H), 3.93 (dd, $J = 14.5, 7.0$ Hz, 3H), 3.83 (d, $J = 3.6$ Hz, 2H), 3.74 (d, $J = 4.4$ Hz, 2H), 3.12 (s, 3H), 2.60 – 2.38 (m, 4H), 2.32 – 2.20 (m, 2H), 1.38 – 1.29 (m, 18H), 1.24 – 1.16 (m, 18H). ^{13}C NMR (101 MHz, CDCl_3): $\delta = 163.72, 163.00, 162.91, 162.82, 162.70, 162.38, 161.93, 161.17, 160.83, 160.53, 159.64, 159.33, 159.22, 150.32, 150.01, 149.23, 149.07, 148.95, 148.69, 148.20, 146.76, 144.98, 138.66, 137.98, 137.47, 136.82, 133.67, 133.52, 133.33, 133.01, 132.82, 132.74, 132.50, 129.14, 127.84, 126.61, 126.28, 125.87, 125.53, 125.28, 123.62,$

122.41, 122.10, 121.94, 121.56, 121.40, 120.17, 116.78, 116.36, 116.10, 115.66, 100.02, 99.48, 99.11, 98.91, 98.33, 97.66, 97.37, 75.24, 75.00, 74.72, 52.03, 28.30, 28.14, 28.03, 19.70, 19.58, 19.54, 19.49, 19.34, 19.22. HRMS (ESI): m/z calcd for $C_{92}H_{92}N_{12}NaO_{14}$ $[M+Na]^+$: 1611.6686, found 1611.6743

2. Crystallographic data

Table S1. Summary of the single-crystal X-ray diffraction measurement and refinement data for TPA-Q₆(*i*-Bu), TPA-Q₆(*n*-He) and Q₆(*i*-Bu)

	TPA-Q ₆ (<i>i</i> -Bu)	TPA-Q ₆ (<i>n</i> -He)	Q ₆ (<i>i</i> -Bu)
Chemical formula	C ₁₀₄ H ₁₀₁ N ₁₃ O ₁₄	C ₁₁₆ H ₁₂₅ N ₁₃ O ₁₄	C ₈₅ H ₈₆ N ₁₂ O ₁₅
M_r	1756.97	1925.28	1535.84
Crystal size [mm ³]	0.28×0.15×0.02	0.32×0.25×0.19	0.31×0.230.31
Crystal system	monoclinic	triclinic	triclinic
Space group	P2 ₁ /n	P -1	P -1
a [Å]	10.36860(10)	16.27079(7)	16.7010(2)
b [Å]	31.9891(3)	24.57400(9)	20.4228(2)
c [Å]	31.1143(2)	28.66463(11)	24.0650(2)
α [°]	90	98.3767(4)	89.1260(10)
β [°]	95.4050(10)	100.3866(3)	76.3960(10)
γ [°]	90	10081.83(8)	87.1740(10)
V [Å ³]	10274.17(15)	10081.83(8)	7968.08(14)
Z	4	4	2
ρ_{calcd} [g cm ⁻³]	1.148	1.268	1.280
μ [mm ⁻¹]	0.629	0.675	0.732
F(000)	3754	4096	3245
θ range [°]	3.110 to 75.569	2.953 to 75.598	2.725 to 75.741
hkl ranges	-12/12, -36/39, -38/38	-20/19, -30/24, -34/35	-19/20, -25/25, -29/29
Reflections collected	203504	135593	31781
Independent reflections	20643	39991	31781
R_{int}	0.0387	0.0239	—
Completeness [%]	99.93 ($\theta = 66.97$)	99.88 ($\theta = 66.97$)	99.85 ($\theta = 68.13$)
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0738$ $wR_2 = 0.2654$	$R_1 = 0.0737$ $wR_2 = 0.2094$	$R_1 = 0.1204$ $wR_2 = 0.3199$
R indices (all data)	$R_1 = 0.0970$ $wR_2 = 0.2779$	$R_1 = 0.0803$ $wR_2 = 0.2201$	$R_1 = 0.1276$ $wR_2 = 0.3236$
Goodness-of-fit on F^2	1.040	1.029	1.058
CCDC	2048310	2048233	2048229

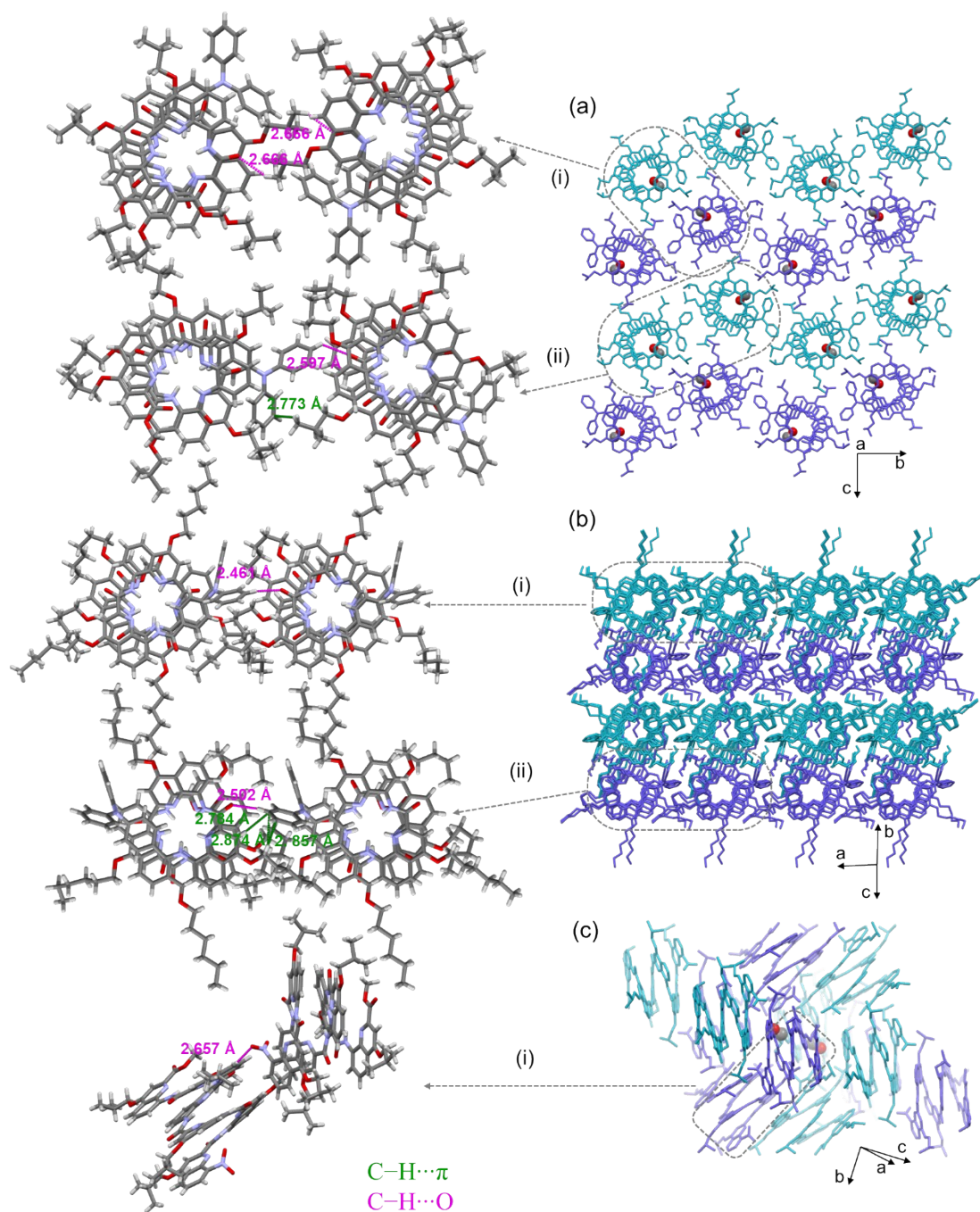


Fig. S1 (a) Assembled crystal structure of TPA-Q₆(*i*-Bu) in which (i) and (ii) are interactions between two helical molecules. (b) Assembled crystal structure TPA-Q₆(*n*-He) in which (i) and (ii) are interactions between two helical molecules. (c) Supramolecular cage of Q₆(*i*-Bu) containing two methanol molecules, where (i) is a weak interaction between a set of dimers. *M*- and *P*-helices are shown in purple and blue, respectively.

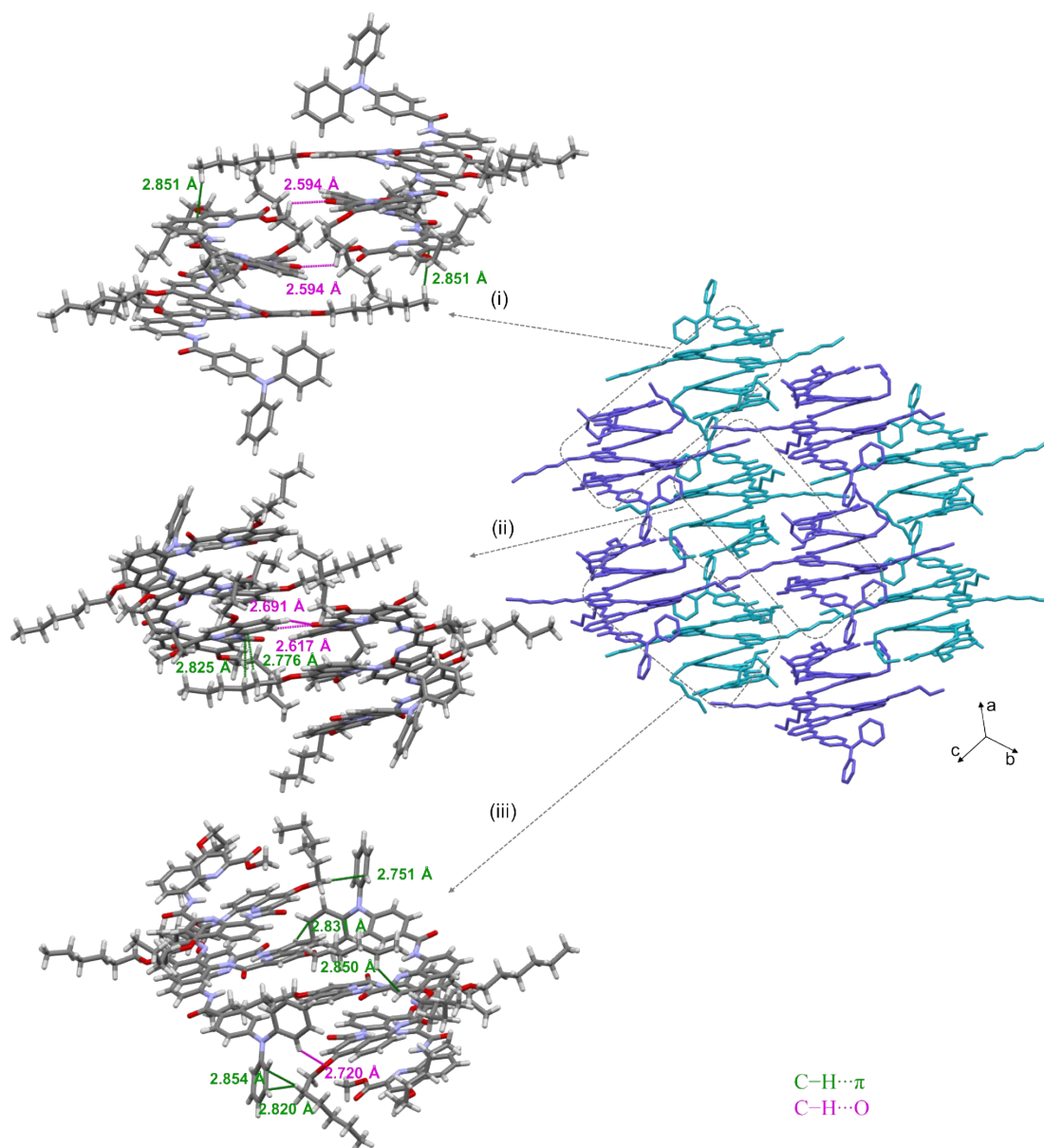


Fig. S2 Assembled crystal structure of TPA-Q₆(*n*-He) in which (i), (ii) and (iii) are interactions between two helical molecules. *M*- and *P*-helices are shown in purple and blue, respectively.

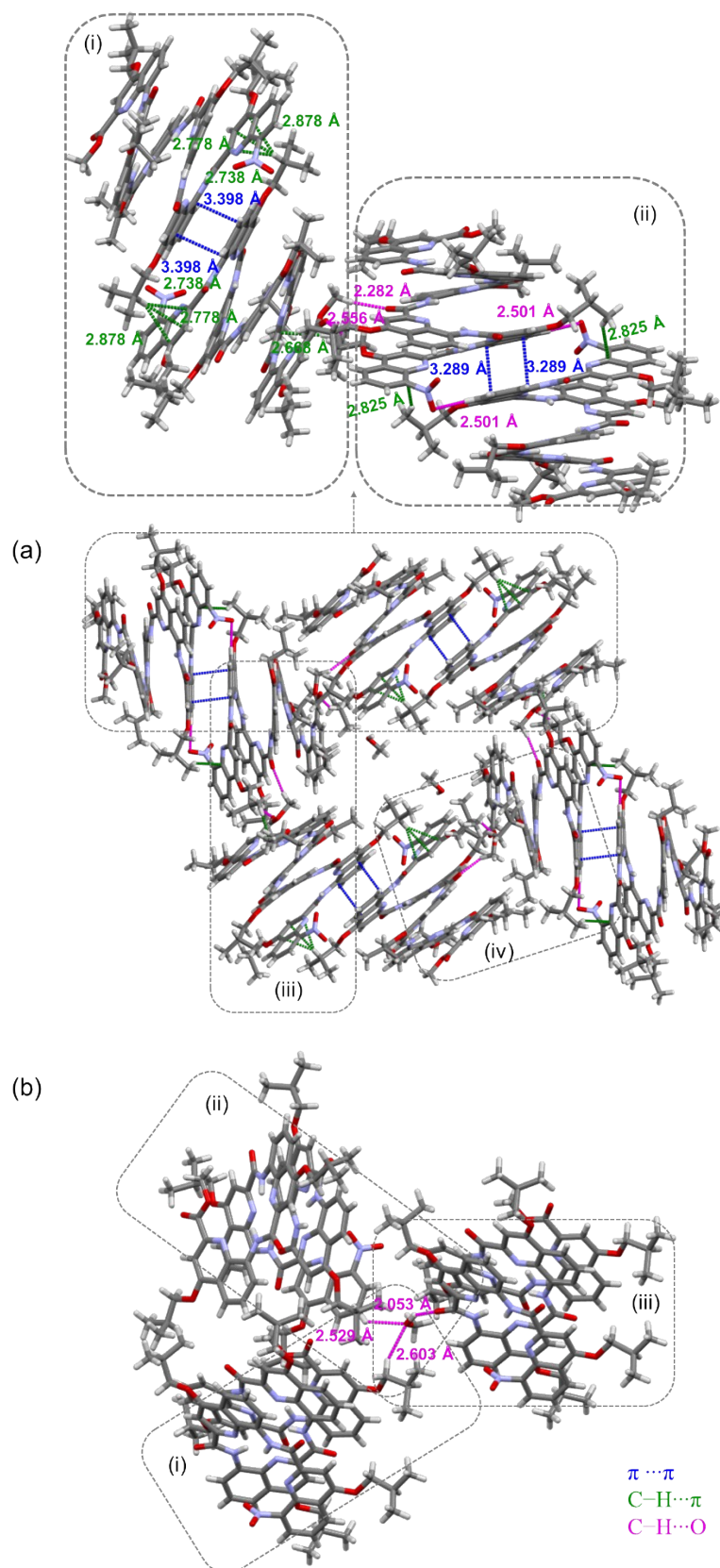


Fig. S3 The interactions between the four pairs of enantiomers in $Q_6(i-Bu)$ crystal: in (a), (i) - (iv) are weak interactions between the dimers; in (b), (i) - (iii) are weak interactions between the dimers and the methanol molecule.

3. Optical properties

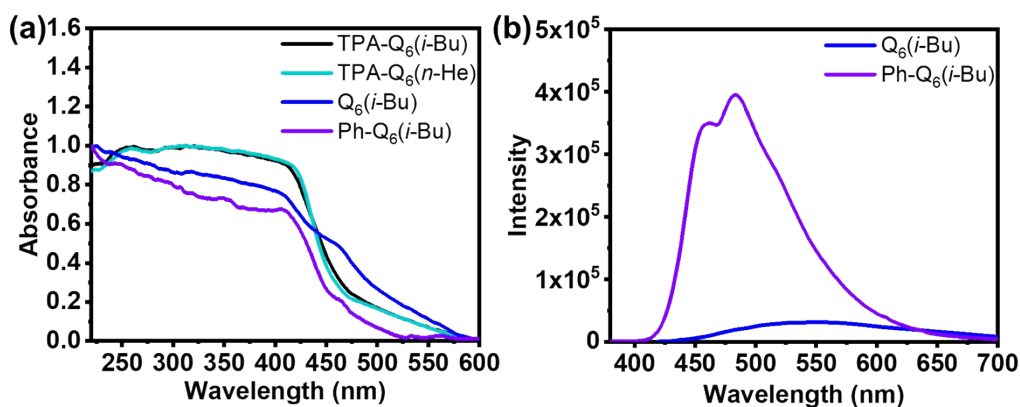


Fig. S4 (a) Absorption spectra of TPA-Q₆(*i*-Bu), TPA-Q₆(*n*-He), Q₆(*i*-Bu) and Ph-Q₆(*i*-Bu) and (b) fluorescence spectrum of Q₆(*i*-Bu) and Ph-Q₆(*i*-Bu) in crystals at room temperature, excited at 360 nm.

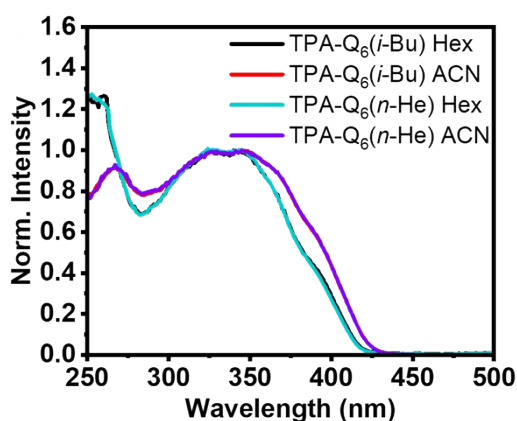


Figure S5. Excitation spectra of TPA-Q₆(*i*-Bu) and TPA-Q₆(*n*-He) in Hex and ACN solutions, respectively.

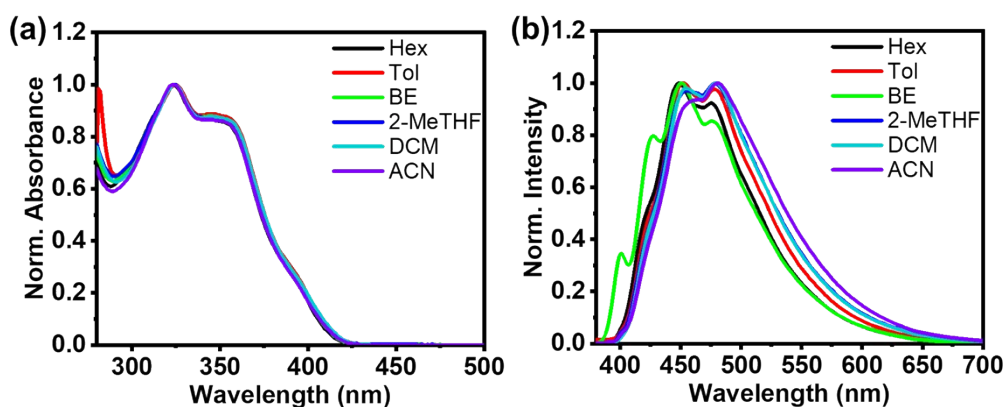


Fig. S6 (a) Absorption spectra and (b) fluorescence spectra of Ph-P₆(*i*-Bu) in different solvents at room temperature, excited at 360 nm.

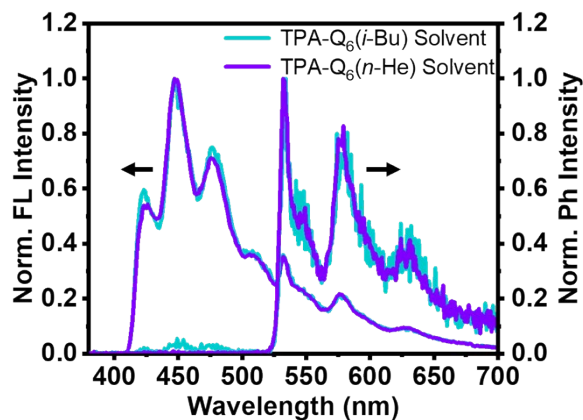


Fig. S7 Fluorescence spectra and phosphorescence spectra in 2-MeTHF solution (1×10^{-5} M) at 77 K, excited at 360 nm.

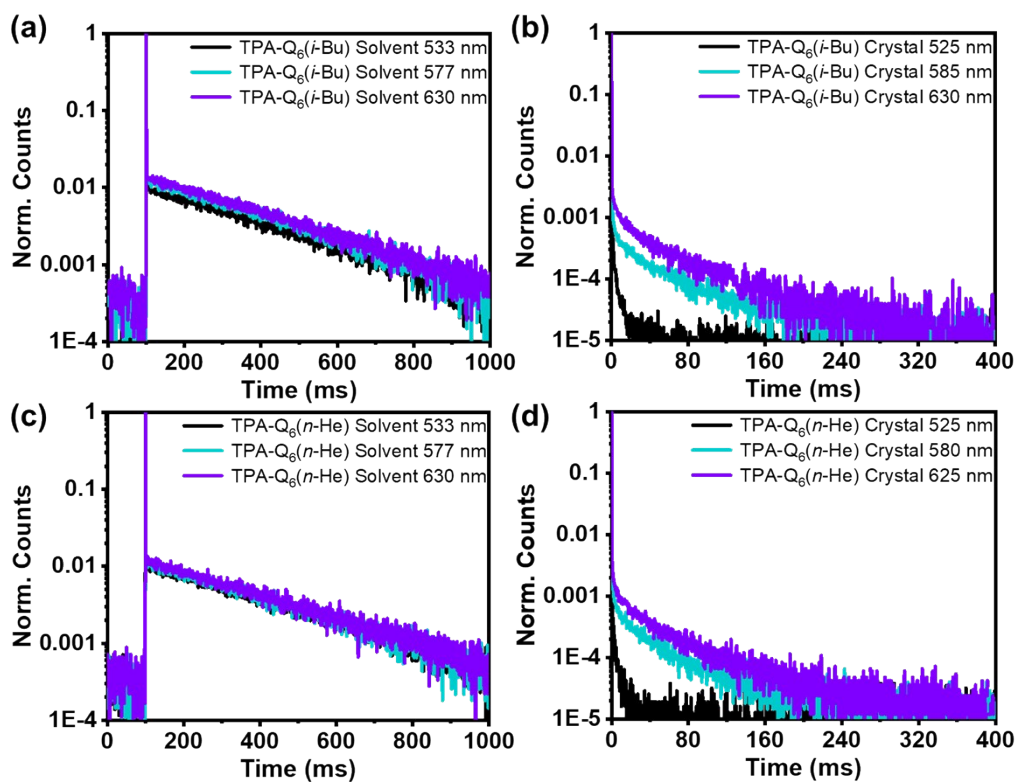


Fig. S8 The decay curves of the phosphorescence at different emission wavelengths in (a) and (c) 2-MeTHF solution (1×10^{-5} M) and (b) and (d) crystals, excited at 360 nm.

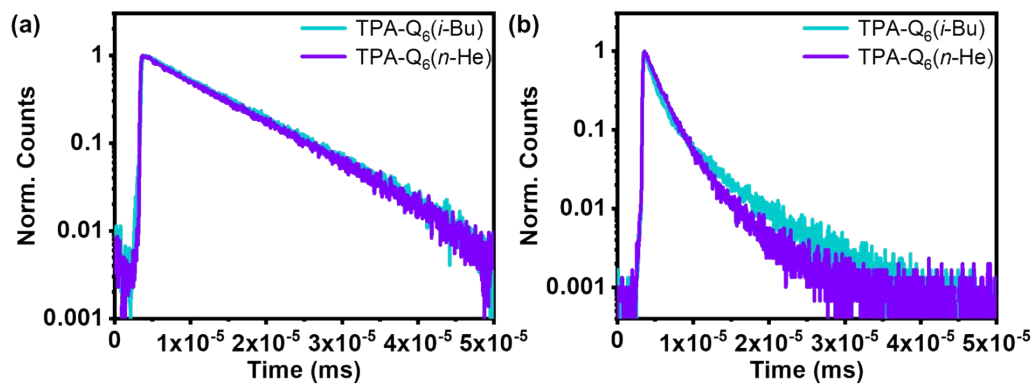
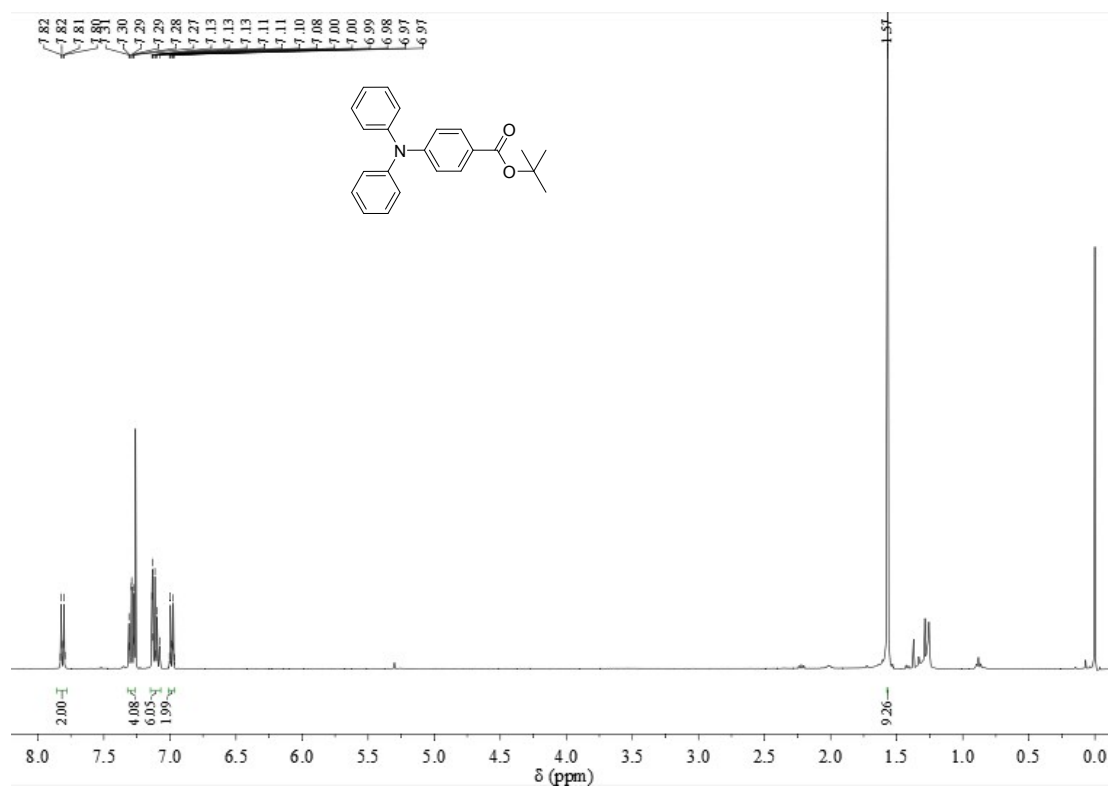
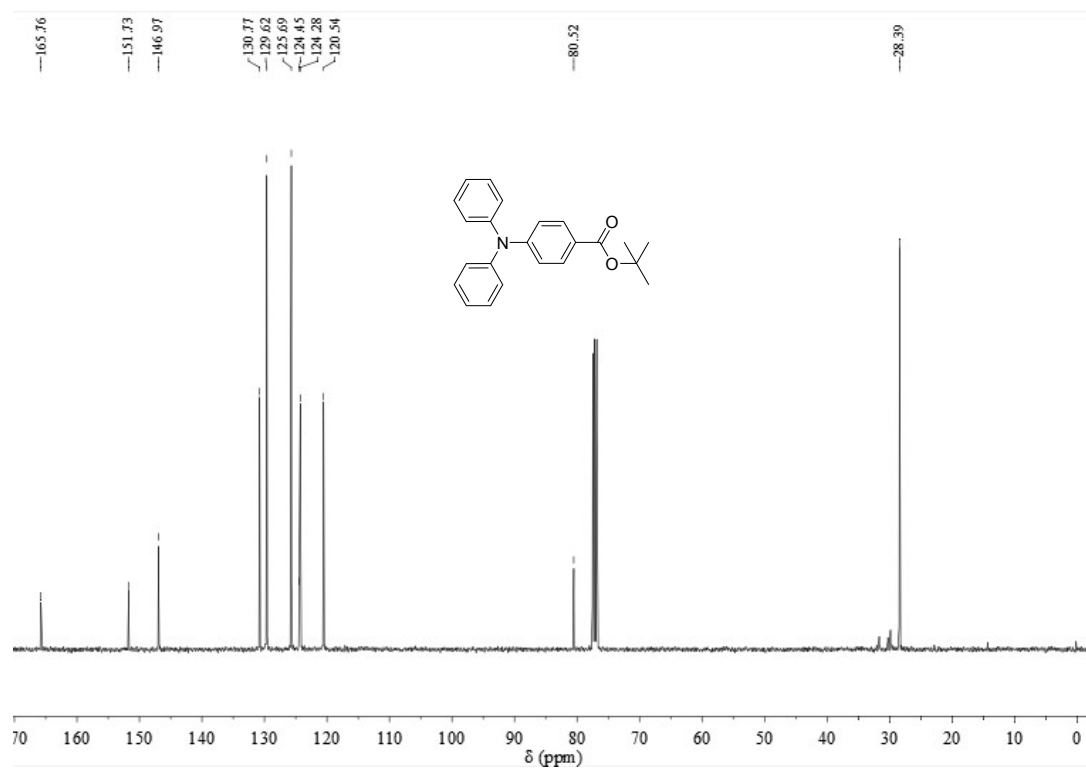


Fig. S9 The decay curves of the transient fluorescence in (a) DCM solutions (5×10^{-4} M) and (b) crystals, excited at 405 nm.

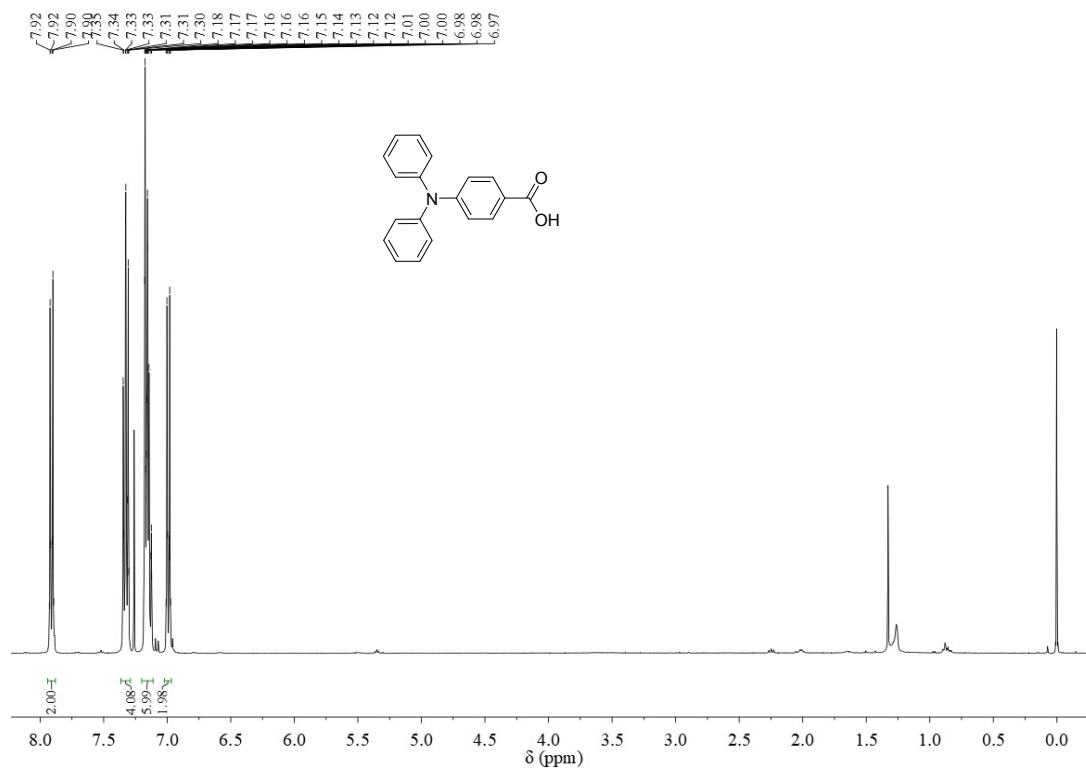
4. NMR spectra



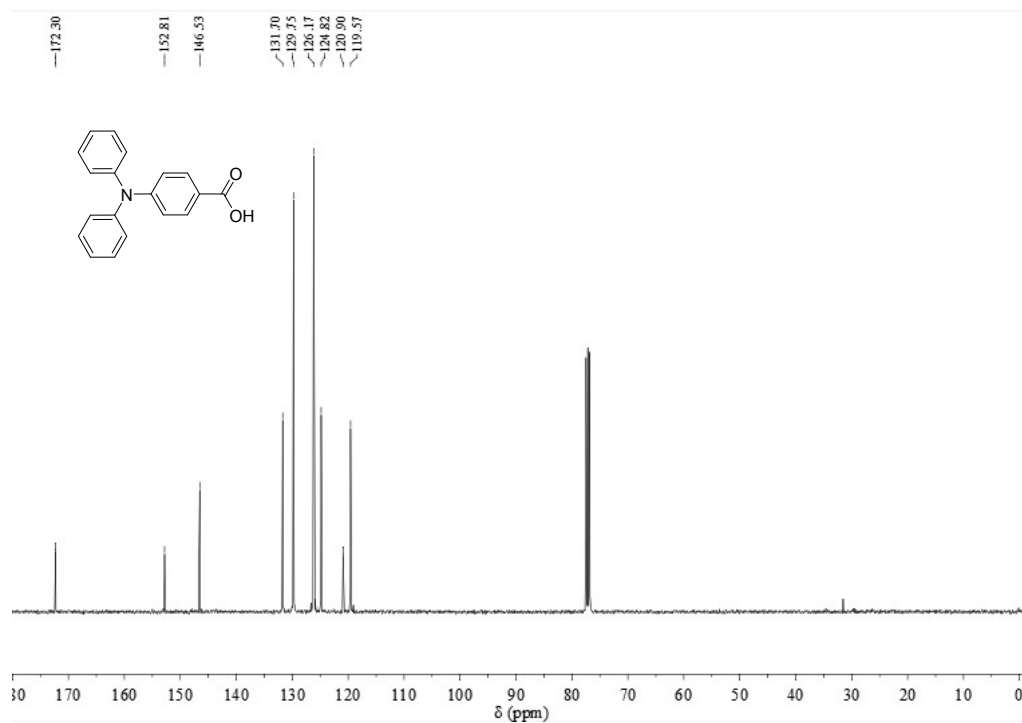
¹H NMR (400 MHz, CDCl₃) spectrum of **3**



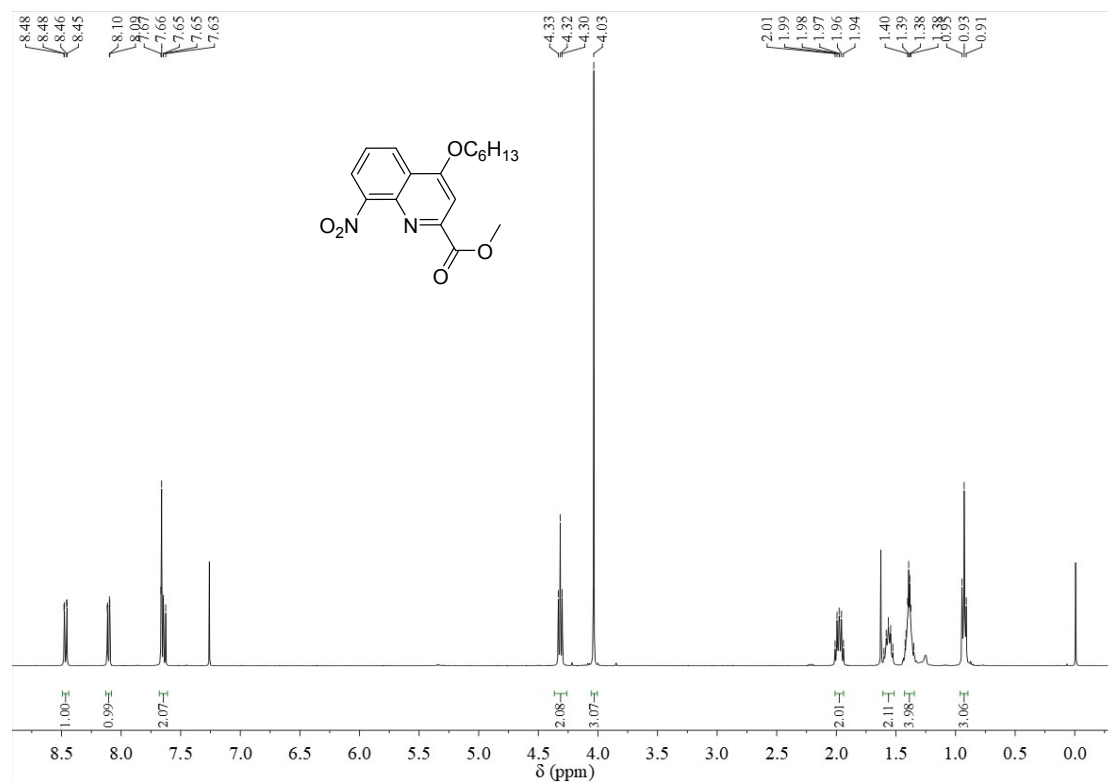
¹³C NMR (101 MHz, CDCl₃) spectrum of **3**



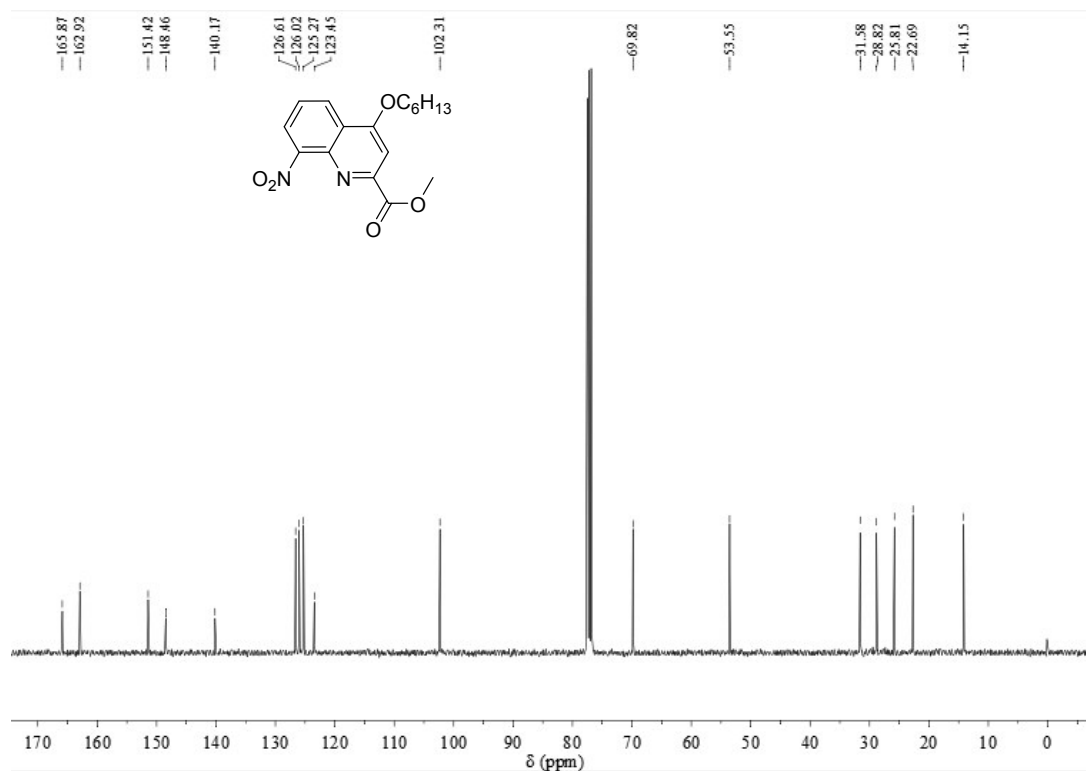
^1H NMR (400 MHz, CDCl_3) spectrum of **1**



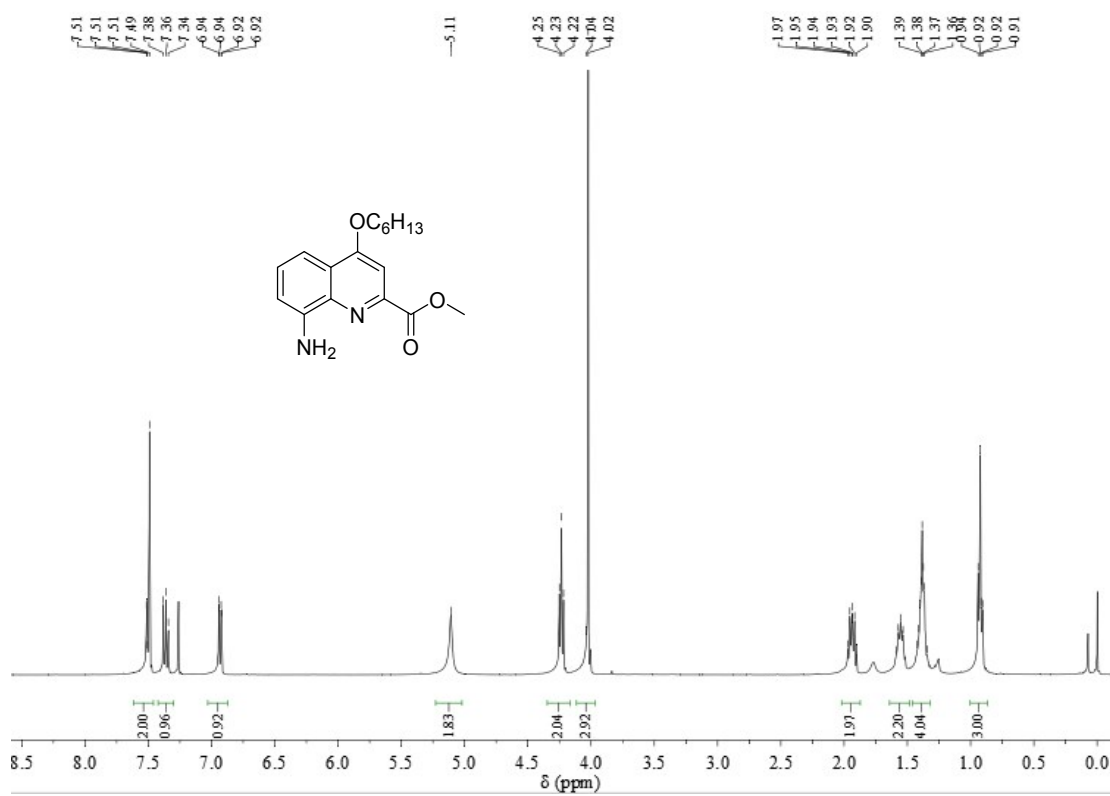
^{13}C NMR (101 MHz, CDCl_3) spectrum of **1**



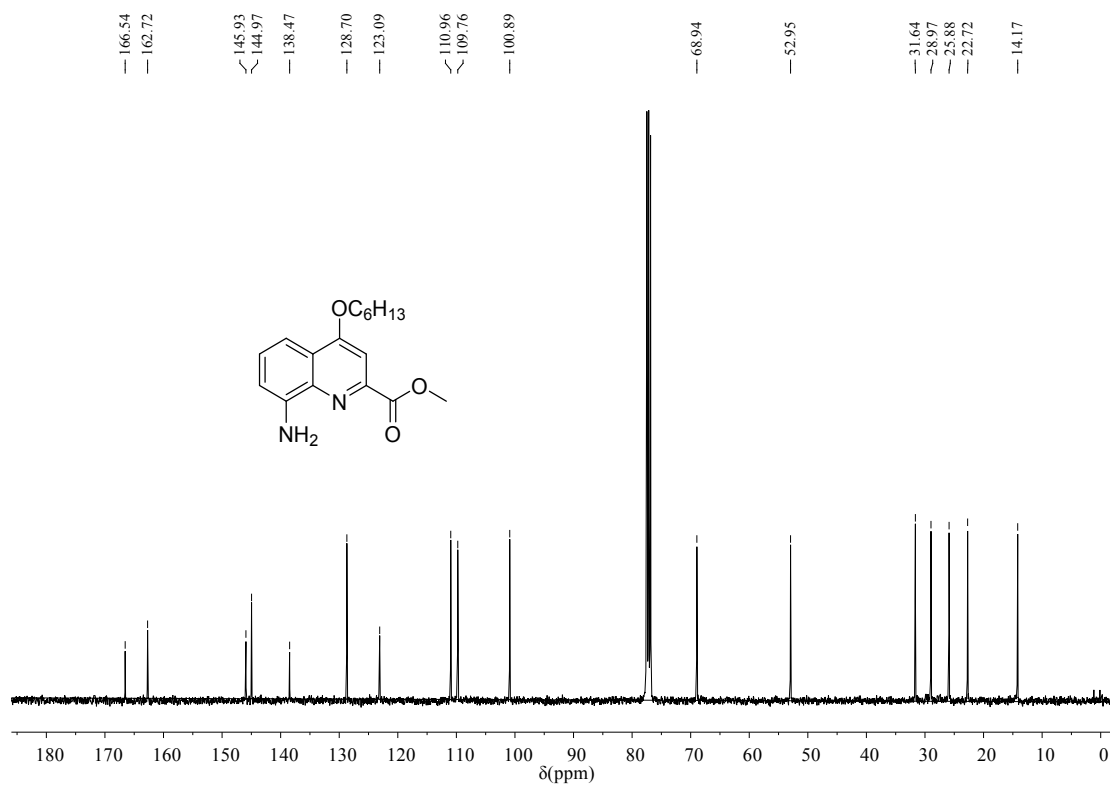
¹H NMR (400 MHz, CDCl₃) spectrum of **6b**



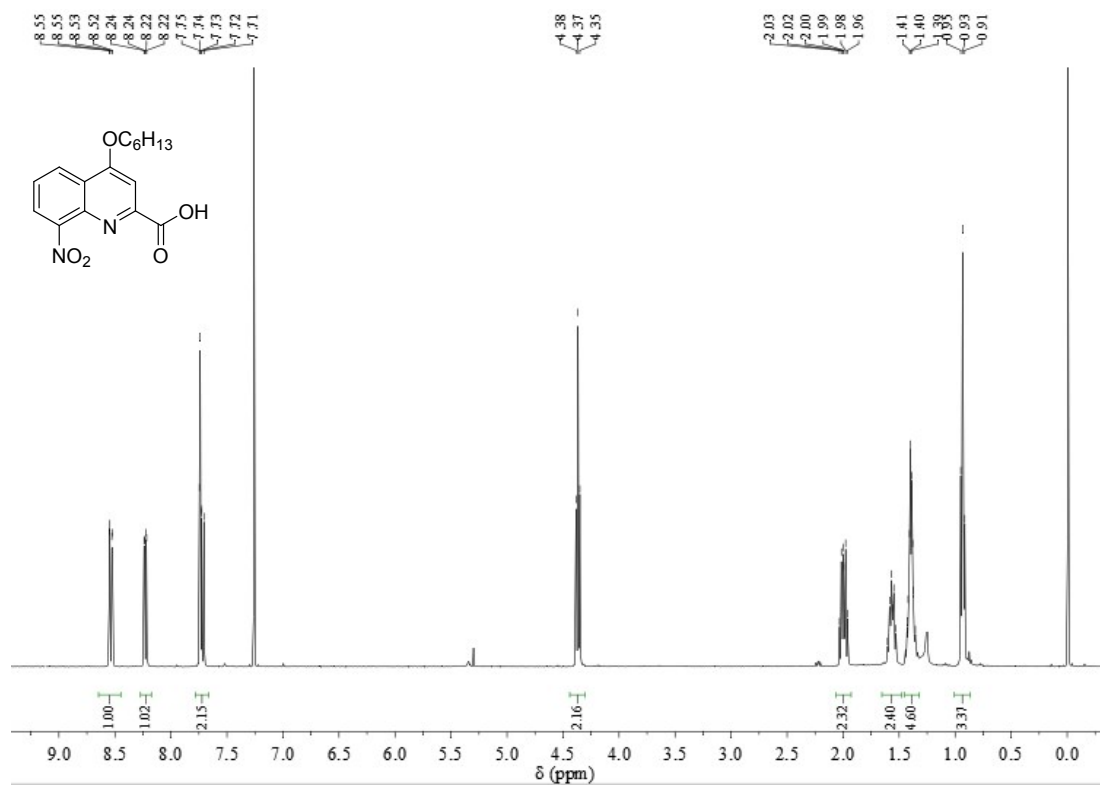
¹³C NMR (101 MHz, CDCl₃) spectrum of **6b**



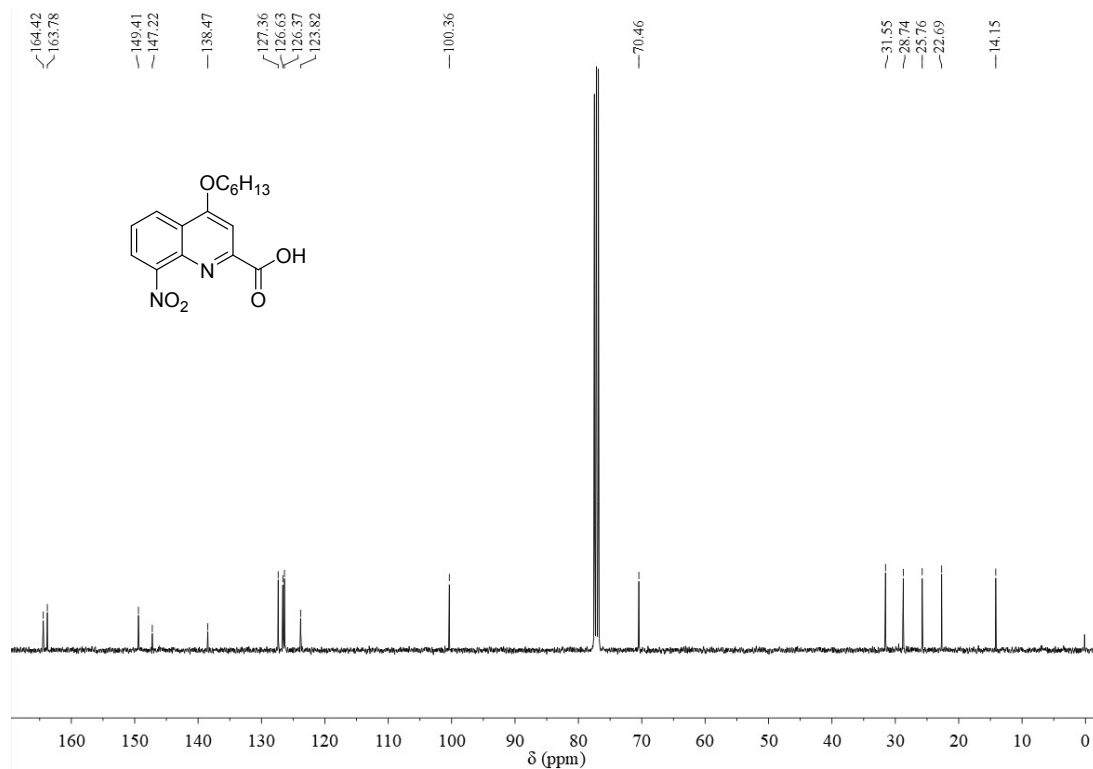
¹H NMR (400 MHz, CDCl₃) spectrum of **7b**



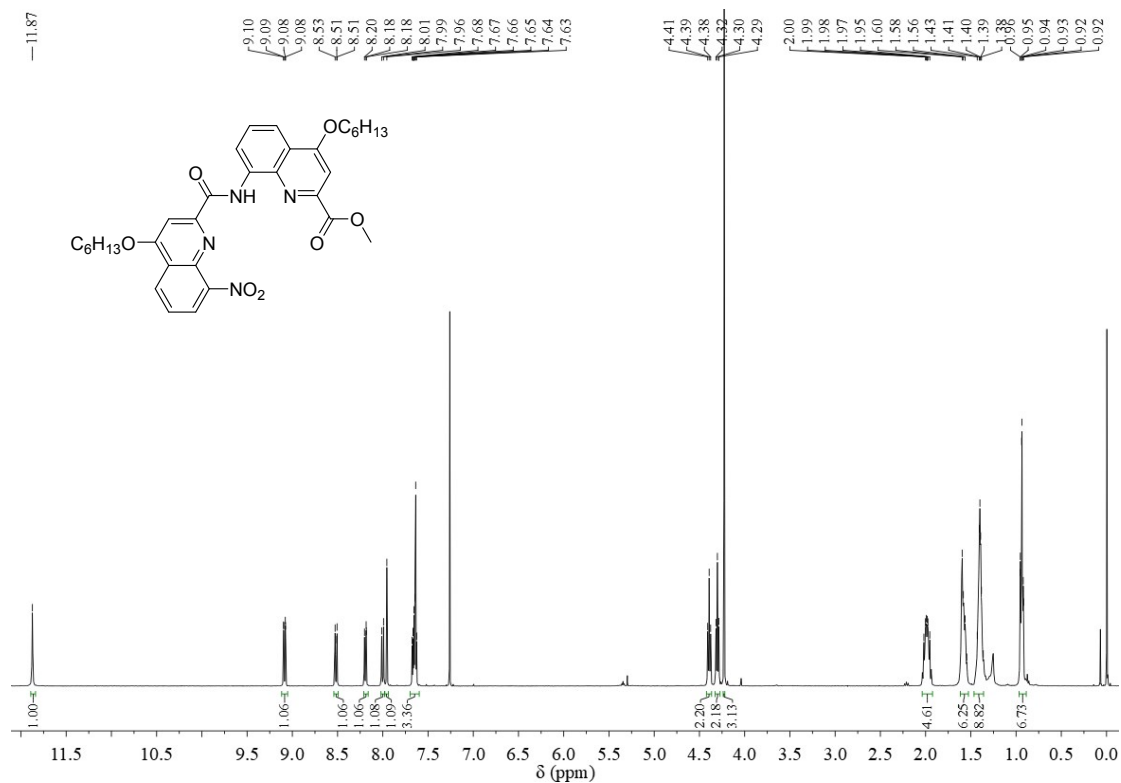
¹³C NMR (101 MHz, CDCl₃) spectrum of **7b**



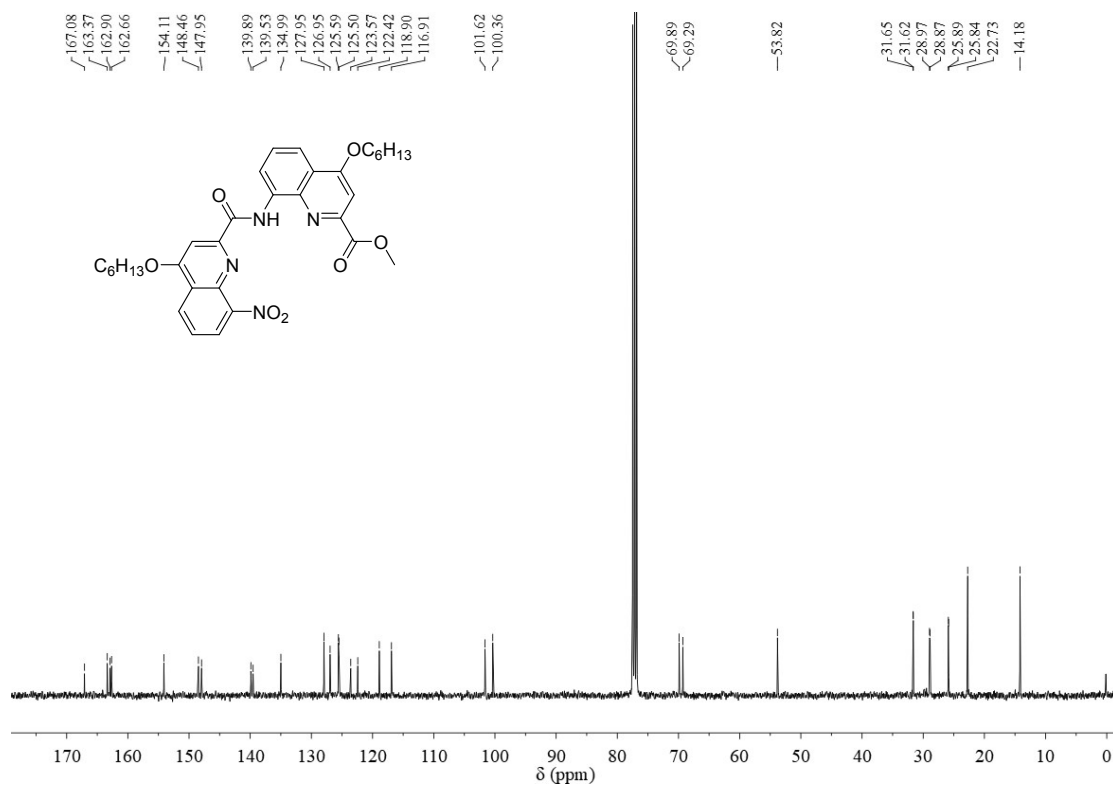
¹H NMR (400 MHz, CDCl₃) spectrum of **8b**



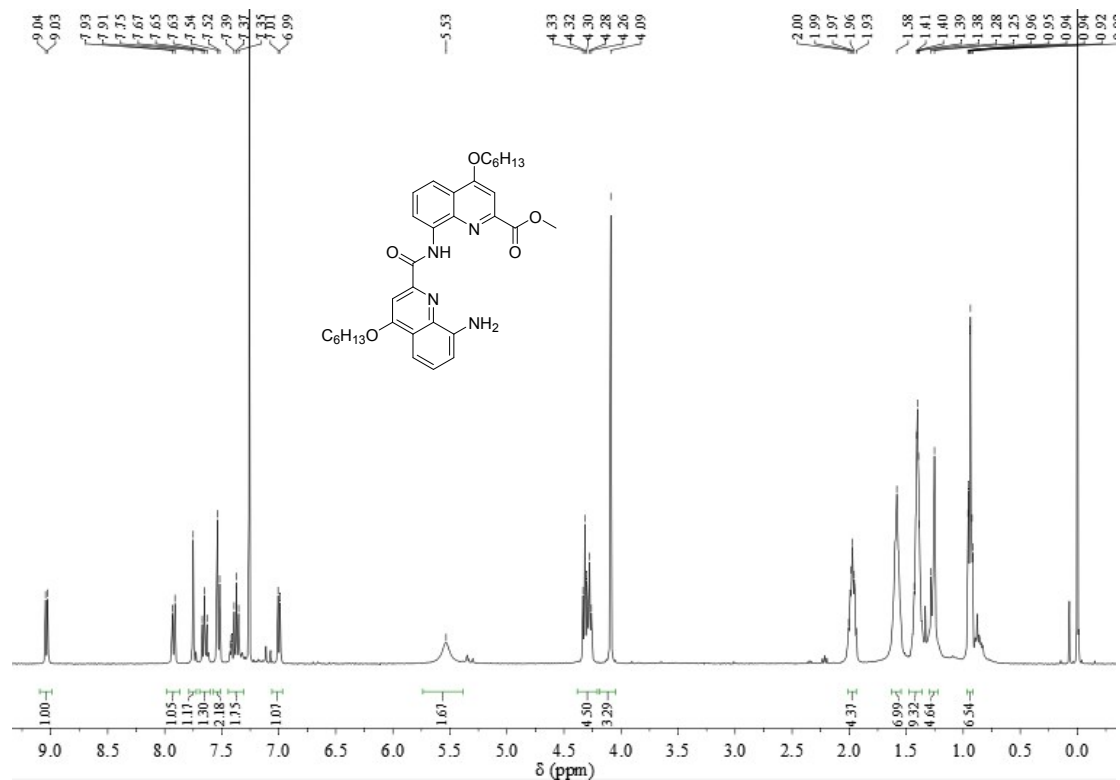
¹³C NMR (101 MHz, CDCl₃) spectrum of **8b**



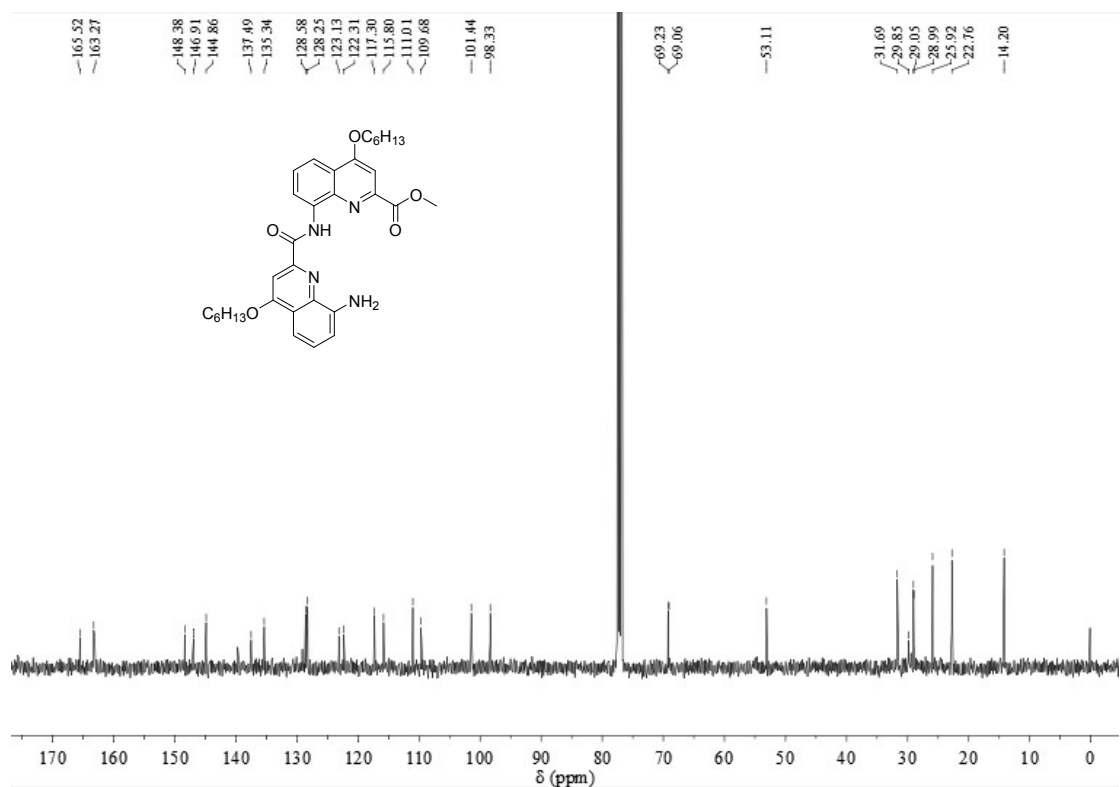
¹H NMR (400 MHz, CDCl₃) spectrum of **10b**



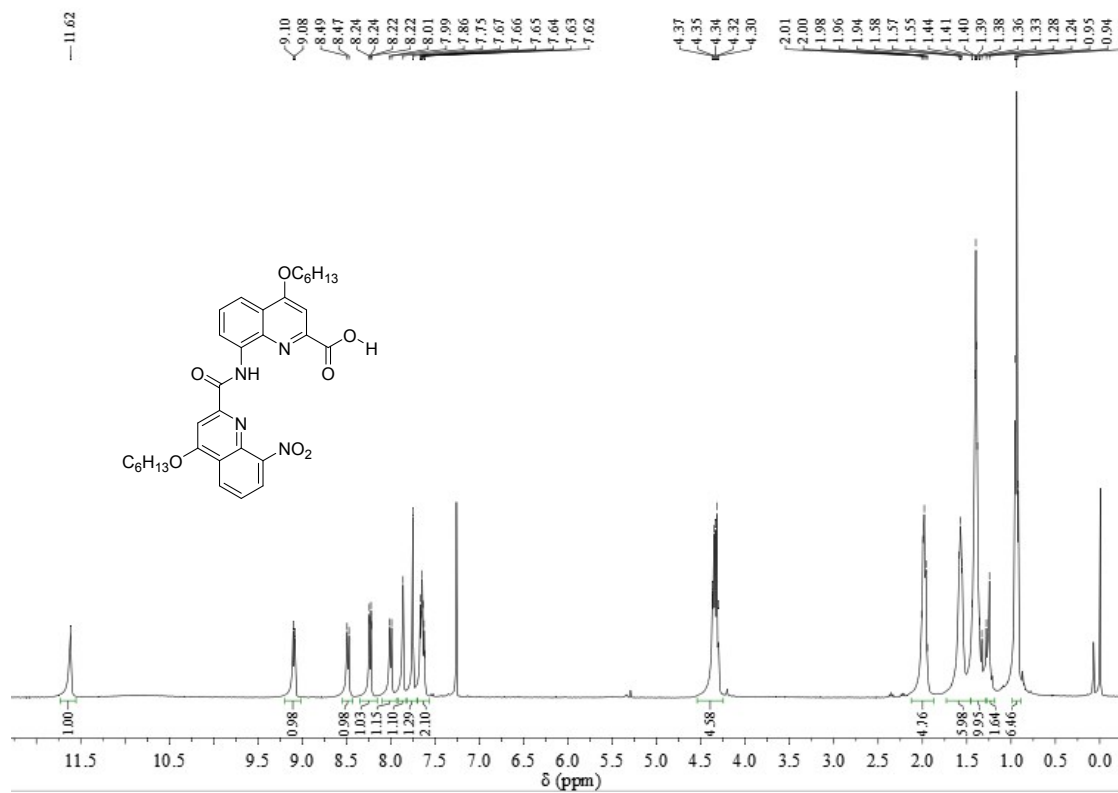
¹³C NMR (101 MHz, CDCl₃) spectrum of **10b**



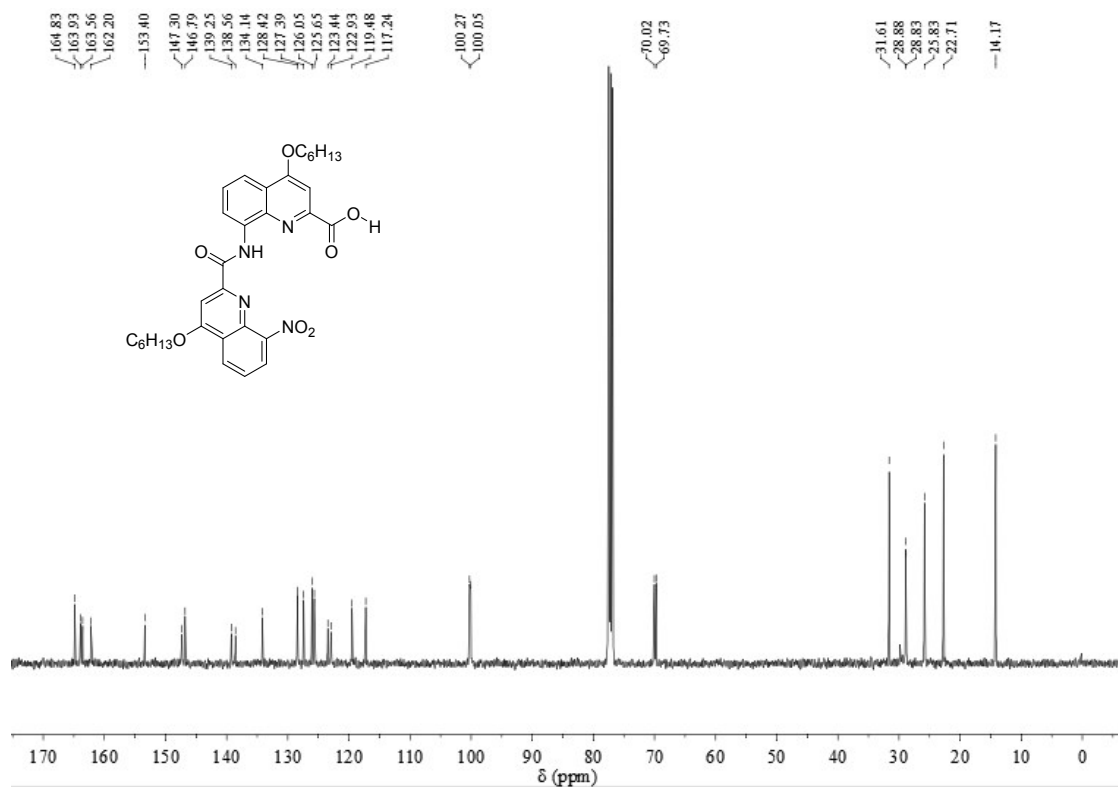
¹H NMR (400 MHz, CDCl₃) spectrum of **11b**



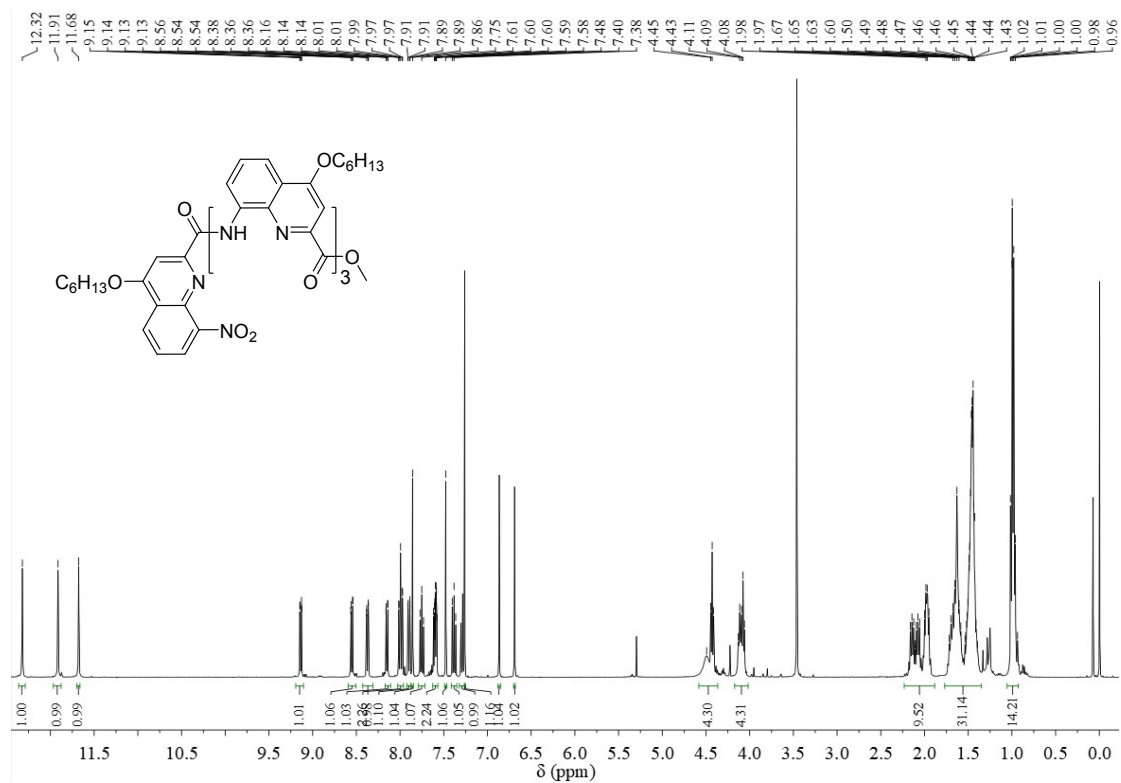
¹³C NMR (101 MHz, CDCl₃) spectrum of **11b**



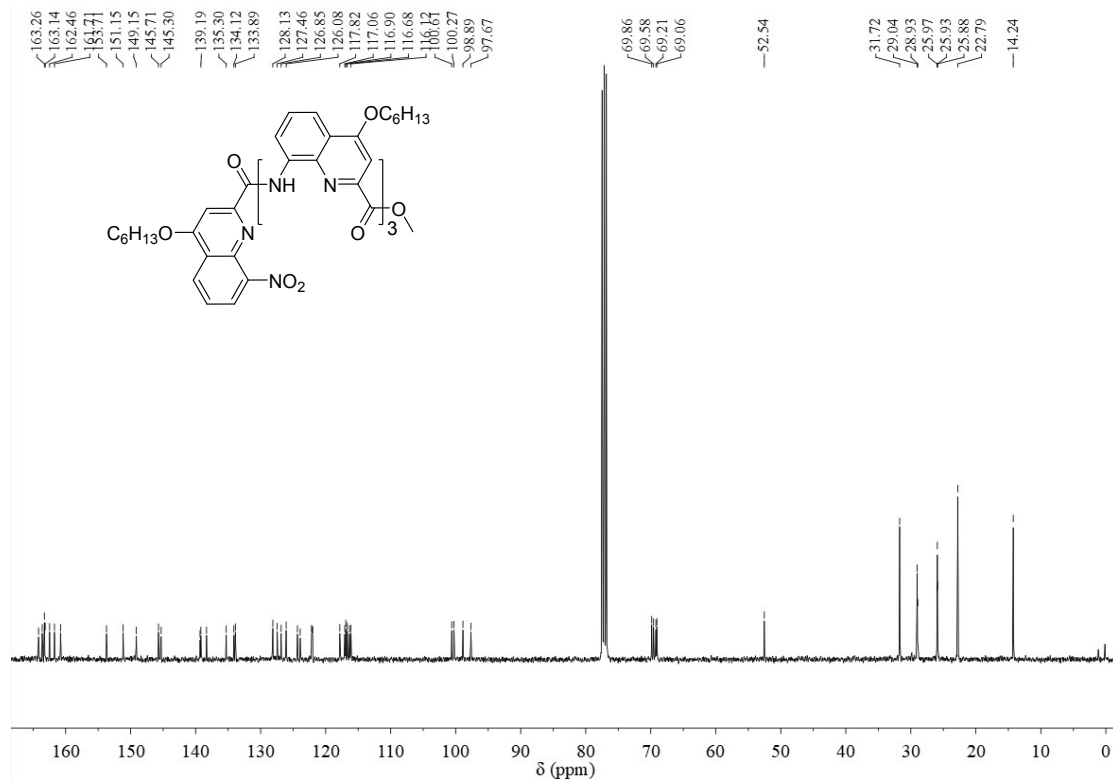
¹H NMR (400 MHz, CDCl₃) spectrum of **12b**



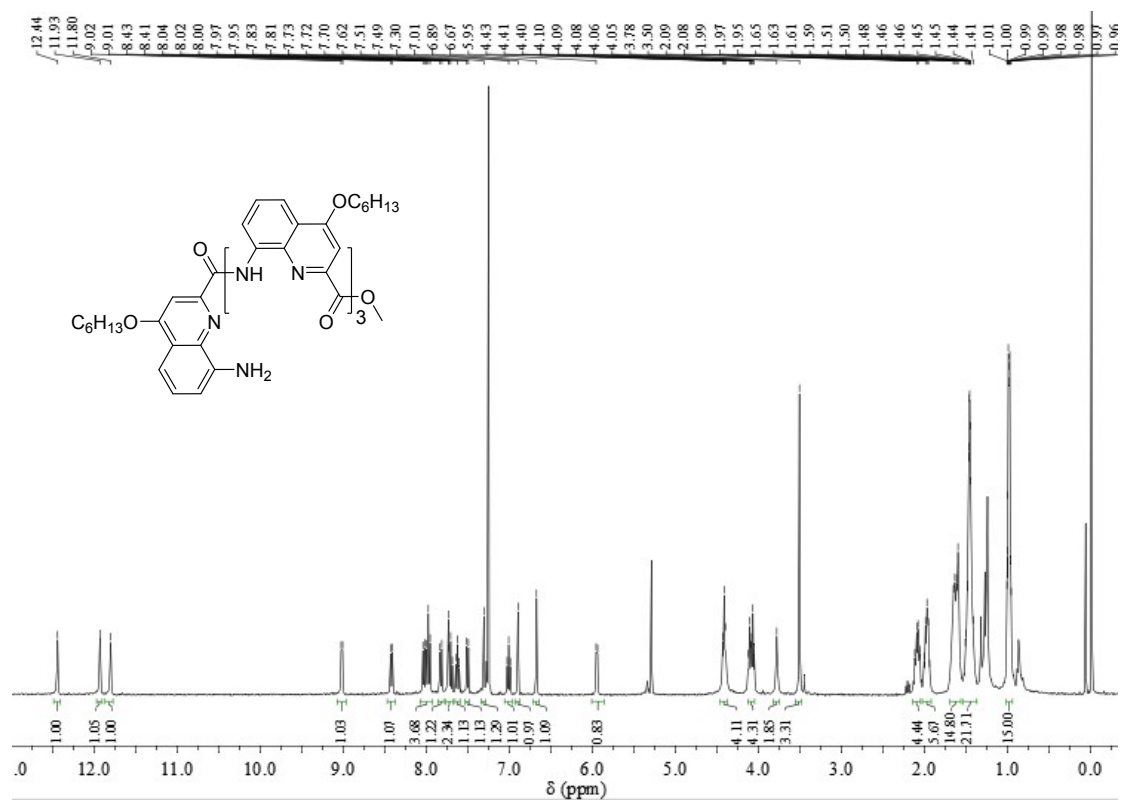
¹³C NMR (101 MHz, CDCl₃) spectrum of **12b**



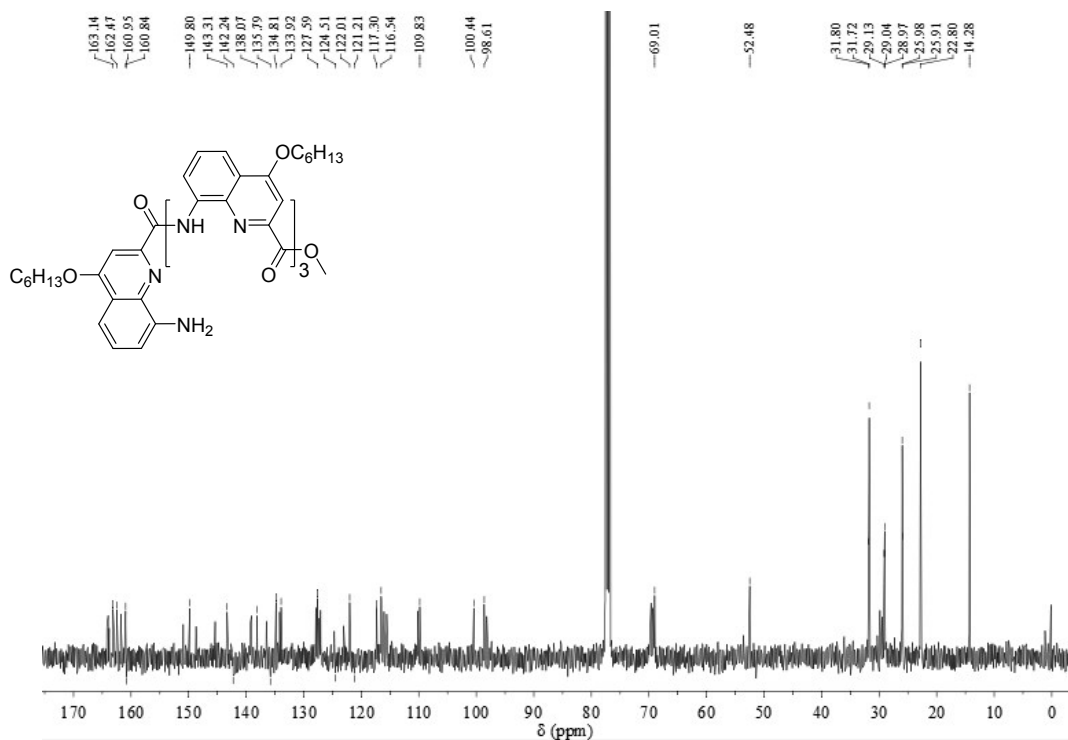
¹H NMR (400 MHz, CDCl₃) spectrum of **14b**



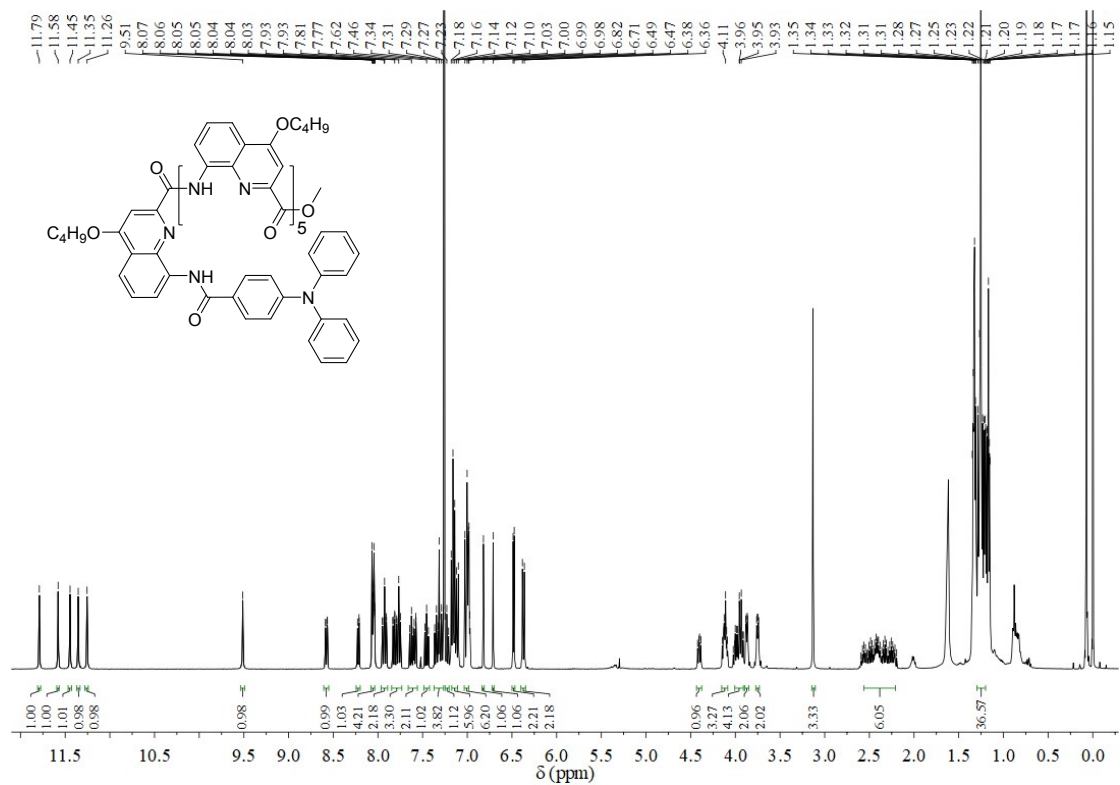
¹³C NMR (101 MHz, CDCl₃) spectrum of **14b**



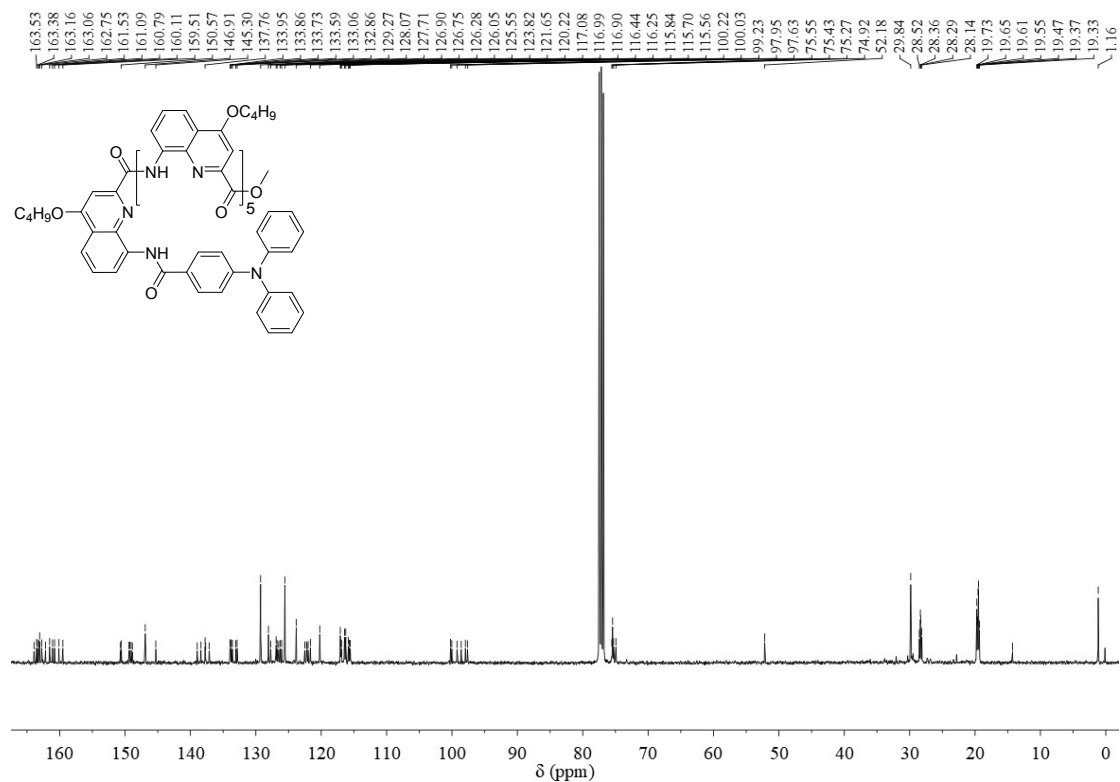
¹H NMR (400 MHz, CDCl₃) spectrum of **15b**



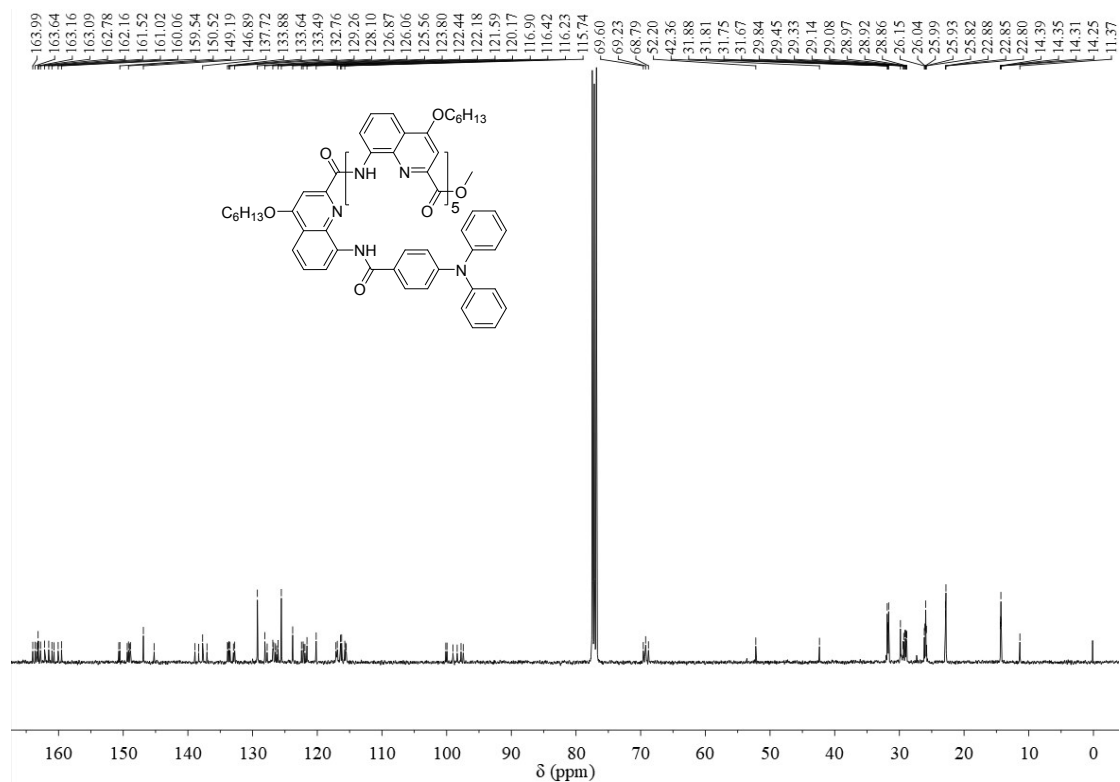
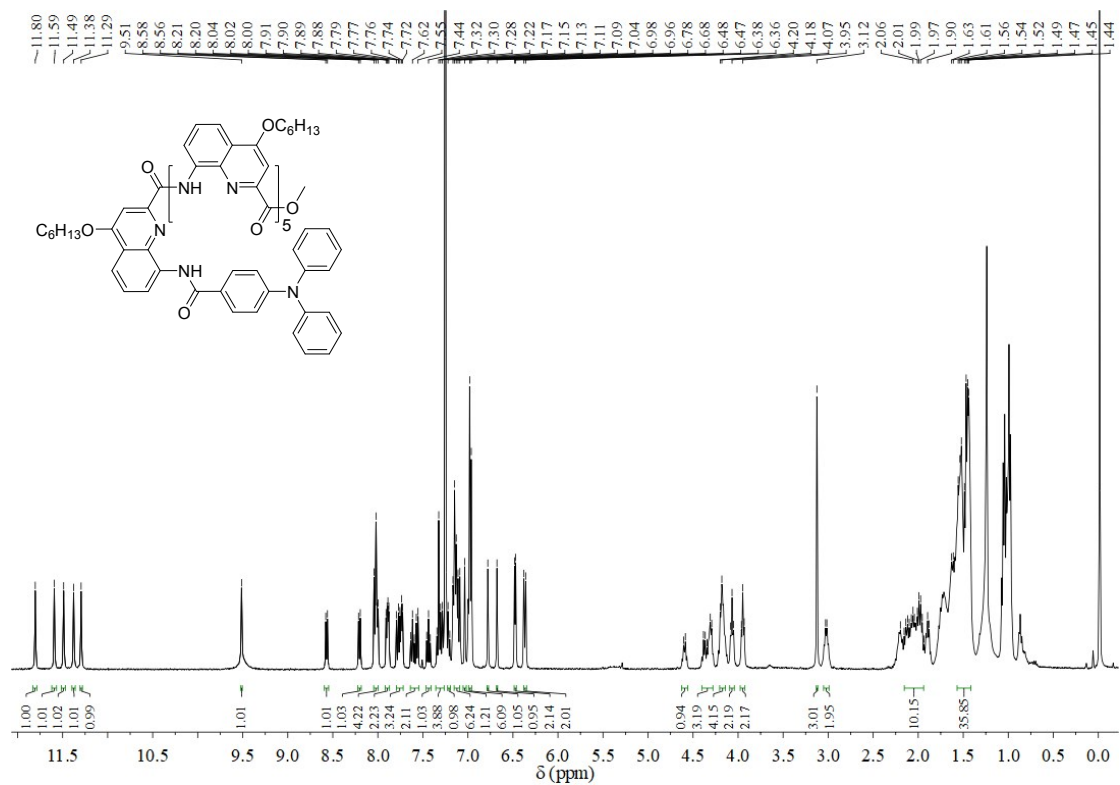
¹³C NMR (101 MHz, CDCl₃) spectrum of **15b**

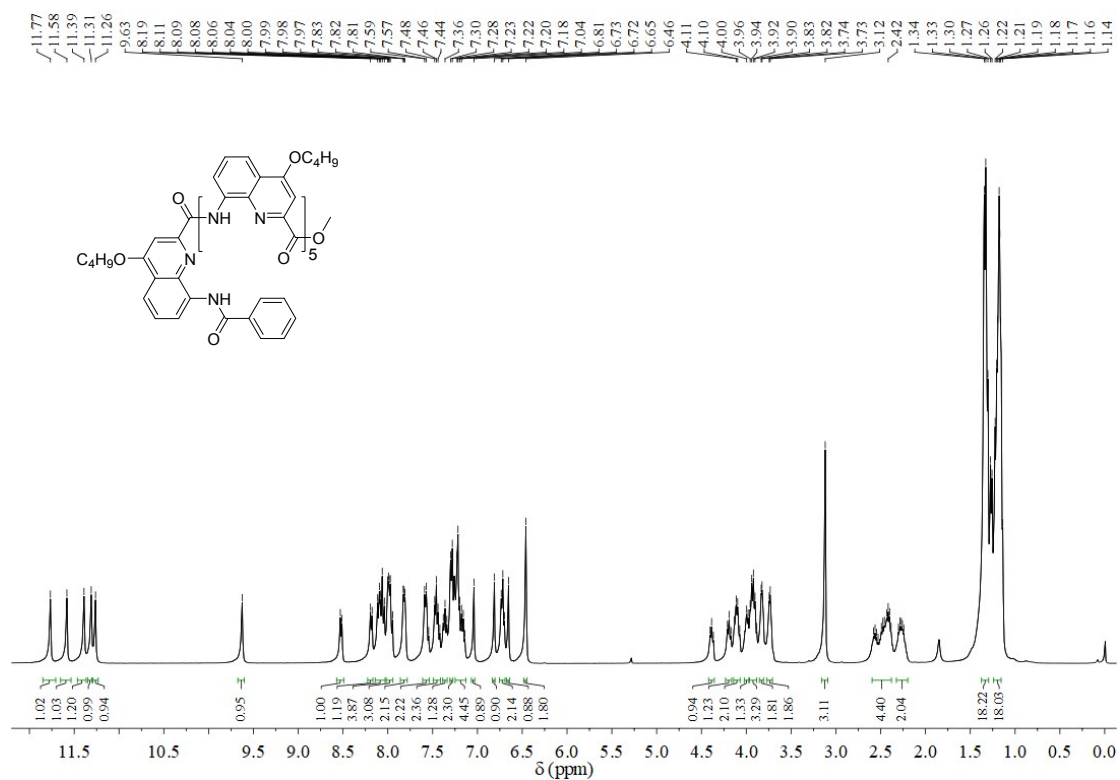


¹H NMR (400 MHz, CDCl₃) spectrum of TPA-Q₆(*i*-Bu)

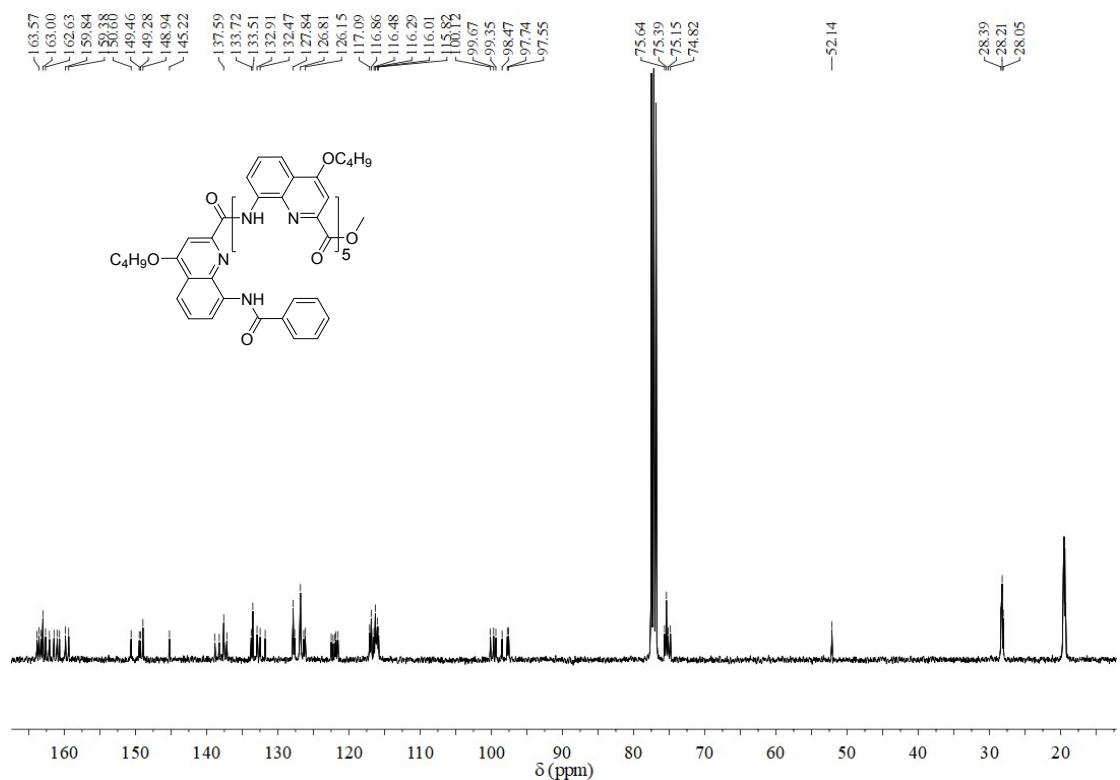


¹³C NMR (101 MHz, CDCl₃) spectrum of TPA-Q₆(*i*-Bu)





¹H NMR (400 MHz, CDCl₃) spectrum of **Ph-Q₆(i-Bu)**



¹³C NMR (101 MHz, CDCl₃) spectrum of **Ph-Q₆(i-Bu)**

5. Theoretical calculations

Table S2. Summary of different methods to calculate the strongest binding energy in **TPA-Q₆(*n*-He)** (Fig. S2(iii)).

Method	D ^a (kJ mol ⁻¹)	M ^b (kJ mol ⁻¹)	P ^c (kJ mol ⁻¹)	ΔE (kJ mol ⁻¹)
PM6-D3	-4466.19687	-2085.54202	-2083.77523	-296.87962
PM6-D3H4	-5467.39443	-2083.03651	-2265.36454	-1118.99338
PM6-D3H4X	-2592.51814	-209.618830	-451.809990	-1931.08932
PM6-DH+	-4107.78911	-1914.56741	-1917.67095	-275.550750
PM6-DH2	-4077.34092	-1900.91142	-1903.92715	-272.502350
PM6-DH2X	-4077.34092	-1900.91142	-1903.92715	-272.502350
PM7	-4258.82326	-1926.85500	-1919.46261	-412.505650

^a Enthalpy of dimer formation. ^b Enthalpy of *M*-helix generation in a dimer. ^c Enthalpy of *P*-helix generation in a dimer.

Table S3. Summary of the strongest three groups of binding energies in **TPA-Q₆(*n*-He)**.

Interaction	Method	D ^a (kJ mol ⁻¹)	M ^b (kJ mol ⁻¹)	P ^c (kJ mol ⁻¹)	ΔE (kJ mol ⁻¹)
Fig. S2(iii)	PM6-DH2	-4077.34092	-1900.91142	-1903.92715	-272.502350
	PM6-DH2X	-4077.34092	-1900.91142	-1903.92715	-272.502350
Fig. S2(ii)	PM6-DH2	-4001.85747	-1895.46477	-1897.5826	-208.8101
	PM6-DH2X	-4001.85747	-1895.46477	-1897.58266	-208.81004
Fig. S2(i)	PM6-DH2	-3973.45214	-1897.70415	-1898.61358	-177.13441
	PM6-DH2X	-3973.45214	-1897.70415	-1898.61358	-177.13441

^a Enthalpy of dimer formation. ^b Enthalpy of *M*-helix generation in a dimer. ^c Enthalpy of *P*-helix generation in a dimer.

Table S4. Summary of the binding energies of **TPA-Q₆(*i*-Bu)**, **TPA-Q₆(*n*-He)** and **Q₆(*i*-Bu)** obtained by the PM6-DH2X semi-empirical method.

Compound	Interaction	ΔE (kJ mol ⁻¹)
TPA-Q₆(<i>i</i>-Bu)	Fig. 3	-264.65
	Fig. 3 ^a	-166.78
	Fig. S1a(i)	-93.45
	Fig. S1a(ii)	-73.93
TPA-Q₆(<i>n</i>-He)	Fig. S2(i)	-177.13
	Fig. S2(ii)	-208.81
	Fig. S2(iii)	-272.50
	Fig. S1b(i)	-199.45
	Fig. S1b(ii)	-187.22
Q₆(<i>i</i>-Bu)	Fig. S3a(i)	-180.65
	Fig. S3a(ii)	-162.47
	Fig. S3a(iii)	-166.54
	Fig. S3a(iv)	-174.28
	Fig. S3b(i)	-21.21
	Fig. S3b(ii)	-32.61
	Fig. S3b(iii)	-31.78
	Fig. S1c(i)	-92.36

^a The bridged methanol molecule of the dimer is ignored in Fig. 3.

Table S5. Atomic coordinates for the optimized structure of **TPA-Q₆(*n*-He)** in Gaussian 09 (Fig. S2(iii), gas phase).

Atom	X	Y	Z
C	-2.60919800	-2.60245700	-4.88896900
C	-5.63571700	-3.80181100	-0.64445900
C	-4.70060500	-4.46868400	2.63916900
C	9.52461500	-2.80666000	3.35613100
C	0.57224000	-9.66028800	3.08871900
C	-0.42988100	-0.99106800	-2.11576900
C	-12.12567000	-3.98960900	2.38077300
C	-3.13735400	2.78386800	-3.63598700
C	8.02619700	8.69073200	2.49375900
C	-9.82637800	7.02039900	-2.25453200
C	-7.94579900	-3.79992300	0.20960500
C	9.43028800	2.20179900	-0.87512800
C	-4.92544500	-2.91852600	-4.20572600
C	8.20612200	1.48485900	-3.95460100
C	3.21575600	0.53555100	4.04268400
C	7.01470200	1.13383600	-3.33372400
C	-2.36999300	-2.11505100	-1.28031600
C	0.06143400	-0.85603900	1.67599000

C	8.94418600	2.06616100	2.80503400
C	-1.15834100	-2.16205700	-1.99289400
C	12.70091600	2.58628800	-2.45300200
C	-7.11811200	-4.49526200	-3.66693600
C	2.49207500	-1.51708600	-4.24013800
C	-5.99350800	-3.82205500	3.02017200
C	-3.28539800	-3.31539700	-1.32096000
C	11.60927100	1.78896100	-1.76124100
C	1.28639200	-2.00634300	-3.45418800
C	2.37298900	-1.11020700	0.06368000
C	9.21514200	0.86143200	-0.60368000
C	-7.90915000	-5.21266800	0.25309900
C	9.15303000	0.49273700	-4.28237300
C	7.97918400	0.48483300	-0.05186900
C	-4.79793900	-4.32045100	-4.39490400
C	6.77128900	-0.24481800	-3.00594500
C	0.41762200	-2.06279600	1.11897300
C	3.48477700	-0.83475400	3.46521100
C	-3.61771000	-3.83321100	2.01407600
C	4.56104700	-2.18760900	-5.57268400
C	14.99581500	2.47704700	-3.57516100
C	-5.94351300	-5.11477200	-4.06279000
C	13.88228400	1.70107700	-2.86405000
C	1.56282900	-2.20296800	0.30850500
C	-2.51950500	-3.99398000	-5.11955300
C	-5.62855700	-5.18516500	-0.61914200
C	3.32472000	-2.67254500	-4.80683600
C	2.58650200	-1.87515800	3.76754800
C	-6.77370300	-5.87625800	-0.16727800
C	6.71770600	-2.82961000	-6.78029600
C	-3.56887300	-4.85027500	-4.85354600
C	4.44321000	-0.96113200	6.69472100
C	-2.45195800	-4.53097200	1.72524900
C	8.93631900	-0.84167400	-4.01117100
C	5.38031100	-1.82783200	-2.08112000
C	7.73424400	-1.22752800	-3.37514500
C	4.10972000	-2.18278900	-1.35204400
C	7.73022400	-0.97297500	0.24581800
C	5.45365000	-3.32732700	-6.07353300
C	17.28826300	2.37943200	-4.69766000
C	9.42528200	-0.36848800	2.98245300
C	16.18096100	1.59650100	-3.98641800
C	4.84776300	-2.21093900	2.23020100
C	10.63097200	-0.43485500	2.30253400

C	-4.57848300	-5.83542000	2.93481200
C	-6.82123400	-7.30800900	-3.68115600
C	2.86602900	-3.14195700	3.28735300
C	5.98979700	-2.35062900	1.37197600
C	6.22837100	-2.89058800	-2.44687900
C	7.41455100	-2.59104100	-3.08631100
C	8.85098100	-1.56468600	3.53395100
C	-2.30818500	-5.88423800	2.08340000
C	5.89448100	-2.40124800	5.53826700
C	0.87068700	-4.16768500	4.21298800
C	4.06022600	-3.35738000	2.52800600
C	-3.41282200	-6.53441800	2.66546400
C	1.12482000	-4.13609700	5.72541200
C	7.14318600	-2.52910100	4.71392800
C	-0.86718300	-6.16136600	-0.54265400
C	-0.09241200	-5.80876300	-1.64828000
C	11.27795100	-1.67889500	2.14406600
C	6.34769100	-3.60339400	0.90642600
C	-0.28667400	-6.22725600	0.72596900
C	-6.28836400	-8.73095400	-3.71568100
C	1.27191800	-5.55935600	-1.50045100
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C	4.45401300	-4.62826500	2.04662400
C	1.08125300	-5.95895000	0.88056800
C	1.85666000	-5.64321700	-0.23208400
C	10.75187400	-2.84691300	2.65462500
C	-7.25315000	-9.74448900	-3.07869600
C	2.33382100	-4.97832700	6.16022900
C	-0.90332500	-7.53494300	4.11796000
C	-10.12883200	-10.21748900	-5.73147200
C	5.58038000	-4.73355400	1.25877300
C	7.68790100	-3.82627500	4.57193100
C	-0.64476300	-7.58853200	2.73684100
C	-8.70177700	-10.09583000	-5.18930900
C	8.89972700	-3.96435800	3.91980500
C	8.06397900	-4.89461700	-3.26471300
C	-0.44627500	-8.54549900	4.96066300
C	2.26088600	-6.45655100	5.76098800
C	10.21005500	-4.83952400	-0.37467200
C	0.09616600	-8.67092800	2.23203900
C	9.17294400	-5.67069700	-3.95388700
C	9.18308700	-5.54873300	0.51108200
C	9.16771800	-5.49302800	-5.47578000
C	0.30221500	-9.61069700	4.45794000

C	3.53247300	-7.25074400	6.09763400
C	4.75503400	-6.84374500	5.26329600
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C	8.00283800	-6.90033900	3.15130300
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C	8.67284100	-7.61792000	1.96576200
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C	-6.81554200	-3.08238900	-0.26468400
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C	-8.39153600	-2.37451900	-3.15639300
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C	-8.99923500	-1.63890800	0.57343100
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H	-1.61855300	5.09164000	-4.51945400
H	8.90835500	9.13783100	2.01699400
H	-3.16564200	4.90489900	-5.39221800
H	6.87466400	8.91089300	4.30271500
H	-7.77151500	3.19579000	0.28465400
H	7.18590500	8.83573200	1.80314400
H	8.50164100	10.63763600	6.34175400
H	-7.05009500	4.51403700	4.64985900
H	-10.08967800	2.98132600	1.07011000
H	-11.16954100	3.18137200	-2.01179500
H	-7.32542900	4.68540500	-4.60488300
H	-5.02715700	5.86677300	-1.70099300
H	-7.97017200	4.73911800	3.14763700
H	9.13437000	12.10601200	5.58729100
H	-9.15399600	4.67703900	5.96424900
H	-6.92356000	5.48178700	-0.13814900
H	-10.42971000	3.56076800	2.69567100
H	8.34900600	11.37265100	3.21479400
H	-2.23911700	7.15314500	-5.78386800
H	7.94111300	12.21887500	6.88887400
H	6.21552200	11.13659000	5.40628600
H	-2.02565800	7.43330800	-4.07169500
H	-5.19631200	5.95472800	-5.61213700
H	6.64951300	11.02290500	2.94083700
H	-11.66941900	3.68720800	1.43762300
H	-9.64735700	4.60461600	-0.78291900
H	-9.02268200	5.25857300	1.51035100
H	-4.47361100	7.42698900	-3.69979800
H	-7.96920500	6.01358500	-2.77601700
H	-4.71617200	7.20350700	-6.74740700
H	-7.58317200	6.02930300	-6.49832100
H	6.80852000	12.64337300	4.72947100
H	-10.42585400	6.04864500	7.30761300
H	-7.90434700	6.80465500	5.50060300

H	-8.98132400	6.44750000	-4.17553700
H	12.40710900	-6.45913900	-8.04341500
H	9.14352900	-8.53635900	2.34272900
H	11.40117900	-6.65885600	-9.48537200
H	11.37423300	-7.88394500	-8.20895900
H	-8.74140500	6.97316600	3.96390900
H	-11.25134300	5.27095200	-0.58127700
H	-3.98046600	8.66798500	-4.84006700
H	-10.61534200	5.94124000	1.78921000
H	-8.64711300	6.88647000	-0.45057000
H	-6.84349400	7.51077200	-4.56535800
H	-7.17710900	7.32448200	-7.62265300
H	-10.92456900	7.22609800	5.15634000
H	-8.48707200	7.55505400	-6.45743400
H	-9.18958600	7.23645500	7.68386900
H	-10.87632100	6.94451700	-2.56370300
H	-6.40307500	8.76581300	-5.70799600
H	-10.25015300	7.55292200	-0.21099100
H	-9.50664200	8.04637200	-2.47619000
H	-9.76340700	8.47907300	5.56130900
H	-11.32900500	7.75223800	8.89556400
H	-12.19149800	7.85204600	7.35410000
H	-10.95135800	9.04759500	7.75041900
N	-4.55170100	-2.99046700	-0.94490200
N	6.99257800	1.32676000	0.20495900
N	5.61857200	-0.55330500	-2.34796000
N	3.53429200	-1.13315400	-0.70892200
N	8.66975400	0.78176000	3.17311100
N	4.56071400	-0.97413500	2.70789800
N	6.62615300	-1.16515900	1.02502900
N	7.68512400	-1.43466900	4.21574800
N	-1.09084900	-6.56307100	1.86331500
N	4.28456000	1.37023700	3.91370900
N	-6.06126200	-2.44899100	2.89687700
N	6.65046300	2.48806700	3.46312900
N	2.92957500	1.17801200	0.47386600
N	-6.07836300	-2.32759900	-3.81255300
N	-2.81100200	-1.05294900	-0.61842600
N	5.99169800	2.02032000	-3.00244500
N	-3.97665200	-0.75310100	-3.97784400
N	-6.77377400	-1.72568600	-0.35090700
N	4.91711900	2.90308700	0.56721700
N	-5.72678200	0.19494900	2.49615000
N	-8.32020400	-1.04082100	-3.43540100

N	-3.68699600	1.05946200	0.82515700
N	-4.70568400	1.34852800	-2.48849400
N	-6.72722200	0.92728300	-0.77006200
N	-7.59321900	1.34955400	-4.25613900
N	1.12772400	6.32129900	-2.23389500
O	-2.91754700	-4.42851100	-1.68992000
O	9.98657900	2.45189100	2.27855800
O	-6.93103500	-4.49234300	3.45126000
O	5.56466100	-1.13081400	5.80705200
O	-5.76999800	-6.44840100	-4.14871200
O	3.67126300	-3.33537600	-1.37127400
O	8.45876600	-1.86170500	-0.19253400
O	2.08909400	-4.22624800	3.44329100
O	5.27436300	-3.36344600	5.95802000
O	8.32141100	-3.49892200	-3.49011300
O	9.58533100	-5.11969900	3.77219500
O	0.70773300	-0.85615800	-2.81377900
O	10.55276300	2.69912900	-1.42550100
O	2.14457000	0.81926800	4.57943300
O	-10.08761600	-3.70984500	1.17770300
O	-9.33864900	-2.95485000	-2.63163500
O	-2.04469700	0.33653400	-4.60259400
O	-0.48618500	1.62144600	2.78294700
O	6.90002700	3.99946000	-3.70337000
O	3.48050300	4.60968600	1.13872100
O	-5.49921100	1.39121900	-5.88432000
O	7.07528300	6.60799500	3.15046600
O	-8.60825200	1.15692700	0.54256900
O	-3.92291900	3.15267000	1.75759000
O	-8.35119400	2.97064000	4.16817000
O	-5.46033000	3.64679100	-5.91832400
O	-3.34536800	5.17632100	-3.35082000
O	-9.61713000	4.79167000	-3.09991200
H	-16.85840600	-5.33994800	4.26120300

Table S6. Atomic coordinates for the optimized structure of **TPA-Q₆(*i*-Bu)** in MOPAC2016 (Fig. 3, gas phase).

Atom	X	Y	Z
O	8.733584326	9.197707465	6.357030494
O	8.450614135	3.416870070	11.321343465
O	8.067669440	7.541456014	14.581381763
O	5.919965360	14.913127978	14.162444338
O	5.943545850	13.349746782	9.058355087
O	5.482332410	6.500734506	5.593352243

O	5.331959370	5.207669242	10.731624502
O	4.308268348	8.960167546	17.372947376
O	3.309101710	12.685937359	13.719447939
O	2.214351190	12.734381431	6.173809020
O	2.188793564	7.571370072	7.270673584
O	0.618412506	9.102225567	14.010695820
O	1.055665885	7.610293705	15.647371031
O	2.360832247	3.270128121	13.554904817
N	9.319946599	15.240307824	8.501390153
N	8.542497019	8.824107992	8.623069742
H	8.486826462	9.266970395	9.560823406
N	8.150550323	7.549726063	11.048568925
N	7.298674945	9.128040748	13.089275137
H	7.144691155	9.319611637	12.073083134
N	6.388213181	11.440827995	11.942549928
N	5.376938899	11.135246959	9.458478507
H	5.279758171	10.425875683	10.219175462
N	5.158896496	8.417076807	9.259953545
N	4.599456780	7.224213674	11.592460922
H	4.345455742	8.206465383	11.334680540
N	3.875895973	9.273745145	13.251675442
N	2.513914062	11.304566034	12.044558982
H	2.338767125	10.308435883	11.791905078
N	2.105361319	10.281614459	9.523453549
N	1.536780827	7.647930644	9.487923447
H	1.320467633	8.293287075	10.281829131
N	1.293111195	7.043024531	12.152118576
C	9.653419115	16.130604035	7.415337673
C	10.617469329	15.776218948	6.455924684
H	11.126080636	14.805149288	6.514391000
C	10.921611514	16.674912998	5.433491803
H	11.674972407	16.410415508	4.690511446
C	10.272732664	17.911378372	5.354750810
H	10.517579956	18.606244177	4.554110280
C	9.308327113	18.252776777	6.309509837
H	8.798353952	19.213212422	6.245597889
C	8.993188605	17.371858826	7.343770404
H	8.237362950	17.632874524	8.083100432
C	9.472264399	15.736348888	9.846281779
C	10.478839063	16.670966901	10.153991761
H	11.137698325	17.047002206	9.373352859
C	10.633726273	17.097688396	11.473657842
H	11.416994671	17.814310698	11.716049253
C	9.799855182	16.607573157	12.482169485

H	9.943940094	16.922033508	13.512655657
C	8.780892009	15.701709289	12.163495159
H	8.128707783	15.320074245	12.950879981
C	8.595697315	15.278057903	10.849683820
H	7.786040441	14.588193623	10.591049126
C	9.175190221	13.842745061	8.263059658
C	8.711147727	13.390300629	7.006495509
H	8.459352316	14.101704689	6.222659985
C	8.549988952	12.028216275	6.785522407
H	8.198052099	11.660993991	5.817225523
C	8.832278404	11.097771091	7.800982653
C	9.285770938	11.554104127	9.046724075
H	9.535764378	10.841094757	9.848873017
C	9.472627190	12.908656790	9.277949108
H	9.888043212	13.230022983	10.234397323
C	8.696475381	9.650158147	7.486886140
C	8.516758784	7.406163292	8.633149543
C	8.675056266	6.622944641	7.503698878
H	8.808503545	7.096966028	6.521022205
C	8.692268272	5.209865071	7.604378670
H	8.825137823	4.632306400	6.688242492
C	8.569137866	4.575204790	8.819311071
H	8.593287933	3.489919884	8.909620945
C	8.414878639	5.346336134	10.003206387
C	8.357290145	6.759235777	9.924690448
C	8.330217698	4.770140873	11.328731864
C	8.169413498	5.565344683	12.449572954
H	8.112617864	5.179716637	13.463016467
C	8.058103160	6.966581971	12.241332519
C	7.826254639	7.879704104	13.437342360
C	7.087563302	10.237977151	13.945242577
C	7.312040799	10.233954825	15.309804721
H	7.655882043	9.317874489	15.802683259
C	7.098035897	11.410919743	16.072406205
H	7.287993750	11.362077780	17.146642964
C	6.678346716	12.583961350	15.488218490
H	6.516446615	13.492144184	16.068159983
C	6.438786426	12.630215733	14.086849486
C	6.624628560	11.461411341	13.309504358
C	5.972006580	12.548991813	11.334938532
C	5.757704219	13.779920319	12.006883446
H	5.412927888	14.637839424	11.434911756
C	6.002560641	13.811455331	13.370278448
C	5.773607942	12.424809501	9.826157539

C	5.369484249	10.579587193	8.149691508
C	5.446845370	11.314436396	6.983573719
H	5.506475254	12.408161566	7.029252603
C	5.481144096	10.652611742	5.727402340
H	5.560444361	11.265423938	4.828927383
C	5.452995024	9.280375992	5.636206911
H	5.512415386	8.764359381	4.675968108
C	5.359580359	8.491137275	6.816279437
C	5.285734351	9.130323818	8.077498566
C	5.138209562	7.083307882	9.217187381
C	5.245611048	6.335516342	8.019343827
H	5.241667254	5.249371988	8.074886848
C	5.354007245	7.043466228	6.831598224
C	5.041352322	6.380837017	10.563538703
C	4.658902753	6.978696103	12.985066249
C	5.045328997	5.781308399	13.559726094
H	5.295063599	4.924855225	12.922008020
C	5.154865801	5.669401213	14.969716559
H	5.496496509	4.720015424	15.382564382
C	4.868147249	6.726562460	15.801885302
H	4.974299600	6.652632577	16.884612719
C	4.435461105	7.964366223	15.250571654
C	4.310703087	8.097746012	13.845963444
C	3.556003682	10.311994301	14.022647670
C	3.675836616	10.304949189	15.437891246
H	3.438663220	11.213245332	15.985776096
C	4.127685720	9.141161545	16.032947466
C	3.114421362	11.566449623	13.280117711
C	2.437182602	12.224644062	10.961105514
C	2.569849421	13.592733372	11.094243185
H	2.697302273	14.035808803	12.088600154
C	2.584350261	14.426828164	9.944894341
H	2.712147784	15.499533208	10.090495323
C	2.459917316	13.905747008	8.678687087
H	2.499511043	14.536336178	7.789009163
C	2.283308251	12.504525769	8.502703606
C	2.169071585	11.859908260	7.213345477
C	2.022684457	10.486382018	7.105872097
H	1.959226772	9.954867118	6.158840676
C	2.000438750	9.738175122	8.309961268
C	2.254386990	11.655005348	9.636737684
C	1.920192771	8.219784484	8.269531639
C	1.731290719	6.293971288	9.869066903
C	2.048296049	5.275163908	8.987789253

H	2.110051762	5.480125448	7.912336369
C	2.331840909	3.973555934	9.472245721
H	2.587046983	3.198221126	8.748776463
C	2.314684571	3.691635876	10.819436863
H	2.569336207	2.702772596	11.202319924
C	1.976337813	4.710309169	11.751279852
C	1.649250962	6.010089075	11.290510263
C	1.298337553	6.804863677	13.459834263
C	1.639515587	5.551654662	14.042539299
H	1.639065221	5.458274896	15.126834098
C	1.986445508	4.524789660	13.186929980
C	8.489472024	2.720189473	12.610385251
H	9.399940501	3.040244841	13.147575085
C	8.526595129	1.242442601	12.182396644
H	7.696049212	1.080321752	11.446470168
C	8.295458459	0.356513590	13.409292869
H	8.335682198	-0.704835070	13.136792237
H	7.315036173	0.534880372	13.864941442
H	9.056000867	0.518516834	14.181101358
C	9.853302324	0.921030092	11.494285657
H	10.706823128	1.021577486	12.188619824
H	10.032945832	1.619123483	10.663902956
H	9.865514822	-0.095004679	11.091426409
C	5.389905673	16.150646713	13.571707914
H	4.332080804	15.971199481	13.317786962
H	5.971556945	16.402815883	12.670019892
C	5.573947365	17.166581719	14.713214914
H	5.215173250	16.683811569	15.660351770
C	7.052913769	17.521179405	14.882635194
H	7.648058604	16.617831044	15.074872760
H	7.207898460	18.204280282	15.723647033
H	7.466638611	18.005523735	13.990151108
C	4.722854804	18.406334649	14.429532284
H	5.025656547	18.910663436	13.504485216
H	4.816799546	19.139556045	15.240194173
H	3.658803065	18.157748752	14.341068245
C	5.669814231	5.048152721	5.487651693
H	4.672706120	4.591494575	5.591384913
H	6.344107250	4.697075949	6.286224459
C	6.269290257	4.892993835	4.078848734
H	5.696190478	5.569042544	3.391171758
C	7.736092374	5.325423395	4.065870360
H	7.842804313	6.348861653	4.459009785
H	8.144778627	5.325450806	3.051035250

H	8.369893157	4.674009651	4.678003440
C	6.102570790	3.446291177	3.608606537
H	6.630931468	2.740028018	4.258328881
H	6.513382796	3.316447607	2.600262693
H	5.049796638	3.145883183	3.571605371
C	4.360215610	10.155405652	18.223682139
H	3.318491703	10.419940657	18.463921574
H	4.857197492	10.980509375	17.685118705
C	5.161121505	9.672635203	19.445807268
H	4.737205352	8.684377636	19.763759748
C	4.997816904	10.677922723	20.588542607
H	5.391785763	11.667030747	20.328390263
H	5.537600493	10.343996113	21.483304367
H	3.948322378	10.804822741	20.876257188
C	6.632690691	9.468472397	19.077009017
H	6.723238465	8.779958007	18.222566909
H	7.194169509	9.036467050	19.911061282
H	7.124406894	10.408946024	18.798380005
C	2.265182612	12.182842683	4.812223417
H	1.284117693	11.726391659	4.602569212
H	3.065531809	11.425434682	4.759664227
C	2.547960961	13.433477740	3.962895025
H	1.982234137	14.288879196	4.420141823
C	4.038933569	13.776596576	3.982960912
H	4.407093951	13.863650408	5.015893772
H	4.231547361	14.734907106	3.488939812
H	4.645235330	13.023641402	3.467708953
C	2.039691242	13.206618661	2.536662393
H	2.548656637	12.369171781	2.046791626
H	2.213825142	14.092562623	1.914493115
H	0.963134039	13.003664071	2.513681493
C	0.937301939	7.985934051	14.320644914
C	2.608875437	3.017179361	14.979178223
H	1.629430907	2.977816846	15.481945160
H	3.224630793	3.835504482	15.390044356
C	3.345024819	1.665099320	14.989874517
H	3.529120973	1.397765571	16.061926494
C	4.693483079	1.790246570	14.274739410
H	4.564966155	2.215853748	13.266460627
H	5.176626428	0.814422345	14.156257382
H	5.383086047	2.442933673	14.818828692
O	18.886674916	8.931077006	6.526989594
O	17.926862912	3.195512585	11.452122152
O	18.120576406	7.404370850	14.715109469

O	16.245332878	14.870410499	14.087074737
O	16.272883775	13.216986696	9.038275935
O	15.145424245	6.393650622	5.662210886
O	15.053822068	5.179298000	10.847874383
O	14.291174650	9.082339833	17.427203027
O	13.695916131	12.877308505	13.744886199
O	12.155427454	12.828518438	6.171695593
O	12.075466552	7.705077433	7.470801049
O	10.713744455	9.244982211	14.318245300
O	11.180688985	7.721633236	15.919482599
O	11.717561426	3.279313760	13.650642850
N	19.798102679	14.925355615	8.666007987
N	18.439204285	8.592158639	8.758935812
H	18.268682341	9.049194292	9.670685277
N	18.121706801	7.337541281	11.196266774
N	17.401825176	8.994953753	13.197665843
H	17.186649095	9.152776347	12.188903929
N	16.741615300	11.336780838	11.950908796
N	15.632750790	11.031475696	9.477260128
H	15.483072177	10.346099399	10.250345658
N	15.168900545	8.352336255	9.315318298
N	14.521986079	7.272659928	11.665448252
H	14.319103410	8.261668211	11.387701828
N	13.986096431	9.410202024	13.297365653
N	12.925777623	11.539325851	12.026267885
H	12.556097909	10.579105253	11.805461711
N	12.392656111	10.480056142	9.591459668
N	11.578518237	7.897938183	9.719773211
H	11.406078160	8.578455297	10.497901143
N	11.278892915	7.234507539	12.410723814
C	19.754884972	15.869484099	7.570901623
C	20.569587383	15.643182432	6.446149167
H	21.190914560	14.749034335	6.392962908
C	20.570070137	16.575636245	5.409137821
H	21.199429525	16.408239784	4.535502795
C	19.777191521	17.726172992	5.487093771
H	19.790405023	18.451292880	4.676373010
C	18.966998818	17.940484445	6.606504898
H	18.344497211	18.832754101	6.664522999
C	18.945261440	17.015436278	7.652031844
H	18.304674910	17.175955376	8.518317838
C	19.859413237	15.488402843	9.995473895
C	20.861510948	16.439176080	10.271683373
H	21.562890463	16.739079046	9.494928861

C	20.946990702	16.985190907	11.552228295
H	21.720612135	17.720010503	11.772153189
C	20.053454911	16.591810862	12.554197188
H	20.133668645	17.016644260	13.552467616
C	19.062226444	15.649194711	12.270594709
H	18.368903104	15.338194776	13.055947278
C	18.951427656	15.099486344	10.992913073
H	18.163578244	14.377482397	10.762070950
C	19.462471946	13.560363768	8.451339557
C	18.887604102	13.141987331	7.229478049
H	18.592525984	13.870755277	6.476003604
C	18.664778178	11.790451072	6.999101445
H	18.230954443	11.456237566	6.051091003
C	18.981374464	10.833391417	7.978872004
C	19.527793971	11.255016816	9.202091976
H	19.779616387	10.525636305	9.976354199
C	19.774234846	12.600733906	9.442765276
H	20.227950668	12.903306229	10.385924452
C	18.773938889	9.399346086	7.647486091
C	18.354416924	7.176421668	8.772065978
C	18.400707620	6.388161225	7.635071903
H	18.513970600	6.854746351	6.647327004
C	18.302473190	4.977281941	7.734178013
H	18.335004980	4.398841879	6.805141764
C	18.163185115	4.348503713	8.948412185
H	18.081104855	3.265063336	9.033222337
C	18.120155883	5.122461547	10.140689832
C	18.203847370	6.535427556	10.066083121
C	17.964810696	4.555549099	11.465106020
C	17.887787102	5.361281822	12.588623372
H	17.770080474	4.980502656	13.598773860
C	17.960353142	6.766095494	12.389583721
C	17.850858839	7.718415230	13.573976556
C	17.291344796	10.148866108	14.009760575
C	17.481035522	10.169804727	15.380174560
H	17.745906861	9.247560073	15.908360462
C	17.327351307	11.381015288	16.105283055
H	17.497625890	11.352614919	17.183439796
C	16.980503040	12.555532648	15.480993781
H	16.846163981	13.486897589	16.031770262
C	16.772283688	12.574162773	14.073006871
C	16.941175251	11.383281569	13.324260014
C	16.329656571	12.437568515	11.320487875
C	16.112486677	13.678063481	11.967565950

H	15.765571290	14.523562066	11.376993958
C	16.346082119	13.741463891	13.332875346
C	16.089859099	12.305461175	9.818701108
C	15.485747595	10.481972414	8.175064013
C	15.531667755	11.205191950	7.000854355
H	15.659781057	12.292973795	7.031156294
C	15.429933470	10.537529098	5.750391139
H	15.470744588	11.142072376	4.843834785
C	15.297182823	9.170729797	5.673005050
H	15.243776155	8.649272141	4.716145258
C	15.227096641	8.394247404	6.864206849
C	15.290129484	9.042635708	8.120211519
C	14.996152839	7.029010935	9.290478269
C	14.970752171	6.266569184	8.097678991
H	14.858070767	5.187382806	8.161737958
C	15.102260362	6.952522604	6.898368856
C	14.861948463	6.365447713	10.653290351
C	14.533121361	7.042332692	13.063230224
C	14.785263918	5.818920014	13.653438630
H	14.946450927	4.934329375	13.028153499
C	14.859197804	5.708810669	15.068268111
H	15.086703091	4.733568574	15.494073566
C	14.676296206	6.800857095	15.883661433
H	14.753226019	6.726478970	16.968548474
C	14.382398561	8.072074901	15.313298680
C	14.292899664	8.203275997	13.906451330
C	13.757791523	10.484018555	14.053498643
C	13.849755898	10.475954626	15.471211948
H	13.685014852	11.404622992	16.012284789
C	14.174729001	9.278203968	16.081859453
C	13.448700474	11.769759907	13.294052458
C	12.845900293	12.451896108	10.939953996
C	13.017985594	13.817198410	11.030256071
H	13.183142599	14.284970836	12.005395342
C	12.992880157	14.613968578	9.852747892
H	13.161347372	15.685929907	9.959282821
C	12.770157639	14.064955865	8.614674828
H	12.757844981	14.675176683	7.708348144
C	12.535882151	12.665150276	8.484622706
C	12.228164681	11.990607885	7.243805667
C	12.011145330	10.622090511	7.203447364
H	11.777497314	10.069118008	6.292878604
C	12.106087857	9.907967547	8.422208168
C	12.591381269	11.848345587	9.640453809

C	11.913278858	8.399636197	8.452941681
C	11.608451856	6.527392977	10.086405104
C	11.792047052	5.499071828	9.175035973
H	11.842942169	5.720951741	8.100419522
C	11.932542398	4.160912139	9.611877650
H	12.096816965	3.386651642	8.862722857
C	11.886654529	3.839439593	10.949819352
H	12.028705028	2.817530411	11.301263575
C	11.651197089	4.857163354	11.909676388
C	11.501072042	6.209151976	11.497800372
C	11.220216490	6.932339718	13.704726367
C	11.365560188	5.619086630	14.232862979
H	11.306348159	5.473909231	15.309590398
C	11.586742137	4.601779546	13.330110960
C	17.671636085	2.499268307	12.717804779
H	18.440955555	2.791292433	13.449030451
C	17.754756050	1.018262186	12.306778669
H	17.117090688	0.884232828	11.392351758
C	17.208631183	0.134118457	13.430366802
H	17.270440111	-0.925917092	13.157667898
H	16.148718006	0.351573334	13.647982414
H	17.771231957	0.257605341	14.362244402
C	19.193556751	0.636931372	11.953766929
H	19.860456256	0.700712515	12.820530145
H	19.593431922	1.310177382	11.182106725
H	19.252580016	-0.385203026	11.566117069
C	15.490230100	15.991214369	13.503473785
H	14.481265535	15.618979972	13.253626760
H	16.016373036	16.337113590	12.599279065
C	15.476732878	17.031940230	14.634148450
H	15.196949551	16.503985937	15.583467556
C	16.863155430	17.653109514	14.814738980
H	17.608890831	16.875094458	15.026929294
H	16.879249765	18.364784250	15.646299720
H	17.195978252	18.189160856	13.918758182
C	14.418625091	18.093030384	14.318497321
H	14.637577758	18.627443541	13.386888322
H	14.365195124	18.843849351	15.115956302
H	13.420153951	17.651079110	14.221673882
C	15.228362612	4.934256978	5.549187253
H	14.189016040	4.567499095	5.544300089
H	15.785291413	4.512082277	6.401349977
C	15.953617727	4.738069980	4.204136079
H	15.447795496	5.393957166	3.448621523

C	17.417449464	5.168832417	4.312082565
H	17.486609427	6.224349819	4.620696754
H	17.936261526	5.074764458	3.352909950
H	17.971476095	4.576164347	5.053045870
C	15.824090629	3.277901123	3.765095210
H	16.302271090	2.592745662	4.473965727
H	16.308674968	3.121271336	2.793528959
H	14.777028135	2.974281112	3.656994392
C	14.522621861	10.255539431	18.277874538
H	13.528369558	10.632459833	18.564748614
H	15.085042712	11.026317466	17.724248793
C	15.315432683	9.665446561	19.458141904
H	14.832218884	8.692215755	19.738947409
C	15.245908084	10.620410553	20.652070802
H	15.686629313	11.597579280	20.423146707
H	15.800829797	10.212779186	21.506955807
H	14.215033997	10.786978339	20.982758118
C	16.761319131	9.381585428	19.046495040
H	16.791245938	8.730675717	18.158995401
H	17.310796559	8.869935386	19.843394269
H	17.313218184	10.298149941	18.803024163
C	11.834948806	12.216556941	4.872675489
H	10.833204239	11.758523481	4.952031795
H	12.597228619	11.450342468	4.653102117
C	11.873976101	13.404496947	3.899202805
H	11.194155127	14.200751849	4.300446045
C	13.291771046	13.973088602	3.803143999
H	13.685520890	14.206600683	4.803104590
H	13.315919166	14.892232697	3.210872437
H	13.987159304	13.266639846	3.337335347
C	11.351788235	12.949998802	2.534412642
H	11.966794752	12.150899445	2.103524138
H	11.357706034	13.780164434	1.818355937
H	10.321690317	12.580871076	2.594660847
C	10.988601923	8.103681151	14.617018247
C	12.127678865	2.952865041	15.021813516
H	11.196313756	2.787686410	15.586680829
H	12.703097687	3.786857369	15.458362416
C	12.985091578	1.682336274	14.879090112
H	13.298330819	1.374402486	15.909659694
C	12.170864768	0.547890400	14.253980731
H	11.347126832	0.233895672	14.900916948
H	12.792291114	-0.328662110	14.046765260
H	11.728294300	0.872204767	13.290154251

C	14.235261999	1.990494709	14.053467719
H	13.964089713	2.375899969	13.059078076
H	14.850208943	1.087426766	13.901296184
H	14.860281047	2.751153804	14.533981242
O	10.312572358	10.213018999	11.769512847
C	9.811968234	11.387694132	12.434215884
H	10.544221681	12.187582472	12.293808986
H	8.876969161	11.646803262	11.927983075
H	9.652786170	11.195652375	13.499918492
H	10.454422075	9.496630556	12.451183874
C	0.792667218	8.635627047	16.640548580
H	-0.265665814	8.571002529	16.907206250
H	1.450686875	8.352303142	17.469319889
H	1.036413646	9.632415705	16.250708805
C	10.950948328	8.738547862	16.934308471
H	9.921390737	8.610792302	17.282641494
H	11.695475376	8.494551551	17.701338674
H	11.107009179	9.745020956	16.525212719
C	2.469974426	0.581098405	14.354865331
H	2.977993537	-0.388325575	14.342262370
H	1.523927995	0.459011828	14.892443315
H	2.223103359	0.840232261	13.315100376
H	16.666199110	2.794400324	13.064289307
H	7.583372033	2.978233148	13.180660647

Table S7. Atomic coordinates for the optimized structure of **TPA-Q₆(*i*-Bu)** in MOPAC2016 (Fig. 3^a, gas phase).

Atom	X	Y	Z
O	8.871569756	9.172118995	6.469870457
O	8.438320646	3.292907836	11.343612269
O	8.048386484	7.406635753	14.630500106
O	6.175491148	14.873949357	14.110463742
O	6.051079893	13.265671944	9.038017326
O	5.483226933	6.411559038	5.610770641
O	5.295808446	5.136847729	10.759141685
O	4.378850980	9.000053846	17.370322511
O	3.553703941	12.723789414	13.666448964
O	2.280004978	12.729429831	6.133920528
O	2.186213837	7.585374880	7.259745783
O	0.821239571	9.143031030	14.050332704
O	1.078339628	7.588713210	15.668551078
O	2.279495111	3.238688223	13.555752329
N	9.482534364	15.142901605	8.750882221
N	8.457302494	8.730622259	8.691420630

H	8.285653445	9.148659557	9.623061049
N	8.156904916	7.429149141	11.091688849
N	7.425609425	9.037917393	13.115686769
H	7.299672943	9.229250319	12.097010084
N	6.658820072	11.374086564	11.920436242
N	5.532151667	11.047961036	9.470870619
H	5.460660332	10.340398310	10.235595851
N	5.221045181	8.344662955	9.271810773
N	4.693257855	7.197539548	11.613306489
H	4.475528817	8.185860838	11.347233292
N	4.022573103	9.287301945	13.239240966
N	2.715479507	11.344297845	12.010984488
H	2.522991275	10.348324467	11.768097035
N	2.231849514	10.307826473	9.510181619
N	1.666055492	7.677368975	9.510878571
H	1.496433266	8.328765839	10.311151473
N	1.385764606	7.065032512	12.168404671
C	9.745626071	16.040575402	7.646985045
C	10.679832739	15.708148385	6.651217229
H	11.203600139	14.744308408	6.681559428
C	10.939741103	16.621865710	5.629572905
H	11.674204857	16.376172314	4.862200018
C	10.272429615	17.850097440	5.585568669
H	10.485836213	18.558687295	4.788469977
C	9.330822882	18.166609753	6.570754585
H	8.803790216	19.119624689	6.532166469
C	9.059841194	17.269294606	7.603460424
H	8.321901918	17.511862230	8.367051950
C	9.678352007	15.675419456	10.075169110
C	10.684261099	16.637272457	10.301768258
H	11.311173795	16.982777253	9.481984078
C	10.875776148	17.137370324	11.589956570
H	11.655246069	17.876508313	11.766077942
C	10.079757203	16.696530369	12.651749691
H	10.246101478	17.079784459	13.654655546
C	9.071869617	15.755561264	12.417406035
H	8.450467321	15.404869651	13.244973291
C	8.854265053	15.255288931	11.134140902
H	8.052290179	14.536891414	10.948344476
C	9.253248313	13.760009448	8.511643572
C	8.819199449	13.336861894	7.231662226
H	8.608013303	14.064586378	6.450681910
C	8.635994025	11.985165509	6.976232043
H	8.321333134	11.646573618	5.984600743

C	8.854142243	11.025784723	7.980647816
C	9.234378894	11.452813509	9.262903122
H	9.397060811	10.728334622	10.067641103
C	9.452712796	12.799026047	9.527855444
H	9.818138020	13.084446820	10.515721489
C	8.729914754	9.592088948	7.608031721
C	8.495573301	7.311527039	8.678850102
C	8.680366645	6.545482347	7.542074844
H	8.811883103	7.032291656	6.566295217
C	8.722796160	5.131078431	7.632170962
H	8.877485444	4.564349303	6.713660279
C	8.595505467	4.480553821	8.838111801
H	8.638453146	3.395180152	8.916951869
C	8.419374040	5.233433058	10.031072288
C	8.351022636	6.646957701	9.962475517
C	8.329237943	4.648347205	11.351957151
C	8.165870088	5.437790550	12.478240963
H	8.107391076	5.047051859	13.490117907
C	8.069277365	6.839905234	12.283952483
C	7.862418242	7.761018421	13.478746018
C	7.280952717	10.173717163	13.951744921
C	7.462442975	10.169523538	15.322007502
H	7.743264401	9.241345084	15.830694389
C	7.291208176	11.364922594	16.067434822
H	7.464053647	11.323253921	17.142673701
C	6.925520984	12.545320791	15.462612967
H	6.788021983	13.465217929	16.029993638
C	6.706068861	12.583962692	14.057234407
C	6.884182042	11.406699260	13.289690676
C	6.209380776	12.472419835	11.312946627
C	5.988461940	13.704563006	11.977819555
H	5.619433863	14.550116850	11.401428892
C	6.261551788	13.757992585	13.335358942
C	5.937795656	12.341502311	9.818593962
C	5.459708531	10.499853297	8.162038292
C	5.518935800	11.235268225	6.995493669
H	5.597631808	12.327816050	7.039404184
C	5.515542560	10.573807223	5.737984081
H	5.579132877	11.187620471	4.839459784
C	5.468508437	9.202316221	5.645168630
H	5.503454550	8.686827225	4.684143627
C	5.388800401	8.411535786	6.826287353
C	5.345621932	9.052586755	8.087464124
C	5.168986149	7.011397860	9.233917063

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C	10.994920728	8.206668784	14.315594116
C	10.884676826	8.906917198	16.614605733
H	9.819344073	8.830306762	16.855314830
H	11.123558796	9.899415031	16.211295455
H	11.526574689	8.639389833	17.460132449
C	12.117260893	3.091391069	14.994914103
H	11.207721446	3.011204833	15.611124954
H	12.738258138	3.939655520	15.332311976
C	12.926539763	1.781832176	14.942429159
H	13.321602783	1.600937138	15.975827302

C	12.020746189	0.611753176	14.557571294
H	11.217773282	0.462222786	15.286053895
H	12.579988448	-0.325337614	14.480051628
H	11.541825906	0.793608149	13.575143475
C	14.109933726	1.920537853	13.980375228
H	13.766259961	2.220485211	12.977745313
H	14.659477553	0.977780486	13.871693603
H	14.815921676	2.687591618	14.317078416

^aThe dimer form of the methanol molecule is ignored in Fig. 3.

Table S8. Atomic coordinates for the optimized structure of **TPA-Q₆(*i*-Bu)** in MOPAC2016 (Fig. S1a(i), gas phase).

Atom	X	Y	Z
O	8.690600724	9.122999176	6.581020952
O	7.941231899	3.374783613	11.512575773
O	7.920142024	7.601185370	14.765858286
O	5.701904891	14.959056702	14.179836518
O	5.802109079	13.335047016	9.116353138
O	5.153699701	6.525439894	5.640920011
O	4.992952146	5.203308560	10.784091449
O	4.138566552	9.059673310	17.400865216
O	3.128149605	12.744599441	13.737792704
O	2.047829881	12.810341320	6.195333498
O	1.909377923	7.655220295	7.296116552
O	0.455760298	9.242210068	14.054261609
O	0.811814507	7.716162267	15.681208920
O	1.881311563	3.325587219	13.580236933
N	9.278239343	15.153020074	8.746450578
N	8.219866781	8.770789173	8.806079458
H	8.016842033	9.221658606	9.713874366
N	7.933616966	7.518258939	11.249462745
N	7.099129892	9.139309280	13.246931045
H	6.883981584	9.289834267	12.238577492
N	6.289462629	11.457678331	12.015487165
N	5.206964203	11.131805030	9.532497482
H	5.090739579	10.430284186	10.293983265
N	4.918318636	8.417056417	9.321497788
N	4.336307800	7.242879277	11.645486488
H	4.092295196	8.225932684	11.384806889
N	3.674422366	9.320537056	13.280030954
N	2.356318669	11.368660662	12.054489660
H	2.168087387	10.375372303	11.797498841
N	1.895418338	10.367555459	9.547896974
N	1.281225568	7.746399941	9.518950046

H	1.082172555	8.397349302	10.312066714
N	1.038935351	7.156592191	12.184923933
C	9.341670043	16.095458208	7.655687613
C	10.174771294	15.830832569	6.553186048
H	10.750791143	14.905788250	6.509974603
C	10.254511784	16.766906681	5.522273254
H	10.895970193	16.568223951	4.663557592
C	9.525646316	17.959574376	5.585189391
H	9.595517987	18.684339680	4.776217927
C	8.706458416	18.217980928	6.688471463
H	8.140345495	19.147148557	6.738588433
C	8.604809263	17.291922871	7.727603406
H	7.959792283	17.487826422	8.582587431
C	9.346436664	15.695489524	10.084419742
C	10.373853767	16.608503154	10.391751409
H	11.095681146	16.899687093	9.630574790
C	10.451580183	17.134507737	11.680893675
H	11.242034425	17.842171036	11.925502068
C	9.532112567	16.749628483	12.663250977
H	9.607329396	17.153524743	13.671206846
C	8.519761042	15.837848709	12.348361982
H	7.809758385	15.531450814	13.120498678
C	8.407603263	15.317038676	11.058651076
H	7.604354386	14.621079548	10.799212331
C	9.029058716	13.776651026	8.516291834
C	8.516675175	13.333869179	7.275214814
H	8.221870375	14.050033713	6.509917182
C	8.357197666	11.973776350	7.040102480
H	7.976023680	11.621507792	6.076416302
C	8.675954358	11.030411703	8.031410400
C	9.161061177	11.475249935	9.273135596
H	9.417611955	10.755924623	10.055073904
C	9.341401820	12.828709441	9.520659864
H	9.744205335	13.147530202	10.481302663
C	8.538258280	9.588879981	7.697927672
C	8.204410374	7.352655798	8.825920866
C	8.309461537	6.560074554	7.695370753
H	8.417133457	7.025921400	6.707184324
C	8.281334035	5.147809139	7.802384887
H	8.364199387	4.561626309	6.886667442
C	8.154242740	4.522367032	9.021831664
H	8.125615762	3.436932312	9.114041580
C	8.055768052	5.301668545	10.206343026
C	8.068901477	6.715562823	10.124188811

C	7.916069950	4.732896562	11.531797065
C	7.792063711	5.538508186	12.651446545
H	7.694367260	5.154896697	13.662971039
C	7.793658477	6.944371091	12.444062925
C	7.628943122	7.897134611	13.621992367
C	6.938561060	10.291614584	14.061360361
C	7.154937557	10.320489142	15.426444166
H	7.480677865	9.412575266	15.948346246
C	6.968876687	11.523657706	16.155921729
H	7.171492610	11.504749753	17.228896075
C	6.560165807	12.682048702	15.538868580
H	6.417966373	13.612890424	16.092559136
C	6.308558240	12.688583540	14.139827378
C	6.506451428	11.505195910	13.385877949
C	5.838774723	12.550184061	11.395847888
C	5.581472330	13.780767812	12.049313306
H	5.195635061	14.614784685	11.467632133
C	5.831312257	13.846152812	13.411443733
C	5.628149424	12.414953563	9.892905231
C	5.173317480	10.580505374	8.222864549
C	5.261803044	11.320508862	7.061249057
H	5.343935385	12.413088153	7.110139679
C	5.279231975	10.666356663	5.800034186
H	5.366988018	11.282687359	4.905306736
C	5.212436579	9.296921173	5.700408424
H	5.254624910	8.785019102	4.737534858
C	5.099788081	8.503731200	6.877538625
C	5.053680887	9.134639764	8.143309326
C	4.843492806	7.084218553	9.269197898
C	4.907386344	6.343298808	8.065354646
H	4.860783649	5.257504231	8.110591009
C	5.043169220	7.057690632	6.883589725
C	4.735791018	6.380651405	10.616197256
C	4.386233430	7.002624273	13.040244505
C	4.727237840	5.797757886	13.623985856
H	4.931932151	4.924885577	12.993675317
C	4.836849364	5.696960163	15.035337086
H	5.131736225	4.732682336	15.455862903
C	4.604630813	6.776330143	15.856050522
H	4.717510649	6.710382301	16.938756375
C	4.212897066	8.023349421	15.293861965
C	4.082738820	8.142539779	13.889001173
C	3.377745161	10.372644777	14.040498872
C	3.508965906	10.382673495	15.453675791

H	3.291666673	11.308208495	15.987430837
C	3.944790950	9.218852965	16.062772651
C	2.941495082	11.622270437	13.293632292
C	2.268177455	12.300498724	10.982487118
C	2.421461017	13.665828464	11.121938735
H	2.552951628	14.104669163	12.117669266
C	2.441712615	14.502072871	9.973347618
H	2.585710236	15.572664131	10.120173607
C	2.305931459	13.986082325	8.706187725
H	2.350750356	14.617966436	7.818130239
C	2.109967115	12.587186142	8.525333515
C	1.984129362	11.942202689	7.237746961
C	1.812678991	10.570707379	7.132412579
H	1.738470925	10.038317244	6.186045766
C	1.775637069	9.824154623	8.335827449
C	2.073421494	11.737278572	9.657729467
C	1.664189247	8.306584443	8.294888945
C	1.442324209	6.388086087	9.901482510
C	1.733425706	5.361000269	9.022179103
H	1.804462429	5.563264345	7.946755340
C	1.976876055	4.051081676	9.507976510
H	2.219701181	3.269988865	8.787079742
C	1.933071281	3.767989090	10.854047865
H	2.151808159	2.771494045	11.239080200
C	1.614610234	4.795802340	11.783230919
C	1.345537719	6.108472889	11.322661189
C	1.014563601	6.912967400	13.491763747
C	1.278629359	5.640943474	14.072442646
H	1.248644277	5.538773935	15.155811579
C	1.585915945	4.601375426	13.216561647
C	7.719702485	2.651660945	12.768955020
H	6.738960758	2.952307980	13.170342286
H	8.528594934	2.911038284	13.469415304
C	7.754293748	1.181981623	12.309568967
H	7.023941960	1.072755168	11.465429211
C	7.322676122	0.269321338	13.458629711
H	7.962819813	0.382127847	14.339764992
H	7.375386680	-0.784284921	13.155290674
H	6.283564117	0.464308980	13.770492379
C	9.148282371	0.819254714	11.793324809
H	9.462220139	1.524641631	11.010920787
H	9.169156203	-0.186833262	11.362780169
H	9.905436025	0.855448796	12.583100026
C	5.088621346	16.143916806	13.554899629

H	4.108133795	15.841702833	13.149377707
H	5.756900413	16.493630935	12.751984854
C	4.963946780	17.139086196	14.719583463
H	4.658270516	16.567250494	15.637310845
C	6.293222506	17.833173370	15.015364066
H	7.079595613	17.104532930	15.241763571
H	6.190536531	18.487760956	15.895705717
H	6.637829939	18.454848416	14.184863822
C	3.867175441	18.151868954	14.383496121
H	4.083831075	18.707825429	13.468994815
H	3.763167176	18.878189904	15.216230789
H	2.888731980	17.668953451	14.275586376
C	5.274038223	5.068642428	5.512627040
H	4.257871045	4.654627079	5.614883641
H	5.938574166	4.676556071	6.300131918
C	5.860919347	4.910507882	4.097348983
H	5.287980961	5.590933306	3.413891198
C	7.330610224	5.334491823	4.077011139
H	7.448445929	6.348745363	4.489876590
H	7.726015203	5.354939389	3.055846436
H	7.967076779	4.662921036	4.662944522
C	5.677252093	3.464737921	3.630504880
H	6.197800330	2.754088005	4.281950842
H	6.082577641	3.322463848	2.621084020
H	4.620146249	3.178660275	3.597647221
C	4.187676812	10.275395582	18.225228888
H	3.146672026	10.588284693	18.399696240
H	4.747655307	11.062272522	17.690655587
C	4.900826466	9.801859066	19.504272718
H	4.417948617	8.846537939	19.838006621
C	4.720965689	10.864451737	20.591411496
H	5.167871571	11.823661332	20.306009278
H	5.207245275	10.555961997	21.525583139
H	3.665254645	11.042087515	20.821461316
C	6.378386223	9.523344425	19.224109933
H	6.490836007	8.830965786	18.375808784
H	6.868737933	9.058996458	20.086791324
H	6.937970879	10.434419231	18.982251493
C	2.037694339	12.248734228	4.836766447
H	1.047190893	11.795333628	4.668720515
H	2.831511906	11.486862602	4.757881328
C	2.290449855	13.490675856	3.965123054
H	1.700554294	14.338815811	4.404405984
C	3.772290424	13.870981441	3.982022953

H	4.133305277	13.995093883	5.013442480
H	3.944952010	14.817978750	3.459555180
H	4.399384856	13.114811609	3.497807110
C	1.794300104	13.216835245	2.543069138
H	2.327840332	12.379932849	2.079236942
H	1.948397127	14.089875375	1.897824749
H	0.723559192	12.985068591	2.521190376
C	0.714812209	8.106001584	14.358808778
C	0.600786836	8.743702090	16.685056946
H	-0.456353983	8.715773269	16.963197585
H	0.880758070	9.732725901	16.299472768
H	1.254005282	8.424288777	17.504929231
C	2.134268132	3.048368174	14.998935539
H	1.151572839	2.846878470	15.455285083
H	2.613498919	3.919641216	15.475695767
C	3.060977543	1.818920940	14.983805408
H	3.266437210	1.550943406	16.051266085
C	2.376310321	0.631504436	14.302749656
H	1.440363857	0.359537233	14.803604306
H	3.020439409	-0.254616471	14.295353027
H	2.127399166	0.868754577	13.258026747
C	4.381638173	2.166673281	14.292797575
H	4.200617077	2.556469039	13.278994400
H	5.029825633	1.279544010	14.191201792
H	4.940238118	2.929966588	14.848752264
O	-1.241736613	22.871363330	24.400518527
O	-0.502202035	28.616446426	19.462384720
O	-0.489615963	24.386066697	16.214939978
O	1.725553632	17.028299652	16.800135498
O	1.644060567	18.657593560	21.863918649
O	2.295059653	25.468168451	25.334347185
O	2.447922165	26.790159050	20.189238314
O	3.288430514	22.921770267	13.576778480
O	4.308874974	19.245460285	17.240413381
O	5.401119412	19.180861751	24.782265185
O	5.536678430	24.334986084	23.679534164
O	6.989267817	22.745461135	16.922887474
O	6.623062918	24.267103579	15.294076735
O	5.556632589	28.660782080	17.392383138
N	-1.829799929	16.841460905	22.234946682
N	-0.774864252	23.224523369	22.174650564
H	-0.572969739	22.772579196	21.268000399
N	-0.491632659	24.473751254	19.730653234
N	0.343372189	22.851871046	17.731781832

H	0.564286087	22.703533671	18.739797762
N	1.152749746	20.533338292	18.963400431
N	2.237960558	20.860233657	21.443318174
H	2.350757255	21.561858234	20.681117602
N	2.525615995	23.576557061	21.653352812
N	3.106033076	24.749637025	19.329049490
H	3.351616037	23.766963769	19.590388288
N	3.766790278	22.670828444	17.696639636
N	5.081992381	20.621071474	18.923651108
H	5.269892611	21.614038489	19.180490746
N	5.548097367	21.622187481	21.428447982
N	6.164765121	24.244107255	21.456441761
H	6.363664874	23.592604487	20.663977048
N	6.403054842	24.831563012	18.789649521
C	-1.904125096	15.899966106	23.325436696
C	-2.728491283	16.176154978	24.431589637
H	-3.291114260	17.109178793	24.478875756
C	-2.816915556	15.240187368	25.463238661
H	-3.452177485	15.448514667	26.324666050
C	-2.107335610	14.036423036	25.395795202
H	-2.185622946	13.311883631	26.203791453
C	-1.297724630	13.766677078	24.287359516
H	-0.746848118	12.828863470	24.233494244
C	-1.186399030	14.691805459	23.248932771
H	-0.549644503	14.486870908	22.390147590
C	-1.910733128	16.301848903	20.896297715
C	-2.940389965	15.388881752	20.596564620
H	-3.656967745	15.094898576	21.362675651
C	-3.028425819	14.864944851	19.306878963
H	-3.820541646	14.156482516	19.067278215
C	-2.117076548	15.251358846	18.317823099
H	-2.200557837	14.848675924	17.309315545
C	-1.101282907	16.161400049	18.625817297
H	-0.398526487	16.470156995	17.848319633
C	-0.980782894	16.681392172	19.915368022
H	-0.175404400	17.376767843	20.168738231
C	-1.583312041	18.218471175	22.465110975
C	-1.065227029	18.660851088	23.704425349
H	-0.765955049	17.943864066	24.466755778
C	-0.905787732	20.020252705	23.939566185
H	-0.521296025	20.372432022	24.901495058
C	-1.229415107	20.964538434	22.950395404
C	-1.718287477	20.520263454	21.710400320
H	-1.978308874	21.239351484	20.928848959

C	-1.899373012	19.166917049	21.462436113
H	-2.305898873	18.848067887	20.503029952
C	-1.091350907	22.405426450	23.283773467
C	-0.759976607	24.641930668	22.153745981
C	-0.864321188	25.435721862	23.283835740
H	-0.970869535	24.970468880	24.272506530
C	-0.836526737	26.847840809	23.175183571
H	-0.918617523	27.434907991	24.090713261
C	-0.711189794	27.471789122	21.954846612
H	-0.683176110	28.557109897	21.861600502
C	-0.613901243	26.691551450	20.771431225
C	-0.626149134	25.277557894	20.855359965
C	-0.476386462	27.258029608	19.444757069
C	-0.353908389	26.451823686	18.326264336
H	-0.258306520	26.834019938	17.313745832
C	-0.353947189	25.046332412	18.534910997
C	-0.191896785	24.092565750	17.357757779
C	0.500125145	21.699041657	16.918225772
C	0.280977589	21.669063828	15.553250687
H	-0.043180676	22.577620467	15.032127926
C	0.461956821	20.464280803	14.825083649
H	0.257919621	20.484125454	13.752961486
C	0.870684924	19.305582002	15.441279517
H	1.007866013	18.374236201	14.888178753
C	1.125209164	19.300307641	16.841317364
C	0.930370617	20.485218324	17.593667744
C	1.601214990	19.440477359	19.583436611
C	1.853497618	18.208347049	18.930561640
H	2.236234306	17.373275985	19.513197605
C	1.600567671	18.142452151	17.569319689
C	1.815956443	19.575945243	21.086232635
C	2.273959072	21.412616017	22.752515826
C	2.187533344	20.673168715	23.914684444
H	2.106029225	19.580703125	23.866226624
C	2.171853977	21.327610818	25.175586435
H	2.085806615	20.711141552	26.071885814
C	2.237652400	22.697566442	25.274897763
H	2.197334331	23.210082145	26.238076718
C	2.348124963	23.489997298	24.097216725
C	2.392616904	22.858728624	22.831928693
C	2.600298120	24.909412342	21.705007449
C	2.537473628	25.650590576	22.909207457
H	2.583330949	26.736129506	22.865312720
C	2.403603282	24.936548465	24.091414169

C	2.706503362	25.611576880	20.357417500
C	3.053649498	24.987891202	17.934081410
C	2.710751099	26.191594781	17.348747086
H	2.506001240	27.065359890	17.978068895
C	2.598865880	26.290402590	15.937248587
H	2.303641196	27.254155429	15.515630563
C	2.828931061	25.209698447	15.118017242
H	2.713895419	25.273560010	14.035535654
C	3.221923563	23.963432176	15.681303569
C	3.356204314	23.846690534	17.086107493
C	4.060089614	21.616864963	16.937190279
C	3.924996168	21.603650617	15.525004100
H	4.139289970	20.675939935	14.993362059
C	3.487486673	22.766238025	14.914694346
C	4.496469277	20.366896517	17.684785484
C	5.171496087	19.688853656	19.994807663
C	5.018061050	18.324005164	19.855993197
H	4.884577364	17.885003971	18.860824928
C	5.000096996	17.487678652	21.005357961
H	4.855867663	16.417222060	20.858831921
C	5.138480277	18.003744162	22.271667642
H	5.095341721	17.372139823	23.160049855
C	5.335131144	19.403165339	22.452398503
C	5.463339282	20.048428001	23.739150776
C	5.635046527	21.420255450	23.843954787
H	5.711120717	21.952629219	24.790445888
C	5.670158231	22.165912553	22.640436297
C	5.369941229	20.252795497	21.319676032
C	5.781536278	23.683705622	22.680863980
C	6.001487110	25.601703729	21.072900532
C	5.709924984	26.629506569	21.951885016
H	5.639936308	26.427952308	23.027782868
C	5.464261978	27.938214301	21.465030324
H	5.220720511	28.719923850	22.185267766
C	5.506432940	28.220250997	20.118544221
H	5.285754016	29.216179686	19.732520428
C	5.825103620	27.192146564	19.190420582
C	6.096288076	25.879900095	19.651869037
C	6.425582595	25.073779577	17.482670312
C	6.159963770	26.345344255	16.901538686
H	6.188886030	26.446475786	15.818192508
C	5.852373823	27.384895213	17.757049165
C	-0.284412101	29.338312949	18.204438804
H	0.695523681	29.037754511	17.800738064

H	-1.095044299	29.077036860	17.506552371
C	-0.319259285	30.808760086	18.661940115
H	0.409934266	30.918845163	19.507626508
C	0.114508738	31.719754366	17.512165382
H	-0.525962560	31.607668115	16.630630776
H	0.065180235	32.773053821	17.814701271
H	1.153817497	31.520373687	17.199519366
C	-1.714623420	31.171854664	19.174837423
H	-2.032062621	30.463313390	19.953321381
H	-1.735190830	32.176634879	19.609197579
H	-2.469475838	31.139682536	18.382196154
C	2.329797133	15.839742630	17.426343733
H	3.307070511	16.137215619	17.843336837
H	1.651641405	15.489488766	18.221603673
C	2.462953543	14.849180368	16.258728973
H	2.775791247	15.424267729	15.345849706
C	1.135172514	14.157949255	15.949723946
H	0.349563374	14.888065417	15.723880197
H	1.243165243	13.507966651	15.066344921
H	0.785081640	13.531064787	16.774032169
C	3.555153119	13.833657711	16.599528284
H	3.328092961	13.268637157	17.505485201
H	3.669523288	13.115798289	15.761182006
H	4.532288827	14.315438597	16.722905527
C	2.167683820	26.924447374	25.463460960
H	3.183283693	27.342148621	25.367898312
H	1.508233497	27.314377223	24.670939940
C	1.570564816	27.079096147	26.874068994
H	2.143139901	26.402031189	27.561570841
C	0.103963820	26.645805760	26.884755648
H	-0.004288899	25.628520311	26.477436808
H	-0.301204848	26.630286103	27.901965734
H	-0.532311027	27.308483628	26.288557375
C	1.742127677	28.525815179	27.341426769
H	1.222628690	29.233274417	26.685437729
H	1.327614083	28.666136306	28.347360687
H	2.796856783	28.819309605	27.381577519
C	3.246722814	21.703856993	12.754987355
H	4.289448672	21.391647332	12.588979103
H	2.682730879	20.918153937	13.287536421
C	2.543312673	22.172430791	11.468810484
H	3.026638794	23.128220572	11.136237753
C	2.735064490	21.107457533	10.386099896
H	2.288563057	20.147610500	10.671573512

H	2.256370981	21.412293129	9.446717457
H	3.793065814	20.932875344	10.164694272
C	1.062613148	22.447529308	11.736386529
H	0.940984325	23.143611015	12.580222864
H	0.578853235	22.908730028	10.868242937
H	0.503781259	21.535118862	11.975648843
C	5.408980344	19.742093989	26.140967922
H	6.397670260	20.198446193	26.310340233
H	4.612883759	20.501339930	26.219078827
C	5.158394568	18.498467545	27.011544189
H	5.755033586	17.653096334	26.574894620
C	3.678875517	18.110350823	26.985999269
H	3.324121820	17.989330267	25.951859166
H	3.509556966	17.159917507	27.503551911
H	3.044864692	18.860306410	27.470678105
C	5.645407271	18.775129035	28.435455279
H	5.100089934	19.604755773	28.900067176
H	5.499713348	17.898014193	29.078201695
H	6.713554014	19.020050033	28.462352582
C	6.725549430	23.879756726	16.617083109
C	6.835618333	23.238981339	14.291684741
H	7.895619030	23.257009749	14.023371486
H	6.543655386	22.252043092	14.673616841
H	6.193371351	23.564533521	13.466033466
C	5.305315756	28.937476767	15.973816255
H	6.287850499	29.143927973	15.518992396
H	4.830648691	28.064150260	15.494763979
C	4.371793966	30.163518366	15.988046801
H	4.171269580	30.432982101	14.920308257
C	5.048290508	31.350984398	16.675597477
H	5.982542498	31.632071014	16.177804307
H	4.397992156	32.232061279	16.687491985
H	5.297410381	31.109825574	17.719685521
C	3.048967173	29.808160760	16.669660231
H	3.226649788	29.413419208	17.683988281
H	2.396636457	30.690843058	16.770879973
H	2.497516881	29.043493523	16.108840254

Table S9. Atomic coordinates for the optimized structure of **TPA-Q₆(*i*-Bu)** in MOPAC2016 (Fig. S1a(ii), gas phase).

Atom	X	Y	Z
O	8.651666719	9.235262396	6.337887887
O	7.980167737	3.442920504	11.251611974
O	8.088382804	7.662988393	14.525471606

O	6.005538958	15.050867371	13.940703966
O	5.838770780	13.355346493	8.891702515
O	5.109255771	6.496115567	5.542772965
O	5.059176711	5.240325105	10.699662192
O	4.272700379	9.121236257	17.302190748
O	3.385048717	12.834284164	13.579147936
O	2.012622497	12.677497963	6.068646950
O	1.883321819	7.573964127	7.309477954
O	0.655417416	9.215604946	14.109952513
O	0.984776110	7.682168734	15.736879632
O	1.976455923	3.273716796	13.621793811
N	9.329949512	15.250084898	8.563644917
N	8.292426376	8.863865343	8.581303015
H	8.117468885	9.307502836	9.499228951
N	8.031272566	7.589571460	11.014604070
N	7.206745235	9.191314041	13.031308155
H	6.953161107	9.338873772	12.031251076
N	6.415553920	11.511256313	11.807812707
N	5.287072352	11.155599335	9.366948226
H	5.198626542	10.461960278	10.141571066
N	4.985117430	8.440127874	9.201465939
N	4.437731242	7.294152103	11.551878103
H	4.199325605	8.278604463	11.289987690
N	3.826576830	9.393551007	13.182961383
N	2.492477948	11.434009851	11.970606875
H	2.270882064	10.437710540	11.757141122
N	1.973943610	10.340442070	9.502765055
N	1.396279586	7.704376278	9.565579654
H	1.240902183	8.366428655	10.358342338
N	1.170605906	7.118914116	12.239758104
C	9.350238878	16.220618385	7.496191894
C	10.053650333	15.947348018	6.306567800
H	10.573896345	14.998467065	6.185204802
C	10.072074180	16.900570948	5.289737400
H	10.601930688	16.688936106	4.359494138
C	9.425465793	18.129505663	5.460199161
H	9.454300698	18.892281733	4.675404574
C	8.743579736	18.401369892	6.648831381
H	8.246705715	19.370909536	6.765217816
C	8.693576223	17.452849969	7.670088578
H	8.142472525	17.654233484	8.586162904
C	9.564964285	15.717512169	9.908262848
C	10.632291680	16.598523975	10.161884370
H	11.263804463	16.943996365	9.345490106

C	10.877774918	17.011805188	11.475196859
H	11.709826008	17.687815759	11.675409828
C	10.075665838	16.554064286	12.523309228
H	10.285942935	16.866659623	13.544247863
C	9.004293134	15.691550489	12.261813363
H	8.374225093	15.339421862	13.082980816
C	8.735052190	15.280216008	10.957170270
H	7.896604349	14.611918167	10.745930372
C	9.101125043	13.869087563	8.311809346
C	8.479512231	13.450782551	7.113118568
H	8.103281760	14.182891402	6.399683231
C	8.303005023	12.094865547	6.865046452
H	7.838937103	11.760411583	5.932430364
C	8.716746336	11.131348659	7.801555531
C	9.322112345	11.551339513	8.997442609
H	9.658902585	10.819285950	9.735690746
C	9.520369875	12.901343320	9.254726222
H	10.020635752	13.200774631	10.175451965
C	8.553675484	9.692567470	7.463058112
C	8.255657604	7.445353739	8.587389062
C	8.327759803	6.661539347	7.448669481
H	8.415980806	7.135540192	6.461037458
C	8.285809590	5.249315206	7.544268656
H	8.342622745	4.671125327	6.618551953
C	8.175520730	4.612067619	8.759762303
H	8.138286426	3.526163357	8.839800437
C	8.107122554	5.380484834	9.953449440
C	8.138335710	6.795360156	9.881627205
C	7.977866326	4.802152154	11.276714732
C	7.880541638	5.600315530	12.403551380
H	7.787178071	5.212054778	13.414264736
C	7.898945050	7.007350771	12.206749744
C	7.761451530	7.954597097	13.391404831
C	7.072493747	10.345593564	13.847624445
C	7.293229293	10.371262441	15.211182559
H	7.603735244	9.459694288	15.735761797
C	7.126835759	11.580051769	15.938835427
H	7.321876936	11.559708413	17.011638983
C	6.741177546	12.746235872	15.319712182
H	6.601494933	13.675528865	15.873618198
C	6.501430850	12.758279535	13.918334136
C	6.661866938	11.564542618	13.171335800
C	5.979880915	12.607472892	11.181536156
C	5.786549964	13.855785805	11.824984311

H	5.420653917	14.694363244	11.237464003
C	6.061454210	13.924550251	13.180309586
C	5.709231570	12.448618310	9.691463808
C	5.200762344	10.589889874	8.065901824
C	5.237177507	11.314411052	6.892645163
H	5.305668785	12.408847490	6.925444592
C	5.215169352	10.644166537	5.641280382
H	5.262415466	11.246249299	4.734871679
C	5.156749868	9.268807128	5.563098613
H	5.169061431	8.744771686	4.607340562
C	5.087774296	8.493216738	6.752975396
C	5.084565715	9.141017574	8.010531297
C	4.900618073	7.108457601	9.169897273
C	4.927634785	6.349639467	7.975117716
H	4.877545879	5.264851464	8.039024049
C	5.032179135	7.046545711	6.779430192
C	4.811119549	6.419447738	10.524936197
C	4.490770784	7.058094678	12.948497097
C	4.813325324	5.850670714	13.536477182
H	5.001988686	4.972093252	12.909190645
C	4.919729365	5.752169631	14.948559258
H	5.199919156	4.787378740	15.374154232
C	4.705416757	6.839020732	15.765148066
H	4.812890110	6.775934423	16.848461710
C	4.338987140	8.090912225	15.197219742
C	4.210185287	8.209165805	13.793227252
C	3.555658373	10.457725245	13.939374815
C	3.691826909	10.469230777	15.353273137
H	3.498849341	11.395837106	15.888351302
C	4.093458163	9.294298578	15.962495463
C	3.140319940	11.709765857	13.178934718
C	2.399808115	12.321216998	10.861566556
C	2.577899944	13.688767908	10.945116270
H	2.752454843	14.158833935	11.920364387
C	2.568268101	14.483663602	9.767814380
H	2.729532672	15.556531370	9.872352242
C	2.380290733	13.925950207	8.524227740
H	2.397658018	14.526917308	7.613994165
C	2.162999065	12.524672331	8.402055936
C	1.984263179	11.842571418	7.139273301
C	1.804843005	10.469116798	7.084439567
H	1.692841565	9.907028114	6.158405045
C	1.812149473	9.760930329	8.310832548
C	2.158362553	11.713431048	9.563879311

C	1.698903845	8.242892350	8.310142225
C	1.532796531	6.343689584	9.949679376
C	1.791096653	5.310380189	9.067719123
H	1.846779658	5.509098436	7.989477950
C	2.020171037	3.998009839	9.551557068
H	2.238256247	3.212728045	8.827554507
C	1.993636359	3.716756611	10.898670614
H	2.200537321	2.716828479	11.282497692
C	1.705890331	4.750923484	11.830593844
C	1.452015070	6.067349822	11.372375325
C	1.159444694	6.874361914	13.546002754
C	1.412201931	5.598094279	14.124205894
H	1.395027384	5.496011915	15.207555292
C	1.694195091	4.554918064	13.263736053
C	7.750732278	2.723199671	12.509309726
H	6.759903105	3.014605906	12.894994997
H	8.543564799	2.994298346	13.223384694
C	7.808411787	1.250255896	12.062348347
H	7.088589306	1.124906527	11.211766213
C	7.385471871	0.345081802	13.220794744
H	8.026329455	0.473629248	14.099923871
H	7.449384299	-0.711447854	12.933770034
H	6.346386540	0.534436726	13.535969515
C	9.211113304	0.897904488	11.563006641
H	9.528485629	1.599425622	10.778473348
H	9.243350481	-0.110435951	11.139168430
H	9.959122062	0.945565878	12.361357961
C	5.452613257	16.262630732	13.315813023
H	4.408479480	16.048027965	13.032859551
H	6.059974949	16.508089272	12.429110248
C	5.563083067	17.309997901	14.436245036
H	5.143683382	16.856911894	15.372456553
C	7.026312052	17.679588954	14.688192860
H	7.617014118	16.788442759	14.938812372
H	7.123614190	18.383612975	15.520169295
H	7.487460969	18.153839533	13.804226894
C	4.732580243	18.537632161	14.055589503
H	5.071764195	18.991276930	13.116280394
H	4.802009660	19.313185492	14.828595115
H	3.670782665	18.292852651	13.940060139
C	5.216222750	5.037621656	5.436370872
H	4.189281346	4.640992831	5.519834470
H	5.854642714	4.644219698	6.243717464
C	5.834163730	4.847761462	4.038885710

H	5.271314948	5.508457540	3.326619731
C	7.300512446	5.278606285	4.037800189
H	7.399605363	6.318901853	4.386498730
H	7.732636440	5.232109017	3.032926668
H	7.918500633	4.652930392	4.692412107
C	5.664916260	3.390725419	3.605214071
H	6.179717897	2.699594544	4.281722733
H	6.085282328	3.230274836	2.604786935
H	4.610710711	3.095000843	3.564547171
C	4.361836070	10.326790517	18.136673388
H	3.336225667	10.695577590	18.286689080
H	4.980416592	11.084479383	17.626205889
C	5.009811780	9.790947226	19.425354638
H	4.478260387	8.846069410	19.708156676
C	4.831682000	10.819265762	20.544261625
H	5.327429501	11.769131120	20.314755916
H	5.264805754	10.452820726	21.483342018
H	3.775759331	11.033380690	20.741134134
C	6.483935408	9.461039209	19.185109042
H	6.596322913	8.798799147	18.313406783
H	6.922047257	8.943498410	20.044399442
H	7.087994349	10.356489321	19.004270286
C	1.912032393	12.071993367	4.731624046
H	0.901923703	11.643090101	4.635441229
H	2.676956817	11.284893126	4.633587846
C	2.150160618	13.274728869	3.804408739
H	1.653139341	14.164566980	4.274009230
C	3.645408049	13.567821064	3.676789374
H	4.105783415	13.674441673	4.669335758
H	3.820920241	14.504316732	3.134237482
H	4.179475751	12.779313785	3.137372584
C	1.508573904	13.007562598	2.442403296
H	1.956678644	12.145145575	1.937079857
H	1.631942840	13.869560863	1.775862446
H	0.432944118	12.822059934	2.525740955
C	0.891525771	8.072343846	14.414452405
C	0.808016604	8.717372449	16.739339334
H	-0.251904477	8.740128703	17.006503914
H	1.137878429	9.692662103	16.359523849
H	1.438120402	8.370189239	17.565633483
C	2.215959131	2.985719877	15.041119440
H	1.227646187	2.822745300	15.498323722
H	2.730870080	3.837233673	15.516125462
C	3.092821134	1.720107009	15.025330728

H	3.294035205	1.443729461	16.092680437
C	2.353422958	0.564318329	14.350038910
H	1.411454430	0.333200265	14.858514969
H	2.956325608	-0.349003707	14.337486668
H	2.106197036	0.815270255	13.307803376
C	4.421517135	2.019774516	14.327596839
H	4.244703620	2.453306914	13.330645006
H	5.023467390	1.109315525	14.182405786
H	5.026992592	2.731668167	14.897033853
O	5.317896970	25.018193307	9.101578439
O	6.097647164	19.132034374	4.370036782
O	6.139223180	23.274443683	0.972828221
O	8.120422065	30.704074676	1.501952341
O	8.181982622	29.047089539	6.589081305
O	8.806362707	22.077015278	9.791630093
O	9.091331153	21.031198297	4.608813143
O	9.915821946	25.038211047	-1.880003063
O	10.798134438	28.711623964	1.818700175
O	11.924209292	28.780337531	9.365079410
O	12.131809367	23.636361733	8.289129902
O	13.560458197	25.069682882	1.479845916
O	13.171237586	23.510999756	-0.108848713
O	12.233957855	19.142741006	2.139149523
N	4.645291501	30.977845554	6.799795225
N	5.785998119	24.605134993	6.885295219
H	6.008481144	25.032168181	5.970987176
N	6.109122864	23.276430232	4.486100353
N	6.941034073	24.848805195	2.464297099
H	7.160245228	25.017565415	3.470778859
N	7.686271277	27.192774222	3.676145971
N	8.822405000	26.868482691	6.117897965
H	8.959439731	26.192347090	5.336768181
N	9.128668508	24.166541918	6.220257170
N	9.744467661	23.107584455	3.843978956
H	9.977777827	24.082470077	4.138703879
N	10.359322076	25.258187775	2.246237170
N	11.591254222	27.342767254	3.503563900
H	11.795992911	26.351390063	3.753738213
N	12.077945176	26.333535308	6.013047869
N	12.717448128	23.708199653	6.053708571
H	12.886238713	24.347006699	5.243960565
N	13.002834696	23.039078521	3.402707659
C	4.655790683	31.939436970	7.880749025
C	3.831516902	31.717610191	8.998436282

H	3.217204330	30.818999425	9.056018461
C	3.811314246	32.659873996	10.026704749
H	3.175942406	32.493609190	10.896899209
C	4.594594779	33.815758120	9.943760368
H	4.572394019	34.547439815	10.748362588
C	5.407773402	34.031130291	8.826200979
H	6.017582506	34.933336359	8.763305904
C	5.448549860	33.097450968	7.790954705
H	6.088153115	33.258406692	6.923738073
C	4.553619396	31.500209547	5.458198764
C	3.567589192	32.469564380	5.186089675
H	2.908195551	32.817898969	5.981229868
C	3.438436974	32.965439699	3.892014815
H	2.677242423	33.715240712	3.675428033
C	4.275715979	32.503961466	2.868012242
H	4.157054065	32.887065729	1.858053584
C	5.250790817	31.543207169	3.144713898
H	5.899510859	31.176041717	2.345557042
C	5.406440621	31.045414384	4.441321486
H	6.181731196	30.307315995	4.660858181
C	4.933033394	29.610076591	7.051683476
C	5.500037054	29.209912320	8.282910430
H	5.822267670	29.950767076	9.012250212
C	5.679953219	27.858438859	8.552900865
H	6.102455636	27.539214542	9.510136358
C	5.326222774	26.884998025	7.603612699
C	4.785714341	27.287057608	6.371075002
H	4.501091920	26.545358136	5.620916555
C	4.582507282	28.631796519	6.091993278
H	4.131803319	28.920967796	5.144332517
C	5.470847516	25.454012905	7.973339312
C	5.779925903	23.188565610	6.905129678
C	5.614875152	22.428890991	8.051745097
H	5.489000226	22.926171602	9.023897878
C	5.598929543	21.015603506	7.982781453
H	5.459830515	20.461149046	8.918160908
C	5.763687109	20.351626448	6.788312945
H	5.750183220	19.262588641	6.728111349
C	5.938248890	21.095329060	5.590443846
C	5.942812700	22.510159396	5.631496813
C	6.114852000	20.484562574	4.287862355
C	6.263661983	21.253851195	3.145142356
H	6.383217796	20.836371453	2.149371878
C	6.260174647	22.664712433	3.308610432

C	6.425524233	23.593031322	2.110235651
C	7.062785545	25.997834663	1.640019132
C	6.849120114	26.010820138	0.274259163
H	6.555692562	25.090188901	-0.243352946
C	7.007584347	27.214152860	-0.462036290
H	6.815189794	27.182333442	-1.535400844
C	7.384293752	28.388582853	0.146568545
H	7.514986877	29.314901050	-0.414003434
C	7.617565935	28.414714174	1.549925752
C	7.455774434	27.229261191	2.307893299
C	8.115294249	28.295218941	4.292162831
C	8.318352755	29.534347141	3.636548182
H	8.678703442	30.382761839	4.214807100
C	8.051820752	29.589402887	2.277068465
C	8.362894052	28.149625148	5.790535174
C	8.855705525	26.272045160	7.408725747
C	8.763415331	26.962168383	8.600043769
H	8.683528004	28.055317572	8.597347329
C	8.742063643	26.250447720	9.830130291
H	8.656256737	26.825990900	10.752531946
C	8.798687902	24.876621897	9.871132395
H	8.754278041	24.324629694	10.811485456
C	8.913103382	24.131153826	8.663392057
C	8.976400835	24.823565487	7.430211270
C	9.209412631	22.833338908	6.208425767
C	9.119287132	22.034258952	7.371782275
H	9.172292402	20.949464563	7.269545005
C	8.958741910	22.685400270	8.586862120
C	9.341307021	22.199968182	4.830814880
C	9.703753866	22.911078348	2.439141066
C	9.385894066	21.714636972	1.828055063
H	9.188301683	20.825266095	2.438888573
C	9.288620679	21.636141460	0.414961233
H	9.014559588	20.675800343	-0.027751244
C	9.503823146	22.736413206	-0.380684848
H	9.403814762	22.692576464	-1.466500773
C	9.859927742	23.980588957	0.211182553
C	9.983622034	24.078740886	1.619182217
C	10.615264266	26.333909154	1.502317796
C	10.482730254	26.365182265	0.088867981
H	10.666509396	27.301558541	-0.432835126
C	10.092954064	25.193608814	-0.538762320
C	11.010148555	27.595320474	2.259345250
C	11.673006599	28.267753716	4.581231611

C	11.506037404	29.632891441	4.449755850
H	11.364273651	30.073201768	3.456667747
C	11.487849958	30.465914547	5.601230890
H	11.337825175	31.535859566	5.456620647
C	11.637975997	29.947461213	6.864338186
H	11.595403597	30.575956529	7.755538798
C	11.846915769	28.548833555	7.038190940
C	11.989160250	27.908729583	8.325494631
C	12.176885212	26.538937369	8.430680195
H	12.265367856	26.008867010	9.377214069
C	12.214901291	25.794149351	7.226246050
C	11.884477979	27.701597195	5.903544224
C	12.348562273	24.277801537	7.276266068
C	12.629427474	22.331601043	5.712422109
C	12.399090527	21.318839154	6.627520126
H	12.318920172	21.553636540	7.697003238
C	12.239402792	19.981348403	6.188693631
H	12.054787585	19.207584465	6.937019460
C	12.291256022	19.658540874	4.851430625
H	12.146701041	18.634301932	4.505017583
C	12.524490875	20.672388638	3.884348528
C	12.737547534	22.010326016	4.301396642
C	13.026972278	22.751918565	2.103905397
C	12.788827462	21.455896065	1.566928261
H	12.802641092	21.321263893	0.486703969
C	12.521567363	20.433915657	2.457383125
C	6.343182744	18.334182129	3.167208729
H	7.230733865	18.728809651	2.647170250
H	5.448798214	18.405959391	2.529131605
C	6.573894287	16.928555143	3.757032587
H	7.452963341	16.989134290	4.454005001
C	6.895248923	15.949944717	2.628471786
H	6.073873840	15.861578320	1.910261474
H	7.087504865	14.946208054	3.028196662
H	7.794084082	16.260055736	2.070920566
C	5.361407321	16.482427662	4.574812959
H	5.117406910	17.230651399	5.341882875
H	5.556412880	15.540044972	5.099339637
H	4.464902333	16.351779734	3.960849262
C	8.732599448	31.904527056	2.093257848
H	9.765581217	31.644780606	2.381649308
H	8.139511652	32.202633160	2.972620774
C	8.673868168	32.925580447	0.944949937
H	9.025820217	32.411345729	0.011894583

C	7.240128679	33.410947173	0.720586559
H	6.578344947	32.569148133	0.478842626
H	7.185138951	34.122824073	-0.109222905
H	6.829175325	33.910947224	1.605473479
C	9.616052531	34.088839111	1.264361129
H	9.333010423	34.605810364	2.188464545
H	9.600949423	34.835732182	0.461126866
H	10.653752300	33.754106791	1.373172870
C	8.611069385	20.621145961	9.796329298
H	9.611907288	20.166797308	9.708540624
H	7.976283780	20.329072185	8.943113560
C	7.938983677	20.336573603	11.152006282
H	8.629242292	20.694141525	11.960212404
C	6.611242585	21.083840309	11.281407641
H	6.748332238	22.158720131	11.087243713
H	6.188785670	20.979802516	12.284797924
H	5.862357686	20.720030713	10.564140824
C	7.742050847	18.826153941	11.284859443
H	6.954374767	18.448675011	10.624823669
H	7.464893873	18.558648702	12.319606737
H	8.661529552	18.269427461	11.053781576
C	9.804150993	26.251977653	-2.699021090
H	10.825025065	26.627142188	-2.864592153
H	9.193735626	27.004500276	-2.168475588
C	9.132771775	25.728773154	-3.979760711
H	9.659175489	24.786450790	-4.282500034
C	9.287567794	26.767754731	-5.093655020
H	8.790393229	27.713003993	-4.847136078
H	8.841777726	26.408101909	-6.029192923
H	10.339093423	26.991675519	-5.303272033
C	7.662398566	25.396636633	-3.715951874
H	7.564618515	24.725021251	-2.849245847
H	7.212491078	24.884756652	-4.572430095
H	7.059302050	26.290944750	-3.523330081
C	11.950610677	28.226193114	10.725957557
H	12.930703483	27.746488163	10.878561115
H	11.136241459	27.490016292	10.823254366
C	11.750035701	29.479918980	11.592990374
H	12.353257602	30.308869726	11.135156028
C	10.279757535	29.901012368	11.602674672
H	9.904759892	30.029014766	10.576885572
H	10.142517365	30.855531006	12.122031785
H	9.639932208	29.166443951	12.103222993
C	12.271123909	29.209409917	13.006617351

H	11.728527084	28.393795025	13.497703547
H	12.158205020	30.096514632	13.641625707
H	13.335424199	28.949123094	13.007188178
C	13.297176874	23.926557293	1.204034033
C	13.349511472	24.523892814	-1.133579713
H	14.404247485	24.522348139	-1.420687915
H	13.046043240	25.512786104	-0.766811194
H	12.697280836	24.175593445	-1.941957660
C	11.931705081	18.817819352	0.740685341
H	12.892625452	18.525194489	0.287471853
H	11.510599332	19.697421666	0.225484158
C	10.922341854	17.656191371	0.815076463
H	10.711555884	17.341239971	-0.239890837
C	11.521460915	16.469590386	1.571311600
H	12.411891559	16.075889123	1.071483416
H	10.806325217	15.646853989	1.662676878
H	11.820095391	16.764499698	2.587543167
C	9.616988028	18.125138416	1.463044174
H	9.811220148	18.568602936	2.452944301
H	8.917056612	17.286376821	1.612245479
H	9.109256074	18.880782469	0.853021967

Table S10. Atomic coordinates for the optimized structure of **TPA-Q₆(*n*-He)** in MOPAC2016 (Fig. S2(i), gas phase).

Atom	X	Y	Z
O	3.698346349	7.746996524	16.76886179
O	2.867443872	7.330013953	20.57612467
O	-4.288585553	4.55302317	20.98082663
O	0.141351804	2.606230179	24.59735557
O	-1.939567349	1.729694636	24.71515267
O	-0.520868948	4.689293752	17.70573692
O	7.557270646	5.623678211	22.57825351
O	-2.333171771	-1.180020806	22.3573949
O	-0.749309164	-0.494639079	17.27941287
O	-1.924668389	3.526865306	14.16272417
O	2.776669266	-0.325997575	23.53014036
O	4.482414104	-2.838573124	22.2999919
O	6.769645095	1.639667636	20.3207154
O	5.555072466	4.609143774	14.98721067
N	9.250981888	-0.195582833	17.12315627
N	3.89710044	3.216723752	15.75761235
H	3.680764152	2.379151003	16.32483848
N	1.416519322	2.087104855	16.18536558
N	1.296958461	0.162538278	18.13014893

H	2.044409042	0.881164433	18.07170101
N	3.636610095	0.227780596	19.63828583
N	2.827223778	1.905065473	22.96227648
H	2.265179853	2.677808903	22.53552549
N	3.601195603	4.414677171	22.35829015
N	1.517922008	5.997585492	21.91002023
H	1.542392598	5.221740735	22.61261087
N	-0.520670446	4.347911182	22.74461504
N	0.712230832	1.447706943	21.31369173
N	0.357230699	3.339463106	19.36607527
H	1.225633052	3.130703621	19.91029435
N	2.804618327	4.245358226	18.80336784
N	4.755106489	2.653500924	19.81675039
H	3.723446224	2.490722278	19.76662356
C	10.30811509	-0.455140175	16.17930516
C	11.62623551	-0.638991727	16.63771244
H	11.85279671	-0.577211127	17.70160324
C	12.63948037	-0.897582809	15.71362404
H	13.66152745	-1.042840902	16.06348621
C	12.3568991	-0.96678509	14.34542598
H	13.15394358	-1.165302492	13.6321415
C	11.04520873	-0.777777343	13.89718495
H	10.82320233	-0.834764051	12.83133386
C	10.01541161	-0.525250967	14.80329013
H	8.994500862	-0.388580934	14.44735924
C	9.183817806	-0.954887496	18.34590485
C	9.542213573	-2.315977898	18.35344662
H	9.852599045	-2.811967224	17.43522423
C	9.491978705	-3.026360184	19.55438784
H	9.769369645	-4.079995079	19.56525137
C	9.081841954	-2.403096449	20.73760906
H	9.046783466	-2.967528827	21.66600475
C	8.719495983	-1.05219044	20.71912807
H	8.397814739	-0.554319714	21.63520232
C	8.774212994	-0.320714622	19.53320258
H	8.487797101	0.737689081	19.53290895
C	8.238420055	0.758019181	16.80300075
C	8.579112522	1.919222297	16.07596148
H	9.614142785	2.104406639	15.79193009
C	7.58849025	2.828956654	15.72700948
H	7.841000903	3.734244477	15.16303301
C	6.24595477	2.601596449	16.08088478
C	5.919326707	1.462598123	16.83482506
H	4.883516164	1.27560474	17.1404147

C	6.898902899	0.54509675	17.19658535
H	6.629502813	-0.340226205	17.77296712
C	5.248584348	3.583613902	15.57415027
C	2.770127721	3.85788891	15.18117356
C	2.83703222	5.025263333	14.43923484
H	3.799997146	5.535030441	14.29778085
C	1.669671535	5.564341337	13.84389098
H	1.764385989	6.483294495	13.26444606
C	0.44822888	4.942628113	13.96804778
H	-0.452270046	5.341075884	13.50085269
C	0.339665487	3.74576969	14.72589329
C	1.484526274	3.209333302	15.36790399
C	0.240170964	1.484114397	16.35023875
C	-0.957326996	1.892177669	15.70152963
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C	4.214702772	-2.542248352	31.64915423

C	5.428033448	-2.583471336	32.30849914
H	5.611479177	-3.339453478	33.08341267
C	6.440225603	-1.639522899	31.99568217
H	7.381106978	-1.698428649	32.55452979
C	6.261198919	-0.688093807	31.01874425
H	7.031698467	0.044792331	30.77633994
C	5.035837945	-0.63439984	30.29754718
C	3.995370303	-1.540349074	30.6190091
C	2.585359603	-0.655157858	28.96918437
C	3.558169813	0.284846937	28.54566936
H	3.31322835	0.978837608	27.74541193
C	4.775412448	0.282109869	29.20875199
C	5.847719383	1.663792885	27.5497273
H	5.603789918	0.85420476	26.83337034
H	5.09694492	2.469901585	27.50985254
C	7.27541302	2.173705456	27.39583586
H	7.38597166	2.616082773	26.38433007
H	7.45393171	3.000155275	28.1140606
C	8.329302823	1.083234944	27.62688735
H	8.228038319	0.705570017	28.66659756
H	9.338618422	1.532646787	27.56434507
C	8.21493341	-0.089025698	26.64692006
H	7.176427678	-0.492798627	26.65920648
H	8.391298473	0.252508981	25.60890608
C	9.194642876	-1.211496767	27.01446327
H	10.23634556	-0.852980036	26.91502728
H	9.068028439	-1.477384333	28.08234581
C	8.990933511	-2.449294787	26.14610404
H	9.28301247	-2.261714241	25.1069886
H	9.5844366	-3.295772973	26.50622922
H	7.930608355	-2.766649178	26.12917877
C	1.23397385	-0.718396239	28.28191543
C	-0.691175924	-2.320492408	28.02395777
C	-1.626360217	-1.471326558	27.46962582
H	-1.340636044	-0.461393541	27.15803008
C	-2.977148629	-1.896251348	27.33794456
H	-3.694805218	-1.186388313	26.91372436
C	-3.387904538	-3.142877992	27.74955785
H	-4.430119626	-3.455956119	27.67809592
C	-2.445765548	-4.060097935	28.30079179
C	-1.093776255	-3.660212561	28.41506501
C	-2.751154604	-5.38611534	28.79386758
C	-1.762823953	-6.21920668	29.30513347
H	-1.958438419	-7.21075226	29.70821963

C	-0.437484258	-5.723014335	29.32565748
C	0.741025958	-6.515943802	29.8835011
C	-4.504977545	-6.973909862	29.30310266
H	-3.964841473	-7.798854914	28.8098323
H	-4.264152969	-6.930681856	30.38048803
C	-6.002141646	-6.990592542	29.01884945
H	-6.181367336	-7.156155352	27.93706649
H	-6.432964684	-5.99067959	29.23730095
C	-6.718572016	-8.06194777	29.84796518
H	-7.814218612	-7.906935227	29.76689678
H	-6.490789979	-7.925884517	30.92399183
C	-6.367588686	-9.496353147	29.43191862
H	-5.270138289	-9.620815606	29.36090063
H	-6.689820885	-10.19656677	30.22814023
C	-7.019006315	-9.900084195	28.10199491
H	-6.723191487	-9.188678273	27.30586029
H	-8.12085126	-9.820408525	28.18358036
C	-6.633206671	-11.31837382	27.69010035
H	-6.908086899	-12.05394774	28.45466277
H	-7.136130987	-11.61074559	26.76127788
H	-5.55488678	-11.41504569	27.51950626
C	3.250025146	-6.272264627	29.94938473
C	3.525329395	-7.224039887	30.91319553
H	2.739721749	-7.9119525	31.24719587
C	4.816160308	-7.296825844	31.49651206
H	4.992288178	-8.047828591	32.26797003
C	5.818174218	-6.430000357	31.12472405
H	6.804736789	-6.45879616	31.59528105
C	5.579053168	-5.449450918	30.12386904
C	4.300966197	-5.36608764	29.51438723
C	4.958311436	-3.574974645	28.16177709
C	6.264324516	-3.537617687	28.72726741
H	6.965196074	-2.776325247	28.38641684
C	6.566130909	-4.482433695	29.69027727
C	8.760973448	-3.549814763	30.14198313
H	9.158406138	-3.609384721	29.11466053
H	8.255792568	-2.581681874	30.30980532
C	9.815793966	-3.862123989	31.19932708
H	10.16338986	-4.90965319	31.07180377
H	10.70410721	-3.226317942	31.01125396
C	9.321697682	-3.657008253	32.6385368
H	10.19188943	-3.533917791	33.31047123
H	8.742614088	-2.709118315	32.71212308
C	8.457213681	-4.833244161	33.10937837

H	9.024245822	-5.78010927	33.02768614
H	7.592482651	-4.947934131	32.41493443
C	7.944655585	-4.659416804	34.54178432
H	8.770438258	-4.823658788	35.26267046
H	7.599924887	-3.613962853	34.70848821
C	6.794286449	-5.616083755	34.84141546
H	6.369404922	-5.433975457	35.83774457
H	5.959579345	-5.484791579	34.1315335
H	7.105793727	-6.661840496	34.78716944
C	4.646328217	-2.598394825	27.05764419
C	2.899590705	-1.820212867	25.59268168
H	3.344803438	-0.823406374	25.68096994
H	3.167238352	-2.278782609	24.63147484
H	1.814425879	-1.799319974	25.73630415
C	0.794311221	-8.562539977	35.28509595
H	1.380357094	-9.166768618	34.57388101
H	1.440577577	-7.845834712	35.82100644
C	-0.074947348	-9.393847818	36.22299276
H	-0.778347414	-10.01335312	35.62974495
H	-0.722524095	-8.720320103	36.82348303
C	0.781767169	-10.27635251	37.13534225
H	1.42479112	-10.94376115	36.52877118
H	1.473027375	-9.651491301	37.73385625
C	-0.099879003	-11.11465079	38.0700046
H	-0.797386912	-11.73654914	37.47574258
H	-0.740689204	-10.45106066	38.68311759
C	0.747380149	-12.01007999	38.9836466
H	1.392553677	-12.66936049	38.37022957
H	1.436274087	-11.38728098	39.58780738
C	-0.124727093	-12.8577622	39.90630774
H	0.487895177	-13.49394289	40.55506247
H	-0.752169514	-12.23409852	40.55356166
H	-0.794535935	-13.51393338	39.33896254

Table S11. Atomic coordinates for the optimized structure of TPA-Q₆(*n*-He) in MOPAC2016 (Fig. S2(ii), gas phase).

Atom	X	Y	Z
O	-2.205875558	13.59991002	24.00755333
O	5.356250309	14.56035171	23.89818517
O	3.683046595	18.62635303	20.9019149
O	-2.444008656	20.06972762	16.49888704
O	-3.839009551	15.5160855	18.97940288
O	0.266053525	9.983933665	22.47727298
O	3.989206975	13.34089298	20.73596659

O	4.130442848	19.39346989	16.02316258
O	-0.752924207	17.4331733	15.23085898
O	-4.453784905	11.08438476	17.42851708
O	0.497662669	9.623968901	18.15644159
O	2.97478538	14.56768203	14.41507392
O	4.969499691	15.61963689	14.5350889
O	7.649727258	12.05896126	17.29785206
N	-6.127438135	18.03242735	21.51176852
N	-0.614181593	14.88736526	22.96757941
H	-0.443738188	15.67627836	22.32054587
N	1.806020141	15.996974	22.29029745
N	1.691193801	17.68255093	20.19519589
H	1.048008448	16.87534665	20.34008687
N	-0.808823326	17.29632733	19.11760498
N	-1.68754704	14.76479206	19.34143854
H	-0.680724074	15.0277993	19.25477205
N	0.512684912	13.4134862	20.15179076
N	2.746122038	14.4186333	19.11491529
H	1.794690935	14.48084635	18.68851469
N	1.874297418	16.09178163	17.13372468
N	-0.340605298	15.24043114	15.82803907
H	0.396774879	14.59857264	16.19299633
N	-0.667521396	12.69708215	16.81376568
N	1.632947636	11.56668633	17.66953469
H	1.553864658	12.51478574	17.24035003
N	3.658731409	12.91221839	16.42056893
C	-6.279425323	18.44760804	20.13761602
C	-5.989978788	17.57722039	19.07425415
H	-5.590482619	16.57176918	19.26310373
C	-6.212859075	18.00323328	17.7643276
H	-6.014496078	17.31778576	16.94036579
C	-6.708903931	19.28530914	17.50784682
H	-6.909166093	19.60073633	16.48691073
C	-6.956283897	20.16140611	18.57099979
H	-7.320274153	21.16853629	18.37115272
C	-6.743928473	19.75418776	19.88737534
H	-6.93990595	20.43210655	20.71778832
C	-7.276633654	18.12764755	22.37649023
C	-8.584018495	18.13346248	21.85647001
H	-8.757568795	18.01466463	20.78804113
C	-9.665289246	18.29459197	22.72436099
H	-10.67871624	18.30618828	22.32369594
C	-9.459162296	18.43358778	24.09973856
H	-10.30674074	18.55528045	24.76951798

C	-8.156950963	18.41481	24.61258605
H	-7.995332439	18.52135808	25.68519415
C	-7.062006071	18.26664238	23.76292399
H	-6.049116004	18.26339622	24.1640959
C	-5.080404418	17.11151951	21.86180316
C	-3.745685809	17.45717431	21.57065986
H	-3.524988194	18.36898691	21.01507901
C	-2.712909713	16.63460525	22.01175456
H	-1.679268303	16.92651556	21.7944021
C	-2.989698925	15.45757219	22.72619142
C	-4.327426918	15.09805147	22.96966421
H	-4.536767554	14.16499313	23.50482278
C	-5.370276135	15.91607827	22.54864074
H	-6.403397008	15.63264214	22.74765854
C	-1.945159512	14.55361017	23.29190954
C	0.558020861	14.28818162	23.50290996
C	1.822762053	14.91169165	23.15462678
C	3.030559398	14.38989135	23.68132846
C	2.993384259	13.24150188	24.51855405
H	3.935114845	12.85306541	24.90509781
C	1.785881082	12.65438911	24.81937241
H	1.745322108	11.77417984	25.46278757
C	0.563511258	13.16934426	24.31671823
H	-0.379771618	12.67349728	24.58313511
C	4.248479188	15.07809381	23.30637883
C	4.223744368	16.16063478	22.44126136
H	5.109907598	16.70522018	22.12911802
C	2.959198774	16.57284633	21.94860204
C	2.850772346	17.74383657	20.98093038
C	1.197319315	18.67993047	19.31514248
C	1.900798135	19.81179642	18.94826525
H	2.904836981	19.99047621	19.35312085
C	1.331403442	20.74739038	18.04578171
H	1.919133037	21.62805873	17.78508867
C	0.078416116	20.55618801	17.51208167
H	-0.367154347	21.266682	16.81556146
C	-0.674446864	19.40149872	17.86539161
C	-0.129467551	18.45455827	18.76598447
C	-1.986514382	19.10125883	17.33174537
C	-2.654659462	17.93632095	17.68107345
H	-3.643857803	17.68188491	17.30940184
C	-2.002544012	17.04758354	18.56972591
C	-2.639254172	15.7201229	18.97575492
C	-3.681282157	19.81056719	15.74748193

H	-4.515218588	19.89869669	16.46504257
H	-3.631291459	18.79958581	15.3091007
C	-3.66161006	20.91496165	14.69712484
H	-2.862741897	20.71459641	13.95432048
H	-3.373436332	21.87565183	15.1744359
C	-5.022214406	21.04955821	14.00568811
H	-5.337709966	20.06489879	13.60632567
H	-5.795894358	21.34161339	14.74326114
C	-4.989441698	22.06584073	12.85557867
H	-4.156145985	21.83060805	12.16484324
H	-5.912053353	21.95957008	12.25121836
C	-4.863433569	23.51455586	13.34745744
H	-5.708983806	23.75928283	14.01933212
H	-3.94861966	23.6253821	13.96311206
C	-4.824802489	24.5047503	12.18572034
H	-3.981647674	24.30945793	11.51334288
H	-4.723330404	25.53458476	12.54716691
H	-5.739615169	24.45972828	11.58406854
C	-1.908627599	13.52906583	20.01203018
C	-3.142349526	12.97960855	20.28916887
H	-4.057482688	13.48524531	19.95954153
C	-3.230622889	11.76671653	21.02669449
H	-4.225728304	11.37900211	21.24810179
C	-2.109546761	11.11272974	21.48196027
H	-2.174285276	10.19285661	22.06677942
C	-0.816666832	11.64412971	21.20955177
C	0.425739496	11.06983114	21.67953919
C	1.64999803	11.63187666	21.33400494
H	2.609105258	11.21679609	21.6393086
C	1.634034756	12.81633649	20.56499484
C	10.64987097	13.58251348	28.29459409
H	10.27690174	12.5666632	28.46825387
H	10.96128843	13.98647399	29.26462952
H	11.5476703	13.50038022	27.67179559
C	2.924556289	13.5238183	20.17615012
C	3.660574972	15.39358133	18.64348239
C	4.961511301	15.53265411	19.08484015
H	5.377578231	14.80576219	19.79782166
C	5.751703977	16.62385005	18.63953788
H	6.763130174	16.72166749	19.03449325
C	5.256477514	17.55597663	17.75723069
H	5.846580372	18.41506085	17.43125842
C	3.939894379	17.41124292	17.23771255
C	3.140952737	16.31915656	17.65166547

C	1.389928012	16.92775388	16.21473135
C	2.081692952	18.07882311	15.75583363
H	1.593002722	18.74791388	15.05210064
C	3.34056832	18.31901683	16.28331731
C	-0.005344727	16.59564356	15.7032037
C	-1.663149494	14.70980021	15.86614479
C	-2.787716325	15.39098014	15.44316792
H	-2.690914063	16.38743472	14.99947119
C	-4.076954648	14.81847588	15.61209671
H	-4.940775087	15.39332498	15.27913715
C	-4.246206256	13.58383277	16.19386645
H	-5.236244799	13.15289758	16.35518418
C	-3.110519306	12.83774194	16.6174616
C	-1.813349319	13.38187031	16.43766541
C	-0.793084889	11.50216021	17.39142598
C	-2.037492431	10.8769709	17.65353464
H	-2.034272401	9.903047147	18.15401234
C	-3.186362978	11.54498885	17.26428292
C	-4.633405399	9.831387252	18.18548963
H	-4.369643472	10.05018191	19.23545311
H	-3.963912825	9.058305121	17.7682384
C	-6.111678648	9.519093406	17.99143082
H	-6.66787204	10.47184294	17.84673053
H	-6.525194757	9.071089231	18.91642112
C	-6.344606185	8.588322546	16.79630281
H	-5.810039577	7.624050695	16.96719719
H	-5.896810134	9.030937641	15.88445178
C	-7.832588163	8.306268026	16.56636634
H	-8.255609592	7.767795	17.43619696
H	-8.391909151	9.260361177	16.50417993
C	-8.078540515	7.499981649	15.28212761
H	-9.149848749	7.577255284	15.00869115
H	-7.526242058	7.958092844	14.43770687
C	-7.694657126	6.028299727	15.40860387
H	-7.970931979	5.469027419	14.50828828
H	-8.19312792	5.552722615	16.25919551
H	-6.604782449	5.902589249	15.55485575
C	0.48837064	10.78582445	17.7782303
C	2.964699833	11.1380393	17.94091656
C	3.282710461	10.09892967	18.79602553
H	2.498092852	9.496963186	19.27854495
C	4.640783709	9.776138709	19.04854503
H	4.838772107	8.936472767	19.72100341
C	5.664152717	10.48981339	18.46744773

H	6.712191459	10.25675506	18.65753334
C	5.368338639	11.5682822	17.58919801
C	4.018277937	11.89355637	17.30032124
C	4.626698015	13.61105403	15.84216818
C	6.015692375	13.40544936	16.08650149
H	6.740031568	14.05221314	15.59487283
C	6.371514428	12.39543188	16.95933232
C	8.706531142	13.04855388	17.06846032
H	8.70767652	13.32552716	16.00159024
H	9.596863852	12.43204382	17.29539569
C	8.540723522	14.24390729	18.00143719
H	7.461201468	14.49883476	18.09643293
H	9.010797391	15.1367463	17.54188549
C	9.132851319	14.01493346	19.39767502
H	10.22478418	13.84898918	19.31108188
H	9.024683581	14.94399687	19.99177519
C	8.507307349	12.83764923	20.15671119
H	9.180186685	12.55119941	20.99680083
H	8.449394887	11.94984031	19.49401883
C	7.110346466	13.14142828	20.70418035
H	6.398906497	13.34327137	19.87120371
H	7.126629394	14.07971783	21.30409827
C	6.562955281	11.99993385	21.55592511
H	6.463471114	11.07723306	20.97551236
H	5.550954929	12.25162236	21.91591351
H	7.193779394	11.78696187	22.429282
C	4.248692656	14.70850824	14.88482468
C	2.530633149	15.57056238	13.45571409
H	2.99357309	15.35928941	12.4874509
H	2.794746841	16.57619043	13.80068801
H	1.446098707	15.41065415	13.4359715
C	3.826108756	20.25392285	14.88351391
H	4.533406026	21.08218099	15.09086819
H	2.78711194	20.61204226	14.97042423
C	4.112186517	19.56519234	13.55134195
H	4.286006504	20.345343	12.78227738
H	3.218455413	19.0033378	13.21226538
C	5.305086319	18.60091875	13.5905984
H	5.07649343	17.74620082	14.26887839
H	5.437917309	18.14684024	12.58988309
C	6.612450188	19.25712238	14.0496981
H	6.478795074	19.67466832	15.06830946
H	6.858354441	20.11378262	13.39631576
C	7.782143074	18.25989356	14.05561193

H	7.816840811	17.71842117	13.08948444
H	8.73615048	18.81838464	14.12592046
C	7.691087661	17.25318669	15.20073081
H	6.727518124	16.71382852	15.17412036
H	7.754376769	17.74652165	16.1754524
H	8.487658869	16.50723534	15.14182575
C	6.661779183	15.13479983	23.54044669
H	6.678277866	16.18631035	23.86513948
H	6.774641881	15.0592781	22.4341598
C	7.641025729	14.22815404	24.27612582
H	7.149541347	13.24167155	24.4437574
H	8.513910189	14.02163733	23.62450998
C	8.101095607	14.81080338	25.61574954
H	7.225806773	14.94118881	26.28388226
H	8.521918872	15.8243744	25.46861525
C	9.143481329	13.90475139	26.28340147
H	8.730046497	12.88618407	26.41899824
H	10.02362212	13.78974949	25.6213451
C	9.588564907	14.46497194	27.64175683
H	8.714937312	14.56033508	28.31671898
H	9.983148173	15.49219873	27.51698092
C	1.495176159	9.434554214	23.07765924
H	1.986513606	10.24342724	23.64631871
H	2.139011676	9.083308619	22.24563594
C	1.009776594	8.298027516	23.96650017
H	0.387167965	7.591966047	23.37899879
H	0.332636943	8.67583401	24.75650773
C	2.223344142	7.585735736	24.57726013
H	3.049049575	7.537012342	23.83756848
H	2.61756749	8.180712342	25.42423766
C	1.893287116	6.164310675	25.04669358
H	1.455236622	5.571530757	24.21590369
H	1.110915866	6.186884026	25.82758564
C	3.156730033	5.469782955	25.57575985
H	3.941055306	5.475575838	24.79247953
H	3.573067721	6.04234368	26.42740093
C	2.878260937	4.033027445	26.00655328
H	2.364281992	3.470862029	25.21066885
H	2.239714005	3.998764131	26.89519681
H	3.807153126	3.500219203	26.23716144
C	-0.708786637	12.84167527	20.46206381
O	3.722901243	7.910505534	16.61623353
O	2.897792182	7.769524582	20.73540343
O	-4.50696181	5.494827636	20.93267126

O	-0.201019624	2.979318399	24.33865125
O	-2.202592808	1.969902831	24.05519533
O	-0.59881154	5.06706915	17.69891522
O	7.492397006	5.779585468	22.37361961
O	-2.345478817	-1.116401144	21.9109483
O	-0.894068311	-0.295485113	17.30332523
O	-2.029688357	3.75659471	14.19974052
O	2.727463149	-0.199759638	23.25560914
O	4.637112006	-2.80419747	21.94947004
O	6.687942379	1.816489438	20.20080945
O	5.493006975	4.645750546	14.95228772
N	9.067705639	-0.167746499	17.22532972
N	3.796572338	3.327619949	15.76629356
H	3.557978554	2.515588032	16.36059429
N	1.292946716	2.259424266	16.20628297
N	1.158554491	0.348307325	18.14606685
H	1.887670439	1.087900843	18.11498964
N	3.539393484	0.393051542	19.54302409
N	2.730499846	2.074286152	22.85624254
H	2.156692175	2.852122444	22.4590456
N	3.522613124	4.588574959	22.17746034
N	1.477686008	6.064457105	21.40012726
H	1.454862645	5.132425038	21.8789537
N	-0.682174989	4.735622248	22.4039517
N	0.610626669	1.710880374	21.2013596
N	0.272351979	3.656050065	19.30357743
H	1.140375239	3.417396628	19.83338112
N	2.740840401	4.474095079	18.70373143
N	4.676299353	2.819167802	19.67473871
H	3.644988117	2.663209019	19.62114067
C	10.175586	-0.377080939	16.33233404
C	11.46288807	-0.611292543	16.8514218
H	11.63135667	-0.61710678	17.92717196
C	12.52222898	-0.834411919	15.97148696
H	13.52074375	-1.017786754	16.36777191
C	12.31418784	-0.82022413	14.58857079
H	13.14544113	-0.99371325	13.90985241
C	11.03285702	-0.581436479	14.08047448
H	10.8698586	-0.570688001	13.00275825
C	9.957604939	-0.361979719	14.9409409
H	8.959257954	-0.187971653	14.54121825
C	9.001001076	-0.926191066	18.44707989
C	9.298788112	-2.302121913	18.42235124
H	9.542015869	-2.794182082	17.48180765

C	9.279060835	-3.023870845	19.61584178
H	9.510421735	-4.088558666	19.60317107
C	8.962596968	-2.392755053	20.82366228
H	8.9700518	-2.961372484	21.74941455
C	8.652475393	-1.0286348	20.83520884
H	8.409935582	-0.528468241	21.77271068
C	8.666095491	-0.288383603	19.65358256
H	8.408836383	0.777708132	19.67123061
C	8.081518207	0.817461949	16.91721159
C	8.464508309	2.014518851	16.27598434
H	9.516755017	2.22086205	16.08193695
C	7.490019603	2.929482188	15.89541893
H	7.771802633	3.863208103	15.3954008
C	6.128414084	2.668025606	16.13176243
C	5.761388753	1.495519713	16.81309946
H	4.708717834	1.284693752	17.03343445
C	6.723686827	0.576265031	17.21608622
H	6.4289064	-0.332929551	17.74110095
C	5.15605405	3.650606993	15.57472897
C	2.685284524	3.979553657	15.1691622
C	2.779848417	5.123719797	14.39497385
H	3.755712667	5.602259287	14.23493265
C	1.62483355	5.677247008	13.78824719
H	1.740310071	6.576020295	13.18028767
C	0.385457134	5.099322811	13.94402893
H	-0.506505604	5.515005028	13.47588233
C	0.247878058	3.927940236	14.73565651
C	1.383661111	3.372166613	15.37844136
C	0.09973206	1.699783062	16.40144048
C	-1.096119904	2.143452958	15.77673192
H	-2.018062314	1.604971241	15.98215247
C	-1.008433575	3.23805409	14.93597197
C	-3.323519972	3.06118163	14.25560267
H	-3.704532721	3.157463618	15.29588787
H	-3.171391594	2.003860893	13.98571782
C	-4.158961629	3.827839636	13.23709148
H	-3.774189124	3.642179741	12.2138822
H	-4.031301204	4.919827394	13.39752413
C	-5.637263814	3.437541555	13.3368266
H	-5.753931621	2.344910545	13.19339667
H	-6.012613978	3.649487563	14.3583396
C	-6.501597784	4.190835293	12.31713697
H	-7.564903764	4.128937359	12.62295371
H	-6.252594742	5.270464788	12.32707968

C	-6.348990455	3.634675818	10.89460944
H	-6.603805539	2.556721562	10.88211347
H	-5.289677276	3.695431044	10.57559358
C	-7.231296233	4.38344291	9.899178306
H	-7.126442098	3.972117033	8.8889145
H	-6.971697474	5.446909373	9.84662305
H	-8.291121026	4.317874142	10.1692579
C	0.041696566	0.484268925	17.31497592
C	1.4373125	-0.73913219	19.0166525
C	2.715855638	-0.712350713	19.7042513
C	3.067700336	-1.7916777	20.5521771
C	2.157024759	-2.866471675	20.74492126
H	2.450748585	-3.677940188	21.4111675
C	0.938551725	-2.853813184	20.10648953
H	0.22407866	-3.664230693	20.25469031
C	0.571951422	-1.795164308	19.23667523
H	-0.406260862	-1.819540237	18.73862576
C	4.35192253	-1.700355015	21.2148382
C	5.15938306	-0.583907364	21.06534046
H	6.125856869	-0.473661794	21.54815401
C	4.685638078	0.454682013	20.22628094
C	5.823827576	-2.790081903	22.81622603
H	5.86371824	-1.836519465	23.3673377
H	6.704646595	-2.908525537	22.16242297
C	5.552069147	-3.992254365	23.71387035
H	4.666680965	-3.782467216	24.35014994
H	5.254118188	-4.857826615	23.08415684
C	6.764081787	-4.352071741	24.57721116
H	7.070055007	-3.481664878	25.18934344
H	7.632837134	-4.59641077	23.93491347
C	6.435784531	-5.542496624	25.48940149
H	5.568659641	-5.297527703	26.13423033
H	6.11772017	-6.410059366	24.87876863
C	7.633220287	-5.939009125	26.36310632
H	8.505883432	-6.177012285	25.72368336
H	7.944313232	-5.0812253	26.99116974
C	7.305833398	-7.136713188	27.25234445
H	7.035118347	-8.01819936	26.65954261
H	6.46505337	-6.924048704	27.92277616
H	8.161587715	-7.413470485	27.87849737
C	5.483646238	1.740225619	20.04255817
C	5.104238569	4.065597527	19.13978419
C	6.414980524	4.490907457	19.07859021
H	7.217846875	3.866531881	19.48670715

C	6.732690465	5.727750112	18.4540319
H	7.781806012	6.019238926	18.40865051
C	5.760441021	6.518432139	17.88883437
H	5.998107856	7.451740347	17.37316432
C	4.395718154	6.114696905	17.94419744
C	4.052002709	4.905430187	18.59231522
C	1.763219354	5.224845145	18.1831946
C	1.987760217	6.433172298	17.48810026
H	1.138225051	6.991244509	17.09300476
C	3.306007502	6.844762515	17.33399787
C	0.352650467	4.674411813	18.34616901
C	-0.842970621	2.829584353	19.58805902
C	-2.09091478	2.966213102	19.0113007
H	-2.284120783	3.78355554	18.3039255
C	-3.124001887	2.042814568	19.32080756
H	-4.096775648	2.188292798	18.84172479
C	-2.913377661	0.9907226	20.18089551
H	-3.693524492	0.262357191	20.4158793
C	-1.64673206	0.833699781	20.81188186
C	-0.611899673	1.761770724	20.54641743
C	0.827897431	0.751099148	22.10109371
C	-0.11805445	-0.260232131	22.41338465
H	0.154334016	-1.047449064	23.11079266
C	-1.339655056	-0.212464586	21.76087454
C	-2.469524625	-1.771065732	23.22132064
H	-2.215574458	-1.041900637	24.01148304
H	-1.765969929	-2.619100581	23.22698276
C	-3.932631681	-2.205985692	23.27436048
H	-4.15992861	-2.567663582	24.29714298
H	-4.086812968	-3.06867662	22.59438577
C	-4.906214045	-1.087915269	22.87327514
H	-4.667334663	-0.759279681	21.83735246
H	-5.93239449	-1.500566473	22.83869723
C	-4.854859874	0.121005012	23.81257535
H	-3.834445116	0.56764183	23.7989946
H	-5.026938011	-0.191783829	24.85816172
C	-5.879530142	1.189807375	23.40685596
H	-6.905414256	0.808557467	23.57254206
H	-5.798872559	1.396361752	22.32174675
C	-5.667174705	2.47954653	24.19556397
H	-5.697776655	2.299071967	25.27656862
H	-6.432700965	3.226362122	23.96931729
H	-4.674687324	2.913730821	23.97863958
C	2.185378045	0.786422266	22.79006989

C	4.097994001	2.405575363	23.07611565
C	5.044637304	1.549505138	23.60016995
H	4.759739114	0.538662258	23.90832542
C	6.398737404	1.968988907	23.7110194
H	7.120032897	1.260330108	24.11736401
C	6.805226235	3.218632222	23.30541375
H	7.848665368	3.531082203	23.36294331
C	5.854703884	4.138747122	22.77845215
C	4.497950403	3.744698783	22.67658697
C	6.172789323	5.463299454	22.29192151
C	5.185939294	6.306121702	21.8001128
H	5.378389633	7.306313033	21.42110833
C	3.859851538	5.811553704	21.76638928
C	2.716942651	6.668964393	21.23503069
C	7.911431759	7.046998613	21.74878971
H	7.414750532	7.873497101	22.28330658
H	7.604976235	7.023985062	20.68730594
C	9.422799694	7.037696788	21.93674812
H	9.673766682	7.188961965	23.00647394
H	9.816828131	6.029859698	21.68593637
C	10.10432897	8.100354024	21.06759488
H	11.20317923	7.987408503	21.16730556
H	9.883477972	7.907673236	19.99827876
C	9.69982292	9.539625334	21.41315103
H	8.598809753	9.65074472	21.36569926
H	10.09906842	10.22432783	20.63755185
C	10.20790653	9.980332401	22.79279975
H	9.922541274	9.23033677	23.55725051
H	11.31520732	10.00833216	22.79522867
C	9.654568435	11.34580362	23.18794035
H	9.876268454	12.10900655	22.42294744
H	10.07344264	11.68704302	24.13973069
H	8.556689847	11.32262891	23.29407917
C	0.195510171	6.547157487	21.02081066
C	-0.023998642	7.628672461	20.19026118
H	0.815795353	8.233788554	19.81539818
C	-1.343809917	7.952781067	19.78492102
H	-1.464186101	8.816501847	19.11311402
C	-2.424593725	7.19969028	20.18226998
H	-3.438462728	7.422498951	19.84995851
C	-2.233079414	6.084839143	21.04383321
C	-0.93022821	5.774202577	21.50928795
C	-1.704963158	3.990295363	22.80479081
C	-3.045017717	4.166395111	22.35735951

H	-3.817621869	3.479119401	22.72099308
C	-3.292329044	5.198161153	21.47302226
C	-5.527535116	4.433466706	20.93810758
H	-6.033557461	4.494353505	21.91586502
H	-5.040481885	3.450146403	20.8154014
C	-6.440122923	4.789008678	19.7696973
H	-6.704895099	5.866902933	19.82291338
H	-7.395746738	4.239437864	19.88476101
C	-5.818283211	4.476668187	18.40176311
H	-6.623529408	4.405200399	17.6456619
H	-5.328708678	3.47978997	18.42015405
C	-4.801324296	5.545976754	17.9829592
H	-5.266182253	6.555497804	18.04425623
H	-3.960349035	5.560404097	18.70805951
C	-4.272514835	5.324332014	16.56384468
H	-5.095094852	5.487260053	15.82830262
H	-3.952259082	4.265167576	16.43907349
C	-3.101798032	6.244052217	16.23799659
H	-2.661649239	5.998942796	15.26233161
H	-2.284034152	6.126596696	16.96919044
H	-3.387040216	7.300237549	16.23054248
C	-1.439779443	2.871125105	23.77648585
C	0.177545881	1.938086896	25.28196614
H	-0.098073389	0.949618571	24.90150829
H	-0.308560246	2.138691291	26.23973414
H	1.270352	2.073702491	25.33847076
C	2.749421096	8.591347633	15.74431248
H	2.082508761	9.182238127	16.39482414
H	2.172560238	7.835689415	15.186803
C	3.677825925	9.417234485	14.86407089
H	4.443174552	9.91226763	15.50074628
H	4.252946074	8.744745365	14.19541378
C	2.906987768	10.46085501	14.05429643
H	2.424949396	11.19583321	14.73320163
H	2.081870711	9.984671097	13.49225754
C	3.849549469	11.19115987	13.08850549
H	4.65405048	11.69436667	13.66037207
H	4.358884849	10.46174	12.43002778
C	3.085784788	12.21753247	12.2435699
H	2.551948047	12.91837133	12.92099366
H	2.301139297	11.7084436	11.65146979
C	4.017900695	12.99237107	11.31535841
H	3.461016769	13.70943153	10.70307096
H	4.551244448	12.32129486	10.6319406

H	4.774917831	13.55002449	11.87928813
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Table S12. Atomic coordinates for the optimized structure of TPA-Q₆(*n*-He) in MOPAC2016 (Fig. S2(iii), gas phase).

Atom	X	Y	Z
O	-2.256221086	14.032181783	24.210099481
O	5.277496477	14.873321819	23.939330427
O	3.636767104	19.012941781	21.066939846
O	-2.306642988	20.666201496	16.504997507
O	-3.879116823	16.127037465	18.996367089
O	0.124455679	10.479405169	22.407724000
O	3.921247643	13.804061501	20.745375061
O	4.124924692	19.906243351	16.099685350
O	-0.710343630	17.933770577	15.178061400
O	-4.604867991	11.764668065	17.494956945
O	0.298717740	10.350301119	18.670175747
O	2.944041567	14.955179450	14.293391741
O	4.769960194	16.235569604	14.680264595
O	7.526350723	12.590225957	17.353789255
N	-6.320126965	18.284637239	21.657059653
N	-0.698180103	15.310995459	23.110318710
H	-0.540120829	16.080623739	22.438908171
N	1.737417677	16.370230964	22.354147498
N	1.685158708	18.088493651	20.235425542
H	1.025730068	17.289540471	20.337564677
N	-0.815561931	17.826642456	19.132495243
N	-1.737381812	15.350504476	19.360390846
H	-0.726578528	15.593398745	19.255500285
N	0.455120538	13.952364654	20.160163329
N	2.725516685	14.865434036	19.079076782
H	1.792772661	14.910879645	18.610975193
N	1.882643101	16.571326031	17.120078246
N	-0.358583763	15.755385920	15.861262645
H	0.354784710	15.109220855	16.263743444
N	-0.764120975	13.242823446	16.906901549
N	1.513018585	11.926067214	17.494750409
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H	-12.592401283	28.428453752	10.325324560
C	-4.170624149	24.068812578	17.196511703
C	-2.775976314	22.921535925	18.952757726
C	-1.480527843	22.972709385	19.603923079
C	-1.112077098	21.935099891	20.494137704
C	-2.019029433	20.872565489	20.755360379
H	-1.707054146	20.088566108	21.447509701
C	-3.251493671	20.863173126	20.146762646
H	-3.962346780	20.050860489	20.346868842
C	-3.640902612	21.885713028	19.245666954
H	-4.634345498	21.845399912	18.783160982
C	0.190436186	22.043705165	21.119993657
C	1.001343730	23.148275590	20.893248754
H	1.987164216	23.264199676	21.334849585
C	0.499963550	24.154923832	20.035630262
C	1.701529378	20.953222684	22.705080227
H	1.854501321	21.934156620	23.175937710
H	2.534398837	20.700651149	22.018575005
C	1.362404706	19.849096302	23.701192585
H	0.605027889	20.212981325	24.424170149
H	0.860823955	19.015203037	23.159199841
C	2.602009875	19.327239368	24.432088258
H	3.096749746	20.145887446	24.987158098
H	3.347835401	18.959283219	23.696386474
C	2.213195334	18.198907157	25.397420365
H	1.545104795	18.588511328	26.189243937

H	1.618988781	17.430540590	24.862178549
C	3.444676934	17.542923611	26.034188508
H	4.146466553	17.210171694	25.244093208
H	4.000260430	18.285216215	26.638095338
C	3.055783593	16.349898153	26.904182852
H	2.510341106	15.591654805	26.326186933
H	2.412344843	16.650166447	27.738173617
H	3.939988694	15.860734395	27.324903461
C	1.263155097	25.452467506	19.803087240
C	0.801818877	27.779233366	18.939903172
C	2.106516114	28.222108191	18.841136413
H	2.929644333	27.598976386	19.210496049
C	2.388185499	29.478189542	18.242017490
H	3.430926887	29.787056643	18.165703141
C	1.386163201	30.277128357	17.743261475
H	1.595322893	31.233140617	17.261049110
C	0.029211545	29.856526250	17.835655355
C	-0.277406326	28.617130117	18.446630389
C	-2.580495814	28.906050174	18.102920531
C	-2.393201160	30.148732969	17.450379164
H	-3.263810591	30.680281493	17.074654929
C	-1.091967776	30.607943720	17.313608118
C	-3.980836826	28.327374957	18.254528072
C	-5.160332097	26.446241234	19.446856408
C	-6.396097122	26.564414079	18.841274450
H	-6.584719868	27.377210411	18.127433627
C	-7.428106149	25.634327990	19.135759022
H	-8.392268291	25.767470081	18.631427191
C	-7.236135248	24.607581242	20.028846843
H	-8.018714711	23.883466855	20.259383009
C	-5.985656615	24.472817926	20.697634192
C	-4.937929294	25.380560365	20.410815699
C	-3.510650958	24.381371149	21.986026241
C	-4.484823609	23.418027432	22.351091619
H	-4.240683285	22.655164453	23.086793039
C	-5.713187263	23.480515651	21.710635167
C	-6.895153945	22.124871809	23.327379777
H	-6.631252509	22.932142947	24.037479311
H	-6.203635498	21.270168513	23.414093661
C	-8.360159456	21.712984650	23.408205418
H	-8.560690615	21.304427426	24.419509388
H	-8.548995662	20.874779049	22.702462058
C	-9.330960246	22.855163881	23.085914101
H	-9.120235745	23.227293998	22.060873916

H	-10.361831758	22.452834057	23.065379659
C	-9.237229420	24.016602904	24.080471288
H	-8.224052076	24.476906901	24.021110842
H	-9.332644281	23.647566156	25.118218191
C	-10.308098061	25.080354869	23.804064439
H	-11.308688164	24.683391756	24.063300676
H	-10.347350097	25.304586741	22.720914273
C	-10.037316370	26.359172839	24.592911826
H	-9.993315574	26.160891765	25.671172427
H	-10.817267870	27.109209042	24.430590068
H	-9.071004308	26.805222452	24.313753110
C	-2.139893793	24.413694121	22.651074967
C	-0.214711423	26.028193957	22.875612885
C	0.753815904	25.162666547	23.342831156
H	0.481180531	24.142942152	23.638025186
C	2.111314516	25.580212128	23.403384544
H	2.852456523	24.863315828	23.759562788
C	2.499406488	26.840291855	23.010213416
H	3.544533543	27.152196246	23.024903036
C	1.525688724	27.773345620	22.553012040
C	0.167437758	27.378670976	22.498870457
C	1.817732547	29.113444452	22.091486031
C	0.811484234	29.965282733	21.657646055
H	0.990990918	30.970859457	21.285293438
C	-0.514929568	29.469362724	21.677358876
C	-1.695859757	30.298159942	21.186113945
C	3.557359143	30.717330612	21.580384477
H	3.012266225	31.520573016	22.103765931
H	3.313422737	30.711710618	20.503583669
C	5.054975750	30.731654917	21.861462350
H	5.232855013	30.811081755	22.953406809
H	5.495373447	29.755954490	21.565684298
C	5.759295181	31.871987482	21.119683555
H	6.855915590	31.738499630	21.219658884
H	5.555111763	31.797007809	20.032972969
C	5.365242530	33.270202114	21.614179484
H	4.265611699	33.392338825	21.584715508
H	5.763148255	34.027871742	20.909799645
C	5.882638331	33.562793652	23.029743226
H	5.489029846	32.805403395	23.737154382
H	6.984983127	33.457590414	23.055494760
C	5.486186467	34.959898732	23.500172844
H	5.872326753	35.738482295	22.832158999
H	5.878633499	35.165405772	24.502602317

H	4.397245447	35.077595281	23.546471351
C	-4.210409065	30.085557394	21.153984418
C	-4.490679568	31.084984547	20.240130458
H	-3.693212206	31.757445562	19.902295990
C	-5.801317415	31.224913470	19.717643503
H	-5.982338627	32.008974095	18.981288214
C	-6.819781819	30.384558953	20.105801632
H	-7.825131724	30.467350318	19.684634409
C	-6.573040228	29.359995644	21.059181532
C	-5.272543386	29.199334149	21.598447243
C	-5.932514351	27.375920590	22.904940978
C	-7.273507662	27.435523345	22.429425072
H	-7.999738400	26.708118331	22.799395355
C	-7.577694208	28.419158635	21.508340278
C	-9.796685515	27.556027439	21.047780836
H	-10.206243607	27.589995351	22.072067998
H	-9.300167800	26.588421590	20.855340168
C	-10.834192828	27.915883450	19.989994273
H	-11.145619566	28.973517928	20.127420095
H	-11.745793900	27.310898767	20.167900931
C	-10.338226984	27.704442017	18.552767508
H	-11.207755496	27.611987824	17.875219204
H	-9.787877430	26.739761698	18.478772882
C	-9.435026999	28.854380073	18.089298344
H	-9.984297513	29.813246820	18.140876398
H	-8.586929115	28.962094645	18.803943850
C	-8.895898155	28.638408316	16.672920351
H	-9.714020406	28.757405353	15.933232327
H	-8.532426176	27.591971300	16.555060296
C	-7.755911871	29.598797875	16.348972683
H	-7.355650947	29.416588215	15.342884971
H	-6.904901355	29.467134192	17.039141383
H	-8.067516735	30.644378126	16.409476126
C	-5.580948889	26.297990788	23.895998061
C	-3.845734564	25.495700697	25.352521441
H	-3.998416430	24.487157503	24.955780047
H	-4.365356861	25.623221378	26.305333812
H	-2.779191924	25.750249031	25.421604272
C	-1.744534838	32.537742909	15.990753837
H	-2.295542940	33.103482086	16.759855694
H	-2.420200625	31.859376068	15.441811244
C	-0.900147614	33.411473387	15.068895107
H	-0.209634824	34.034643666	15.673243574
H	-0.240470263	32.763687341	14.452591621

C	-1.779680665	34.291069803	14.176075768
H	-2.419570522	34.947398974	14.797930526
H	-2.472495957	33.662554111	13.582977286
C	-0.918632129	35.144141840	13.235169933
H	-0.228962338	35.779617299	13.824642282
H	-0.270557937	34.489701067	12.619548916
C	-1.784730853	36.022877423	12.323163519
H	-2.430336831	36.681061650	12.937538646
H	-2.473189388	35.387256494	11.732136402
C	-0.932218465	36.870614708	11.381913778
H	-1.558839032	37.493963310	10.734127230
H	-0.307516315	36.247226429	10.731655955
H	-0.262724173	37.539786854	11.934540627

Table S13. Atomic coordinates for the optimized structure of TPA-Q₆(*n*-He) in MOPAC2016 (Fig. S1b(i), gas phase).

Atom	X	Y	Z
O	3.634089944	8.015623942	16.524149682
O	3.177628293	7.496224029	20.410866616
O	-4.023833081	4.965793325	21.087601980
O	0.434277401	2.790179988	24.526458005
O	-1.493479530	1.652602901	24.278787664
O	-0.499692293	4.932502593	17.681888007
O	7.919481439	5.571071951	21.984687468
O	-1.933954039	-1.258095827	21.981665371
O	-0.643875941	-0.511676326	17.264319898
O	-2.006351392	3.555724670	14.231965488
O	3.146422018	-0.290622163	23.130574561
O	5.133247875	-2.696869507	21.813163417
O	6.953483814	1.889512495	19.788514501
O	5.474378479	4.625872717	14.650953922
N	9.481082297	0.177437254	16.911249089
N	3.868171729	3.284114824	15.614023144
H	3.685674024	2.468543555	16.221580071
N	1.405289994	2.157873155	16.159774284
N	1.381227614	0.247340803	18.095351270
H	2.075510259	1.019392390	18.042604733
N	3.816161828	0.386762107	19.360704262
N	3.134334661	1.980884031	22.731735353
H	2.545256075	2.769008141	22.380795754
N	3.922319599	4.499158068	22.066069540
N	1.868820246	6.139452010	21.762540425
H	1.909634297	5.332987765	22.430140721
N	-0.179203550	4.515132487	22.629565462

N	0.942190025	1.614797049	21.156904723
N	0.460818064	3.612564086	19.321380892
H	1.350469581	3.420395544	19.827885541
N	2.884118547	4.492134311	18.578953895
N	4.901673228	2.852211873	19.376142578
H	3.869642857	2.688897813	19.414125837
C	10.492023847	-0.110901478	15.920368041
C	11.799807388	-0.394346677	16.367110930
H	12.031710161	-0.419365979	17.432703567
C	12.793902736	-0.664446977	15.431731170
H	13.813888966	-0.892315483	15.778426218
C	12.505409988	-0.641954078	14.061432867
H	13.290687496	-0.857110646	13.338958418
C	11.209557018	-0.360697261	13.627640590
H	10.977021408	-0.357838879	12.562155552
C	10.190426861	-0.106016415	14.551845860
H	9.176457345	0.088983538	14.204939715
C	9.372509925	-0.711351595	18.046519337
C	9.668072602	-2.082148099	17.930146225
H	9.944377998	-2.510934892	16.967524730
C	9.629576565	-2.885424601	19.067897788
H	9.856531020	-3.949781338	18.982121565
C	9.280224696	-2.345339868	20.309917014
H	9.256252603	-2.982969437	21.188716951
C	8.971253039	-0.983335765	20.412499783
H	8.692770556	-0.548717582	21.372306315
C	9.007628585	-0.164295637	19.286116460
H	8.741014732	0.896619864	19.368686164
C	8.371641183	1.007117365	16.553246380
C	8.629821711	2.219586579	15.878471370
H	9.654725022	2.498148472	15.612145995
C	7.575927321	3.055735529	15.526587477
H	7.767606783	4.006116690	15.010201985
C	6.250263355	2.692987049	15.818740052
C	5.993220731	1.488505196	16.494243255
H	4.967885801	1.189394086	16.740829710
C	7.042505778	0.650989249	16.868790487
H	6.840747571	-0.278930556	17.401549776
C	5.203381906	3.626292006	15.322543625
C	2.717866487	3.928822216	15.097031308
C	2.748667177	5.101075593	14.367268283
H	3.702134657	5.615312636	14.181697819
C	1.556276424	5.645346260	13.825855681
H	1.622943386	6.571219226	13.257081812

C	0.342179825	5.013473500	13.984263874
H	-0.579265780	5.409351035	13.556762853
C	0.266972996	3.811934613	14.739446697
C	1.437759547	3.277698399	15.341812541
C	0.243148662	1.543690088	16.358233137
C	-0.978926666	1.941590759	15.753306174
H	-1.873690376	1.353031953	15.947500528
C	-0.950790851	3.059433054	14.936339684
C	-3.265158239	2.796782052	14.265518486
H	-3.631292753	2.804388463	15.314557915
H	-3.063083601	1.767435689	13.923934777
C	-4.160521320	3.583070088	13.314280313
H	-3.807940422	3.465707889	12.271663540
H	-4.070525214	4.669823504	13.535139979
C	-5.620446469	3.128601249	13.436921315
H	-5.695682588	2.043755191	13.228370135
H	-5.974512646	3.266656317	14.478752186
C	-6.550798219	3.897033621	12.485345961
H	-7.600581738	3.736500960	12.796306898
H	-6.375470701	4.985996333	12.572457720
C	-6.384511010	3.457796333	11.024150833
H	-6.622823027	2.378898312	10.927761832
H	-5.326954902	3.563140823	10.710619838
C	-7.281678995	4.276279635	10.098068441
H	-7.192786643	3.944143935	9.058769527
H	-7.023965630	5.340364211	10.126807422
H	-8.340744761	4.185404781	10.376292428
C	0.256095112	0.325967381	17.272915133
C	1.738537063	-0.822918351	18.957306305
C	3.043063554	-0.741325168	19.582769648
C	3.473713793	-1.792614592	20.433801818
C	2.614262197	-2.897288304	20.679414592
H	2.966233520	-3.687522586	21.342985592
C	1.373122641	-2.939491992	20.093831308
H	0.698073275	-3.777262906	20.283837798
C	0.927095990	-1.911394851	19.222877006
H	-0.070541577	-1.976031515	18.771409841
C	4.775280268	-1.630487086	21.046891504
C	5.537750866	-0.499818654	20.828610226
H	6.520468723	-0.338625468	21.267164683
C	4.998615692	0.502458104	19.983304907
C	6.362337475	-2.552366953	22.610553974
H	6.344110985	-1.578655477	23.127715202
H	7.212468292	-2.612698027	21.907212970

C	6.263469849	-3.738621889	23.569873209
H	5.373791037	-3.596667709	24.223055069
H	6.068634501	-4.663063085	22.994748919
C	7.533964982	-3.879927100	24.414825870
H	7.736804373	-2.933480618	24.952699359
H	8.405085802	-4.071524961	23.759917583
C	7.391173068	-5.034020770	25.425037877
H	6.519042570	-4.844960184	26.086519317
H	7.158923812	-5.978614520	24.901267689
C	8.653409953	-5.210652601	26.270007351
H	9.527599679	-5.424003068	25.622134489
H	8.896970632	-4.278206128	26.814076805
C	8.485168053	-6.351872810	27.278614608
H	8.271710379	-7.303583459	26.772668822
H	7.651377750	-6.152365639	27.971019959
H	9.384795117	-6.491715667	27.887670301
C	5.752996274	1.798334126	19.718168496
C	5.276448542	4.109148845	18.816400595
C	6.568559511	4.542232184	18.629879294
H	7.415977283	3.915648375	18.939397648
C	6.823870077	5.785053054	17.992571016
H	7.863177469	6.082430263	17.854366982
C	5.797546441	6.577699480	17.525593530
H	5.985619927	7.518595605	17.008955070
C	4.446493602	6.163058011	17.700951518
C	4.175827217	4.944836931	18.367868683
C	1.858826909	5.211257443	18.115017016
C	2.007534979	6.428999455	17.412136239
H	1.118881896	6.939121667	17.052389536
C	3.300858349	6.888916487	17.202616602
C	0.475624579	4.603456608	18.330262147
C	-0.593579458	2.705268275	19.592714111
C	-1.846572273	2.775207541	19.023041257
H	-2.093222675	3.579854034	18.312103264
C	-2.827038006	1.798110300	19.326650095
H	-3.805743497	1.888771061	18.850999773
C	-2.571636617	0.761466338	20.200819813
H	-3.308712495	-0.001614279	20.442069235
C	-1.294957225	0.673372847	20.824155757
C	-0.297966008	1.634983434	20.540934078
C	1.203567373	0.661925635	22.056498952
C	0.291677978	-0.366648742	22.401410687
H	0.591948086	-1.134705012	23.103553266
C	-0.945922387	-0.347664910	21.782662429

C	-2.021099480	-1.879417279	23.313521810
H	-1.733048771	-1.132799080	24.077358031
H	-1.324720795	-2.734078695	23.316594156
C	-3.486817517	-2.303744199	23.418359619
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H	10.540722776	2.389880925	18.634642164
C	10.773436426	4.549557180	18.525949314
H	10.161117599	5.456614683	18.688247659
H	11.646285157	4.643418230	19.220179350
C	11.269732080	4.517917728	17.077446354
H	10.438524311	4.776849525	16.391875228
H	11.589876570	3.490994882	16.784022697
C	12.439183627	5.477049011	16.865630153
H	12.792407185	5.476118765	15.829742575
H	13.312232384	5.194002267	17.481079886

H	12.172916023	6.505440953	17.128676029
C	14.860067460	1.936976931	24.407668079
C	16.612534750	1.214352959	25.876625808
H	16.510662908	0.201843214	25.471455151
H	16.074642748	1.319259055	26.821133868
H	17.665027176	1.516946606	25.960644627
C	18.554933472	8.585154170	16.213989388
H	18.012258793	9.256457189	16.898841989
H	17.865439926	7.859827055	15.749836064
C	19.420210365	9.321354969	15.194623910
H	20.147560377	9.972275876	15.720740409
H	20.037368314	8.587471073	14.637625869
C	18.560166092	10.138278370	14.224825149
H	17.928285679	10.848879864	14.791318260
H	17.860444991	9.472596937	13.680489052
C	19.433094074	10.899022484	13.218932553
H	20.141247718	11.559917964	13.762768729
H	20.058890463	10.188081698	12.642532567
C	18.575699962	11.729263171	12.254762851
H	17.941013281	12.433516423	12.829619521
H	17.880654177	11.065822208	11.699896171
C	19.429669228	12.517099238	11.263069649
H	18.799375138	13.110524910	10.588054215
H	20.054362712	11.859532242	10.651642996
H	20.094634452	13.220817664	11.775049701

Table S14. Atomic coordinates for the optimized structure of **TPA-Q₆(*n*-He)** in MOPAC2016 (Fig. S1b(ii), gas phase).

Atom	X	Y	Z
O	-2.623754243	13.825772547	23.932756932
O	4.905582850	14.784713381	23.908579802
O	3.263132442	18.821537186	20.819675084
O	-2.853992099	20.054757268	16.304476111
O	-4.152230793	15.558124622	18.891756619
O	0.015889544	10.107883480	22.413338751
O	3.706902972	13.495380159	20.705937143
O	4.042954763	19.542531649	16.028418054
O	-0.810129566	17.609586971	15.042555816
O	-4.678487904	11.443496501	17.315625490
O	0.211902747	10.090183888	18.583216702
O	2.878716691	14.648346143	14.188343334
O	4.688634125	15.950801923	14.567183742
O	7.429537602	12.467037547	17.434958532
N	-6.594284656	18.143477909	21.355098693

N	-1.039095332	15.055405816	22.817451001
H	-0.863272848	15.815392511	22.138178636
N	1.396328827	16.176483977	22.176851750
N	1.345363661	17.797559590	20.025153625
H	0.723642836	16.971592056	20.156056614
N	-1.133628553	17.351434831	18.944585594
N	-1.988065785	14.818812041	19.218482589
H	-0.983129116	15.082632138	19.097585399
N	0.245468459	13.515482006	20.055911982
N	2.506779046	14.550853296	19.040534356
H	1.585607084	14.581509382	18.551921538
N	1.737182182	16.234309788	17.010378918
N	-0.423847256	15.403230459	15.604757793
H	0.294544006	14.749276773	15.985875420
N	-0.834218401	12.917268721	16.709606633
N	1.437727102	11.609346655	17.346447610
H	1.366737653	12.431422667	16.705060219
N	3.470252588	13.104751848	16.285166653
C	-6.791258825	18.556653477	19.997208502
C	-6.348676938	17.746524342	18.935771001
H	-5.794451293	16.818387782	19.128066552
C	-6.602177539	18.138867961	17.622301244
H	-6.277437985	17.498233822	16.800652695
C	-7.287578111	19.326227138	17.350964322
H	-7.528868749	19.601485244	16.323768796
C	-7.687627070	20.150335314	18.409073780
H	-8.205398508	21.086664016	18.202343705
C	-7.438170018	19.781435624	19.729162089
H	-7.742022068	20.434282010	20.548390564
C	-7.605920758	18.372210995	22.353777528
C	-8.957663602	18.531509084	22.004557601
H	-9.293678019	18.460755295	20.968486479
C	-9.896652248	18.813017643	22.999382285
H	-10.945198487	18.974087968	22.710206567
C	-9.513399230	18.881022978	24.340857975
H	-10.254449000	19.086775853	25.110490709
C	-8.169894950	18.699870754	24.686377363
H	-7.865811133	18.759263562	25.731345930
C	-7.209696773	18.455804882	23.705304215
H	-6.161618174	18.345983913	23.980903315
C	-5.520839224	17.240238004	21.686660668
C	-4.190708036	17.611205064	21.413827732
H	-3.977578434	18.533888741	20.871957325
C	-3.150348968	16.800404308	21.862417670

H	-2.118401489	17.109081613	21.663847306
C	-3.419100842	15.616720812	22.568330530
C	-4.752117529	15.229599432	22.786391128
H	-4.960088580	14.299046980	23.338321241
C	-5.801611896	16.028703046	22.346464605
H	-6.833035384	15.725315786	22.525036876
C	-2.366148153	14.742949046	23.166785209
C	0.130120529	14.473919302	23.382028122
C	1.397621796	15.099432399	23.051648106
C	2.594901034	14.591526521	23.614677134
C	2.546972274	13.448371019	24.458534547
H	3.483169957	13.071651048	24.870036155
C	1.337350460	12.856337432	24.739361326
H	1.287082913	11.978212558	25.384318842
C	0.124342116	13.363286146	24.207347850
H	-0.821922928	12.868864447	24.463760522
C	3.817711575	15.287324623	23.270531505
C	3.807941017	16.362858376	22.395985587
H	4.698435136	16.911307117	22.103789266
C	2.555022345	16.756621257	21.859615775
C	2.459268079	17.912269229	20.869310961
C	0.844629838	18.769926150	19.119730206
C	1.530515391	19.905393386	18.733135852
H	2.526949682	20.111539399	19.141940666
C	0.951031270	20.807259241	17.802189710
H	1.526792027	21.688810419	17.520277023
C	-0.298789348	20.588054400	17.270409098
H	-0.748752123	21.274075217	16.551949784
C	-1.039047441	19.434532275	17.650911862
C	-0.475181472	18.513046721	18.567567370
C	-2.356555231	19.112949645	17.143350666
C	-3.004285085	17.943807391	17.520405825
H	-3.995861731	17.668567381	17.169394313
C	-2.330092531	17.081291133	18.414308103
C	-2.952030447	15.761994528	18.855022421
C	-4.180661572	19.803622766	15.719406276
H	-4.917454358	19.947079317	16.531453027
H	-4.212806043	18.774440502	15.322014074
C	-4.278943978	20.856242772	14.624782347
H	-3.598005233	20.602154434	13.787483299
H	-3.910647969	21.832020064	15.005847974
C	-5.724575006	20.977801860	14.133538886
H	-6.116188721	19.965959738	13.867921509
H	-6.374168904	21.343609097	14.953291324

C	-5.849724191	21.901275127	12.916695203
H	-5.115417409	21.608952480	12.141172285
H	-6.842712270	21.758332697	12.447451663
C	-5.662610745	23.380255907	13.283411421
H	-6.480276160	23.705671992	13.955623559
H	-4.727112310	23.510764075	13.863517937
C	-5.623047094	24.269896944	12.043747841
H	-4.777083504	24.019165893	11.393071780
H	-5.521700446	25.326156793	12.317769549
H	-6.535647812	24.175228579	11.444990725
C	-2.185493481	13.614774933	19.948447479
C	-3.411039481	13.076217235	20.275521537
H	-4.341321524	13.560750565	19.926200453
C	-3.486581715	11.907515433	21.079446384
H	-4.475897491	11.533426400	21.348656971
C	-2.354057591	11.275883581	21.537128017
H	-2.403188244	10.388592186	22.170157956
C	-1.068814182	11.790584470	21.202309699
C	0.183138845	11.210800226	21.638595806
C	1.400841357	11.776856130	21.288984876
H	2.363461818	11.385885318	21.608209262
C	1.371491090	12.944217159	20.487563664
C	10.253038512	13.915109584	28.370261948
H	9.825023022	12.943334150	28.641734943
H	10.629759704	14.375591392	29.290778205
H	11.116233340	13.723266287	27.722832734
C	2.658537737	13.661521274	20.108069115
C	3.431659819	15.545306095	18.626202173
C	4.691570947	15.714142463	19.165837491
H	5.066411686	14.999636406	19.913398620
C	5.493374472	16.820021228	18.781251673
H	6.467134168	16.939789075	19.256907200
C	5.054452844	17.735802768	17.854133603
H	5.653682588	18.602875350	17.567839885
C	3.782793681	17.566616576	17.239529422
C	2.970477165	16.465380614	17.601633892
C	1.305207531	17.071627094	16.066625542
C	2.021259697	18.217781077	15.637301854
H	1.581405998	18.875446043	14.892450929
C	3.244456606	18.465238670	16.239821916
C	-0.076340429	16.759638255	15.512161086
C	-1.757444876	14.903674256	15.635102489
C	-2.851189556	15.591754575	15.146642688
H	-2.719190069	16.571251722	14.672653752

C	-4.154904627	15.041855418	15.273748146
H	-4.995144400	15.609691781	14.873081634
C	-4.362393535	13.832106386	15.891165326
H	-5.357710328	13.401406531	15.992828367
C	-3.263822054	13.094483312	16.414324307
C	-1.950280466	13.605515021	16.260371875
C	-1.002603289	11.748572225	17.330619347
C	-2.270653995	11.166836572	17.582577083
H	-2.308767309	10.230566224	18.138193885
C	-3.392108692	11.847176335	17.134153420
C	-4.893047826	10.217661351	18.110637486
H	-4.555006956	10.435582738	19.139405301
H	-4.295747859	9.404475300	17.663716827
C	-6.391899131	9.977647859	18.017652550
H	-6.942111035	10.923289682	18.263811642
H	-6.697376497	9.253090183	18.798027316
C	-6.800674683	9.470088589	16.630109102
H	-6.340476137	8.482661811	16.433950825
H	-6.395168070	10.150452907	15.853291579
C	-8.323355514	9.374301384	16.492734678
H	-8.741145245	8.718059435	17.279434013
H	-8.769732508	10.375567365	16.670318801
C	-8.762176830	8.874395859	15.110650896
H	-9.834039661	9.120373025	14.965015771
H	-8.221193753	9.426944761	14.317780859
C	-8.556937339	7.372642224	14.927195425
H	-8.895013829	7.044851480	13.938206990
H	-9.113998513	6.796794742	15.675147444
H	-7.501487673	7.095206832	15.021692634
C	0.253816852	11.045589401	17.828032411
C	2.760718231	11.283455040	17.746879617
C	3.080837695	10.272506299	18.635400920
H	2.289737424	9.642654591	19.059500141
C	4.430545757	10.052783521	19.010190940
H	4.645259257	9.249809133	19.715718938
C	5.450511763	10.827295842	18.506188417
H	6.491282372	10.670397065	18.794815487
C	5.158942795	11.873370450	17.588861985
C	3.818649318	12.105715919	17.189447219
C	4.434209568	13.877348031	15.799622957
C	5.808463775	13.766041274	16.157006569
H	6.524311863	14.471925739	15.739626170
C	6.159922669	12.758390490	17.034527186
C	8.466429759	13.487977424	17.255142046

H	8.463957793	13.829038688	16.206956971
H	9.368603883	12.878109773	17.449471809
C	8.269117584	14.622304926	18.254313513
H	7.181154468	14.836961529	18.352946457
H	8.717691494	15.552733658	17.852409281
C	8.860629696	14.325380566	19.637721578
H	9.953744416	14.171201204	19.548765982
H	8.742455522	15.219839654	20.280855488
C	8.236919502	13.103699009	20.327099347
H	8.877787464	12.799053288	21.176244556
H	8.228031268	12.241817359	19.627976231
C	6.811192567	13.364347806	20.821158336
H	6.124717678	13.533237193	19.960399732
H	6.776653570	14.308531687	21.410959397
C	6.269252491	12.215150231	21.665309703
H	6.260285112	11.273651287	21.107193256
H	5.223261220	12.423661580	21.947753641
H	6.844079344	12.064223308	22.581969501
C	4.052871616	14.948835385	14.814829725
C	2.404118187	15.603522830	13.198016123
H	2.933469575	15.415510986	12.260318326
H	2.566082578	16.632031378	13.540450459
H	1.338294601	15.352313750	13.123995762
C	3.752304899	20.457453428	14.927305386
H	4.437346241	21.284168852	15.203901288
H	2.703882942	20.790442386	15.002709992
C	4.086904346	19.853975741	13.565555379
H	4.275992196	20.680489610	12.850290257
H	3.209605772	19.305089153	13.167019539
C	5.284313400	18.896256979	13.585062955
H	5.034631110	18.006077110	14.209313580
H	5.449838515	18.498218282	12.565993385
C	6.574565406	19.530831941	14.116524299
H	6.395134826	19.948102894	15.127830953
H	6.870040555	20.383523609	13.477814508
C	7.726009401	18.515224957	14.183470589
H	7.835457675	18.006003012	13.205742172
H	8.678178633	19.056224096	14.347297900
C	7.529022638	17.474956017	15.284787097
H	6.564300966	16.951004768	15.164058577
H	7.515937697	17.936809849	16.277085314
H	8.320066913	16.721546823	15.270541440
C	6.221702961	15.376654147	23.621636911
H	6.206421947	16.423790392	23.960678729

H	6.389488335	15.313847890	22.522523283
C	7.170107656	14.469297361	24.396458281
H	6.634370653	13.521057038	24.635069073
H	8.016331888	14.170751719	23.745284394
C	7.691102683	15.107520351	25.687803961
H	6.841292219	15.344932447	26.358764604
H	8.180799681	16.075226099	25.465205195
C	8.678508408	14.175023238	26.401785966
H	8.185649849	13.213107690	26.643135650
H	9.517950752	13.921884457	25.725395907
C	9.224722507	14.812839038	27.686431690
H	8.391533633	15.025703700	28.384951389
H	9.682606561	15.794907285	27.456582500
C	1.220821951	9.416033125	22.892688488
H	1.790729975	10.118285572	23.524192021
H	1.813570646	9.105212349	22.015941154
C	0.633548194	8.241958799	23.669280426
H	0.048321009	7.595599396	22.983256569
H	-0.101064717	8.616051466	24.412432162
C	1.739792526	7.437816468	24.359176610
H	2.488284134	7.101989268	23.614094324
H	2.289493947	8.082863843	25.072776879
C	1.162804893	6.222338913	25.096387236
H	0.638457073	5.558887694	24.380958970
H	0.391727978	6.548215442	25.821390301
C	2.262694434	5.437368490	25.824609214
H	3.039872792	5.118953782	25.102019656
H	2.775400963	6.096938063	26.552957889
C	1.702002245	4.214927091	26.546569001
H	1.229949361	3.513892456	25.848740068
H	0.946114170	4.493714875	27.289787233
H	2.493250017	3.668924832	27.072967167
C	-0.972875475	12.955872768	20.405459316
O	-18.172051446	13.723899166	24.088549991
O	-10.622908564	14.509920343	23.848813511
O	-12.267493540	18.718444056	21.017728534
O	-18.347106236	20.250922487	16.577468449
O	-19.689051622	15.630242836	18.937291761
O	-15.677879354	10.050233357	22.372650421
O	-11.866335624	13.321669529	20.706612375
O	-11.243527329	19.449843153	16.151001131
O	-16.181348829	17.888593458	15.153130421
O	-20.678865429	12.066649332	17.152385952
O	-15.913702871	10.268288715	18.523938401

O	-13.084754709	14.696526929	14.178444784
O	-11.148685645	15.837053290	14.414186611
O	-8.612260592	12.401099161	17.490385160
N	-22.166980215	17.959183694	21.379033246
N	-16.594637826	14.975820884	22.985009350
H	-16.424446006	15.756032350	22.328591078
N	-14.152308585	16.062441583	22.297932325
N	-14.163399750	17.730955310	20.141297231
H	-14.798156844	16.909774634	20.229868195
N	-16.649415530	17.396692040	19.065467939
N	-17.537129679	14.900878675	19.325708150
H	-16.529049540	15.154776771	19.224091410
N	-15.336028026	13.501540523	20.098242646
N	-13.047398015	14.513956604	19.120544778
H	-13.973383151	14.602745283	18.648632634
N	-13.752096060	16.283394103	17.127184875
N	-16.027143429	15.662739840	15.738548071
H	-15.385609014	14.937159704	16.127234434
N	-16.703100233	13.168412458	16.665885690
N	-14.590630425	11.598419460	17.172575840
H	-14.613984821	12.389398774	16.487820146
N	-12.510561288	13.073803449	16.194145728
C	-22.303553771	18.281136367	19.977815601
C	-21.969445909	17.347791424	18.982223183
H	-21.572369247	16.360987664	19.251094430
C	-22.136817058	17.688285262	17.640284573
H	-21.884878336	16.956857044	16.871864751
C	-22.639628961	18.944166776	17.283916027
H	-22.794361184	19.193799053	16.237481468
C	-22.956275084	19.874632554	18.279909128
H	-23.341546805	20.855655079	18.003766906
C	-22.789203395	19.555304607	19.627741591
H	-23.035061791	20.279064973	20.404633176
C	-23.336785140	18.047443696	22.215324906
C	-24.632345346	17.971007304	21.672262546
H	-24.779387907	17.803823801	20.606284231
C	-25.736262311	18.107143623	22.515462156
H	-26.741402442	18.050827137	22.097839147
C	-25.563084839	18.304445247	23.888459037
H	-26.427304056	18.404710841	24.539884780
C	-24.271640006	18.374002019	24.423328082
H	-24.134736014	18.527688979	25.493404471
C	-23.154994896	18.249908435	23.598528699
H	-22.150566864	18.313956733	24.015908702

C	-21.097381936	17.091670173	21.797193749
C	-19.768743756	17.467518951	21.519854698
H	-19.563939498	18.365644623	20.936053752
C	-18.721052611	16.689225592	22.005990766
H	-17.692134705	17.000372830	21.796821425
C	-18.977790967	15.529195070	22.753219709
C	-20.308999127	15.147899199	22.999995342
H	-20.500745462	14.233484387	23.572642217
C	-21.366354444	15.918756461	22.530813453
H	-22.393911188	15.615516998	22.729970755
C	-17.919603062	14.654936220	23.339094221
C	-15.422090266	14.352717616	23.494195741
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C	-12.950593172	14.391766804	23.637951241
C	-12.999520811	13.226417147	24.450780930
H	-12.059028129	12.810950212	24.813922474
C	-14.214662133	12.661387159	24.760422354
H	-14.268243808	11.767293877	25.383046609
C	-15.429752833	13.218574681	24.287974497
H	-16.380773351	12.743619180	24.564328344
C	-11.718291509	15.052213957	23.261976987
C	-11.726038412	16.137460119	22.399856521
H	-10.820295447	16.633310111	22.057053914
C	-12.984452413	16.603403469	21.944814998
C	-13.069584022	17.802100895	21.009454373
C	-14.635717926	18.749986795	19.269731300
C	-13.914454619	19.870684014	18.906887568
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C	-14.476964635	20.819448774	18.011577203
H	-13.874476585	21.687797736	17.744433715
C	-15.743951748	20.664511694	17.497651213
H	-16.180169188	21.388336587	16.808212087
C	-16.520044991	19.526460018	17.854448331
C	-15.968981190	18.555759297	18.726451386
C	-17.857679570	19.261032382	17.366536035
C	-18.531675870	18.098063456	17.712561390
H	-19.539854984	17.862814198	17.376592423
C	-17.860796341	17.175558219	18.548212766
C	-18.491706719	15.845632822	18.942316298
C	-19.681309525	20.054849714	15.989316207
H	-20.414117619	20.205858058	16.802099799
H	-19.750909983	19.033171830	15.578433098
C	-19.738705442	21.126710635	14.908679450
H	-18.948843898	20.939365508	14.151939901

H	-19.489658185	22.116384427	15.343756486
C	-21.123552990	21.157204655	14.253213323
H	-21.396504844	20.139994262	13.907604491
H	-21.890335542	21.437366880	15.002384075
C	-21.181608292	22.119973830	13.059767449
H	-20.338598685	21.919763316	12.369793490
H	-22.099186776	21.915371291	12.473519254
C	-21.167925985	23.593334391	13.489054073
H	-22.021718186	23.796435096	14.164948455
H	-20.256958640	23.804645717	14.083468053
C	-21.226717383	24.531853071	12.286319147
H	-20.370301607	24.387925854	11.617446135
H	-21.222392504	25.581028494	12.602846986
H	-22.135088301	24.375067983	11.693581558
C	-17.765902612	13.681248086	20.016575824
C	-19.009811655	13.175804863	20.337710425
H	-19.916596068	13.705731149	20.023893503
C	-19.114882577	11.983673393	21.102609217
H	-20.111714274	11.627980038	21.364894057
C	-17.998645791	11.305792121	21.534686348
H	-18.073130791	10.398432758	22.137055695
C	-16.701296275	11.793388753	21.210713405
C	-15.465882553	11.164450012	21.627304355
C	-14.232254168	11.697490443	21.286162627
H	-13.281819443	11.270079277	21.594473647
C	-14.227813231	12.883500619	20.509388785
C	-3.960121354	14.374600113	26.838352726
H	-4.106057785	13.414494172	27.342418984
H	-3.286169605	14.977365169	27.454741837
H	-3.433131373	14.161149461	25.893405815
C	-12.916595318	13.564574473	20.139873859
C	-12.087180038	15.486377857	18.732838935
C	-10.834068980	15.610174954	19.302192789
H	-10.504559749	14.885942537	20.060083185
C	-9.976072101	16.677075569	18.929811804
H	-8.999360287	16.753745795	19.414976873
C	-10.355641710	17.601680717	17.986075118
H	-9.704249297	18.430223602	17.696623647
C	-11.629707887	17.494998679	17.363895513
C	-12.502514934	16.435786435	17.714803373
C	-14.142837886	17.164062501	16.205554709
C	-13.360097095	18.272196756	15.787066681
H	-13.770622484	18.965430547	15.058189036
C	-12.116869642	18.432436283	16.374142314

C	-15.542859244	16.972268054	15.642105426
C	-17.399155766	15.284044829	15.678670800
C	-18.409480457	16.084046532	15.181389324
H	-18.171441473	17.059431302	14.741408245
C	-19.764948998	15.666063842	15.270962170
H	-20.532151059	16.328536110	14.870171281
C	-20.111231297	14.471717270	15.857202578
H	-21.151251457	14.160334235	15.967947711
C	-19.095955089	13.603395182	16.350391421
C	-17.735835579	13.984004701	16.234116605
C	-16.994714000	11.997271170	17.235325059
C	-18.316873135	11.537611881	17.450003616
H	-18.465043437	10.592176599	17.969723849
C	-19.356141105	12.346293793	17.015704254
C	-21.047594656	10.920855135	18.001653782
H	-20.837828338	11.223872968	19.043034841
H	-20.433775760	10.046845337	17.724651872
C	-22.531917571	10.734459024	17.718378985
H	-23.001900925	11.729843657	17.560124446
H	-23.025805952	10.308865172	18.614312532
C	-22.776209226	9.840557644	16.497130613
H	-22.221270039	8.887585487	16.605449439
H	-22.360790639	10.329936106	15.593232645
C	-24.268126378	9.547044440	16.298331534
H	-24.685162261	9.067385548	17.204908756
H	-24.824612189	10.496867010	16.174564526
C	-24.522255559	8.649795806	15.078494154
H	-25.606645390	8.649379220	14.849250972
H	-24.028147344	9.082131085	14.185937033
C	-24.047424623	7.212840152	15.283935566
H	-24.262875662	6.595617236	14.404672616
H	-24.538073709	6.743567421	16.144078331
H	-22.966237282	7.165678451	15.459703009
C	-15.805860248	11.179759082	17.724665459
C	-13.292027872	11.272082933	17.644059510
C	-13.019088581	10.275871838	18.563555922
H	-13.832008790	9.650854119	18.950499017
C	-11.694151603	10.080894306	19.030779880
H	-11.517665518	9.300891202	19.771184102
C	-10.653345084	10.858055439	18.576435366
H	-9.636367937	10.736566467	18.955080163
C	-10.891878097	11.869675480	17.606117998
C	-12.207629065	12.089225224	17.130237666
C	-11.526638114	13.848997478	15.753816915

C	-10.171438002	13.737060684	16.173274796
H	-9.434608498	14.439990229	15.788539796
C	-9.861409344	12.733771718	17.071679088
C	-7.497359375	13.299447694	17.168341522
H	-7.583045208	13.627772196	16.119945762
H	-6.641133780	12.594286049	17.277867505
C	-7.467555058	14.450107453	18.160999715
H	-8.510827083	14.769034322	18.370765698
H	-6.967084538	15.326673648	17.698496758
C	-6.754231714	14.113923508	19.473453462
H	-5.660980875	13.973759762	19.274628408
H	-6.800288820	14.996736238	20.143460681
C	-7.299578032	12.878957487	20.197487067
H	-6.618488461	12.615564189	21.028772575
H	-7.292315950	12.005933167	19.505322811
C	-8.718193576	13.089316875	20.735215588
H	-9.431727412	13.203798556	19.889101259
H	-8.773319011	14.047292002	21.301797901
C	-9.186295113	11.943227958	21.626686779
H	-9.114946645	10.978052575	21.117097026
H	-10.245988827	12.095860983	21.893658579
H	-8.611420653	11.879932574	22.554546646
C	-11.858472380	14.908469862	14.737193240
C	-13.520303183	15.663026623	13.180800059
H	-13.012353979	15.442191160	12.238674067
H	-13.306587180	16.685067509	13.514336225
H	-14.597765470	15.463643391	13.121804341
C	-11.525073633	20.436406998	15.112913086
H	-10.730389659	21.170571057	15.354659917
H	-12.518670592	20.876859278	15.300810593
C	-11.388650955	19.873938707	13.700150998
H	-11.159318312	20.710621566	13.008981855
H	-12.361249719	19.462419051	13.359530927
C	-10.327986317	18.775598385	13.563234623
H	-10.635689365	17.885751217	14.161735296
H	-10.301046789	18.425864294	12.513565608
C	-8.928532876	19.216667169	14.004759977
H	-8.945788254	19.485585446	15.083547665
H	-8.629907047	20.133047628	13.462533699
C	-7.879012529	18.118126390	13.774830283
H	-7.886031326	17.806505083	12.711684797
H	-6.866524780	18.548451258	13.955073498
C	-8.096130081	16.896680142	14.663158163
H	-9.044081118	16.391310549	14.407984062

H	-8.184598276	17.168794786	15.721653875
H	-7.290730596	16.167187959	14.554912361
C	-9.310545162	15.113886795	23.561405209
H	-9.340049221	16.169056189	23.884163836
H	-9.139444550	15.038076896	22.464806696
C	-8.361034090	14.234113190	24.366166927
H	-8.959004410	13.498597442	24.951072485
H	-7.746433836	13.617751687	23.679059920
C	-7.466277750	15.047566889	25.307044741
H	-8.044992875	15.365759266	26.195148522
H	-7.140017384	15.987204658	24.814757013
C	-6.235466838	14.241788001	25.738176313
H	-6.540788369	13.340020688	26.300686633
H	-5.690344739	13.870481709	24.841374288
C	-5.281750305	15.093967238	26.588428350
H	-5.761661333	15.351183068	27.550989842
H	-5.084323370	16.058354748	26.079244987
C	-14.514098448	9.311217187	22.876457766
H	-13.932048232	9.983775021	23.528842904
H	-13.910686647	8.980698992	22.015346817
C	-15.185490694	8.163471563	23.624435373
H	-15.770863552	7.547557664	22.910766183
H	-15.936836896	8.575912325	24.330847546
C	-14.160987683	7.302835791	24.368272014
H	-13.406862934	6.906641547	23.660187934
H	-13.602107055	7.921528343	25.097575087
C	-14.854576095	6.142069614	25.093927555
H	-15.386055953	5.502531319	24.362413184
H	-15.637511917	6.532832713	25.773282598
C	-13.853050161	5.296594144	25.891824952
H	-13.065068977	4.907050037	25.217791389
H	-13.331917859	5.932094628	26.634818666
C	-14.540779252	4.134219564	26.603957653
H	-15.026147739	3.454806305	25.894108223
H	-15.312713729	4.483949104	27.299264444
H	-13.822556881	3.543076161	27.183092653
C	-16.571788498	12.974049389	20.442799648

Table S15. Atomic coordinates for the optimized structure of **Q₆(*t*-Bu)** in MOPAC2016 (Fig. S3a(i), gas phase).

Atom	X	Y	Z
O	10.894521214	17.249141780	15.800336297
O	10.228041373	15.759896882	14.389081752
O	16.660166270	13.947074695	14.481447079

O	15.569750440	18.176745208	11.541454128
O	11.410710154	24.587072445	12.626614416
O	9.715367586	21.320960103	16.519452402
O	12.791610789	15.321303488	20.163582256
O	16.509861606	16.521728323	16.522606560
O	17.623461469	22.566776315	11.893325630
O	13.839371800	24.329728838	15.129319432
O	10.497994793	21.737504645	21.568272859
O	14.639331515	18.491809141	21.039695175
O	21.147422631	18.236302932	16.969972425
O	19.227180652	22.929174361	15.531570558
O	17.722483345	23.201178022	17.201980455
N	13.553583333	16.677081346	13.997201127
N	11.020581257	16.202629393	15.212655919
N	14.102143912	19.201275132	13.019204552
H	13.492683254	19.023776719	13.849813643
N	12.342941386	20.879093419	14.236477133
N	11.720509690	20.194385922	16.770549746
H	12.635291979	20.007274139	16.301655033
N	13.583317515	18.282761680	17.376268744
N	15.929740028	18.739998152	16.224778487
H	15.242025266	19.477683539	16.512111381
N	15.644745502	21.291299705	15.306578537
N	14.135663459	22.857751671	16.884268423
H	14.714608692	22.048309182	17.206922124
N	13.839594420	21.356216689	19.139915410
N	15.962182620	19.795819976	19.660340092
H	15.982573318	20.680839963	19.101192517
N	17.923081892	20.683572814	17.963445320
C	12.196953123	15.344025157	15.518701131
C	12.082883080	14.329009918	16.444187782
H	11.152384634	14.176695528	16.997618146
C	13.182843709	13.465555202	16.689486543
H	13.069281124	12.680522822	17.438569831
C	14.361308185	13.617216180	15.993908663
H	15.215752095	12.953327212	16.159143893
C	14.502707522	14.662628294	15.041477239
C	15.720612193	14.904500209	14.301033771
C	15.834735235	16.012231387	13.473356893
H	16.735846370	16.250932603	12.909770800
C	14.724565185	16.882552233	13.380800797
C	13.430397037	15.573630701	14.822393153
C	18.001797611	14.186319219	13.926090282
H	18.480402031	14.942754782	14.572523660

H	17.917254350	14.555973028	12.892024937
C	18.660032481	12.799345424	14.019128927
H	18.503896165	12.414776240	15.060098262
C	18.000028070	11.827149801	13.039059389
H	16.918062535	11.771062950	13.222392199
H	18.405823200	10.815900385	13.144795135
H	18.143719666	12.130542687	11.996180504
C	20.160232397	12.941300295	13.756355189
H	20.368996033	13.340107883	12.757240725
H	20.662233037	11.968354189	13.819130993
H	20.644615034	13.599371831	14.486870197
C	14.851194273	18.143914649	12.523451386
C	13.884028517	20.463753925	12.394965118
C	14.485752497	20.885903275	11.226637448
H	15.199206602	20.237483768	10.702568931
C	14.160818039	22.156706954	10.680727748
H	14.619639298	22.444524534	9.730167964
C	13.275941926	23.003206704	11.308717572
H	13.031950942	23.985539472	10.895636156
C	12.637763067	22.600008068	12.513510953
C	11.648232922	23.388806334	13.216716346
C	11.028147409	22.912471549	14.363224944
H	10.244174537	23.451608477	14.888325624
C	11.430359369	21.642315794	14.840086692
C	12.935644745	21.331864530	13.066793557
C	10.319124103	25.410943301	13.164754205
H	10.481583698	25.566837416	14.241777817
H	9.375814063	24.861980155	12.978792655
C	10.452469197	26.699898250	12.337130429
H	10.623942833	26.401962329	11.268992391
C	11.662439427	27.510710072	12.803978582
H	11.533077435	27.908336023	13.815065196
H	11.859434260	28.356324048	12.139381014
H	12.565085827	26.879109571	12.813510274
C	9.152903931	27.502503739	12.430938170
H	8.290396366	26.910322486	12.106584592
H	9.199638818	28.391036066	11.791064661
H	8.959383858	27.845522984	13.453187408
C	10.826408912	21.055877546	16.109560196
C	11.414845633	19.302975388	17.827814430
C	10.265063091	19.351737824	18.594078504
H	9.509960852	20.123800676	18.400637745
C	10.049262114	18.391102093	19.616057083
H	9.133270354	18.469645483	20.203038431

C	10.950132679	17.380846678	19.863795501
H	10.780928678	16.632425229	20.637520620
C	12.146137329	17.296966344	19.097001227
C	13.152028605	16.271101939	19.257468452
C	14.328230321	16.283532332	18.523094673
H	15.115811364	15.544185798	18.631095379
C	14.500272893	17.340095396	17.594102101
C	12.405370397	18.273128671	18.103509257
C	13.672030089	14.164772926	20.340253013
H	14.481118615	14.482140893	21.019450463
H	14.085619789	13.850276721	19.369144789
C	12.738423463	13.109870823	20.961204374
H	12.271841170	13.560858010	21.874696775
C	11.619526917	12.733498988	19.986574373
H	11.088168851	13.634468764	19.647695921
H	10.883022563	12.077216106	20.461647531
H	11.999006715	12.216234757	19.099305993
C	13.566379402	11.890053356	21.368806285
H	14.034815449	11.402529593	20.507085589
H	12.937827434	11.136906909	21.858639473
H	14.360498173	12.151881899	22.076749526
C	15.757458131	17.457662755	16.743709103
C	16.806034651	19.149287245	15.184777872
C	17.801715133	18.367291466	14.635896704
H	18.006860211	17.374718093	15.047613654
C	18.541113937	18.843725804	13.519683736
H	19.308049222	18.195304161	13.098465937
C	18.290882759	20.076558303	12.963714792
H	18.827397928	20.433041672	12.081745052
C	17.298904379	20.925431356	13.532056859
C	16.574769729	20.486814451	14.663846932
C	16.957521605	22.238606573	13.024452452
C	16.031824461	23.040491400	13.675348525
H	15.733388067	24.024092020	13.315582598
C	15.409518318	22.516431857	14.833984060
C	17.259751467	23.827438211	11.224205906
H	17.225819855	24.641826794	11.963666542
H	16.265581614	23.675814959	10.764891519
C	18.388427606	23.990085525	10.195513145
H	18.554041779	22.993844280	9.706630305
C	19.684165716	24.409647801	10.893988436
H	19.610653649	25.410036608	11.332107366
H	20.528950479	24.417363001	10.199657724
H	19.925641623	23.711957988	11.709288675

C	17.947060328	24.999894542	9.134999995
H	17.021556372	24.683022364	8.634260782
H	18.714767231	25.120011218	8.363560296
H	17.761108801	25.990078048	9.565413366
C	14.381984911	23.343707650	15.595925211
C	13.014828617	23.145810534	17.707313863
C	12.059289166	24.107615962	17.436868397
H	12.160876753	24.748980139	16.554018424
C	10.925455499	24.242633509	18.281912781
H	10.181697600	24.998343049	18.025201742
C	10.746130192	23.437395113	19.382629462
H	9.865793193	23.521685226	20.021055709
C	11.720303707	22.452204581	19.707521165
C	11.616570222	21.537851335	20.822966241
C	12.589950373	20.581342169	21.067290094
H	12.538380673	19.856446168	21.875134503
C	13.697959481	20.539488362	20.182583175
C	12.861442592	22.305101695	18.882236239
C	10.245329555	20.823221326	22.688542319
H	11.084194298	20.906100879	23.398819517
H	10.171374250	19.796680357	22.294316098
C	8.922081922	21.365556788	23.255944865
H	8.973836261	22.486604645	23.218902197
C	7.740100747	20.911996953	22.397979357
H	7.908291825	21.162585980	21.340594036
H	6.811856684	21.404676759	22.706318141
H	7.571374852	19.832342417	22.460098993
C	8.772755124	20.922831459	24.712590930
H	8.751654197	19.831908649	24.809104818
H	7.837935230	21.302035534	25.142599388
H	9.592054560	21.296124119	25.337284601
C	14.788395184	19.492920028	20.360064672
C	17.057214634	18.925118157	19.420327426
C	17.182131535	17.660928136	19.968218030
H	16.423524396	17.288024186	20.666195081
C	18.279678457	16.835605216	19.617451325
H	18.337523956	15.840319261	20.057601550
C	19.245499579	17.263283578	18.733712322
H	20.083618032	16.628265293	18.447067154
C	19.158306798	18.562388543	18.165007583
C	20.122498804	19.096243402	17.226315342
C	19.965418446	20.355555960	16.682497954
H	20.640479461	20.784590839	15.945652255
C	18.830727412	21.114134802	17.097223214

C	18.071577975	19.407842504	18.500578633
C	18.646001110	22.484910174	16.498662454
C	17.422779268	24.539908213	16.717143835
H	17.311355553	24.538106108	15.626802068
H	18.225588974	25.212154238	17.031517269
H	16.475609219	24.762119119	17.224681499
C	22.271702804	18.733768720	16.167451213
H	22.569636774	19.730219642	16.530806848
H	21.929063932	18.786426425	15.120999580
C	23.358983120	17.668989613	16.396565019
H	22.897863127	16.662718239	16.222293385
C	24.489406058	17.886940596	15.388349888
H	24.134814883	17.826305140	14.353976466
H	25.272754181	17.128730586	15.508338487
H	24.970541888	18.863672455	15.517228905
C	23.870397129	17.721712192	17.837943714
H	24.394830285	18.657544401	18.058530219
H	24.562290006	16.899856602	18.048058315
H	23.034234435	17.640428479	18.546890858
O	13.490752540	23.637939649	7.596304925
O	14.151732136	25.127475141	9.007647717
O	7.721204069	26.939935123	8.910422339
O	8.812914282	22.712247077	11.856421144
O	12.971570875	16.301978503	10.771689330
O	14.665687216	19.568565548	6.877974481
O	11.588551276	25.571187629	3.239673213
O	7.870208339	24.364427598	6.873729694
O	6.762340995	18.324469367	11.509148149
O	10.540518929	16.560093302	8.266830151
O	13.883517685	19.153803424	1.831699865
O	9.740755187	22.399325521	2.360961959
O	3.229375009	22.648185083	6.423867816
O	5.162001896	17.960740891	7.869083605
O	6.651660985	17.682828140	6.187333638
N	10.827572996	24.210632203	9.398803453
N	13.363860608	24.686602839	8.186873488
N	10.277530458	21.686680121	10.375515282
H	10.886542105	21.863089064	9.543986337
N	12.037443069	20.007859382	9.158736674
N	12.659823067	20.693235640	6.624869807
H	11.743917727	20.878078922	7.092556996
N	10.795984553	22.603472136	6.020634704
N	8.448397636	22.145603611	7.172240228
H	9.134944884	21.407611355	6.882933888

N	8.733686815	19.595382380	8.089942494
N	10.240610037	18.027826029	6.509885647
H	9.660390295	18.836126915	6.187820687
N	10.538739100	19.532515543	4.256392630
N	8.416727186	21.092891768	3.736053167
H	8.396140874	20.206473861	4.293540244
N	6.456520919	20.203572639	5.432561718
C	12.185998796	25.543362114	7.878212179
C	12.300442334	26.557951283	6.952263620
H	13.231353697	26.710302284	6.399112362
C	11.200829430	27.421518638	6.705819614
H	11.314977623	28.206387810	5.956504176
C	10.021573870	27.269749595	7.400507756
H	9.167428319	27.933405109	7.233986663
C	9.878745005	26.224286267	8.352474523
C	8.660562490	25.982463095	9.089724545
C	8.544730530	24.873025422	9.917381147
H	7.642484860	24.634100015	10.477399099
C	9.655640091	24.004196597	10.012904540
C	10.952075760	25.313017972	8.572631119
C	6.376383945	26.695213632	9.455824637
H	5.905148591	25.938363306	8.804948459
H	6.455367986	26.324158095	10.489702030
C	5.713912909	28.079620780	9.360438615
H	5.875018326	28.466789621	8.321171336
C	6.363215528	29.053086310	10.346553522
H	7.445483600	29.117025789	10.167591232
H	5.950769166	30.061933512	10.242748364
H	6.217473503	28.744830247	11.387718967
C	4.212178698	27.931852865	9.612965361
H	3.998318021	27.528675556	10.609286721
H	3.707030694	28.902840926	9.549884817
H	3.735237879	27.274309737	8.877198639
C	9.531010901	22.743775999	10.870410171
C	10.496982137	20.423588460	10.999947620
C	9.894711885	20.001954795	12.168920820
H	9.181219416	20.650218275	12.692548922
C	10.220241528	18.731267895	12.714786921
H	9.761200603	18.443738477	13.665567033
C	11.103974884	17.884624691	12.087391780
H	11.348325140	16.902139119	12.500000953
C	11.742679618	18.287191025	10.881493142
C	12.732173102	17.499012545	10.179233760
C	13.351855127	17.974493159	9.031903276

H	14.135116843	17.434778928	8.506713946
C	12.949329174	19.244555687	8.555000875
C	11.444283151	19.555550869	10.328481472
C	14.060108801	15.475526510	10.231780231
H	13.900120056	15.325734478	9.153725832
H	15.005529407	16.019603778	10.423003921
C	13.919015444	14.182878754	11.052100642
H	13.750326061	14.475345145	12.122036034
C	12.703466620	13.383004713	10.580803967
H	12.827557693	12.995350035	9.565052852
H	12.504192945	12.531278719	11.236884753
H	11.803681115	14.018885511	10.580990866
C	15.213209693	13.372290812	10.952674768
H	16.078810380	13.954254888	11.287433608
H	15.157827365	12.475682517	11.580318142
H	15.407597372	13.040843060	9.926918978
C	13.554502238	19.831595065	7.286020317
C	12.965266814	21.585758441	5.568825576
C	14.116063896	21.538944359	4.802914611
H	14.870917961	20.766651658	4.996190772
C	14.331639973	22.500414106	3.782584429
H	15.247985794	22.423703219	3.195757706
C	13.429714327	23.510469062	3.535628080
H	13.599146923	24.259467517	2.762485850
C	12.233657161	23.591717358	4.301523239
C	11.225986148	24.618683914	4.142801604
C	10.050615133	24.603354399	4.874698018
H	9.261563406	25.341985931	4.767706972
C	9.878284720	23.545839029	5.802625465
C	11.974716913	22.615586684	5.293078695
C	10.700731182	26.721615264	3.057449181
H	9.889156791	26.394552472	2.386195240
H	10.291852338	27.042480856	4.028395660
C	11.625785667	27.774877496	2.421091420
H	12.090176831	27.317274424	1.509927173
C	12.747320892	28.166872115	3.386635499
H	13.281465599	27.271506530	3.736241788
H	13.481084496	28.817802373	2.899868218
H	12.370015291	28.695886116	4.267761228
C	10.789298099	28.986070768	2.005324987
H	10.322484329	29.480070080	2.864120131
H	11.411546152	29.737287366	1.504516710
H	9.993361130	28.712865500	1.303894908
C	8.620319284	23.428446441	6.652149543

C	7.572102430	21.736780614	8.211296378
C	6.576633517	22.519176051	8.761214493
H	6.370554188	23.511002182	8.348135126
C	5.839036514	22.043119490	9.878449109
H	5.071837625	22.691549212	10.299939734
C	6.091022885	20.811637481	10.435581561
H	5.556275447	20.455871722	11.318898061
C	7.082449477	19.961972590	9.866484429
C	7.803823843	20.399214199	8.732719613
C	7.425179620	18.649722924	10.375057954
C	8.347626131	17.846291350	9.721460047
H	8.646954187	16.863207623	10.082891414
C	8.968203844	18.369422672	8.562786845
C	7.116948537	17.059927132	12.175728261
H	7.167038388	16.249814986	11.432423506
H	8.102335061	17.212286303	12.652678422
C	5.970461729	16.888210459	13.182792667
H	5.796737628	17.880358761	13.677718580
C	4.686769644	16.475866906	12.457603555
H	4.764835543	15.475618916	12.019266105
H	3.828356589	16.471087026	13.135271728
H	4.464806487	17.176174475	11.638598004
C	6.392223720	15.868296678	14.241240688
H	7.306017178	16.182131209	14.764121426
H	5.609092476	15.738883227	14.995523560
H	6.589509795	14.882972730	13.804677197
C	9.996765894	17.541212211	7.800474669
C	11.363243036	17.741838238	5.688627511
C	12.318373064	16.780839759	5.958818160
H	12.216616273	16.138391018	6.841330269
C	13.453093789	16.646338510	5.114881030
H	14.196407731	15.890479023	5.371058494
C	13.632652736	17.452332496	4.013735783
H	14.513332031	17.368738879	3.376218313
C	12.658350789	18.437287703	3.690061555
C	12.762864012	19.352909404	2.574314237
C	11.789867274	20.307804305	2.329531602
H	11.841446518	21.032919404	1.521489679
C	10.680785851	20.349558721	3.213386387
C	11.516637922	18.583670916	4.513459188
C	14.133172811	20.062694474	0.706267210
H	13.287782700	19.985823204	0.003430472
H	14.219274784	21.089131086	1.097799339
C	15.446488986	19.507417795	0.127995080

H	15.386129792	18.387018065	0.171493886
C	16.640590805	19.955431873	0.972109972
H	16.480681082	19.712164694	2.032343096
H	17.561144270	19.452957757	0.657450682
H	16.818209322	21.032937647	0.902099933
C	15.584885892	19.941362200	-1.332315851
H	15.617265874	21.031717385	-1.434160968
H	16.510603387	19.549169433	-1.770640873
H	14.754317801	19.574544870	-1.946091473
C	9.591270444	21.397028750	3.036448400
C	7.321894326	21.962067132	3.975930255
C	7.196632223	23.227332893	3.428610074
H	7.955462711	23.600997006	2.731658389
C	6.097282704	24.051463292	3.779533312
H	6.039974563	25.046827301	3.338925701
C	5.131799434	23.623202389	4.660590169
H	4.292251958	24.256639840	4.947190597
C	5.219339300	22.323015520	5.229914267
C	4.254761006	21.788312027	6.167282322
C	4.411768386	20.528939381	6.709770163
H	3.735546692	20.098861273	7.445439927
C	5.547269985	19.771818319	6.296962772
C	6.306249065	21.478772724	4.894854645
C	5.734343227	18.401058879	6.897656405
C	6.955098616	16.345311939	6.672707812
H	7.081472848	16.350358396	7.761635993
H	6.146725568	15.673919146	6.371700440
H	7.894416727	16.119323980	6.152401267
C	2.103430641	22.148456832	7.222684938
H	1.812801833	21.148151815	6.863721662
H	2.441375897	22.103651300	8.271055927
C	1.010932638	23.205347721	6.982356530
H	1.464871527	24.215274675	7.154095280
C	-0.123598210	22.985560073	7.985722253
H	0.225035168	23.055566567	9.021608822
H	-0.911723552	23.737244130	7.856645600
H	-0.596897580	22.004722436	7.860674974
C	0.507547236	23.142154147	5.538679772
H	-0.006511970	22.200427326	5.319050336
H	-0.191575300	23.956172364	5.321929205
H	1.346242540	23.229022695	4.833433362

Table S16. Atomic coordinates for the optimized structure of **Q₆(*i*-Bu)** in MOPAC2016 (Fig. S3a(ii), gas phase).

Atom	X	Y	Z
O	-0.917858433	14.177021367	3.998487878
O	-0.964539707	15.144328528	2.067404727
O	5.329673366	16.790421640	2.705434558
O	4.139454976	12.470571196	-0.090474788
O	-0.451530914	6.388220995	1.095486029
O	-2.161954214	9.979535041	4.705461415
O	1.193645492	15.987541489	8.153417987
O	4.981463202	14.274312993	4.816284097
O	5.924532941	7.978342317	0.517923153
O	2.032241313	6.443801266	3.689548152
O	-1.834120706	9.095813074	9.786874224
O	2.294298117	12.495285773	9.339614857
O	8.964906944	12.373566597	5.589064938
O	7.091417881	7.653609220	4.360573032
O	5.455182052	7.451934337	5.907658473
N	2.094976580	14.222031557	2.171157149
N	-0.474302882	14.939121334	3.164136933
N	2.533410348	11.621565085	1.353007762
H	1.888318316	11.882121049	2.133451289
N	0.596566272	10.129843495	2.540007011
N	-0.118539027	11.040980038	4.954265786
H	0.827771821	11.138609967	4.522316501
N	1.868037286	12.816830226	5.569109319
N	4.230732389	12.102049430	4.575550999
H	3.469147217	11.438118407	4.848025268
N	3.824368613	9.523519270	3.749564817
N	1.906721712	8.242928945	5.128373932
H	2.374486703	9.137121016	5.399277566
N	1.522328703	9.673506693	7.418501597
N	3.695996397	11.030357691	8.221249534
H	3.725107791	10.115137467	7.712874522
N	5.715686273	9.997394263	6.670386560
C	0.735120882	15.731174668	3.515197893
C	0.632815840	16.794377064	4.387377929
H	-0.316602097	17.030282305	4.877345789
C	1.768743292	17.601995289	4.655793257
H	1.663397796	18.434970851	5.350987198
C	2.973697774	17.341070995	4.042193843
H	3.856950976	17.961451781	4.224048925
C	3.105751047	16.236854527	3.157356899
C	4.345210744	15.880854506	2.504211552
C	4.432484931	14.732901072	1.732973254
H	5.345443261	14.419008026	1.229042189

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H	6.692341889	16.081072370	1.256931268
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C	7.450405583	17.765856621	2.485986406
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H	7.510370778	19.741222924	1.564622963
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H	9.294637785	17.045987345	1.549313388
H	9.264467441	16.858430996	3.313292309
H	9.516043851	18.448604076	2.590245712
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C	2.921885237	9.806599882	-0.308679027
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H	1.279304108	6.790096250	-0.573256277
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C	-0.832131917	8.181772074	2.714717517
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C	-5.989553096	8.300642569	-6.833147827
C	-6.941085954	8.868535385	-5.903131934
C	-6.777058980	10.146390095	-5.407626528
H	-7.457303548	10.611803835	-4.696674453
C	-5.628699774	10.876163931	-5.835469225
C	-4.871059870	9.106957679	-7.160485702
C	-5.446243220	12.259536789	-5.263669892
C	-4.161114823	14.279647592	-5.400092586
H	-3.163258270	14.471326891	-5.813425216
H	-4.908782839	14.972878330	-5.792652656
H	-4.153616530	14.283758246	-4.303260415
C	-8.877929703	8.411879410	-4.518361158
H	-8.289908209	8.746016074	-3.646685590
H	-9.510338148	9.230452922	-4.896734136
C	-9.653659414	7.106888202	-4.267119925
H	-9.869469027	6.642756249	-5.266070805
C	-10.977541442	7.420505592	-3.568954450
H	-10.824046262	7.877547010	-2.584655962
H	-11.598732644	8.103651973	-4.159783243
H	-11.564921765	6.507700211	-3.412137010
C	-8.798485730	6.131451572	-3.455352391
H	-7.811974795	6.006455921	-3.926144844
H	-8.636602443	6.479973474	-2.429717303

H	-9.267815410	5.141666538	-3.399641062
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Table S17. Atomic coordinates for the optimized structure of **Q₆(*i*-Bu)** in MOPAC2016 (Fig. S3a(iii), gas phase).

Atom	X	Y	Z
O	-0.762883826	14.155813346	4.346295531
O	-0.899516973	15.017273205	2.368626541
O	5.427205788	16.687696139	2.643656488
O	4.161917688	12.303714268	0.027756068
O	-0.242575180	6.150592268	1.364734017
O	-2.017435783	9.696494850	4.987273321
O	1.248809095	15.885460661	8.259889807
O	5.013008360	14.236808808	4.905535009
O	6.371500579	7.978367372	0.665076458
O	2.323584950	6.352900941	3.652035282
O	-1.646591724	8.927262848	9.734450179
O	2.368543011	12.461210981	9.343164522
O	9.047446361	12.236975819	5.499087124
O	7.061570283	7.406619684	4.628395850
O	5.360080059	7.497201588	6.116551107
N	2.151793826	14.142130617	2.283240925
N	-0.362154835	14.862171927	3.443185650
N	2.437879185	11.566812442	1.382736354
H	1.765867929	11.859983925	2.126828565
N	0.586314033	10.009007255	2.648675058
N	-0.051727793	10.917644912	5.086266891
H	0.852987660	11.078486077	4.589458329
N	1.922178566	12.715101176	5.669168399
N	4.279142420	12.070709088	4.583055255
H	3.521916252	11.392191835	4.826959753
N	4.005261717	9.476974196	3.731072946
N	2.247313373	8.076188958	5.187919512
H	2.727055863	8.954971642	5.486939086
N	1.736902518	9.583077907	7.424301615
N	3.818514883	11.037397717	8.235503050
H	3.866271329	10.109363490	7.742211562
N	5.787764966	9.966017459	6.729931135
C	0.874155777	15.655896467	3.704370984
C	0.829259890	16.723762950	4.575755798
H	-0.088098630	16.962985307	5.122502544
C	1.980350952	17.531233159	4.770359506
H	1.918674074	18.369643499	5.464443033
C	3.147391954	17.262047367	4.091487536
H	4.042373870	17.879028697	4.219216881

C	3.223123219	16.153188716	3.205527701
C	4.423471405	15.790613105	2.488743174
C	4.467449911	14.635286422	1.723330276
H	5.346543523	14.319435006	1.163227676
C	3.303476418	13.831018792	1.677960910
C	2.090639639	15.305476318	3.031363966
C	6.754550765	16.342772824	2.110293443
H	6.659313504	16.067637445	1.048170578
H	7.132751616	15.493378369	2.704861380
C	7.547853090	17.641583992	2.334381848
H	7.288904832	18.023409613	3.357458541
C	7.147011389	18.700382576	1.304068792
H	6.060938831	18.862769421	1.315030076
H	7.425139770	18.411208378	0.284891732
H	7.624769896	19.663101622	1.514174834
C	9.046470408	17.341226273	2.277057637
H	9.342119836	16.905471392	1.315645361
H	9.358167817	16.648239737	3.068873118
H	9.634121670	18.260188070	2.402531877
C	3.354850583	12.506223775	0.916632636
C	2.242962748	10.249575032	0.881553319
C	2.952100847	9.692186211	-0.165024730
H	3.727991282	10.273105974	-0.678397760
C	2.677103504	8.362988239	-0.585212564
H	3.248846161	7.965134769	-1.423790277
C	1.715365375	7.596726303	0.030951451
H	1.499647765	6.575417357	-0.285388787
C	0.972137134	8.132939485	1.119675960
C	-0.032473895	7.396938037	1.860528444
C	-0.684933189	7.966746579	2.942790251
H	-1.461999775	7.457729934	3.507833269
C	-0.320423104	9.287226570	3.310855547
C	1.233223648	9.453560327	1.557396595
C	-0.914251033	5.160428365	2.216012235
H	-1.968762176	5.170538300	1.898362491
H	-0.822029360	5.440239464	3.279003001
C	-0.204424367	3.825152634	1.913124999
H	-0.748395984	3.029407730	2.485492808
C	1.245263910	3.876697576	2.390410997
H	1.321363145	3.999705080	3.480106078
H	1.780485615	4.739457792	1.961678523
H	1.798714862	2.972083058	2.120727617
C	-0.290998117	3.495791711	0.420312674
H	0.146799945	4.299266552	-0.187406347

H	-1.326029954	3.368969639	0.089285397
H	0.248471004	2.573239750	0.182319123
C	-0.928060707	9.973200772	4.533188616
C	-0.324568593	11.869028695	6.103010339
C	-1.486590309	11.921786501	6.848579828
H	-2.282370071	11.187536874	6.676415112
C	-1.665330268	12.946178736	7.814204945
H	-2.597129687	12.956487782	8.380974239
C	-0.712562775	13.917374474	8.025398973
H	-0.855325771	14.715380812	8.754625382
C	0.502952233	13.888969966	7.287899419
C	1.570253749	14.855487007	7.430653675
C	2.768881130	14.714462905	6.748642197
H	3.600328484	15.406711281	6.841487232
C	2.896658338	13.602200315	5.880070868
C	0.724598946	12.846063347	6.353188726
C	2.268849395	16.911351226	8.507194557
H	2.703483740	17.238319779	7.549446011
H	3.040838282	16.454547059	9.148603904
C	1.471361588	18.020116084	9.216434882
H	0.830036997	17.533101388	9.997498760
C	0.557045226	18.744083329	8.224918720
H	-0.081775306	18.026158853	7.692625590
H	1.120999556	19.313857558	7.480315047
H	-0.104462949	19.450927455	8.738144362
C	2.445739929	18.983584778	9.895949523
H	3.115590845	19.469676586	9.177933428
H	3.065501238	18.476620248	10.644691416
H	1.904649840	19.782992131	10.417726611
C	4.174176782	13.369840996	5.090696715
C	5.203010415	11.599862656	3.615297098
C	6.239332669	12.349821551	3.094303617
H	6.434843630	13.355029938	3.482715781
C	7.026635391	11.835948023	2.030910023
H	7.802251855	12.475332345	1.608390467
C	6.806740377	10.579288834	1.519006493
H	7.370812264	10.198872531	0.665047759
C	5.808967703	9.741030923	2.092606453
C	4.995680985	10.241939461	3.136528044
C	5.546745703	8.382235777	1.668497763
C	4.555002436	7.622575926	2.270243212
H	4.313330444	6.606288341	1.965037784
C	3.811730033	8.222481306	3.318718975
C	6.056142975	6.749449099	-0.065677908

H	6.623753704	6.937419664	-0.997374345
H	4.975747762	6.731234298	-0.284710676
C	6.539005701	5.502555838	0.693702433
H	6.345027002	5.656600612	1.787833165
C	8.040065212	5.283243974	0.511697967
H	8.619165601	6.157940157	0.830007424
H	8.307835881	5.068740467	-0.527034962
H	8.391838666	4.423219798	1.106496588
C	5.738238281	4.291359253	0.205834389
H	5.801591799	4.160866537	-0.879234979
H	4.679597120	4.353709757	0.480043483
H	6.130372969	3.361145648	0.645233599
C	2.725871814	7.435935189	4.045427136
C	1.119278815	7.720000289	5.976201783
C	0.266521843	6.670481234	5.692527228
H	0.480973145	6.002579358	4.849496476
C	-0.904040289	6.474176361	6.472650755
H	-1.575513585	5.656970883	6.189320935
C	-1.200276332	7.277958857	7.546585541
H	-2.105895311	7.139624819	8.139863739
C	-0.319135997	8.339788098	7.900615811
C	-0.527968035	9.225906164	9.023729869
C	0.370441700	10.241463318	9.316704748
H	0.231812778	10.951605429	10.128780820
C	1.507317425	10.365434996	8.482792901
C	0.840287230	8.570927746	7.121177600
C	-1.912479616	9.695362503	10.959240270
H	-2.337726383	10.661467321	10.641498956
H	-0.974874602	9.847705883	11.517934102
C	-2.916967545	8.807491304	11.711906037
H	-3.717975921	8.503050570	10.988604845
C	-2.230430075	7.544161014	12.237281704
H	-1.460579848	7.771792497	12.982733463
H	-1.744276896	6.998442598	11.417173693
H	-2.950540968	6.865953341	12.707296215
C	-3.545750690	9.620301283	12.846330192
H	-4.078519331	10.502001859	12.473662357
H	-2.799691357	9.963245462	13.572222196
H	-4.274296265	9.017381234	13.402238568
C	2.573789003	11.423258361	8.748311686
C	4.956882823	11.853882461	8.016347735
C	5.128435665	13.139271195	8.501204716
H	4.364192210	13.586349135	9.145198292
C	6.275621091	13.884705365	8.134114681

H	6.377483472	14.898035018	8.523113611
C	7.236378406	13.367806349	7.286369736
H	8.101822455	13.955150696	6.977339019
C	7.100232751	12.047658955	6.786372317
C	8.016850372	11.423192032	5.851764738
C	7.815144811	10.131954655	5.403691271
H	8.449476192	9.636692574	4.661227418
C	6.671235536	9.439358293	5.895702361
C	5.979666023	11.272365898	7.169826186
C	6.421935037	8.020685808	5.450975013
C	5.041846076	6.105546446	5.823460661
H	4.087114372	5.963249251	6.337496728
H	5.832620351	5.467817169	6.248737079
H	4.962908666	5.960038047	4.742888910
C	9.965357395	11.772867846	4.452026666
H	9.385613617	11.363331751	3.607058390
H	10.606572287	10.996073132	4.899021315
C	10.730214320	13.057415883	4.088471277
H	11.003761895	13.574254227	5.046742480
C	12.008615579	12.686487595	3.335502952
H	11.798836176	12.158835347	2.397732338
H	12.665660654	12.047509755	3.936505452
H	12.585136901	13.583187988	3.076241021
C	9.833756354	13.991721551	3.273819166
H	8.854734071	14.105534108	3.764437393
H	9.662817855	13.619119714	2.259057653
H	10.274190989	14.992779463	3.184279831
O	12.029430803	3.206902798	7.539540012
O	13.269338072	4.921545325	7.979950714
O	6.581966755	6.545160858	8.967974208
O	7.789612055	2.122959995	11.558088129
O	11.974270582	-4.162921794	10.288553890
O	13.538453849	-0.814978081	6.350775407
O	10.308252203	5.517923588	3.476776200
O	6.627815519	3.837463376	6.892331088
O	5.321668405	-2.341006482	11.217890886
O	9.333914708	-3.921636194	8.071909272
O	12.620868701	-1.129782069	1.769752003
O	8.471697158	2.054562729	2.259255615
O	1.953658041	2.523559914	6.279456319
O	3.689537646	-2.241008036	7.738610723
O	5.214676914	-2.544865939	6.092211486
N	9.733225312	3.836217923	9.170261712
N	12.191510756	4.385241383	7.752390259

N	9.317482331	1.255108243	10.052979886
H	9.939020314	1.491719801	9.245148609
N	11.013372481	-0.443489125	8.728924684
N	11.488948821	0.252943804	6.178447821
H	10.575721082	0.376064176	6.673119402
N	9.577747390	2.190364712	5.837709711
N	7.336315886	1.673409292	7.196974221
H	8.052975569	0.964349158	6.919388137
N	7.522680295	-0.933094136	7.993551344
N	8.838019796	-2.560241631	6.270010791
H	8.221632497	-1.777567999	5.957469002
N	9.194436974	-0.893588455	4.104617404
N	7.173642842	0.841209005	3.738602992
H	7.147261395	-0.022197708	4.327933125
N	5.137231140	-0.008370162	5.373196681
C	11.023652617	5.300470546	7.702689652
C	11.126466763	6.462708007	6.961478278
H	12.048472562	6.684578434	6.413563612
C	10.046914122	7.379106346	6.906354506
H	10.158078167	8.288338435	6.308227190
C	8.883152913	7.124812972	7.595503942
H	8.040121065	7.824512542	7.579668520
C	8.747896260	5.934453107	8.359579659
C	7.543101370	5.601741473	9.081750494
C	7.461519804	4.427269500	9.818721691
H	6.577914561	4.134171587	10.382724046
C	8.589343638	3.576472788	9.817679799
C	9.823514700	4.999928021	8.428444392
C	5.244082005	6.237416876	9.500013913
H	4.821883576	5.439308504	8.867524820
H	5.341140186	5.903983938	10.544608579
C	4.498937695	7.576013164	9.359616718
H	4.631453124	7.941981334	8.302382155
C	5.089091265	8.615494739	10.312863199
H	6.148145993	8.790649428	10.080136519
H	4.577880717	9.580398249	10.228859820
H	5.028465676	8.302274528	11.359031433
C	3.012423401	7.328282600	9.633435149
H	2.847231584	6.750023197	10.547714655
H	2.478181367	8.276270925	9.764864776
H	2.530500057	6.803102472	8.801157583
C	8.517583966	2.261934579	10.589379704
C	9.487826465	-0.052500428	10.585538506
C	8.820206826	-0.542709461	11.691886203

H	8.084248549	0.081334099	12.213941736
C	9.086317569	-1.855242483	12.165363116
H	8.536277024	-2.200283666	13.040894033
C	10.016036995	-2.665640239	11.557248150
H	10.236786243	-3.668314228	11.923869749
C	10.714196460	-2.201682554	10.407148998
C	11.696858737	-2.979237219	9.682540279
C	12.278386295	-2.501885571	8.516037918
H	13.013642872	-3.056450491	7.941183050
C	11.880185504	-1.217759540	8.070061885
C	10.434215052	-0.911244769	9.894611871
C	12.862410975	-5.104266378	9.596197331
H	12.409991745	-5.358033624	8.623667142
H	13.842169860	-4.618564602	9.458828876
C	12.909554149	-6.286976563	10.580293559
H	12.965162475	-5.860214511	11.617224161
C	11.634853529	-7.125851822	10.472581281
H	11.554303830	-7.633558967	9.505524877
H	11.594304433	-7.894925906	11.250158502
H	10.743301280	-6.491851367	10.582140002
C	14.163655828	-7.123024021	10.316117956
H	15.080166070	-6.539229063	10.458894437
H	14.215613659	-7.976485760	11.003140031
H	14.179121057	-7.530411286	9.299118124
C	12.431122012	-0.592033457	6.791428595
C	11.762291488	1.277627761	5.233788520
C	12.907876300	1.354053295	4.466451966
H	13.685590074	0.587811511	4.565346339
C	13.096251445	2.443216554	3.574953224
H	14.014942470	2.467508636	2.987591583
C	12.171442207	3.455803593	3.467648715
H	12.320725585	4.305710728	2.801709115
C	10.979940614	3.414463603	4.245525896
C	9.969881559	4.448525454	4.245082319
C	8.809878145	4.330680143	4.995936436
H	8.024943582	5.089348047	5.009023503
C	8.662065333	3.158436442	5.778745581
C	10.743399673	2.309157425	5.099316929
C	9.420030190	6.687492654	3.520455699
H	8.487044238	6.420321446	2.989069596
H	9.182426188	6.927359174	4.571195366
C	10.236886477	7.775915948	2.811068571
H	10.775149277	7.302418736	1.949797169
C	11.281217249	8.379740199	3.759190224

H	12.013725406	7.616449738	4.054013050
H	11.833756285	9.193438567	3.280758699
H	10.825848992	8.770941265	4.678029489
C	9.270811560	8.836004789	2.285554477
H	8.670298395	9.275729039	3.100486982
H	9.794036406	9.644006435	1.768038322
H	8.548127887	8.401791389	1.575010856
C	7.437426873	2.951857444	6.654432798
C	6.408925052	1.227311812	8.174801772
C	5.398144626	2.001310724	8.717894956
H	5.232140956	3.019860137	8.351442776
C	4.586455843	1.481841338	9.757662079
H	3.808124316	2.122829121	10.171426285
C	4.777896769	0.211499290	10.256026247
H	4.172691570	-0.185952070	11.072682505
C	5.783955763	-0.622431232	9.697983572
C	6.583146081	-0.137129578	8.635283314
C	6.054641404	-1.977295825	10.134211298
C	6.979837743	-2.772547400	9.478911436
H	7.221391317	-3.787931858	9.779976524
C	7.678811521	-2.195021935	8.386612625
C	5.539311017	-3.684933777	11.770325960
H	5.391400150	-4.429385428	10.972423912
H	6.572082376	-3.723172322	12.155513606
C	4.474661529	-3.762479928	12.877881452
H	4.428454815	-2.757456876	13.376596778
C	3.100317131	-4.066272224	12.279352958
H	3.056327347	-5.062304985	11.826485714
H	2.313018632	-4.019004724	13.038643447
H	2.848407724	-3.338650166	11.494361605
C	4.890309993	-4.813611090	13.909171255
H	5.832498563	-4.550610529	14.402920662
H	4.130955806	-4.912702156	14.694601532
H	5.013514916	-5.805059543	13.459075248
C	8.706109417	-2.994665757	7.596727152
C	9.978274013	-2.779180024	5.443278644
C	10.920979531	-3.761914591	5.670619266
H	10.797792800	-4.457587056	6.507824048
C	12.074602865	-3.853239927	4.846227074
H	12.804272511	-4.632628496	5.068876341
C	12.285362332	-2.976982358	3.809147565
H	13.183745670	-3.019983074	3.190236959
C	11.323959847	-1.964942480	3.527888034
C	11.476548179	-0.975313998	2.485301050

C	10.517204022	0.004415094	2.278975332
H	10.603305666	0.785285547	1.526076838
C	9.383796983	-0.001848221	3.128650329
C	10.156769431	-1.866357031	4.325921461
C	12.937796491	-0.119515504	0.749956978
H	12.141906317	-0.144117884	-0.011620424
H	12.980905064	0.868317039	1.237771335
C	14.296619308	-0.607119017	0.218161763
H	14.277448633	-1.730440648	0.226296999
C	15.435534417	-0.139460729	1.125699050
H	15.256318682	-0.438393948	2.168223546
H	16.391866593	-0.578809316	0.820805548
H	15.561321356	0.947870861	1.107909786
C	14.487777940	-0.124550748	-1.221335673
H	14.499771635	0.968946872	-1.289122944
H	15.441127270	-0.481533397	-1.630446839
H	13.694630218	-0.489715471	-1.883013201
C	8.320770375	1.079207162	2.975683851
C	6.071237281	1.716668942	3.917428250
C	5.959321866	2.957613411	3.318973957
H	6.754586203	3.319485222	2.653645495
C	4.828737338	3.773634618	3.570590045
H	4.761501887	4.739101189	3.060407585
C	3.838610940	3.379869260	4.440861206
H	2.972776272	4.019302109	4.643838864
C	3.926889601	2.117409272	5.086071186
C	2.950618499	1.629685918	6.033897202
C	3.069181352	0.373367852	6.598713253
H	2.371220152	-0.029774666	7.328091972
C	4.189854557	-0.416261721	6.209336784
C	5.023033441	1.259187417	4.812656291
C	4.309213348	-1.800027469	6.790651372
C	5.415076726	-3.916094282	6.534724683
H	5.514936027	-3.958191457	7.624598590
H	4.571327479	-4.520497321	6.192637637
H	6.348283926	-4.189618845	6.027127095
C	0.877800146	2.118998497	7.194458978
H	0.491212605	1.134737092	6.889542664
H	1.307981478	2.067953657	8.207861019
C	-0.148925021	3.250827001	7.025453461
H	0.406947818	4.225165246	7.089831760
C	-1.170778063	3.180361730	8.161692388
H	-0.696810171	3.288117000	9.143959759
H	-1.912580957	3.983693447	8.073779842

H	-1.723794494	2.234281385	8.160682114
C	-0.819617170	3.165933792	5.651650511
H	-1.401852078	2.247443683	5.528627142
H	-1.498949733	4.012694097	5.488987821
H	-0.060591058	3.183090726	4.854444687

Table S18. Atomic coordinates for the optimized structure of $Q_6(i\text{-Bu})$ in MOPAC2016 (Fig. S3a(iv), gas phase).

Atom	X	Y	Z
O	10.303860917	-2.923754016	15.740937231
O	9.212334102	-4.676948590	15.103553316
O	15.878460232	-6.293870986	14.600748096
O	14.799913608	-1.908156060	11.891702599
O	10.611688625	4.427421446	13.047112142
O	8.771496016	1.033143188	16.794004811
O	11.806118540	-5.151686032	20.187320561
O	15.634968039	-3.695497089	16.787652663
O	17.208095534	2.562052845	12.577632683
O	12.998326942	4.095423696	15.453968407
O	9.393742229	1.288674639	21.610510296
O	13.597914147	-1.898239822	21.211743900
O	20.071753093	-1.978678581	17.063153594
O	18.384349406	2.922311846	16.233356788
O	16.673217764	2.974160058	17.717929914
N	12.747960013	-3.575440973	14.225887540
N	10.218214109	-4.106019536	15.493457705
N	13.214174842	-1.018114767	13.325133612
H	12.554521453	-1.252558409	14.103197447
N	11.435169266	0.651448812	14.558583255
N	10.787206667	-0.078294460	17.075387999
H	11.710835249	-0.246465567	16.613927806
N	12.663501191	-1.998106329	17.636561161
N	14.996729224	-1.498143935	16.468357912
H	14.280382080	-0.780977420	16.733333324
N	14.810272804	1.101160310	15.637602339
N	13.356340908	2.715447166	17.271925902
H	13.965927017	1.945245445	17.625942564
N	12.902411368	1.058509039	19.409536545
N	14.989612857	-0.523247915	19.979063221
H	15.037328963	0.399907878	19.486046984
N	16.965081751	0.462929911	18.383433119
C	11.407448061	-4.975277168	15.708076620
C	11.295534175	-6.064135275	16.548956809
H	10.356011200	-6.265953146	17.074363023

C	12.398262933	-6.935633797	16.742343136
H	12.284554830	-7.779105611	17.424309795
C	13.580729064	-6.724396218	16.069890982
H	14.439458529	-7.390906225	16.195620997
C	13.716361508	-5.619281209	15.186252852
C	14.928395645	-5.339103718	14.452634599
C	15.032434523	-4.198303403	13.669783778
H	15.924001944	-3.937034783	13.102504262
C	13.913858672	-3.334837852	13.613963929
C	12.634988346	-4.704918967	15.017283109
C	17.192573585	-6.058302325	13.980765321
H	17.677227980	-5.252065102	14.557105591
H	17.050845381	-5.758893009	12.930107470
C	17.894424392	-7.418974121	14.133483988
H	17.701264613	-7.786957415	15.174946112
C	17.322039223	-8.436501500	13.144950059
H	16.232908649	-8.519890490	13.259907735
H	17.747004460	-9.433085763	13.306799121
H	17.520327757	-8.162698235	12.102562484
C	19.401451335	-7.227859109	13.943155898
H	19.646126262	-6.833526672	12.950361948
H	19.931610223	-8.183531208	14.041451375
H	19.826188884	-6.545703403	14.688134232
C	14.028422791	-2.031057841	12.825794259
C	13.072185650	0.293266578	12.791791483
C	13.808489292	0.798769660	11.737404997
H	14.567798297	0.178126741	11.247220846
C	13.572997737	2.119271951	11.269466793
H	14.173064663	2.477202929	10.432453363
C	12.615472748	2.924997138	11.839882572
H	12.423528279	3.936397790	11.480132937
C	11.848398277	2.444852045	12.938395272
C	10.831265525	3.216205929	13.621726509
C	10.168563948	2.711196409	14.730842907
H	9.394845610	3.252645009	15.266933601
C	10.529686763	1.413480013	15.173701922
C	12.088554667	1.142394521	13.439896482
C	9.720190300	5.365833592	13.743124386
H	10.129138761	5.546694021	14.750533192
H	8.718530343	4.908720692	13.796632458
C	9.768308292	6.604015623	12.831123790
H	9.819272389	6.237569706	11.771066092
C	11.021356402	7.435299015	13.111733411
H	10.993845613	7.911811058	14.097351715

H	11.145399766	8.230865644	12.369475407
H	11.923477275	6.807348627	13.078073173
C	8.489775098	7.426318021	13.010269456
H	7.591539085	6.841320396	12.782950654
H	8.485303613	8.291676097	12.335867902
H	8.388002206	7.815862910	14.029149485
C	9.896076331	0.783700934	16.410329674
C	10.452737945	-1.052007620	18.052137810
C	9.264966809	-1.082176006	18.758721966
H	8.498302817	-0.319808484	18.574637616
C	9.020700384	-2.117869196	19.697636876
H	8.068993057	-2.108647226	20.231643703
C	9.932943501	-3.124529869	19.918462012
H	9.741217403	-3.932282558	20.625628953
C	11.168474998	-3.126700896	19.213670642
C	12.188249796	-4.145401313	19.354981102
C	13.386643310	-4.071262800	18.663831128
H	14.178068241	-4.811233680	18.745747427
C	13.576204014	-2.952542501	17.811232053
C	11.454070891	-2.076540619	18.307326985
C	12.732109031	-6.268432889	20.402353093
H	13.524125994	-5.903084788	21.077377222
H	13.160524420	-6.588894987	19.439678597
C	11.832501963	-7.337730867	21.049487587
H	11.257430652	-6.844027284	21.876294244
C	10.833006217	-7.894747612	20.033081091
H	10.245071735	-7.080824490	19.586998792
H	10.125711975	-8.584376874	20.507946950
H	11.325545573	-8.438894287	19.220388206
C	12.709037841	-8.442703112	21.642671385
H	13.309737133	-8.949380793	20.879287601
H	12.093198422	-9.211902288	22.125375392
H	13.393441559	-8.058317700	22.407505916
C	14.848094238	-2.787617957	16.990426445
C	15.925573303	-1.063421302	15.488942391
C	16.924422858	-1.849610317	14.947784603
H	17.078236400	-2.868889015	15.318671045
C	17.735009954	-1.347548721	13.895823803
H	18.484125246	-2.011055406	13.463654881
C	17.572243895	-0.071318037	13.409458399
H	18.161988244	0.307483451	12.572519315
C	16.598509088	0.791732918	13.986804497
C	15.768492606	0.306962241	15.025870798
C	16.384373442	2.164429898	13.581027654

C	15.424816741	2.953784723	14.197074890
H	15.199857063	3.974589284	13.897440347
C	14.666635600	2.365266554	15.239938078
C	17.032319359	3.921541668	12.044227154
H	17.004528244	4.644617367	12.885826181
H	16.079775471	3.931687260	11.489507852
C	18.272105168	4.095961826	11.150736419
H	18.506066134	3.095576266	10.698452161
C	19.472389207	4.550282183	11.980882306
H	19.400320914	5.602091296	12.289649442
H	20.409404829	4.457467871	11.420642118
H	19.577543288	3.949389882	12.901077936
C	17.955798353	5.087209734	10.028524557
H	17.113797087	4.758256501	9.410001701
H	18.818175057	5.212341243	9.361322992
H	17.714814080	6.084513943	10.416800614
C	13.587780585	3.159985284	15.962773494
C	12.145449538	2.895751096	17.998842714
C	11.168370895	3.813665894	17.668271169
H	11.304820552	4.474699079	16.803378857
C	9.967241873	3.884300631	18.424142874
H	9.209923126	4.607219031	18.117771328
C	9.743541358	3.054025252	19.496521205
H	8.814881939	3.091367016	20.069057832
C	10.728059828	2.094000715	19.868487011
C	10.562358161	1.134072111	20.937253703
C	11.533844578	0.182555324	21.209505182
H	11.436002651	-0.577629413	21.981857588
C	12.696849002	0.188289849	20.401007513
C	11.930992536	2.004734238	19.126101164
C	9.051939757	0.297269134	22.640544388
H	9.797633755	0.375164371	23.448063056
H	9.074136578	-0.706672919	22.186483996
C	7.644404862	0.747847832	23.068668431
H	7.624614322	1.870705368	23.038658412
C	6.588085749	0.222184303	22.095624812
H	6.821390185	0.519447500	21.063348954
H	5.595538157	0.622180855	22.332009129
H	6.510268875	-0.870003983	22.117397647
C	7.375529725	0.283461959	24.501415939
H	7.416756254	-0.807790633	24.593236185
H	6.377067415	0.594411814	24.833623022
H	8.097695342	0.705067103	25.209749162
C	13.780365310	-0.865483751	20.595683620

C	16.090881927	-1.379496703	19.716909701
C	16.221288375	-2.666799114	20.206674542
H	15.464410595	-3.073831518	20.887387794
C	17.315625495	-3.472225279	19.801766482
H	17.382163738	-4.486034153	20.198950665
C	18.262566500	-3.009548230	18.914556727
H	19.085929086	-3.640443213	18.576421997
C	18.167881160	-1.687179840	18.403844865
C	19.082370818	-1.121187273	17.432625108
C	18.920142823	0.170278729	16.971310231
H	19.542503347	0.616568132	16.189136518
C	17.841108432	0.932114338	17.505160727
C	17.103173026	-0.851019261	18.821832499
C	17.688469469	2.362625635	17.058526498
C	16.469612610	4.382524374	17.409996164
H	16.040641753	4.469721691	16.410165333
H	17.424210386	4.929514000	17.489019016
H	15.763899573	4.701960301	18.195017565
C	21.016374552	-1.530484465	16.032591472
H	21.295930107	-0.470454863	16.201405383
H	20.498990573	-1.643114286	15.065397787
C	22.215315616	-2.477970666	16.198475450
H	21.822561977	-3.524749629	16.272235476
C	23.109082626	-2.356587957	14.962278531
H	22.578345562	-2.629574363	14.042663010
H	23.977555749	-3.021492773	15.041367897
H	23.496423013	-1.337860775	14.835734201
C	22.981653154	-2.154943260	17.482639032
H	23.437043376	-1.159188794	17.455273796
H	23.785074006	-2.878145300	17.664811728
H	22.308114834	-2.179380804	18.350606385
O	23.902345329	6.056997523	18.695917052
O	24.317181802	5.052965586	20.566244873
O	17.886378420	3.622355587	20.842578401
O	19.399338275	8.032903120	23.212248946
O	23.969109490	14.024701776	21.840773115
O	25.489375900	10.495461195	18.068653575
O	21.817667489	4.434526149	15.034400973
O	18.290752879	6.330976135	18.546496405
O	17.411948499	12.686395791	22.732437224
O	21.378229844	14.100194329	19.631800698
O	25.190130768	11.514590790	13.504456673
O	21.047462049	8.236936092	13.624515767
O	14.378468877	7.635318723	17.357681288

O	15.997145136	12.358513174	18.996210979
O	17.553371612	12.765665780	17.406218921
N	21.227037214	6.107058611	20.873041973
N	23.632582283	5.278951999	19.588555767
N	21.090215163	8.706592736	21.786307053
H	21.711107857	8.401147578	21.004734622
N	22.939992695	10.249008499	20.461758087
N	23.415300353	9.466400208	17.939360741
H	22.507675867	9.368983429	18.449007691
N	21.368149728	7.720104713	17.519721042
N	19.156240897	8.448856550	18.796981728
H	19.926364600	9.091965230	18.504109931
N	19.555680557	11.054629265	19.563767979
N	21.279139910	12.469769154	18.002850374
H	20.767224021	11.614837014	17.694502639
N	21.707883685	11.021216657	15.711188799
N	19.664568704	9.414588610	15.054520454
H	19.612611144	10.251648326	15.680014027
N	17.551634447	10.229470118	16.602848427
C	22.375243285	4.488901161	19.455735462
C	22.358676229	3.349112780	18.681165642
H	23.240379568	3.049080956	18.108862300
C	21.191596407	2.542100755	18.627093961
H	21.201023393	1.639380730	18.015397547
C	20.072523208	2.886297437	19.350022856
H	19.171218810	2.263186059	19.352171317
C	20.058975746	4.073477267	20.130835445
C	18.911132912	4.502193430	20.895173085
C	18.942732118	5.693247088	21.606819855
H	18.105593570	6.060998582	22.198103989
C	20.125669430	6.466909762	21.544081500
C	21.210174398	4.909897219	20.176956430
C	16.638925074	3.970625745	21.539367563
H	16.874022660	4.241557347	22.581278591
H	16.194400859	4.822478824	20.999421449
C	15.808206251	2.680926739	21.423323630
H	15.858258981	2.334796441	20.354315491
C	16.389774810	1.585826307	22.319498407
H	17.429585588	1.369589484	22.040322630
H	16.377826410	1.864796230	23.377900862
H	15.828977363	0.649510112	22.220879988
C	14.356815914	2.998574864	21.789824727
H	14.273957016	3.523763019	22.746847276
H	13.868674238	3.614080287	21.015330178

H	13.766830102	2.079569852	21.884949412
C	20.157916636	7.800743566	22.287467946
C	21.344156824	10.012963930	22.290145418
C	20.691782628	10.573923266	23.371557628
H	19.910808536	10.011513632	23.898557877
C	21.024535413	11.883024808	23.812117046
H	20.486332160	12.284064258	24.670926582
C	21.997510516	12.625236270	23.186656468
H	22.266436774	13.628344080	23.519717525
C	22.681814264	12.087036345	22.060266801
C	23.684158695	12.808220489	21.307967448
C	24.270467733	12.256870343	20.178708390
H	25.038059741	12.760090429	19.596087681
C	23.843674908	10.964324432	19.787055192
C	22.356426900	10.789238340	21.595290160
C	24.583692826	15.035045334	20.970636187
H	25.666938927	14.967280361	21.157196941
H	24.348236134	14.822847314	19.912505484
C	23.969471213	16.371570949	21.430602953
H	24.453346478	17.179691526	20.824162581
C	22.465437359	16.380813116	21.154115730
H	22.244065565	16.273020961	20.083309701
H	21.967668977	15.524257276	21.634061265
H	21.988512555	17.296332357	21.510066124
C	24.273989622	16.620287101	22.910352215
H	23.904898024	15.791693127	23.530645509
H	25.349309691	16.711111672	23.093965658
H	23.797003474	17.537786931	23.268564287
C	24.381122675	10.297434143	18.522374363
C	23.609382331	8.481436332	16.935039500
C	24.732551540	8.363215408	16.142379450
H	25.565065623	9.064985892	16.260933854
C	24.821416256	7.308453762	15.193862470
H	25.719862472	7.250078963	14.580081890
C	23.826757418	6.367282938	15.061068511
H	23.902099226	5.544749532	14.350210776
C	22.653836391	6.455187998	15.863086895
C	21.568396718	5.501201615	15.841186333
C	20.420927521	5.688285246	16.599074619
H	19.580437981	4.991385730	16.592238611
C	20.368207161	6.841177857	17.419314331
C	22.515322080	7.536207191	16.767403937
C	20.844600633	3.336156031	15.035591963
H	20.556889237	3.093304061	16.073899052

H	19.952788140	3.683770819	14.469017309
C	21.598663072	2.202462685	14.324825854
H	22.155676780	2.651618299	13.461412743
C	22.618715563	1.544329022	15.258353698
H	23.235346371	2.305063187	15.755051958
H	22.138155508	0.929955525	16.033594433
H	23.301111220	0.892100100	14.700345157
C	20.577491293	1.194022343	13.796858436
H	19.914070494	0.833839253	14.601089187
H	19.924482373	1.646942178	13.036733512
H	21.066293599	0.328997334	13.338806706
C	19.161949277	7.149873912	18.290390332
C	18.271122994	8.986700435	19.768602869
C	17.208084007	8.298135424	20.321913670
H	16.970336828	7.285602530	19.974865848
C	16.434959339	8.891103071	21.353112924
H	15.611181705	8.315613681	21.775295086
C	16.719063837	10.150222522	21.829642072
H	16.145598981	10.604732251	22.639837965
C	17.784672506	10.900750403	21.259949145
C	18.552313797	10.342337697	20.208121416
C	18.143665775	12.239552724	21.676695417
C	19.147032672	12.942203841	21.031935850
H	19.467774400	13.939947985	21.325143539
C	19.814669507	12.301137050	19.956964281
C	17.645320248	14.040081352	23.232735570
H	17.110228218	13.977780433	24.199320500
H	18.724544859	14.182555352	23.406517163
C	17.039374815	15.088870587	22.283373540
H	17.475948116	14.939195703	21.261872836
C	15.525451178	14.907408241	22.177290852
H	15.281323434	13.879507482	21.867926032
H	15.015060266	15.093693343	23.126940267
H	15.089940766	15.580354788	21.430657958
C	17.416752529	16.488805275	22.775877491
H	17.044859180	16.686997681	23.787057703
H	18.501924697	16.641375601	22.781835945
H	16.986537061	17.260340232	22.125495073
C	20.898509103	13.060645953	19.206217455
C	22.409182082	12.813793047	17.209774960
C	23.298484666	13.826987058	17.511892358
H	23.119504171	14.477680091	18.376700568
C	24.464890710	14.016140517	16.722800604
H	25.149618851	14.818061185	17.000218728

C	24.740373689	13.206614890	15.646649311
H	25.649734892	13.323903563	15.054682691
C	23.828937658	12.175157540	15.283117855
C	24.028928660	11.276700110	14.167618472
C	23.092966520	10.304601441	13.852998351
H	23.214214781	9.590365860	13.041196839
C	21.931568504	10.226601307	14.662434761
C	22.647094522	11.984768603	16.040687398
C	25.506389743	10.691200144	12.329805713
H	25.912586549	9.740738530	12.713896581
H	24.597488443	10.513066687	11.734206762
C	26.550048493	11.544755519	11.588976141
H	27.311193264	11.881503449	12.340695626
C	25.893439310	12.784002508	10.975772206
H	25.161440042	12.527605057	10.202643472
H	25.368369899	13.364808070	11.747155666
H	26.637308616	13.443854068	10.516872421
C	27.241121162	10.688010680	10.525801945
H	27.769153506	9.834948654	10.966020142
H	26.531484841	10.296136435	9.788647066
H	27.984100093	11.277485073	9.973645890
C	20.864935186	9.177161135	14.375555521
C	18.545222305	8.547304638	15.132322683
C	18.449652172	7.335188284	14.471181641
H	19.268928570	6.994800857	13.824543321
C	17.305279884	6.518183701	14.641633629
H	17.266593524	5.566299828	14.094471260
C	16.273725407	6.891709833	15.471380515
H	15.382440314	6.272443807	15.602130571
C	16.349611553	8.119595608	16.183685305
C	15.351888894	8.557491526	17.136281755
C	15.439782249	9.801453245	17.731691779
H	14.712178540	10.177831703	18.449033077
C	16.567730423	10.609777382	17.409648891
C	17.457650700	8.981405627	15.991748120
C	16.646603583	11.971844171	18.049258033
C	17.727685298	14.111485584	17.930552156
H	18.700485510	14.400162646	17.514540786
H	16.917135979	14.736975671	17.547494536
H	17.735092865	14.103386315	19.026572406
C	13.394540510	7.915880289	18.412802771
H	13.863754854	8.477550207	19.237378661
H	12.602771798	8.516396388	17.936835936
C	12.920197708	6.517477323	18.844397625

H	12.727694841	5.915427421	17.916054867
C	11.617735705	6.653150253	19.635899337
H	11.748956689	7.239080988	20.551630587
H	10.827677500	7.127730881	19.044892325
H	11.241787336	5.664239777	19.935581915
C	14.002831093	5.811173710	19.659100201
H	14.906787082	5.647963905	19.043161961
H	14.294371421	6.379838507	20.547290435
H	13.664556582	4.816471446	19.996801623

Table S19. Atomic coordinates for the optimized structure of **Q₆(*i*-Bu)** in MOPAC2016 (Fig. S3b(i), gas phase).

Atom	X	Y	Z
O	-0.838802736	14.262049297	4.150120015
O	-0.897273963	15.185513191	2.194406992
O	5.455056203	16.676130959	2.758289504
O	4.160445040	12.297200242	0.081219628
O	-0.647573483	6.401147806	1.289750821
O	-2.249849194	10.001047379	4.912287488
O	1.151002000	16.070776984	8.217841784
O	4.962660715	14.273644953	5.009552680
O	6.046814995	8.038403311	0.659054965
O	1.987057414	6.503083635	3.626016508
O	-1.802101473	9.055823513	9.844626346
O	2.283849067	12.494583446	9.341888518
O	9.063462123	12.275314289	5.755222004
O	7.052978806	7.591237296	4.433623616
O	5.429627220	7.456552689	6.002616862
N	2.144205800	14.209351033	2.257652541
N	-0.397676642	14.991488926	3.283701099
N	2.365986428	11.639237888	1.386441914
H	1.703008788	11.959737815	2.128517041
N	0.406746765	10.189043512	2.617219542
N	-0.214869001	11.095810569	5.078091474
H	0.704244693	11.217621435	4.600712980
N	1.801407632	12.847014931	5.688064474
N	4.150241561	12.142976625	4.639990177
H	3.360919572	11.493985761	4.860136524
N	3.775324987	9.573943116	3.774452310
N	1.901654226	8.232896881	5.151703707
H	2.370517552	9.123241260	5.439935302
N	1.518202084	9.661106440	7.431122951
N	3.684216714	11.036630603	8.212450499
H	3.714252633	10.122262289	7.704057936

N	5.717134606	9.984637235	6.702018472
C	0.838757291	15.760982302	3.605534862
C	0.773605766	16.838350950	4.461611382
H	-0.165865189	17.107277632	4.954542632
C	1.934484153	17.619327396	4.708241008
H	1.855110899	18.468111823	5.387559462
C	3.129121193	17.312210752	4.097267029
H	4.031947681	17.906757498	4.269021168
C	3.223574755	16.192729708	3.224553087
C	4.446730424	15.793159736	2.566908100
C	4.497589767	14.630790410	1.809214258
H	5.396862929	14.277361193	1.306901235
C	3.315959999	13.859272162	1.711201041
C	2.079886666	15.374097211	3.000273644
C	6.787373282	16.354443357	2.224783620
H	6.698148240	16.062368759	1.167110961
H	7.186916084	15.524724594	2.831731709
C	7.545680634	17.678439257	2.428149172
H	7.327404053	18.033425531	3.469974757
C	7.055807376	18.738322339	1.438271667
H	5.963920649	18.846857456	1.493438985
H	7.306079341	18.485869692	0.401883074
H	7.497924766	19.717478947	1.651716385
C	9.048681920	17.431317877	2.286589577
H	9.309781715	17.037576036	1.297654480
H	9.419930590	16.724002260	3.037424497
H	9.613034373	18.363787783	2.413370861
C	3.342536664	12.532878012	0.949963766
C	2.094091639	10.345244786	0.865626784
C	2.769947672	9.760362861	-0.187090665
H	3.591087994	10.295609601	-0.679279398
C	2.405887725	8.462196707	-0.637115625
H	2.955588148	8.043652035	-1.480617365
C	1.389448581	7.753263142	-0.041464438
H	1.100498054	6.757810898	-0.381316556
C	0.681276948	8.316574449	1.058534621
C	-0.362787271	7.632838437	1.789606908
C	-0.988034566	8.225065985	2.876576618
H	-1.796956552	7.754704107	3.431589550
C	-0.548361934	9.516442547	3.262108890
C	1.024509820	9.609943678	1.520852812
C	-1.259354066	5.420321526	2.195629625
H	-2.337132484	5.442822952	1.969194313
H	-1.073601734	5.698760086	3.247822600

C	-0.589461134	4.079216712	1.837627305
H	-1.020759858	3.306726337	2.524644228
C	0.919680784	4.159665024	2.070953859
H	1.162972937	4.476229543	3.095983388
H	1.383840274	4.915705076	1.421995102
H	1.411838334	3.202046252	1.888228589
C	-0.909774560	3.690332137	0.391867225
H	-0.621862763	4.492780111	-0.301220939
H	-1.978308443	3.501939172	0.248118342
H	-0.367480154	2.788307751	0.090457479
C	-1.133565602	10.218251672	4.486233426
C	-0.472725085	12.059714442	6.088468514
C	-1.643952081	12.144045585	6.817108409
H	-2.451798387	11.423937519	6.642729357
C	-1.815718755	13.183689815	7.768211744
H	-2.754730845	13.217326345	8.321988506
C	-0.846761174	14.137911813	7.981184756
H	-0.985389256	14.947876622	8.697397562
C	0.380588772	14.073431479	7.264927244
C	1.465129708	15.019865578	7.410722467
C	2.671837555	14.843907283	6.753597405
H	3.519367639	15.516548219	6.846269719
C	2.791260807	13.712579274	5.907120307
C	0.593735908	13.014018305	6.347331326
C	2.174306889	17.101432512	8.429262425
H	2.505609498	17.483008989	7.450497326
H	3.014757309	16.637050158	8.970749328
C	1.422923104	18.151378291	9.266955706
H	0.846803256	17.602793916	10.058830842
C	0.429127433	18.922492026	8.395002617
H	-0.235909106	18.228685218	7.862032817
H	0.927896730	19.549019443	7.649347182
H	-0.202410333	19.582677514	8.999530972
C	2.431677792	19.085529733	9.938330549
H	3.018257923	19.654068326	9.208348318
H	3.132394738	18.537183804	10.578378599
H	1.921305292	19.817865808	10.576503799
C	4.086794627	13.438598113	5.158882724
C	5.104534572	11.619882474	3.730253012
C	6.224438466	12.298204796	3.289873259
H	6.460801498	13.286441528	3.699293301
C	7.061301852	11.719699024	2.299661339
H	7.928539264	12.288279108	1.963936036
C	6.784726194	10.486996685	1.755327977

H	7.405606786	10.049281823	0.971508130
C	5.660748017	9.743689911	2.213526366
C	4.832769230	10.284079422	3.226548168
C	5.289531762	8.436688997	1.714628726
C	4.244390316	7.723537680	2.281012639
H	3.934143532	6.736129683	1.943743052
C	3.524217516	8.340246516	3.334355623
C	5.758435446	6.747200831	0.037034341
H	6.238985237	6.894740655	-0.948653795
H	4.668694429	6.634051762	-0.089642916
C	6.399058644	5.613751891	0.855699012
H	6.089522343	5.729069204	1.928039416
C	7.923940380	5.709845922	0.797726106
H	8.260725896	6.692130066	1.160774775
H	8.312479177	5.581243887	-0.216964582
H	8.397321370	4.950675732	1.429760687
C	5.890022093	4.268869233	0.330168823
H	6.108554087	4.132512190	-0.734795876
H	4.808087439	4.160883397	0.466699577
H	6.367410142	3.434861693	0.859175638
C	2.398078650	7.581482355	4.025640462
C	0.797194574	7.860491593	5.963799817
C	-0.077410866	6.827195446	5.693390114
H	0.091008915	6.178156619	4.826675271
C	-1.208850631	6.617655412	6.528527398
H	-1.889495623	5.804464738	6.275091228
C	-1.458631348	7.415149210	7.621045687
H	-2.339422624	7.273229853	8.249632280
C	-0.555391119	8.464029431	7.956618041
C	-0.697181354	9.334869743	9.104368310
C	0.237692742	10.320724285	9.381061106
H	0.149932845	11.019869260	10.209049423
C	1.349992982	10.427731762	8.509096463
C	0.578342475	8.686534338	7.139619960
C	-1.956577160	9.717869395	11.147723338
H	-2.395707595	10.708616743	10.948114589
H	-0.977153571	9.815502093	11.642234087
C	-2.907774758	8.771982394	11.902035431
H	-3.792488662	8.576716101	11.241520660
C	-2.215247351	7.438244899	12.193333766
H	-1.358748359	7.552629904	12.866037101
H	-1.841511933	6.985131044	11.264344958
H	-2.901275710	6.722990061	12.658364919
C	-3.379427505	9.453293866	13.189107437

H	-3.914532178	10.387581751	12.987998561
H	-2.546140097	9.683014197	13.863089286
H	-4.065312722	8.802517573	13.746114721
C	2.455887184	11.448342575	8.746002272
C	4.838829177	11.842218461	8.024561180
C	4.989318999	13.118217460	8.535566825
H	4.197460158	13.555398848	9.155116977
C	6.149971096	13.875802828	8.234945288
H	6.226051493	14.883509148	8.644018483
C	7.147412213	13.369518588	7.433093044
H	8.030304069	13.955720713	7.176604942
C	7.033061158	12.055123487	6.902155893
C	8.013129254	11.456384831	6.019408843
C	7.842441052	10.174742733	5.531758239
H	8.547365217	9.685605167	4.862129084
C	6.657750944	9.480222052	5.911221538
C	5.890908178	11.272221636	7.201067035
C	6.440587553	8.100274970	5.347206402
C	5.079523001	6.129011369	5.522273840
H	4.081996571	5.980993995	5.954464831
H	5.806401392	5.414187811	5.916114174
H	5.055867548	6.107898055	4.426739190
C	10.019206593	11.870828892	4.710487668
H	9.463361873	11.593272659	3.802318918
H	10.595459476	11.006656133	5.094835879
C	10.869164526	13.143108237	4.552629686
H	10.989732545	13.591475516	5.575101293
C	12.250181017	12.780572437	4.005956013
H	12.201521370	12.393801665	2.983102337
H	12.734505207	12.004222101	4.622248333
H	12.915076301	13.650333133	3.996097400
C	10.155641907	14.161552674	3.658576541
H	9.140984343	14.357504981	4.031413055
H	10.073375149	13.811244593	2.624324737
H	10.698803072	15.112897888	3.637497402
O	12.452573687	10.184238848	5.720034781
H	12.914540802	9.347182552	5.515496702
C	12.389407244	10.381074117	7.141577803
H	11.860350535	9.549719008	7.617638251
H	13.397376860	10.499505184	7.550643268
H	11.815910573	11.312282636	7.251010366

Table S20. Atomic coordinates for the optimized structure of **Q₆(*i*-Bu)** in MOPAC2016 (Fig. S3b(ii), gas phase).

Atom	X	Y	Z
O	13.224330860	7.975313917	6.036801793
H	14.017730408	7.516132564	5.692982580
C	13.380367965	8.201172682	7.451173406
H	13.455874725	7.236876277	7.977431802
H	14.256573123	8.826576654	7.639272271
H	12.463179835	8.726743265	7.739124215
O	12.042133387	3.378064440	7.333746593
O	12.983741898	5.148935650	8.132774561
O	6.294038646	6.357202210	8.867420388
O	7.826790144	2.146141933	11.599414608
O	12.077138505	-4.094451430	10.350112168
O	13.695595141	-0.765755538	6.466867976
O	10.488437624	5.259257018	2.978409084
O	6.780717158	3.907006080	6.512055785
O	5.344466736	-2.021041275	11.173333981
O	9.428441759	-3.805242434	8.221669586
O	12.842902346	-1.256138196	1.879773672
O	8.605564098	1.879605091	2.199805445
O	2.260385806	2.340294331	6.465462428
O	3.904261244	-2.495619506	7.695621249
O	5.486540096	-2.765887838	6.102352082
N	9.630596166	3.872173570	9.105905809
N	12.025845199	4.538124853	7.678783562
N	9.357812495	1.295337271	10.087974510
H	9.957376646	1.531418144	9.265122174
N	11.117420703	-0.370738830	8.790409558
N	11.649684127	0.290360029	6.206692535
H	10.728622708	0.441979154	6.673842703
N	9.735932204	2.173869590	5.644944375
N	7.460906448	1.746709538	6.965032447
H	8.172590289	1.017339865	6.728090937
N	7.637229531	-0.816816746	7.931714627
N	8.963430414	-2.562829217	6.328806990
H	8.338159924	-1.813897559	5.955059171
N	9.341966570	-1.007379817	4.095144762
N	7.248958991	0.575302402	3.544621496
H	7.209544884	-0.316844056	4.089023702
N	5.296848696	-0.261741301	5.289230896
C	10.774885762	5.323136067	7.514865293
C	10.754595348	6.382879067	6.631328752
H	11.643448664	6.638540071	6.029076263
C	9.588319360	7.178656851	6.497649266
H	9.604763824	8.009823403	5.792125742

C	8.470221182	6.913996033	7.254920895
H	7.563161666	7.519174125	7.169371418
C	8.467159769	5.828817622	8.174336290
C	7.322986213	5.481667090	8.982414789
C	7.348742489	4.360192247	9.797727358
H	6.512965692	4.052301293	10.424653689
C	8.524310074	3.573456016	9.797290795
C	9.615574193	4.991572950	8.290645215
C	5.023588618	6.011094296	9.524285535
H	4.607675528	5.143070358	8.984257895
H	5.214852124	5.760023613	10.579457499
C	4.190197090	7.291730145	9.345064366
H	4.355584124	7.661441650	8.298818866
C	4.647170894	8.376378488	10.322931393
H	5.723862528	8.566210059	10.218506904
H	4.127309052	9.323339140	10.140243402
H	4.462377793	8.096018074	11.365977357
C	2.708484766	6.954778920	9.531085006
H	2.501704671	6.543711273	10.525850731
H	2.087374305	7.852588120	9.424198389
H	2.356887730	6.228895541	8.789330901
C	8.531072775	2.284933334	10.615104950
C	9.567043330	-0.000301454	10.638192600
C	8.910709917	-0.491113965	11.751131968
H	8.167331679	0.124987629	12.272396068
C	9.195340626	-1.795598246	12.234324660
H	8.652709830	-2.142675270	13.113446029
C	10.131821703	-2.597784414	11.625679766
H	10.362791201	-3.598161201	11.993366851
C	10.822965920	-2.128796758	10.473652675
C	11.807652541	-2.905746181	9.750709056
C	12.397369540	-2.424056224	8.592943962
H	13.143451903	-2.972418613	8.025250928
C	11.995859516	-1.139319666	8.144881781
C	10.532017757	-0.843418101	9.954906560
C	12.893058714	-5.071679725	9.618886230
H	12.468585182	-5.211808297	8.611720516
H	13.919908332	-4.676979784	9.559268816
C	12.765575996	-6.317145161	10.514707164
H	12.791510726	-5.966268545	11.581077294
C	11.425793689	-7.013706202	10.268784442
H	11.372924861	-7.471498076	9.275227290
H	11.244734650	-7.803158262	11.004490196
H	10.595679452	-6.294865299	10.341467465

C	13.949365472	-7.254203877	10.268647784
H	14.906551586	-6.765625371	10.484113348
H	13.886744570	-8.138861416	10.914237095
H	13.979979628	-7.614228276	9.234103318
C	12.573582218	-0.533871763	6.870224969
C	11.945678801	1.240384488	5.193560512
C	13.121072442	1.273122325	4.467661859
H	13.904657098	0.529731480	4.657367424
C	13.331578807	2.287981138	3.497609976
H	14.274993310	2.282012093	2.949947856
C	12.395351487	3.267911671	3.262544324
H	12.557697976	4.057746602	2.528768589
C	11.173672200	3.269800622	3.991877554
C	10.144058125	4.276860060	3.853330507
C	8.970347425	4.216920897	4.587331579
H	8.171781069	4.949756650	4.509845151
C	8.815324737	3.123218155	5.477451385
C	10.923266564	2.242769554	4.934355559
C	9.584522996	6.404637364	2.829908562
H	8.747927432	6.072325893	2.193302174
H	9.215892463	6.721332016	3.818623782
C	10.480715838	7.460115403	2.155883648
H	10.938109334	6.988711404	1.247496001
C	11.608652407	7.895884603	3.092538832
H	12.175103091	7.024967182	3.450544524
H	12.315627796	8.560741052	2.585336687
H	11.244415899	8.429587657	3.977858087
C	9.616537557	8.646532602	1.722400533
H	9.139175565	9.142592079	2.574514740
H	10.225839587	9.405290030	1.215957230
H	8.828956417	8.348074567	1.022389217
C	7.573451964	2.995343203	6.347540597
C	6.533158651	1.361286479	7.966395595
C	5.525302921	2.171666312	8.454096657
H	5.364604763	3.163179392	8.017118435
C	4.707200019	1.726628056	9.525270031
H	3.935085815	2.399549593	9.895327574
C	4.883472784	0.486953673	10.095660891
H	4.276870200	0.145293451	10.935379936
C	5.879994944	-0.391859530	9.587781698
C	6.697402728	0.023960116	8.510095593
C	6.115143496	-1.727137992	10.096497922
C	7.042625222	-2.569145611	9.503778900
H	7.262027552	-3.570353298	9.863023049

C	7.771690838	-2.057480261	8.399604115
C	5.440005731	-3.369067951	11.750820167
H	5.282703392	-4.112644815	10.953803422
H	6.445191897	-3.471886953	12.191303797
C	4.311814687	-3.344674271	12.797255050
H	4.276858859	-2.308216270	13.229746847
C	2.961603713	-3.638113104	12.141670652
H	2.895186057	-4.666270820	11.770620660
H	2.136073607	-3.494063089	12.846265662
H	2.788717714	-2.969841969	11.285914383
C	4.621540783	-4.339475113	13.917014300
H	5.548662331	-4.086398179	14.442775764
H	3.818426184	-4.346446211	14.664588391
H	4.715249818	-5.365286899	13.543594324
C	8.808663725	-2.909615221	7.678414045
C	10.131780324	-2.799843058	5.547983441
C	11.087822198	-3.749684475	5.847659568
H	10.952854618	-4.409719003	6.711353078
C	12.268118466	-3.849855797	5.062288026
H	13.008508929	-4.600232689	5.341640843
C	12.491850319	-3.015549169	3.992965069
H	13.409621883	-3.064396016	3.404263259
C	11.514712669	-2.043870424	3.633885970
C	11.669532819	-1.102920873	2.546263754
C	10.687565544	-0.167728550	2.258400770
H	10.771234140	0.573133415	1.465856152
C	9.529830283	-0.165899346	3.076504840
C	10.322911191	-1.939220360	4.392465679
C	13.174096343	-0.291279178	0.821882326
H	12.471074489	-0.454367696	-0.010557503
H	13.071671581	0.730505556	1.222137686
C	14.625124805	-0.674557843	0.479665470
H	14.702596355	-1.792809512	0.546076519
C	15.599693864	-0.065863990	1.489640451
H	15.312379293	-0.330676720	2.517813006
H	16.619067686	-0.434844266	1.331669399
H	15.638972555	1.025876496	1.421757949
C	14.948325133	-0.240679406	-0.951342765
H	14.868644692	0.844456050	-1.080515061
H	15.974341493	-0.518829453	-1.223077198
H	14.281735950	-0.713625527	-1.680985333
C	8.439147666	0.877106810	2.870268290
C	6.173976130	1.466532309	3.799610982
C	6.057080508	2.723258476	3.232721669

H	6.799342466	3.067352012	2.502149246
C	4.995700340	3.582798463	3.611933695
H	4.945570922	4.571451826	3.154925020
C	4.061816612	3.198504027	4.547417661
H	3.258959550	3.864364377	4.864636832
C	4.138426627	1.906445946	5.133773555
C	3.210765241	1.423046844	6.134747723
C	3.332337551	0.153932516	6.663539608
H	2.673283344	-0.246409461	7.430775731
C	4.405567195	-0.657236041	6.190038060
C	5.178954347	1.019899011	4.758616315
C	4.537904678	-2.041949777	6.767990224
C	5.701060331	-4.130417393	6.559176320
H	5.828923846	-4.152649112	7.646579878
H	4.851058835	-4.744701891	6.249469565
H	6.623097920	-4.406801090	6.032049503
C	1.211593644	1.938606376	7.410734549
H	0.838134320	0.935340307	7.149160716
H	1.665992793	1.931615915	8.414853887
C	0.150496746	3.038896017	7.228816321
H	0.674487778	4.029479844	7.256398583
C	-0.851798660	2.966393440	8.382856538
H	-0.374092522	3.136689490	9.353444244
H	-1.634485877	3.726692871	8.268384427
H	-1.357075771	1.994349223	8.425788123
C	-0.541856842	2.896862769	5.871458124
H	-1.112398969	1.965145814	5.794050702
H	-1.236594327	3.722681281	5.686078508
H	0.198345396	2.896305817	5.058732478

Table S21. Atomic coordinates for the optimized structure of **Q₆(*i*-Bu)** in MOPAC2016 (Fig. S3b(iii), gas phase).

Atom	X	Y	Z
O	15.878482575	14.304653695	4.214121404
O	15.832448476	15.144890867	2.220470222
O	22.166526369	16.695517211	2.702248975
O	20.835895390	12.321504457	0.034593418
O	16.069705517	6.407376573	1.279315810
O	14.560334980	9.879614951	5.031250278
O	17.908684075	16.033684919	8.275309920
O	21.676702087	14.292885711	4.969534155
O	22.758588183	8.051296325	0.617940655
O	18.723029488	6.513451415	3.609914724
O	14.908180240	9.052041025	9.805529866

O	19.012627475	12.485896211	9.355395845
O	25.724498016	12.335204968	5.662136378
O	23.777235473	7.643299598	4.357875393
O	22.161497370	7.461729635	5.930111699
N	18.849150908	14.230000813	2.241713829
N	16.325970747	14.996117049	3.317334858
N	19.056050623	11.664109266	1.362115283
H	18.399222632	11.987001070	2.107254648
N	17.136726573	10.178614550	2.642390910
N	16.513282432	11.119583399	5.072487087
H	17.410772815	11.279765513	4.562140949
N	18.535717924	12.852878830	5.691610282
N	20.878202507	12.153831460	4.620256216
H	20.098924845	11.497561916	4.854957051
N	20.500556046	9.589149652	3.744763786
N	18.656090248	8.232513852	5.149066558
H	19.123685426	9.123278718	5.438539428
N	18.251510833	9.662620904	7.430716028
N	20.414386648	11.026584965	8.228808781
H	20.443053458	10.113883405	7.718197490
N	22.430638356	9.994309460	6.672256086
C	17.562998595	15.770852894	3.618388844
C	17.510405949	16.841885030	4.483465123
H	16.578991427	17.103339198	4.995094831
C	18.672941812	17.624088848	4.715140764
H	18.605143081	18.467625686	5.401712583
C	19.856535492	17.327083506	4.077317659
H	20.758859885	17.925501604	4.235426568
C	19.939356863	16.212365230	3.197845200
C	21.152129088	15.817517350	2.519533207
C	21.192922402	14.658765796	1.755750696
H	22.084378461	14.313935171	1.234558942
C	20.011355832	13.885275623	1.672748516
C	18.793867907	15.392655909	2.988241917
C	23.497752768	16.350240604	2.180772066
H	23.412578951	16.068074995	1.119574928
H	23.873981114	15.507931234	2.785119446
C	24.279281535	17.657278760	2.401848682
H	24.046993079	18.016169053	3.438982523
C	23.827167779	18.726279408	1.404122246
H	22.737810275	18.860644691	1.447410929
H	24.084639842	18.464880197	0.371878593
H	24.287760419	19.696121506	1.621034776
C	25.780654442	17.386579999	2.292730703

H	26.055249914	16.969879674	1.317037702
H	26.133216396	16.686768062	3.064098050
H	26.352765128	18.314860351	2.416123432
C	20.027295568	12.558325887	0.912202338
C	18.786064079	10.364577302	0.853173756
C	19.445838299	9.787820377	-0.214295698
H	20.248627697	10.332939786	-0.725976310
C	19.087788345	8.486475701	-0.658405033
H	19.624917398	8.073843127	-1.512404899
C	18.088604996	7.767438402	-0.046594846
H	17.802475345	6.770072208	-0.383162421
C	17.395054478	8.322460004	1.065779052
C	16.361401845	7.626555214	1.801292915
C	15.754456316	8.203590798	2.906659140
H	14.957982137	7.722557567	3.471632368
C	16.197688264	9.491611370	3.297358511
C	17.738068934	9.616123460	1.529052660
C	15.416259170	5.417020921	2.144608587
H	14.355358902	5.431108947	1.846384954
H	15.526004598	5.693615160	3.206429452
C	16.121314845	4.083664833	1.827389773
H	15.675359061	3.308874559	2.503731465
C	17.617945588	4.189721410	2.121402373
H	17.815307275	4.475463982	3.164302075
H	18.089689452	4.976994237	1.515767443
H	18.139833818	3.251053977	1.923138534
C	15.863837324	3.674832323	0.374587498
H	16.175744004	4.467585661	-0.319032744
H	14.802951304	3.478404250	0.190328073
H	16.420799063	2.770017157	0.110295431
C	15.635398794	10.172529858	4.541531873
C	16.255618558	12.074773165	6.092006265
C	15.077209472	12.176181150	6.804136492
H	14.253716344	11.476761734	6.614490661
C	14.906254455	13.218075726	7.754017945
H	13.954979981	13.272873021	8.285508546
C	15.889397290	14.152525908	7.984390451
H	15.755233498	14.965707881	8.697921397
C	17.124493922	14.069798646	7.283030242
C	18.219145170	15.000357711	7.447687023
C	19.424551356	14.826476536	6.785938384
H	20.278035818	15.488859754	6.895815711
C	19.530642530	13.711946961	5.916249452
C	17.331490452	13.016491969	6.358676382

C	18.927706186	17.061918575	8.508832511
H	19.316768841	17.417520719	7.541930940
H	19.731881890	16.601266077	9.106246366
C	18.142362760	18.136047792	9.282453743
H	17.536812419	17.610790650	10.068063261
C	17.179488104	18.883791654	8.357036209
H	16.524448859	18.179734156	7.826062326
H	17.703226603	19.488101489	7.610474833
H	16.534194058	19.563376085	8.925053215
C	19.127588380	19.089270539	9.961048960
H	19.743584567	19.631424618	9.235089782
H	19.801571111	18.561599086	10.645429269
H	18.594023007	19.842418880	10.554031999
C	20.812649337	13.449880805	5.139738839
C	21.811369405	11.645244169	3.680137568
C	22.910781899	12.337119304	3.211748584
H	23.143679728	13.328516476	3.615742437
C	23.729563957	11.770585222	2.199614433
H	24.577153457	12.352818179	1.838799437
C	23.457707902	10.532791666	1.664299517
H	24.064190316	10.102632109	0.865201702
C	22.356128360	9.774531279	2.150184563
C	21.541633395	10.308054631	3.178316505
C	21.996186187	8.459001472	1.665695539
C	20.959251418	7.742431206	2.243425891
H	20.649552912	6.754214930	1.908105907
C	20.249447487	8.355213644	3.305824825
C	22.499522783	6.736183377	0.032512364
H	23.026306905	6.848714148	-0.933717177
H	21.416555226	6.622373133	-0.141558656
C	23.097121178	5.630763181	0.919559972
H	22.761255723	5.800742321	1.976639665
C	24.624341222	5.695786510	0.900952845
H	24.970287327	6.684374300	1.236446254
H	25.037950950	5.517739204	-0.095865277
H	25.063068204	4.954473083	1.577655334
C	22.576006539	4.270855568	0.447655258
H	22.822968234	4.074323271	-0.601387745
H	21.488943505	4.187421671	0.557818481
H	23.022935612	3.457180748	1.031779994
C	19.137416301	7.589535666	4.010787252
C	17.550769151	7.856288697	5.958108379
C	16.684158141	6.816342054	5.684770574
H	16.861374227	6.170074381	4.818212476

C	15.552746911	6.595882553	6.516053815
H	14.880396317	5.775756863	6.260929118
C	15.293878675	7.391181088	7.607835211
H	14.415663943	7.236332872	8.237202174
C	16.184521018	8.450508348	7.942599683
C	16.029746229	9.322694023	9.086248365
C	16.959015090	10.309089292	9.376787695
H	16.862796900	11.001458967	10.210091225
C	18.078044077	10.421842809	8.512933051
C	17.321228741	8.681475270	7.131908532
C	14.740148761	9.709493601	11.108118392
H	14.351561286	10.721021626	10.906841779
H	15.707566498	9.759288081	11.633497929
C	13.724174513	8.797900127	11.817864816
H	12.870494270	8.618906226	11.112966421
C	14.359238892	7.447900918	12.158561177
H	15.180947583	7.543224556	12.876328806
H	14.765782765	6.971946098	11.255245556
H	13.625952025	6.759752184	12.592555107
C	13.203561309	9.509960869	13.067764101
H	12.690528734	10.446492601	12.823386885
H	14.007677415	9.742975076	13.775034434
H	12.484197594	8.878034010	13.603831514
C	19.184049727	11.440798766	8.759262012
C	21.566967193	11.833794454	8.034279823
C	21.728555314	13.099429551	8.568827414
H	20.953834348	13.522566318	9.219267284
C	22.880821041	13.864951838	8.257258960
H	22.969628630	14.861388587	8.690242885
C	23.856080257	13.380339719	7.416479563
H	24.730502300	13.973546001	7.147232003
C	23.730783502	12.076311248	6.864151580
C	24.688753044	11.500404575	5.945225537
C	24.517126347	10.227064210	5.440940791
H	25.201448469	9.757854737	4.736645796
C	23.354539563	9.510772758	5.849844961
C	22.601963100	11.279929815	7.179329449
C	23.156933501	8.130640299	5.277813469
C	21.843363042	6.128593677	5.441658188
H	20.851152349	5.953743712	5.875961238
H	22.589633745	5.429906710	5.828974575
H	21.817239097	6.114489907	4.345897167
C	26.663181308	11.934353807	4.606470280
H	26.099745122	11.588265831	3.724003259

H	27.290557962	11.124281314	5.009566606
C	27.435639649	13.241135946	4.353709242
H	27.677526068	13.692605764	5.352293060
C	28.739164417	12.929628927	3.618270581
H	28.562760245	12.486517924	2.631682015
H	29.369213977	12.233362860	4.184356179
H	29.329041723	13.840832867	3.460649968
C	26.553614555	14.223246828	3.580130687
H	25.580893706	14.337278398	4.083351483
H	26.371263976	13.893319544	2.552331451
H	27.010760426	15.220366529	3.524186353
O	12.105404278	9.792523063	6.769876027
H	12.865944256	9.699021782	6.138844346
C	12.587618189	9.818601596	8.115412685
H	12.930685300	8.819933135	8.412229494
H	13.403621728	10.541372096	8.223436147
H	11.716924895	10.121533134	8.706828038

Table S22. Atomic coordinates for the optimized structure of **Q₆(*i*-Bu)** in MOPAC2016 (Fig. S1c(i), gas phase).

Atom	X	Y	Z
O	13.244814416	23.609737301	7.407857259
O	14.281499380	25.333614471	8.198166491
O	7.641735522	26.866674834	8.865464429
O	8.924356243	22.595841264	11.618219359
O	13.083476740	16.248279083	10.742751318
O	14.584424394	19.134934960	6.492523953
O	11.716118763	25.462776163	3.150865945
O	7.964169605	24.214083491	6.698922239
O	6.470177184	18.182922838	11.244501471
O	10.554349206	16.455225136	8.303068042
O	13.881760493	18.801939573	1.842279188
O	9.829673329	22.185709223	2.309265312
O	3.322291609	22.544821375	6.375585860
O	5.117528662	17.759464841	7.692336182
O	6.656678223	17.519185998	6.051103602
N	10.836027169	24.207262544	9.135378965
N	13.295581140	24.769565707	7.753442399
N	10.436717181	21.649630472	10.145883465
H	11.042183568	21.834274125	9.315849755
N	12.136570630	19.853305194	8.923932459
N	12.696362376	20.467402273	6.384568419
H	11.814449286	20.710669669	6.894906145
N	10.863964296	22.403375425	5.816822881

N	8.561802587	22.013877586	7.077915648
H	9.251958166	21.268241605	6.815810761
N	8.755951568	19.456412513	8.020120638
N	10.119011928	17.729644223	6.424849021
H	9.518318839	18.504409303	6.059742396
N	10.495302675	19.270539378	4.188414485
N	8.452301341	20.907182865	3.655226711
H	8.394407115	20.009244461	4.192707253
N	6.481309625	20.043052069	5.328978514
C	12.085332881	25.620792188	7.588499098
C	12.146618316	26.707548813	6.740111379
H	13.059259686	26.921771043	6.174342588
C	11.025141323	27.563126148	6.592958975
H	11.098593227	28.408932364	5.908804088
C	9.873937618	27.334750235	7.312537846
H	9.000682156	27.988066112	7.218619045
C	9.791221065	26.228972069	8.201811232
C	8.613932634	25.931480490	8.985070563
C	8.565373712	24.799749020	9.784335848
H	7.699343328	24.523130100	10.384261969
C	9.702623122	23.959243131	9.803780674
C	10.893318838	25.333291708	8.331293588
C	6.360331184	26.631852606	9.549357885
H	5.851222821	25.813644846	9.012093301
H	6.547674115	26.352918332	10.598493976
C	5.655663987	27.991683557	9.400211427
H	5.798361924	28.334630599	8.341758978
C	6.283127781	29.027334807	10.335687561
H	7.364954103	29.104483244	10.161069554
H	5.851057836	30.021360645	10.179519650
H	6.139579936	28.771062655	11.391221377
C	4.160547707	27.814425325	9.673404735
H	3.969054832	27.439701883	10.685216588
H	3.630530980	28.770692415	9.587079104
H	3.692447413	27.121840790	8.964919213
C	9.643213691	22.682456581	10.636738727
C	10.606437265	20.373130101	10.753360211
C	9.929463578	19.954300018	11.882445454
H	9.186590729	20.608033141	12.357739222
C	10.193423982	18.677967033	12.447698751
H	9.634577823	18.390652951	13.338456725
C	11.130989623	17.833787771	11.902352429
H	11.357001049	16.860202989	12.338194051
C	11.831780091	18.220949316	10.724764979

C	12.807143951	17.388916730	10.056665482
C	13.387821517	17.776990422	8.856190670
H	14.115106094	17.176719303	8.313210236
C	12.992636114	19.026223684	8.317675654
C	11.555902042	19.473082338	10.121925976
C	13.893602605	15.236837777	10.053999424
H	13.325075853	14.908300347	9.164852563
H	14.852890550	15.701856698	9.757933914
C	14.072799710	14.131719334	11.105400850
H	14.079781974	14.620169026	12.115665925
C	12.903640264	13.144502041	11.052906067
H	12.885863228	12.578391396	10.113903708
H	12.946925892	12.423224447	11.876996284
H	11.942255986	13.670377772	11.129103573
C	15.415895378	13.437096400	10.870544436
H	16.258014662	14.140442174	10.933357408
H	15.597728598	12.657905392	11.616150707
H	15.475603869	12.978205339	9.872886895
C	13.538455432	19.524869601	6.981975583
C	13.007665335	21.355611449	5.322771303
C	14.144367624	21.293722531	4.541172886
H	14.873129670	20.491178999	4.695343604
C	14.377956507	22.283324148	3.548436619
H	15.288050056	22.200848787	2.952842050
C	13.505757097	23.328149138	3.347909976
H	13.690798604	24.097911827	2.598273560
C	12.317194140	23.420577221	4.126182611
C	11.337135685	24.479643196	4.013047366
C	10.168007544	24.466946773	4.757314846
H	9.397817855	25.230056956	4.687600553
C	9.973704669	23.380877234	5.647122801
C	12.038926160	22.415760633	5.084274738
C	10.822758933	26.613479608	2.985771822
H	10.005661566	26.289690569	2.318984778
H	10.422481034	26.922788987	3.965154518
C	11.729332157	27.682173913	2.348751389
H	12.203407912	27.233546824	1.437710555
C	12.841668403	28.099751098	3.313819566
H	13.405375101	27.218986173	3.652664305
H	13.554196409	28.777025341	2.830293474
H	12.453810619	28.611879531	4.199931554
C	10.864073602	28.874360170	1.932932339
H	10.370871646	29.344393481	2.791143183
H	11.470938448	29.649287447	1.449241280

H	10.085505059	28.585098472	1.217757787
C	8.721361057	23.278281824	6.507400657
C	7.630094620	21.620763679	8.072767591
C	6.617577132	22.421038413	8.563982820
H	6.458672857	23.419997177	8.144008855
C	5.789411946	21.952529121	9.617805179
H	5.005720354	22.613843737	9.986436429
C	5.969141658	20.707155929	10.173840985
H	5.350925191	20.349896265	10.999114284
C	6.982392072	19.843253092	9.671842575
C	7.801798231	20.278034408	8.602431541
C	7.237440095	18.509598168	10.172496157
C	8.185999121	17.689682849	9.580867273
H	8.425640376	16.690511757	9.933995178
C	8.911351903	18.215578609	8.482999306
C	6.605096961	16.824000112	11.788669695
H	6.471044199	16.096423091	10.971798893
H	7.613308010	16.741262988	12.227877086
C	5.479067687	16.770753902	12.834794872
H	5.407974371	17.784779319	13.311384887
C	4.138885216	16.457907274	12.167015998
H	4.113173250	15.449006120	11.741476541
H	3.310177245	16.531371470	12.878483083
H	3.937540120	17.162572286	11.346902557
C	5.832026736	15.738129673	13.908112426
H	6.756728916	15.996298090	14.436020001
H	5.039010541	15.670961863	14.662650548
H	5.955879989	14.734370772	13.486403709
C	9.952220701	17.365150423	7.763049915
C	11.237546094	17.416175167	5.598270677
C	12.137707359	16.399037778	5.845012533
H	12.008039166	15.748741395	6.715465337
C	13.242765049	16.195157777	4.973885215
H	13.925675794	15.362027765	5.179547093
C	13.454711633	17.015029516	3.891282914
H	14.284180535	16.871679985	3.196226298
C	12.556784109	18.081580716	3.616460528
C	12.737296504	19.025755417	2.534729016
C	11.812237491	20.026790033	2.291893631
H	11.913420677	20.766507701	1.501637193
C	10.690167266	20.093372229	3.155756305
C	11.423121737	18.272398490	4.439926482
C	14.246850788	19.736048519	0.771359794
H	13.443762606	19.735360720	0.016959400

H	14.367468185	20.739802376	1.208778194
C	15.558840960	19.117614863	0.257329118
H	15.417905976	18.001179935	0.229271491
C	16.714728596	19.424332657	1.212567072
H	16.458869033	19.125669281	2.238865244
H	17.617006969	18.871157388	0.927235286
H	16.973405237	20.486432668	1.224883519
C	15.830345570	19.623741059	-1.159792737
H	15.929833819	20.713475107	-1.196921047
H	16.761115324	19.198679625	-1.555678121
H	15.027970476	19.339750233	-1.850803134
C	9.642256335	21.180713016	2.969948852
C	7.377457173	21.799435456	3.891137209
C	7.272308821	23.066794327	3.347068827
H	8.037266795	23.429601231	2.650457322
C	6.189240847	23.908586747	3.706328216
H	6.145691534	24.906440869	3.268823551
C	5.219900009	23.494040667	4.591796887
H	4.394728384	24.143056281	4.885803815
C	5.286856977	22.189974890	5.153876312
C	4.319102754	21.662320405	6.091063849
C	4.444532737	20.388659929	6.609914431
H	3.756862148	19.963793940	7.337063662
C	5.562289756	19.612869615	6.184214289
C	6.355940868	21.327984356	4.809265468
C	5.720041502	18.225690571	6.750104806
C	6.918626877	16.159359967	6.497323617
H	7.029389006	16.127625836	7.586327151
H	6.098035447	15.517656000	6.164845264
H	7.859062627	15.924492679	5.980857074
C	2.183268613	22.058729212	7.162211431
H	1.867928255	21.071756876	6.787027337
H	2.516193756	21.986414838	8.209956629
C	1.122242653	23.149518003	6.932484158
H	1.608836191	24.143597733	7.108067038
C	-0.013875023	22.954903957	7.938533124
H	0.338089238	23.020929781	8.973433474
H	-0.787616984	23.721201113	7.808253270
H	-0.504847317	21.982260176	7.815579853
C	0.613161730	23.106874141	5.490118998
H	0.079393320	22.176847539	5.266377518
H	-0.070226507	23.936470279	5.282133952
H	1.450590765	23.181156891	4.781653056
O	15.766222618	14.364188044	3.961683406

O	15.615878033	15.338022870	2.036330972
O	21.985260738	16.900809589	2.770684537
O	20.779718110	12.501548829	0.096829350
O	16.186650406	6.452751255	1.271722404
O	14.264041830	10.195174486	4.659180569
O	17.582323792	16.336641415	7.859765910
O	21.511218144	14.348538792	4.936402029
O	22.727285368	8.091325371	0.661269484
O	18.649969671	6.516498169	3.594128870
O	14.760463255	9.110784756	9.726995589
O	18.786084937	12.629080793	9.168170631
O	25.591929013	12.392793748	5.659389523
O	23.673832190	7.700591484	4.382834121
O	22.044341862	7.504947662	5.935789236
N	18.692423584	14.420865118	2.190450263
N	16.144905575	15.148252159	3.112295348
N	18.980786480	11.817617449	1.380062940
H	18.292375807	12.125637722	2.104078185
N	17.047548043	10.296953401	2.583219373
N	16.349343293	11.120853216	5.072652861
H	17.333620498	11.130984208	4.729387275
N	18.345184229	12.928384126	5.618305671
N	20.704977373	12.213015447	4.585723391
H	19.917865728	11.562494024	4.806252065
N	20.386030191	9.616042217	3.733034904
N	18.558976300	8.239715171	5.125361711
H	19.043708534	9.115929326	5.433276549
N	18.099551342	9.726943389	7.345382399
N	20.242087726	11.127653051	8.168091810
H	20.290367895	10.198008587	7.690650548
N	22.279789338	10.068956268	6.653512210
C	17.327111205	15.991706689	3.438913893
C	17.197222324	17.115616738	4.224780062
H	16.232327951	17.399765421	4.669865349
C	18.333910110	17.934444339	4.468416555
H	18.202550781	18.821326043	5.094131045
C	19.560703145	17.617358069	3.933723906
H	20.441468372	18.242565457	4.110219363
C	19.718489163	16.450768755	3.132299151
C	20.972224620	16.027056021	2.552618621
C	21.056350157	14.846299633	1.826081628
H	21.978681336	14.489441167	1.370538853
C	19.885073579	14.065668327	1.693809062
C	18.596932129	15.606362070	2.896674962

C	23.342767596	16.502775175	2.366430815
H	23.326768303	16.153472199	1.321979810
H	23.657672259	15.693060431	3.046661607
C	24.144555178	17.802458080	2.553209635
H	23.897323997	18.214243971	3.566563852
C	23.740343137	18.833216934	1.496332532
H	22.656146010	19.009911092	1.524424154
H	23.991453066	18.504750569	0.481927975
H	24.239296614	19.793796116	1.661570943
C	25.640985667	17.489593935	2.491548037
H	25.925338327	17.021303079	1.542339190
H	25.956944426	16.818550584	3.301778825
H	26.236565889	18.406076610	2.584516708
C	19.943482499	12.730891943	0.952614505
C	18.764557347	10.508829202	0.866770126
C	19.474035394	9.946431773	-0.176494108
H	20.275044494	10.511551560	-0.668786502
C	19.175165677	8.629511263	-0.618738058
H	19.751093856	8.230716331	-1.453941641
C	18.187677607	7.878069403	-0.026357765
H	17.953915153	6.865155970	-0.356021300
C	17.437408224	8.421080008	1.054780054
C	16.405935082	7.698561585	1.767410230
C	15.730049423	8.275772508	2.831622339
H	14.931289718	7.777314182	3.374087036
C	16.102669570	9.590458525	3.205814350
C	17.717264934	9.732845895	1.509975306
C	15.541575859	5.468744898	2.151839011
H	14.469170987	5.507567818	1.905128808
H	15.716731816	5.734291405	3.211049375
C	16.203066280	4.124111762	1.791731835
H	15.741950212	3.345634889	2.453108483
C	17.705039291	4.186996825	2.072620493
H	17.916878872	4.412849198	3.127416686
H	18.178239858	5.002844235	1.506543951
H	18.211031491	3.254221460	1.816269785
C	15.921895470	3.762373814	0.331165800
H	16.264349747	4.561624091	-0.340412984
H	14.853562362	3.614299823	0.144945093
H	16.439538537	2.843218395	0.039457146
C	15.436208892	10.315504783	4.370827776
C	16.020517687	12.228793148	5.898961200
C	14.763580868	12.465480482	6.423975194
H	13.949096866	11.756132593	6.236667468

C	14.507559254	13.659334784	7.145208973
H	13.490172125	13.829510575	7.510055533
C	15.496495181	14.591240045	7.364951248
H	15.304967904	15.536953416	7.877874161
C	16.816582783	14.353193011	6.896232833
C	17.924373351	15.260643644	7.104107400
C	19.171875497	15.009363388	6.556327162
H	20.025233665	15.672712297	6.666612229
C	19.321832050	13.818927720	5.800258258
C	17.091054470	13.179622895	6.152705056
C	18.632262267	17.304138612	8.207089769
H	19.028830753	17.739141176	7.276984762
H	19.422357983	16.765075680	8.755467953
C	17.872693061	18.318235666	9.082267491
H	17.145249243	17.742883311	9.715291671
C	17.083329936	19.297667557	8.217455206
H	16.401337940	18.766317630	7.529856320
H	17.723275316	19.940947692	7.608440088
H	16.454553504	19.958946883	8.825390532
C	18.867436848	19.036087753	9.998386829
H	19.607071471	19.610925414	9.430548871
H	19.403587617	18.337343031	10.649512001
H	18.345881788	19.749828203	10.649663266
C	20.632161912	13.516323189	5.088050782
C	21.661366549	11.698005124	3.672702660
C	22.760969829	12.400306522	3.217921353
H	22.974912309	13.398517302	3.615598399
C	23.607668872	11.838220430	2.227569710
H	24.452046650	12.431315537	1.876034009
C	23.366432644	10.590939524	1.700203216
H	23.996352947	10.163062962	0.918461340
C	22.267224204	9.820734995	2.173040268
C	21.423206863	10.350881932	3.179518345
C	21.940929766	8.494898822	1.693919814
C	20.909413185	7.762099260	2.260989362
H	20.628637591	6.764324957	1.928504669
C	20.169220114	8.371463157	3.303516254
C	22.506386530	6.763786170	0.088454994
H	23.070778179	6.870856698	-0.857343285
H	21.432882100	6.635131299	-0.127812767
C	23.076708102	5.676403517	1.014952457
H	22.722542025	5.877599537	2.060905825
C	24.604344864	5.728701583	1.026286440
H	24.951773200	6.722606562	1.344810386

H	25.037165455	5.521948068	0.043076563
H	25.021403968	5.001106143	1.731422183
C	22.553098755	4.307520009	0.572693055
H	22.817951171	4.078540548	-0.465038603
H	21.463048749	4.236546188	0.662697749
H	22.979214140	3.507628189	1.190830843
C	19.056569701	7.594006165	3.995553835
C	17.428285734	7.884289553	5.906590494
C	16.553940021	6.853935363	5.624627676
H	16.735792468	6.198059764	4.764839852
C	15.403995000	6.654401315	6.436883420
H	14.725990976	5.842151366	6.172545302
C	15.137802755	7.457423668	7.520833068
H	14.247783712	7.317147427	8.136943348
C	16.034116549	8.510578639	7.861533037
C	15.868711008	9.393885085	8.995347160
C	16.788910453	10.395045718	9.270332974
H	16.691645489	11.089034087	10.101921357
C	17.906964535	10.509637025	8.408346185
C	17.180902104	8.730088686	7.062607630
C	14.542436924	9.869194318	10.966091632
H	14.086960679	10.828868759	10.662822769
H	15.500835995	10.034378227	11.483612043
C	13.589394670	8.972625918	11.772216967
H	12.737280870	8.681856802	11.104591411
C	14.304955490	7.697437275	12.224613997
H	15.124638119	7.903913213	12.920872272
H	14.735915841	7.167927058	11.363196197
H	13.618090557	7.007628608	12.725690383
C	13.050487246	9.772244202	12.961773726
H	12.501568295	10.666576280	12.639669413
H	13.850802227	10.097981417	13.636155192
H	12.360278715	9.165065821	13.560122326
C	18.991256016	11.557251029	8.631779412
C	21.394812325	11.934769413	7.969005585
C	21.548540086	13.209679497	8.483523060
H	20.761173624	13.647672954	9.108423857
C	22.708808484	13.967366115	8.182521203
H	22.793483238	14.971036213	8.601063701
C	23.698780689	13.465717871	7.368655613
H	24.580956541	14.051380014	7.106616104
C	23.578727376	12.154096931	6.833992266
C	24.550405836	11.563462443	5.939096193
C	24.386071750	10.282812634	5.452975178

H	25.078299678	9.802597018	4.764038746
C	23.215914514	9.572863830	5.854700732
C	22.443993871	11.363882968	7.142931685
C	23.037399914	8.186846206	5.293628830
C	21.770477061	6.159875771	5.450244800
H	20.780850885	5.953688744	5.875225424
H	22.537395265	5.487088331	5.843112301
H	21.755214786	6.141860486	4.354171076
C	26.546297978	11.972604301	4.625394427
H	25.996397220	11.598766363	3.745830249
H	27.173039077	11.176963576	5.058275802
C	27.318142871	13.274331121	4.346791768
H	27.543720806	13.755861686	5.334923530
C	28.632901892	12.942389197	3.640196619
H	28.468186479	12.473310433	2.663642648
H	29.255028609	12.261660839	4.232470786
H	29.225810470	13.848255581	3.465749564
C	26.454251096	14.234009555	3.525803098
H	25.467428009	14.358201627	3.996349993
H	26.299990494	13.878622584	2.501790234
H	26.915544203	15.227479428	3.458239746
