**Supplementary information**

# A Platinum(II) Molecular Hinge with Motions Visualized by Phosphorescence Changes

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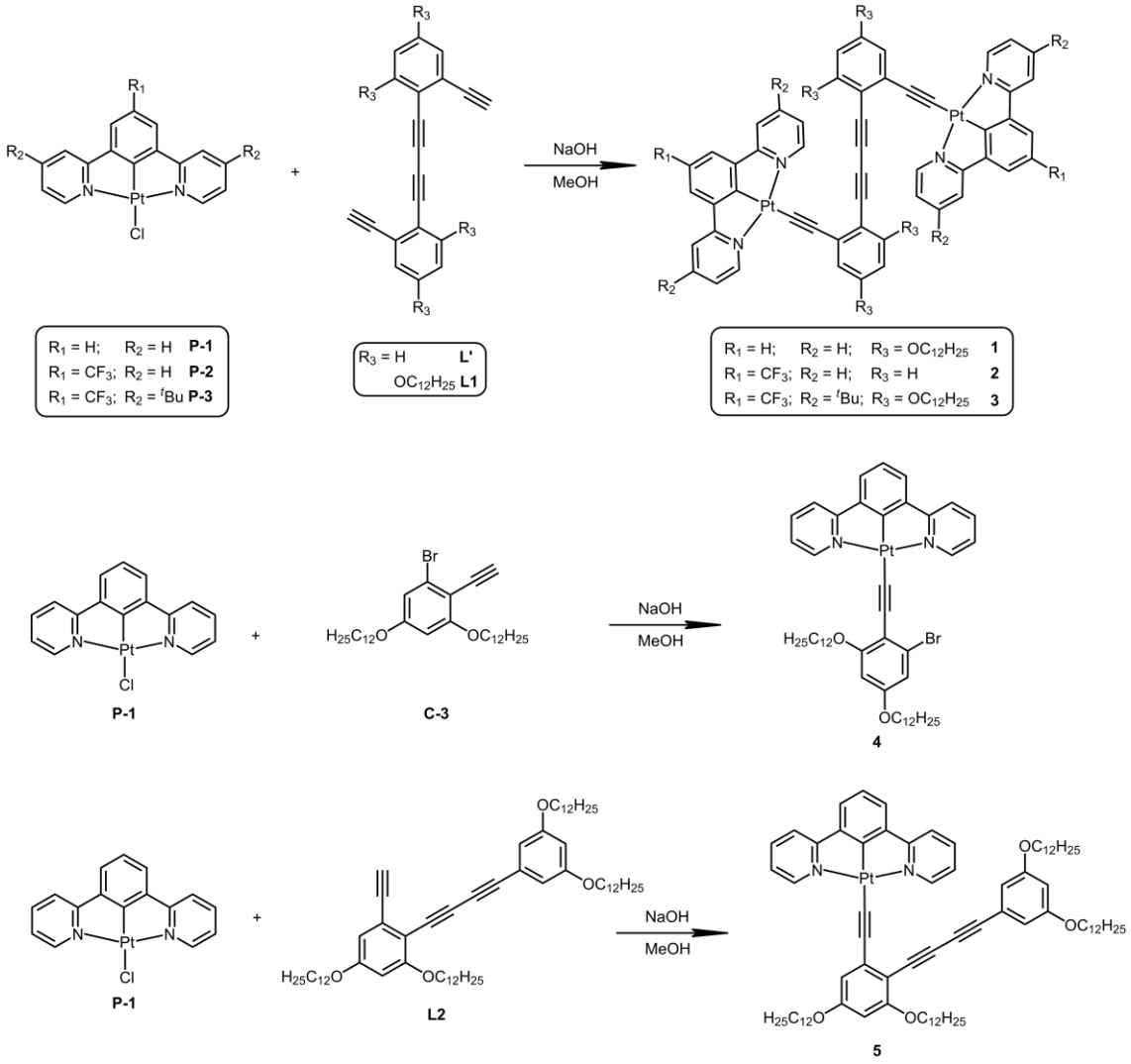
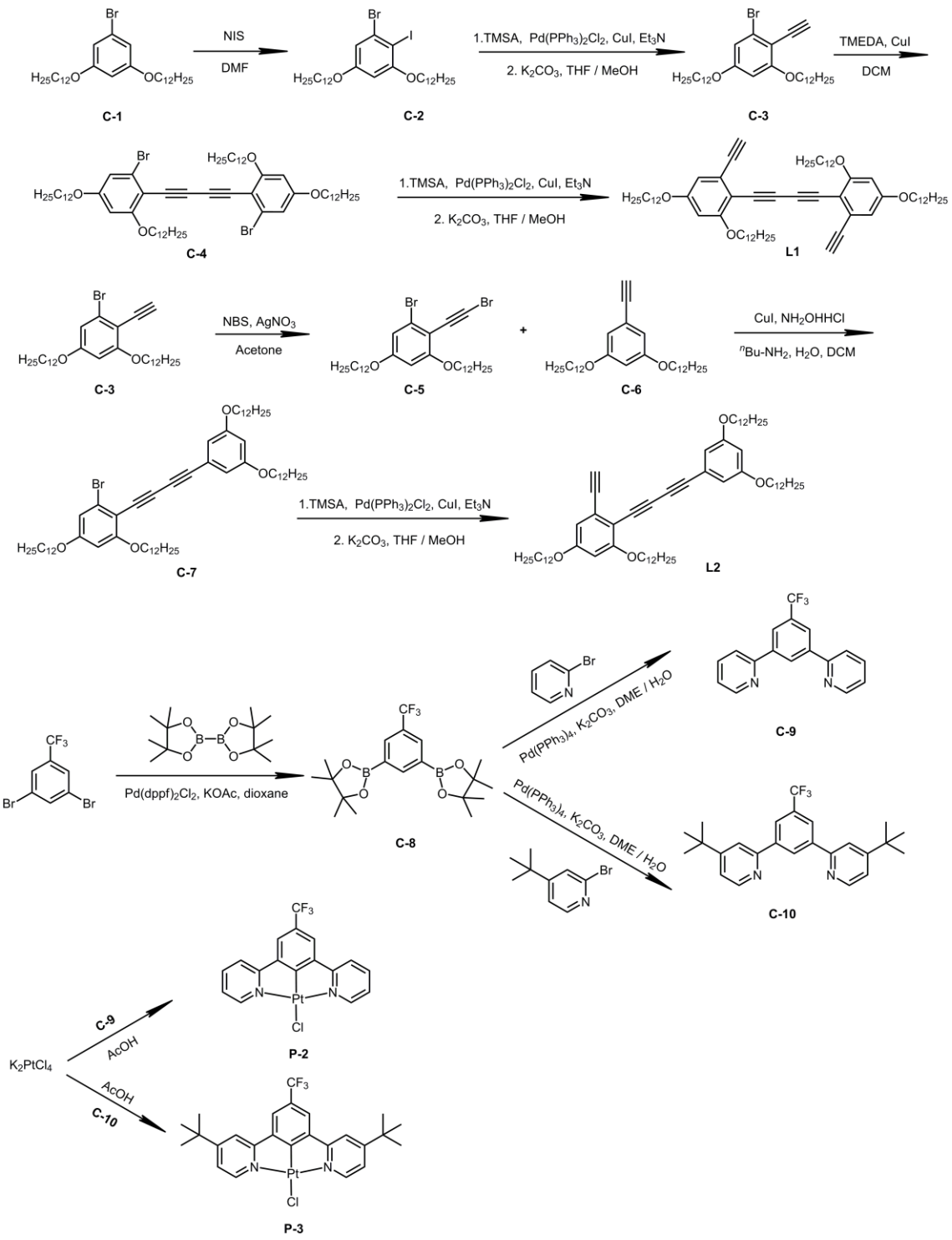
## Material and Methods

The synthetic routes of **1**−**5** were shown in Scheme S1. Complex **6**, chloroplatinum(II) precursors **P-1** and **P-2**, compounds **C-1** and **C-6**, and 1,1'-(1,3-butadiyne-1,4-diyl)bis[2-ethynylbenzene] (**L'**) in Schemes S1 and S2 were synthesized according to the reported literatures (1−4). Compound **L1**, **L2** and **P-3** were synthesized according to Scheme S2.




**Scheme S1.** Synthetic routes of **1**−**5**.




**Scheme S2.** Synthetic routes of ligands and chloroplatinum(II) precursors.

## Experimental Procedures

### Synthesis of alkynylplatinum(II) complexes

Synthesis of **1**. A mixture of **L1** (30 mg, 0.030 mmol) and NaOH (6 mg, 0.15 mmol) in a methanol (50 mL) solution was stirred for 20 minutes at room temperature under nitrogen atmosphere. Subsequently, [(N^C^N)PtCl] (29 mg, 0.064 mmol) was added to the above reaction mixture. The mixture was stirred for 24 hours at room temperature. Slow precipitation with methanol (100 mL) in batches for 10 min afforded the pure product as a yellow solid. Yield: 43 mg, 0.023 mmol, 77 %; $^{1}$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.85–0.90 (m, 12H, $–CH_3$), 1.25–1.52 (m, 72H, $–CH_2–$), 1.75–1.91 (m, 8H, $–CH_2–$), 3.95–4.02 (m, 8H, $–OCH_2–$), 6.28 (d, *J* = 2.1 Hz, 2H, phenyl), 6.59 (d, *J* = 2.1 Hz, 2H, phenyl), 6.71 (t, *J* = 7.6 Hz, 2H, phenyl), 6.96 (d, *J* = 7.6 Hz, 4H, phenyl), 7.26–7.32 (m, 8H, pyridyl), 7.71 (t, *J* = 8.4 Hz, 4H, pyridyl), 9.49 (d, *J* = 6.1 Hz, 4H, pyridyl); MS (MALDI): *m/z*: 1837.914 $[M+H]^+$; elemental analysis calcd (%) for $C_{100}H_{126}N_4O_4Pt_2$: C 65.33, H 6.91, N 3.05; found: C 65.54, H 6.78, N 2.95; mp/°C: complex decomposed before melting.

Synthesis of **2**. A mixture of **L'** (20 mg, 0.080 mmol) and NaOH (8 mg, 0.32 mmol) in a methanol (50 mL) solution was stirred for 20 min at room temperature under nitrogen atmosphere. Subsequently, [(N^C^N-$CF_3$)PtCl] (89 mg, 0.17 mmol) was added to the above reaction mixture. The mixture was stirred for 24 hours at room temperature. Slow precipitation with methanol (100 mL) in batches for 10 min afforded the pure product as an orange solid. Yield: 78 mg, 0.063 mmol, 79 %; $^{1}$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 7.06 (s, 4H, phenyl), 7.15 (t, *J* = 7.6 Hz, 2H, phenyl), 7.24−7.32 (m, 10H, pyridyl and phenyl), 7.40 (d, *J* = 7.6 Hz, 2H, phenyl), 7.55 (d, *J* = 7.7 Hz, 2H, phenyl), 7.78 (t, *J* = 7.5 Hz, 4H, pyridyl), 9.46 (d, *J* = 4.9 Hz, 4H, pyridyl); MS (MALDI): *m/z*: 1237.945 $[M+H]^+$; elemental analysis calcd (%) for $C_{54}H_{28}F_6N_4Pt_2 \bullet 0.5CH_2Cl_2$: C 51.17, H 2.29, N 4.38; found: C 51.07, H 2.50, N 4.32; mp/°C: complex decomposed before melting.

Synthesis of **3**. The procedures were similar to that of **1**, except **P-3** (50 mg, 0.078 mmol) was used in place of [(N^C^N)PtCl] to give the product as a deep-red solid. Yield: 52 mg, 0.024 mmol, 64 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.86–0.89 (m, 12H, –$CH_3$), 1.27–1.49 (m, 108H, –$CH_2$– and –$CH_3$), 1.74–1.81 (m, 4H, –$CH_2$–), 1.88–1.95 (m, 4H, –$CH_2$–), 3.94 (t, $J$ = 6.5 Hz, 4H, –$OCH_2$–), 4.05 (t, $J$ = 6.5 Hz, 4H, –$OCH_2$–), 6.29 (d, $J$ = 1.8 Hz, 2H, phenyl), 6.50 (d, $J$ = 1.8 Hz, 2H, phenyl), 6.94 (s, 4H, phenyl), 7.26 (s, 4H, pyridyl, mixed with solvent peak), 7.34 (d, $J$ = 5.9 Hz, 4H, pyridyl), 9.30 (d, $J$ = 5.9 Hz, 4H, pyridyl); MS (MALDI): *m/z*: 2199.628 $[M+H]^+$; elemental analysis calcd (%) for $C_{118}H_{156}F_6N_4O_4Pt_2$: C 64.48, H 7.10, N 2.55; found: C 64.20, H 6.98, N 2.77; mp/°C: 197−199.

Synthesis of **4**. The procedures were similar to that of **1**, except **C-3** (33 mg, 0.060 mmol) was used in place of **L1** to give the product as a yellow solid. Yield: 25 mg, 0.025 mmol, 47 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.85–0.90 (m, 6H, –$CH_3$), 1.20–1.48 (m, 36H, –$CH_2$–), 1.72–1.80 (m, 2H, –$CH_2$–), 1.89–1.96 (m, 2H, –$CH_2$–), 3.93 (t, $J$ = 6.5 Hz, 2H, −$OCH_2$−), 3.03 (t, $J$ = 6.8 Hz, 2H, −$OCH_2$−), 6.40 (d, $J$ = 1.8 Hz, 1H, phenyl), 6.76 (d, $J$ = 1.8 Hz, 1H, phenyl), 7.17−7.26 (m, 3H, pyridyl and phenyl, mixed with solvent peak), 7.52 (d, $J$ = 7.7 Hz, 2H, phenyl), 7.67 (d, $J$ = 8.0 Hz, 2H, pyridyl), 7.92 (t, $J$ = 7.6 Hz, 2H, pyridyl), 9.79 (d, $J$ = 5.4 Hz, 2H, pyridyl); MS (MALDI): *m/z*: 975.541 $[M+H]^+$; elemental analysis calcd (%) for $C_{48}H_{63}N_2O_2BrPt$: C 59.20 4, H 6.47, N 2.88; found: C 59.49, H 6.20, N 2.75; mp/°C: 121−123.

Synthesis of **5**. The procedures were similar to that of **1**, except **L2** (50 mg, 0.052 mmol) was used in place of **L1** to give the product as a yellow solid. Yield: 45 mg, 0.032 mmol, 66 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.85–0.89 (m, 6H, –$CH_3$), 1.26–1.50 (m, 36H, –$CH_2$–), 1.69–1.88 (m, 4H, –$CH_2$–), 3.83 (t, $J$ = 6.5 Hz, 2H, −$OCH_2$−), 3.97–4.03 (m, 2H, –$OCH_2$–), 6.30 (d, $J$ = 2.0 Hz, 1H, phenyl), 6.41 (s, 1H, phenyl), 6.45 (d, $J$ = 1.4 Hz, 2H, phenyl), 6.73 (d, $J$ = 2.0 Hz,

1H, phenyl), 7.20 (t, *J* = 7.8 Hz, 1H, phenyl), 7.30 (t, *J* = 6.0 Hz, 2H, pyridyl, mixed with solvent peak), 7.50 (d, *J* = 7.8 Hz, 2H, phenyl), 7.64 (d, *J* = 8.2 Hz, 2H, pyridyl), 7.85 (t, *J* = 8.2 Hz, 2H, pyridyl), 9.73 (d, *J* = 6.0 Hz, 2H, pyridyl); MS (MALDI): *m/z*: 1389.135 $[M+H]^+$; elemental analysis calcd (%) for $C_{82}H_{116}N_2O_4Pt$: C 70.94, H 8.36, N 2.02; found: C 70.78, H 8.49, N 2.25; mp/°C: 64−66.

**Synthesis of chloroplatinum(II) precursor complexes**

Synthesis of **P-3**. The compound was synthesized according to the modification of a reported procedure (5). **C-10** (130 mg, 0.31 mmol) and $K_2PtCl_4$ (125 mg, 0.30 mmol) were added into glacial acetic acid (15 mL), and the mixture was heated for 110 ℃ for 3 days. After cooling to room temperature, slow participation with ethanol (30 mL) in batches afforded the pure product as an orange solid. Yield: 110 mg, 0.17 mmol, 57 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 1.43 (s, 18H, $-CH_3$), 7.35 (d, *J* = 6.1 Hz, 2H, pyridyl), 7.69–7.73 (m, 4H, pyridyl and phenyl), 9.24 (d, *J* = 6.1 Hz, 2H, pyridyl); MS (MALDI): *m/z*: 606.278 $[M-Cl]^+$; elemental analysis calcd (%) for $C_{25}H_{26}N_2F_3ClPt$: C 46.80, H 4.06, N 4.37; found: C 46.65, H 4.26, N 4.50; mp/°C: > 300.

**Synthesis of ligand precursors**

Synthesis of **C-2**. The compound was synthesized according to the modification of a reported procedure (6). To a solution of **C-1** (4.4 g, 8.4 mmol) in dry DMF (50 mL) was added *N*-iodosuccinimide (2.0 g, 8.8 mmol). The mixture was heated at 70 ℃ for overnight under nitrogen atmosphere. Upon completion of the reaction, dichloromethane (200 mL) was added into the reaction mixture, which was washed with deionized water for 2 times. The organic layer was dried over anhydrous $MgSO_4$. Removal of the solvent under reduced pressure afforded the crude product, which was purified by column chromatography on silica gel using dichloromethane–petroleum ether (1:20 v / v) as the eluent to give **C-2** as a white solid. Yield: 3.9 g, 6.0 mmol, 71 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.82 (t, *J* = 6.7 Hz, 6H, $-CH_3$), 1.21–1.52 (m, 36H, $-CH_2-$), 1.65–1.80 (m, 4H, $-CH_2-$), 3.81–3.86 (m,

4H, –$OCH_2$–), 6.24 (d, *J* = 2.4 Hz, 1H, phenyl), 6.77 (d, *J* = 2.4 Hz, 1H, phenyl); MS (MALDI): *m/z*: 652.35 $[M]^+$.

Synthesis of **C-3**. The compound was synthesized by a Sonogashira coupling reaction according to the modification of reported procedure (7). **C-2** (1.2 g, 1.8 mmol), $Pd(PPh_3)_2Cl_2$ (66 mg, 0.09 mmol), CuI (18 mg, 0.09 mmol) and trimethylsilylacetylene (TMSA, 1.0 mL, 7.2 mmol) were added to the flask with degassed triethylamine (60 mL), and the mixture was stirred overnight at room temperature under nitrogen atmosphere. Removal of the solvent under reduced pressure afforded the crude product, which was purified by column chromatography on silica gel using dichloromethane–petroleum ether (1:20 v / v) as the eluent to give **C-3-TMS** (0.9 g, 1.45 mmol) as a light-yellow solid. Subsequently, to the THF–methanol (1:1 v / v, 50 mL) solution mixture of **C-3-TMS** (0.5 g, 0.8 mmol) was added $K_2CO_3$ (167 mg, 1.2 mmol). The reaction mixture was stirred for 2 hours at room temperature. Then the reaction mixture was poured into dichloromethane (100 mL) and was washed with deionized water for 2 times. The organic layer was dried over anhydrous $MgSO_4$. Removal of the solvent under reduced pressure afforded the crude product, which was used for subsequent reactions without further purification. Yield: 390 mg, 0.71 mmol, 69 %; $^1$H NMR (400 MHz, $CDCl_3$, 298 K, relative to $Me_4Si$, $\delta$ / ppm): 0.88 (t, *J* = 6.6 Hz, 6H, –$CH_3$), 1.26–1.52 (m, 36H, –$CH_2$–), 1.72–1.85 (m, 4H, –$CH_2$–), 3.90–3.99 (m, 4H, –$OCH_2$–), 6.32 (d, *J* = 1.5 Hz, 1H, phenyl), 6.69 (d, *J* = 1.5 Hz, 1H, phenyl); MS (MALDI): *m/z*: 551.170 $[M+H]^+$.

Synthesis of **C-4**: The compound was synthesized according to the modification of a reported procedure (8). CuI (82 mg, 0.44 mmol) was dispersed in a solution of dichloromethane (50 mL), *N,N,N',N'*-tetramethylethylenediamine (0.16 mL, 1.1 mmol) was added and the mixture was stirred for 5 min. The dichloromethane solution of **C-3** (1.2 g, 2.2 mmol) was then added to the mixture and stirred for overnight at room temperature at the oxygen atmosphere. Upon completion of the reaction, the reaction mixture was washed with deionized water for 2 times and the

organic layer was dried over anhydrous $MgSO_4$. Removal of the solvent under reduced pressure afforded the crude product, which was purified by column chromatography on silica gel using dichloromethane–petroleum ether (1:5 v / v) as the eluent to give **C-4** as a pale-yellow solid. Yield: 900 mg, 0.82 mmol, 75 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.85–0.89 (m, 12H, $–CH_3$), 1.23–1.50 (m, 72H, $–CH_2–$), 1.72–1.86 (m, 8H, $–CH_2–$), 3.91–3.99 (m, 8H, $–OCH_2–$), 6.34 (d, $J$ = 2.0 Hz, 2H, phenyl), 6.70 (d, $J$ = 2.0 Hz, 2H, phenyl); MS (MALDI): *m/z*: 1095.655 $[M+H]^+$.

Synthesis of **C-5** and **C-7**. The compounds were synthesized according to the modification of a reported procedure (9). To a solution of **C-3** (1.32 g, 2.0 mmol) and $AgNO_3$ (0.41 g, 2.4 mmol) in acetone (30 mL) was added. NBS (0.53 g, 3.0 mmol), and the mixture was stirred in the dark at room temperature for overnight. Removal of the solvent under reduced pressure afforded the crude product **C-5** (1.0g, 1.6 mmol) which was used without further purification. CuI (0.3 g, 1.6 mmol) was dispersed in a mixture of butylamine (6 mL) and water (8 mL), and the mixture was stirred for 5 min. Subsequently, $NH_2OH•HCl$ was added in portions until the solution turned colorless. **C-6** (0.6 g, 1.3 mmol) was added and the mixture was stirred for 5 min. The dichloromethane solution of **C-5** (0.8 g, 1.3 mmol) was then added dropwise to the mixture and stirred for another 30 min at room temperature. Upon completion of the reaction, the reaction mixture was washed with deionized water for 2 times and the organic layer was dried over anhydrous $MgSO_4$. Removal of the solvent under reduced pressure afforded the crude product, which was purified by column chromatography on silica gel using dichloromethane–petroleum ether (1:5 v / v) as the eluent to give **C-7** as a yellow solid. Yield: 630 mg, 0.62 mmol, 38 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.85–0.90 (m, 12H, $–CH_3$), 1.24–1.50 (m, 72H, $–CH_2–$), 1.72–1.87 (m, 8H, $–CH_2–$), 3.89–4.00 (m, 8H, $–OCH_2–$), 6.35 (d, $J$ = 1.8 Hz, 1H, phenyl), 6.46 (s, 1H, phenyl), 6.65 (d, $J$ = 2.0 Hz, 2H, phenyl), 6.71 (d, $J$ = 1.8 Hz, 1H, phenyl); MS (MALDI): *m/z*: 1019.942 $[M+H]^+$.

Synthesis of **C-8**. The compounds were synthesized according to the modification of a reported procedure (10). 3,5-Dibromobenzotrifluoride (1.0 g, 3.3 mmol), bispinacolatodiboron (1.8 g, 7.2 mmol), $Pd(dppf)Cl_2$ (178 mg, 0.23 mmol) and KOAc (2.6 g, 26.2 mmol) were added to the flask with degassed dioxane (70 mL), and the mixture was stirred at 110 ℃ for 24 hours under nitrogen atmosphere. Upon cooling to the room temperature, ethyl acetate (150 mL) was added. The reaction mixture was washed with deionized water for 2 times and the organic layer was dried over anhydrous $MgSO_4$. Removal of the solvent under reduced pressure afforded the crude product, which was purified by column chromatography on silica gel using ethyl acetate–petroleum ether (1:15 v / v) as the eluent to give **C-8** as a white solid. Yield: 1.0 g, 2.5 mmol, 78 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 1.35 (s, 24H, $–CH_3$), 8.13 (s 2H, phenyl), 8.41 (s 1H, phenyl); MS (MALDI): *m/z*: 399.55 $[M+H]^+$.

Synthesis of **C-9**. The compounds were synthesized according to the modification of a reported procedure (10). 2-Bromopyridine (1.1 g, 6.7 mmol), **C-8** (1.0 g, 3.0 mmol), $Pd(PPh_3)_4$ (345 mg, 0.30 mmol) and $Na_2CO_3$ (2.1 g, 15.0 mmol) were added to the flask with degassed DME/$H_2O$ mixture (60 mL, 1:1, v/v), and the mixture was stirred at 100 ℃ for 24 hours under nitrogen atmosphere. Upon cooling to the room temperature, ethyl acetate (100 mL) was added. The reaction mixture was washed with deionized water for 2 times and the organic layer was dried over anhydrous $MgSO_4$. Removal of the solvent under reduced pressure afforded the crude product, which was purified by column chromatography on silica gel using ethyl acetate–petroleum ether (1:8 v / v) as the eluent to give **C-9** as a white solid. Yield: 0.7 g, 2.3 mmol, 77 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 7.32 (t, $J$ = 6.2 Hz, 2H, pyridyl), 7.83 (t, $J$ = 7.0 Hz, 2H, pyridyl), 7.89 (d, $J$ = 7.9 Hz, 2H, pyridyl), 8.34 (s, 2H, phenyl), 8.75 (d, $J$ = 4.6 Hz, 2H, pyridyl), 8.83 (s, 1H , phenyl); MS (MALDI): *m/z*: 301.23 $[M+H]^+$;

Synthesis of **C-10**.

The procedures were similar to that of compound **C-9**, except 2-bromo-4-(tert-butyl)pyridine (296 mg, 1.38 mmol) was used in place of 2-Bromopyridine. The crude product was purified by column chromatography on silica gel using ethyl acetate–petroleum ether (1:10 v / v) as the eluent to give the desired product as a gray-white solid. Yield: 130 mg, 0.31 mmol, 50 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 1.40 (s, 18H, $–CH_3$), 7.31 (d, $J$ = 5.2 Hz, 2H, pyridyl), 7.80 (s, 2H, pyridyl), 8.28 (s, 2H, phenyl), 8.65 (d, $J$ = 5.2 Hz, 2H, pyridyl), 8.74 (s, 1H, phenyl); MS (MALDI): *m/z*: 413.34 $[M+H]^+$.

**Synthesis of alkynyl ligands**

Synthesis of **L1**. The procedures were similar to that of compound **C-3**, except **C-4** (200 mg, 0.2 mmol) was used in place of **C-2** with heating at 70 ℃. The crude product was purified by column chromatography on silica gel using dichloromethane–petroleum ether (1:3 v / v) as the eluent to give the desired product as an off-white solid. Yield: 110 mg, 0.11 mmol, 52 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.86–0.89 (m, 12H, $–CH_3$), 1.20–1.47 (m, 72H, $–CH_2–$), 1.73–1.87 (m, 8H, $–CH_2–$), 3.22 (s, 2H, –C≡C–H), 3.93 (t, $J$ = 6.5 Hz, 4H, $–OCH_2–$), 4.00 (t, $J$ = 6.7 Hz, 4H, $–OCH_2–$), 6.44 (d, $J$ = 1.8 Hz, 2H, phenyl), 6.62 (d, $J$ = 1.8 Hz, 2H, phenyl); MS (MALDI): *m/z*: 986.669 $[M]^+$ ; mp/°C: 53−55.

Synthesis of **L2**. The procedures were similar to that of compound **L1**, except **C-7** (400 mg, 0.39 mmol) was used in place of **C-4**. The crude product was purified by column chromatography on silica gel using dichloromethane–petroleum ether (1:3 v / v) as the eluent to give the desired product as a yellow solid. Yield: 275 mg, 0.29 mmol, 74 %; $^1$H NMR (400 MHz, 298 K, $CDCl_3$, relative to $Me_4Si$, $\delta$ / ppm): 0.83–0.90 (m, 12H, $–CH_3$), 1.24–1.51 (m, 72H, $–CH_2–$), 1.72–1.87 (m, 8H, $–CH_2–$), 3.34 (s, 1H, –C≡C–H), 3.89–4.01 (m, 8H, $–OCH_2–$), 6.42 (d, $J$ = 1.3 Hz, 1H, phenyl), 6.46 (s, 1H, phenyl), 6.60 (d, $J$ = 1.3 Hz, 1H, phenyl), 6.65 (d, $J$ = 1.8 Hz, 2H, phenyl); MS (MALDI): *m/z*: 962.981 $[M]^+$ ; mp/°C: 45−47.

**Physical Measurements and Instrumentations**

All $^{1}H$ NMR spectra were recorded on a Bruker DPX 400 FT–NMR spectrometer 400 MHz. Matrix assisted laser desorption ionization time of flight mass were performed on a Bruker ultrafleXtreme MALDI–TOF/TOF mass spectrometer using positive-ion mode (Bruker Daltonics). Elemental analyses of the complexes were performed on a Vario EL elemental analyzer. Melting points (mp) were measured on a Buchi M-560 apparatus with heating rate of 1℃/min.

Electronic absorption spectra and temperature-dependent electronic absorption spectra were recorded using a Shimadzu UV–3600 spectrophotometer and a Varian Cary 50 UV-vis spectrophotometer, respectively, with the monitoring of temperature using the Varian Cary single-cell Peltier thermostat. The photoluminescence spectra were measured on Edinburgh Instruments FS5 and Edinburgh Instruments FLS980 fluorescence spectrophotometers. Emission lifetime measurements were performed using LP980 transient absorption spectrometer (Edinburgh Instruments Ltd, UK). The excitation source was the 355 nm output (third harmonic) of an Nd: YAG laser (Quanta-Ray Lab130 Pulsed Nd:YAG Laser) and the probe light source was a Xe900 450 W xenon arc lamp. All solutions for photophysical studies were prepared under high vacuum in a 10-$cm^3$ round-bottomed flask equipped with a sidearm 1-cm fluorescence cuvette and sealed from the atmosphere by a Rotaflo HP6/6 quick-release Teflon stopper. Solutions were rigorously degassed on a high-vacuum line in a two-compartment cell with no less than four successive freeze-pump-thaw cycles. The emission quantum yields were measured on a Hamamatsu C9920-02G absolute PL quantum yield measurement system. Time-resolved emission spectra were obtained using an Edinburgh Instrument LP980KS transient absorption spectrometer equipped with a R928P photomultiplier tube, with capability for time-resolved emission measurements. Dynamic light scattering spectra were obtained using a Malvern Panalytical Zetasizer Nano ZS90 particle size analyzer. Scanning electron microscope experiments were performed by using ZEISS GeminiSEM 500. The atomic force microscopy measurements were performed on Bruker Dimension Scanfast in a tapping mode. The SEM and AFM samples were

prepared by dropcasting solutions onto silicon wafers and allowing them to dry naturally. Transmission electron micrographs (TEM) were recorded on a FEI Tecnai G2 Spirit. The samples for TEM were prepared by dropcasting solutions on the carbon-coated copper grids.

**Time-Dependent Emission and UV-Vis Spectral Changes**

1. Solutions of **1** in dichloromethane (0.3 mL, $5.4 \times 10^{-4}$ M) were injected into hexane, cyclohexane, decane, or methylcyclohexane (2.7 mL) to yield the respective solution mixtures of **1** in hexane-dichloromethane, cyclohexane-dichloromethane, decane-dichloromethane, methylcyclohexane-dichloromethane (9:1, v/v) ($5.4 \times 10^{-5}$ M). After rapid mixing, the emission intensity at 516 nm was recorded with time.

2. Solutions of **1** in dichloromethane (0.3 mL) were injected into hexane or cyclohexane (2.7 mL) to yield solution mixtures of **1** in hexane-dichloromethane, cyclohexane-dichloromethane (9:1, v/v) respectively. After rapid mixing, the absorbance intensity at 425 nm was recorded with time under different conditions.

**Crystal Structure Determination**

Single crystals of **2** suitable for X-ray diffraction studies were grown by vapor diffusion of diethyl ether into a concentrated dichloromethane solution of **2**. Single-crystal diffraction data of **2** were collected on an Agilent SuperNova X-ray diffractometer using micro-focus dual with X-ray Source of Cu–K$\alpha$ radiation ($\lambda$ = 1.54178 Å) at 150 K. Using Olex2 (11), the structure of the crystal was solved with the ShelXS (12) structure solution program using direct methods and refined with the XL (12) refinement package using least squares minimization. CCDC XXX contains the supplementary crystallographic data for **2**. This can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

**Computational Details**

All the density functional theory (DFT) calculations were performed using the Gaussian 09 suite of programs (13). The ground-state geometries of both the open and closed forms of **1** and **3** were fully optimized by DFT with the hybrid meta exchange-correlation M06 functional (14), which is recommended for application in organometallic and metal coordination compounds and for non-covalent interactions (14, 15), in conjunction with the solvation model density (SMD) continuum method (16) using dichloromethane as the solvent. Vibrational frequencies were then computed for all stationary points to verify that each was a minimum (NIMAG = 0) on the potential energy surface (PES). The lowest-lying triplet excited state ($T_1$) of the open form of **1** has also been optimized with the unrestricted method (UM06) in order to calculate its emission energy. All calculations were performed with the Stuttgart effective core potentials (ECPs) and the associated basis set to describe Pt (17), with two f-type polarization functions ($\zeta$ = 0.70 and 0.14) (18), and the 6-31G(d,p) basis set (19−22) to describe all other atoms. All the DFT calculations were performed with a pruned (99,590) grid for numerical integration. The Cartesian coordinates of the optimized ground-state geometries of the open and closed forms of **1** and **3**, and those of the optimized $T_1$ geometry of the open form of **1**, are given in Tables S3–S7.

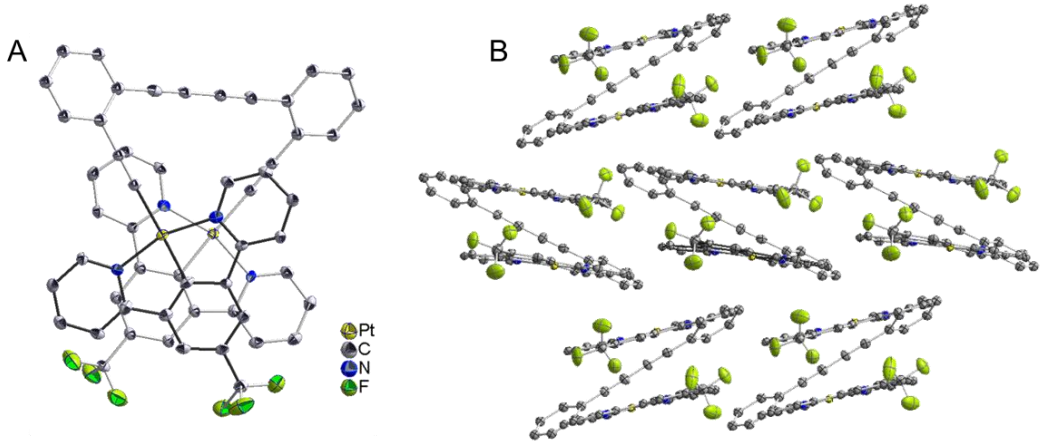



**Figure S1.** (A) Perspective drawing of **2**. Hydrogen atoms and solvent molecules are omitted for clarity. Thermal ellipsoids were shown at the 30 % probability level.(B) Crystal packing of **2** without intermolecular π–π interaction.

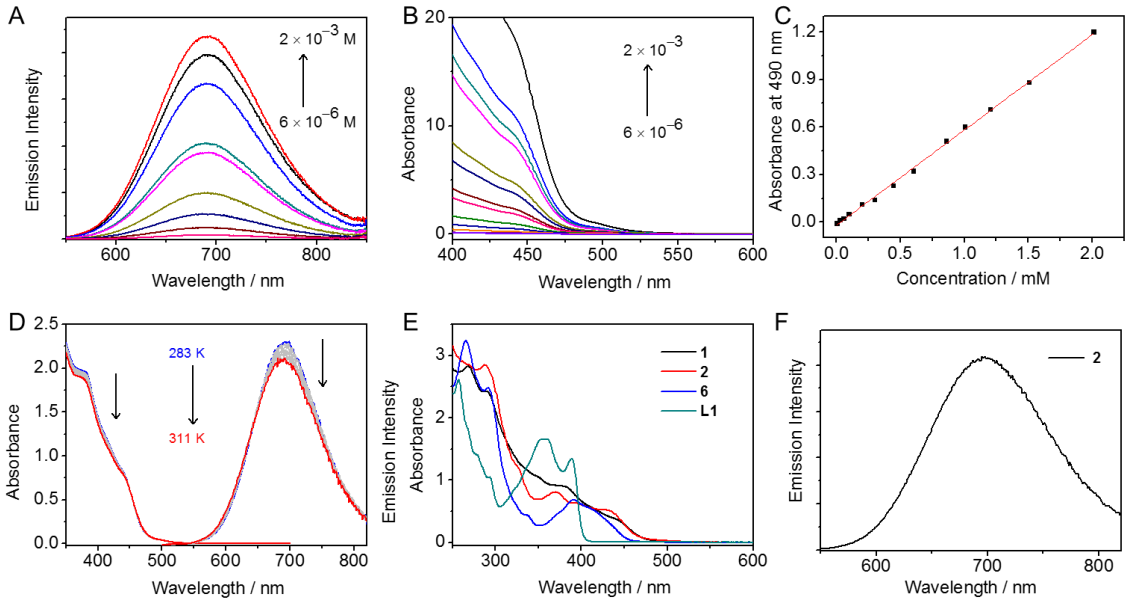



**Figure S2.** Concentration-dependent (A) emission and (B) UV-vis absorption spectra of **1** in dichloromethane from 6.0 × $10^{-6}$ to 2.0 × $10^{-3}$ M. (C) A plot of apparent absorbance at 490 nm as a function of concentration and the solid line gives the linear relationship between absorbance and concentration. The apparent absorbance is the absorbance corrected to 1-cm pathlength equivalence. (D) Temperature-dependent UV-vis absorption and emission spectra of **1** in dichloromethane at 8.2 × $10^{-5}$ M. (E) UV-vis absorption spectra of **1**, **2**, **6** and **L1** in dichloromethane solutions. (F) Emission spectrum of **2** in degassed dichloromethane solution (2.5 × $10^{-5}$ M).

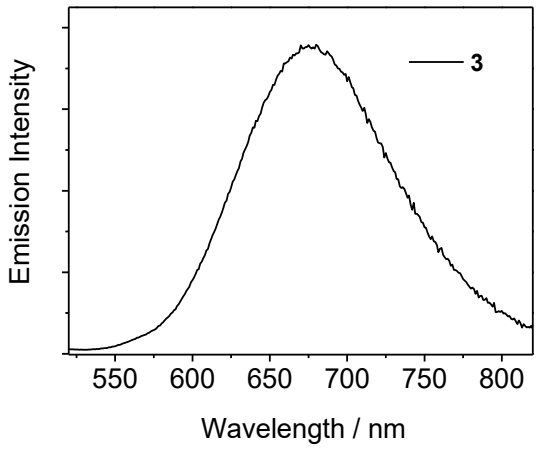



**Figure S3.** Emission spectrum of **3** in degassed dichloromethane solution ($1.3 \times 10^{-5}$ M).

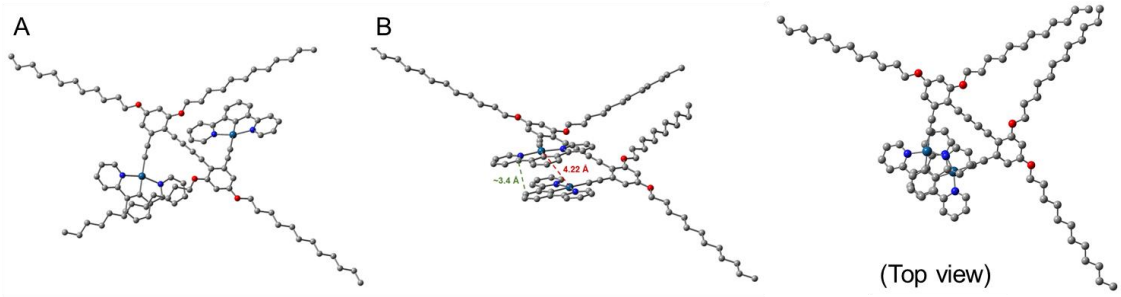



**Figure S4.** Optimized structures of molecular hinge **1** in (A) open form and (B) closed form.

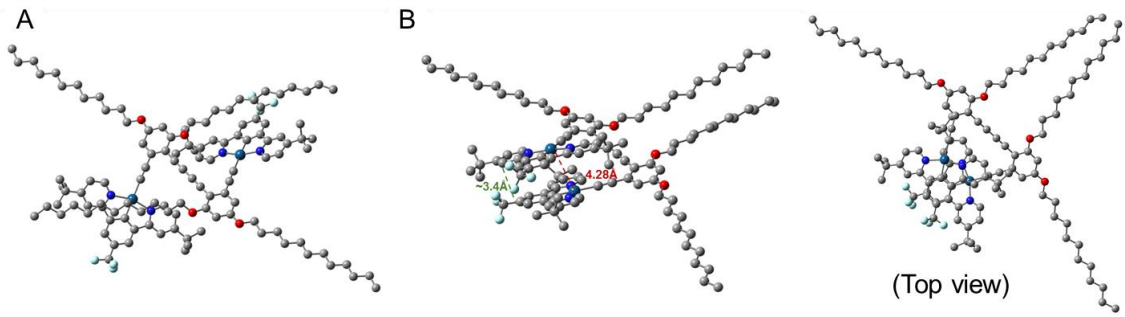



**Figure S5.** Optimized structures of molecular hinge **3** in (A) open form and (B) closed form.

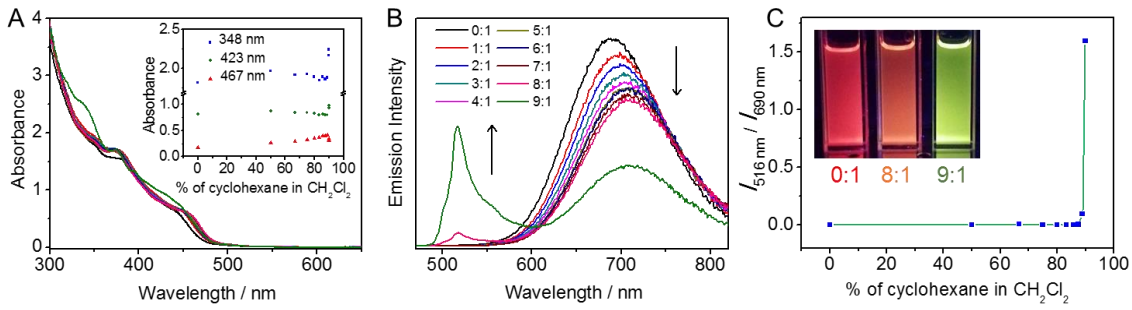



**Figure S6.** Solvent-dependent (A) UV-vis absorption and (B) emission spectra of **1** upon increasing cyclohexane portion in dichloromethane (v/v, $5.6 \times 10^{-5}$ M). Inset of (A): Plots of the corresponding absorbance at 348, 423 and 467 nm upon increasing cyclohexane content. (C) The phosphorescence intensity ratio between 516 and 690 nm ($I_{516}$ / $I_{690}$) upon increasing cyclohexane portion in dichloromethane (v/v, $5.6 \times 10^{-5}$ M). Inset: Photographs of different emission colors in cyclohexane-dichloromethane (0:1, 8:1, 9:1, v/v) mixtures.

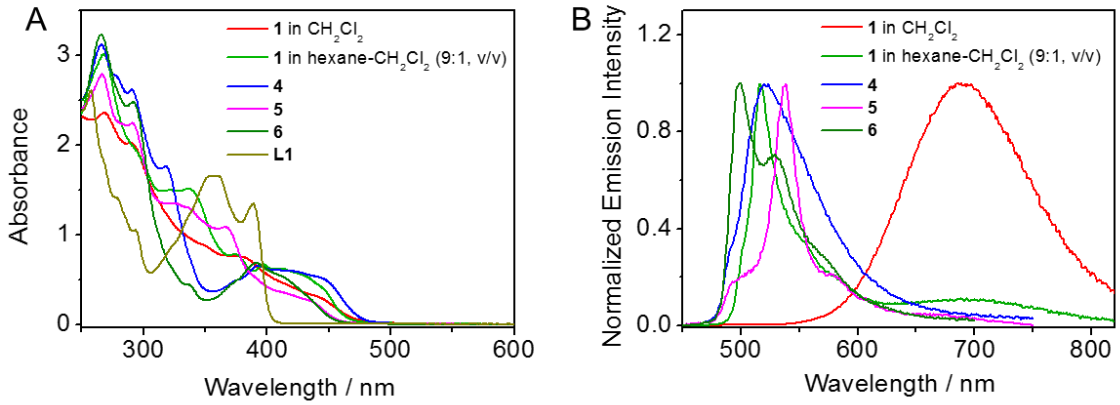



**Figure S7.** (A) UV-vis absorption of **1**, **4**–**6** and **L1** in dichloromethane solutions and UV-vis absorption of **1** in hexane-dichloromethane (9:1, v/v) mixture. (B) Emission spectra of **1**, **4**–**6** in dichloromethane solutions and emission spectrum of **1** in hexane-dichloromethane (9:1, v/v) mixture.

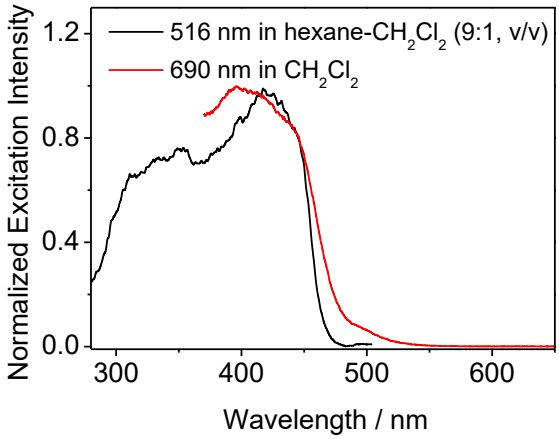



**Figure S8.** Excitation spectra of **1** with emission peaks at 690 nm in dichloromethane and 516 nm in hexane-dichloromethane (9:1, v/v) mixture respectively.

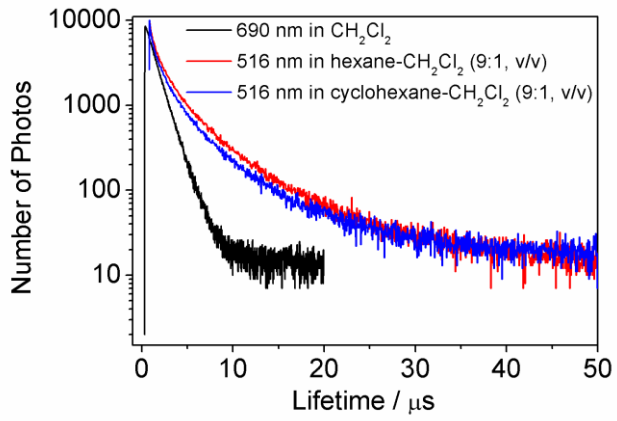



**Figure S9.** Emission decay profiles monitored at 690 nm in dichloromethane solution with closed form ($\tau$ = 1.4 μs) and 516 nm in hexane/cyclohexane-dichloromethane (9:1, v/v) mixtures with open form ($\tau$ = 3.6 μs) after a laser pulse.

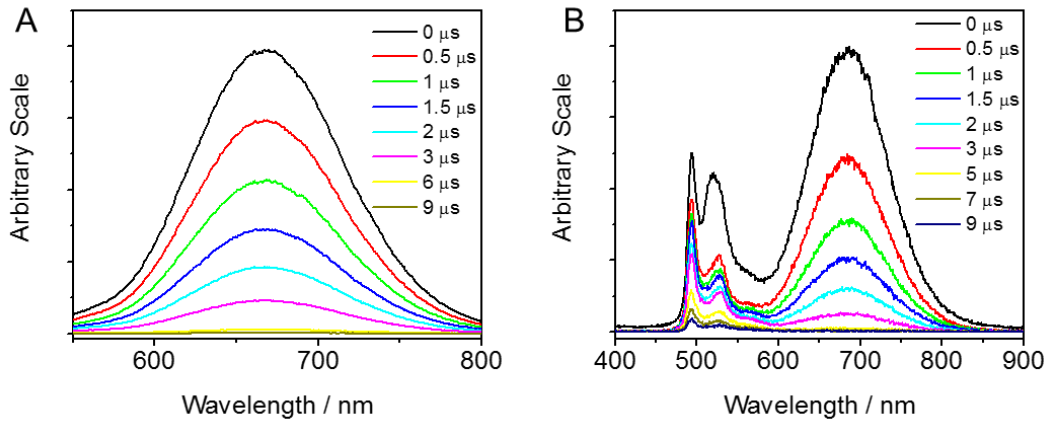



**Figure S10.** Time-resolved emission spectra of **1** in (A) dichloromethane solution (5.7 × $10^{-5}$ M) and (B) hexane-dichloromethane (9:1, v/v) mixture (5.7 × $10^{-5}$ M).

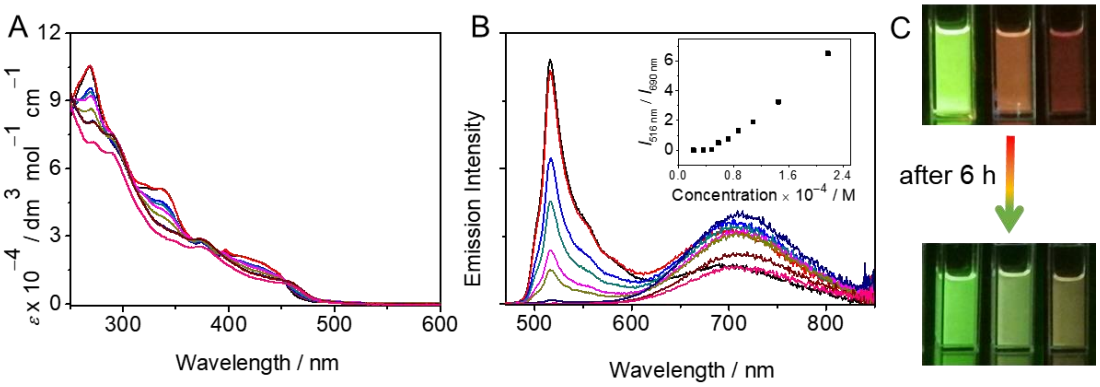



**Figure S11.** Concentration-dependent (A) UV-vis absorption and (B) emission spectra of **1** in cyclohexane-dichloromethane (9:1, v/v) mixtures at different concentrations from 2.2 × $10^{-5}$ to 2.2 × $10^{-4}$ M at room temperature. Inset: A plot of the corresponding phosphorescence intensity ratio between 516 and 690 nm ($I_{516}$ / $I_{690}$) in cyclohexane-dichloromethane (9:1, v/v) mixtures at different concentrations. (C) Photographs of emission color changes in cyclohexane-dichloromethane (9:1, v/v) mixtures at concentrations of 7.2 × $10^{-5}$, 5.8 × $10^{-5}$, 4.8 × $10^{-5}$ M (from left to right).

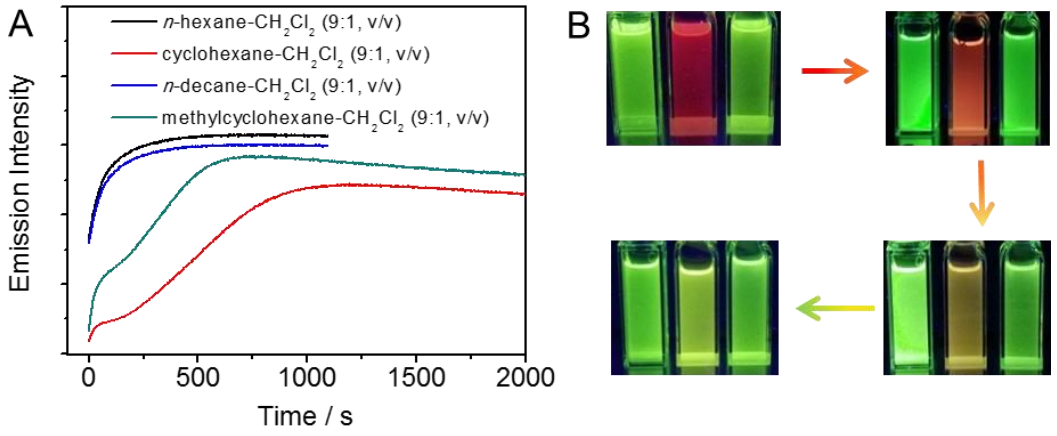



**Figure S12.** (A) Time-dependent emission spectral changes of **1** in *n*-hexane/*n*-decane/cyclohexane/methylcyclohexane-dichloromethane (9:1, v/v) mixtures ($5.4 \times 10^{-5}$ M). (B) Photographs of hexane-dichloromethane, cyclohexane-dichloromethane and decane-dichloromethane (9:1, v/v, left to right) mixtures with increasing time.

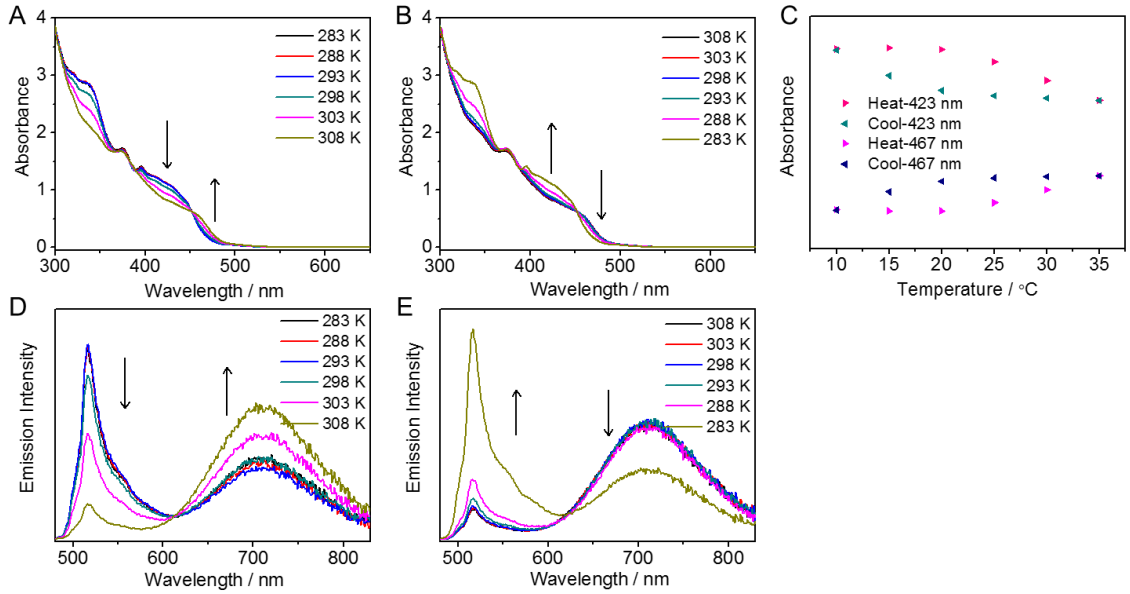



**Figure S13.** Temperature-dependent UV-vis absorption spectra of **1** in cyclohexane-dichloromethane (9:1, v/v) ($5.6 \times 10^{-5}$ M) mixture with (A) heating and (B) cooling processes. (C) Plots of the corresponding absorbance at 423 and 467 nm at different temperatures with heating and cooling processes. Temperature-dependent emission spectra of **1** in cyclohexane-dichloromethane (9:1, v/v) ($5.6 \times 10^{-5}$ M) mixture with (D) heating and (E) cooling processes.

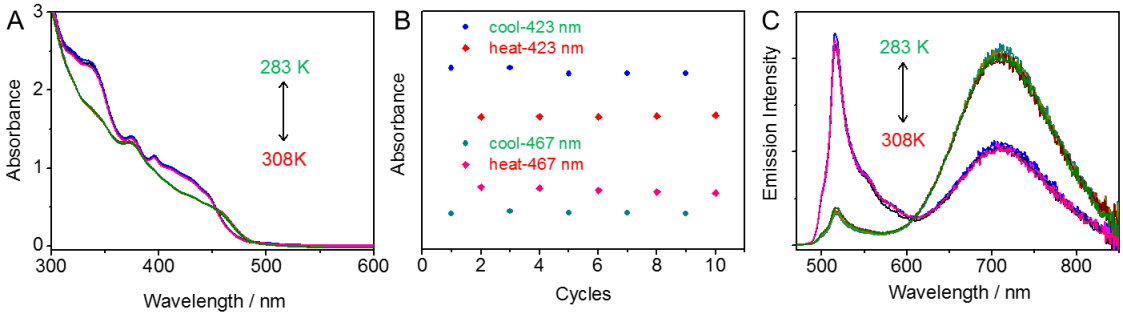



**Figure S14.** (A) Reversible processes of the molecular hinge between open form and closed form with electronic absorption spectra of **1** in cyclohexane-dichloromethane (9:1, v/v) ($5.6 \times 10^{-5}$ M) mixture in 5 cycles. (B) Plots of the corresponding absorbance at 423 and 467 nm with the number of repeating cycles. (C) Reversible processes of the molecular hinge between open form and closed form with emission spectra of **1** in cyclohexane-dichloromethane (9:1, v/v) ($5.6 \times 10^{-5}$ M) mixture in 5 cycles.

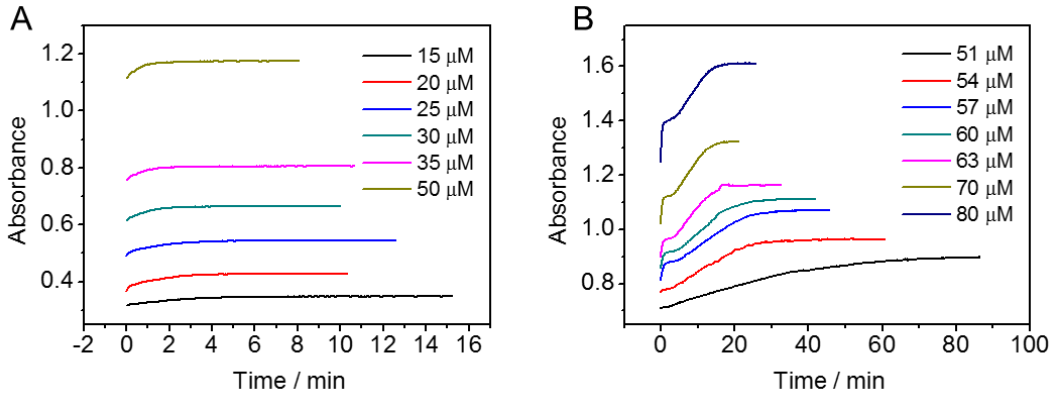



**Figure S15.** (A) Time-dependent UV-vis spectra of complex **1** in hexane-dichloromethane (9:1, v/v) mixtures at different concentrations from 15 to 50 μM at 293 K. (B) Time-dependent UV-vis spectra of complex **1** in cyclohexane-dichloromethane (9:1, v/v) mixtures at different concentrations from 51 to 80 μM at 293 K.

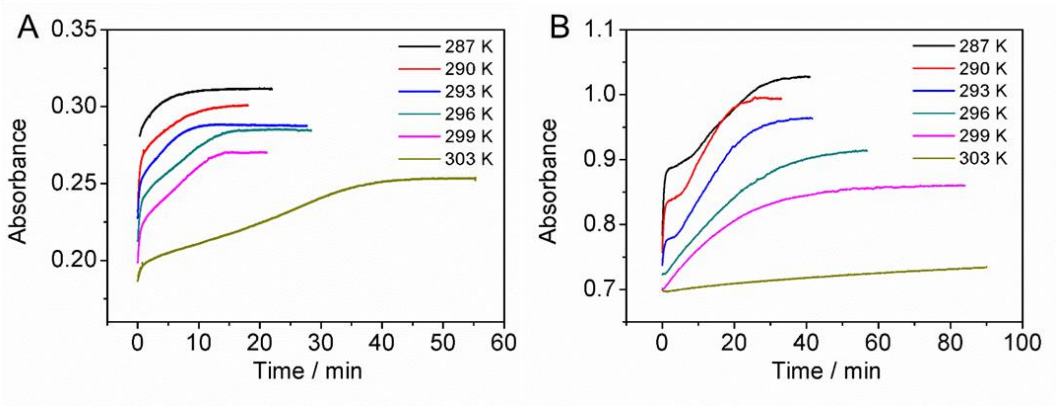



**Figure S16.** Time-dependent UV-vis spectra of complex **1** in (A) hexane-dichloromethane (9:1, v/v) ($1.5 \times 10^{-5}$ M) and (B) cyclohexane-dichloromethane (9:1, v/v) ($5.7 \times 10^{-5}$ M) mixtures at different temperatures.

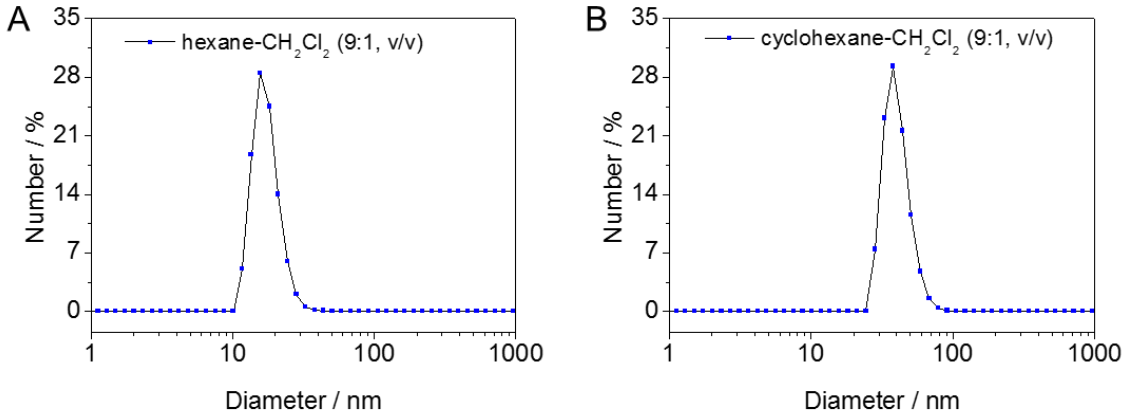



**Figure S17.** DLS studies of **1** in (A) hexane-dichloromethane (9:1, v/v) mixture ($5.7 \times 10^{-5}$ M) and (B) cyclohexane-dichloromethane (9:1, v/v) mixture ($5.7 \times 10^{-5}$ M) respectively.

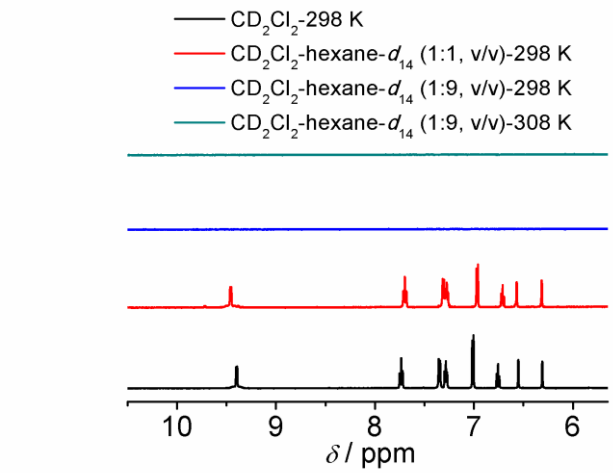



**Figure S18.** $^{1}$H NMR spectra of **1** upon increasing the hexane-$d_{14}$ portion in $CD_2Cl_2$ ($4.6 \times 10^{-4}$ M).

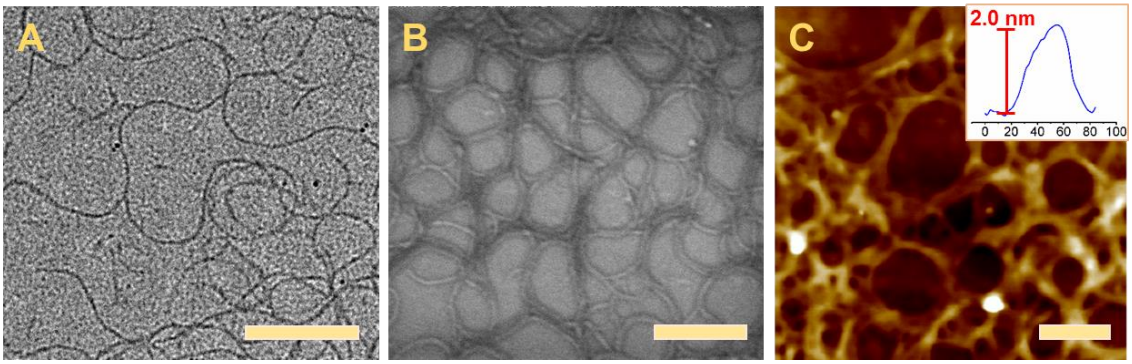



**Figure S19.** (A) TEM, (B) SEM and (C) AFM images of **1** prepared from cyclohexane-dichloromethane (9:1, v/v) mixture ($5.6 \times 10^{-5}$ M). Scale bars: 200 nm.

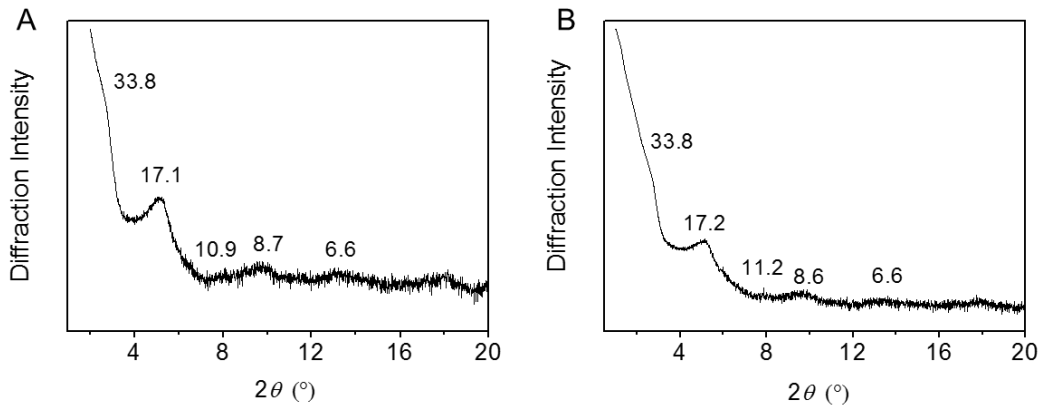



**Figure S20.** XRD patterns of **1** prepared from (A) hexane-dichloromethane (9:1, v/v) mixture and (B) cyclohexane-dichloromethane (9:1, v/v) mixture with the ratio of about 1:1/2:1/3:1/4:1/5.

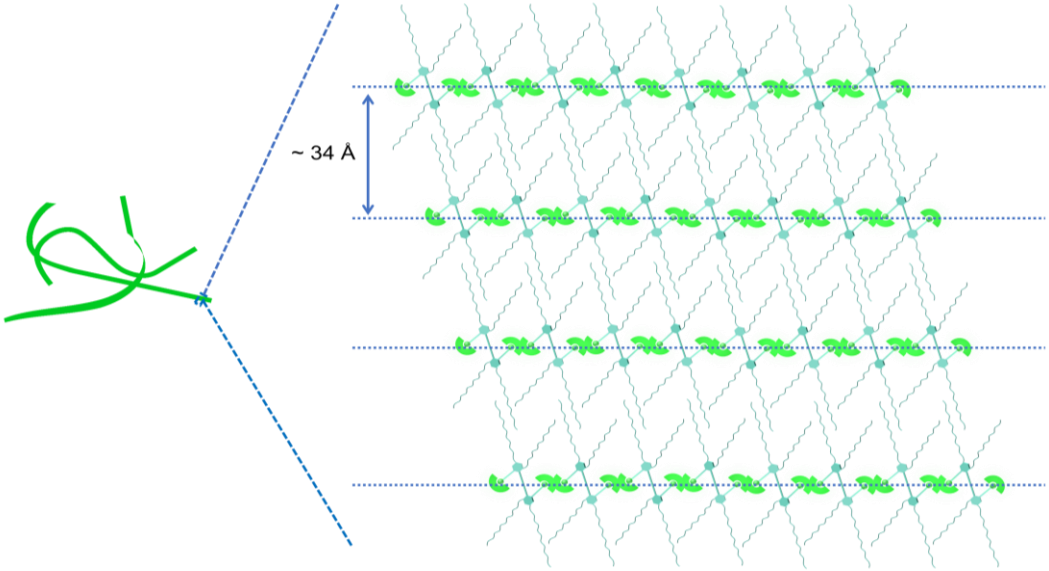



**Figure S21.** Schematic representation of one-dimensional nanofiber formed in hexane/cyclohexane-dichloromethane (9:1, v/v) mixtures.

**Video 1.** A video showing the luminescence changes in hexane-dichloromethane mixture of **1**.

**Video 2.** A video showing the luminescence changes in cyclohexane-dichloromethane mixture of **1**.

**Table S1**. Crystallographic and structural refinement data for complex **2**

| Identification code | Complex **2** |
|---|---|
| Empirical formula | $C_{54}H_{28}F_6N_4Pt_2$ |
| Formula weight | 1236.98 |
| Temperature/K | 150.00 |
| Crystal system | triclinic |
| Space group | $P\bar{1}$ |
| *a*/Å | 10.136 1(2) |
| *b*/Å | 14.9235(3) |
| *c*/Å | 27.9163(6) |
| *α*/° | 97.5834(17) |
| *β*/° | 97.4100(18) |
| *γ*/° | 90.1700(18) |
| *V*/Å $^3$ | 4150.06(16) |
| *Z* | 4 |
| $\rho_{calc}$/g·cm$^{-3}$ | 1.980 |
| $\mu$/mm$^{-1}$ | 13.046 |
| *F*(000) | 2360.0 |
| Crystal size/mm$^3$ | 0.696 × 0.513 × 0.233 |
| Radiation | Cu–K$\alpha$ ($\lambda$ = 1.54184 Å ) |
| 2$\theta$ range for data collection/° | 7.158 to 148.476 |
| Index ranges | $-12 \le h \le 12$, $-18 \le k \le 16$, $-30 \le l \le 34$ |
| Reflections collected | 27688 |
| Independent reflections | 16187 [$R_{int}$ = 0.0849, $R_{sigma}$ = 0.0681] |
| Data/restraints/parameters | 16187/852/776 |
| Goodness-of-fit on $F^2$ | 1.085 |
| Final *R* indexes [$I \ge 2\sigma(I)$] | $R_1$ = 0.0849, $wR_2$ = 0.2293 |
| Final *R* indexes [all data] | $R_1$ = 0.0906, $wR_2$ = 0.2379 |
| Largest diff. peak/hole / e Å $^{-3}$ | 5.51/–4.46 |

**Table S2.** Selected bond distances (Å) and bond angles (°) for **2** with estimated standard deviations (e.s.d.s.) in parentheses

| | | | |
|---|---|---|---|
| Pt(1)–N(1) | 2.033(8) | Pt(1)–C(12) | 1.949(9) |
| Pt(1)–N(2) | 2.039(8) | Pt(1)–C(18) | 2.049(9) |
| Pt(2)–N(3) | 2.045(8) | Pt(2)–C(49) | 1.957(9) |
| Pt(2)–N(4) | 2.035(8) | Pt(2)–C(37) | 2.062(9) |
| C(18)–C(19) | 1.207(13) | C(28)–C(29) | 1.195(15) |
| C(26)–C(27) | 1.184(15) | C(36)–C(37) | 1.212(13) |
| | | | |
| N(1)–Pt(1)–N(2) | 160.2(3) | N(1)–Pt(1)–C(12) | 80.8(4) |
| N(1)–Pt(1)–C(18) | 100.5(3) | N(2)–Pt(1)–C(12) | 79.3(4) |
| N(2)–Pt(1)–C(18) | 99.3(3) | Pt(1)–C(18)–C(19) | 175.0(8) |
| C(12)–Pt(1)–C(18) | 178.2(4) | C(37)–Pt(2)–C(49) | 178.5(4) |
| N(3)–Pt(2)–N(4) | 160.4(3) | N(3)–Pt(2)–C(49) | 80.1(4) |
| N(3)–Pt(2)–C(37) | 99.0(3) | N(4)–Pt(2)–C(49) | 80.3(4) |
| N(4)–Pt(2)–C(37) | 100.6(3) | Pt(2)–C(37)–C(36) | 177.9(8) |
| C(26)–C(27)–C(28) | 178.1(11) | C(27)–C(28)–C(29) | 178.6(12) |

**Table S3**. Cartesian coordinates of the optimized ground-state geometry of the open form of **1** in dichloromethane

| Energy = –4642.03829696 Hartree | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Pt | -1.536839 | -3.138260 | 2.683490 | 54 | C | 3.208195 | 3.877166 | -1.411238 |
| 2 | C | -0.563727 | -4.812014 | 2.953996 | 55 | Pt | 2.059432 | 5.219931 | -2.500905 |
| 3 | C | -1.097882 | -5.764057 | 3.823743 | 56 | C | 0.951137 | 6.449663 | -3.540408 |
| 4 | C | 0.646398 | -5.004361 | 2.283740 | 57 | C | 1.527379 | 7.623843 | -4.027436 |
| 5 | C | -0.396847 | -6.957233 | 4.026828 | 58 | C | -0.390127 | 6.126588 | -3.757530 |
| 6 | C | 1.344730 | -6.198167 | 2.490218 | 59 | C | 0.732679 | 8.505210 | -4.768416 |
| 7 | C | 0.812442 | -7.159939 | 3.355522 | 60 | C | -1.181546 | 7.011260 | -4.496125 |
| 8 | H | -0.773661 | -7.730331 | 4.697130 | 61 | C | -0.609096 | 8.186176 | -4.995274 |
| 9 | H | 2.294093 | -6.394517 | 1.992181 | 62 | H | 1.138538 | 9.432467 | -5.173549 |
| 10 | H | 1.357093 | -8.087805 | 3.515975 | 63 | H | -2.233268 | 6.803738 | -4.692152 |
| 11 | N | 0.104955 | -2.825549 | 1.457942 | 64 | H | -1.226182 | 8.871833 | -5.571870 |
| 12 | C | 1.018642 | -3.854750 | 1.452935 | 65 | N | 3.432993 | 6.719429 | -2.899790 |
| 13 | C | 0.348432 | -1.715585 | 0.747697 | 66 | C | 2.934311 | 7.764004 | -3.642921 |
| 14 | C | 2.193602 | -3.734910 | 0.718391 | 67 | C | 4.707786 | 6.746064 | -2.485971 |
| 15 | C | 1.500829 | -1.555723 | -0.006321 | 68 | C | 3.753357 | 8.842327 | -3.961223 |
| 16 | H | -0.412637 | -0.939682 | 0.804643 | 69 | C | 5.560378 | 7.798304 | -2.779255 |
| 17 | C | 2.439591 | -2.579918 | -0.014182 | 70 | H | 5.032267 | 5.887933 | -1.903034 |
| 18 | H | 2.913271 | -4.549948 | 0.730848 | 71 | C | 5.072268 | 8.861958 | -3.529538 |
| 19 | H | 1.654485 | -0.632068 | -0.557307 | 72 | H | 3.348394 | 9.660516 | -4.551243 |
| 20 | H | 3.362568 | -2.477975 | -0.580377 | 73 | H | 6.584694 | 7.774748 | -2.421494 |
| 21 | N | -2.785343 | -4.083492 | 4.039599 | 74 | H | 5.713917 | 9.703677 | -3.776882 |
| 22 | C | -3.919062 | -3.578243 | 4.545873 | 75 | N | 0.250903 | 4.208962 | -2.479868 |
| 23 | C | -2.353031 | -5.326289 | 4.439769 | 76 | C | -0.774090 | 4.859121 | -3.128276 |
| 24 | C | -4.687655 | -4.264853 | 5.471962 | 77 | C | 0.015212 | 3.043274 | -1.862956 |
| 25 | H | -4.198461 | -2.592061 | 4.183608 | 78 | C | -2.053372 | 4.313097 | -3.125063 |
| 26 | C | -3.090465 | -6.051476 | 5.370048 | 79 | C | -1.239429 | 2.453334 | -1.847062 |
| 27 | C | -4.263081 | -5.520939 | 5.889774 | 80 | H | 0.869786 | 2.590876 | -1.362817 |
| 28 | H | -5.597679 | -3.813951 | 5.854608 | 81 | C | -2.290684 | 3.105316 | -2.479713 |
| 29 | H | -2.737538 | -7.032109 | 5.679590 | 82 | H | -2.858989 | 4.843373 | -3.627380 |
| 30 | H | -4.840634 | -6.084771 | 6.617729 | 83 | H | -1.377532 | 1.508889 | -1.328431 |
| 31 | C | -2.563104 | -1.364428 | 2.356040 | 84 | H | -3.291386 | 2.679447 | -2.467582 |
| 32 | C | -3.128774 | -0.297477 | 2.102538 | 85 | O | 7.634443 | 0.193757 | 0.357024 |
| 33 | C | -3.706306 | 0.957358 | 1.754361 | 86 | O | 3.477048 | -0.421396 | 2.532554 |
| 34 | C | -5.099164 | 1.104524 | 1.663351 | 87 | C | 8.473735 | 0.879925 | -0.565387 |
| 35 | C | -2.861745 | 2.053701 | 1.458768 | 88 | H | 8.045087 | 0.818460 | -1.578830 |
| 36 | C | -5.640848 | 2.323242 | 1.261776 | 89 | H | 8.535757 | 1.946014 | -0.292985 |
| 37 | H | -5.729666 | 0.252289 | 1.895823 | 90 | C | 9.836532 | 0.233860 | -0.519696 |
| 38 | C | -3.439920 | 3.283986 | 1.053798 | 91 | H | 9.735507 | -0.833018 | -0.767707 |
| 39 | C | -4.815337 | 3.414563 | 0.949299 | 92 | H | 10.221832 | 0.284205 | 0.509321 |
| 40 | H | -5.285530 | 4.342293 | 0.637617 | 93 | C | 10.811972 | 0.901628 | -1.476233 |
| 41 | C | -1.456184 | 1.931612 | 1.492349 | 94 | H | 10.412926 | 0.854453 | -2.502435 |
| 42 | C | -0.237663 | 1.847185 | 1.449284 | 95 | H | 10.893134 | 1.973117 | -1.231591 |
| 43 | C | 1.110205 | 1.711092 | 1.328265 | 96 | C | 12.195035 | 0.270226 | -1.442848 |
| 44 | C | 2.309259 | 1.549509 | 1.155701 | 97 | H | 12.112408 | -0.802592 | -1.682627 |
| 45 | C | 3.677013 | 1.272947 | 0.944999 | 98 | H | 12.593801 | 0.319505 | -0.416341 |
| 46 | C | 4.441325 | 1.988898 | -0.006456 | 99 | C | 13.177519 | 0.927339 | -2.399218 |
| 47 | C | 4.281826 | 0.206763 | 1.659114 | 100 | H | 12.778065 | 0.876805 | -3.425681 |
| 48 | C | 5.787257 | 1.651174 | -0.216910 | 101 | H | 13.257755 | 2.000821 | -2.160577 |
| 49 | C | 5.605376 | -0.132546 | 1.430319 | 102 | C | 14.561502 | 0.298085 | -2.365070 |
| 50 | C | 6.356132 | 0.598340 | 0.496388 | 103 | H | 14.480398 | -0.776003 | -2.601009 |
| 51 | H | 6.356933 | 2.214164 | -0.949329 | 104 | H | 14.961440 | 0.350374 | -1.338844 |
| 52 | H | 6.092484 | -0.946053 | 1.959468 | 105 | C | 15.544702 | 0.951498 | -3.323565 |
| 53 | C | 3.821839 | 3.022864 | -0.766157 | 106 | H | 15.144397 | 0.899071 | -4.349692 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 107 | H | 15.625980 | 2.025639 | -3.087888 | 160 | H | -21.765911 | -0.099560 | -0.235488 |
| 108 | C | 16.928489 | 0.321750 | -3.289871 | 161 | H | -22.443418 | -1.346999 | 0.821620 |
| 109 | H | 16.846617 | -0.752711 | -3.523991 | 162 | H | -21.899406 | 0.194140 | 1.502876 |
| 110 | H | 17.329600 | 0.375330 | -2.264133 | 163 | C | -3.026630 | 5.482882 | 0.215935 |
| 111 | C | 17.911147 | 0.972999 | -4.250452 | 164 | H | -3.738703 | 5.971762 | 0.900062 |
| 112 | H | 17.508775 | 0.920631 | -5.275813 | 165 | H | -3.557885 | 5.273777 | -0.729422 |
| 113 | H | 17.994404 | 2.047199 | -4.015606 | 166 | C | -1.818288 | 6.355173 | -0.022778 |
| 114 | C | 19.294009 | 0.341451 | -4.219499 | 167 | H | -1.345053 | 6.585950 | 0.942647 |
| 115 | H | 19.698366 | 0.394007 | -3.194846 | 168 | H | -1.078445 | 5.780323 | -0.602610 |
| 116 | H | 19.211254 | -0.733024 | -4.453830 | 169 | C | -2.166682 | 7.637299 | -0.760060 |
| 117 | C | 20.276572 | 0.991319 | -5.182191 | 170 | H | -2.593713 | 7.384973 | -1.746570 |
| 118 | H | 19.868594 | 0.940470 | -6.203564 | 171 | H | -2.957079 | 8.180847 | -0.216685 |
| 119 | H | 20.360072 | 2.063098 | -4.944346 | 172 | C | -0.962133 | 8.544722 | -0.955994 |
| 120 | C | 21.650380 | 0.344776 | -5.142969 | 173 | H | -0.548502 | 8.824349 | 0.026671 |
| 121 | H | 22.348116 | 0.817154 | -5.844142 | 174 | H | -0.167399 | 7.978069 | -1.471661 |
| 122 | H | 22.091422 | 0.414069 | -4.139776 | 175 | C | -1.279423 | 9.796922 | -1.756967 |
| 123 | H | 21.592713 | -0.721056 | -5.400726 | 176 | H | -2.058984 | 10.382653 | -1.241895 |
| 124 | O | -6.961827 | 2.558563 | 1.133266 | 177 | H | -1.713914 | 9.498719 | -2.726411 |
| 125 | O | -2.561798 | 4.263494 | 0.779150 | 178 | C | -0.065073 | 10.676100 | -2.010651 |
| 126 | C | -7.877234 | 1.498349 | 1.387348 | 179 | H | 0.339605 | 11.038279 | -1.051241 |
| 127 | H | -7.660890 | 0.649389 | 0.718492 | 180 | H | 0.734301 | 10.063060 | -2.463925 |
| 128 | H | -7.764072 | 1.144359 | 2.424801 | 181 | C | -0.363388 | 11.856963 | -2.920679 |
| 129 | C | -9.269278 | 2.028881 | 1.147971 | 182 | H | -1.165804 | 12.470636 | -2.478686 |
| 130 | H | -9.325058 | 2.429557 | 0.125142 | 183 | H | -0.766615 | 11.480135 | -3.876494 |
| 131 | H | -9.452893 | 2.873739 | 1.828010 | 184 | C | 0.848703 | 12.731736 | -3.198480 |
| 132 | C | -10.331228 | 0.958483 | 1.344016 | 185 | H | 1.245396 | 13.123019 | -2.247170 |
| 133 | H | -10.134675 | 0.116016 | 0.661137 | 186 | H | 1.655104 | 12.111277 | -3.625231 |
| 134 | H | -10.258807 | 0.545725 | 2.363179 | 187 | C | 0.553865 | 13.889462 | -4.139497 |
| 135 | C | -11.739031 | 1.482693 | 1.108091 | 188 | H | -0.246956 | 14.514363 | -3.710693 |
| 136 | H | -11.801118 | 1.915181 | 0.095972 | 189 | H | 0.150808 | 13.494987 | -5.087235 |
| 137 | H | -11.939809 | 2.314666 | 1.802905 | 190 | C | 1.768559 | 14.756084 | -4.431614 |
| 138 | C | -12.814417 | 0.419878 | 1.267592 | 191 | H | 2.169499 | 15.156402 | -3.485573 |
| 139 | H | -12.615926 | -0.408766 | 0.567741 | 192 | H | 2.571583 | 14.130142 | -4.855659 |
| 140 | H | -12.751249 | -0.018152 | 2.277410 | 193 | C | 1.475314 | 15.907940 | -5.381489 |
| 141 | C | -14.219276 | 0.952926 | 1.034036 | 194 | H | 0.672917 | 16.530937 | -4.957052 |
| 142 | H | -14.275884 | 1.403536 | 0.029224 | 195 | H | 1.075958 | 15.505249 | -6.325286 |
| 143 | H | -14.420474 | 1.774145 | 1.741870 | 196 | C | 2.699311 | 16.762551 | -5.662094 |
| 144 | C | -15.300854 | -0.106990 | 1.171090 | 197 | H | 2.475776 | 17.590839 | -6.344328 |
| 145 | H | -15.103655 | -0.924722 | 0.458071 | 198 | H | 3.099703 | 17.195324 | -4.735866 |
| 146 | H | -15.242703 | -0.562813 | 2.173423 | 199 | H | 3.501535 | 16.166244 | -6.116574 |
| 147 | C | -16.703530 | 0.434282 | 0.943088 | 200 | C | 3.932741 | -1.596300 | 3.190791 |
| 148 | H | -16.757577 | 0.899681 | -0.055122 | 201 | H | 4.823128 | -1.370337 | 3.799416 |
| 149 | H | -16.903034 | 1.245746 | 1.662596 | 202 | H | 4.219931 | -2.353092 | 2.439973 |
| 150 | C | -17.788152 | -0.624502 | 1.064065 | 203 | C | 2.795710 | -2.090601 | 4.051843 |
| 151 | H | -17.593605 | -1.431408 | 0.338074 | 204 | H | 2.567804 | -1.331091 | 4.813939 |
| 152 | H | -17.729815 | -1.096405 | 2.058975 | 205 | H | 1.893944 | -2.182435 | 3.425045 |
| 153 | C | -19.190325 | -0.077815 | 0.846964 | 206 | C | 3.098099 | -3.424907 | 4.713280 |
| 154 | H | -19.246933 | 0.403707 | -0.143556 | 207 | H | 3.279771 | -4.186138 | 3.934352 |
| 155 | H | -19.388928 | 0.722052 | 1.579735 | 208 | H | 4.032060 | -3.355314 | 5.294871 |
| 156 | C | -20.275763 | -1.138356 | 0.953177 | 209 | C | 1.965690 | -3.892137 | 5.614558 |
| 157 | H | -20.208889 | -1.626615 | 1.937745 | 210 | H | 1.800587 | -3.147813 | 6.410704 |
| 158 | H | -20.081824 | -1.928763 | 0.211667 | 211 | H | 1.030764 | -3.922232 | 5.028051 |
| 159 | C | -21.670715 | -0.572611 | 0.750931 | 212 | C | 2.208540 | -5.259346 | 6.232853 |

| | | | | |
|---|---|---|---|---|
| 213 | H | 2.394156 | -5.989229 | 5.426609 |
| 214 | H | 3.128324 | -5.236862 | 6.840735 |
| 215 | C | 1.045986 | -5.745750 | 7.083279 |
| 216 | H | 0.884639 | -5.050071 | 7.923250 |
| 217 | H | 0.121241 | -5.711022 | 6.480364 |
| 218 | C | 1.237567 | -7.156115 | 7.617244 |
| 219 | H | 2.163966 | -7.203029 | 8.213416 |
| 220 | H | 1.392285 | -7.845750 | 6.769325 |
| 221 | C | 0.068965 | -7.645388 | 8.457981 |
| 222 | H | -0.080003 | -6.961564 | 9.309961 |
| 223 | H | -0.858334 | -7.585811 | 7.862333 |
| 224 | C | 0.247055 | -9.064545 | 8.974363 |
| 225 | H | 1.179213 | -9.125253 | 9.560225 |
| 226 | H | 0.384850 | -9.749452 | 8.121040 |
| 227 | C | -0.915563 | -9.547882 | 9.826865 |
| 228 | H | -1.849900 | -9.483458 | 9.244304 |
| 229 | H | -1.049735 | -8.866025 | 10.683090 |
| 230 | C | -0.739451 | -10.969599 | 10.339193 |
| 231 | H | 0.196332 | -11.032317 | 10.915938 |
| 232 | H | -0.610953 | -11.649349 | 9.482621 |
| 233 | C | -1.905353 | -11.433227 | 11.195161 |
| 234 | H | -2.846117 | -11.406993 | 10.629409 |
| 235 | H | -1.767159 | -12.457964 | 11.559022 |
| 236 | H | -2.034070 | -10.785109 | 12.072084 |

**Table S4**. Cartesian coordinates of the optimized ground-state geometry of the closed form of **1** in dichloromethane

| Energy = –4642.04582043 Hartrees | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Pt | -3.020472 | -3.593160 | 1.447847 | 54 | C | 1.917646 | -3.016856 | -0.528916 |
| 2 | C | -2.453559 | -5.378089 | 2.007680 | 55 | Pt | 0.458826 | -4.470731 | -0.776867 |
| 3 | C | -3.332127 | -6.448623 | 1.835464 | 56 | C | -0.920208 | -5.822376 | -1.081095 |
| 4 | C | -1.182860 | -5.533728 | 2.565857 | 57 | C | -0.667048 | -7.140912 | -0.699207 |
| 5 | C | -2.917470 | -7.727349 | 2.223513 | 58 | C | -2.124823 | -5.430664 | -1.669345 |
| 6 | C | -0.770345 | -6.813069 | 2.946807 | 59 | C | -1.657438 | -8.105538 | -0.913417 |
| 7 | C | -1.643963 | -7.892821 | 2.773910 | 60 | C | -3.113602 | -6.396678 | -1.877020 |
| 8 | H | -3.563508 | -8.596167 | 2.097256 | 61 | C | -2.865862 | -7.721479 | -1.500687 |
| 9 | H | 0.218876 | -6.986874 | 3.371795 | 62 | H | -1.507352 | -9.146423 | -0.627019 |
| 10 | H | -1.318728 | -8.888311 | 3.068944 | 63 | H | -4.074919 | -6.138647 | -2.322771 |
| 11 | N | -1.117916 | -3.178341 | 2.155794 | 64 | H | -3.638956 | -8.469849 | -1.662031 |
| 12 | C | -0.441612 | -4.271741 | 2.643253 | 65 | N | 1.396392 | -6.152849 | -0.005109 |
| 13 | C | -0.525402 | -1.976517 | 2.154507 | 66 | C | 0.648755 | -7.304436 | -0.077261 |
| 14 | C | 0.839659 | -4.122211 | 3.163605 | 67 | C | 2.607216 | -6.180831 | 0.571203 |
| 15 | C | 0.751816 | -1.780117 | 2.657851 | 68 | C | 1.154040 | -8.494191 | 0.440609 |
| 16 | H | -1.108175 | -1.159905 | 1.731499 | 69 | C | 3.148493 | -7.338997 | 1.105270 |
| 17 | C | 1.440038 | -2.870260 | 3.176510 | 70 | H | 3.139404 | -5.232724 | 0.594469 |
| 18 | H | 1.356934 | -4.994497 | 3.556317 | 71 | C | 2.407274 | -8.514540 | 1.034839 |
| 19 | H | 1.190092 | -0.786902 | 2.629713 | 72 | H | 0.550463 | -9.396476 | 0.381393 |
| 20 | H | 2.441430 | -2.748438 | 3.581825 | 73 | H | 4.133005 | -7.311871 | 1.561488 |
| 21 | N | -4.691631 | -4.704125 | 0.927654 | 74 | H | 2.803058 | -9.441232 | 1.442463 |
| 22 | C | -5.794278 | -4.227838 | 0.331570 | 75 | N | -1.029592 | -3.305563 | -1.619309 |
| 23 | C | -4.592851 | -6.046935 | 1.207309 | 76 | C | -2.170761 | -3.994021 | -1.957532 |
| 24 | C | -6.857764 | -5.042323 | -0.022354 | 77 | C | -0.968730 | -1.980793 | -1.811651 |
| 25 | H | -5.800266 | -3.157238 | 0.140035 | 78 | C | -3.248115 | -3.318510 | -2.521551 |
| 26 | C | -5.638584 | -6.903745 | 0.873662 | 79 | C | -2.019514 | -1.264437 | -2.363468 |
| 27 | C | -6.775622 | -6.402814 | 0.256871 | 80 | H | -0.041128 | -1.499292 | -1.506828 |
| 28 | H | -7.729651 | -4.609569 | -0.502674 | 81 | C | -3.174372 | -1.947153 | -2.726840 |
| 29 | H | -5.546819 | -7.963604 | 1.097497 | 82 | H | -4.141206 | -3.875872 | -2.793010 |
| 30 | H | -7.592604 | -7.069964 | -0.005847 | 83 | H | -1.924358 | -0.190622 | -2.494007 |
| 31 | C | -3.615468 | -1.677916 | 0.914652 | 84 | H | -4.016076 | -1.413977 | -3.161928 |
| 32 | C | -3.925321 | -0.517053 | 0.633876 | 85 | O | 7.338302 | -0.487509 | -0.425599 |
| 33 | C | -4.227764 | 0.836304 | 0.311186 | 86 | O | 3.762256 | 2.545984 | 0.190823 |
| 34 | C | -5.563377 | 1.255790 | 0.199587 | 87 | C | 7.847204 | -1.805496 | -0.597920 |
| 35 | C | -3.180314 | 1.765117 | 0.109319 | 88 | H | 7.524809 | -2.442574 | 0.241928 |
| 36 | C | -5.851929 | 2.582650 | -0.109654 | 89 | H | 7.444810 | -2.245347 | -1.524696 |
| 37 | H | -6.350484 | 0.526287 | 0.361154 | 90 | C | 9.352316 | -1.716354 | -0.654320 |
| 38 | C | -3.504336 | 3.114616 | -0.188369 | 91 | H | 9.713787 | -1.216362 | 0.256192 |
| 39 | C | -4.824123 | 3.518914 | -0.300883 | 92 | H | 9.643441 | -1.078033 | -1.501376 |
| 40 | H | -5.094783 | 4.543370 | -0.538475 | 93 | C | 9.997055 | -3.087245 | -0.785432 |
| 41 | C | -1.819590 | 1.386607 | 0.155575 | 94 | H | 9.700668 | -3.715708 | 0.069995 |
| 42 | C | -0.624082 | 1.130325 | 0.132063 | 95 | H | 9.609029 | -3.595035 | -1.683163 |
| 43 | C | 0.705235 | 0.843401 | 0.073349 | 96 | C | 11.514289 | -3.018279 | -0.858843 |
| 44 | C | 1.897778 | 0.584161 | -0.002512 | 97 | H | 11.897803 | -2.485942 | 0.027045 |
| 45 | C | 3.272061 | 0.273031 | -0.101772 | 98 | H | 11.810411 | -2.408288 | -1.727876 |
| 46 | C | 3.704110 | -1.060744 | -0.309625 | 99 | C | 12.174804 | -4.384708 | -0.949873 |
| 47 | C | 4.243636 | 1.303880 | -0.010619 | 100 | H | 11.882739 | -4.990093 | -0.075787 |
| 48 | C | 5.074422 | -1.346595 | -0.415966 | 101 | H | 11.786627 | -4.922092 | -1.830850 |
| 49 | C | 5.593087 | 1.010238 | -0.131192 | 102 | C | 13.691625 | -4.312713 | -1.029098 |
| 50 | C | 6.004659 | -0.315701 | -0.329472 | 103 | H | 14.076412 | -3.760275 | -0.155785 |
| 51 | H | 5.378357 | -2.376119 | -0.576735 | 104 | H | 13.983716 | -3.719504 | -1.911447 |
| 52 | H | 6.359558 | 1.776287 | -0.075049 | 105 | C | 14.359393 | -5.677349 | -1.094414 |
| 53 | C | 2.754106 | -2.115104 | -0.427685 | 106 | H | 14.069194 | -6.268497 | -0.209927 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 107 | H | 13.974368 | -6.232498 | -1.965847 | 160 | H | -22.043568 | 2.271392 | -2.561643 |
| 108 | C | 15.876045 | -5.601071 | -1.173939 | 161 | H | -22.942558 | 1.265647 | -1.415252 |
| 109 | H | 16.258808 | -5.038092 | -0.306444 | 162 | H | -22.259630 | 2.812137 | -0.891741 |
| 110 | H | 16.166388 | -5.016133 | -2.062444 | 163 | C | -2.637160 | 5.297947 | -0.668915 |
| 111 | C | 16.548663 | -6.963975 | -1.225418 | 164 | H | -3.290911 | 5.776607 | 0.077644 |
| 112 | H | 16.257650 | -7.548755 | -0.336944 | 165 | H | -3.126797 | 5.387687 | -1.652541 |
| 113 | H | 16.167894 | -7.527588 | -2.093352 | 166 | C | -1.263707 | 5.923803 | -0.669419 |
| 114 | C | 18.065196 | -6.884153 | -1.301328 | 167 | H | -0.839489 | 5.828321 | 0.341118 |
| 115 | H | 18.357298 | -6.300833 | -2.190505 | 168 | H | -0.612609 | 5.337687 | -1.334187 |
| 116 | H | 18.445582 | -6.318587 | -0.434327 | 169 | C | -1.256949 | 7.381497 | -1.096914 |
| 117 | C | 18.741769 | -8.246021 | -1.348802 | 170 | H | -1.569544 | 7.463127 | -2.150187 |
| 118 | H | 18.445602 | -8.827766 | -0.462127 | 171 | H | -1.997587 | 7.951207 | -0.512682 |
| 119 | H | 18.363663 | -8.807398 | -2.217209 | 172 | C | 0.119129 | 8.003150 | -0.914292 |
| 120 | C | 20.255796 | -8.145464 | -1.418309 | 173 | H | 0.375148 | 7.988102 | 0.158196 |
| 121 | H | 20.733306 | -9.131384 | -1.456355 | 174 | H | 0.872869 | 7.368509 | -1.409742 |
| 122 | H | 20.573761 | -7.589161 | -2.310015 | 175 | C | 0.239487 | 9.424036 | -1.439201 |
| 123 | H | 20.657039 | -7.616203 | -0.543923 | 176 | H | -0.569128 | 10.044185 | -1.018344 |
| 124 | O | -7.100735 | 3.072132 | -0.248711 | 177 | H | 0.086990 | 9.429027 | -2.530904 |
| 125 | O | -2.446434 | 3.926061 | -0.345946 | 178 | C | 1.581760 | 10.055005 | -1.104071 |
| 126 | C | -8.201380 | 2.183831 | -0.091765 | 179 | H | 1.691912 | 10.095963 | -0.006679 |
| 127 | H | -8.104578 | 1.341587 | -0.795877 | 180 | H | 2.396417 | 9.401267 | -1.462088 |
| 128 | H | -8.203868 | 1.767601 | 0.928744 | 181 | C | 1.768815 | 11.450374 | -1.677045 |
| 129 | C | -9.469850 | 2.954897 | -0.361878 | 182 | H | 0.919888 | 12.086176 | -1.375397 |
| 130 | H | -9.420703 | 3.377376 | -1.376321 | 183 | H | 1.735012 | 11.405102 | -2.778113 |
| 131 | H | -9.532183 | 3.805042 | 0.332964 | 184 | C | 3.066749 | 12.103685 | -1.230080 |
| 132 | C | -10.698539 | 2.069673 | -0.222706 | 185 | H | 3.078968 | 12.157908 | -0.127444 |
| 133 | H | -10.594664 | 1.193310 | -0.883130 | 186 | H | 3.918993 | 11.457235 | -1.504495 |
| 134 | H | -10.750085 | 1.670239 | 0.803072 | 187 | C | 3.279738 | 13.496744 | -1.800588 |
| 135 | C | -11.996199 | 2.791343 | -0.550903 | 188 | H | 2.402759 | 14.123096 | -1.566721 |
| 136 | H | -11.944401 | 3.183718 | -1.579786 | 189 | H | 3.325203 | 13.442148 | -2.900953 |
| 137 | H | -12.103298 | 3.672310 | 0.102796 | 190 | C | 4.533524 | 14.173872 | -1.270113 |
| 138 | C | -13.220957 | 1.901161 | -0.410072 | 191 | H | 4.475844 | 14.232224 | -0.168623 |
| 139 | H | -13.096521 | 1.008767 | -1.045822 | 192 | H | 5.413117 | 13.543612 | -1.488248 |
| 140 | H | -13.282344 | 1.525498 | 0.624733 | 193 | C | 4.760188 | 15.568759 | -1.832927 |
| 141 | C | -14.523250 | 2.597534 | -0.772822 | 194 | H | 3.859617 | 16.178145 | -1.660397 |
| 142 | H | -14.461497 | 2.970090 | -1.808817 | 195 | H | 4.876463 | 15.505326 | -2.925789 |
| 143 | H | -14.651036 | 3.491103 | -0.139664 | 196 | C | 5.968128 | 16.256517 | -1.220214 |
| 144 | C | -15.741910 | 1.698533 | -0.632205 | 197 | H | 6.137424 | 17.251975 | -1.646783 |
| 145 | H | -15.605127 | 0.799627 | -1.256217 | 198 | H | 5.840161 | 16.379186 | -0.134872 |
| 146 | H | -15.809126 | 1.334348 | 0.406433 | 199 | H | 6.882922 | 15.668711 | -1.378378 |
| 147 | C | -17.046784 | 2.380537 | -1.012867 | 200 | C | 4.685882 | 3.629136 | 0.211378 |
| 148 | H | -16.978976 | 2.744578 | -2.051542 | 201 | H | 5.210457 | 3.683335 | -0.756803 |
| 149 | H | -17.186589 | 3.278877 | -0.388918 | 202 | H | 5.444562 | 3.458430 | 0.991898 |
| 150 | C | -18.260998 | 1.475059 | -0.874604 | 203 | C | 3.939464 | 4.911913 | 0.489680 |
| 151 | H | -18.117027 | 0.574706 | -1.494908 | 204 | H | 3.115951 | 5.024665 | -0.230529 |
| 152 | H | -18.330918 | 1.114183 | 0.165055 | 205 | H | 3.482751 | 4.854187 | 1.488534 |
| 153 | C | -19.567322 | 2.149874 | -1.262574 | 206 | C | 4.887524 | 6.100965 | 0.407291 |
| 154 | H | -19.497905 | 2.512061 | -2.301922 | 207 | H | 5.795252 | 5.882202 | 0.993902 |
| 155 | H | -19.714277 | 3.049362 | -0.641632 | 208 | H | 5.227345 | 6.223568 | -0.633672 |
| 156 | C | -20.780218 | 1.241122 | -1.127017 | 209 | C | 4.293387 | 7.409437 | 0.906385 |
| 157 | H | -20.847510 | 0.880995 | -0.088734 | 210 | H | 3.353657 | 7.624904 | 0.371224 |
| 158 | H | -20.630518 | 0.343610 | -1.747082 | 211 | H | 4.018092 | 7.299797 | 1.967954 |
| 159 | C | -22.076489 | 1.929490 | -1.518690 | 212 | C | 5.256050 | 8.577812 | 0.748403 |

| | | | | |
|---|---|---|---|---|
| 213 | H | 6.240727 | 8.288753 | 1.153034 |
| 214 | H | 5.420967 | 8.773879 | -0.324864 |
| 215 | C | 4.803032 | 9.858672 | 1.431774 |
| 216 | H | 3.824843 | 10.171925 | 1.027625 |
| 217 | H | 4.637182 | 9.660946 | 2.503679 |
| 218 | C | 5.805488 | 10.992195 | 1.277098 |
| 219 | H | 5.949038 | 11.210480 | 0.204511 |
| 220 | H | 6.789345 | 10.657112 | 1.646762 |
| 221 | C | 5.410666 | 12.270673 | 1.999009 |
| 222 | H | 4.447568 | 12.635134 | 1.601281 |
| 223 | H | 5.231537 | 12.052299 | 3.064782 |
| 224 | C | 6.456142 | 13.368099 | 1.875966 |
| 225 | H | 6.676681 | 13.543484 | 0.808539 |
| 226 | H | 7.402141 | 13.021316 | 2.324241 |
| 227 | C | 6.041794 | 14.681658 | 2.518775 |
| 228 | H | 5.745479 | 14.505769 | 3.566403 |
| 229 | H | 5.137982 | 15.065493 | 2.013182 |
| 230 | C | 7.132347 | 15.741440 | 2.474354 |
| 231 | H | 7.467185 | 15.869887 | 1.432439 |
| 232 | H | 8.011041 | 15.378140 | 3.029086 |
| 233 | C | 6.677160 | 17.076347 | 3.037496 |
| 234 | H | 6.346516 | 16.974248 | 4.079698 |
| 235 | H | 7.475311 | 17.827364 | 3.015480 |
| 236 | H | 5.828933 | 17.477305 | 2.465979 |

**Table S5**. Cartesian coordinates of the optimized ground-state geometry of the open form of **3** in dichloromethane

| Energy = –5944.48838658 Hartrees | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Pt | 4.608124 | 2.604801 | -0.470329 | 54 | C | -6.601867 | -5.386206 | -0.866860 |
| 2 | C | 4.845309 | 4.473266 | -0.986428 | 55 | C | -4.260941 | -5.833378 | -1.440552 |
| 3 | C | 6.077785 | 5.083021 | -0.747445 | 56 | C | -6.932073 | -6.708816 | -1.167799 |
| 4 | C | 3.773890 | 5.148343 | -1.580561 | 57 | C | -4.588267 | -7.153827 | -1.735944 |
| 5 | C | 6.250214 | 6.420715 | -1.106715 | 58 | C | -5.918746 | -7.571502 | -1.592474 |
| 6 | C | 3.941280 | 6.485293 | -1.930451 | 59 | H | -7.951072 | -7.080277 | -1.077502 |
| 7 | C | 5.178597 | 7.100109 | -1.689877 | 60 | H | -3.840456 | -7.870116 | -2.076599 |
| 8 | H | 7.190806 | 6.943499 | -0.938129 | 61 | N | -6.842100 | -3.124708 | -0.146770 |
| 9 | H | 3.137059 | 7.069107 | -2.378564 | 62 | C | -7.484758 | -4.308530 | -0.405415 |
| 10 | N | 2.737391 | 3.019494 | -1.253065 | 63 | C | -7.561572 | -2.078017 | 0.283599 |
| 11 | C | 2.580586 | 4.303439 | -1.723697 | 64 | C | -8.863155 | -4.412371 | -0.246432 |
| 12 | C | 1.698880 | 2.178986 | -1.313527 | 65 | C | -8.931358 | -2.137495 | 0.452703 |
| 13 | C | 1.371664 | 4.704841 | -2.268915 | 66 | H | -7.000260 | -1.168127 | 0.481270 |
| 14 | C | 0.472050 | 2.542684 | -1.848460 | 67 | C | -9.626222 | -3.320297 | 0.169846 |
| 15 | H | 1.871420 | 1.180424 | -0.916053 | 68 | H | -9.332859 | -5.365823 | -0.476414 |
| 16 | C | 0.283084 | 3.827333 | -2.357869 | 69 | H | -9.450353 | -1.244030 | 0.789028 |
| 17 | H | 1.289441 | 5.723703 | -2.643433 | 70 | N | -2.959460 | -3.851006 | -1.139276 |
| 18 | H | -0.321649 | 1.801516 | -1.853064 | 71 | C | -2.954013 | -5.168735 | -1.534484 |
| 19 | N | 6.564709 | 2.916162 | 0.135073 | 72 | C | -1.821328 | -3.151392 | -1.208979 |
| 20 | C | 7.368261 | 2.026565 | 0.728910 | 73 | C | -1.786580 | -5.754508 | -1.996936 |
| 21 | C | 7.038333 | 4.186738 | -0.094116 | 74 | C | -0.634339 | -3.696396 | -1.675189 |
| 22 | C | 8.659964 | 2.332859 | 1.128090 | 75 | H | -1.877746 | -2.116134 | -0.875744 |
| 23 | H | 6.945329 | 1.036824 | 0.883297 | 76 | C | -0.592817 | -5.028067 | -2.091326 |
| 24 | C | 8.321242 | 4.535558 | 0.296417 | 77 | H | -1.821608 | -6.798640 | -2.301439 |
| 25 | C | 9.170090 | 3.615485 | 0.920760 | 78 | H | 0.244776 | -3.058847 | -1.702618 |
| 26 | H | 9.248644 | 1.554427 | 1.602584 | 79 | O | -5.189049 | 4.687420 | 0.638357 |
| 27 | H | 8.654866 | 5.554665 | 0.107668 | 80 | O | -0.690639 | 3.312745 | 1.163503 |
| 28 | C | 4.375279 | 0.602753 | 0.013745 | 81 | C | -6.566485 | 4.396759 | 0.426026 |
| 29 | C | 4.240584 | -0.603288 | 0.234567 | 82 | H | -6.702666 | 3.930131 | -0.563009 |
| 30 | C | 4.080347 | -2.001975 | 0.455747 | 83 | H | -6.916481 | 3.678623 | 1.185064 |
| 31 | C | 5.207517 | -2.829903 | 0.433010 | 84 | C | -7.336859 | 5.690713 | 0.519465 |
| 32 | C | 2.778704 | -2.545134 | 0.672825 | 85 | H | -6.961804 | 6.389461 | -0.242677 |
| 33 | C | 5.059086 | -4.206815 | 0.602381 | 86 | H | -7.140185 | 6.153666 | 1.497529 |
| 34 | H | 6.180002 | -2.377762 | 0.265037 | 87 | C | -8.830132 | 5.466814 | 0.338822 |
| 35 | C | 2.661465 | -3.947652 | 0.855126 | 88 | H | -9.016094 | 4.983678 | -0.634077 |
| 36 | C | 3.792924 | -4.752757 | 0.813582 | 89 | H | -9.188631 | 4.757098 | 1.101962 |
| 37 | H | 3.684467 | -5.825183 | 0.954691 | 90 | C | -9.640198 | 6.750720 | 0.427627 |
| 38 | C | 1.672196 | -1.665234 | 0.633717 | 91 | H | -9.295716 | 7.456038 | -0.346185 |
| 39 | C | 0.738976 | -0.875917 | 0.618639 | 92 | H | -9.440477 | 7.242402 | 1.393742 |
| 40 | C | -0.318751 | -0.021121 | 0.624076 | 93 | C | -11.135810 | 6.521532 | 0.277059 |
| 41 | C | -1.268068 | 0.749508 | 0.638052 | 94 | H | -11.334753 | 6.025226 | -0.687199 |
| 42 | C | -2.305694 | 1.706540 | 0.653730 | 95 | H | -11.475624 | 5.815730 | 1.053046 |
| 43 | C | -3.651945 | 1.350643 | 0.404146 | 96 | C | -11.956059 | 7.798945 | 0.365544 |
| 44 | C | -1.986729 | 3.066835 | 0.908204 | 97 | H | -11.625940 | 8.501495 | -0.417470 |
| 45 | C | -4.647419 | 2.340339 | 0.395909 | 98 | H | -11.748768 | 8.300690 | 1.325226 |
| 46 | C | -2.976244 | 4.037587 | 0.888656 | 99 | C | -13.452391 | 7.561542 | 0.233939 |
| 47 | C | -4.305960 | 3.669667 | 0.630765 | 100 | H | -13.659660 | 7.056259 | -0.723960 |
| 48 | H | -5.672836 | 2.042573 | 0.201963 | 101 | H | -13.780715 | 6.860530 | 1.019237 |
| 49 | H | -2.761577 | 5.084942 | 1.078567 | 102 | C | -14.277199 | 8.836187 | 0.320183 |
| 50 | C | -4.001112 | -0.006901 | 0.152860 | 103 | H | -13.955063 | 9.534501 | -0.470009 |
| 51 | C | -4.306784 | -1.179972 | -0.075259 | 104 | H | -14.064288 | 9.345417 | 1.274728 |
| 52 | Pt | -4.806891 | -3.138076 | -0.535602 | 105 | C | -15.773951 | 8.594705 | 0.200901 |
| 53 | C | -5.273541 | -4.976236 | -0.997512 | 106 | H | -15.986615 | 8.080516 | -0.751091 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 107 | H | -16.096257 | 7.900400 | 0.994619 | 160 | C | -0.657890 | -5.174427 | 1.812307 |
| 108 | C | -16.599179 | 9.869351 | 0.280289 | 161 | H | -0.798639 | -5.670956 | 0.837735 |
| 109 | H | -16.382315 | 10.387889 | 1.229082 | 162 | H | -0.264963 | -5.935530 | 2.501963 |
| 110 | H | -16.281649 | 10.561295 | -0.517536 | 163 | C | -1.992597 | -4.632971 | 2.302547 |
| 111 | C | -18.097427 | 9.628557 | 0.170352 | 164 | H | -1.879933 | -4.211468 | 3.314194 |
| 112 | H | -18.310788 | 9.102669 | -0.773140 | 165 | H | -2.304088 | -3.792312 | 1.656327 |
| 113 | H | -18.413890 | 8.945367 | 0.973699 | 166 | C | -3.091777 | -5.681805 | 2.297720 |
| 114 | C | -18.904040 | 10.913889 | 0.238316 | 167 | H | -3.175517 | -6.105457 | 1.280839 |
| 115 | H | -19.981786 | 10.727977 | 0.164744 | 168 | H | -2.811145 | -6.523517 | 2.952243 |
| 116 | H | -18.723875 | 11.444518 | 1.182633 | 169 | C | -4.445695 | -5.131664 | 2.713531 |
| 117 | H | -18.629399 | 11.596545 | -0.576643 | 170 | H | -4.678309 | -4.250141 | 2.087174 |
| 118 | O | 6.075869 | -5.089474 | 0.589042 | 171 | H | -4.398463 | -4.766376 | 3.752841 |
| 119 | O | 1.505706 | -4.631871 | 1.011886 | 172 | C | -5.565710 | -6.147916 | 2.572012 |
| 120 | C | 7.406510 | -4.609226 | 0.428012 | 173 | H | -5.596245 | -6.501551 | 1.526461 |
| 121 | H | 7.505656 | -4.092699 | -0.540429 | 174 | H | -5.341875 | -7.037036 | 3.184994 |
| 122 | H | 7.640301 | -3.881032 | 1.221324 | 175 | C | -6.934145 | -5.606114 | 2.950902 |
| 123 | C | 8.328117 | -5.801334 | 0.503514 | 176 | H | -7.135065 | -4.682503 | 2.377613 |
| 124 | H | 8.045668 | -6.519797 | -0.279908 | 177 | H | -6.933291 | -5.307460 | 4.012272 |
| 125 | H | 8.171189 | -6.308894 | 1.466696 | 178 | C | -8.053096 | -6.603698 | 2.700559 |
| 126 | C | 9.790835 | -5.415048 | 0.352516 | 179 | H | -8.087425 | -6.839079 | 1.621459 |
| 127 | H | 9.942563 | -4.904058 | -0.611977 | 180 | H | -7.818229 | -7.554742 | 3.206592 |
| 128 | H | 10.062690 | -4.683227 | 1.130316 | 181 | C | -9.418599 | -6.114565 | 3.152175 |
| 129 | C | 10.716885 | -6.617994 | 0.442433 | 182 | H | -9.630526 | -5.144769 | 2.667380 |
| 130 | H | 10.439723 | -7.348600 | -0.335141 | 183 | H | -9.398116 | -5.909910 | 4.235243 |
| 131 | H | 10.554329 | -7.129398 | 1.405438 | 184 | C | -10.539372 | -7.092354 | 2.838285 |
| 132 | C | 12.189509 | -6.267137 | 0.302100 | 185 | H | -10.575097 | -7.264557 | 1.747574 |
| 133 | H | 12.356547 | -5.760091 | -0.662581 | 186 | H | -10.306994 | -8.074935 | 3.281120 |
| 134 | H | 12.468111 | -5.535796 | 1.078738 | 187 | C | -11.906233 | -6.631750 | 3.323275 |
| 135 | C | 13.099080 | -7.481797 | 0.401147 | 188 | H | -12.096211 | -5.609159 | 2.958459 |
| 136 | H | 12.817657 | -8.211611 | -0.376061 | 189 | H | -11.895057 | -6.560927 | 4.421531 |
| 137 | H | 12.924593 | -7.989256 | 1.364463 | 190 | C | -13.027270 | -7.549762 | 2.868734 |
| 138 | C | 14.577310 | -7.150937 | 0.268558 | 191 | H | -14.004455 | -7.224412 | 3.243845 |
| 139 | H | 14.755299 | -6.645661 | -0.695196 | 192 | H | -13.086729 | -7.580610 | 1.771944 |
| 140 | H | 14.861055 | -6.422546 | 1.046219 | 193 | H | -12.864185 | -8.578687 | 3.215690 |
| 141 | C | 15.473828 | -8.374956 | 0.371419 | 194 | C | -0.250821 | 4.655598 | 1.327235 |
| 142 | H | 15.188504 | -9.101942 | -0.407062 | 195 | H | -0.826672 | 5.151265 | 2.124701 |
| 143 | H | 15.290771 | -8.880860 | 1.333976 | 196 | H | -0.421331 | 5.215657 | 0.391004 |
| 144 | C | 16.955518 | -8.057351 | 0.244246 | 197 | C | 1.217554 | 4.612729 | 1.671884 |
| 145 | H | 17.140441 | -7.551217 | -0.717795 | 198 | H | 1.342918 | 4.161708 | 2.666998 |
| 146 | H | 17.243064 | -7.332917 | 1.024245 | 199 | H | 1.729319 | 3.945740 | 0.960757 |
| 147 | C | 17.842738 | -9.288004 | 0.346295 | 200 | C | 1.861541 | 5.989061 | 1.629134 |
| 148 | H | 17.555132 | -10.011671 | -0.434584 | 201 | H | 1.819918 | 6.373637 | 0.594439 |
| 149 | H | 17.655198 | -9.795678 | 1.307183 | 202 | H | 1.284479 | 6.700303 | 2.242591 |
| 150 | C | 19.327380 | -8.979649 | 0.222784 | 203 | C | 3.308487 | 5.959628 | 2.093616 |
| 151 | H | 19.614433 | -8.261486 | 1.006376 | 204 | H | 3.349066 | 5.662025 | 3.154153 |
| 152 | H | 19.512570 | -8.469641 | -0.735273 | 205 | H | 3.842890 | 5.168576 | 1.537076 |
| 153 | C | 20.193166 | -10.223852 | 0.320815 | 206 | C | 4.041156 | 7.276969 | 1.895683 |
| 154 | H | 19.944425 | -10.941165 | -0.472421 | 207 | H | 3.956169 | 7.576883 | 0.837191 |
| 155 | H | 21.260738 | -9.990917 | 0.233443 | 208 | H | 3.551009 | 8.075505 | 2.476408 |
| 156 | H | 20.043467 | -10.735311 | 1.280918 | 209 | C | 5.513502 | 7.185745 | 2.265138 |
| 157 | C | 0.346367 | -4.065484 | 1.625247 | 210 | H | 5.620817 | 7.004919 | 3.346936 |
| 158 | H | -0.089628 | -3.295083 | 0.979834 | 211 | H | 5.938742 | 6.295404 | 1.770080 |
| 159 | H | 0.623779 | -3.593359 | 2.580474 | 212 | C | 6.333092 | 8.400569 | 1.857016 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 213 | H | 6.016556 | 9.286636 | 2.430477 | 266 | C | 0.666805 | -5.694797 | -2.623943 |
| 214 | H | 6.122837 | 8.636513 | 0.800030 | 267 | C | -11.581475 | -2.880770 | 1.665516 |
| 215 | C | 7.827595 | 8.174582 | 2.021751 | 268 | H | -11.297015 | -1.839068 | 1.853365 |
| 216 | H | 8.067266 | 8.002005 | 3.084268 | 269 | H | -12.674256 | -2.942943 | 1.749129 |
| 217 | H | 8.095551 | 7.236111 | 1.504663 | 270 | H | -11.145489 | -3.499238 | 2.461002 |
| 218 | C | 8.695182 | 9.295335 | 1.472291 | 271 | C | -11.721916 | -2.420161 | -0.788376 |
| 219 | H | 8.493973 | 10.229405 | 2.021631 | 272 | H | -11.392683 | -1.384393 | -0.642514 |
| 220 | H | 8.408250 | 9.494308 | 0.425546 | 273 | H | -11.421958 | -2.733703 | -1.796563 |
| 221 | C | 10.180345 | 8.972992 | 1.533105 | 274 | H | -12.818590 | -2.434379 | -0.740369 |
| 222 | H | 10.369572 | 8.037716 | 0.976153 | 275 | C | -11.702427 | -4.760792 | 0.037601 |
| 223 | H | 10.469469 | 8.759332 | 2.576184 | 276 | H | -11.295106 | -5.493098 | 0.746701 |
| 224 | C | 11.073060 | 10.070882 | 0.975977 | 277 | H | -12.792113 | -4.746178 | 0.165667 |
| 225 | H | 10.905801 | 10.998652 | 1.544302 | 278 | H | -11.495446 | -5.114784 | -0.980314 |
| 226 | H | 10.769885 | 10.292557 | -0.058961 | 279 | C | 1.059442 | -6.835736 | -1.677951 |
| 227 | C | 12.544930 | 9.697282 | 1.013905 | 280 | H | 0.273894 | -7.598113 | -1.605102 |
| 228 | H | 12.734647 | 8.785331 | 0.431618 | 281 | H | 1.968581 | -7.326815 | -2.048979 |
| 229 | H | 13.182646 | 10.489499 | 0.605182 | 282 | H | 1.262025 | -6.451506 | -0.670106 |
| 230 | H | 12.876705 | 9.501773 | 2.042176 | 283 | C | 1.834552 | -4.717557 | -2.724518 |
| 231 | C | 5.295338 | 8.547920 | -2.036388 | 284 | H | 1.614056 | -3.884589 | -3.404461 |
| 232 | C | -6.221251 | -8.996385 | -1.922846 | 285 | H | 2.110283 | -4.302202 | -1.746490 |
| 233 | F | 6.514151 | 9.046880 | -1.792345 | 286 | H | 2.714058 | -5.242831 | -3.116227 |
| 234 | F | 5.024309 | 8.780732 | -3.330426 | 287 | C | 0.386726 | -6.260072 | -4.021007 |
| 235 | F | 4.421346 | 9.292652 | -1.334051 | 288 | H | 1.295980 | -6.732093 | -4.414842 |
| 236 | F | -7.509950 | -9.309159 | -1.749180 | 289 | H | -0.402522 | -7.020922 | -4.011222 |
| 237 | F | -5.913678 | -9.287245 | -3.198599 | 290 | H | 0.088129 | -5.466748 | -4.718152 |
| 238 | F | -5.503650 | -9.844387 | -1.166837 | | | | | |
| 239 | C | 10.559969 | 4.041622 | 1.371163 | | | | | |
| 240 | C | 11.391207 | 2.859785 | 1.862360 | | | | | |
| 241 | H | 10.943098 | 2.375946 | 2.739120 | | | | | |
| 242 | H | 11.526271 | 2.102543 | 1.079295 | | | | | |
| 243 | H | 12.386272 | 3.213864 | 2.157977 | | | | | |
| 244 | C | 10.400224 | 5.042567 | 2.522217 | | | | | |
| 245 | H | 11.386671 | 5.394815 | 2.852142 | | | | | |
| 246 | H | 9.812295 | 5.919259 | 2.222278 | | | | | |
| 247 | H | 9.898586 | 4.578718 | 3.381186 | | | | | |
| 248 | C | 11.305267 | 4.708777 | 0.210336 | | | | | |
| 249 | H | 11.416564 | 4.021384 | -0.637852 | | | | | |
| 250 | H | 10.799186 | 5.612459 | -0.149443 | | | | | |
| 251 | H | 12.309359 | 5.005474 | 0.539819 | | | | | |
| 252 | C | -1.008077 | 4.271984 | -3.031900 | | | | | |
| 253 | C | -2.099958 | 3.208762 | -2.943094 | | | | | |
| 254 | H | -2.351488 | 2.964310 | -1.901463 | | | | | |
| 255 | H | -3.010896 | 3.584490 | -3.424916 | | | | | |
| 256 | H | -1.814291 | 2.282064 | -3.456546 | | | | | |
| 257 | C | -0.700001 | 4.534515 | -4.512003 | | | | | |
| 258 | H | 0.038671 | 5.334685 | -4.643061 | | | | | |
| 259 | H | -0.312780 | 3.630988 | -5.000264 | | | | | |
| 260 | H | -1.617532 | 4.835675 | -5.034011 | | | | | |
| 261 | C | -1.533948 | 5.557488 | -2.385695 | | | | | |
| 262 | H | -2.417146 | 5.908280 | -2.934801 | | | | | |
| 263 | H | -1.839210 | 5.377819 | -1.346165 | | | | | |
| 264 | H | -0.795666 | 6.368196 | -2.393910 | | | | | |
| 265 | C | -11.144034 | -3.360711 | 0.277372 | | | | | |

**Table S6**. Cartesian coordinates of the optimized ground-state geometry of the closed form of **3** in dichloromethane

| Energy = –5944.50391589 Hartrees | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Pt | -2.588530 | -2.552894 | 1.164861 | 54 | C | -0.204323 | -5.971161 | -1.415358 |
| 2 | C | -1.998857 | -4.379903 | 1.516334 | 55 | C | -1.743026 | -4.203051 | -2.137492 |
| 3 | C | -2.873361 | -5.431646 | 1.227446 | 56 | C | -1.191662 | -6.925128 | -1.647669 |
| 4 | C | -0.702904 | -4.587075 | 1.995404 | 57 | C | -2.735465 | -5.157353 | -2.364005 |
| 5 | C | -2.433385 | -6.738427 | 1.417410 | 58 | C | -2.440993 | -6.503169 | -2.120459 |
| 6 | C | -0.259351 | -5.896703 | 2.182974 | 59 | H | -1.025150 | -7.984499 | -1.453518 |
| 7 | C | -1.133023 | -6.950152 | 1.892955 | 60 | H | -3.728180 | -4.877899 | -2.715234 |
| 8 | H | -3.062637 | -7.596984 | 1.182470 | 61 | N | 1.863873 | -5.008108 | -0.721981 |
| 9 | H | 0.748637 | -6.115647 | 2.533558 | 62 | C | 1.144445 | -6.165622 | -0.870384 |
| 10 | N | -0.670439 | -2.202647 | 1.848450 | 63 | C | 3.103641 | -5.076168 | -0.214677 |
| 11 | C | 0.036905 | -3.331889 | 2.189375 | 64 | C | 1.693883 | -7.389944 | -0.500401 |
| 12 | C | -0.077725 | -1.009471 | 1.957001 | 65 | C | 3.686627 | -6.269638 | 0.164292 |
| 13 | C | 1.334054 | -3.224127 | 2.666373 | 66 | H | 3.625361 | -4.126462 | -0.116284 |
| 14 | C | 1.219022 | -0.859369 | 2.424336 | 67 | C | 2.983969 | -7.473703 | 0.022923 |
| 15 | H | -0.675534 | -0.152285 | 1.652169 | 68 | H | 1.084800 | -8.280932 | -0.625603 |
| 16 | C | 1.960790 | -1.979116 | 2.800588 | 69 | H | 4.697602 | -6.249015 | 0.563437 |
| 17 | H | 1.863042 | -4.138308 | 2.931027 | 70 | N | -0.679630 | -2.071040 | -1.931824 |
| 18 | H | 1.631906 | 0.143915 | 2.469856 | 71 | C | -1.823979 | -2.743971 | -2.293129 |
| 19 | N | -4.268910 | -3.609809 | 0.577868 | 72 | C | -0.658307 | -0.737394 | -2.021851 |
| 20 | C | -5.401810 | -3.091388 | 0.080538 | 73 | C | -2.923962 | -2.046817 | -2.766798 |
| 21 | C | -4.157077 | -4.971565 | 0.686761 | 74 | C | -1.739915 | -0.001703 | -2.483355 |
| 22 | C | -6.460673 | -3.877301 | -0.331601 | 75 | H | 0.265959 | -0.254201 | -1.709532 |
| 23 | H | -5.435712 | -2.005623 | 0.019968 | 76 | C | -2.910658 | -0.650961 | -2.876128 |
| 24 | C | -5.200546 | -5.800323 | 0.286310 | 77 | H | -3.808240 | -2.614402 | -3.052179 |
| 25 | C | -6.382293 | -5.273202 | -0.233086 | 78 | H | -1.646275 | 1.079711 | -2.513332 |
| 26 | H | -7.348538 | -3.386644 | -0.722949 | 79 | O | 7.731414 | 0.513726 | -0.079516 |
| 27 | H | -5.065202 | -6.873847 | 0.385174 | 80 | O | 4.195420 | 3.642278 | 0.193267 |
| 28 | C | -3.186123 | -0.601922 | 0.811355 | 81 | C | 8.218707 | -0.816859 | -0.214384 |
| 29 | C | -3.479028 | 0.578468 | 0.606161 | 82 | H | 7.766011 | -1.459227 | 0.559466 |
| 30 | C | -3.801539 | 1.942113 | 0.357286 | 83 | H | 7.931504 | -1.224751 | -1.196976 |
| 31 | C | -5.146492 | 2.342611 | 0.297164 | 84 | C | 9.719814 | -0.772492 | -0.069644 |
| 32 | C | -2.773001 | 2.893205 | 0.158612 | 85 | H | 9.970844 | -0.310447 | 0.896430 |
| 33 | C | -5.463830 | 3.673550 | 0.040249 | 86 | H | 10.133792 | -0.116754 | -0.849684 |
| 34 | H | -5.917291 | 1.593984 | 0.451593 | 87 | C | 10.345119 | -2.155437 | -0.163465 |
| 35 | C | -3.125813 | 4.249371 | -0.069942 | 88 | H | 9.935554 | -2.799871 | 0.631257 |
| 36 | C | -4.455493 | 4.631732 | -0.143644 | 89 | H | 10.057215 | -2.628731 | -1.116089 |
| 37 | H | -4.750330 | 5.658538 | -0.337304 | 90 | C | 11.861609 | -2.119120 | -0.055296 |
| 38 | C | -1.408066 | 2.528304 | 0.148052 | 91 | H | 12.147895 | -1.619234 | 0.884589 |
| 39 | C | -0.214324 | 2.271299 | 0.082161 | 92 | H | 12.268867 | -1.491844 | -0.865112 |
| 40 | C | 1.112324 | 1.979967 | -0.009380 | 93 | C | 12.505664 | -3.495395 | -0.109504 |
| 41 | C | 2.302298 | 1.712892 | -0.097974 | 94 | H | 12.111320 | -4.116721 | 0.711662 |
| 42 | C | 3.674713 | 1.384626 | -0.161586 | 95 | H | 12.207653 | -4.004015 | -1.041243 |
| 43 | C | 4.093934 | 0.051239 | -0.395181 | 96 | C | 14.023204 | -3.447153 | -0.023473 |
| 44 | C | 4.659253 | 2.387669 | 0.036462 | 97 | H | 14.319627 | -2.920636 | 0.898939 |
| 45 | C | 5.460258 | -0.271009 | -0.374138 | 98 | H | 14.416004 | -2.838553 | -0.854855 |
| 46 | C | 6.005365 | 2.056759 | 0.056995 | 99 | C | 14.677472 | -4.819655 | -0.050779 |
| 47 | C | 6.401675 | 0.725601 | -0.136451 | 100 | H | 14.294716 | -5.424215 | 0.788280 |
| 48 | H | 5.752878 | -1.301529 | -0.550605 | 101 | H | 14.374234 | -5.352334 | -0.967393 |
| 49 | H | 6.779173 | 2.798737 | 0.225349 | 102 | C | 16.195446 | -4.761141 | 0.019989 |
| 50 | C | 3.135898 | -0.970082 | -0.648846 | 103 | H | 16.497585 | -4.217316 | 0.930470 |
| 51 | C | 2.300274 | -1.849607 | -0.871472 | 104 | H | 16.577042 | -4.164710 | -0.825372 |
| 52 | Pt | 0.859226 | -3.282903 | -1.266032 | 105 | C | 16.856856 | -6.130498 | 0.009397 |
| 53 | C | -0.499618 | -4.626677 | -1.662437 | 106 | H | 16.482472 | -6.724116 | 0.859991 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 107 | H | 16.549953 | -6.678447 | -0.896997 | 160 | C | -1.000180 | 7.180990 | -0.075544 |
| 108 | C | 18.374875 | -6.064895 | 0.069023 | 161 | H | -0.644058 | 6.925878 | 0.933574 |
| 109 | H | 18.749318 | -5.476620 | -0.785367 | 162 | H | -0.259232 | 6.774654 | -0.778878 |
| 110 | H | 18.682171 | -5.510384 | 0.971457 | 163 | C | -1.092515 | 8.690778 | -0.226457 |
| 111 | C | 19.041626 | -7.432473 | 0.068451 | 164 | H | -1.276299 | 8.949102 | -1.281481 |
| 112 | H | 18.670864 | -8.015757 | 0.925559 | 165 | H | -1.962172 | 9.070769 | 0.334240 |
| 113 | H | 18.729626 | -7.986663 | -0.830352 | 166 | C | 0.162242 | 9.393190 | 0.268429 |
| 114 | C | 20.557167 | -7.344581 | 0.120480 | 167 | H | 0.267133 | 9.213866 | 1.351128 |
| 115 | H | 21.027878 | -8.334451 | 0.122823 | 168 | H | 1.049979 | 8.933921 | -0.197069 |
| 116 | H | 20.950447 | -6.792741 | -0.743500 | 169 | C | 0.168450 | 10.889302 | 0.000555 |
| 117 | H | 20.891163 | -6.816672 | 1.023517 | 170 | H | -0.790837 | 11.325863 | 0.324778 |
| 118 | O | -6.723108 | 4.147044 | -0.045686 | 171 | H | 0.226906 | 11.067533 | -1.085808 |
| 119 | O | -2.088357 | 5.092929 | -0.199776 | 172 | C | 1.306887 | 11.613551 | 0.701766 |
| 120 | C | -7.804481 | 3.240273 | 0.137252 | 173 | H | 1.166910 | 11.532580 | 1.792450 |
| 121 | H | -7.763084 | 2.449997 | -0.631014 | 174 | H | 2.260052 | 11.101014 | 0.485075 |
| 122 | H | -7.721950 | 2.752671 | 1.121957 | 175 | C | 1.420597 | 13.078875 | 0.312389 |
| 123 | C | -9.091625 | 4.021457 | 0.041275 | 176 | H | 0.431301 | 13.558714 | 0.400214 |
| 124 | H | -9.142231 | 4.519566 | -0.937968 | 177 | H | 1.694959 | 13.152564 | -0.753865 |
| 125 | H | -9.081232 | 4.817084 | 0.800725 | 178 | C | 2.426744 | 13.850057 | 1.151663 |
| 126 | C | -10.305224 | 3.127182 | 0.241209 | 179 | H | 2.118752 | 13.816103 | 2.209892 |
| 127 | H | -10.320758 | 2.345713 | -0.535688 | 180 | H | 3.405726 | 13.341861 | 1.107465 |
| 128 | H | -10.213747 | 2.596184 | 1.202665 | 181 | C | 2.589045 | 15.298546 | 0.718717 |
| 129 | C | -11.618263 | 3.893864 | 0.216461 | 182 | H | 1.602574 | 15.791909 | 0.718900 |
| 130 | H | -11.716438 | 4.425000 | -0.744410 | 183 | H | 2.939722 | 15.329838 | -0.327544 |
| 131 | H | -11.596199 | 4.676467 | 0.992453 | 184 | C | 3.548150 | 16.089515 | 1.593991 |
| 132 | C | -12.832151 | 3.004064 | 0.432565 | 185 | H | 3.205601 | 16.053396 | 2.641651 |
| 133 | H | -12.865010 | 2.231108 | -0.353060 | 186 | H | 4.538157 | 15.599952 | 1.586913 |
| 134 | H | -12.718219 | 2.459518 | 1.384587 | 187 | C | 3.702463 | 17.540671 | 1.164082 |
| 135 | C | -14.146848 | 3.768278 | 0.446252 | 188 | H | 2.716508 | 18.030320 | 1.181589 |
| 136 | H | -14.267189 | 4.309407 | -0.506851 | 189 | H | 4.036489 | 17.571895 | 0.113723 |
| 137 | H | -14.108977 | 4.544044 | 1.228939 | 190 | C | 4.678784 | 18.310518 | 2.036591 |
| 138 | C | -15.357051 | 2.877273 | 0.679252 | 191 | H | 4.781361 | 19.354732 | 1.718153 |
| 139 | H | -15.401711 | 2.106667 | -0.108226 | 192 | H | 4.353122 | 18.315144 | 3.085406 |
| 140 | H | -15.228137 | 2.329362 | 1.627506 | 193 | H | 5.678287 | 17.854633 | 2.010585 |
| 141 | C | -16.672358 | 3.639847 | 0.714920 | 194 | C | 5.140016 | 4.708677 | 0.196939 |
| 142 | H | -16.806155 | 4.184676 | -0.234341 | 195 | H | 5.798657 | 4.613244 | -0.681545 |
| 143 | H | -16.624626 | 4.412753 | 1.499966 | 196 | H | 5.773197 | 4.645484 | 1.096627 |
| 144 | C | -17.879023 | 2.747183 | 0.960058 | 197 | C | 4.399014 | 6.024023 | 0.149918 |
| 145 | H | -17.930669 | 1.977194 | 0.172352 | 198 | H | 3.686701 | 6.001452 | -0.687711 |
| 146 | H | -17.739948 | 2.198496 | 1.906453 | 199 | H | 3.807308 | 6.153424 | 1.067660 |
| 147 | C | -19.194840 | 3.507865 | 1.008978 | 200 | C | 5.378330 | 7.175775 | -0.027078 |
| 148 | H | -19.338291 | 4.054880 | 0.062215 | 201 | H | 6.118901 | 7.159638 | 0.789118 |
| 149 | H | -19.142649 | 4.279424 | 1.795256 | 202 | H | 5.952009 | 7.014473 | -0.954460 |
| 150 | C | -20.399717 | 2.613713 | 1.261641 | 203 | C | 4.729672 | 8.550958 | -0.085008 |
| 151 | H | -20.251262 | 2.066080 | 2.205250 | 204 | H | 3.937388 | 8.553231 | -0.851775 |
| 152 | H | -20.452822 | 1.846630 | 0.473531 | 205 | H | 4.227586 | 8.768396 | 0.872326 |
| 153 | C | -21.704648 | 3.388873 | 1.315742 | 206 | C | 5.741085 | 9.642156 | -0.403813 |
| 154 | H | -21.889133 | 3.918506 | 0.371758 | 207 | H | 6.569952 | 9.595286 | 0.321735 |
| 155 | H | -22.564589 | 2.735166 | 1.502004 | 208 | H | 6.193965 | 9.430516 | -1.386785 |
| 156 | H | -21.683211 | 4.143355 | 2.113237 | 209 | C | 5.168863 | 11.051059 | -0.413756 |
| 157 | C | -2.325004 | 6.492801 | -0.296702 | 210 | H | 4.281353 | 11.088084 | -1.069110 |
| 158 | H | -3.051944 | 6.805073 | 0.469231 | 211 | H | 4.808506 | 11.310940 | 0.596644 |
| 159 | H | -2.751989 | 6.733732 | -1.283948 | 212 | C | 6.178660 | 12.089795 | -0.879067 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 213 | H | 6.483886 | 11.857105 | -1.912749 | 266 | C | -3.936448 | 1.598943 | -3.413692 |
| 214 | H | 7.094991 | 12.006968 | -0.271350 | 267 | C | -3.100162 | 1.903136 | -4.055917 |
| 215 | C | 5.662260 | 13.517843 | -0.815583 | 268 | H | -4.842290 | 2.080551 | -3.802482 |
| 216 | H | 4.709882 | 13.590677 | -1.369720 | 269 | H | -3.759012 | 1.992842 | -2.403877 |
| 217 | H | 5.418844 | 13.771929 | 0.230477 | 270 | H | -5.349026 | -0.250669 | -2.541328 |
| 218 | C | 6.644404 | 14.541720 | -1.363206 | 271 | C | -5.607865 | -1.316002 | -2.591329 |
| 219 | H | 6.876565 | 14.301657 | -2.414049 | 272 | H | -5.158997 | 0.007945 | -1.491048 |
| 220 | H | 7.599471 | 14.459239 | -0.818115 | 273 | H | -6.221201 | 0.320925 | -2.886049 |
| 221 | C | 6.132065 | 15.969979 | -1.270793 | 274 | H | -4.392189 | -0.373865 | -4.851635 |
| 222 | H | 5.899227 | 16.206543 | -0.217726 | 275 | C | -3.538152 | -0.143913 | -5.501622 |
| 223 | H | 5.173441 | 16.050417 | -1.812474 | 276 | H | -4.584460 | -1.451974 | -4.912088 |
| 224 | C | 7.103607 | 17.006276 | -1.814615 | 277 | H | -5.272158 | 0.145456 | -5.253183 |
| 225 | H | 7.332884 | 16.771521 | -2.865568 | 278 | H | 3.633907 | -8.788712 | 0.429194 |
| 226 | H | 8.058559 | 16.926375 | -1.272506 | 279 | C | 4.903803 | -8.990265 | -0.406235 |
| 227 | C | 6.567017 | 18.423328 | -1.707167 | 280 | H | 5.633784 | -8.187213 | -0.248142 |
| 228 | H | 6.365710 | 18.691229 | -0.660785 | 281 | H | 5.383842 | -9.937174 | -0.127660 |
| 229 | H | 7.271574 | 19.161854 | -2.107108 | 282 | H | 4.671016 | -9.031207 | -1.477922 |
| 230 | H | 5.624034 | 18.532062 | -2.259847 | 283 | C | 4.008247 | -8.727635 | 1.915087 |
| 231 | C | -0.696118 | -8.368500 | 2.046381 | 284 | H | 4.467194 | -9.676998 | 2.219642 |
| 232 | C | -3.467548 | -7.562480 | -2.345544 | 285 | H | 4.728559 | -7.928928 | 2.128101 |
| 233 | F | -4.663635 | -7.066279 | -2.688868 | 286 | H | 3.123033 | -8.564051 | 2.541703 |
| 234 | F | -3.105316 | -8.420073 | -3.312840 | 287 | C | 2.711753 | -9.984003 | 0.206469 |
| 235 | F | -3.661257 | -8.314662 | -1.242673 | 288 | H | 1.790724 | -9.908631 | 0.797089 |
| 236 | F | -1.437886 | -9.034835 | 2.944764 | 289 | H | 2.438728 | -10.098506 | -0.850463 |
| 237 | F | 0.582411 | -8.482091 | 2.429466 | 290 | H | 3.228451 | -10.901315 | 0.513812 |
| 238 | F | -0.816512 | -9.055967 | 0.891335 | | | | | |
| 239 | C | 3.382998 | -1.892606 | 3.338117 | | | | | |
| 240 | C | 3.899339 | -0.456252 | 3.372021 | | | | | |
| 241 | H | 3.292364 | 0.181871 | 4.026865 | | | | | |
| 242 | H | 4.924296 | -0.449441 | 3.763210 | | | | | |
| 243 | H | 3.923300 | -0.002095 | 2.372022 | | | | | |
| 244 | C | 3.404927 | -2.451024 | 4.766155 | | | | | |
| 245 | H | 2.745689 | -1.873010 | 5.426530 | | | | | |
| 246 | H | 3.087986 | -3.500301 | 4.804122 | | | | | |
| 247 | H | 4.423681 | -2.395305 | 5.171555 | | | | | |
| 248 | C | 4.314671 | -2.724687 | 2.448263 | | | | | |
| 249 | H | 4.060218 | -3.792230 | 2.470134 | | | | | |
| 250 | H | 4.265227 | -2.380781 | 1.406085 | | | | | |
| 251 | H | 5.350797 | -2.621986 | 2.798004 | | | | | |
| 252 | C | -7.556158 | -6.137148 | -0.670279 | | | | | |
| 253 | C | -8.768477 | -5.789073 | 0.201699 | | | | | |
| 254 | H | -9.056800 | -4.735552 | 0.105844 | | | | | |
| 255 | H | -9.629433 | -6.400740 | -0.097608 | | | | | |
| 256 | H | -8.562268 | -5.989391 | 1.260938 | | | | | |
| 257 | C | -7.265857 | -7.628348 | -0.525138 | | | | | |
| 258 | H | -6.417515 | -7.943257 | -1.145187 | | | | | |
| 259 | H | -7.058810 | -7.906383 | 0.516234 | | | | | |
| 260 | H | -8.143643 | -8.200805 | -0.848494 | | | | | |
| 261 | C | -7.879972 | -5.843366 | -2.139635 | | | | | |
| 262 | H | -8.724507 | -6.464916 | -2.463582 | | | | | |
| 263 | H | -8.158653 | -4.795534 | -2.301915 | | | | | |
| 264 | H | -7.023915 | -6.072658 | -2.786163 | | | | | |
| 265 | C | -4.131575 | 0.084825 | -3.411757 | | | | | |

**Table S7**. Cartesian coordinates of the optimized $T_1$ geometry of the open form of **1** in dichloromethane

| Energy = –4641.95790161 Hartrees | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Pt | 3.671448 | 3.390323 | -0.874539 | 54 | C | -4.024170 | -2.138761 | -0.588695 |
| 2 | C | 3.427858 | 5.288124 | -1.273955 | 55 | Pt | -3.665803 | -4.107758 | -1.113475 |
| 3 | C | 4.469987 | 6.172881 | -0.989146 | 56 | C | -3.224394 | -5.956099 | -1.569441 |
| 4 | C | 2.208970 | 5.713482 | -1.807116 | 57 | C | -4.125409 | -6.965853 | -1.226783 |
| 5 | C | 4.286676 | 7.534513 | -1.248984 | 58 | C | -1.985790 | -6.225543 | -2.156203 |
| 6 | C | 2.029227 | 7.076264 | -2.064772 | 59 | C | -3.773613 | -8.295719 | -1.476859 |
| 7 | C | 3.070316 | 7.967798 | -1.786140 | 60 | C | -1.636787 | -7.557248 | -2.402190 |
| 8 | H | 5.070689 | 8.262438 | -1.037721 | 61 | C | -2.534291 | -8.573501 | -2.060356 |
| 9 | H | 1.094320 | 7.456715 | -2.475544 | 62 | H | -4.442619 | -9.115819 | -1.216987 |
| 10 | H | 2.928178 | 9.027342 | -1.986668 | 63 | H | -0.678338 | -7.819020 | -2.849553 |
| 11 | N | 1.746825 | 3.372891 | -1.643476 | 64 | H | -2.258566 | -9.607980 | -2.250530 |
| 12 | C | 1.259823 | 4.612589 | -1.992030 | 65 | N | -5.356591 | -5.085353 | -0.411015 |
| 13 | C | 0.962305 | 2.292849 | -1.761569 | 66 | C | -5.341941 | -6.447687 | -0.597968 |
| 14 | C | -0.047568 | 4.739961 | -2.450412 | 67 | C | -6.419706 | -4.506091 | 0.166207 |
| 15 | C | -0.342365 | 2.370128 | -2.224050 | 68 | C | -6.428779 | -7.218104 | -0.195631 |
| 16 | H | 1.409463 | 1.347175 | -1.460600 | 69 | C | -7.525790 | -5.231237 | 0.581175 |
| 17 | C | -0.855711 | 3.615682 | -2.567203 | 70 | H | -6.361348 | -3.427341 | 0.286631 |
| 18 | H | -0.424282 | 5.726854 | -2.708660 | 71 | C | -7.528407 | -6.610103 | 0.393749 |
| 19 | H | -0.938612 | 1.464005 | -2.292792 | 72 | H | -6.401020 | -8.293988 | -0.353114 |
| 20 | H | -1.880683 | 3.712978 | -2.917236 | 73 | H | -8.363256 | -4.717123 | 1.042141 |
| 21 | N | 5.491484 | 4.146926 | -0.234087 | 74 | H | -8.381197 | -7.209405 | 0.705381 |
| 22 | C | 6.488191 | 3.437293 | 0.314577 | 75 | N | -1.816118 | -3.844759 | -2.015918 |
| 23 | C | 5.631257 | 5.505460 | -0.396466 | 76 | C | -1.203636 | -5.011802 | -2.409653 |
| 24 | C | 7.673202 | 4.022123 | 0.730638 | 77 | C | -1.200467 | -2.670594 | -2.214290 |
| 25 | H | 6.307688 | 2.369829 | 0.412726 | 78 | C | 0.062364 | -4.970827 | -2.984500 |
| 26 | C | 6.804625 | 6.136181 | 0.004599 | 79 | C | 0.054263 | -2.579873 | -2.797272 |
| 27 | C | 7.831533 | 5.394391 | 0.571241 | 80 | H | -1.742526 | -1.790162 | -1.874398 |
| 28 | H | 8.450329 | 3.405245 | 1.170500 | 81 | C | 0.697941 | -3.751722 | -3.178414 |
| 29 | H | 6.902384 | 7.210048 | -0.134644 | 82 | H | 0.544686 | -5.901105 | -3.273359 |
| 30 | H | 8.748678 | 5.884813 | 0.886884 | 83 | H | 0.514117 | -1.604274 | -2.929536 |
| 31 | C | 3.928504 | 1.370724 | -0.492041 | 84 | H | 1.691050 | -3.717691 | -3.619370 |
| 32 | C | 4.063709 | 0.151266 | -0.334434 | 85 | O | -6.227089 | 3.424500 | 0.205994 |
| 33 | C | 4.172438 | -1.256449 | -0.227528 | 86 | O | -1.549004 | 2.992943 | 0.769810 |
| 34 | C | 5.427441 | -1.872357 | -0.281278 | 87 | C | -7.520452 | 2.875004 | -0.020346 |
| 35 | C | 2.963821 | -2.055646 | -0.130012 | 88 | H | -7.552122 | 2.393881 | -1.011438 |
| 36 | C | 5.527174 | -3.261029 | -0.279588 | 89 | H | -7.732683 | 2.099623 | 0.733284 |
| 37 | H | 6.308230 | -1.241554 | -0.353916 | 90 | C | -8.526418 | 3.995953 | 0.067240 |
| 38 | C | 3.113607 | -3.491222 | -0.151205 | 91 | H | -8.268426 | 4.769912 | -0.670415 |
| 39 | C | 4.366310 | -4.055946 | -0.222296 | 92 | H | -8.452065 | 4.466615 | 1.058544 |
| 40 | H | 4.460435 | -5.138828 | -0.217649 | 93 | C | -9.943704 | 3.498609 | -0.170476 |
| 41 | C | 1.748419 | -1.425038 | -0.052585 | 94 | H | -10.006564 | 3.026133 | -1.164113 |
| 42 | C | 0.655664 | -0.814079 | 0.077618 | 95 | H | -10.182270 | 2.705692 | 0.556801 |
| 43 | C | -0.500036 | -0.208766 | 0.190394 | 96 | C | -10.983592 | 4.603262 | -0.069577 |
| 44 | C | -1.613838 | 0.384600 | 0.250052 | 97 | H | -10.742973 | 5.399577 | -0.792859 |
| 45 | C | -2.785706 | 1.074451 | 0.253856 | 98 | H | -10.922257 | 5.072494 | 0.926004 |
| 46 | C | -4.069605 | 0.443074 | -0.005832 | 99 | C | -12.402112 | 4.111995 | -0.310750 |
| 47 | C | -2.768611 | 2.503210 | 0.501503 | 100 | H | -12.464045 | 3.649126 | -1.309557 |
| 48 | C | -5.234571 | 1.224113 | -0.013031 | 101 | H | -12.637429 | 3.308753 | 0.407010 |
| 49 | C | -3.923034 | 3.238254 | 0.457148 | 102 | C | -13.447087 | 5.210638 | -0.197422 |
| 50 | C | -5.165105 | 2.594575 | 0.206361 | 103 | H | -13.209827 | 6.016393 | -0.911778 |
| 51 | H | -6.181625 | 0.732890 | -0.215058 | 104 | H | -13.386874 | 5.670130 | 0.803109 |
| 52 | H | -3.931893 | 4.310238 | 0.630477 | 105 | C | -14.865612 | 4.720814 | -0.442672 |
| 53 | C | -4.099820 | -0.937050 | -0.299028 | 106 | H | -14.927920 | 4.268054 | -1.446162 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 107 | H | -15.100122 | 3.909909 | 0.266808 | 160 | H | 21.617317 | -6.503875 | -0.050747 |
| 108 | C | -15.911320 | 5.817564 | -0.317684 | 161 | H | 22.573500 | -5.256096 | 0.763475 |
| 109 | H | -15.673802 | 6.631167 | -1.023078 | 162 | H | 21.479439 | -6.286503 | 1.698667 |
| 110 | H | -15.851225 | 6.266302 | 0.687772 | 163 | C | 0.888243 | -4.117177 | 0.598703 |
| 111 | C | -17.330236 | 5.331695 | -0.568557 | 164 | H | 0.198998 | -3.487742 | 0.018647 |
| 112 | H | -17.392896 | 4.890474 | -1.577184 | 165 | H | 1.133558 | -3.581943 | 1.528451 |
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| 121 | H | -21.841728 | 6.703808 | -0.733283 | 174 | H | -1.306239 | -7.212363 | 2.429281 |
| 122 | H | -20.806660 | 7.471184 | 0.480423 | 175 | C | -3.227630 | -6.226356 | 2.505363 |
| 123 | H | -20.619080 | 7.884204 | -1.228786 | 176 | H | -3.775532 | -5.469268 | 1.915705 |
| 124 | O | 6.686821 | -3.945001 | -0.325000 | 177 | H | -3.051940 | -5.767706 | 3.492798 |
| 125 | O | 2.079894 | -4.361572 | -0.153930 | 178 | C | -4.104384 | -7.457118 | 2.667543 |
| 126 | C | 7.909657 | -3.215910 | -0.334121 | 179 | H | -4.291874 | -7.901468 | 1.673555 |
| 127 | H | 7.974242 | -2.606305 | -1.250266 | 180 | H | -3.566993 | -8.226959 | 3.245848 |
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| 129 | C | 9.042038 | -4.210332 | -0.263381 | 182 | H | -5.926212 | -6.323103 | 2.791053 |
| 130 | H | 8.967917 | -4.903117 | -1.114357 | 183 | H | -5.246576 | -6.757202 | 4.354843 |
| 131 | H | 8.924439 | -4.815538 | 0.647501 | 184 | C | -6.380856 | -8.328977 | 3.412337 |
| 132 | C | 10.399522 | -3.524788 | -0.260703 | 185 | H | -6.591755 | -8.686146 | 2.389140 |
| 133 | H | 10.522244 | -2.942933 | -1.188444 | 186 | H | -5.888422 | -9.170013 | 3.927777 |
| 134 | H | 10.440322 | -2.793560 | 0.562989 | 187 | C | -7.691163 | -8.001669 | 4.111289 |
| 135 | C | 11.553128 | -4.505639 | -0.118974 | 188 | H | -8.148452 | -7.117377 | 3.634562 |
| 136 | H | 11.511342 | -5.241723 | -0.938462 | 189 | H | -7.485425 | -7.703409 | 5.152406 |
| 137 | H | 11.424730 | -5.083551 | 0.810957 | 190 | C | -8.687535 | -9.149817 | 4.100445 |
| 138 | C | 12.916991 | -3.833270 | -0.109570 | 191 | H | -8.912183 | -9.428613 | 3.056651 |
| 139 | H | 13.054646 | -3.269383 | -1.046980 | 192 | H | -8.225526 | -10.042146 | 4.554850 |
| 140 | H | 12.948607 | -3.084055 | 0.698881 | 193 | C | -9.985468 | -8.829286 | 4.826391 |
| 141 | C | 14.067618 | -4.812191 | 0.066443 | 194 | H | -10.439206 | -7.933033 | 4.375498 |
| 142 | H | 14.037515 | -5.561887 | -0.741576 | 195 | H | -9.757456 | -8.558093 | 5.868666 |
| 143 | H | 13.925341 | -5.375914 | 1.003406 | 196 | C | -10.976040 | -9.980497 | 4.796585 |
| 144 | C | 15.433334 | -4.143185 | 0.084715 | 197 | H | -11.906013 | -9.737212 | 5.323402 |
| 145 | H | 15.581186 | -3.586652 | -0.855660 | 198 | H | -11.239723 | -10.248386 | 3.764861 |
| 146 | H | 15.458700 | -3.387369 | 0.887304 | 199 | H | -10.553547 | -10.877517 | 5.268357 |
| 147 | C | 16.581506 | -5.121731 | 0.278626 | 200 | C | -1.392781 | 4.391967 | 0.971750 |
| 148 | H | 16.557854 | -5.877303 | -0.524182 | 201 | H | -2.081041 | 4.738320 | 1.759169 |
| 149 | H | 16.430837 | -5.678658 | 1.218376 | 202 | H | -1.650501 | 4.926156 | 0.039975 |
| 150 | C | 17.947592 | -4.453528 | 0.303171 | 203 | C | 0.043597 | 4.635083 | 1.365522 |
| 151 | H | 18.101441 | -3.900963 | -0.638638 | 204 | H | 0.232092 | 4.164516 | 2.341528 |
| 152 | H | 17.968178 | -3.694159 | 1.102569 | 205 | H | 0.701970 | 4.127748 | 0.643122 |
| 153 | C | 19.094834 | -5.430761 | 0.507943 | 206 | C | 0.386789 | 6.114607 | 1.418786 |
| 154 | H | 19.076436 | -6.190890 | -0.290885 | 207 | H | 0.259769 | 6.553077 | 0.413241 |
| 155 | H | 18.941134 | -5.983324 | 1.449905 | 208 | H | -0.323199 | 6.644269 | 2.075373 |
| 156 | C | 20.461316 | -4.762012 | 0.534976 | 209 | C | 1.809599 | 6.363442 | 1.894236 |
| 157 | H | 20.475576 | -4.000638 | 1.330279 | 210 | H | 1.933090 | 5.957445 | 2.911466 |
| 158 | H | 20.614990 | -4.214832 | -0.408033 | 211 | H | 2.505362 | 5.794170 | 1.253222 |
| 159 | C | 21.595181 | -5.750175 | 0.747467 | 212 | C | 2.202102 | 7.831860 | 1.875949 |

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|---|---|---|---|---|
| 213 | H | 2.026531 | 8.238114 | 0.865202 |
| 214 | H | 1.543299 | 8.402343 | 2.551773 |
| 215 | C | 3.653931 | 8.068603 | 2.258361 |
| 216 | H | 3.838654 | 7.678480 | 3.272850 |
| 217 | H | 4.301707 | 7.478775 | 1.585673 |
| 218 | C | 4.064178 | 9.530959 | 2.192405 |
| 219 | H | 3.426801 | 10.122790 | 2.870175 |
| 220 | H | 3.864211 | 9.918630 | 1.178423 |
| 221 | C | 5.525643 | 9.762435 | 2.542021 |
| 222 | H | 5.731618 | 9.348418 | 3.542951 |
| 223 | H | 6.161539 | 9.189246 | 1.845671 |
| 224 | C | 5.931948 | 11.227360 | 2.509649 |
| 225 | H | 5.298046 | 11.795888 | 3.210153 |
| 226 | H | 5.722090 | 11.644400 | 1.510574 |
| 227 | C | 7.394706 | 11.457286 | 2.855510 |
| 228 | H | 8.031363 | 10.900476 | 2.147714 |
| 229 | H | 7.607509 | 11.029341 | 3.849315 |
| 230 | C | 7.793542 | 12.925450 | 2.844532 |
| 231 | H | 7.157749 | 13.476651 | 3.554473 |
| 232 | H | 7.576499 | 13.351809 | 1.852906 |
| 233 | C | 9.257115 | 13.139870 | 3.188973 |
| 234 | H | 9.911278 | 12.622536 | 2.474779 |
| 235 | H | 9.530892 | 14.201257 | 3.179292 |
| 236 | H | 9.489776 | 12.747203 | 4.187667 |

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