

Templating Conformations with Cucurbiturils

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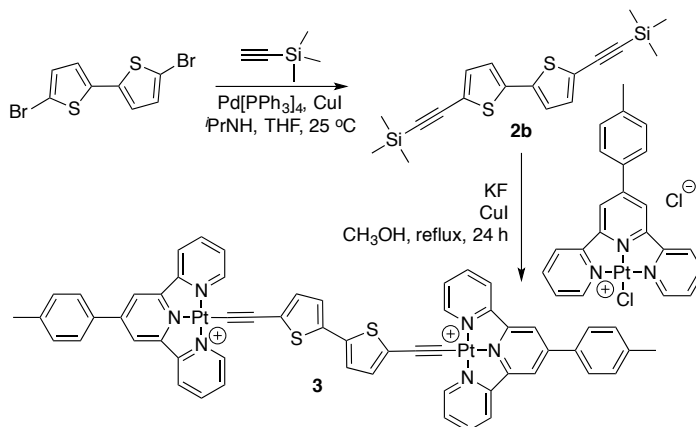
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1. Generalities

Starting materials were purchased from Sigma-Aldrich (St. Louis, MO), AK Scientific (Union City, CA), Oakwood Chemicals (West Columbia, SC), Fischer Scientific (Hampton, NH), Alfa Aesar (Ward Hill, MA), and TCI America (Portland, OR). Cucurbit[8]uril (CB[8])¹ and terpyridyl platinum(II) chlorides² were prepared using known procedures. Characterization by nuclear magnetic resonance spectroscopy (NMR) was carried out using Bruker 500, 700 and 850 MHz spectrometers, available at Ohio University in the first case, and at The Ohio State University, Columbus, OH in the latter two cases. Products were characterized by high resolution mass spectrometry (HRMS) performed at the COSMIC facility of the Old Dominion University (Norfolk, VA) using a Bruker Daltonics 12 Tesla APEX-Qe FTICR mass spectrometer with an Apollo II Ion Funnel.

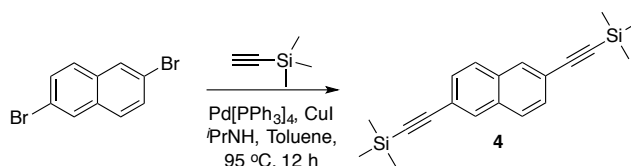
2. Preparation of the Pt(II) complexes and their precursors



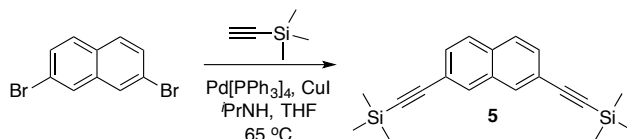
5,5'-Bis[2-(trimethylsilyl)ethynyl]-2,2'-dithiophene (2b).³ 5,5'-Dibromo-2,2'-dithiophene (0.50 g, 1.5 mmol) and trimethylsilylacetylene (0.43 mL, 0.29 g, 6.2 mmol) were dissolved in a mixture of dry THF (15 mL) and diisopropylamine (8.0 mL). Pd[PPh₃]₄ (86 mg, 80 μmol) and CuI (15 mg, 80 μmol) were then added. The reaction mixture was then stirred overnight at 25 °C, then later treated with water (25 mL), and extracted with CH₂Cl₂ (3 × 15 mL). The combined organic layers were washed with brine (15 mL) and dried over Na₂SO₄. After removal of the solvents under vacuum, the dark-brown crude product was purified by column chromatography (hexanes) affording a flaky yellow solid (0.28 g, 51%). ¹H NMR (500 MHz, CDCl₃): δ = 7.11 (d, *J* = 3.8 Hz, 2H), 6.99 (d, *J* = 3.8 Hz, 2H), 0.25 (s, 18H) ppm. ¹³C NMR (125 MHz, CDCl₃): δ = 138.1, 133.6, 123.9, 122.7, 100.7, 97.3, 0.0 ppm. HRMS (ESI) *m/z* calcd for C₁₈H₂₂S₂Si₂ H⁺ 359.077422, found 359.077248.

Dithiophene 3.² Chloro[4'-(4-methylphenyl)-2,2':6',2''-terpyridine]platinum(II) chloride (15 mg, 24 μmol), 5,5'-bis[2-(trimethylsilyl)ethynyl]-2,2'-dithiophene (**2b**; 4.8 mg, 14 μmol), CuI (3.0 mg, 16 μmol) and KF (6.3 mg, 0.11 mmol) were dissolved in degassed methanol (6.0 mL), and the reaction mixture was stirred at reflux under argon for 24 h. The mixture was then centrifuged. The

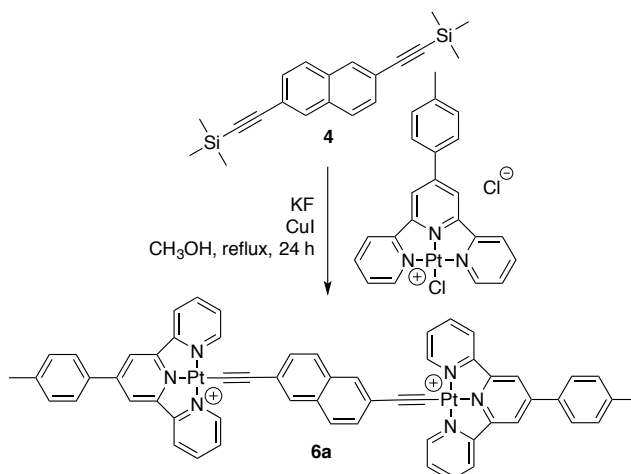
precipitate was separated from the solvent and washed with methanol (4.0 mL) and diethyl ether (4.0 mL). The resulting black solid was dried under high vacuum (12 mg, 72%). ^1H NMR (500 MHz, DMSO- d_6): δ = 9.09 (d, J = 4.4 Hz, 4H), 8.97 (s, 4H), 8.84 (d, J = 8.1 Hz, 4H), 8.55 (t, J = 7.9 Hz, 4H), 8.08 (d, J = 7.9 Hz, 4H), 7.95 (t, J = 6.7 Hz, 4H), 7.48 (d, J = 7.9 Hz, 4H), 7.26 (d, J = 3.7 Hz, 2H), 7.19 (d, J = 3.7 Hz, 2H), 2.44 (s, 6H). ppm. ^{13}C NMR (214 MHz, DMSO- d_6): δ = 158.1, 154.2, 153.5, 152.5, 141.9, 135.0, 131.4, 129.9, 129.6, 127.6, 126.0, 123.7, 120.2, 107.6, 21.0 ppm. HRMS (ESI) m/z calcd for $(\text{C}_{56}\text{H}_{38}\text{N}_6\text{Pt}_2\text{S}_2)^{2+}$ 624.094194, found 624.093466.



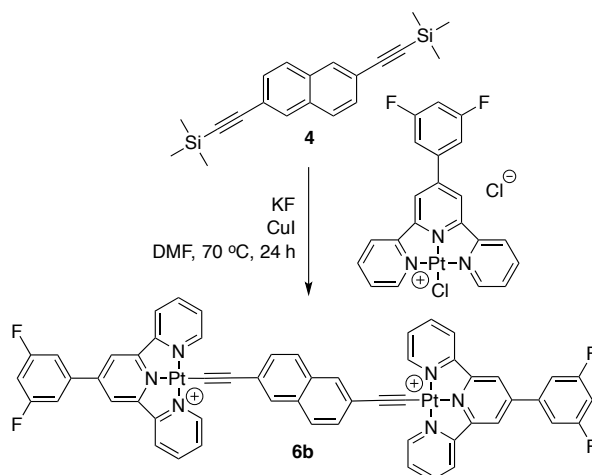
2,6-Bis[2-(trimethylsilyl)ethynyl]naphthalene (4).⁴ 2,6-Dibromonaphthalene (0.50 g, 1.8 mmol) and trimethylsilylacetylene (0.97 mL, 0.67 g, 7.0 mmol) were dissolved in a 1:1 mixture of dry toluene (6.0 mL) and diisopropylamine (6.0 mL). $\text{Pd}[\text{PPh}_3]_4$ (51 mg, 44 μmol) and CuI (8.3 mg, 44 μmol) were then added to the reaction mixture. The brown solution was stirred overnight at 95 °C. The solvent was removed under vacuum, and the resulting brown solid was purified by column chromatography (hexanes) to afford an off-white solid (0.44 g, 79%). ^1H NMR (500 MHz, CDCl_3): δ = 8.08 – 8.05 (m, 2H), 7.82 (d, J = 8.4 Hz, 2H), 7.62 (dd, J = 8.4, 1.5 Hz, 2H), 0.41 (s, 18H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ = 132.5, 131.9, 129.4, 127.8, 121.5, 105.3, 95.6, 0.1 ppm. HRMS (ESI) m/z calcd for $(\text{C}_{20}\text{H}_{24}\text{Si}_2)^+ \text{H}^+$ 641.290584, found 641.289965



2,7-bis[2-(trimethylsilyl)ethynyl]naphthalene (5).⁵ 2,7-Dibromonaphthalene (0.50 g, 1.8 mmol) and trimethylsilylacetylene (0.97 mL, 0.67 g, 7.0 mmol) were dissolved in a mixture of dry THF (25 mL) and diisopropylamine (6.0 mL). $\text{Pd}[\text{PPh}_3]_4$ (0.20 g, 0.18 mmol) and CuI (33 mg, 0.18 mmol) were added to the reaction mixture, which was stirred overnight at 65 °C. The solvent was then removed under vacuum and the resulting brown solid was dissolved in ethyl acetate (50 mL). The solution was then consecutively washed with citric acid (1.0 M in water, 10 mL), concentrated NaHCO_3 (10 mL), and brine (10 mL). The solvent was removed from the combined organic layers, and the resulting solid was purified by column chromatography (hexanes) to afford a white solid (0.53 g, 94%). ^1H NMR (500 MHz, CDCl_3): δ = 7.88 (d, J = 1.4 Hz, 2H), 7.68 (d, J = 8.5 Hz, 2H), 7.46 (dd, J = 8.4, 1.5 Hz, 2H), 0.25 (s, 18H) ppm. ^{13}C NMR (125 MHz, CDCl_3): δ = 132.5, 132.4, 131.8, 129.7, 127.9, 121.3, 105.2, 95.3, 0.1 ppm. HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{24}\text{Si}_2^+$ 320.141105, found 320.140863.

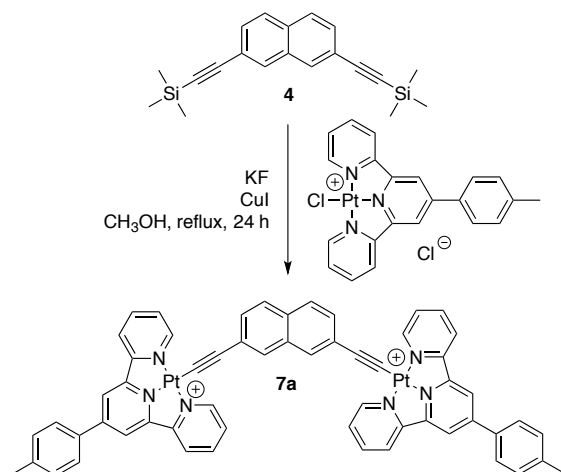


2,6-Disubstituted naphthalene 6a. Prepared similarly to dithiophene **3** with 2,6-bis[2-(trimethylsilyl)ethynyl]naphthalene (**4**; 3.5 mg, 11 μmol). Red solid (14 mg, 84%). ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ = 9.20 (d, J = 5.3 Hz, 4H), 8.88 (s, 4H), 8.82–8.73 (m, 4H), 8.48 (t, J = 8.1 Hz, 4H), 8.02–7.90 (m, J = 9.1 Hz, 10H), 7.69–7.60 (m, 2H), 7.55 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 7.7 Hz, 4H), 2.42 (s, 6H) ppm. ^{13}C NMR (214 MHz, $\text{DMSO}-d_6$): δ = 158.4, 154.3, 153.8, 152.6, 141.9, 141.7, 131.8, 131.4, 130.2, 130.0, 129.9, 129.6, 127.6, 127.0, 126.0, 124.0, 120.8, 120.4, 100.9, 21.0 ppm. HRMS (ESI) m/z calcd for $(\text{C}_{58}\text{H}_{40}\text{N}_6\text{Pt}_2)^{2+}$ 605.129948, found 605.129419.

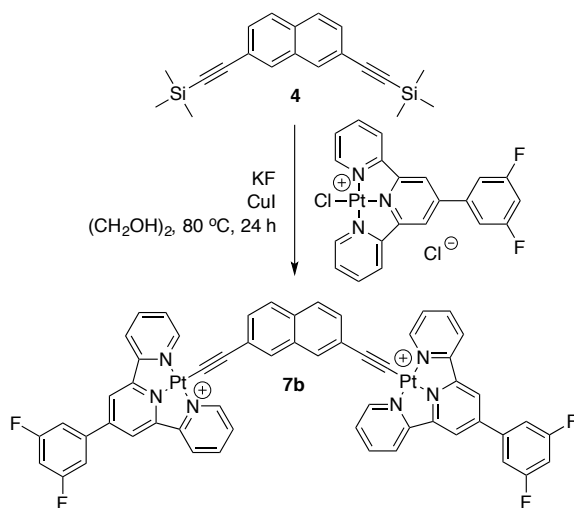


2,6-Disubstituted naphthalene 6b. Chloro[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride (15 mg, 25 μmol), 2,6-bis[2-(trimethylsilyl)ethynyl]naphthalene (3.5 mg, 11 μmol), CuI (3.0 mg, 16 μmol) and KF (6.3 mg, 0.11 mmol) were mixed with dry, degassed DMF (6.0 mL). The solution was stirred at 70 $^{\circ}\text{C}$ for 24 h. Centrifugation and removal of the filtrate afforded a dark red, almost black solid, which was then washed consecutively with dichloromethane (2×5.0 mL) and acetonitrile (5.0 mL) with sonication, and dried under high vacuum (7.4 mg, 45%). ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ = 9.28 (d, J = 5.4 Hz, 4H), 9.04 (s, 4H), 8.81 (d, J = 8.0 Hz, 4H), 8.55 (t, J = 8.0 Hz, 4H), 8.06 – 7.95 (m, 10H), 7.75–7.68 (s, 2H), 7.63 – 7.55 (m, 4H) ppm. ^{13}C NMR (176 MHz, $\text{DMSO}-d_6$): δ = 163.8, 162.3, 158.2, 154.5, 154.1, 149.6, 152.1, 138.2, 132.7, 131.7, 131.5, 130.2–129.9 (t, 24.7 Hz), 129.6, 128.7, 128.6, 127.0, 126.1,

123.9, 121.4, 111.2, 111.1, 106.7, 104.7, 100.5 ppm. HRMS (ESI) m/z calcd for $(C_{56}H_{32}F_4N_6Pt_2)^{2+}$ 627.095454, found 627.094662.



2,7-Disubstituted naphthalene 7a. Prepared similarly to dithiophene **3** with 2,7-bis[2-(trimethylsilyl)ethynyl]naphthalene (**5**; 3.5 mg, 11 μ mol). Red solid (15 mg, 91%). 1H NMR (500 MHz, DMSO- d_6): δ = 9.09 (d, J = 4.4 Hz, 4H), 8.97 (s, 4H), 8.84 (d, J = 8.1 Hz, 4H), 8.55 (t, J = 7.9 Hz, 4H), 8.08 (d, J = 7.9 Hz, 4H), 7.95 (t, J = 6.7 Hz, 4H), 7.48 (d, J = 7.9 Hz, 4H), 7.26 (d, J = 3.7 Hz, 2H), 7.19 (d, J = 3.7 Hz, 2H), 2.44 (s, 6H) ^{13}C NMR (214 MHz, DMSO- d_6): δ = 158.3, 154.2, 153.7, 152.5, 141.8, 141.7, 133.0, 131.9, 130.0, 129.9, 129.7, 129.5, 128.6, 127.7, 127.5, 125.9, 124.7, 120.4, 104.12, 100.85, 21.0 ppm. HRMS (ESI) m/z calcd for $(C_{58}H_{40}N_6Pt_2)^{2+}$ 605.129948, found 605.129383.



2,7-Disubstituted naphthalene 7b. Chloro[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride (10 mg, 16 μ mol), 2,7-bis[2-(trimethylsilyl)ethynyl]naphthalene (2.6 mg, 8.2 μ mol), CuI (3.0 mg, 16 μ mol) and KF (3.8 mg, 66 mmol) were mixed with degassed ethylene glycol (6.0 mL). The solution was stirred at 80 $^{\circ}C$ for 24 h under an argon atmosphere. Water (5.0 mL) was then added. The precipitate was separated by centrifugation and washed with acetone (3 $\times$ 4.0 mL). The dark red solid was then dried under vacuum (2.6 mg, 25%). 1H NMR

(500 MHz, DMSO- d^6): δ = 9.29 – 9.16 (m, 4H), 9.05 (s, 4H), 8.80 (d, J = 7.9 Hz, 4H), 8.62 – 8.50 (m, 4H), 8.12 – 7.82 (m, 12H), 7.68 – 7.54 (m, 4H). ^{13}C NMR (176 MHz, DMSO- d^6): δ = 163.8, 162.4, 158.4, 154.4, 154.2, 149.7, 142.1, 138.3, 132.9, 130.2, 129.9, 129.7, 127.5, 126.1, 124.5, 121.5, 111.3, 111.2, 106.7, 104.6, 100.4. HRMS (ESI) m/z calcd for $(\text{C}_{56}\text{H}_{32}\text{F}_4\text{N}_6\text{Pt}_2)^{2+}$ 627.095454, found 627.095993.

3. Characterization of the Pt complexes/CB[8] assemblies

3 $\mathbf{2}$ ·CB[8] $\mathbf{2}$. ^1H NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 5:2): δ = 9.41 (d, J = 5.6 Hz, 8H), 8.98 (d, J = 8.0 Hz, 8H), 8.57 (t, J = 7.8 Hz, 8H), 8.45 (s, 8H), 7.92 (t, J = 6.6 Hz, 8H), 7.38 (d, J = 3.2 Hz, 4H), 7.33 (d, J = 3.2 Hz, 4H), 7.09 (d, J = 7.7 Hz, 8H), 6.56 (d, J = 7.7 Hz, 8H), 6.15 (d, J = 15.2 Hz, 16H), 5.98 (d, J = 15.2 Hz, 16H), 5.67 (s, 32H), 4.43 (d, J = 15.0 Hz, 16H), 4.36 (d, J = 15.2 Hz, 16H), 2.23 (s, 12H) ppm.

6 $\mathbf{a2}$ ·CB[8] $\mathbf{2}$. ^1H NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 5:2): δ = 9.58 (d, J = 5.5 Hz, 8H), 8.99 (d, J = 8.0 Hz, 8H), 8.54 (t, J = 7.9 Hz, 8H), 8.46 (s, 8H), 7.94 (t, J = 5.9 Hz, 12H), 7.71 (d, J = 8.2 Hz, 4H), 7.62 (d, J = 8.4 Hz, 4H), 7.08 (d, J = 7.7 Hz, 8H), 6.54 (d, J = 7.8 Hz, 8H), 6.12 (d, J = 15.3 Hz, 16H), 5.97 (d, J = 15.2 Hz, 16H), 5.65 (s, 32H), 4.41 (d, J = 15.2 Hz, 16H), 4.35 (d, J = 15.3 Hz, 16H), 2.21 (s, 12H) ppm.

6 $\mathbf{b2}$ ·CB[8] $\mathbf{2}$. ^1H NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 5:2): δ = 9.65 (d, J = 5.7 Hz, 8H), 9.01 (d, J = 8.0 Hz, 8H), 8.60 (s, 8H), 8.55 (t, J = 7.7 Hz, 8H), 8.01 (t, J = 6.7 Hz, 8H), 7.97 (s, 4H), 7.73 (d, J = 8.1 Hz, 4H), 7.64 (d, J = 8.3 Hz, 4H), 6.94 (d, J = 6.7 Hz, 8H), 6.85-6.80 (s, 4H), 6.11 (d, J = 15.4 Hz, 16H), 5.99 (d, J = 15.3 Hz, 16H), 5.67 (s, 32H), 4.50-4.30 (m, 32H) ppm.

7 $\mathbf{a2}$ ·CB[8] $\mathbf{2}$. ^1H NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 5:2): δ = 9.60 (d, J = 5.5 Hz, 8H), 9.01 (d, J = 8.1 Hz, 8H), 8.58 (t, J = 7.8 Hz, 8H), 8.47 (s, 8H), 8.02 (s, 4H), 7.97 (t, J = 6.7 Hz, 8H), 7.81-7.71 (m, 8H), 7.10 (d, J = 7.7 Hz, 8H), 6.57 (d, J = 7.6 Hz, 8H), 6.15 (d, J = 15.2 Hz, 16H), 5.99 (d, J = 15.0 Hz, 16H), 5.67 (s, 32H), 4.43 (d, J = 15.2 Hz, 16H), 4.37 (d, J = 15.2 Hz, 16H), 2.23 (s, 12H) ppm.

7 $\mathbf{b2}$ ·CB[8] $\mathbf{2}$. ^1H NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 5:2): δ = 9.64 (d, J = 5.6 Hz, 8H), 9.00 (d, J = 8.2 Hz, 8H), 8.62 – 8.52 (m, 16H), 8.01 (t, J = 6.4 Hz, 8H), 7.97 (s, 4H), 7.72 (s, 8H), 6.95-6.90 (m, 8H), 6.85-6.79 (m, 4H), 6.10 (d, J = 15.2 Hz, 16H), 5.98 (d, J = 15.3 Hz, 16H), 5.66 (s, 32H), 4.48-4.31 (m, 32H) ppm.

4. General experimental procedure for self-sorting assays

Stock solutions of each 2:2 homoternary Pt complex/CB[8] assembly (0.50 mM with respect to the assembly) were prepared in a 5:2 $\text{D}_2\text{O}:\text{CD}_3\text{CN}$ mixture saturated in free CB[8]. For each self-sorting experiment, solutions of CB[8]-secured Pt dimers bearing tolyl and 3,5-difluoroaryl terpyridyl heads (0.30 mL each) were combined and heated to 40 °C, and the self-sorting process was monitored by ^1H and ^{19}F NMR spectroscopy over time. Ratio α (see equations 1) that corresponds to the concentration of CB[8]-secured heterodimers [AB] relative to the concentration

of CB[8]-secured homodimers bearing tolyl heads [AA] was obtained by integrating relevant ^1H NMR signals (**6a**·**6b**·CB[8]₂: 7.20 (d, heteroternary), 7.10 (d, homoternary); **7a**·**7b**·CB[8]₂: 7.20 (d, heteroternary), 7.10 (d, homoternary); **3**·**6b**·CB[8]₂: 7.15 (d, heteroternary), 7.06 (d, homoternary); **3**·**7b**·CB[8]₂: 9.40 (d, homoternary), 9.09 (d, heteroternary) ppm). Similarly, ratio β (see equations 1) that corresponds to the concentration of CB[8]-secured heterodimers [AB] relative to the concentration of CB[8]-secured homodimers bearing difluoroaryl heads [BB] was obtained by integrating relevant ^{19}F NMR signals (**6a**·**6b**·CB[8]₂: -106.70 (s, homoternary), -107.75 (s, heteroternary); **7a**·**7b**·CB[8]₂: -106.70 (s, homoternary), -107.75 (s, heteroternary); **3**·**6b**·CB[8]₂: -106.71 (s, homoternary), -107.79 (s, heteroternary); **3**·**7b**·CB[8]₂: -106.70 (s, homoternary), -107.79 (s, heteroternary) ppm). Both ratios are used to calculate the equilibrium constant K and the free energy term of the self-sorting process ΔG (see equation 2). Self-sorting was monitored before and after equilibrium was reached, until at least 3 free energy terms ΔG returned a standard deviation of less than 0.02 kcal/mol (all cases but one), or until the standard deviation remained steady after 7 measurements (pair **6a**₂·CB[8]₂ and **6b**₂·CB[8]₂; standard deviation 0.09 kcal/mol; see Figure S1).

$$\text{Let } \alpha = \frac{[\text{AB}]}{[\text{AA}]} \text{ and } \beta = \frac{[\text{AB}]}{[\text{BB}]} \quad (1)$$

$$\Delta G = -RT \ln K = \frac{[\text{AB}]^{1/2} [\text{BA}]^{1/2}}{[\text{AA}]^{1/2} [\text{BB}]^{1/2}} = \frac{[\text{AB}]/2}{[\text{AA}]^{1/2} [\text{BB}]^{1/2}} = \frac{\sqrt{\alpha\beta}}{2} \quad (2)$$

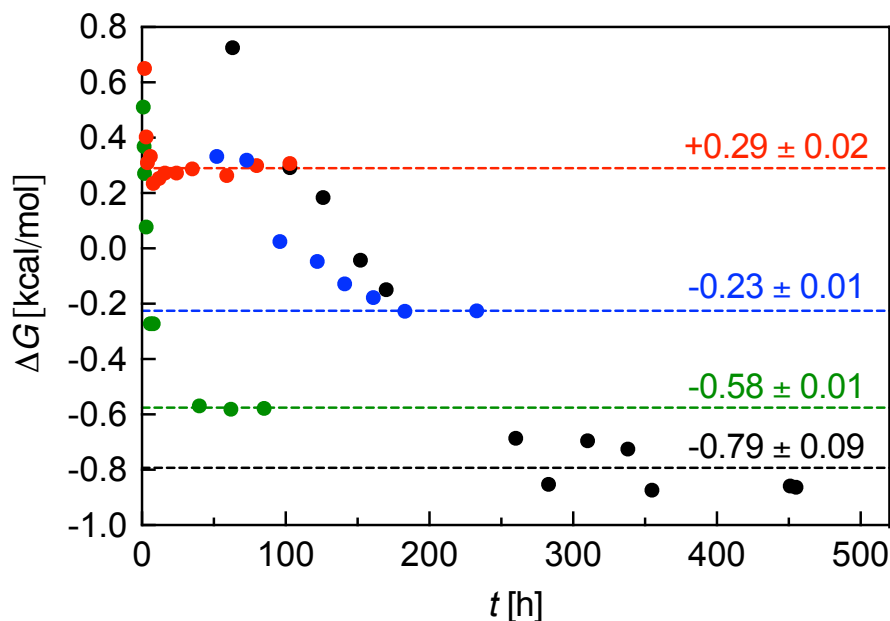


Figure S1. Free energy term ΔG [kcal/mol] of the self-sorting process as a function of time [h], between pairs of assemblies **3**₂·CB[8]₂ and **6b**₂·CB[8]₂ (in blue), **3**₂·CB[8]₂ and **7b**₂·CB[8]₂ (in red), **6a**₂·CB[8]₂ and **6b**₂·CB[8]₂ (in black), and **7a**₂·CB[8]₂ and **7b**₂·CB[8]₂ (in green). Average ΔG terms at equilibrium used in the narrative are displayed with dashed lines of the relevant color.

5. ^1H and ^{13}C NMR spectra of the Pt(II) complexes and their precursors.

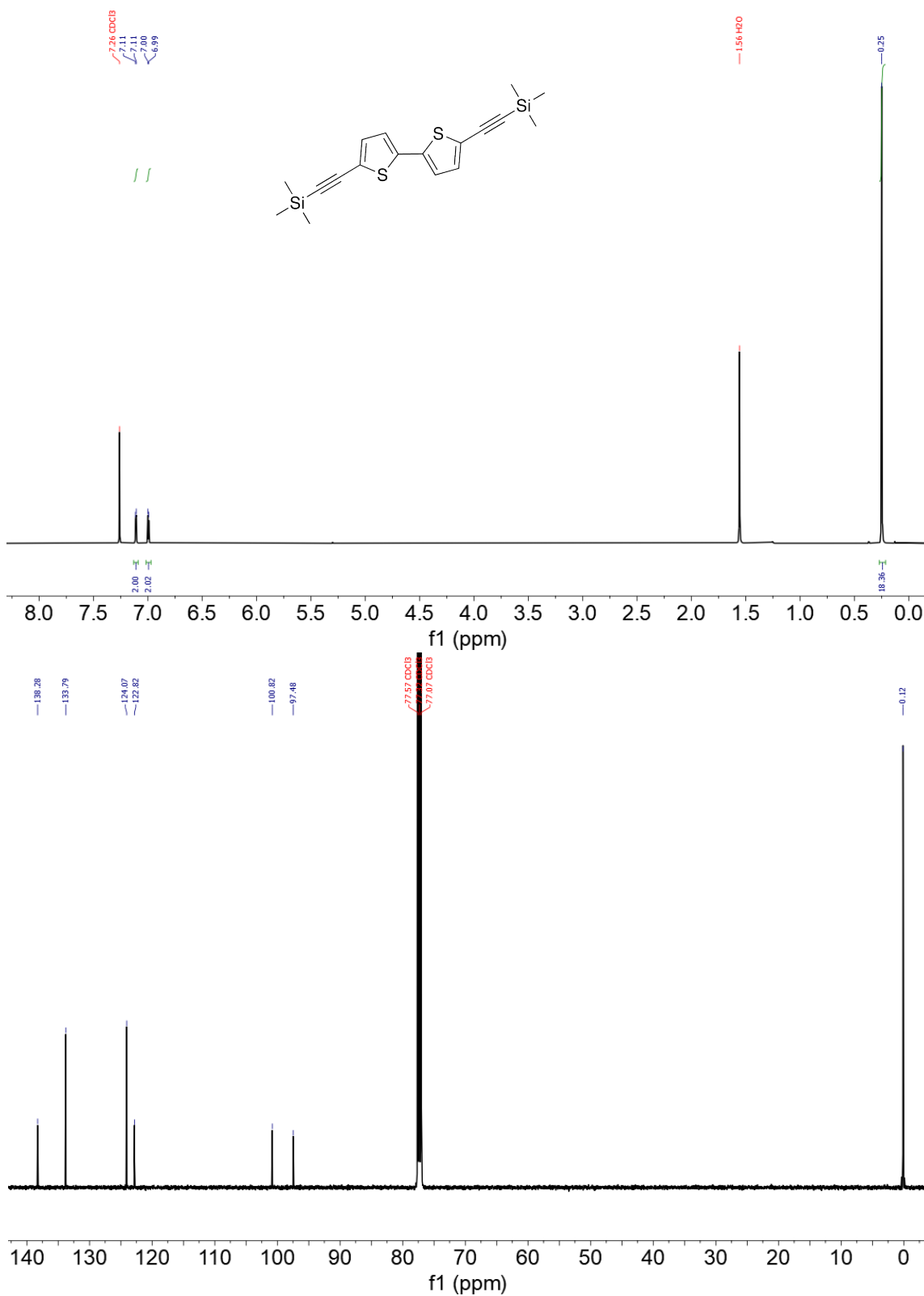


Figure S2. (top) ^1H NMR and (bottom) ^{13}C NMR spectra of dithiophene **2b** in CDCl_3 .

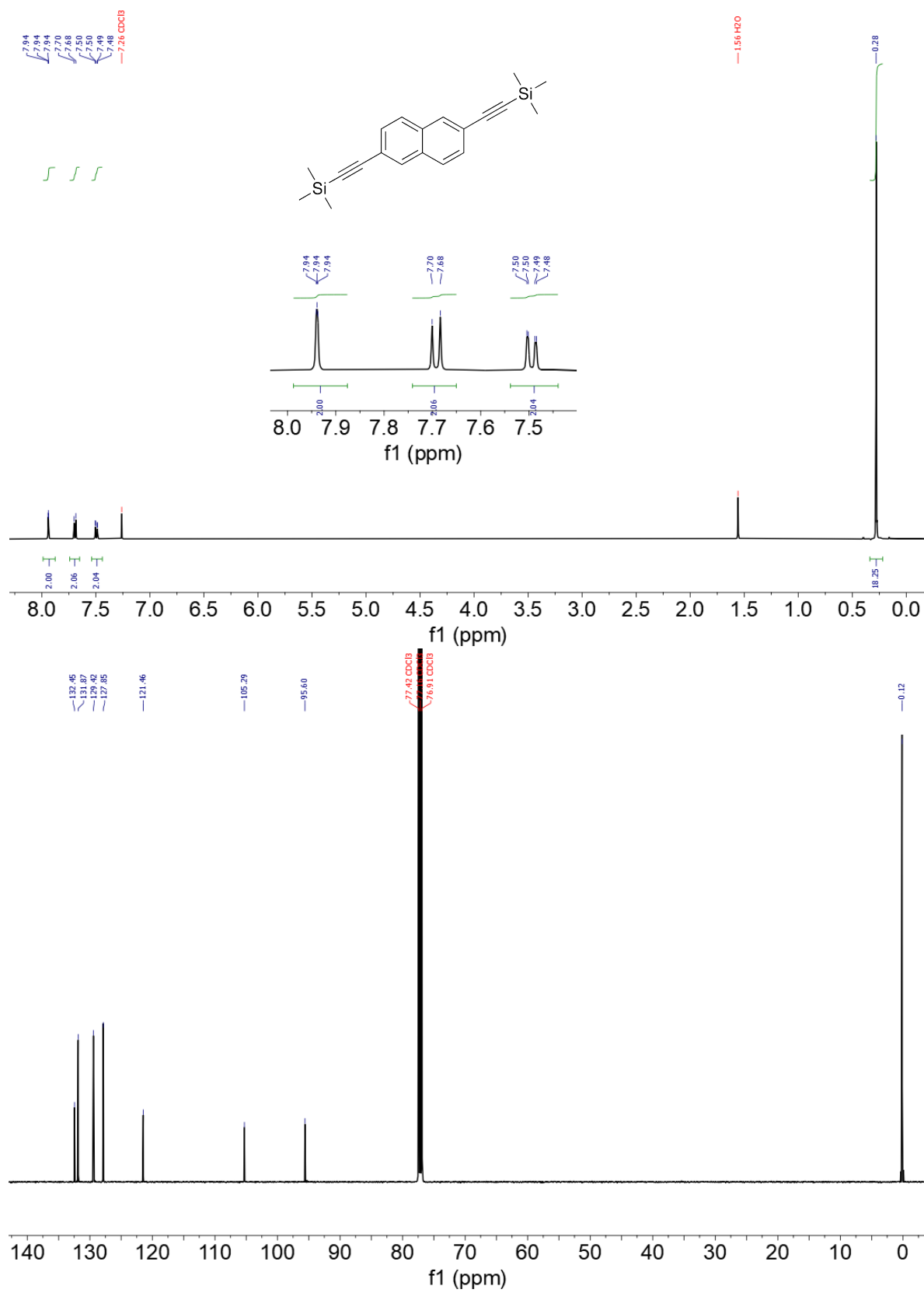


Figure S3. (top) ^1H NMR and (bottom) ^{13}C NMR spectra of naphthalene **4** in CDCl_3 .

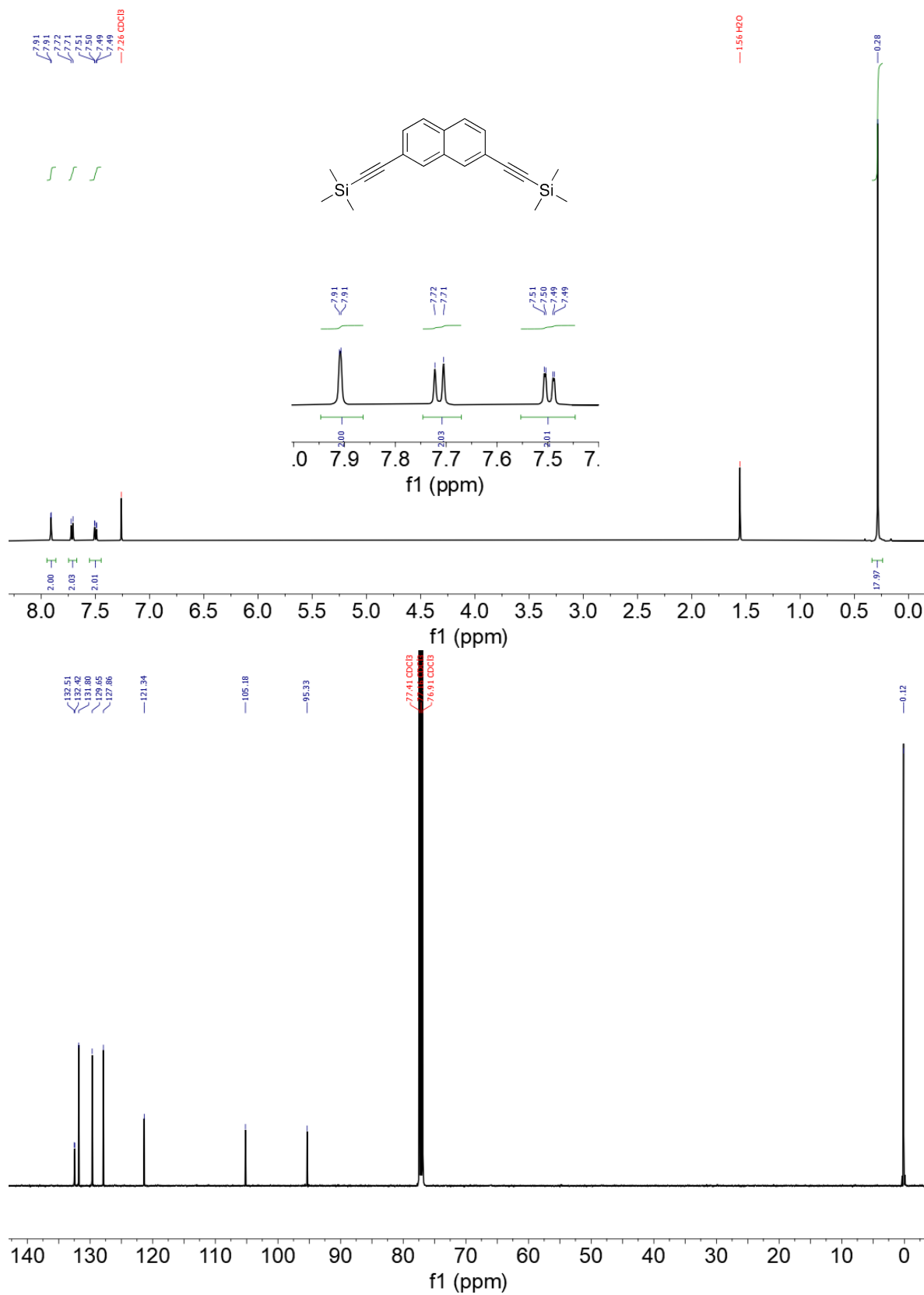


Figure S4. (top) ^1H NMR and (bottom) ^{13}C NMR spectra of naphthalene **5** in CDCl_3 .

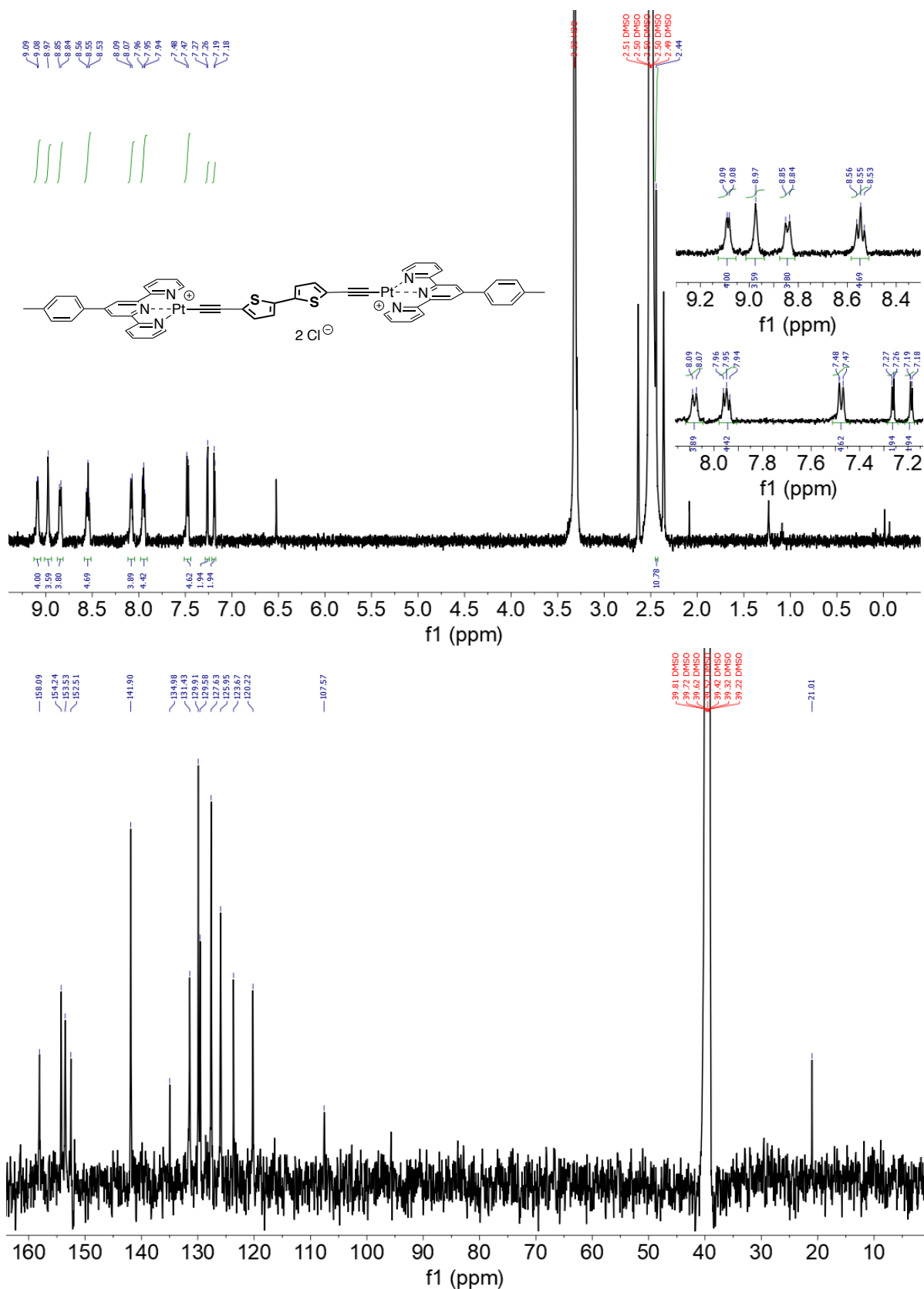


Figure S5. (top) ^1H NMR and (bottom) ^{13}C NMR spectra of dithiophene **3** in $\text{DMSO}-d_6$.

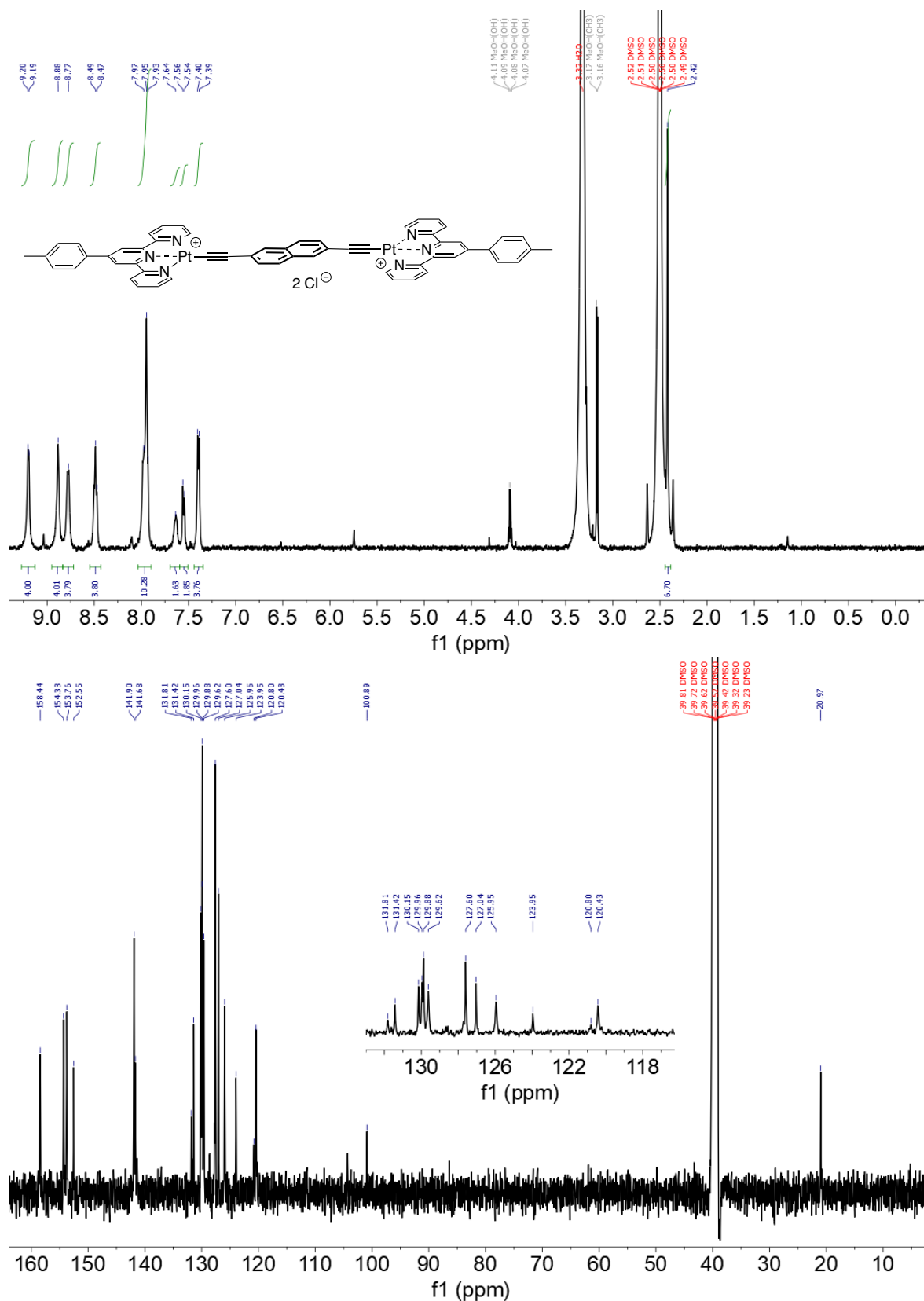


Figure S6. (top) ¹H NMR and (bottom) ¹³C NMR spectra of naphthalene **6a** in DMSO-*d*⁶.

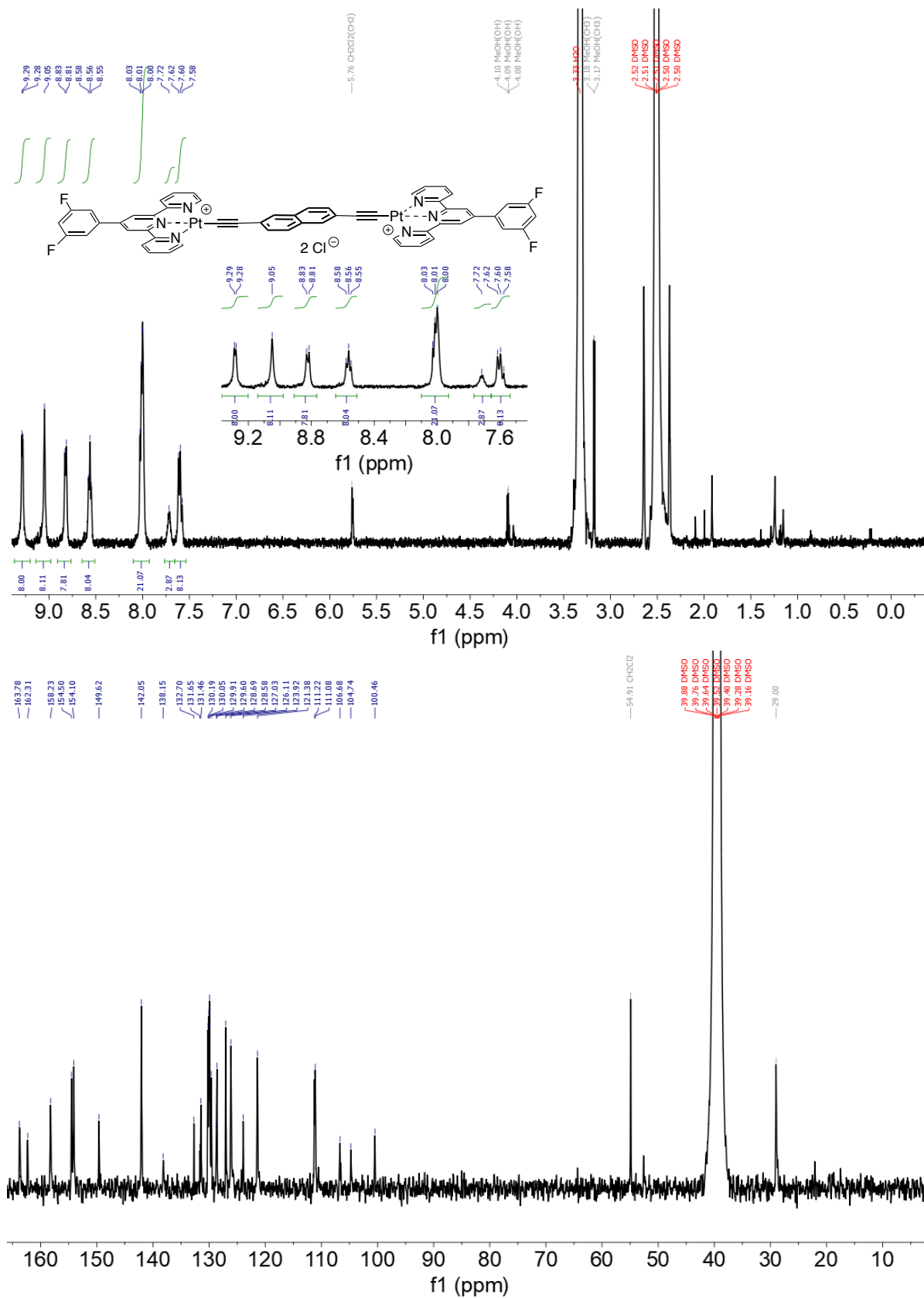


Figure S7. (top) ¹H NMR and (bottom) ¹³C NMR spectra of naphthalene **6b** in DMSO-*d*⁶.

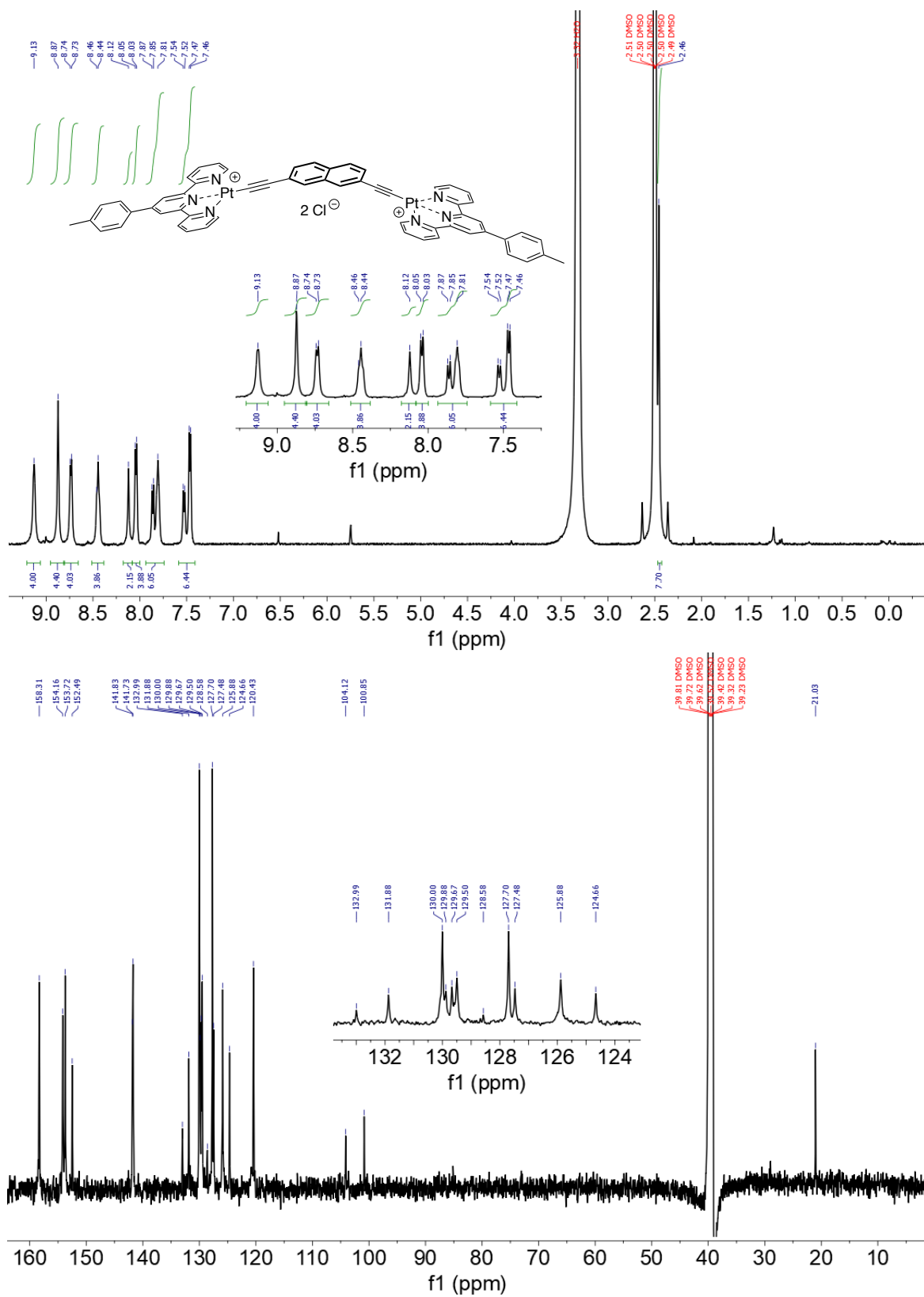


Figure S8. (top) ^1H NMR and (bottom) ^{13}C NMR spectra of naphthalene **7a** in $\text{DMSO-}d^6$.

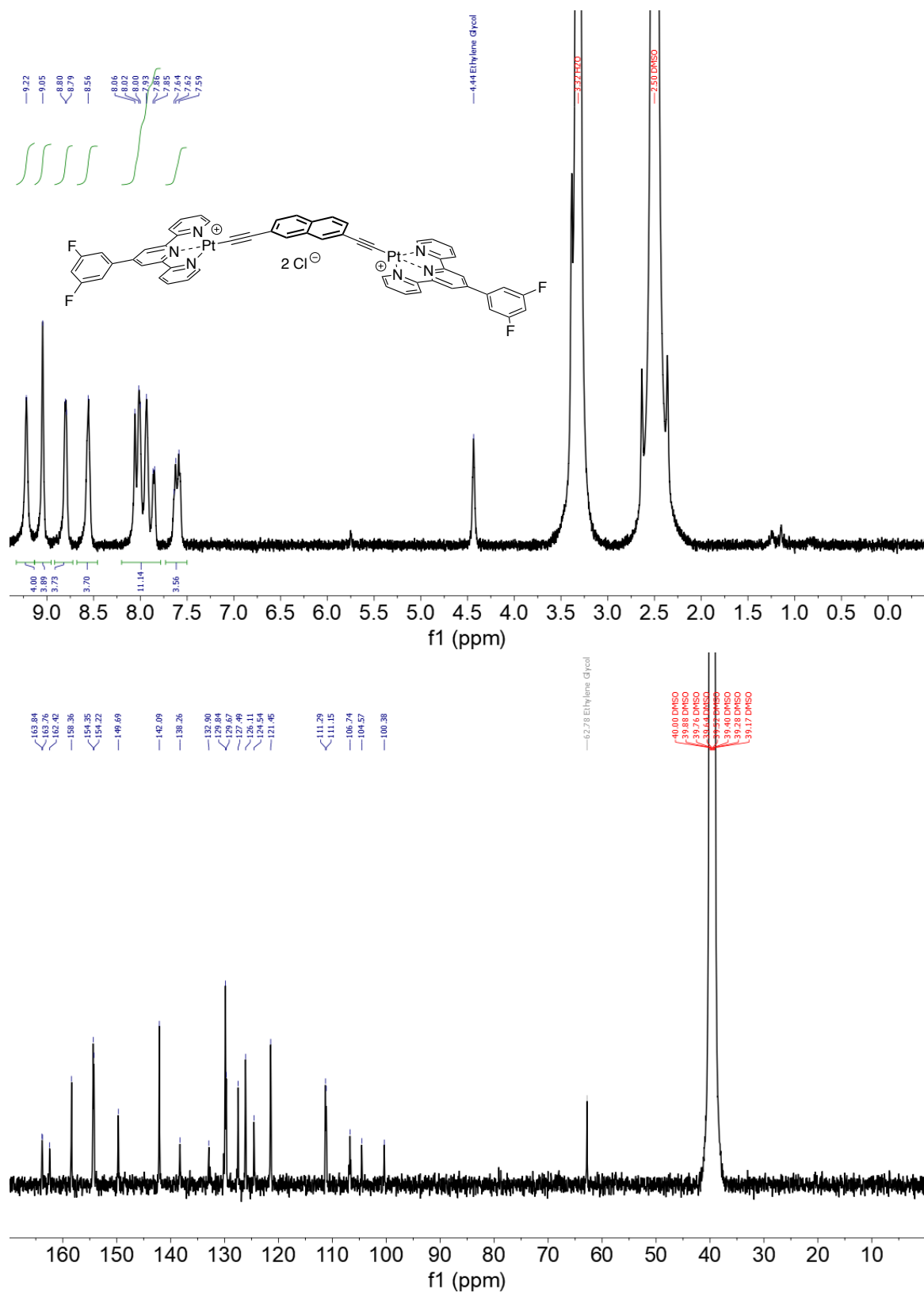


Figure S9. (top) ¹H NMR and (bottom) ¹³C NMR spectra of naphthalene **7b** in DMSO-*d*⁶.

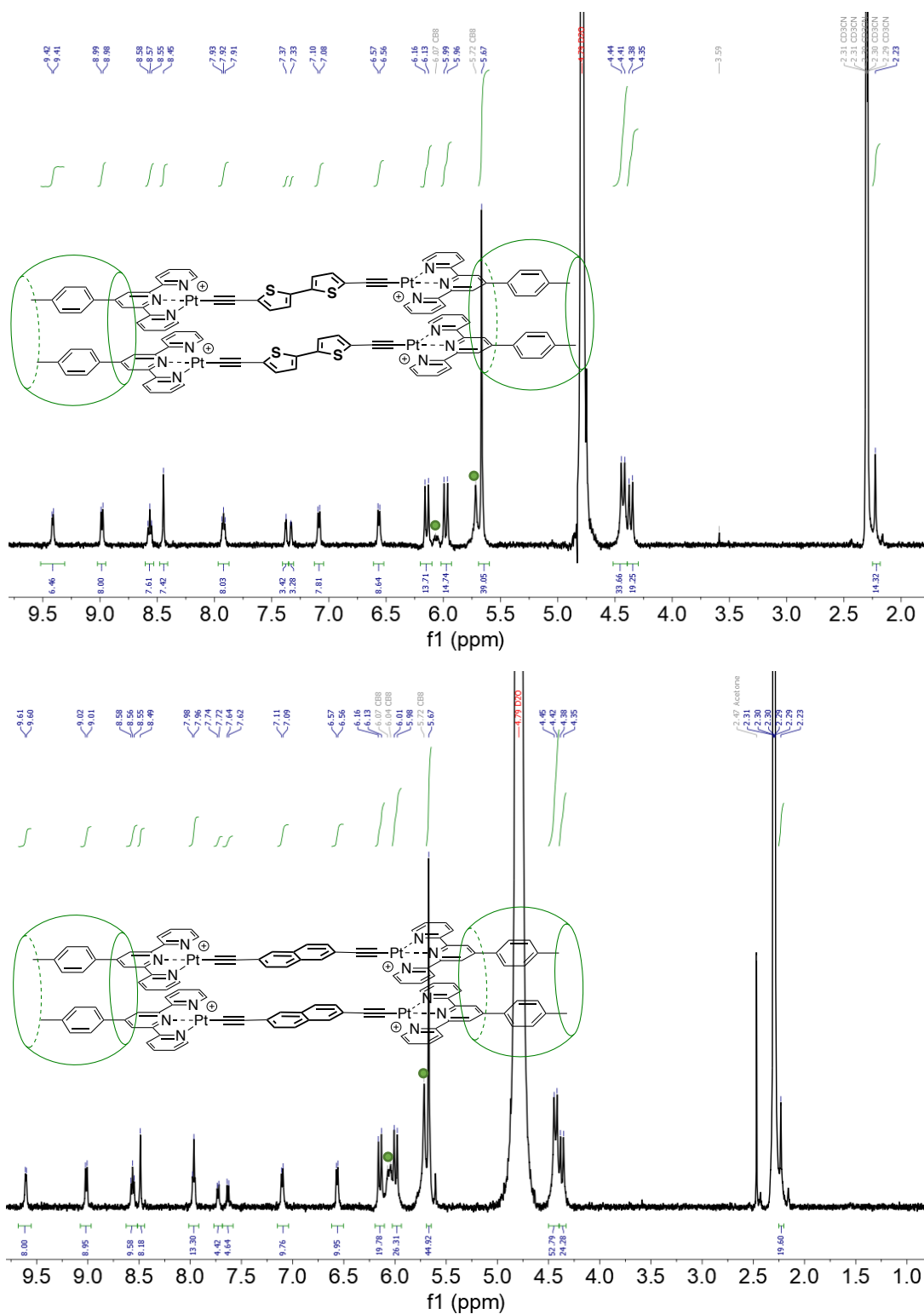
6. ^1H NMR spectra of the Pt complexes/CB[8] assemblies

Figure S10. ^1H NMR spectra of assemblies $3_2\cdot\text{CB}[8]_2$ (top) and $6a_2\cdot\text{CB}[8]_2$ (bottom) in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (5:2). Excess free CB[8] is highlighted with green circles.

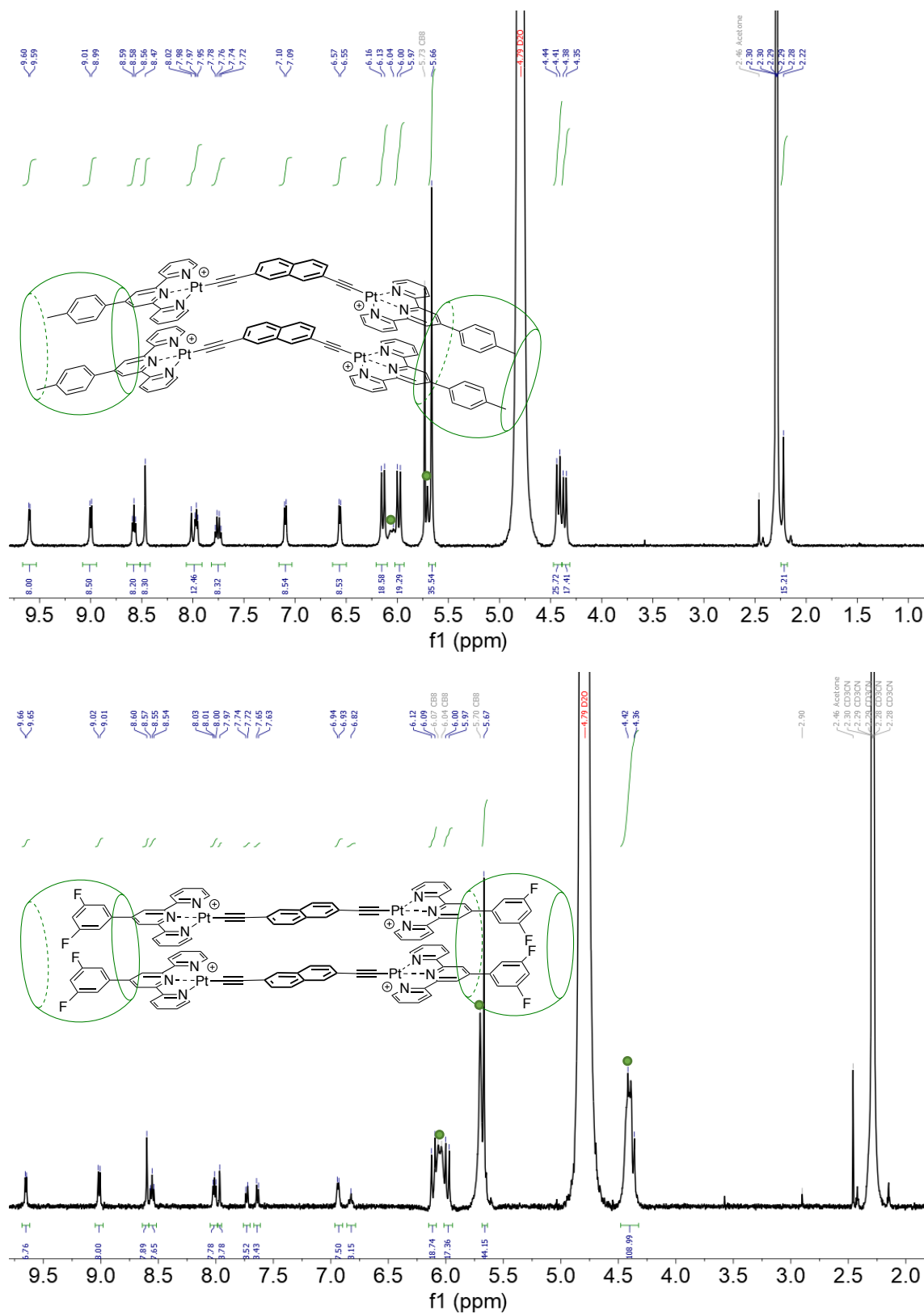


Figure S11. ^1H NMR spectra of assemblies $7\text{a}_2\cdot\text{CB}[8]_2$ (top) and $6\text{b}_2\cdot\text{CB}[8]_2$ (bottom) in $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ (5:2).

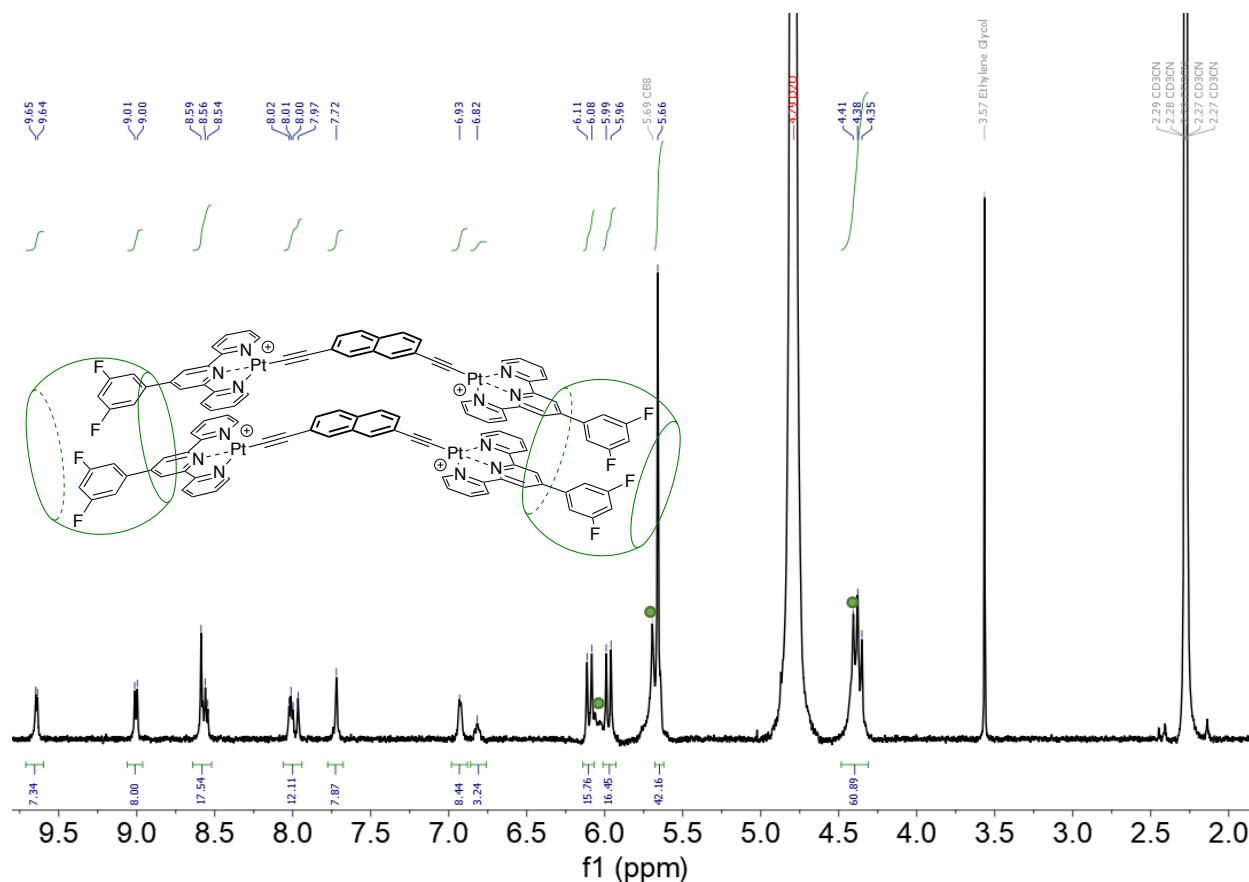
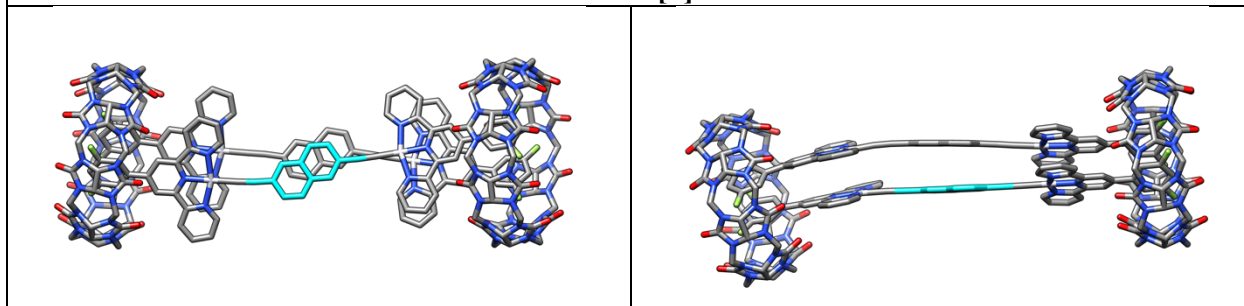


Figure S12. ¹H NMR spectrum of assembly **7b2**·**CB[8]**₂ in D₂O/CD₃CN (5:2).

7. Computational details

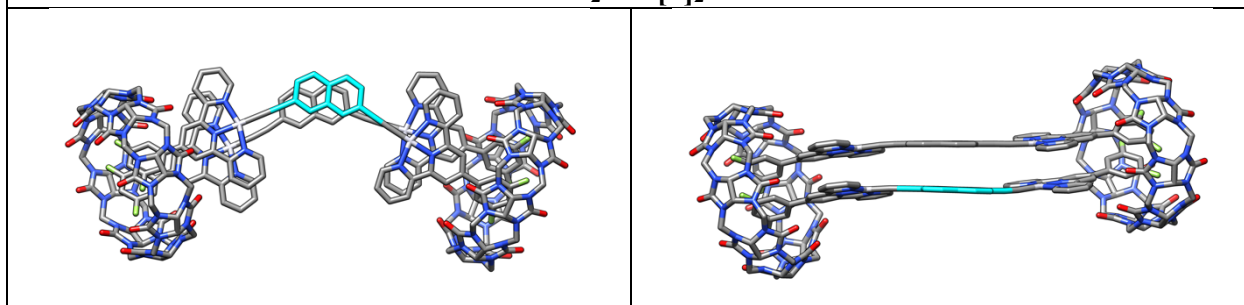
Calculations were carried out with the TURBOMOLE suite of programs (version 7.2).⁶⁻⁹ Energy profiles of dithiophenes **2a** and **2b** along the SCCS dihedral angle were obtained at the B3LYP-D3^{ATM} level with def2-TZVP basis sets. Enthalpic and entropic contributions were obtained after vibrational analysis at the same level of theory. The energy profile of dithiophene **3** was obtained at the B97-3c level¹⁰ with def2-mTZVP basis sets in conjunction with default COSMO solvation parameters. That same level of theory was used to exhaustively screen the conformations of all CB[8]-secured Pt dimers. The m4 grid was used throughout this study. Convergence criteria were 10⁻⁸ Hartree for dithiophenes **2a**, **2b** and **3**, and 10⁻⁶ Hartree for all CB[8]-secured assemblies.

Quaternary assemblies are displayed as orthographic projections (left) along a normal to the naphthyl and dithiophene units in grey, and (right) after a 90° rotation. Pt dimers of complexes **8a** and **8b** are displayed as orthographic projections (left) along a normal to the terpyridyl NNN plane in the background, and (right) along the Pt-CCH axis.

6b₂·CB[8]₂

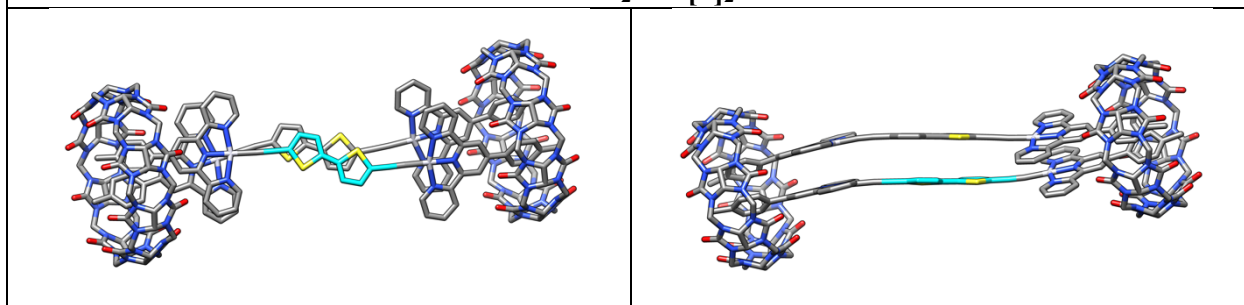
H	-0.33663	11.16462	0.46723	C	-4.97710	12.77639	-0.03744	C	-1.34290	-13.91813	-0.25451
C	-0.26290	10.11344	0.68915	C	-5.77181	15.27231	-1.04288	C	-0.61577	-16.61557	0.00928
C	-0.08808	7.44812	1.28534	C	-6.18271	12.90175	-0.73093	C	-0.48250	-14.50818	-1.18134
C	-1.40088	9.35585	0.89291	C	-4.17084	13.89948	0.15225	C	-1.83893	-14.67948	0.80593
C	0.98393	9.51937	0.78683	C	-4.58322	15.11184	-0.35682	C	-1.46000	-15.99992	0.91299
C	1.07278	8.17187	1.09472	C	-6.54268	14.13967	-0.121930	C	-0.13439	-15.83113	-1.02098
N	-1.29574	8.01673	1.18552	H	-6.82347	12.05492	-0.92474	H	-0.09323	-13.95760	-2.02170
H	1.87080	10.11117	0.61972	H	-3.24625	13.84501	0.70313	H	-2.47250	-14.25037	1.56618
H	2.02629	7.67526	1.18456	H	0.93505	9.17564	-2.62093	C	-2.95733	12.17619	-3.02150
H	-0.08515	6.39634	1.52118	C	0.69565	8.15523	-2.36236	C	-3.01034	14.94009	-3.49984
C	-2.76380	9.88057	0.81935	C	0.03245	5.58139	-1.70172	C	-4.03923	12.75375	-3.68755
C	-5.46475	10.46866	0.75636	C	-0.62607	7.78176	-2.19327	C	-1.90053	12.98208	-2.59263
C	-3.16756	11.15564	0.47751	C	1.70009	7.21507	-2.19668	C	-1.95888	14.33805	-2.83611
N	-3.69839	8.95300	1.09372	C	1.36480	5.91568	-1.85352	C	-4.04077	14.11435	-3.90686
C	-5.01991	9.20506	1.09359	N	-0.94218	6.48153	-1.87534	H	-4.85805	12.15823	-4.05672
C	-4.53238	11.45763	0.42234	H	2.73354	7.49944	-2.32581	H	-1.05302	12.58182	-2.05707
H	-2.43227	11.90195	0.23268	H	2.12186	5.16067	-1.70811	N	6.10500	-12.21531	1.28724
H	-6.51679	10.70413	0.78474	H	-0.29551	4.58712	-1.44361	C	6.86450	-13.30140	1.85876
C	-5.81726	8.03314	1.45555	C	-1.76202	8.69442	-2.32343	C	6.35754	-13.35786	3.31886
C	-7.12588	5.71598	2.14408	C	-4.15322	10.05553	-2.52491	N	5.42666	-12.25883	3.39754
C	-7.19270	8.04523	1.60739	C	-1.74278	10.03818	-2.64404	C	5.33860	-11.56010	2.21903
N	-5.10828	6.87096	1.65286	N	-2.94242	8.08890	-2.10141	H	7.93269	-13.10010	1.77519
C	-5.75401	5.74519	1.98018	C	-4.12970	8.71029	-2.21575	H	7.14874	-13.23514	4.05880
C	-7.85377	6.87971	1.96009	C	-2.95062	10.73876	-2.73285	N	6.56148	-14.61069	1.34139
H	-7.73944	8.96335	1.45278	H	-0.81313	10.53229	-2.87832	N	5.77452	-14.67520	3.42271
H	-5.13755	4.87002	2.10742	H	-5.09509	10.56955	-2.60435	C	5.97039	-15.42294	2.28097
H	-8.92640	6.88219	2.08319	C	-5.26408	7.81907	-1.97790	O	4.71883	-10.52016	2.03770
H	-7.60572	4.78706	2.41042	C	-7.24841	5.98476	-1.47154	O	5.69857	-16.60620	2.14226
Pt	-3.09432	7.10569	1.44567	C	-6.58533	8.22247	-1.99076	N	0.77744	-14.14432	-4.89791
C	-2.47858	5.28516	1.75859	N	-4.94432	6.50693	-1.71733	C	1.63413	-15.10147	-5.55791
C	-2.07867	4.13141	1.83468	C	-5.91527	5.62009	-1.47141	C	3.05976	-14.62295	-5.18601
H	-2.69779	-10.61517	3.62434	C	-7.58708	7.30136	-1.73368	N	2.82083	-13.45411	-4.37227
C	-2.77124	-9.54934	3.47312	H	-6.84492	9.24585	-2.20198	C	1.48640	-13.17806	-4.23059
C	-2.89564	-6.83970	3.09517	H	-5.59046	4.61140	-1.27425	H	1.43916	-15.10544	-6.63012
C	-1.74475	-8.87087	2.84138	H	-8.61847	7.61982	-1.73429	H	3.67387	-14.36400	-6.04838
C	-3.87910	-8.84945	3.92477	H	-7.99948	5.23839	-1.26457	N	1.58030	-16.44143	-5.02903
C	-3.94467	-7.48085	3.72716	Pt	-2.94387	6.15014	-1.71338	N	3.62097	-15.75022	-4.48562
N	-1.82035	-7.50856	2.66755	C	-2.94253	4.20962	-1.50999	C	2.76514	-16.82719	-4.44698
H	-4.68377	-9.37072	4.42108	C	-2.92359	2.98748	-1.44662	O	1.00676	-12.21940	-3.63575
H	-4.79374	-6.90329	4.05790	H	-5.40245	-11.67425	1.36538	O	3.02666	-17.93956	-4.01235
H	-2.89395	-5.77839	2.90810	C	-5.44023	-10.60987	1.43305	N	-3.43305	-15.47479	-3.64878
C	-0.54557	-9.51095	2.29906	C	-5.45659	-7.90487	0.76637	C	-2.95856	-16.68732	-4.25357
C	1.82835	-10.31397	1.13943	C	-4.37486	-9.97947	0.57599	C	-1.70473	-16.23784	-5.03366
C	-0.19305	-10.84590	2.34585	C	-6.53369	-9.86332	1.60265	N	-1.49784	-14.88312	-4.56192
N	0.27508	-8.63776	1.68754	C	-6.54196	-8.49580	1.38501	C	-2.57946	-14.41664	-3.84416
C	1.44548	-8.98884	1.12724	N	-4.39863	-8.62057	0.36614	H	-3.73148	-17.12513	-4.88560
C	1.00654	-11.26425	1.75496	H	-7.36880	-10.34611	2.08781	H	1.83684	-16.24551	-6.11602
C	-0.83665	-11.55148	2.84417	H	-7.37361	-7.88044	1.69128	N	-2.43590	-17.68149	-3.33511
C	2.77887	-10.59802	0.72332	H	-5.40675	-6.84521	0.57609	N	-0.70355	-17.19215	-4.64480
C	2.18040	-7.85059	0.57901	C	-3.17749	-10.67045	0.09791	C	-1.14897	-18.05342	-3.67057
C	3.39010	-5.58604	-0.39973	C	-0.81927	-11.59910	-0.99485	O	-2.75838	-13.26547	-3.47602
C	3.40399	-7.95240	-0.05922	C	-2.88325	-12.01657	0.18502	O	-0.53042	-19.00035	-3.20686
N	1.57324	-6.62634	0.72489	N	-2.30075	-9.84370	-0.50010	N	-5.62076	-15.85163	0.31727
C	2.16777	-5.52807	0.24250	C	-1.14671	-10.25845	-1.05325	C	-5.64609	-17.24551	-0.05374
C	4.01725	-6.81167	-0.55096	C	-1.68839	-12.49766	-0.36325	C	-5.12646	-17.23385	-1.50997
H	3.86315	-8.92180	-0.17666	H	-3.59118	-12.69016	0.63722	N	-4.93790	-15.83302	-1.79045
H	1.63483	-4.60246	0.38884	O	0.10011	-11.94243	-1.43758	C	-5.27937	-15.03090	-0.72968
H	4.97076	-6.88160	-1.05261	C	-0.37680	-9.16407	-1.64613	H	-6.65564	-17.64477	0.04637
H	3.83279	-4.67596	-0.77371	C	0.90205	-6.96430	-2.69044	H	-5.82443	-17.67145	-2.22391
Pt	-0.21761	-6.72471	1.68633	C	0.84869	-9.31899	-2.26899	N	-4.70500	-18.08930	0.63806
C	-0.65252	-4.82518	1.76255	N	-0.94721	-7.91713	-1.54491	N	-3.91715	-18.02328	-1.44491
C	-0.90203	-3.62923	1.83842	C	-0.31748	-6.85119	-2.05141	C	-3.73360	-18.58725	-0.19946
C	-1.65101	-2.79078	1.83735	C	1.49317	-8.21211	-2.79776	O	-5.30973	-13.80752	-0.72526
H	-3.58664	1.98900	2.25574	H	1.29078	-10.29874	-2.35437	O	-2.87806	-19.40845	0.09714
C	-2.54721	1.75678	2.06741	H	-0.82261	-5.90750	-1.92417	C	-0.60948	-13.97593	-5.23692
C	0.12647	1.16614	1.53346	H	2.44809	-8.32693	-3.28809	H	-0.71913	-14.09668	-6.31665
C	-2.14240	0.41574	2.03862	H	1.37332	-6.08098	-3.09215	H	-0.90165	-12.96882	-4.95880
C	-0.29161	2.46511	1.56940	Pt	-2.74126	-7.92126	-0.58300	C	0.53335	-17.37370	-5.35920
C	-0.77626	0.10064	1.76048	C	-3.16496	-6.02267	-0.68726	H	0.90277	-18.36828	-5.13432
C	-3.04961	-0.64757	2.25648	C	-3.37266	-4.81869	-0.75516	H	0.32427	-17.30301	-6.42724
H	0.40878	3.26841	1.38658	C	-2.82598	1.58343	-1.37181	N	-4.29394	-14.93453	4.50751
H	0.65169	-1.47997	1.47660	H	-4.88589	1.24990	-0.90599	C	-4.76489	-16.26862	4.82172
H	1.16142	0.93605	1.31492	C	-3.92576	0.78547	-1.08773	C	-5.46229	-16.71435	3.51390
C	-2.38442	-1.94589	2.20694	C	-1.43733	-0.39954	-1.52898	N	-5.44119	-15.52432	2.70353
H	-4.08822	-0.41498	2.45184	C	-3.81629	-0.61082	-1.01128	C	-4.75128	-14.49535	3.28924
H	-3.34465	-2.74979	2.35447	C	-1.56774	0.95617	-1.59395	H	-5.42981	-16.24095	5.68473
C	-1.28398	-2.27454	1.91768	C	-2.54682	-1.22686	-1.24147	H	-6.48738	-17.05511	3.65674
C	-0.37933	-1.24423	1.70462	C	-4.91996	-1.44223	-0.70320	N	-3.73491	-17.25374	5.00939
C	1.41043	-12.67341	1.77803	H	-0.70880	1.57781	-1.80161	N	-4.62676	-17.80045	3.05070
C	2.18895	-15.36969	1.81099	H	-1.46510	-3.07980	-1.30488	C	-3.67208	-18.15697	3.97436
C	2.26113	-13.12723	0.78896	H	-0.47045	-0.85983	-1.68528	O	-4.59326	-13.37290	2.82183
C	0.94198	-13.52769	2.77716	C	-4.78183	-2.79786	-0.61927	O	-2.93073	-19.12689	3.91044
C	1.33783	-14.84738	2.76604	H	-5.88406	-0.98376	-0.52322	N	-0.42644	-13.55113	6.46361
C	2.62219	-14.50189	0.82714	H	-5.63263	-3.41889	-0.37509	C	-0.64501	-14.71619	7.29008
H	2.61926	-12.55599	-0.02039	C	-3.52235	-3.42099	-0.84629	C	-2.08232	-15.15817	6.92019
H	0.29206	-13.17797	3.56205	C	-2.43194	-2.62011	-1.15390	N	-2.48674	-14.18602	5.93333

C	-1.52233	-13.24156	5.69696	C	1.14815	17.36759	-1.72174	H	-8.16592	13.95870	4.40919
H	-0.52305	-14.45940	8.34228	H	3.65463	15.63064	-2.01505	H	-7.37424	12.54468	3.68438
H	-2.77327	-15.15127	7.76313	H	3.06631	16.01963	0.30817	C	-10.52154	12.01733	-0.05656
N	0.15432	-15.86726	6.95522	N	2.18982	14.14602	-1.98949	H	-10.18416	11.02457	0.02153
N	-1.90741	-16.49991	6.42180	N	1.55559	14.58975	0.08945	H	-11.59066	12.10120	0.13822
O	-0.59946	-16.92120	6.49603	C	1.58281	13.61697	-0.87993	C	-3.28208	17.84155	3.11466
O	-1.62631	-12.27264	4.95293	O	0.51674	18.35235	-2.07667	H	-3.11912	18.04324	4.17506
O	-0.18879	-18.04422	6.24074	O	1.17418	12.46880	-0.76447	H	-3.45940	18.77813	2.59743
C	-3.85245	-14.01476	5.52188	N	-4.45149	13.88599	-7.78447	C	-2.85142	14.35606	3.97023
H	-4.49532	-14.11764	6.39779	C	-3.74273	12.65982	-8.04305	H	-2.76227	13.27507	3.95143
H	-3.95417	-13.01234	5.12035	C	-2.25973	13.04302	-7.84219	H	-2.66651	14.71479	4.98543
C	-3.00824	-17.41210	6.24012	N	-2.32772	14.40894	-7.37395	C	-10.01081	14.00399	-5.75614
H	-3.70407	-17.29102	7.07118	C	-3.60649	14.91801	-7.44915	H	-10.79738	13.47805	-6.29875
H	-2.60421	-18.41842	6.25779	H	-3.96635	12.29944	-9.04772	H	-10.06536	15.06239	-5.98660
C	-4.97812	-18.64547	1.94011	H	-1.66976	12.98691	-8.75765	C	-9.19527	10.74688	-4.54661
H	-4.40626	-19.56180	2.03864	N	-3.94713	11.60511	-7.07618	H	-8.77611	9.87077	-4.06365
H	-6.04205	-18.88110	1.99459	N	-1.78337	12.08079	-6.88249	H	-10.05148	10.44538	-5.15242
O	0.62079	-12.59808	6.71929	C	-2.76621	11.20101	-6.49147	C	-11.05129	15.31435	-1.16163
H	0.72720	-12.48309	7.79992	O	-3.92627	16.08572	-7.27937	H	-12.05370	15.08391	-0.80021
H	0.32185	-11.64882	6.28722	O	-2.61470	10.22160	-5.77679	H	-11.03322	16.33297	-1.53387
C	1.52528	-16.01108	7.36716	N	-8.73303	13.52294	-6.21848	N	-1.84068	14.89876	3.10096
H	1.77531	-17.06424	7.29969	C	-8.49731	12.13821	-6.53975	C	-1.33227	16.24328	3.24278
H	1.61788	-15.68708	8.40448	C	-7.17362	12.16873	-7.34164	C	0.01165	16.21180	2.48156
C	-4.76073	-15.32369	-3.12268	N	-6.81559	13.56549	-7.34278	N	0.08826	14.85472	1.99874
H	-5.45772	-15.82987	-3.79187	C	-7.76882	14.35462	-6.74059	C	-0.97629	14.08989	2.40063
H	-4.99190	-14.26432	-3.10027	H	-9.33851	11.72950	-7.09980	H	-11.22541	16.49162	4.30476
C	-3.31162	-18.58191	-2.62675	H	-7.27305	11.79882	-8.36205	H	0.87646	16.44111	3.10435
H	-2.72134	-19.43991	-2.32397	N	-8.18537	11.28987	-5.41429	N	-2.08629	17.26216	2.56292
H	-4.10428	-18.91449	-3.30176	N	-6.29611	11.30920	-6.58235	N	-0.15488	17.21803	1.46283
C	-6.23445	-15.35680	1.51726	C	-6.91598	10.77444	-5.47842	C	-1.36494	17.86675	1.55909
H	-7.18812	-15.86265	1.66947	O	-7.77803	15.57660	-6.71067	O	-1.12395	12.89178	2.19360
H	-6.41361	-14.29639	1.37672	O	-6.42651	9.96279	-4.70277	O	-1.71940	18.83267	0.89906
N	2.48066	-15.27975	6.57837	N	-10.74217	14.44949	-2.26733	C	0.95559	17.74818	0.71182
C	2.78420	-13.89207	6.79412	C	-11.09285	13.04905	-2.30679	H	0.66643	18.72829	0.34827
C	4.11402	-13.68834	6.03654	C	-10.68610	12.62463	-3.74078	H	1.81078	17.85222	1.38083
N	4.26406	-14.92609	5.29775	N	-10.24386	13.85421	-4.34556	C	1.29722	14.28318	1.46958
C	3.36505	-15.88416	5.71812	C	-10.29906	14.92062	-3.47930	H	1.21801	13.20508	1.55930
H	2.85176	-13.68009	7.86151	H	-12.15311	12.91651	-2.09353	H	2.13839	14.63110	2.07122
H	4.97047	-13.53233	6.69304	H	-11.50269	12.18821	-4.31560	C	0.90625	12.37709	-4.66610
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C	2.57873	-12.07095	5.33200	C	-9.46245	11.37101	-2.18314	C	0.73743	14.04486	-6.29964
C	3.37586	-17.06663	5.40796	O	-10.04603	16.08439	-3.75442	N	0.29581	12.75012	-5.83849
O	2.12086	-11.06580	4.80970	O	-8.70656	10.52950	-1.71322	H	2.75370	14.62827	-5.57031
C	4.93171	-11.74280	4.64607	C	-5.80735	14.10227	-8.21760	H	1.18719	13.95917	-7.28905
H	4.54841	-10.74600	4.45703	H	-5.92831	13.65992	-9.20831	N	-0.26971	15.07950	-6.29297
H	5.75698	-11.68176	5.35679	H	-5.96826	15.17268	-8.28374	N	1.19993	15.76584	-4.77017
C	5.51994	-15.29418	4.69654	C	-5.09516	10.74005	-7.13410	C	0.05378	16.11551	-5.44205
H	5.50930	-16.36859	4.54914	C	-4.85825	9.84691	-6.56617	O	-0.55382	17.17029	-5.33413
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C	4.75314	-12.03118	-1.82345	C	-8.81508	12.57901	1.63127	C	-1.17297	15.26806	-7.39685
O	3.99265	-11.11341	-1.53152	O	-8.95064	17.17772	-0.46449	H	-0.62742	15.10502	-8.32967
O	5.78126	-16.94175	-1.62819	O	-8.33705	11.45558	1.73606	H	-1.52531	16.29326	-7.36635
C	7.15612	-15.12208	0.13254	N	-4.46607	17.03319	2.98173	F	-0.95899	15.11892	-2.38302
H	8.17628	-14.74114	0.06561	C	-4.78454	15.96973	3.89763	F	-5.09887	14.66660	-4.53499
H	7.18489	-16.20388	0.20493	C	-6.29493	15.73390	3.67596	F	0.73173	-16.38202	-1.89505
C	6.38817	-11.66483	-0.00903	N	-6.60447	16.59040	2.55201	F	-1.90137	-16.71476	1.96664
H	5.95454	-10.67136	-0.04066	C	-5.55317	17.42404	2.23522	H	-0.33481	-17.65116	0.11343
H	7.46770	-11.58602	-0.13887	H	-4.53549	16.26279	4.91811	H	-3.02725	16.00305	-3.68029
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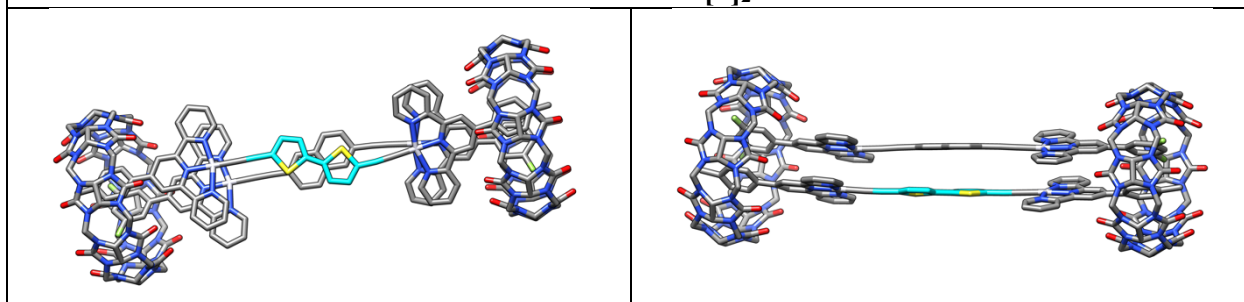
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H	2.11334	5.51281	-2.36831	C	-2.02273	8.96578	-4.49504	C	-6.28703	13.48992	-1.95347
H	0.03152	4.82228	-1.19152	C	-2.33613	6.29657	-3.97251	C	-4.90115	13.55485	-3.92669
C	-1.65199	8.93652	-0.94520	C	-3.14886	8.49530	-3.84373	C	-4.94541	14.92998	-3.87589
C	-3.83707	10.24617	0.11890	C	-1.04152	8.07362	-4.89569	C	-6.30010	14.86808	-1.95597
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Pt	-2.46924	6.31336	-0.13166	N	-6.85803	6.91652	-1.78244	C	-10.92691	-13.88625	-0.51747
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C	-8.42375	-8.51228	5.72862	C	-11.22168	-4.30817	2.11637	C	-13.25409	-8.81452	0.61949
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H	-3.48132	-6.00928	4.13522	C	-5.60848	-8.45256	1.64940	H	-17.42738	-7.04584	2.58357
H	-3.60479	-10.19800	5.07296	C	-3.00952	-7.94036	0.91284	N	-17.10758	-8.28297	5.45443
H	-2.29101	-8.18760	4.36236	C	-4.69016	-9.48756	1.62200	N	-17.04923	-8.95499	3.34078
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C	-4.14591	-3.13261	3.44701	C	-3.38117	-9.23250	1.24580	O	-17.64023	-10.48623	4.97435
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C	-1.19615	-0.80113	1.49875	C	-5.26168	-3.34286	0.07101	N	-13.44628	-6.92204	8.94214
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H	0.23070	1.89734	0.00336	H	-5.77129	1.50901	-1.16479	C	-15.66872	-7.02438	8.18319
O	0.00964	-2.58179	1.60771	C	-4.76099	1.28161	-1.77359	N	-14.77350	-6.37302	7.25452
H	0.71973	-0.43518	0.58586	C	-2.17329	0.70842	-2.35946	C	-13.50342	-6.23805	7.75405
C	-3.17038	-2.33782	2.81219	C	-4.26348	-0.02081	-1.32191	H	-15.01936	-7.08021	10.30480
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C	-1.89963	-2.89135	2.48946	C	-2.93460	-0.31473	-1.75864	N	-14.82014	-8.90689	9.30650
C	-0.94897	-2.14324	1.85459	C	-5.02493	-1.03866	-0.71714	N	-16.25094	-8.25936	7.72925
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H	-9.53108	-10.42113	7.27703	C	-2.42543	-1.61237	-1.55555	N	-11.60800	-8.04741	10.04442
H	-12.36249	-7.93276	5.16990	C	-9.72459	-10.89632	3.23238	C	-10.29352	-8.20327	9.67014
C	-2.87811	12.45104	-0.55083	C	-11.08593	-13.14353	4.21566	H	-10.37561	-9.84864	12.21014

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C	-12.53735	-11.30452	10.54335	C	0.80251	12.67901	-3.76663	C	-0.04122	16.28019	2.66614
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H	-12.69068	-6.46379	10.81149	C	-7.42795	14.87581	-7.40640	H	0.33657	11.64609	2.63364
H	-11.64109	-6.09350	9.42865	C	-6.03953	14.76330	-8.07298	H	1.14843	12.93169	3.54610
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C	-17.40044	-8.31643	6.86114	H	-6.08127	14.67324	-9.15866	C	-10.71535	12.95275	-1.79757
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H	-7.89900	-8.87740	9.77680	O	-6.33699	11.69850	-6.37183	H	-8.68444	17.11245	3.06821
C	-10.49493	-12.41770	11.37621	N	-9.86565	15.96276	-2.73326	N	0.81938	13.30335	1.53685
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H	-10.12319	-12.22111	12.38380	C	-9.86415	14.92176	-4.84174	C	2.01101	14.65199	0.02646
C	-14.91445	-7.23989	1.52889	N	-8.94320	16.03165	-4.76086	N	1.64082	13.77006	-0.52300
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H	-16.12784	-5.08339	6.36461	O	-8.45062	17.72362	-3.25434	O	0.75549	11.37517	0.25181
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C	-7.64142	-17.14946	4.45393	N	-1.19158	15.59501	3.19617	F	-4.25112	15.63246	-4.79306
H	-6.79422	-17.74907	4.12047	C	-1.05696	14.39362	3.99773	F	-6.94095	15.50928	-0.95836
H	-8.43038	-17.80939	4.79800	C	-2.45865	14.23749	4.62632	F	-9.07522	-13.87881	5.16688
C	-5.47759	-14.57819	3.41855	N	-3.10413	15.48382	4.32303	F	-13.06437	-12.28108	3.29471
C	-4.94438	-13.67008	3.15804	C	-2.35167	16.27921	3.49445	H	-11.60598	-14.00750	4.59735
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C	-10.77666	-15.92222	0.95393	H	-2.43993	14.07156	5.70370	H	-2.77589	-0.80393	-0.80393
H	-10.52528	-16.47060	0.04261	N	-0.87809	13.17372	3.26032	H	-1.69881	-3.92064	2.75241
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N	0.76738	15.81060	-5.10851	C	-4.31604	15.92930	4.95668	F	-4.32147	15.22220	1.27103
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C	0.79619	16.55945	-3.95540	H	-4.18810	12.37048	5.48785				
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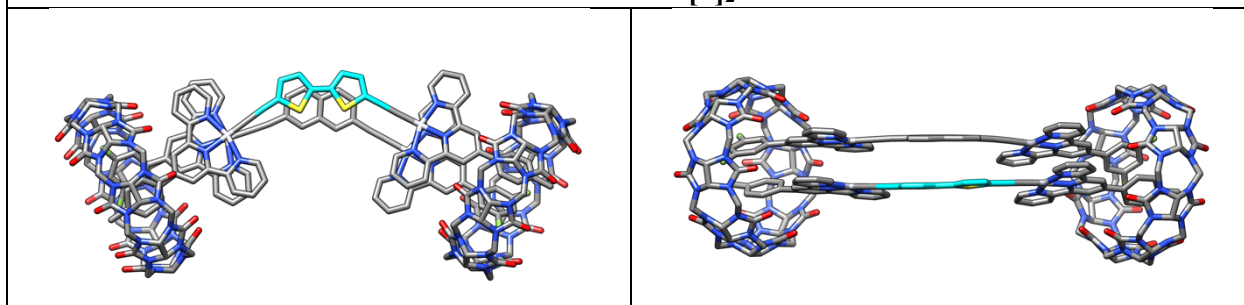
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H	-7.45204	8.30101	0.84804	C	-6.11657	5.66772	-2.94118	H	3.00323	-14.76336	-5.58002
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C	-5.84444	-8.05788	3.02861	C	-3.68990	-10.65931	-0.21043	C	-2.86475	-13.92912	-2.75520
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C	-1.81007	-16.13040	2.28241	C	1.12893	-13.29997	-0.05385	C	-4.82448	-14.45471	4.69724
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H	-2.59098	-16.71137	1.80945	C	0.88048	-15.67761	-0.40052	N	-5.07092	-17.74783	3.88736
H	1.19498	-16.47446	2.77301	C	2.84414	-14.84155	0.67106	C	-3.97882	-14.52487	4.52489
C	-2.31434	13.16206	-1.37269	H	2.95983	-12.73432	0.93131	O	-4.72475	-13.25543	4.47157
C	-2.45397	15.96330	-1.66957	H	-0.54935	-14.23459	-1.02581	O	-3.38147	-19.29948	4.19540
C	-3.13814	13.93305	-0.54719	C	-5.43244	12.97532	-3.36330	C	-6.41111	-14.94855	2.88159
C	-1.54880	13.82319	-2.33796	C	-6.14245	15.66040	-2.87041	H	-7.41344	-15.34289	3.04803
C	-1.62193	15.19568	-2.48092	C	-6.35074	13.30640	-2.35917	H	-6.45031	-13.86463	2.88449
C	-3.19607	15.30437	-0.68851	C	-4.90139	14.01239	-4.13243	C	-5.71938	-18.39177	2.77748
H	-3.70896	13.46169	0.23945	C	-5.25843	15.32585	-3.89322	H	-6.79268	-18.42135	2.96632
H	-0.90540	13.26277	-3.00086	C	-6.69447	14.62070	-2.12044	H	-5.34062	-19.40630	2.71611
H	-1.02642	15.68022	-3.24323	H	-6.77197	12.53241	-1.73370	C	-4.47942	-18.06519	-1.92822
H	-3.83189	15.87852	-0.02729	H	-4.22748	13.79272	-4.94695	H	-4.10447	-19.07588	-1.81022
C	-0.51673	-18.25551	2.62327	N	4.18805	-13.34640	5.71113	H	-5.33682	-18.07715	-2.60239
H	-1.27364	-18.77925	3.20324	C	4.52383	-14.50906	6.15869	C	-3.56737	-14.44484	6.81309
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H	-3.31053	-17.93506	7.60659	H	-12.09224	13.51019	-2.86255	N	1.85384	17.05597	-2.01882
C	-1.05268	-13.70790	-4.41531	H	-11.43238	13.81432	-5.17079	C	1.12347	17.62896	-1.00354
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H	-1.19670	-12.66783	-4.14380	N	-9.67227	12.80149	-4.68856	O	0.49683	18.67550	-1.06920
C	-0.35433	-17.26269	-4.34157	C	-9.55121	11.98664	-3.59207	C	2.10210	17.73445	-3.26285
H	-0.09143	-18.27267	-4.04691	O	-9.89911	17.02999	-3.06158	H	1.75664	18.75714	-3.15640
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C	-0.11383	-15.53703	7.68402	H	-9.83536	13.43858	2.75536	C	-2.05101	15.55663	-8.15413
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C	7.13509	-13.96339	1.89356	H	-6.89025	13.86217	4.50879	C	-5.54642	16.80738	-7.94015
N	6.81486	-15.27401	1.37977	N	-4.15321	13.21908	3.22164	H	-5.71047	16.79264	-9.02020
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H	4.75690	-11.55323	4.55995	N	0.11369	14.05062	1.78105	C	-3.30009	-3.26017	-1.44094
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C	7.24252	-15.73259	0.08401	C	-0.85745	13.09861	2.00082	H	-4.40677	-0.66051	-1.53717
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C	6.58509	-12.27921	0.07850	C	-3.44373	16.41583	3.58081	C	-1.98859	-0.98846	1.48870
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N	1.82117	14.75634	-4.52198	H	0.45753	18.26960	1.32475	H	0.41649	-0.21742	0.14644
C	0.97267	13.92313	-5.20742	C	1.38122	13.72589	1.17988	H	0.58946	2.21649	-0.73954
O	-0.21602	18.77427	-4.64140	H	1.37648	12.66383	0.95752	H	3.80085	-15.00699	1.14815
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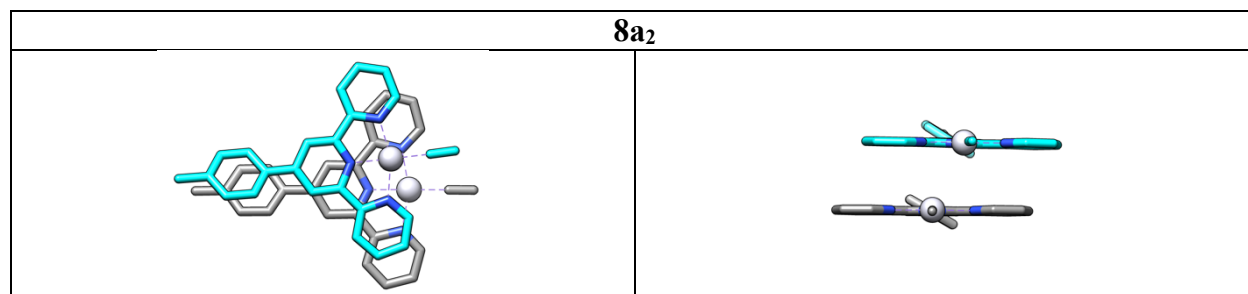
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N	-0.17262	-9.22943	2.24406	C	-5.03241	-7.88823	-1.87036	N	0.98415	-17.44072	-3.72770
C	1.13705	-9.46094	2.43194	N	-2.74153	-8.37199	-1.46344	C	0.03270	-18.25674	-3.15641
C	0.62221	-11.80498	2.63569	H	-6.37214	-9.56443	-1.86194	O	-0.80763	-13.26985	-3.66374
H	-1.47387	-12.27900	2.47424	H	-5.78757	-7.14620	-2.07867	O	0.25195	-19.25429	-2.48544
H	2.59781	-10.97741	2.84694	H	-3.40970	-6.46293	-1.80682	N	-5.32180	-15.54297	-1.32843
C	1.94768	-8.25306	2.39202	C	-1.90873	-10.58538	-1.04187	C	-5.36981	-16.91103	-1.78152
C	3.28943	-5.85788	2.25153	C	0.47825	-11.89620	-0.60875	C	-4.31454	-16.94635	-2.91593
C	3.31895	-8.22661	2.57770	C	-1.92169	-11.94930	-0.83398	N	-3.80475	-15.59423	-2.94733
N	1.25898	-7.08772	2.14870	N	-0.73708	-9.92406	-1.00353	C	-4.46945	-14.76982	-2.07412
C	1.92069	-5.92698	2.07376	C	0.44911	-10.53199	-0.81619	H	-6.37698	-17.16144	-2.11513
C	3.99634	-7.01967	2.51305	C	-0.71809	-12.62808	-0.59840	H	-4.73103	-17.21161	-3.88812
H	3.84857	-9.14685	2.77239	H	-2.84472	-12.49960	-0.90951	N	-4.89313	-17.90269	-0.84909
H	1.31666	-5.05679	1.87271	H	1.41936	-12.39039	-0.44150	N	-3.38507	-17.95859	-2.47848
H	5.06598	-6.99069	2.65746	C	1.57312	-9.59668	-0.84139	C	-3.78205	-18.56552	-1.31150
H	3.78352	-4.90105	2.18424	C	3.53787	-7.67238	-0.92150	C	-4.35538	-13.55277	-1.99997
Pt	-0.75069	-7.36164	1.95422	C	2.89383	-9.95992	-0.65762	O	-3.26357	-19.54491	-0.79421
C	-1.31305	-5.50360	1.77167	N	1.24498	-8.27827	-1.05632	C	1.75514	-14.32072	-4.44020
C	-1.62432	-4.32478	1.66522	C	2.20684	-7.34773	-1.09440	H	2.05316	-14.50827	-5.47438
C	-1.75747	2.03762	0.56788	C	3.88473	-8.99426	-0.69545	H	1.51369	-13.26994	-4.32333
H	-3.79091	1.49910	0.93680	H	3.16042	-10.98963	-0.49322	C	2.35833	-17.84729	-3.85251
C	-2.77108	1.14432	0.88072	H	1.87563	-6.33639	-1.26451	H	2.45498	-18.83242	-3.40965
C	-0.13953	0.23158	0.68814	H	4.91404	-9.28080	-0.54288	H	2.61219	-17.90495	-4.91348
C	-2.50728	-0.21699	1.09688	H	4.28098	-6.89120	-0.95932	N	-5.43455	-14.78949	3.10586
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C	-1.16369	-0.69374	1.00120	C	-0.77135	-6.05683	-1.63013	C	-6.36194	-16.42506	1.69585
C	-3.52979	-1.14828	1.39458	C	-0.80153	-4.84957	-1.84712	N	-5.94151	-15.24057	0.99183
H	0.36808	2.24308	0.22804	C	-0.71200	-14.06205	-1.31680	N	-5.41704	-18.25674	1.82593
O	0.11700	-2.41174	1.11441	C	-0.64099	-16.79615	-0.37463	H	-6.95712	-16.04367	3.80183
H	0.87891	-0.12570	0.60638	C	0.40294	-14.84942	-0.60869	H	-7.41285	-16.63195	1.49551
C	-3.24788	-2.47083	1.58591	C	-1.81087	-14.67971	0.29438	N	-5.20488	-17.16307	3.60369
H	-4.55163	-0.79724	1.46099	C	-1.77177	-16.01819	0.63117	N	-5.56163	-17.60247	1.45672
H	-4.04213	-3.17194	1.80154	C	0.43008	-16.18997	-0.27774	C	-4.94283	-18.06304	2.59656
C	-1.91385	-2.95677	1.49240	H	1.24677	-14.42043	-1.12805	O	-5.03114	-13.17324	1.49180
C	-0.89952	-2.05417	2.69080	H	-2.69080	-14.10216	0.54125	O	-4.30412	-19.09882	2.70260
C	1.05677	-13.19743	2.77919	H	-2.62519	-16.46596	1.12385	N	-2.32515	-13.79350	6.28530
C	1.85615	-15.87963	2.96612	H	1.30685	-16.77639	-0.51815	C	-2.87153	-14.97534	6.91232
C	2.30591	-13.59238	2.29470	C	-5.32083	12.83226	-3.47645	C	-4.12834	-15.28860	6.06496
C	0.21007	-14.14460	3.35540	C	-5.55555	15.64351	-3.39939	N	-4.13433	-15.23989	5.07366
O	0.62691	-15.45570	3.43276	C	-6.23838	13.45631	-2.62653	C	-3.10543	-13.34825	5.24470
C	2.66634	-14.91890	2.39316	C	-4.55091	13.64488	-4.31601	H	-0.91399	-14.77695	7.96128
H	2.98190	-12.89795	1.81932	C	-4.67412	15.01804	-4.28231	H	-0.55996	-15.27257	6.63746
H	-0.75006	-13.87162	3.76105	C	-6.35287	14.83316	-2.59469	N	-2.07293	-16.16736	6.78111

N	-3.87356	-16.61373	5.55651	N	1.79262	13.78284	-2.19370	H	-10.13957	12.32018	2.18560
C	-2.69632	-17.14257	6.03781	C	1.18572	13.04183	-3.17610	C	-0.83197	16.46541	3.12952
O	-2.92444	-12.32421	4.59811	O	0.50710	18.02792	-3.13204	H	-0.18162	16.44977	4.00704
O	-2.29806	-18.28516	5.86825	O	0.71412	11.91646	-3.04583	H	-1.10569	17.49142	2.90894
C	-5.28342	-13.94505	4.26082	N	-6.67950	15.94331	-7.34898	C	-0.35839	12.90866	3.20847
H	-6.17878	-14.03053	4.87899	C	-6.48313	14.76714	-8.16575	H	-0.37496	11.84113	3.01713
H	-5.18887	-12.92212	3.91288	C	-4.97114	14.80732	-8.49374	H	0.24170	13.10520	4.09791
C	-4.91230	-17.43236	4.98624	N	-4.52065	16.02964	-7.87501	C	-10.53107	16.17234	-2.90680
H	-5.82534	-17.29675	5.56798	C	-5.54463	16.71381	-7.26166	H	-11.60075	16.05067	-3.08715
H	-4.59302	-18.46622	5.06005	H	-7.12181	14.81224	-9.04848	H	-10.30589	17.22796	-2.80031
C	-5.67510	-18.38886	0.25698	H	-4.75823	14.82572	-9.56299	C	-10.50081	12.60419	-3.14714
H	-5.33418	-19.39253	0.48721	N	-6.64877	13.50325	-7.49568	H	-10.24782	11.54979	-3.17587
H	-6.72282	-18.42619	-0.04243	N	-4.46944	13.59018	-7.90235	H	-11.57339	12.72004	-3.30903
C	-1.37971	-12.93325	6.94832	C	-5.47444	12.79792	-7.39463	C	-9.52892	15.89548	1.84910
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H	-0.74765	-17.50744	7.57627	C	-10.20755	14.50701	-4.77978	C	0.83732	14.86083	2.13145
H	-1.20995	-16.18135	8.65935	C	-9.39431	14.59849	-6.09301	C	1.67421	14.94965	0.83324
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C	3.42399	-12.36381	6.53725	C	-7.98724	16.46649	-7.04820	H	-1.31490	14.90082	-8.98356
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C	3.81859	-15.93612	6.89152	C	-7.93217	12.90220	-7.26088	C	-1.36245	16.89272	-6.64552
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C	6.55885	-16.58107	1.07885	N	-6.54107	15.41324	3.77257	C	0.93631	13.19290	-5.62221
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C	7.34787	-14.38867	1.35903	C	-8.35984	14.06890	3.14925	H	0.74798	12.13544	-5.47219
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N	6.57166	-15.99919	-0.16676	C	-7.32851	16.16328	2.93352	H	0.72078	17.82106	-5.56356
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C	5.77342	-12.81659	0.62277	C	-6.95681	12.34502	2.41584	C	-3.26562	16.65286	-8.20642
O	5.02657	-11.84657	0.62111	O	-7.16462	17.34124	2.65015	H	-3.09417	16.54237	-9.27840
O	6.27982	-17.74511	1.32632	O	-6.55942	11.35750	1.80979	H	-3.34481	17.70727	-7.96526
C	7.17432	-15.92025	3.37626	N	-2.04372	15.74874	3.42741	S	-2.20208	1.54142	-2.81516
H	8.15184	-15.54254	3.67622	C	-2.03604	14.52327	4.19823	C	-2.78998	-0.04668	-2.37136
H	7.15988	-16.99890	3.48972	C	-3.52494	14.32987	4.56460	C	-4.13980	0.00964	-2.06930
C	6.66658	-12.48198	2.89290	N	-4.14217	15.55452	4.13224	C	-4.69632	1.28457	-2.18170
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H	7.71885	-12.47512	3.17612	H	-1.38312	14.62468	5.06543	H	-4.69767	-0.85578	-1.74371
C	6.39365	-16.74892	-1.37895	H	-3.69645	14.17556	5.63017	H	-5.73003	1.51462	-1.97349
H	7.22625	-16.53558	-2.05072	N	-1.70857	13.33052	3.46418	C	-1.92446	-1.17403	-2.31818
H	6.40717	-17.80158	-1.11809	N	-3.89237	13.14462	3.81901	C	-0.54620	-1.22270	-2.42578
C	5.68722	-13.27585	-1.79268	C	-2.79631	12.51243	3.27257	C	-0.00674	-2.50327	-2.27448
H	6.58913	-13.29710	-2.40672	O	-3.50334	17.51745	3.08220	C	-0.95314	-3.48754	-2.04438
H	5.29401	-12.26504	-1.77413	O	-2.78974	11.41217	2.74105	S	-2.56459	-2.77795	-2.02885
N	1.18939	16.20772	-4.39158	C	-5.45888	15.96604	4.54162	H	0.05484	-0.33856	-2.57746
C	1.96018	15.00717	-4.19403	H	-5.59626	15.68842	5.58692	H	1.04923	-2.72286	-2.31340
C	2.30775	15.03830	-2.68644	H	-5.51192	17.04535	4.45024	F	-1.58024	15.38394	-2.52256
N	1.62542	16.21809	-2.21455	C	-5.12657	12.44710	4.05557	F	-4.82519	15.33812	0.85857
C	1.03449	16.93014	-3.23115	H	-5.32506	12.42116	5.12897	F	-0.20418	-16.36746	3.97632
H	2.83474	15.00604	-4.84483	H	-5.00283	11.43271	3.69069	F	3.85068	-15.30668	1.87779
C	3.37661	15.10840	-2.48470	C	-9.26023	12.33716	1.54018	H	2.16499	-16.91061	3.03213
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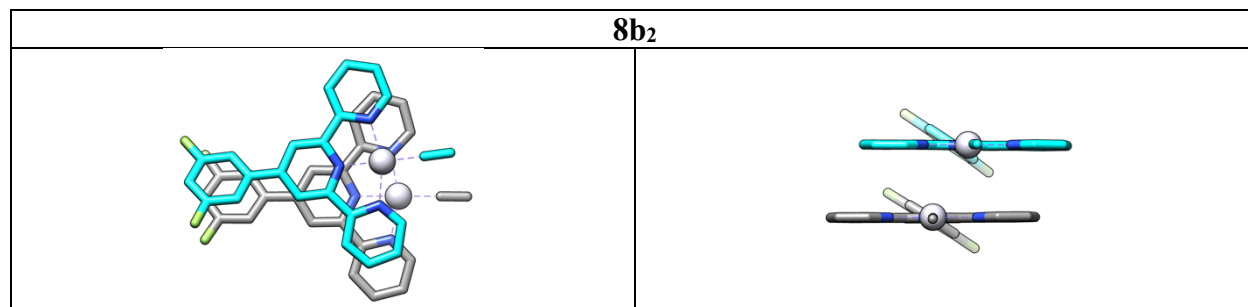
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H	7.16501	2.82454	-4.95857	H	0.97213	8.75611	-8.36976	H	8.86323	10.01408	-10.42296
H	5.43690	1.32908	-3.93012	C	0.36175	7.97559	-7.95031	C	8.95480	10.09039	-11.50465
H	3.16457	2.25437	-3.50790	C	-1.18411	5.97947	-6.89713	H	9.81936	9.68904	-10.02408
C	4.10534	6.31686	-5.06897	C	0.88054	6.71069	-7.74933	H	8.65666	11.01524	-10.04280
C	2.86677	8.76265	-5.42491	C	-0.95573	8.24029	-7.61910	N	6.12872	-12.82113	0.48035
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C	2.18819	7.69624	-4.86793	H	-1.35346	9.23235	-7.76884	N	5.74235	-12.48616	2.63699
C	4.19402	8.59304	-5.83344	H	-2.77147	7.39479	-6.82032	C	5.53381	-11.97474	1.38209
H	5.83866	7.20478	-5.93646	H	-1.74166	5.15607	-6.48166	H	7.97284	-13.71030	0.89818
H	2.39509	9.72902	-5.50335	C	2.25794	6.32562	-8.05433	H	7.45152	-13.51200	3.25369
C	0.81065	7.66129	-4.37704	C	4.75302	5.21186	-8.46117	N	6.51610	-15.20106	0.85046
C	-1.75138	7.37915	-3.42178	C	3.26576	7.10600	-8.58412	N	5.91269	-14.90007	2.97272
C	-0.03919	8.75349	-4.36941	N	2.52231	5.04512	-7.73383	C	5.96717	-15.82250	1.94714
N	0.38046	6.44535	-3.89981	C	3.71749	4.46243	-7.94170	O	4.95298	-10.93014	-1.11423
C	-0.87077	6.31432	-3.44417	C	4.54328	6.56135	-8.77743	O	5.62206	-16.99233	2.01506
C	-1.32931	8.61468	-3.88343	H	3.07033	8.13502	-8.83145	N	-0.02560	-15.24619	-4.74630
O	0.31180	9.70485	-4.73973	H	5.70532	4.75350	-8.67128	C	0.70242	-16.39910	-5.21126
H	-1.13944	5.33071	-3.09394	C	3.72767	3.04853	-7.56989	C	2.18304	-15.96377	-5.10245
H	-1.99829	9.46213	-3.87329	C	3.54261	0.41751	-6.79119	N	2.10141	-14.66093	-4.47934
H	-2.75134	7.23073	-3.04457	C	4.81920	2.21122	-7.72424	C	0.80400	-14.22739	-4.34989
Pt	1.81607	4.99979	-3.95579	N	2.55362	2.56375	-7.04150	H	0.39780	-16.65742	-6.22530
C	0.84458	3.53223	-3.11611	C	2.47519	1.28394	-6.65674	H	2.68971	-15.89118	-6.06486
C	0.21596	2.61888	-2.59916	C	4.72671	0.88424	-7.33834	N	0.62886	-17.55827	-4.35086
H	-2.56688	-10.68236	3.23354	H	5.73358	2.59972	-8.14640	N	-2.77998	-16.99438	-4.29603
C	-2.64237	-9.65466	2.91652	H	1.52899	0.97645	-6.24141	C	1.87130	-17.94321	-3.89152
C	-2.79060	-7.04573	2.09978	H	5.57431	0.22597	-7.45671	O	0.44999	-13.11913	-3.96982
C	-1.63335	-9.08846	2.15965	H	3.43588	-0.60670	-6.46897	O	2.12135	-18.96181	-3.26456
C	-3.74281	-8.89148	3.27347	Pt	1.06523	3.95448	-6.96527	N	-4.14008	-16.03078	-2.86567
C	-3.81801	-7.57258	2.85988	C	-0.39122	2.85524	-6.29846	C	-3.85575	-17.35388	-3.35503
N	-1.72410	-7.77565	1.75827	C	-1.31267	2.16062	-5.88121	C	-2.61137	-17.15155	-4.25003
H	-4.53373	-9.32830	3.86426	H	-5.39986	-11.63270	1.24185	N	-2.29767	-15.75191	-4.07852
H	-4.66003	-6.94822	3.11466	C	-5.41329	-10.62619	0.85661	C	-3.25262	-15.09013	-3.33480
H	-2.80017	-6.30509	1.73761	C	-5.37067	-8.07399	-0.13126	H	-4.71812	-17.75160	-3.89115
C	-0.43765	-9.80355	1.71213	C	-4.34340	-10.17240	0.10498	H	-2.79260	-17.37243	-5.30241
C	1.91561	-10.78245	0.64608	C	-6.48085	-9.78155	1.11050	N	-3.40397	-18.30335	-2.36415
C	-0.09280	-11.12115	1.94100	C	-6.45867	-8.48964	0.61101	N	-1.64756	-18.07348	-3.70547
N	0.38073	-9.03382	0.97232	N	-4.33842	-8.88844	-0.38638	C	-2.14290	-18.77936	-2.63382
H	1.54059	-9.46933	0.45053	H	-7.31885	-10.12818	1.69671	O	-3.31653	-13.88403	-3.15468
C	1.09374	-11.62800	1.39738	H	-7.26858	-7.79991	0.79147	O	-1.57380	-19.69186	-2.05127
H	-0.73927	-11.75018	2.52814	H	-5.29846	-7.08015	-0.54223	N	-5.92068	-15.62507	1.28309
H	2.85367	-11.13622	0.25557	C	-3.17229	-10.98140	-0.23008	C	-6.11946	-17.04792	1.13425
C	2.26151	-8.43111	-0.28464	C	-0.88857	-12.20641	-1.17622	C	-5.81631	-17.29870	-0.36366
C	3.43754	-6.35226	-1.64336	C	-2.93020	-12.29720	0.10355	N	-5.50507	-15.98251	-0.86705
C	3.49291	-8.61952	-0.88700	N	-2.27437	-10.31680	-0.98149	C	-5.65195	-15.00790	0.08615
N	1.63163	-7.21205	-0.36012	C	-1.15205	-10.88167	-1.46520	H	-7.13573	-17.31710	1.42335
C	2.20871	-6.20569	-1.02830	C	-1.78145	-12.93905	-0.37904	H	-6.65849	-17.72098	-0.91270
C	4.08946	-7.57186	-1.56925	H	-3.65738	-12.84096	0.68006	N	-5.16752	-17.88758	1.81510
H	3.97547	-9.58151	-0.81776	H	-0.00112	-12.67128	-1.56999	N	-4.72068	-18.23716	-0.33368
H	1.65574	-5.28066	-1.05429	C	-0.35260	-9.94863	-2.26045	C	-4.40934	-18.63687	0.94589
H	5.05022	-7.71008	-2.04220	C	0.99173	-8.03344	-3.70958	O	-5.59418	-13.79956	-0.10012
H	3.86615	-5.51439	-2.17106	C	0.88183	-10.24608	-2.80736	O	-3.63056	-19.52580	1.25457
Pt	-0.14994	-7.16440	0.62103	N	-0.89595	-8.69546	-2.42923	C	-1.43074	-15.05156	-4.98836
C	-0.64765	-5.31028	0.28318	C	-0.23546	-7.76919	-3.13314	H	-1.65265	-15.36710	-6.00970
C	-0.94913	-4.15171	0.03215	C	1.55891	-9.28543	-3.54042	H	-1.63902	-13.99176	-4.88714
C	-2.01678	1.88623	-1.93812	H	1.31320	-11.22332	-2.67012	C	-0.47345	-18.48459	-4.42457
H	-3.92787	1.15486	-1.36823	H	-0.71631	-6.80794	-3.21292	H	-0.13931	-19.42631	-4.00319
C	-2.86892	0.94361	-1.44007	H	2.52315	-9.51595	-3.96773	H	-0.73907	-18.63496	-5.47313
C	-0.14316	0.38438	-1.66264	H	1.48870	-7.25906	-4.27271	N	-3.97911	-14.20705	5.07737
C	-2.39772	-0.31919	-1.02647	Pt	-2.68141	-8.45015	-1.48334	C	-4.48382	-15.44617	5.63591
C	-0.62344	1.62210	-2.05912	C	-3.14678	-6.64871	-2.04465	C	-5.37083	-16.00800	4.50262
C	-1.00365	-0.60842	-1.15354	C	-3.49683	-5.53167	-2.41233	N	-5.41532	-14.93310	3.54785
C	-3.25503	-1.31288	-0.51245	C	-1.52430	-14.33979	-0.04950	C	-4.59357	-13.88779	3.88646
H	0.51487	-2.11243	-0.89289	C	-0.93018	-17.00696	0.64771	H	-5.02596	-15.25155	6.56092
O	0.91132	0.16439	-1.76433	C	-0.77523	-15.15766	-0.90210	H	-6.37784	-16.27296	4.82371
C	-2.77717	-2.53895	-0.14829	C	-2.00069	-14.89621	1.14067	N	-3.49770	-16.47289	5.83441
H	-4.31130	-1.09597	-0.42447	C	-1.70812	-16.20435	1.47843	N	-4.64970	-17.18797	-0.47336
H	-3.44640	-3.30157	0.22169	C	-0.49413	-16.46433	-0.56237	C	-3.60766	-17.49524	4.92228
H	-1.39728	-2.85391	-0.29135	H	-0.43246	-14.77512	-1.85161	O	-4.45001	-12.84668	3.25635
C	-0.53647	-1.88337	-0.77870	H	-2.56745	-14.28993	1.83292	O	-2.92481	-18.50791	4.88787
C	1.46538	-13.03229	1.58848	H	-2.06458	-16.60207	2.41887	N	0.16531	-12.88844	6.40870
C	2.11859	-15.73982	1.90687	H	0.09131	-17.07357	-1.23837	C	-0.03281	-13.90310	7.41985
C	2.21245	-13.69349	0.61158	C	5.64522	7.39201	-9.25795	C	-1.52494	-14.28677	7.25863
C	1.04583	-13.72585	2.72334	C	7.76279	9.07706	-10.04984	N	-1.98164	-13.42068	6.19802
C	1.37485	-15.05783	2.85008	C	6.96168	7.12100	-8.87530	C	-0.99562	-12.58582	5.74076
C	2.50866	-15.02710	0.78995	C	5.41292	8.50487	-10.21216	H	0.21216	-13.50473	8.40444
H	2.53225	-13.20112	-0.29667	C	6.45253	9.32074	-10.46640	H	-2.11735	-14.12583	8.15926
H	0.48246	-13.24180	3.50351	C	7.99696	7.95061	-9.26543	N	0.65847	-15.14572	7.19180
C	4.91377	9.68794	-6.49035	H	7.18074	6.27410	-8.24080	N	-1.47893	-15.68981	6.92842

C	-0.19810	-16.19450	6.95732	C	9.56620	4.98470	-7.01937	C	10.06427	11.88803	-3.74888
O	-1.13024	-11.70479	4.89977	O	12.37463	8.68916	-8.90943	H	10.38024	11.97961	-2.70825
O	0.11518	-17.36973	6.83868	O	8.45141	4.55266	-6.75848	H	10.65760	12.55775	-4.36156
C	-3.37167	-13.19906	5.90768	N	5.73668	9.07326	-14.14063	C	7.68465	9.48807	-2.50459
H	-3.91880	-13.13806	6.85018	C	5.14264	7.76761	-14.30805	H	6.90172	8.74699	-2.38536
H	-3.45462	-12.25120	5.38722	C	6.33641	6.79837	-14.14608	H	8.14682	9.68194	-1.53401
C	-2.64218	-16.53578	6.98875	N	7.45572	7.67873	-13.92541	C	2.46277	13.76423	-12.48829
H	-3.23006	-16.26788	7.86753	C	7.10376	9.00528	-13.98431	H	1.54130	13.98642	-13.02730
H	-2.29671	-17.55880	7.08954	H	4.65669	7.69711	-15.28186	H	3.24494	14.43403	-12.82859
C	-5.25030	-18.18190	3.21885	H	6.51475	6.17669	-15.02429	C	0.47696	11.25885	-10.90924
C	-4.73210	-19.11898	3.39177	N	4.23436	7.36365	-13.26406	H	0.06506	10.45013	-10.31514
H	-6.30030	-18.29728	3.49355	N	5.95601	5.97644	-13.02304	H	-0.30902	11.67105	-11.54460
C	1.29377	-11.99449	6.41395	C	4.68551	6.25893	-12.57459	C	3.02165	15.90275	-8.12692
H	1.52727	-11.73638	7.44909	O	7.86953	9.95799	-13.94097	H	2.23248	16.57707	-7.79409
H	1.00869	-11.09547	5.87803	O	4.05686	5.62607	-11.74054	H	3.80784	16.48160	-8.59964
C	2.05465	-15.33145	7.48497	N	2.86636	12.41949	-12.81432	N	8.68126	8.93825	-3.38639
H	2.23133	-16.39879	7.55941	C	1.92778	11.34023	-12.97248	C	10.05496	9.38900	-3.38168
H	2.27825	-14.86384	8.44451	C	2.75260	10.23943	-13.67868	C	10.81271	8.25133	-4.10830
C	-5.40037	-15.67998	-2.26943	N	4.08700	10.79399	-13.71941	N	9.77619	7.29242	-4.40176
H	-6.19632	-16.20007	-2.80446	C	4.11708	12.10416	-13.28841	C	8.54606	7.68727	-3.94041
H	-5.53441	-14.60946	-2.38117	H	1.06044	11.67185	-13.54374	H	10.39340	9.55423	-2.35883
C	-4.31567	-18.99194	-1.48960	H	2.40310	10.01307	-14.68609	H	11.59375	7.79052	-3.50333
H	-3.81906	-19.89066	-1.14012	N	1.50684	10.70237	-11.74622	N	10.32527	10.54599	-4.19581
H	-5.20592	-19.27201	-2.05627	N	2.59624	9.09108	-12.82247	N	11.38715	8.90733	-5.25769
C	-6.34026	-14.89401	2.44739	C	1.83629	9.36852	-11.71117	C	11.15285	10.26488	-5.25737
H	-7.29708	-15.28611	2.79195	O	5.07796	12.85764	-13.34806	O	7.51280	7.03212	-3.99191
H	-6.46766	-13.85149	2.15302	O	1.49579	8.56371	-10.85467	O	11.62840	11.07734	-6.03623
N	2.96087	-14.80110	6.50168	N	2.48869	15.01292	-9.12133	C	12.43409	8.06733	-6.04355
C	3.36827	-13.42409	6.47067	C	1.17917	14.41044	-9.03546	H	12.96063	9.10636	-6.55298
C	4.61829	-13.43437	5.56581	C	1.04134	13.67261	-10.39217	H	13.12532	7.79103	-5.37541
H	4.60944	-14.77275	5.00934	N	2.25387	14.01711	-11.08909	C	10.05374	5.94100	-4.80538
C	3.70918	-15.59008	5.66105	C	3.08427	14.82047	-10.34363	H	9.17911	5.34142	-4.57725
H	3.56252	-13.06230	7.48077	H	0.41960	15.17441	-8.87204	H	10.90124	5.57124	-4.22583
H	5.54876	-13.25427	6.10493	H	0.16913	13.97888	-10.96947	C	7.97735	4.33794	-10.70594
N	2.47143	-12.52133	5.77698	N	1.03885	13.35276	-8.06646	N	9.30207	4.43248	-10.35706
N	4.36902	-12.37410	4.62925	N	0.92620	12.28346	-10.00709	C	10.12823	4.88568	-11.44935
C	3.11565	-11.82712	4.77319	C	0.89513	12.11823	-8.64406	C	9.10391	5.19421	-12.56897
O	3.61799	-16.80284	5.53866	O	4.13747	15.31288	-10.72100	N	7.83290	4.87443	-11.96142
O	2.66493	-10.87972	4.14711	O	0.73064	11.06194	-8.04691	H	10.84863	4.11311	-11.71950
C	5.40630	-11.76977	3.83802	C	5.09007	10.26955	-14.61020	H	9.25018	4.59453	-13.46791
H	5.06895	-10.78204	3.54346	H	4.62989	10.06397	-15.57993	N	9.33254	6.58841	-12.85877
H	6.30051	-11.67483	4.45469	H	5.85154	11.03183	-14.73315	N	10.80009	6.14582	-11.25280
H	5.76473	-15.31614	4.34346	C	2.84799	7.74539	-13.26851	C	10.38726	7.10675	-12.14483
H	5.66979	-16.39651	4.35470	H	2.32212	7.07196	-12.60024	O	10.89250	8.20811	-12.30146
H	6.66370	-15.03127	4.89601	H	2.44946	7.63476	-14.27921	O	7.09186	3.82627	-10.03295
C	5.38208	-16.76398	-2.04368	N	5.12119	14.71492	-5.45231	C	9.83558	3.81146	-9.17467
N	6.09306	-15.73184	-1.47993	C	3.87434	14.59092	-4.73356	H	10.67448	3.17377	-9.45289
C	6.16484	-14.57341	-2.34046	C	2.80623	14.91488	-5.80493	H	9.04901	3.20132	-8.74358
C	5.22106	-14.94479	-3.50937	N	3.58394	15.25799	-6.96662	C	11.99257	6.28685	-10.46288
N	4.84686	-16.30432	-3.22426	C	4.93670	15.18000	-6.73767	H	12.52199	7.16413	-10.81883
H	7.19396	-14.39074	-2.64871	H	3.85768	15.27320	-3.88342	H	12.62017	5.40659	-10.60778
H	5.69137	-14.87557	-4.49008	H	2.14959	15.74106	-5.53212	C	6.61744	4.73474	-12.71987
N	4.15377	-13.97207	-3.39660	N	3.53478	13.25470	-4.30806	H	6.84101	4.21626	-13.65416
N	5.58272	-13.36625	-1.81085	N	2.05051	13.68805	-5.89608	H	5.93316	4.13332	-12.13063
C	4.40922	-13.02520	-2.43420	C	2.42949	12.76289	-4.95734	C	8.81823	7.23217	-14.03665
O	3.72564	-12.03556	-2.19249	O	5.82076	15.49946	-7.51827	H	8.89192	6.54204	-14.87913
O	5.28092	-17.89890	-1.60220	O	1.86132	11.70509	-4.71419	H	9.43699	8.10105	-14.23270
C	6.93550	-15.91353	-0.32928	N	8.68971	12.30326	-3.84645	S	-1.83574	-0.30966	-4.84065
H	7.95014	-15.59791	-0.57502	C	7.70890	11.98330	-2.84345	C	-3.48009	-0.67391	-4.37481
H	6.93914	-16.97305	-0.09744	C	6.56315	12.98173	-3.11944	C	-4.29930	0.41567	-4.61854
C	6.27620	-12.48640	-0.90959	N	6.98022	13.63901	-4.33845	C	-3.63318	1.51509	-5.16578
H	5.88441	-11.48417	-1.04422	C	8.27228	13.30849	-4.68670	C	-2.27688	1.31364	-5.36226
H	7.33412	-12.49278	-1.17305	H	8.14130	12.08174	-1.84729	H	-5.35515	0.41252	-4.39438
C	4.20506	-17.16682	-4.17869	H	6.42495	13.71470	-2.32388	H	-4.11290	2.44975	-5.41334
H	4.65492	-17.00147	-5.15799	N	7.06752	10.69484	-2.98573	C	-3.83120	-1.92630	-3.79605
H	4.38768	-18.19051	-3.87073	N	5.39882	12.14375	-3.23358	C	-5.05244	-2.30864	-3.26758
C	3.21145	-13.74587	-4.45920	C	5.69773	10.80792	-3.09789	C	-5.05950	-2.59912	-2.73344
H	3.73687	-13.80819	-5.41418	O	8.93854	13.83857	-5.56404	C	-3.84359	-4.25651	-2.82621
H	2.81113	-12.74490	-4.34060	O	4.89321	9.88945	-3.05505	S	-2.66513	-3.21722	-3.62145
N	11.75319	6.46055	-9.05321	C	6.37792	14.87331	-4.76960	H	-5.91125	-1.65502	-3.25274
C	11.58419	5.34329	-8.15225	H	6.22722	15.51853	-3.90036	H	-5.92118	-4.05706	-2.27210
C	11.66189	6.00119	-6.75333	H	7.06898	15.35447	-5.45301	F	8.29602	10.88444	-6.93769
N	11.98286	7.37480	-7.04226	C	4.06000	12.65606	-3.11018	F	4.25437	12.45562	-8.71996
C	12.06067	7.62792	-8.39116	H	4.04112	13.39530	-2.30754	F	0.93909	-15.73267	3.93297
H	12.35523	4.59359	-8.32769	H	3.41136	11.82632	-2.84983	F	3.17954	-15.67622	-0.18256
H	12.41867	5.56057	-6.10462	C	0.83873	13.57224	-6.65966	H	2.36585	-16.78234	2.02488
N	10.27959	4.73378	-8.16344	H	0.28695	12.72664	-6.26289	H	6.82297	12.51982	-8.33766
N	10.34040	5.78047	-6.20665	H	0.24686	14.47878	-6.53373	H	-2.39296	2.84303	-2.26975



H	0.97617	9.91011	-1.78302	C	-3.38692	15.29151	-0.70592	H	-7.36030	5.19589	-1.77341
C	0.88498	8.84388	-1.65424	C	-3.87622	13.16634	0.34280	H	-10.24899	8.22336	-0.83260
C	0.60804	6.14477	-1.31500	C	-2.37630	13.25477	-1.52633	H	-9.61789	5.80698	-0.92950
C	-0.28903	8.30746	-1.15865	C	-2.55470	14.62032	-1.60294	Pt	-4.91841	6.79021	-2.81389
C	1.93984	8.00817	-1.98552	C	-4.04104	14.53773	0.26641	C	-4.88107	4.83978	-2.66944
C	1.79719	6.64211	-1.81551	H	-4.38006	12.62100	1.12713	C	-4.86877	3.62786	-2.55569
N	-0.41142	6.94893	-0.99068	H	-1.74299	12.77052	-2.25471	C	-5.19811	12.92089	-3.47894
H	2.85636	8.42373	-2.37396	H	-1.40555	9.90942	-4.52246	C	-5.44209	15.69669	-3.91797
H	2.59093	5.95670	-2.06522	C	-1.59735	8.86571	-4.33388	C	-5.97940	13.71537	-2.63737
H	0.44370	5.09116	-1.16283	C	-2.12687	6.22708	-3.84170	C	-4.52583	13.54375	-4.53667
C	-1.46721	9.09964	-0.79668	C	-2.81851	8.47143	-3.82017	C	-4.64910	14.90273	-4.74929
C	-3.86161	10.21424	0.00863	C	-0.62708	7.91524	-4.61344	C	-6.09386	15.07615	-2.85453
C	-1.62852	10.46942	-0.86682	C	-0.89647	6.58076	-4.36477	H	-6.47541	13.27926	-1.78347
N	-2.48304	8.34537	-0.34355	N	-3.06795	7.14083	-3.58099	H	-3.92777	12.95838	-5.21956
C	-3.65722	8.84962	0.07235	H	0.32383	8.21988	-5.02111	H	-4.83046	2.57213	-2.43434
C	-2.84217	11.05162	-0.46956	H	-0.16983	5.81136	-4.56923	H	-1.59212	2.20777	0.06537
H	-0.81334	11.09319	-1.19199	H	-2.38703	5.20670	-3.61609	H	-4.13066	15.35663	-5.58294
H	-4.80611	10.63338	0.31007	C	-3.91075	9.39138	-3.48920	H	-6.69242	15.66945	-2.17737
C	-4.58577	7.81443	0.53332	C	-6.18270	10.76340	-2.72986	H	-2.05062	15.17671	-2.38070
C	-6.19047	5.72278	1.30665	C	-3.95328	10.76385	-3.64706	H	-4.68858	15.03200	0.97728
C	-5.86011	8.06989	1.00423	N	-4.97841	8.76120	-2.97080	C	-3.57381	16.76897	-0.80886
N	-4.11781	6.52374	0.46956	C	-6.10192	9.39176	-2.58796	H	-2.61799	17.29017	-0.77450
C	-4.90719	5.50961	0.83678	C	-5.10448	11.47549	-3.27635	H	-4.20334	17.15318	-0.01149
C	-6.67076	7.01741	1.40028	H	-3.10383	11.28752	-4.05119	H	-4.03725	17.02388	-1.76024
H	-6.21688	9.08506	1.06696	H	-7.08922	11.27970	-2.46368	C	-5.59209	17.16160	-4.17606
H	-4.48398	4.52473	0.73911	C	-7.12966	8.47124	-2.09348	H	-4.62398	17.65088	-4.27565
H	-7.66427	7.21140	1.77248	C	-8.93628	6.57801	-1.25059	H	-6.14281	17.65498	-3.37991
H	-6.79276	4.87673	1.59565	C	-8.36822	8.86850	-1.62560	H	-6.12877	17.33537	-5.10899
Pt	-2.22233	6.38661	-0.25428	N	-6.79973	7.13656	-2.12869				
C	-1.93822	4.45526	-0.12136	C	-7.68468	6.22145	-1.71901				
C	-1.74413	3.25793	-0.01046	C	-9.28173	7.91681	-1.19873				
C	-3.03442	12.49835	-0.55032	H	-8.61976	9.91610	-1.59470				



H	0.96512	10.03552	-1.84815	C	-1.69114	3.38901	0.02544	N	-6.85487	7.02045	-2.14033
C	0.88413	8.97082	-1.70125	C	-3.05577	12.60723	-0.62290	C	-7.73487	6.10712	-1.71687
C	0.63386	6.27460	-1.31547	C	-3.40212	15.38744	-0.76441	C	-9.34955	7.80029	-1.24352
C	-0.28462	8.43019	-1.19833	C	-3.86007	13.26122	0.31239	H	-8.70152	9.79621	-1.67803
C	1.94778	8.13992	-2.01699	C	-2.43231	13.34150	-1.63329	H	-7.40272	5.08308	-1.74761
C	1.81883	6.77586	-1.82270	C	-2.61979	14.70678	-1.67778	H	-10.32182	8.10647	-0.89079
N	-0.39415	7.07375	-1.00723	C	-4.00762	14.62938	0.21963	H	-9.66953	5.69416	-0.93026
Pt	2.86054	8.55790	-2.41143	H	-4.33413	12.73223	1.12303	Pt	-4.96718	6.67631	-2.80740
H	2.62004	6.09439	-2.05882	H	-1.82466	12.87001	-2.38783	C	-4.91189	4.73143	-2.61667
H	0.48058	5.22225	-1.14473	H	-1.45862	9.78569	-4.54004	C	-4.88510	3.52310	-2.47246
C	-1.47066	9.21591	-0.85052	C	-1.64659	8.74411	-4.33665	C	-5.24656	12.80063	-3.50368
C	-3.87821	10.32137	-0.06365	C	-2.16700	6.11012	-3.80866	C	-5.41138	15.57726	-3.86380
C	-1.64157	10.58507	-0.93310	C	-2.86915	8.35059	-3.82606	C	-5.97842	13.58049	-2.60692
N	-2.48393	8.46037	-0.39396	C	-0.66592	7.79422	-4.59631	C	-4.59695	13.40651	-4.58102
C	-3.66486	8.95716	0.01189	C	-0.93429	6.46281	-4.32812	C	-4.69785	14.77350	-4.73250
C	-2.85932	11.15473	-0.54133	N	-3.11443	7.02265	-3.56923	C	-6.03820	14.94317	-2.80816
H	-0.83023	11.21394	-1.25829	H	0.28178	8.09747	-5.00301	H	-6.46696	13.15179	-1.74759
H	-4.82461	10.73941	0.23430	H	-0.20239	5.69400	-4.51528	H	-4.04752	12.83188	-5.30888
C	-4.58524	7.91984	0.48277	H	-2.42256	5.09200	-3.56858	F	-2.02044	15.41263	-2.66139
C	-6.17008	5.82421	1.28329	C	-3.96699	9.26948	-3.51402	F	-4.77428	15.26286	1.13488
C	-5.86713	8.16851	0.93561	C	-6.25084	10.64291	-2.78210	H	-3.53383	16.45573	-0.81736
N	-4.10082	6.63406	0.44691	C	-4.01091	10.64228	-3.67968	H	-4.83764	2.47040	-2.32915
C	-4.88010	5.61763	0.82805	N	-5.03932	8.64310	-3.00061	H	-1.52846	2.34168	0.11672
C	-6.66778	7.11371	1.34635	C	-6.16940	9.27079	-2.63322	H	-5.47084	16.64494	-3.99910
H	-6.23724	9.17987	0.97582	C	-5.16574	11.34639	-3.31770	F	-4.07646	15.35816	-5.78144
H	-4.44475	4.63617	0.75237	H	-3.16134	11.16747	-4.08225				
H	-7.66689	7.30237	1.70593	H	-7.15845	11.16202	-2.52491				
H	-6.76340	4.97627	1.58496	C	-7.19611	8.35243	-2.13461				
Pt	-2.20168	6.50687	-0.26758	C	-8.99236	6.46381	-1.26373				
C	-1.89709	4.58254	-0.10066	C	-8.44095	8.75039	-1.68469				

8a·8b											
H	0.85096	10.57451	-2.03378	C	-3.00868	13.17792	-0.40667	C	-9.40121	7.42489	-1.26809
C	0.76111	9.50763	-1.90964	C	-3.25814	15.97049	-0.29238	H	-8.67658	9.39798	-1.67980
C	0.48789	6.80551	-1.57907	C	-3.77536	13.77292	0.59779	H	-7.56957	4.63922	-1.82544
C	-0.39783	8.96991	-1.38238	C	-2.36826	13.97850	-1.35340	H	-10.35819	7.76522	-0.90492
C	1.80395	8.67058	-2.27673	C	-2.50993	15.34699	-1.27249	H	-9.79924	5.32889	-0.97202
C	1.66594	7.30468	-2.10517	C	-3.88005	15.14708	0.62680	Pt	-5.08617	6.14495	-2.90785
N	-0.52129	7.60910	-1.22741	H	-4.26009	13.19030	1.36410	C	-5.13077	4.19093	-2.82388
H	2.70970	9.08624	-2.68945	H	-1.79912	13.55639	-2.16461	C	-5.17385	2.97437	-2.78820
H	2.45307	6.61989	-2.37654	H	-1.45053	9.15312	-4.55585	C	-5.03024	12.30660	-3.27099
H	0.32386	5.75133	-1.43165	C	-1.68264	8.11410	-4.38748	C	-5.04905	15.12104	-3.45355
C	-1.55215	9.76346	-0.95263	C	-2.32144	5.48811	-3.95379	C	-5.76899	13.08186	-2.37126
C	-3.89576	10.88077	-0.00975	C	-2.91596	7.75706	-3.87561	C	-4.29142	12.96726	-4.25678
C	-1.68603	11.13941	-0.94143	C	-0.75291	7.13109	-4.68969	C	-4.30765	14.34709	-4.34556
N	-2.56574	9.00777	-0.49760	C	-1.07442	5.80456	-4.46191	C	-5.77161	14.45952	-2.45995
C	-3.72204	9.50883	-0.03150	N	-3.22555	6.43258	-3.67694	H	-6.32259	12.61027	-1.57292
C	-2.86582	11.71751	-0.45748	H	0.20890	7.40341	-5.09472	H	-3.72583	12.40223	-4.98286
H	-0.87060	11.76302	-1.26586	H	-0.37631	5.01145	-4.67577	H	-3.73579	14.83268	-5.12399
H	-4.81930	11.30278	0.34799	H	-2.62246	4.47473	-3.75179	H	-6.33632	15.03400	-1.73906
C	-4.65828	8.46695	0.39890	C	-3.96106	8.71532	-3.50702	C	-5.08716	16.60957	-3.56496
C	-6.26386	6.36188	1.14140	C	-6.16782	10.16796	-2.70426	H	-5.10291	17.08076	-2.58469
C	-5.92501	8.71459	0.89343	C	-3.92452	10.09406	-3.58817	H	-5.98870	16.93207	-4.08760
N	-4.20563	7.17469	0.27832	N	-5.06378	8.11954	-3.02213	H	-4.23373	16.99124	-4.11845
C	-4.99408	6.15473	0.63321	C	-6.16094	8.78900	-2.62894	F	-1.89633	16.11852	-2.19781
C	-6.73554	7.65574	1.27467	C	-5.03773	10.84698	-3.18508	F	-4.61786	15.72212	1.60494
H	-6.27607	9.72905	0.98916	H	-3.04042	10.59026	-3.95013	H	-3.35278	17.04313	-0.24696
H	-4.58073	5.17008	0.49484	H	-7.05139	10.71958	-2.43127	H	-5.19377	1.91191	-2.73904
H	-7.72096	7.84666	1.66918	C	-7.23157	7.90274	-2.16512	H	-1.79176	2.84379	-0.53080
H	-6.86271	5.51177	1.42506	C	-9.09598	6.07536	-1.30424				
Pt	-2.32528	7.04500	-0.48322	C	-8.45805	8.34280	-1.70271				
C	-2.07289	5.10611	-0.47151	N	-6.94696	6.55886	-2.19847				
C	-1.91032	3.90000	-0.49462	C	-7.85915	5.67557	-1.77574				

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