Supplementary Information

iso-TEtraQuinoline (*i*-TEQ): An Inherently Chiral N4 Macrocyclic Quinoline Tetramer

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Table of Contents

1. General methods

1-1. Reactions and purifications

Unless otherwise noted, all reactions were carried out under an inert atmosphere and were stirred with Teflon-coated magnetic stir bars. All work-up and purification procedures were carried out with reagent-grade solvents under ambient atmosphere. Thin layer chromatography (TLC) was performed on Merck TLC plates (0.25 mm) pre-coated with silica gel 60 F254 and visualized by UV quenching. Flash column chromatography was performed on a Biotage Isolera Spektra One.

1-2. Characterizations

Infrared (IR) spectra were recorded on a JASCO FT/IR-4700 Fourier transform infrared spectrophotometer. NMR spectra were recorded on a Bruker AVANCE500 or a Bruker AVANCE NEO 600. Chemical shifts (δ) are given in ppm relative to residual solvent peaks[1]. Data for ^{1}H NMR are reported as follows: chemical shift (multiplicity, coupling constants where applicable, number of hydrogens). Abbreviations are as follows: s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet), br (broad). High resolution mass spectra (ESI) were measured on JEOL JMS-T100LP. Melting points were measured on a Yanagimoto Seisakusho Micro Melting Point Apparatus. HPLC analysis was conducted on a JASCO HPLC system or Shimadzu HPLC system NexeraXR equipped with Daicel chiral-stationary-phase columns. Optical rotation was measured using a 2 mL cell with a 0.5 dm path length on a JASCO polarimeter P-1030. Single-crystal X-ray data were collected on a Rigaku R-AXIS RAPID II imaging plate area detector with graphite-monochromated Cu-K**α** radiation. UV-Visible absorption spectra were recorded using a 0.1 dm cell on a Jasco V-660 spectrophotometer. Fluorescence emission spectra were recorded using a 0.1 dm cell on a Jasco FP-8600 spectrofluorometer, with which absolute fluorescence quantum yields were measured with a Jasco ILF-835 unit (100 mm integrating sphere). Circular dichroism (CD) spectra were recorded on a JASCO J-1100 spectrometer. Circularly polarized luminescence (CPL) spectra were recorded on a JASCO CPL-200S at room temperature. TG-DTA analysis was performed on a TG-DTA8122 apparatus.

1-3. Solvents and reagents

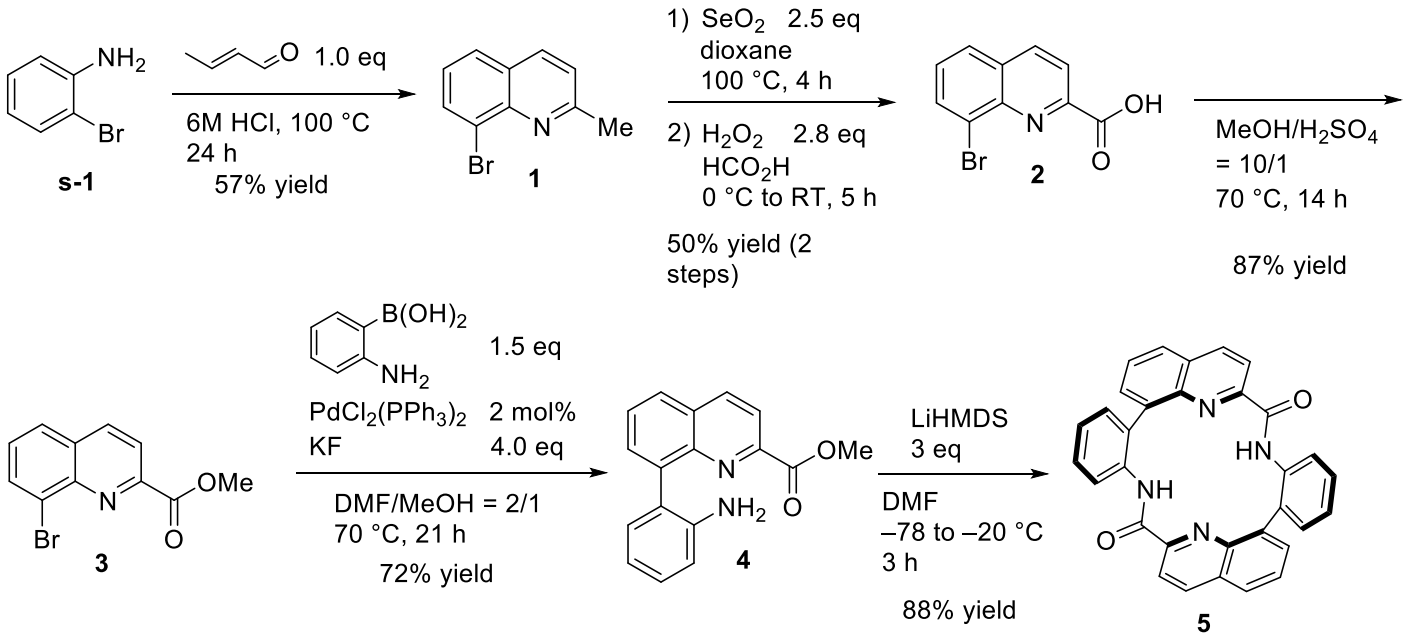
Unless otherwise noted, materials were purchased from commercial suppliers and were used without purification. THF, toluene, and CH_2Cl_2 were purified by passing through a solvent purification system (Glass Contour). Anhydrous 1,2-dichloroethane, methanol and LiHMDS were purchased from Sigma-Aldrich or Kanto Chemical. 2-Bromoaniline **s-1,** trifluoromethanesulfonic anhydride, 4-ethynylanisole and pyridine･HCl were purchased from Tokyo Chemical Industry. 2-aminophenyl boronic acid was purchased from Combi-Blocks Inc.

1-4. Computational investigations

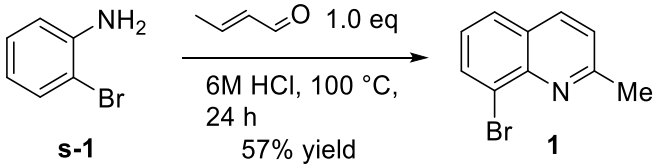
All quantum chemical calculations were performed using the Gaussian 16 program[2]. Density functional theory (DFT) calculations employed an ultrafine integral grid (99 radial shells, 590 angular points). Structural optimizations were conducted at the level of theory specified in the corresponding section. Frequency calculations confirmed the identity of geometry minima (no imaginary frequencies) and transitions states (one imaginary frequency). All transition state structures were verified to connect the reactant and the product of interest by performing IRC calculations. Zero-point energies and thermal corrections were obtained at 298 K and are unscaled.

2. Preparation of *iso*-TEtraQuinoline (*i*-TEQ) **6**

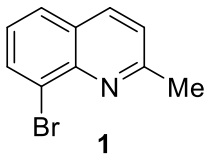
Synthetic route for substrate **5**.



2-1. Synthesis of 8-bromo-2-methylquinoline (**1**)

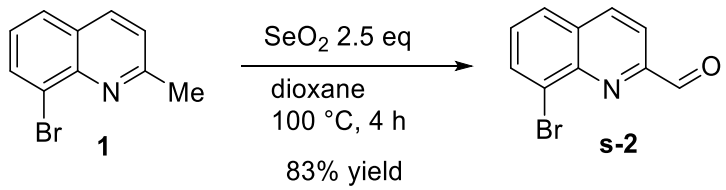


To a two-necked flask were added 2-bromoaniline **s-1** (43.0 g, 250 mmol), 6 M HCl (125 mL) under N_2 and heated to 100 °C. Then crotonaldehyde (21.0 mL, 250 mmol, 1.0 eq) was added dropwise and stirred for 24 h. After the starting material was consumed, $ZnCl_2$ (34 g, 1 eq) was added to quench the reaction, and the formed solid was filtered, washed with 3 M HCl and Et_2O. The residue was dissolved in $NH_3 \bullet H_2O$, and extracted with Et_2O for 3 times, washed with brine, and dried over anhydrous Na_2SO_4. The solution was evaporated under the reduced pressure to afford the title product (31.6 g, 57% yield) as a yellow solid.

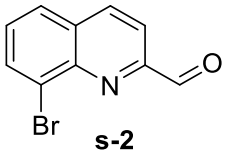


8-Bromo-2-methylquinoline (1). ^{1}H NMR (500 MHz, $CDCl_3$) **δ** 8.03 (**d**, *J* = 8.5 Hz, 1H), 8.02 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.74 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.33 (dd, *J* = 7.9, 7.7 Hz, 1H), 2.82 (s, 3H). The spectroscopic data is in agreement with that previously reported.[3]

2-2. Synthesis of 8-bromoquinoline-2-carbaldehyde (**s-2**)

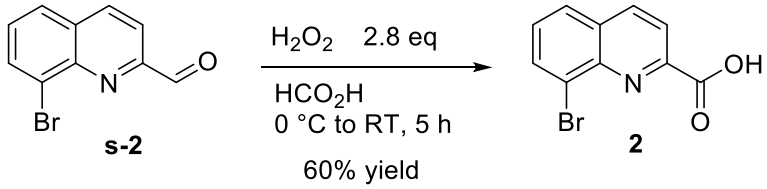


To a flask were added 8-bromo-2-methylquinoline **1** (14.4 g, 66 mmol), Se_2O (18.0 g, 165 mmol, 2.5 eq), and dioxane (120 mL) and the resulting mixture was stirred at 100 ˚C for 4 h. After the starting material was consumed, the reaction mixture was filtered through a pad of celite®, and the volatiles were evaporated under the reduced pressure. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: *n*-hexane/ethyl acetate = 10/1) to afford the title product (12.9 g, 83% yield) as a yellow solid.

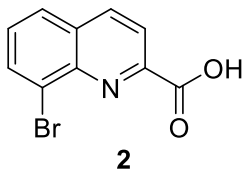


8-Bromoquinoline-2-carbaldehyde (s-2). ^{1}H NMR (500 MHz, $CDCl_3$) **δ** 10.32 (s, 1H), 8.34 (d, *J* = 8.1 Hz, 1H), 8.17 (d, *J* = 6.3 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 9.4 Hz, 1H), 7.62–7.51 (m, 1H). The spectroscopic data is in agreement with that previously reported.[3]

2-3. Synthesis of 8-bromoquinoline-2-carboxylic acid (**2**)

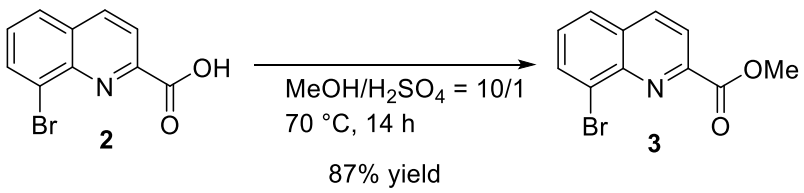


To a two-necked flask were added 8-bromoquinoline-2-carbaldehyde **s-2** (11.3 g, 47.9 mmol), H_2O_2 (19.6 mL, 134 mmol, 2.8 eq), and HCO_2H (200 mL) under N_2 and the resulting mixture was stirred at 0 ˚C for 2 h. Then the resulting mixture was stirred at room temperature for 3 h. After the starting material was consumed, sat. $Na_2S_2O_3$ was added to quench the reaction. The reaction mixture was extracted with CH_2Cl_2, the solution was evaporated under reduced pressure. The residue was basified by 1 M NaOH and washed with CH_2Cl_2. Then the aqueous phase was acidified by 3 M HCl and extracted with ethyl acetate, washed with brine and dried over anhydrous Na_2SO_4. The solution was evaporated under the reduced pressure to afford the title product (7.3 g, 60% yield) as a yellow solid.

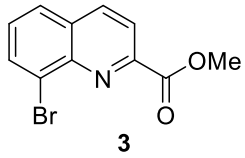


8-Bromoquinoine-2-carboxylic acid (2). ^{1}H NMR (500 MHz, $CDCl_3$) **δ** 11.32 (s, 1H), 8.45 (d, *J* = 8.4 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 7.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.61–7.54 (m, 1H).

2-4. Synthesis of methyl 8-bromoquinoline-2-caroxylate (**3**)

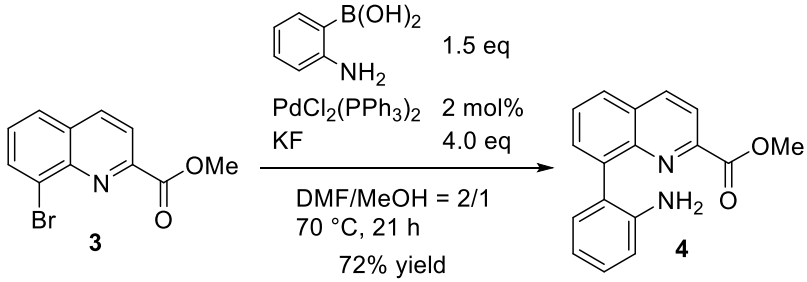


To a two-necked flask were added 8-bromoquinoline-2-carboxylic acid **2** (7.3 g, 29.0 mmol), methanol (80 mL), H_2SO_4 (8 mL) and the resulting mixture was stirred at 70 ˚C for 14 h. After the starting material was consumed, the reaction mixture was concentrated under the reduced pressure and $NaHCO_3$ was added to quench the reaction. The reaction mixture was extracted with CH_2Cl_2, washed with brine and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: *n*-hexane/ethyl acetate = 70/30) to afford the title product (6.7 g, 87% yield) as a yellow solid.

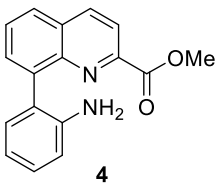


Methyl 8-bromoquinoline-2-carboxylate (3). ^{1}H NMR (500 MHz, $CDCl_3$) **δ** 8.32 (d, *J* = 7.5, 1H), 8.26 (d, *J* = 7.5 Hz, 1H), 8.14 (dd, *J* = 6.2, 1.2, 1H), 7.86 (dd, *J* = 7.0, 1.2 Hz, 1H), 7.51 (dd, *J* = 7.6, 7.6 Hz, 1H), 4.09 (s, 3H). The spectroscopic data is in agreement with that previously reported.[4]

2-5. Synthesis of methyl 8-(2-aminophenyl)quinoline-2-carboxylate (**4**)

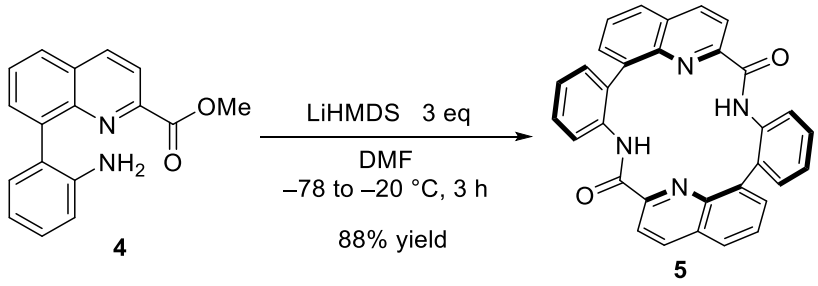


To a two-necked flask were added methyl 8-bromoquinoline-2-carboxylate **3** (6.5 g, 24.4 mmol), 2-aminophenyl boronic acid (5.0 g, 36.6 mmol, 1.5 eq), $PdCl_2(PPh_3)_2$ (343 mg, 0.49 mmol, 2 mol%), KF (5.6 g, 97.6 mmol, 4.0 eq), and DMF/MeOH (2/1, 200 mL) under N_2 atmosphere and the resulting mixture was stirred at 70 ˚C for 21 h. After the starting material was consumed, NH_4Cl (sat.) was added to quench the reaction. The reaction mixture was extracted with ethyl acetate for 3 times, washed with brine and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: *n*-hexane/ethyl acetate = 80/20 to 60/40) to afford the title product (4.9 g, 72% yield) as a yellow solid.

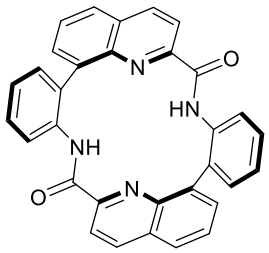


Methyl 8-(2-aminophenyl)quinoline-2-carboxylate (4). m.p. 135 ˚C. **IR** (film): 3853, 3649, 3445, 3362, 3022, 2954, 2927, 2360, 1947, 1719, 1284, 1127, 750 cm^{-1}. **^{1}H NMR** (600 MHz, $CDCl_3$) **δ** 8.24 (d, *J* = 8.5 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.77 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.70 (dd, *J* = 7.1, 1.5 Hz, 1H), 7.60 (dd, *J* = 8.1, 7.2 Hz, 1H), 7.18–7.14 (m, 2H), 6.82 (m, 1H), 6.78 (dd, *J* = 8.4, 1.2 Hz, 1H), 4.06 (br, 2H), 3.84 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) **δ** 165.79, 147.54, 145.37, 145.17, 141.00, 137.98, 132.91, 132.41, 129.45, 128.81, 128.78, 127.37, 126.62, 120.71, 118.96, 117.26, 52.76. **HRMS** (ESI) *m/z* calcd for $C_{17}H_{15}O_2N_2$ $[M+H]^+$: 279.1134, found 279.1135.

2-6. Synthesis of cyclic diamide (**5**)



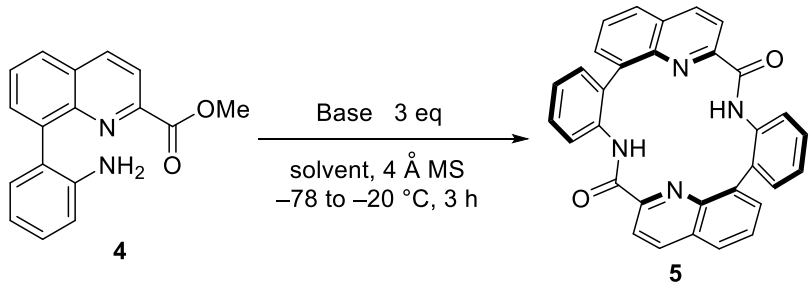
To a three-necked flask were added methyl 8-(2-aminophenyl) quinoline-2-carboxylate **4** (112 mg, 0.40 mmol), DMF (120 mL) under N_2 atmosphere. Then LiHMDS (1.2 mL, 1.2 mmol, 3.0 eq) was added at –78 ˚C and stirred for 2 h. After the starting material was consumed, NH_4Cl (sat.) was added to quench the reaction, and the reaction mixture was extracted with CH_2Cl_2 for 3 times. The solvent was azeotroped with toluene under the reduced pressure. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: toluene/ethyl acetate = 85/15 to 70/30) to afford the title product (86.7 mg, 88% yield) as a white solid.



5

3,7-Diaza-1(8,2),5(2,8)-diquinolina-2,6(1,2)-dibenzenacyclooctaphane-4,8-dione (5). m.p. >300 ˚C. **IR** (film): 3227, 3079, 3058, 1679, 1515, 1438, 770 cm^{-1}. **^{1}H NMR** (500 MHz, $CDCl_3$) **δ** 11.08 (s, 2H), 8.26 (d, *J* = 8.5 Hz, 2H), 7.93–7.86 (m, 6H), 7.83 (dd, *J* = 7.3, 1.5 Hz, 2H), 7.71 (dd, *J* = 7.9, 7.5 Hz, 2H), 7.58–7.54 (m, 2H), 7.39–7.33 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) **δ** 165.29, 153.42, 144.13, 139.39, 139.00, 135.17, 134.93, 134.66, 133.62, 129.26, 128.95, 128.45, 128.16, 126.35, 126.17, 120.08. **HRMS** (ESI) *m/z* calcd for $C_{32}H_{20}O_2N_4Na$ $[M+Na]^+$: 515.1484, found 515.1481.

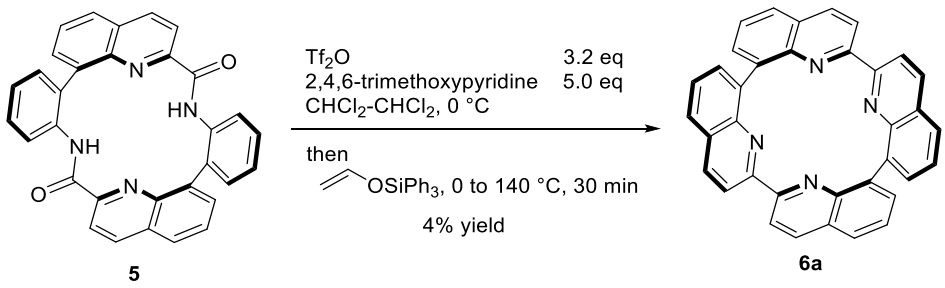
Optimized conditions for the synthesis of **5**.



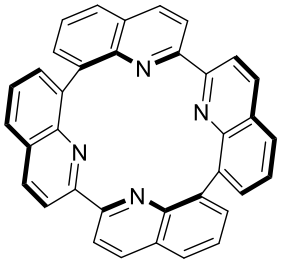
Entry	Base	Solvent	Conc. (mM)	Yield of **5** (%)[a]
1[b]	NaHMDS	THF	10	4
2[b]	NaHMDS	toluene	10	5
3[b]	NaHMDS	DMF	10	21
4	NaHMDS	DMF	25	60
5	NaHMDS	DMF	50	30
6	NaHMDS	DMF	100	40
7	LiHMDS	DMF	100	60
8	LiHMDS	DMF	25	60
9	LiHMDS	DMF	10	75
10	LiHMDS	DMF	3.3	88

[a]Isolated yields. All reactions were performed on 0.05 mmol scale.[b]0.072 mmol scale, in the absence of 4 Å molecular sieves.

2-7. Synthesis of *iso*-TEtraQuinoline (*i*-TEQ) **6a**



To a sealed tube were added cyclic diamide **5** (26.9 mg, 0.06 mmol), 2,4,6-trimethoxypyridine (50.0 mg, 0.30 mmol, 5.0 eq) and tetrachloroethane (1.5 mL) under N_2. Tf_2O (31.0 μL, 0.19 mmol, 3.2 eq) was added at 0 ˚C dropwise, and the resulting mixture was stirred for 5 min at 0 ˚C. After adding triphenyl(vinyloxy)silane (90.7 mg, 0.30 mmol, 5 eq), the resulting mixture was stirred at 140 ˚C for 30 min. Et_3N was added to quench the reaction, and the mixture was filtered through a long pad of basic Al_2O_3 (eluent: CH_2Cl_2). The filtrate was concentrated, and the resulting residue was filtered again through a pad of silica gel (eluent: *n*-hexane/ethyl acetate = 1/1). Volatiles were evaporated under the reduced pressure and the resulting residue was washed by methanol for 4 times (centrifuged to remove the solvent by decanting or pipetting) to afford the title product (1.2 mg, 4% yield) as a white solid.



1,23:8,10:11,13:20,22-Tetraethenotetrabenzo[*e*,*g*,*m*,*o*][1,4,9,12]tetraazacyclohexadecine (6a). m.p. >300 ˚C. **IR** (film): 3038, 2954, 2918, 2844, 1588, 1438, 1389, 1314 cm^{-1}. **^{1}H NMR** (500 MHz, $CDCl_3$) **δ** 8.04 (dd, *J* = 7.0, 1.4 Hz, 4H), 7.91 (d, *J* = 8.4 Hz, 4H), 7.82 (dd, *J* = 8.2, 1.3 Hz, 4H), 7.66 (dd, *J* = 8.1, 7.1 Hz, 4H), 7.06 (d, *J* = 8.3 Hz, 4H). **^{13}C NMR** (151 MHz, $CDCl_3$) **δ** 157.89, 146.45, 139.84, 135.15, 129.45, 127.49, 126.66, 125.85, 119.51. **HRMS** (ESI) *m/z* calcd for $C_{36}H_{21}N_4$ $[M+H]^+$: 509.1766, found 509.1766.

Chiral resolution of ***i*-TEQ 6a** was performed with preparative CHIRALPAK IB N-5 column (ϕ 2 cm x 25 cm), *n*-hexane/CH_2Cl_2 = 50/50, flow rate 7.5 mL/min, detection at 254 nm. For (+)-**6a**, t_R = 12.25 min, $[\alpha]_D^{23}$ 69.9 (*c* 0.050, $CHCl_3$). For (–)-**6a**, t_R = 17.13 min, $[\alpha]_D^{23}$ –68.9 (*c* 0.050, $CHCl_3$).

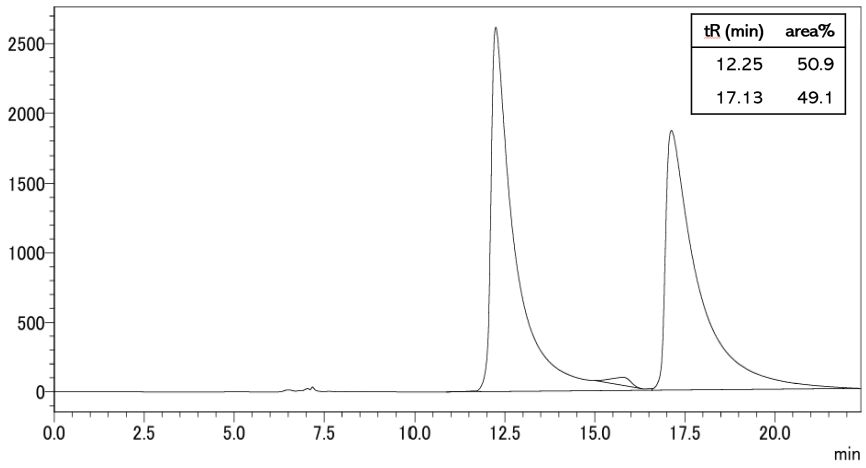
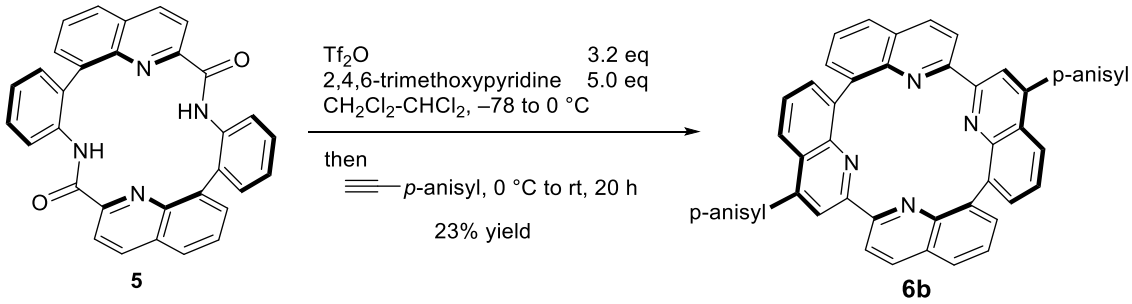
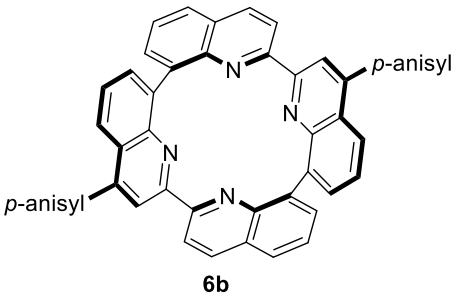


Figure S1. HPLC traces of racemic ***i*-TEQ 6a**.

2-8. Synthesis of ***i*-TEQ 6b**



To a sealed tube were added cyclic diamide **5** (148 mg, 0.10 mmol), 2,4,6-trimethoxypyridine (254 μL, 0.50 mmol, 5.0 eq) and dichloroethane (1.5 mL) under N_2. Tf_2O (213 μL, 1.3 mmol, 3.2 eq) was added at –78 ˚C dropwise, and the resulting mixture was stirred for 5 min at 0 ˚C. After adding 4-ethynylanisole (132 mg, 1.0 mmol, 10 eq), the resulting mixture was stirred at room temperature for 20 h. Et_3N was added to quench the reaction, and the mixture was filtered through a long pad of basic Al_2O_3 (eluent: CH_2Cl_2). The filtrate was concentrated, and the resulting residue was filtered through a pad of silica gel (eluent: hexane/ethyl acetate = 1/1). Volatiles were evaporated under reduced pressure and the resulting residue was washed by Et_2O for 4 times (centrifuged to remove the solvent by decanting or pipetting) to afford the title product (50.2 mg, 23% yield) as a white solid.



26,29-Bis(4-methoxyphenyl)-1,23:8,10:11,13:20,22-tetraethenotetrabenzo [*e*,*g*,*m*,*o*][1,4,9,12]tetraazacyclohexadecine (6b). m.p. >300 ˚C. **IR** (film): 3042, 3000, 2953, 2932, 2901, 2831, 1605, 1490, 1245 cm^{-1}. **^{1}H NMR** (500 MHz, $CDCl_3$) **δ** 8.06 (dd, *J* = 7.0, 1.4 Hz, 2H), 8.02 (dd, *J* = 7.0, 1.4 Hz, 2H), 7.94 (dd, *J* = 8.5, 1.3 Hz, 2H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.80 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.66 (dd, *J* = 8.1, 7.1 Hz, 2H), 7.58 (dd, *J* = 8.5, 7.0 Hz, 2H), 7.30–7.27 (m, 4H), 7.10 (d, *J* = 8.3 Hz, 2H), 7.03 (s, 2H), 6.95 (d, *J* = 8.7 Hz, 4H), 3.86 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) **δ** 159.43, 157.80, 157.32, 147.27, 147.06, 146.50, 140.25, 139.98, 135.17, 131.09, 130.94, 129.29, 127.42, 126.68, 125.82, 125.64, 125.59, 125.41, 119.50, 119.44, 113.68, 55.35. one carbon was overlapped. **HRMS** (ESI) *m/z* calcd for $C_{48}H_{29}N_4O_2$ $[M+H]^+$: 721.2604, found 721.2598.

Chiral resolution of ***i*-TEQ 6b** was performed with preparative CHIRALPAK IB N-5 column (ϕ 2 cm x 25 cm), *n*-hexane/CH_2Cl_2 = 30/70, flow rate 7.5 mL/min, detection at 254 nm. For (–)-**6b**, t_R = 4.82 min, $[\alpha]_D^{23}$ –52.2 (*c* 0.050, $CHCl_3$). For (+)-**6b**, t_R = 7.15 min, $[\alpha]_D^{23}$ 52.1 (*c* 0.050, $CHCl_3$).

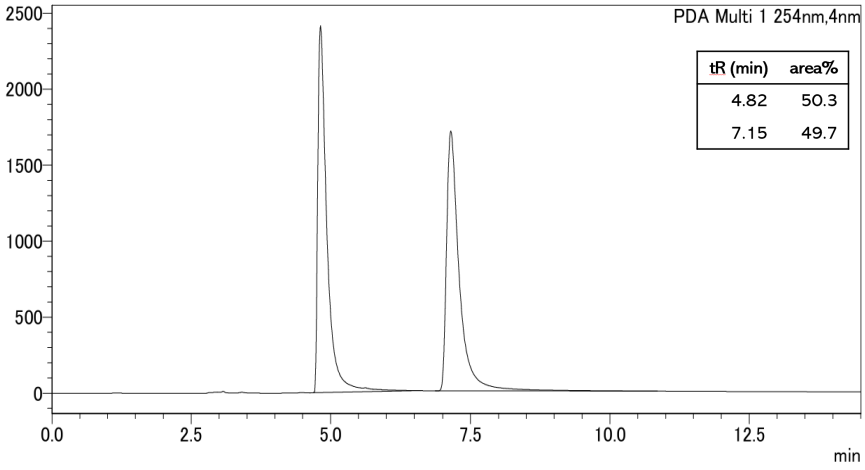
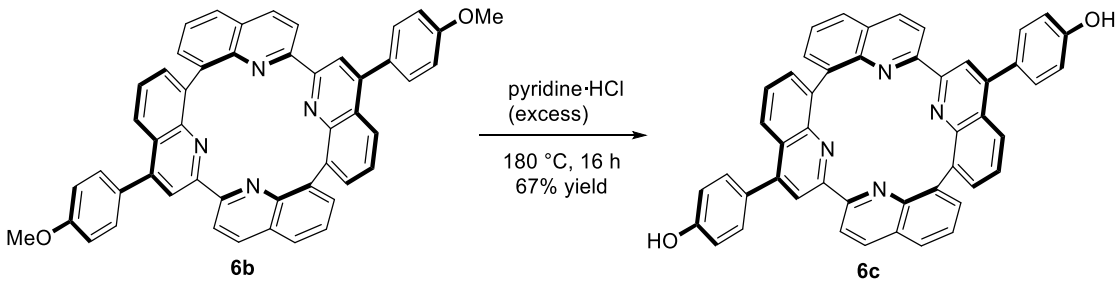
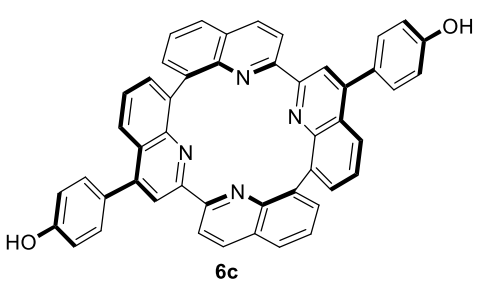


Figure S2. HPLC traces of racemic ***i*-TEQ 6b**.

2-9. Synthesis of ***i*-TEQ 6c**

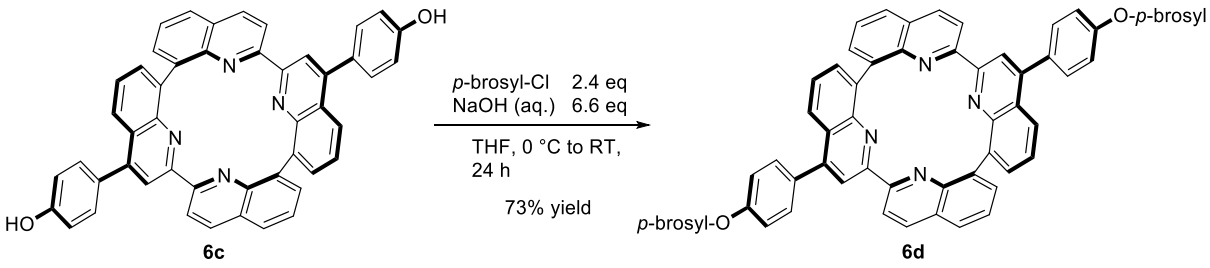


To a sealed tube were added ***i*-TEQ 6b** (50.0 mg, 0.069 mmol), pyridine HCl (3.2 g, 27.7 mmol, 400 eq) under N_2 and the resulting mixture was stirred at 180 ˚C for 16 h. After the starting material was consumed, 2 M NaOH was added to quench the reaction. The reaction mixture was extracted with CH_2Cl_2, washed with brine and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: CH_2Cl_2/methanol = 95/5) to afford the title product (32.0 mg, 67% yield) as a yellow solid.

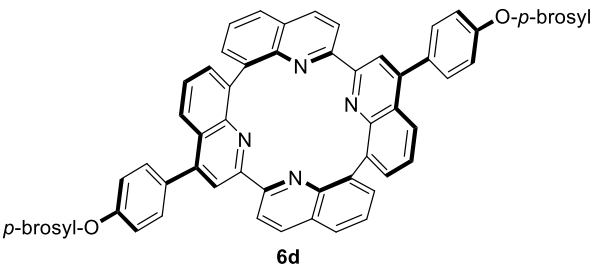


4,4'-(1,23:8,10:11,13:20,22-Tetraethenotetrabenzo[*e*,*g*,*m*,*o*][1,4,9,12] tetraazacyclohexadecine-26,29-diyl)diphenol (6c). **m.p.** >300 ˚C. **IR** (film): 3354, 3034, 2919, 2860, 2844, 2339, 1489, 1269, 767 cm^{-1}. **^{1}H NMR** (600 MHz, DMSO-d_6) **δ** 9.74 (s, 2H), 8.17 (d, *J* = 8.4 Hz, 2H), 8.0–7.96 (m, 6H), 7.94 (dd, *J* = 8.5, 1.3 Hz, 2H), 7.72 (dd, *J* = 8.1, 7.1 Hz, 2H), 7.66 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.25–7.20 (m, 4H), 7.17 (d, *J* = 8.3 Hz, 2H), 6.99 (s, 2H), 6.87–6.85 (m, 4H). **^{13}C NMR** (126 MHz, DMSO-d_6) **δ** 157.85, 157.74, 157.45, 147.21, 146.24, 145.44, 139.94, 139.83, 135.90, 130.83, 130.79, 130.65, 128.07, 128.03, 126.56, 126.25, 125.51, 124.93, 119.63, 119.03, 115.44. one carbon was overlapped. **HRMS** (ESI) *m/z* calcd for $C_{50}H_{33}N_4O_2$ $[M+H]^+$: 693.2291, found 693.2296.

2-10. Synthesis of ***i*-TEQ 6d**



To a sealed tube were added ***i*-TEQ 6c** (20.0 mg, 0.028 mmol), NaOH (7.4 mg, 0.185 mmol, 6.6 eq, 15% in water), and THF (1.0 mL) under N_2. 4-Brosyl chloride (17.7 mg, 0.070 mmol, 2.4 eq dissolved in THF) was added at 0 ˚C and the resulting mixture was stirred for 24 h at room temperature. After the starting material was consumed, the reaction mixture was extracted with ethyl acetate, washed with brine and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: CH_2Cl_2/methanol = 70/30) to afford the title product (23.1 mg, 73% yield) as a white solid.

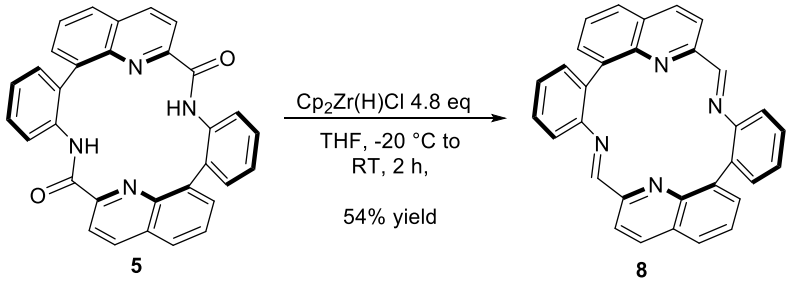


6d

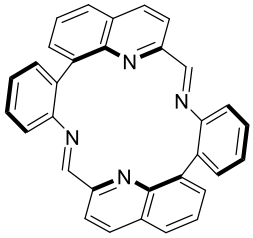
1,23:8,10:11,13:20,22-Tetraethenotetrabenzo[*e*,*g*,*m*,*o*][1,4,9,12] tetraazacyclohexadecine-26,29-diylbis(4,1-phenylene) bis(4-bromobenzenesulfonate) (6d). **m.p.** >300 ˚C. **IR** (film): 3038, 2954, 2922, 2844, 2340, 1574, 1488, 1373, 751 cm^{-1}. **^{1}H NMR** (600 MHz, DMSO-d_6) **δ** 8.20 (d, *J* = 8.4 Hz, 2H), 8.01 (dd, *J* = 9.9, 3.0 Hz, 6H), 7.85 (d, *J* = 8.7 Hz, 4H), 7.80 (d, *J* = 8.7 Hz, 4H), 7.76–7.70 (m, 4H), 7.70–7.65 (m, 2H), 7.36 (d, *J* = 8.4 Hz, 4H), 7.16 (dd, *J* = 13.0, 8.5 Hz, 6H), 7.02 (s, 2H). **^{13}C NMR** (151 MHz, DMSO-d_6) **δ** 157.58, 157.31, 148.81, 146.00, 145.57, 145.37, 139.97, 139.51, 136.80, 136.01, 133.43, 132.99, 131.21, 130.92, 130.87, 130.18, 129.39, 128.15, 126.82, 126.59, 126.34, 124.93, 124.35, 122.31, 119.62, 119.44. **HRMS** (ESI) *m/z* calcd for $C_{60}H_{35}O_6N_4Br_2S_2$ $[M+H]^+$: 1131.0344, found 1131.0273.

3. Derivatization cyclic diamide 5

3-1. Synthesis of 8



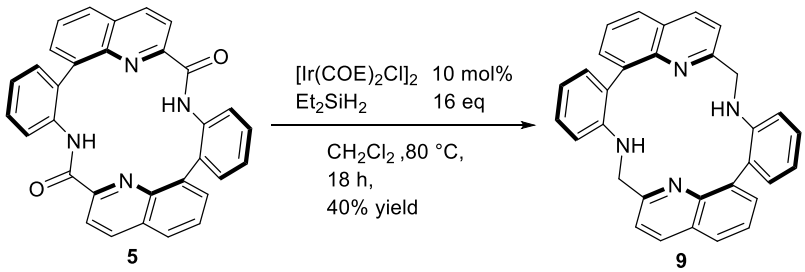
To a sealed tube were added $Cp_2Zr(H)Cl$ (49.5 mg, 0.192 mmol, 4.8 eq), and THF (0.5 mL) under N_2. The mixture was stirred for 5 min at –20 ˚C. Cyclic diamide **5** (19.7 mg, 0.04 mmol) in THF (0.5 mL) was added dropwise and heated to room temperature. After the starting material was consumed, hexane was added to the reaction mixture and then, filtered through celite. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: *n*-hexane/ethyl acetate = 80/20) to afford the title product (10.0 mg, 54% yield) as a white solid.



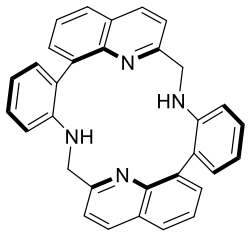
8

(3*Z*,7*Z*)-3,7-Diaza-1(8,2),5(2,8)-diquinolina-2,6(1,2)-dibenzenacyclooctaphane-3,7-diene (8). **m.p.** >300 ˚C. **IR** (film): 2949, 2912, 2844, 1629, 1498, 1430, 1328, 771 cm^{-1}. **^{1}H NMR** (600 MHz, $CDCl_3$) **δ** 8.65 (d, *J* = 0.6 Hz, 2H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.88 (dd, *J* = 7.1, 1.5 Hz, 2H), 7.77 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.65 (dd, *J* = 8.1, 7.2 Hz, 2H), 7.59 (dd, *J* = 7.5, 1.4 Hz, 2H), 7.54–7.47 (m, 4H), 7.40 (td, *J* = 7.6, 1.2 Hz, 2H), 6.94 (dd, *J* = 7.7, 1.1 Hz, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) **δ** 166.99, 154.14, 153.88, 144.69, 140.01, 136.47, 132.27, 131.19, 131.10, 129.15, 128.61, 128.02, 127.35, 125.49, 118.13, 117.16. **HRMS** (ESI) *m/z* calcd for $C_{32}H_{21}N_4$ $[M+H]^+$: 461.1766, found 461.1763.

3-2. Synthesis of 9



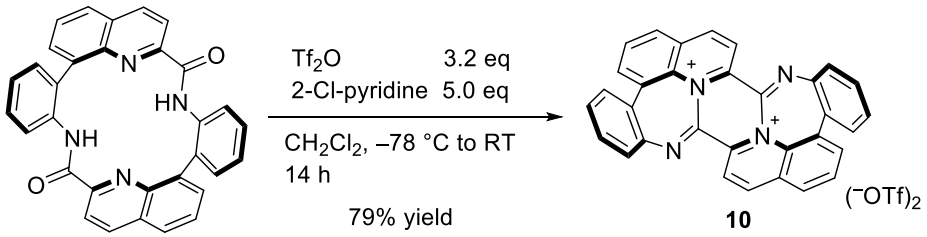
To a sealed tube were added $[Ir(COE)_2Cl]_2$ (9.0 mg, 0.010 mmol, 10 mol%), and Et_2SiH_2 (0.21 mL, 1.6 mmol, 16 eq). The reaction mixture was stirred for 5 min at room temperature. Cyclic diamide **5** (49.3 mg, 0.10 mmol) in CH_2Cl_2 (1.0 mL) was added and the reaction mixture was stirred for 24 h at –20 ˚C. After the starting material was consumed, 1 M HCl (in dioxane) was added to the reaction mixture at room temperature, and white precipitant formed immediately. After stirring at room temperature for 1 h, Na_2CO_3 aq was added and the reaction mixture was extracted with CH_2Cl_2 3 times, washed with brine and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: CH_2Cl_2/methanol = 70/30) to afford the title product (17.2 mg, 40% yield) as a yellow solid.



9

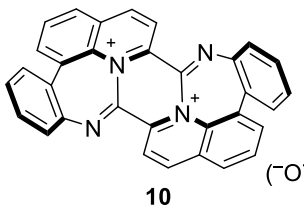
3,7-Diaza-1(8,2),5(2,8)-diquinolina-2,6(1,2)-dibenzenacyclooctaphane (9). m.p. >300 ˚C. **IR** (film): 3311, 3276, 2956, 2907, 2857, 1595, 1499, 1061, 1006, 741 cm^{-1}. **^{1}H NMR** (600 MHz, $CDCl_3$) **δ** 8.04 (d, *J* = 8.4 Hz, 2H), 7.74 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.71 (dd, *J* = 7.2, 1.4 Hz, 2H), 7.58 (dd, *J* = 7.9, 7.4 Hz, 2H), 7.43 (td, *J* = 8.0, 1.6 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.25 (dd, *J* = 9.6, 1.6 Hz, 2H), 7.04 (d, *J* = 7.9 Hz, 2H), 6.98 (m, 2H), 5.21 (d, *J* = 10.7 Hz, 2H), 4.53 (t, *J* = 10.1 Hz, 2H), 4.41 (d, *J* = 9.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) **δ** 158.97, 147.52, 144.92, 140.11, 137.78, 132.73, 132.39, 129.12, 128.42, 127.59, 127.24, 127.05, 122.37, 118.96, 111.89, 52.78. **HRMS** (ESI) *m/z* calcd for $C_{32}H_{25}N_4$ $[M+H]^+$: 465.2079, found 465.2087.

3-3. Synthesis of **10**



5 **10**

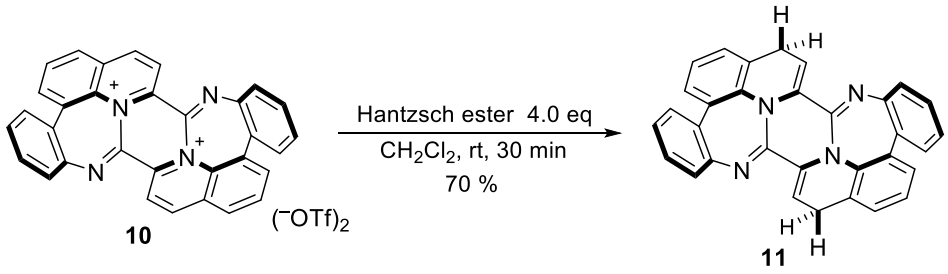
To a sealed tube were added cyclic diamide **5** (200 mg, 0.41 mmol), 2-chloropyridine (170 µL, 2.0 mmol, 5.0 eq), and CH_2Cl_2 (15 mL) under N_2. Tf_2O (213 µL, 1.3 mmol, 3.2 eq) was added at –78 ˚C, and the resulting mixture was stirred for 15 min at 0 °C. Then the resulting mixture was stirred at room temperature for 14 h. After the starting material was consumed, the resulting residue was washed by CH_2Cl_2 for 3 times (centrifuged to remove the solvent by decanting or pipetting) to afford title product (245 mg, 79% yield) as a reddish brown solid.



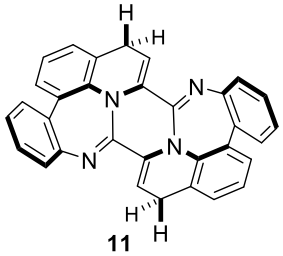
10

Dimeric benzo[4,5][1,3]diazepino[6,7,1-*ij*]quinolin-7-ium trifluoromethanesulfonate (10). m.p. >273 ˚C (decomposed). **IR** (film): 3128, 3081, 2918, 2854, 1273, 1252, 1224, 1156, 1028 cm^{-1}. **^{1}H NMR** (600 MHz, CD_3CN) **δ** 9.31 (d, *J* = 8.6 Hz, 2H), 8.62 (d, *J* = 8.5 Hz, 2H), 8.60 (dd, *J* = 7.7, 1.4 Hz, 2H), 8.39 (dd, *J* = 8.1, 1.2 Hz, 2H), 8.23 (t, *J* = 7.8 Hz, 2H), 7.80–7.75 (m, 2H), 7.72–7.68 (m, 2H), 7.63 (dd, *J* = 7.8, 1.3 Hz, 2H), 7.57 (dd, *J* = 8.0, 1.3 Hz, 2H). **^{13}C NMR** (151 MHz, CD_3CN) **δ** 153.60, 146.39, 144.04, 141.29, 139.97, 135.79, 135.50, 134.06, 133.93, 133.35, 132.68, 132.61, 132.56, 131.61, 131.23, 125.09, 122.00 (q, *J* = 321.6 Hz). **^{19}F NMR** (471 MHz, $CDCl_3$) **δ** –79.31.

3-4. Synthesis of **11**



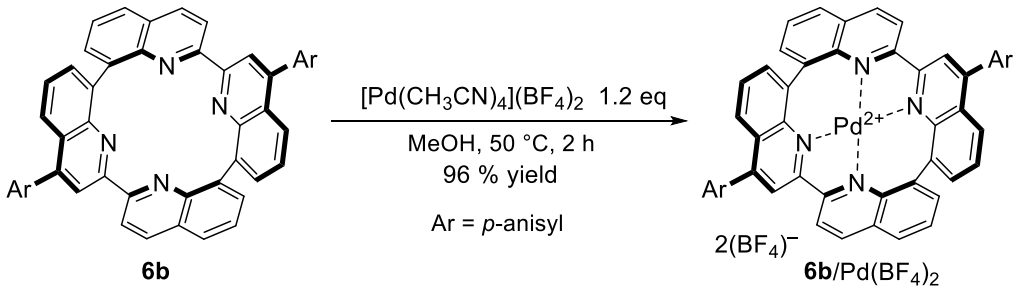
To a sealed tube were added **10** (75.7 mg, 0.10 mmol), Hantzsch ester (101 mg, 0.40 mmol, 4.0 eq), CH_2Cl_2 (15 mL) under N_2 and the resulting mixture was stirred at room temperature for 30 min. After the starting material was consumed, the reaction mixture was evaporated under the reduced pressure. The residue was purified by column chromatography on silica gel (Biotage RediSep prepacked column, eluent: *n*-hexane/ethyl acetate = 60/40) to afford the title product (32.0 mg, 72% yield) as a light yellow solid.



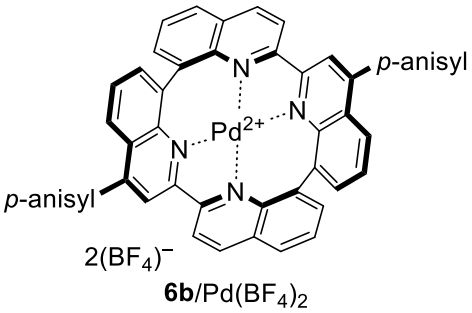
Dimeric 4*H*-benzo[4,5][1,3]diazepino[6,7,1-*ij*]quinoline (11). m.p. >197 ˚C (decomposed). **IR** (film): 3062, 2980, 2926, 2889, 1737, 1645, 1239, 1222, 772, 753 cm^{-1}. **^{1}H NMR** (500 MHz, $CDCl_3$) **δ** 7.28–7.24 (m, 2H), 7.23–7.18 (m, 6H), 7.19–7.17 (m, 4H), 7.14–7.11 (m, 4H), 6.99–6.97 (m, 2H), 5.67 (d, *J* = 1.4 Hz, 2H), 3.72 (dd, *J* = 21.9, 3.1 Hz, 2H), 3.50 (dd, *J* = 22.0, 4.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) **δ** 154.43, 145.93, 142.96, 136.08, 135.92, 134.33, 130.54, 130.45, 129.34, 129.13, 128.71, 128.62, 126.69, 126.36, 123.94, 105.00, 26.45. **HRMS** (ESI) *m/z* calcd for $C_{32}H_{21}N_4$ $[M+H]^+$: 461.1766, found 461.1768.

4. Preparation of *i*-TEQ/Pd complex

4-1. Synthesis of **6b**/$Pd(BF_4)_2$.



To a sealed tube were added ***i*-TEQ 6b** (10.0 mg, 0.014 mmol), $[Pd(CH_3CN)_4](BF_4)_2$ (7.39 mg, 0.0166 mmol, 1.2 eq) and dried methanol (3 mL) under argon atmosphere. The mixture was stirred at 50 ˚C for 2 h. After the reaction was complete, the resulting mixture was filtered through celite for two times (eluent: methanol). The filtrate was evaporated under the reduced pressure, the title product was obtained the title product as a red solid (13.4 mg, 96% yield).



6b/$Pd(BF_4)_2$

26,29-Bis(4-methoxyphenyl)-1,23:8,10:11,13:20,22-tetraethenotetrabenzo [*e*,*g*,*m*,*o*][1,4,9,12]tetraazacyclohexadecine palladium (II) tetrafluoroborate (6b/$Pd(BF_4)_2$). m.p. >300 ˚C. **IR** (film): 3071, 3026, 3018, 2970, 2923, 2847, 1505, 1018 cm^{-1}. **^{1}H NMR** (600 MHz, $CDCl_3$) **δ** 9.08 (d, *J* = 8.5 Hz, 2H), 8.69 (d, *J* = 8.5 Hz, 2H), 8.38 (s, 2H), 8.33 (dd, *J* = 8.5, 1.2 Hz, 2H), 8.20 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.89–7.84 (m, 2H), 7.81–7.76 (m, 6H), 7.36 (dd, *J* = 7.2, 1.3 Hz, 2H), 7.29 (dd, *J* = 7.2, 1.2 Hz, 2H), 7.18 (d, *J* = 8.8 Hz, 4H), 3.93 (s, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) **δ** 162.46, 162.15, 161.01, 157.77, 146.95, 146.06, 145.49, 140.04, 139.81, 132.22, 132.05, 131.93, 130.59, 129.88, 129.69, 129.29, 129.26, 128.33, 126.83, 122.04, 121.74, 115.18, 55.64. **^{19}F NMR** (471 MHz, $CDCl_3$) **δ** –152.42. **HRMS** (ESI) *m/z* calcd for $C_{50}H_{32}N_4O_2Pd$ $[M]^{2+}$:826.1560, found 826.1574.

5. Racemization protocol

5-1. Racemization protocol of (–)-*i*-TEQ 6b

To a 1 mL vial was added (–)-**6b** solution (0.1 mL, 1.0 mg/mL in diphenyl ether) under argon, and the mixture was heated at 220 ˚C for 24 h. Then the mixture was cooled down, and CH_2Cl_2 (0.1 mL) was added to the mixture, and it was directly injected into the HPLC system to determine the enantiomer excess. CHIRALPAK IC column (*ϕ* 0.46 cm x 25 cm), *n*-hexane/ethyl acetate = 7/3, flow rate 1.0 mL/min, detection at 254 nm.

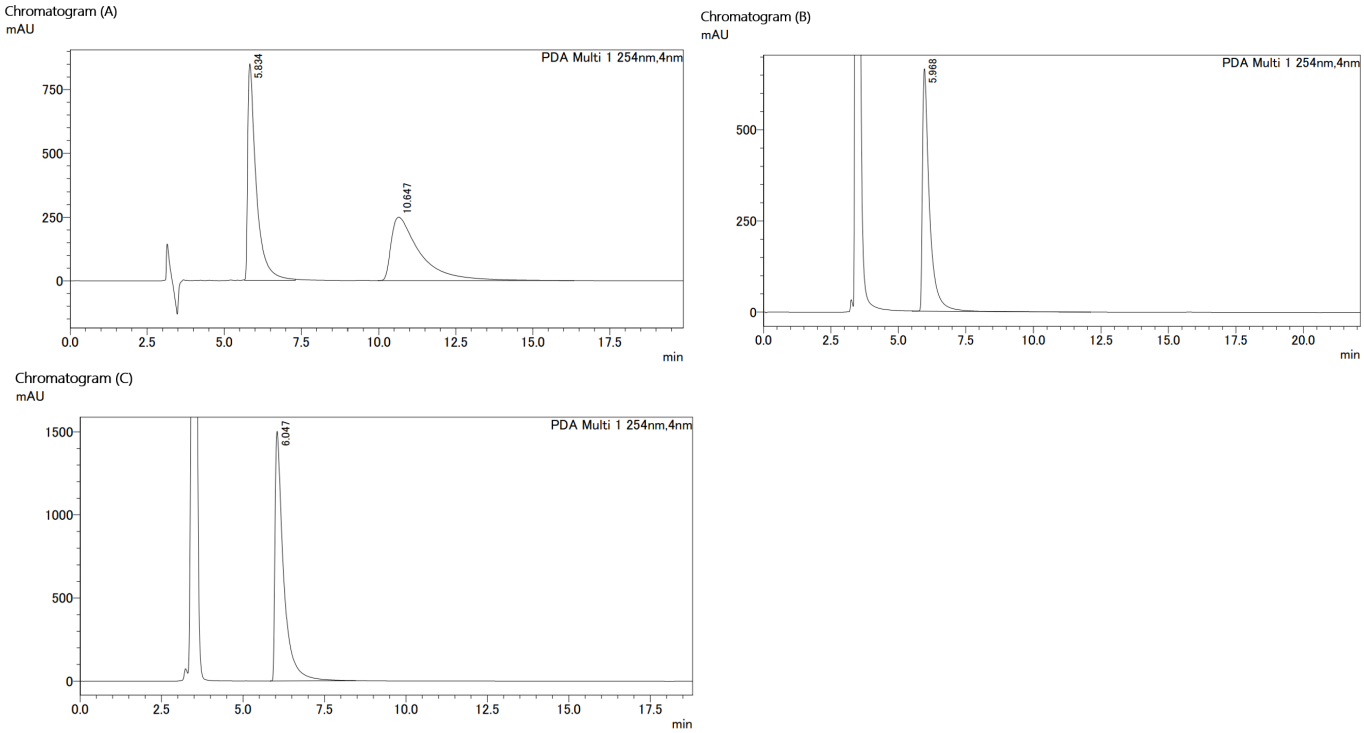


Figure S3. HPLC traces of *i*-TEQ 6b. (A) racemic. (B) enantiopure (–)-**6b** after heated at 140 ˚C for 56 h. (C) enantiopure (–)-**6b** after heated at 220 ˚C for 24 h.

5-2. Racemization protocol of (–)-*i*-TEQ 6b with metal salts

To a sealed tube were added (–)-**6b** (1.50 mg, 0.0021 mmol), $Pd(CH_3CN)_4(BF_4)_2$ (1.65 mg, 0.0021 mmol, 1.0 eq), and diphenyl ether (1.0 mL) under N_2, and the mixture was heated at 100 ˚C. Then 50 μL of the mixture was taken at 2, 4, 8,

20, 30 h. For each analysis, the sample was cooled down, and Na_2S was added to remove Pd salt. The mixture was filtered, then directly injected into the HPLC system to determine the enantiomer excess. CHIRALPAK IC column (ϕ0.46 cm x 25 cm), hexane/ethyl acetate = 70/30, flow rate 1.0 mL/min, detection at 254 nm.

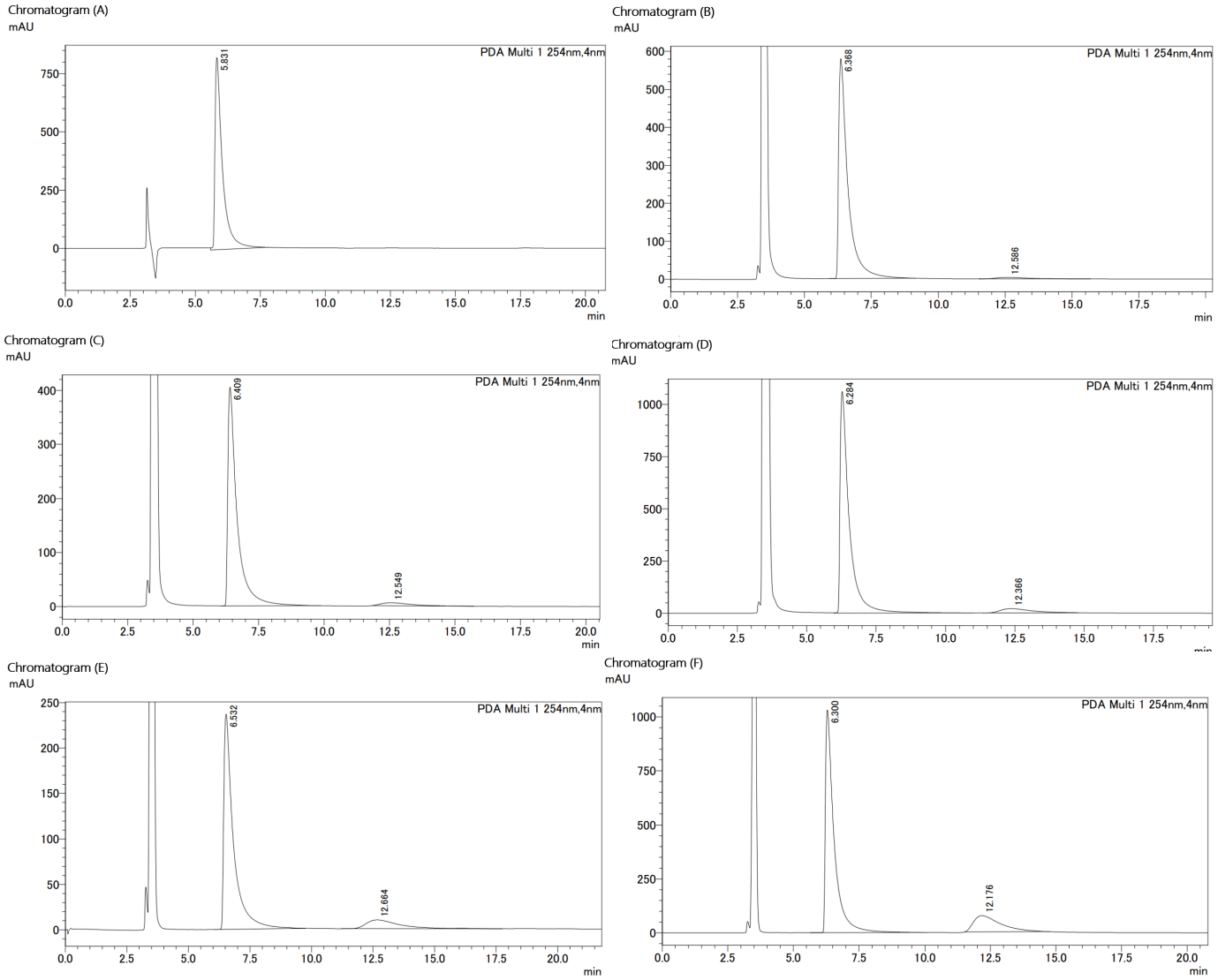


Figure S4. HPLC traces of (–)-**6b** + $[Pd(CH_3CN)_4](BF_4)_2$ before heating, and after heating at 100 ˚C for (A) 0 h, (B) 2 h, (C) 4 h, (D) 8 h, (E) 20 h, (F) 30 h.

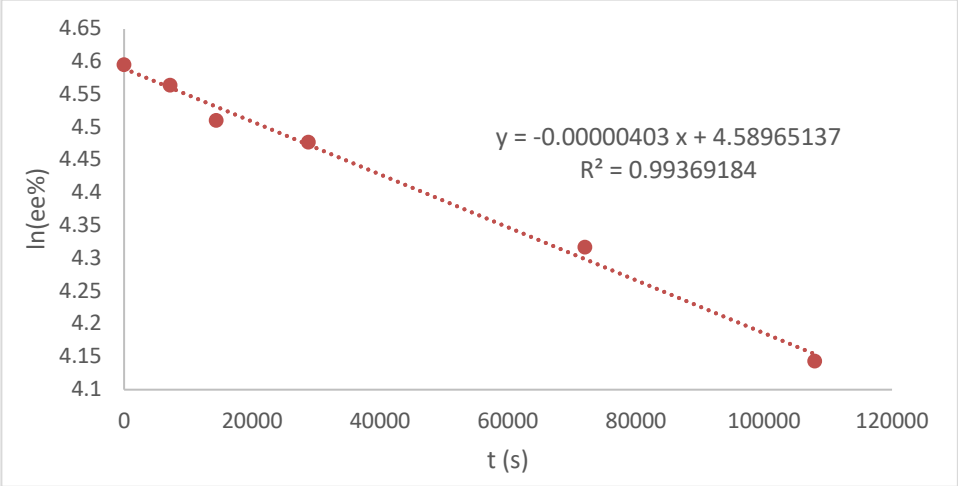


Figure S5. Plots of ln (ee%) vs time at 100 ˚C for (–)-**6b** + $[Pd(CH_3CN)_4](BF_4)_2$

With similar procedure, the racemization at 140 ˚C was also performed in the presence of 1 eq of $[Pd(CH_3CN)_4](BF_4)_2$. The sampling time was changed to 15, 30, 60, 90, 150 min for each analysis.

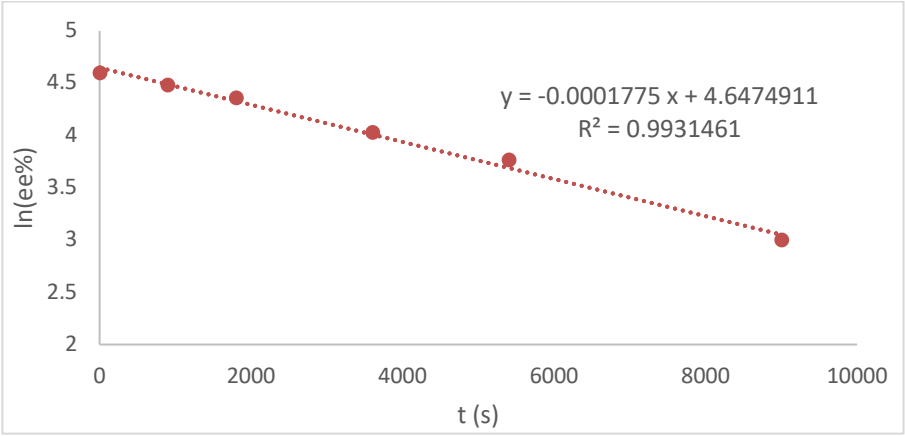


Figure S6. Plots of ln (ee%) vs time at for (–)-**6b** + $[Pd(CH_3CN)_4](BF_4)_2$

With similar procedure, the racemization at 140 ˚C was performed in the presence of 1 eq of $CuCl_2$. The sampling time was changed to 2, 4, 8, 20, 30 h for each analysis.

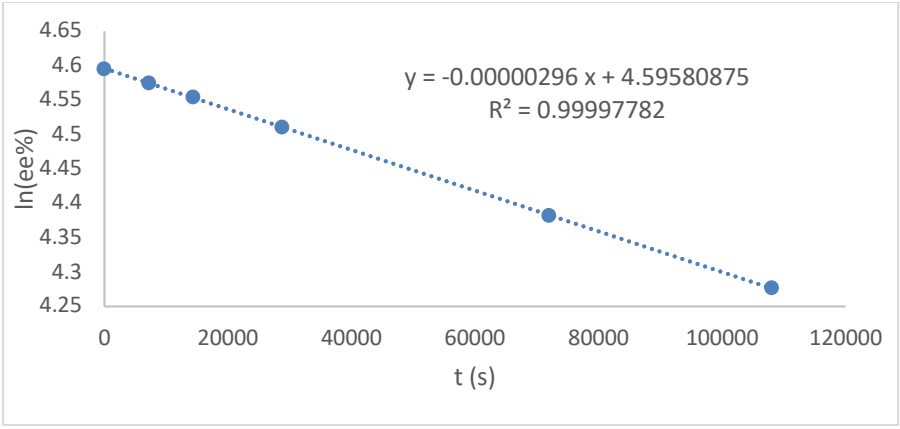


Figure S7. Plots of ln (ee%) vs time at 140 ˚C for (–)-**6b** + $CuCl_2$

With similar procedure, the racemization at 140 ˚C was performed in the presence of 1 eq of $CoCl_2$. The sampling time was changed to 8, 22, 32, 46, 56 h for each analysis.

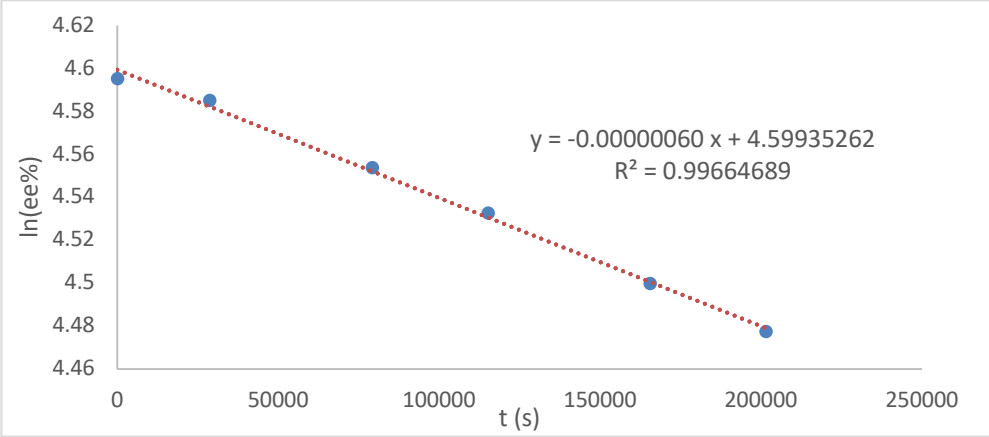


Figure S8. Plots of ln (ee%) vs time 140 ˚C for (–)-**6b** + $CoCl_2$

With similar procedure, the racemization at 160 ˚C was performed in the presence of 1 eq of TFA. The sampling time was changed to 8, 22, 32, 46, 56 h for each analysis.

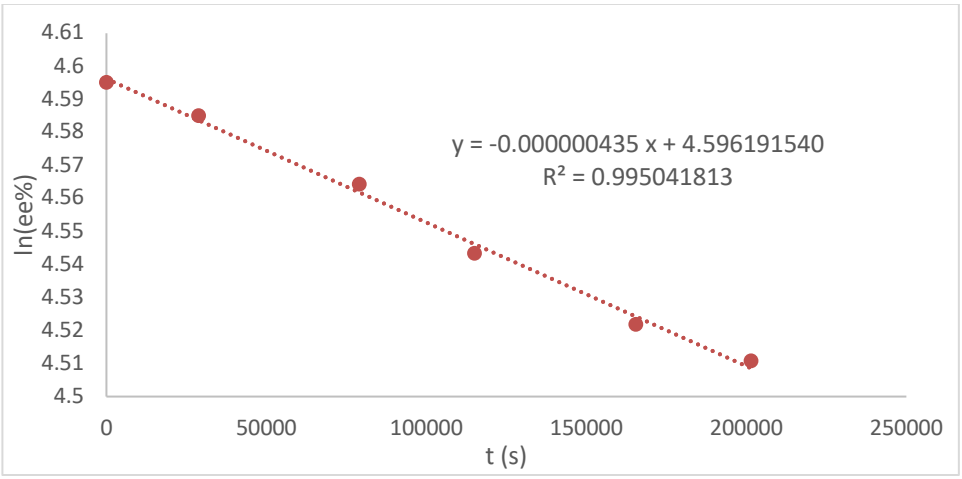


Figure S9. Plots of ln (ee%) vs time 160 ˚C (–)-**6b** + TFA

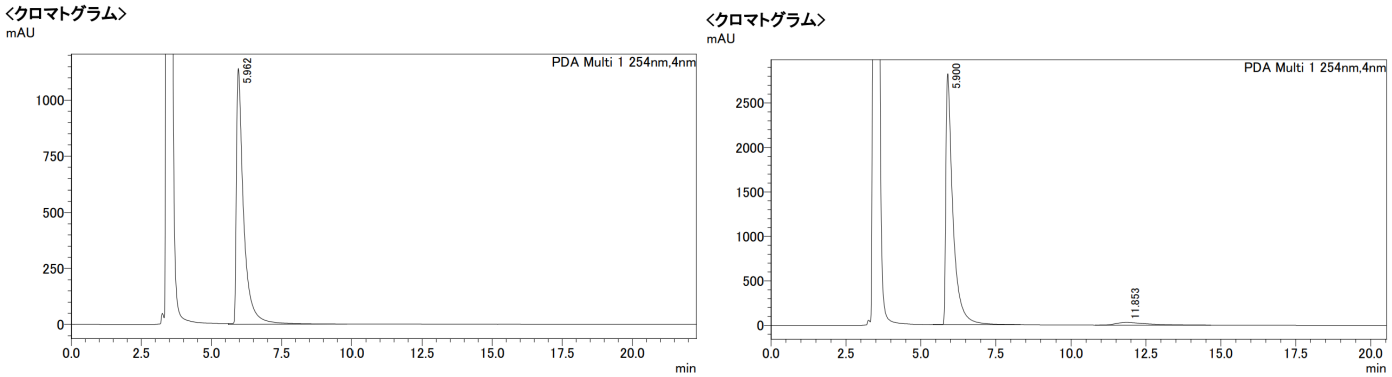


Figure S10. HPLC traces of (–)-**6b** + TFA after heating at 140 ˚C for 56 h, and after heating at 160 ˚C for 56 h in order.

5-3. Racemization protocol of (–)-**TEQ 7b** with $Pd(CH_3CN)_4(BF_4)_2$

To a sealed tube were added (–)-**TEQ 7b** (0.50 mg, 0.0007 mmol), $[Pd(CH_3CN)_4](BF_4)_2$ (0.55 mg, 0.0007 mmol, 1.0 eq), and diphenyl ether (1.0 mL) under N_2, and the mixture was heated at 140 ˚C for 24 h. Then the mixture was cooled down, and Na_2S was added to remove Pd salt. The mixture was filtered, purified by preparative thin layer chromatography (eluent: *n*-hexane/ethyl acetate = 1/3), and injected into the HPLC system to determine the enantiomer excess. CHIRALPAK IC column (ϕ 0.46 cm x 25 cm), ethyl acetate/dichloromethane/diethyl amine = 1/9/0.1, flow rate 1.0 mL/min, detection at 254 nm.

The enantiomeric excess of (–)-**TEQ 7b** was 88% on average over two measurements.

6. Inversion Barriers of *i*-TEQs

Table S1. Relative Gibbs free energy of ***i*-TEQs**, those transition states (TS), and intermediates (Int) calculated at the B3LYP-D3/6-31G(d,p)-SDD(Co, Cu, Pd) or B3LYP-D3/6-311+G(2d,p)-SDD(Co, Cu, Pd)/SMD(diethyl ether) level of theory. [a]Not calculated.

	B3LYP-D3 6-31G(d,p) –	B3LYP-D3 6-311+G(2d,p) SMD(Et_2O)
***i*-TEQ 6a**	62.0	58.0
***i*-TEQ 6a**•$1H^+$	47.5	50.8
***i*-TEQ 6a**•$2H^+$	44.5	46.3
***i*-TEQ 6a**•$4H^+$	62.9	–[a]
***i*-TEQ 6a**/Pd(II)	33.9	33.3
***i*-TEQ 6a**/Co(II)	32.7	30.6
***i*-TEQ 6a**/Cu(II)	36.8	34.4

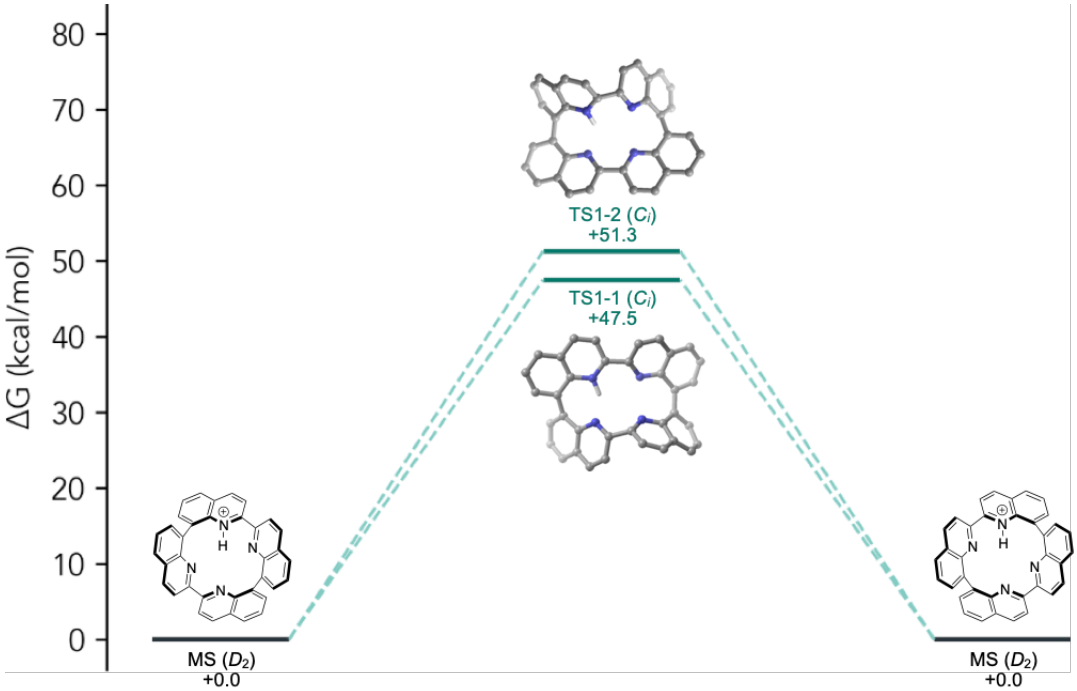


Figure S11. Inversion pathway of ***i*-TEQ 6a**•H^+ calculated at the B3LYP-D3/6-31G(d,p) level of theory.

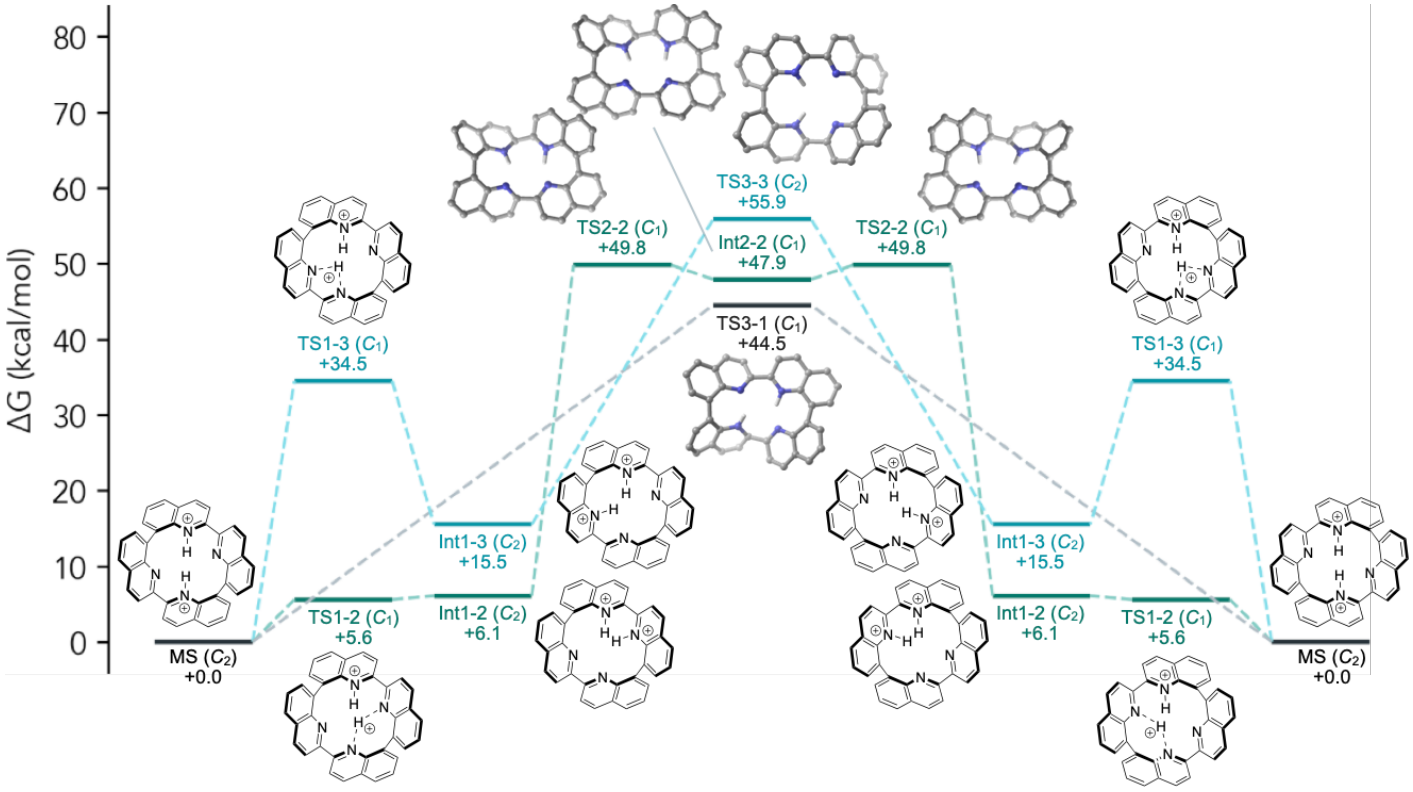


Figure S12. Inversion pathway of ***i*-TEQ 6a**•2H⁺ calculated at the B3LYP-D3/6-31G(d,p) level of theory.

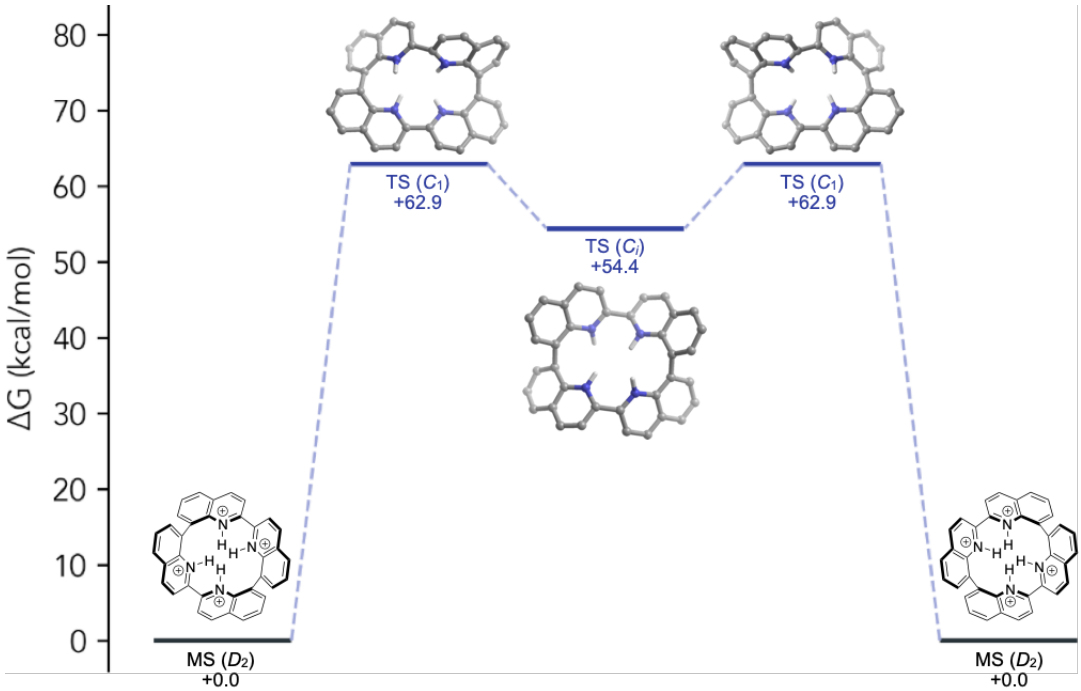


Figure S13. Inversion pathway of ***i*-TEQ 6a**•4H⁺ calculated at the B3LYP-D3/6-31G(d,p) level of theory.

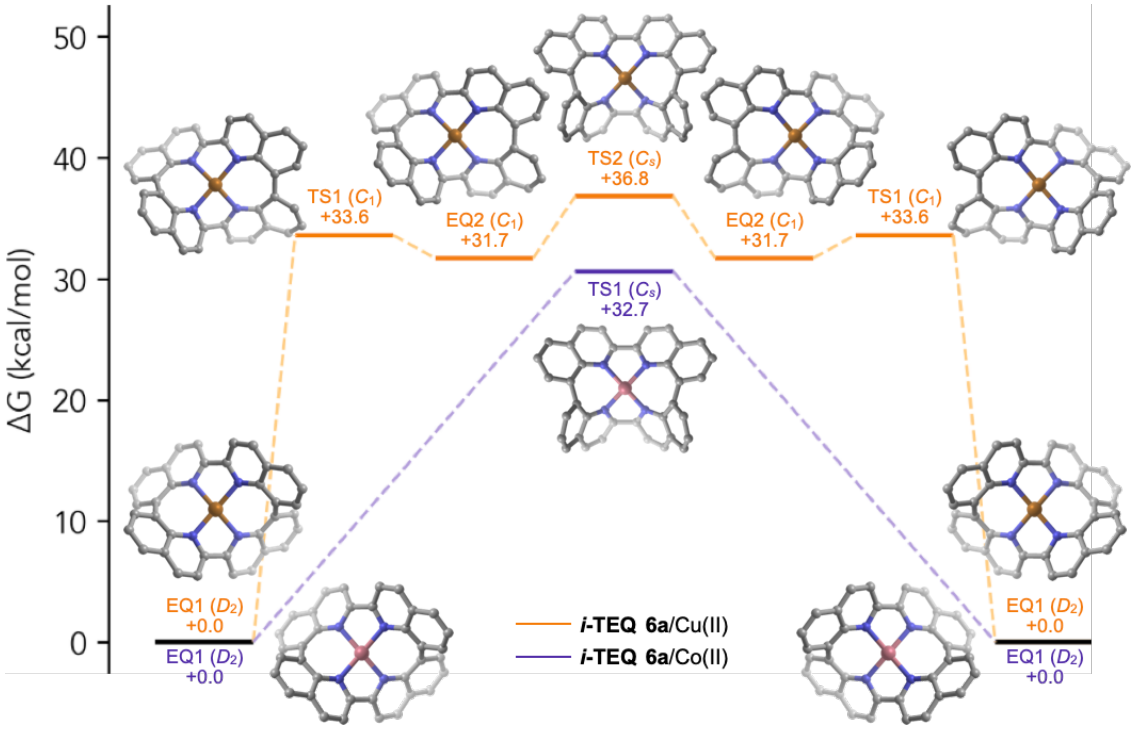


Figure S14. Inversion pathway of ***i*-TEQ 6a**/Co(II) and ***i*-TEQ 6a**/Cu(II) calculated at the B3LYP-D3/6-31G(d,p)-SDD(Co, Cu) level of theory.

Table S2. Single point calculations on the intermediates (Int) and transition states (TS) of ***i*-TEQ 6a**/Pd(II) calculated with B3LYP-D3 functionals, designated basis, solvation model density (SMD) model (diethyl ether), and SDD(Pd). Each structure was optimized at the B3LYP-D3/6-31G(d,p)-SDD(Pd) level of theory. [a]Not calculated.

	B3LYP-D3 6-31G(d,p)	B3LYP-D3 6-31++G(d,p)	B3LYP-D3 6-311+G(2d,p)	B3LYP-D3 def2-TZVP	B3LYP-D3 def2-TZVPP	B3LYP-D3 may-cc-pVTZ	B3LYP-D3 def2-QZVP	B3LYP-D3 aug-cc-pVTZ
EQ1 (D_2)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1 (C_1)	**33.1**	**33.1**	**32.7**	**32.5**	**32.4**	**32.4**	**32.4**	**32.4**
Int (C_1)	30.0	30.1	29.5	29.7	29.7	29.6	29.7	–[a]
TS2 (C_s)	31.3	31.2	30.8	30.8	30.8	30.7	30.8	–[a]

Table S3. Relative Gibbs free energy of ***i*-TEQ 6a**/Pd(II), transition states (TS), and intermediates (Int) calculated with designated functionals, 6-31G(d,p) level of theory as basis, integral equation formalism polarizable continuum model (IEFPCM) model (diethyl ether), and SDD(Pd).

	B3LYP-D3 6-31G(d,p)	B3LYP-D3BJ 6-31G(d,p)	CAM-B3LYP-D3 6-31G(d,p)	**ω**B97XD 6-31G(d,p)	M06-2X 6-31G(d,p)
EQ1 (D_2)	0.0	0.0	0.0	0.0	0.0
TS1 (C_1)	**35.9**	**35.0**	**36.9**	**37.2**	**37.0**
Int (C_1)	31.6	30.9	32.2	32.3	30.5
TS2 (C_s)	32.6	31.9	33.8	33.8	33.3

7. Physical properties

7-1. Absorption spectra of ***i*-TEQ 6b** and **6b** + 4 equiv TFA .

All spectra were recorded using 2.0×10^{-5} mol/L solution in CH_2Cl_2.

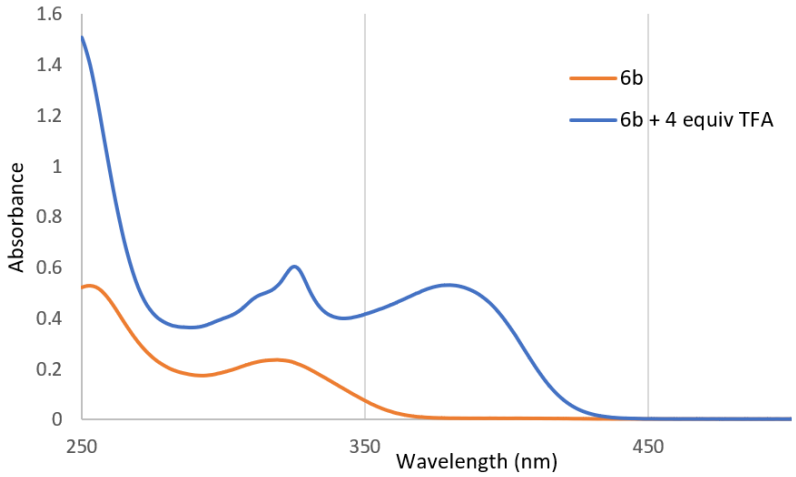


Figure S15. Absorption spectra of ***i*-TEQ 6b** with or without 4 equiv TFA in CH_2Cl_2.

7-2. CD spectra of non-substituted ***i*-TEQ 6a.**

Both spectra were recorded using 5.0×10^{-5} mol/L solution in CH_2Cl_2.

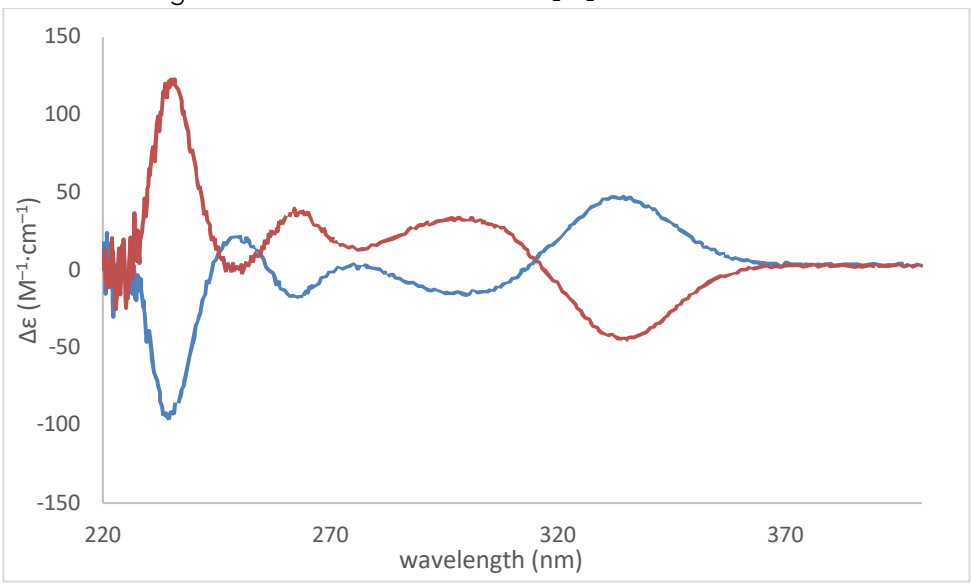


Figure S16. CD spectra of ***i*-TEQ 6a** in CH_2Cl_2.

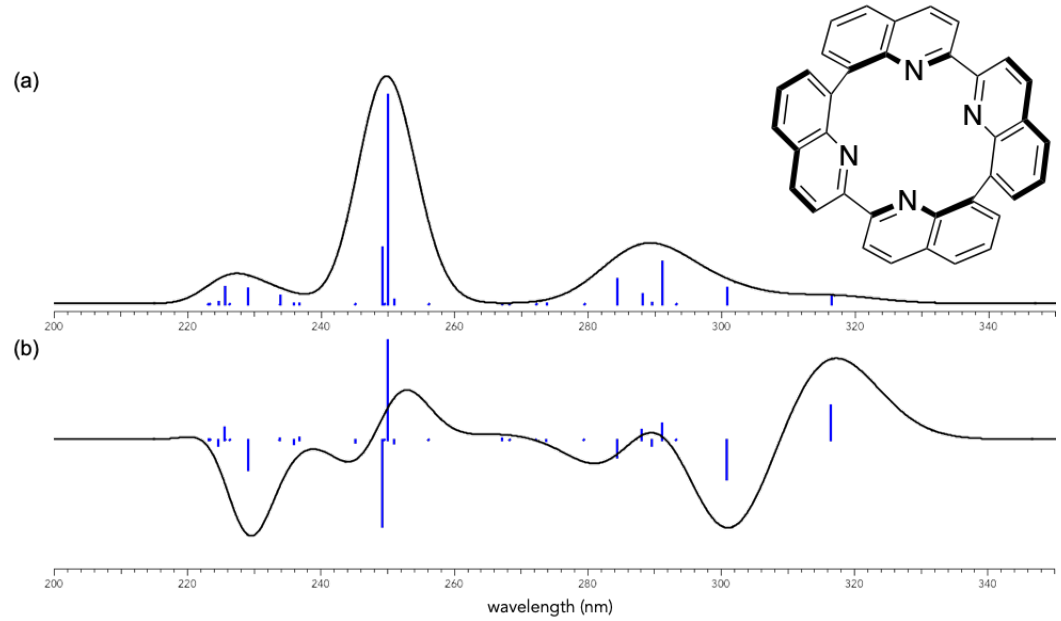


Figure S17. TD-DFT calculations on the (a) UV-Vis or (b) ECD spectra of (+)-***i*-TEQ 6a** at the CAM-B3LYP-D3/6-311+G(2d,p)/SMD(dichloromethane)//B3LYP-D3/6-31G(d,p) level of theory (NState = 30).

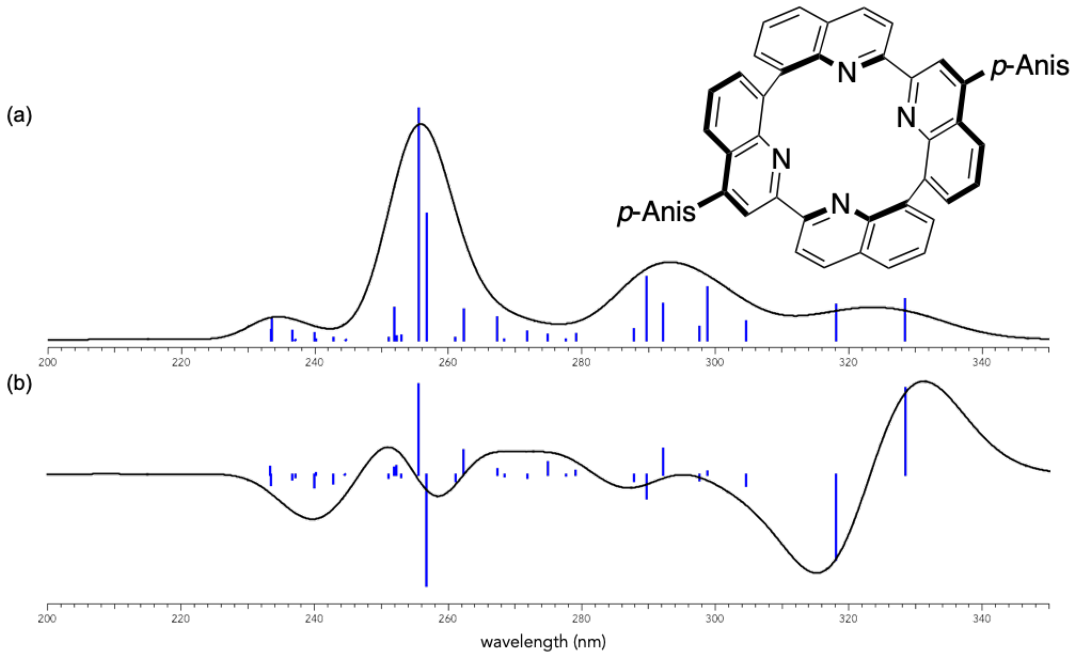


Figure S18. TD-DFT calculations on the (a) UV-Vis or (b) ECD spectra of (–)-***i*-TEQ 6b** at the CAM-B3LYP-D3/6-311+G(2d,p)/SMD(dichloromethane)//B3LYP-D3/6-31G(d,p) level of theory (NState = 30).

Table S4. Electronic absorption on ***i*-TEQ 6** calculated at the CAM-B3LYP-D3/6-311+G(2d,p)/SMD(dichloromethane)//6-31G(d,p)/SMD(dichloromethane) level of theory. *f* denotes oscillator strength. H and L denote the HOMO and LUMO, respectively. [a]Molecular orbitals involved in the transition.

Cmpd.	States	E_x	λ_{max}	*f*	MO[a]			Coefficients	Wave functions			(%)
***i*-TEQ 6a** (G → S_n)	1	3.92	316	0.0969	128	→	133	-0.11976	H–4	→	L	3
					130	→	134	0.21554	H–2	→	L+1	9
					131	→	135	-0.25768	H–1	→	L+2	13
					132	→	133	0.58830	H	→	L	69
	2	4.13	300	0.1660	129	→	134	0.18444	H–3	→	L+1	7
					131	→	133	0.53144	H–1	→	L	56
					132	→	135	-0.36569	H	→	L+2	27
***i*-TEQ 6b** (G → S_n)	1	3.78	328	0.2343	184	→	190	-0.14995	H–4	→	L+1	4
					185	→	191	-0.11211	H–3	→	L+2	3
					186	→	189	0.18383	H–2	→	L	7
					187	→	190	0.16047	H–1	→	L+1	5
					187	→	191	-0.21071	H–1	→	L+2	9
					188	→	189	0.56092	H	→	L	63
	2	3.90	318	0.2025	182	→	190	-0.12297	H–6	→	L+1	3
					185	→	189	0.11737	H–3	→	L	3
					186	→	190	-0.13626	H–2	→	L+1	4
					187	→	189	0.46348	H–1	→	L	43
					187	→	192	0.10856	H–1	→	L+3	2
					188	→	190	0.32032	H	→	L+1	21
					188	→	191	-0.26583	H	→	L+2	14

7-3. CD spectra of *p*-anisyl ***i*-TEQ 6b.**

Both spectra were recorded using 5.0×10^{-5} mol/L solution in CH_2Cl_2.

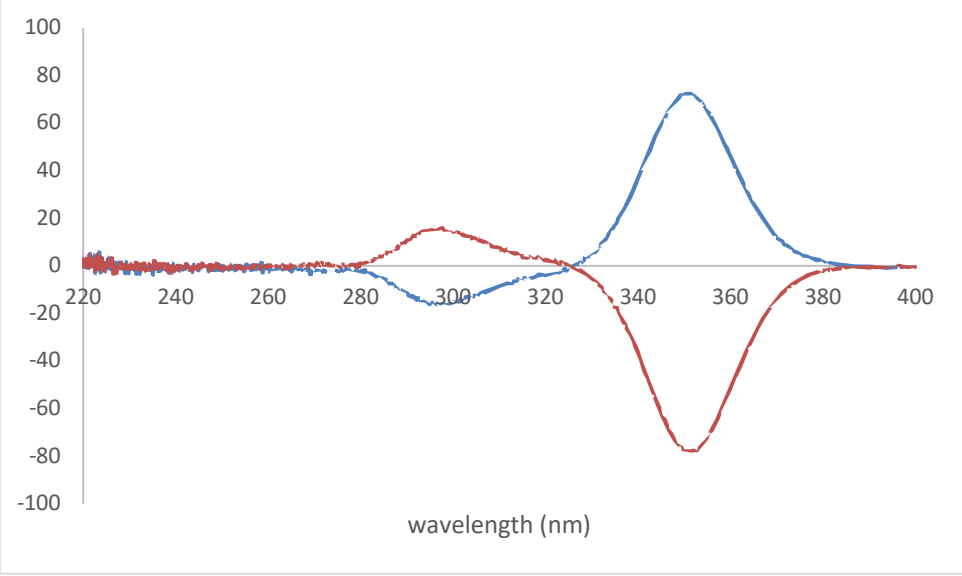
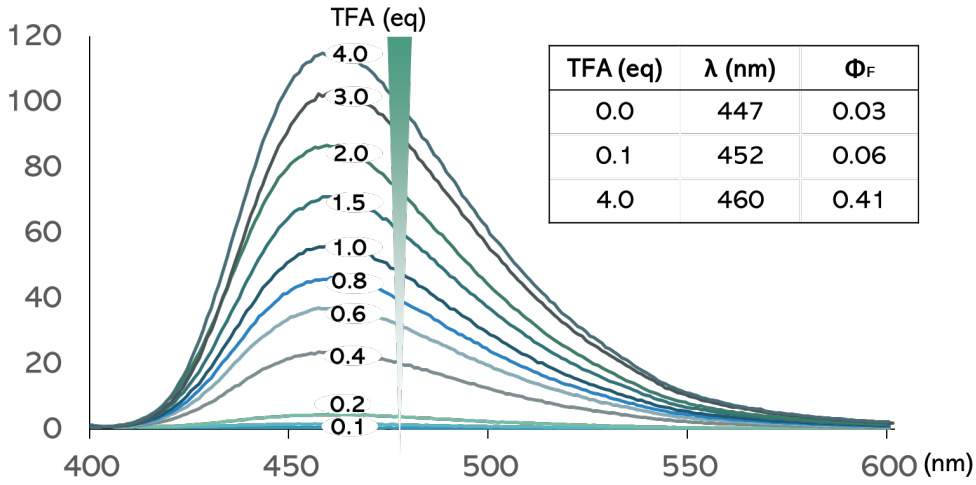


Figure S19. CD spectra of ***i*-TEQ 6b** in CH_2Cl_2.

7-4. Fluorescence spectra of ***i*-TEQ 6b** and **6b** + TFA.

All spectra were recorded using 2.0×10^{-5} mol/L solution in CH_2Cl_2 for emission with excitation at 385.5 nm.



TFA (eq)	λ (nm)	Φ_F
0.0	447	0.03
0.1	452	0.06
4.0	460	0.41

Figure S20. Fluorescence spectra of ***i*-TEQ 6b** with TFA (0.0 – 4.0 eq) in CH_2Cl_2.

7-5. CPL spectra of (+)-***i*-TEQ 6b** and (–)-***i*-TEQ 6b** + 4 equiv of trifluoroacetic acid (TFA) solution

Preparation of TFA solution (50 mL, 5.0×10^{-3} mol/L)

To a 50 mL volumetric flask was added TFA (18.6 μL, 0.25 mmol) and diluted to the volume by dichloromethane.

Preparation of (+)-***i*-TEQ 6b** solution (10 mL, 2.0×10^{-4} mol/L)

To a 10 mL volumetric flask was added (+)-***i*-TEQ 6b** (1.44 mg, 0.002 mmol) and diluted to the volume by dichloromethane.

Preparation of (+)-***i*-TEQ 6b** + 4 equiv TFA solution (10 mL, 2.0×10^{-5} mol/L)

To a 20 mL volumetric flask was added (+)-***i*-TEQ 6b** solution (2 mL, 2.0×10^{-4} mol/L), TFA solution (0.32 mL, 5.0×10^{-3} mol/L) and diluted to the volume by dichloromethane.

(–)-***i*-TEQ 6b** + 4 equiv TFA solution was prepared with similar procedure.

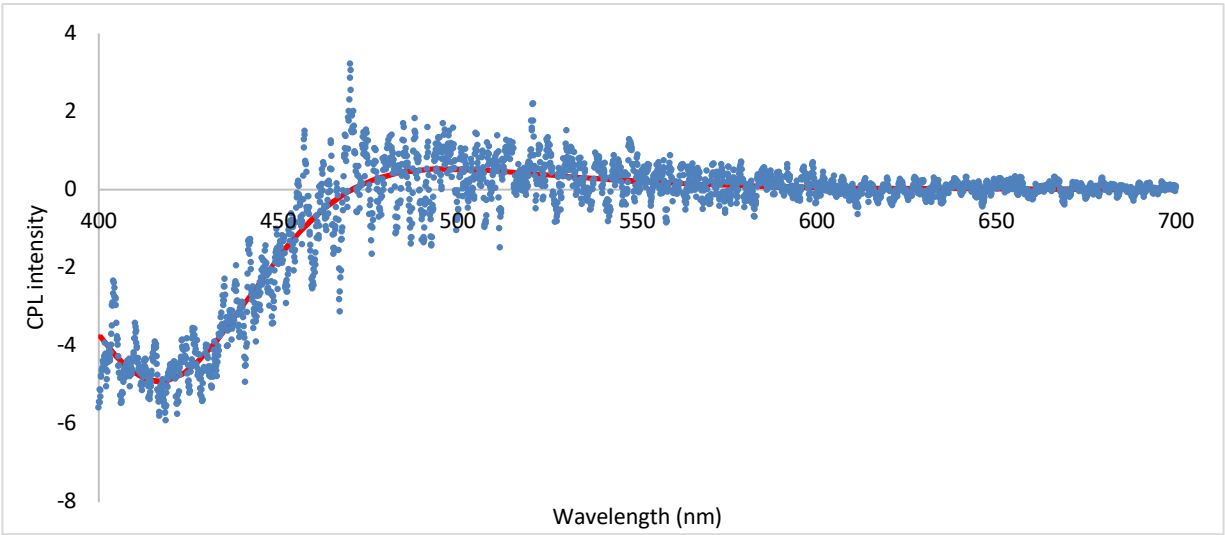


Figure S21. CPL spectra of (+)-***i*-TEQ 6b** + 4 equiv TFA (excited at 350 nm).
$g_{lum} = -5.04 \times 10^{-3}$ at 412 nm

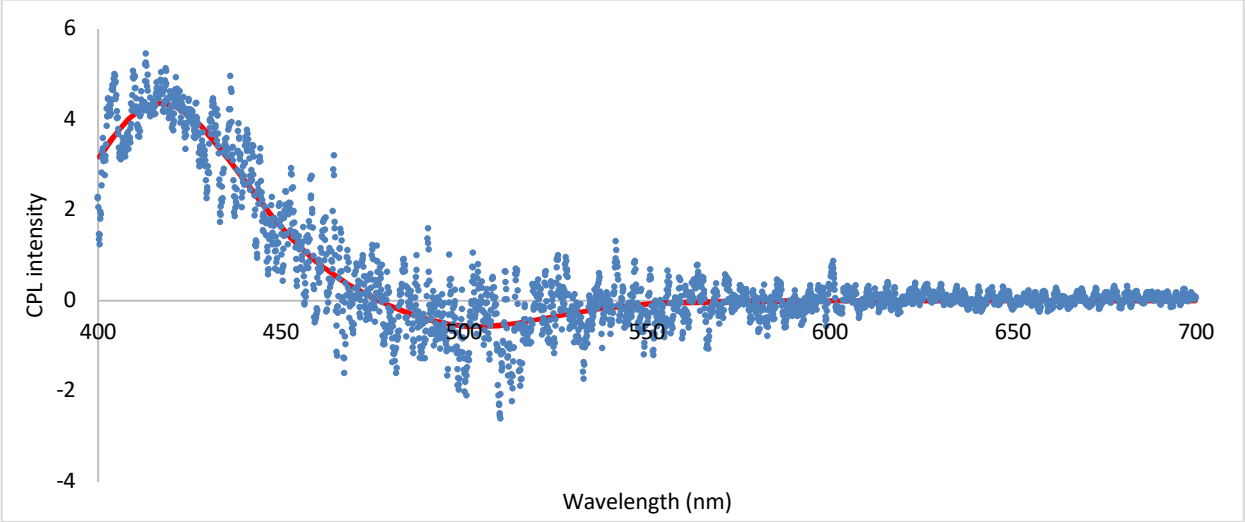


Figure S22. CPL spectra of (–)-***i*-TEQ 6b** + 4 equiv TFA (excited at 350 nm).
g_{lum} = 4.90 x 10^{-3} at 411 nm

7-6. The arrangement of electric and magnetic transition dipole moments of S_4 symmetric **TEQ 7a**, and D_2 symmetric ***i*-TEQ 6a**.

TD-DFT calculations on **TEQ 7a** and ***i*-TEQ 6a** were performed at the CAM-B3LYP-D3/6-311+G(2d,p)/SMD(dichloro-methane)//6-31G(d,p)/SMD(dichlromethane) level of theory. For the S_4 symmetrical **TEQ 7a**, |cos**θ**|, where **θ** is defined as the angle between electric and magnetic transition dipole moments, is low in both the transition from ground (G) state to first excited singlet (S_1) state and the transition from S_1 to G, in other words both transition dipole moments are almost perpendicular. In contrast, for the D_2 symmetrical ***i*-TEQ 6a** and ***i*-TEQ 6a**·$4H^+$, |cos**θ**| is quite high, in other words both transition dipole moments are almost parallel. Although |cos**θ**| decreases due to symmetry breaking in the excited state, |cos**θ**| of ***i*-TEQ 6a**·$4H^+$ in the transition from S_1 to G is 3.27 times higher than that of **TEQ 7a**•$4H^+$. Considering following equation, D_2 symmetrical architecture of ***i*-TEQ 6a** results in a higher CPL intensity.

$$g = \frac{4|\mu||m|\cos\theta}{|\mu|^2+|m|^2}$$

Table S5. Detailed information within the transitions from the ground state (G) to the first excited singlet state (S_1) and from S_1 to G.

		|μ| ($\times10^{-18}$ esu•cm)	|m| ($\times10^{-20}$ erg•Gauss^{-1})	|cos**θ**|	|g| ($\times10^{-2}$)
TEQ 7a	G → S_1	0.00	6.40	**0.00**	**0.000**
***i*-TEQ 6a**	G → S_1	308.44	5.50	**1.00**	**7.134**
TEQ 7a•$4H^+$	G → S_1	11.92	6.68	0.20	34.300
***i*-TEQ 6a**•$4H^+$	G → S_1	193.66	1.06	1.00	2.187
TEQ 7a	S_1 → G	584.61	5.94	0.07	0.265
***i*-TEQ 6a**	S_1 → G	493.86	4.90	0.17	0.691
TEQ 7a•$4H^+$	S_1 → G	664.95	5.93	**0.10**	**0.343**
***i*-TEQ 6a**•$4H^+$	S_1 → G	249.83	1.39	**0.31**	**0.701**

7-7. Homodesmotic Reaction of S_4 symmetric **TEQ 7a**, and D_2 symmetric ***i*-TEQ 6a**

Opened structures gave local minima with no imaginary frequency. Enthalpy of homodesmotic reaction of non-substituted **TEQ 7a** or ***i*-TEQ 6a** with four biphenyl or 2-phenylpyridine molecules to give opened 2,8-diphenylquinoline, 2-phenyl-8-(2-pyridyl)quinoline, or 2-(2-pyridyl)-8-phenylquinoline were evaluated, suggesting that strain of the cyclic architecture of **TEQ 7a** and ***i*-TEQ 6a** and is in a reasonable level.

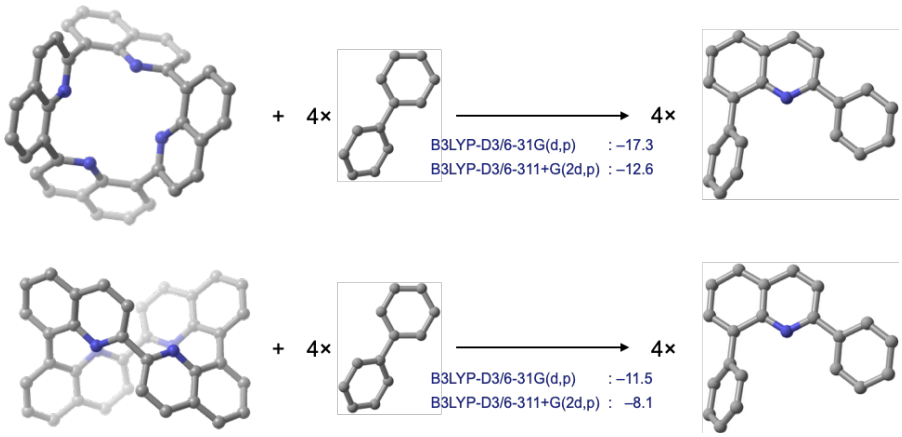


Figure S23. Homodesmotic reaction of **TEQ 7a** and ***i*-TEQ 6a** with biphenyl.

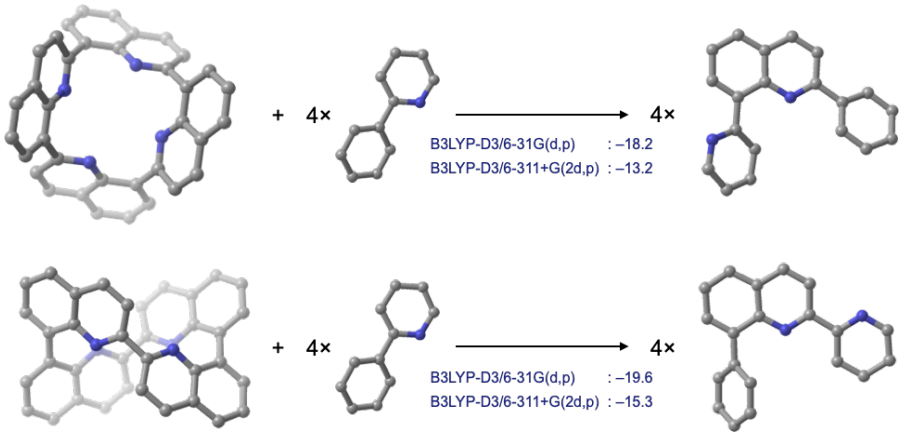
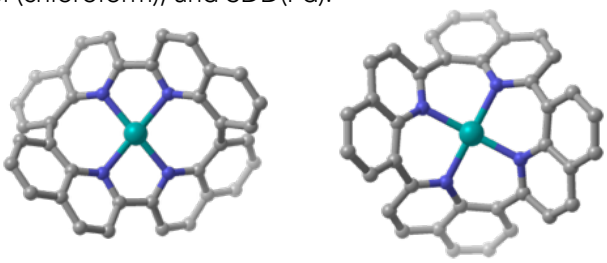


Figure S24. Homodesmotic reaction of **TEQ 7a** and ***i*-TEQ 6a** with 2-phenylpyridine.

8. Thermal Stability of *i*-TEQ **6a** compared to TEQ **7a**

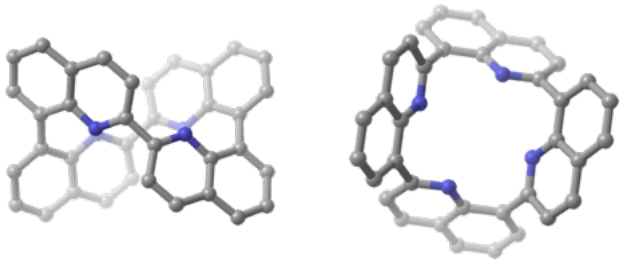
Table S6. Relative Gibbs free energy, enthalpy, and entropy of *i*-TEQ **6a**/Pd(II), compared to those of TEQ **7a**/Pd(II), calculated with designated functionals, 6-31G(d,p) level of theory as basis, integral equation formalism polarizable continuum model (IEFPCM) model (chloroform), and SDD(Pd).



i-TEQ/Pd (D_2) TEQ/Pd (S_4)

	B3LYP-D3	B3LYP-D3BJ	CAM-B3LYP-D3	ωB97XD	M06-2X
	6-31G(d,p)	6-31G(d,p)	6-31G(d,p)	6-31G(d,p)	6-31G(d,p)
ΔG (kcal•mol^{-1})	+20.6	+22.3	+22.9	+22.5	+22.3
ΔH (kcal•mol^{-1})	+22.1	+23.4	+23.7	+23.1	+23.5
ΔS (cal•mol^{-1}•K^{-1})	+6.6	+3.9	+2.6	+2.2	+4.2

Table S7. Relative Gibbs free energy, enthalpy, and entropy of *i*-TEQ **6a**, compared to those of TEQ **7a**, calculated with designated functionals, 6-31G(d,p) level of theory as basis, integral equation formalism polarizable continuum model (IEFPCM) model (chloroform).



i-TEQ (D_2) TEQ (S_4)

	B3LYP-D3	M06-2X
	6-31G(d,p)	6-31G(d,p)
ΔG (kcal•mol^{-1})	–2.2	–2.3
ΔH (kcal•mol^{-1})	–3.1	–2.9
ΔS (cal•mol^{-1}•K^{-1})	–2.8	–1.9

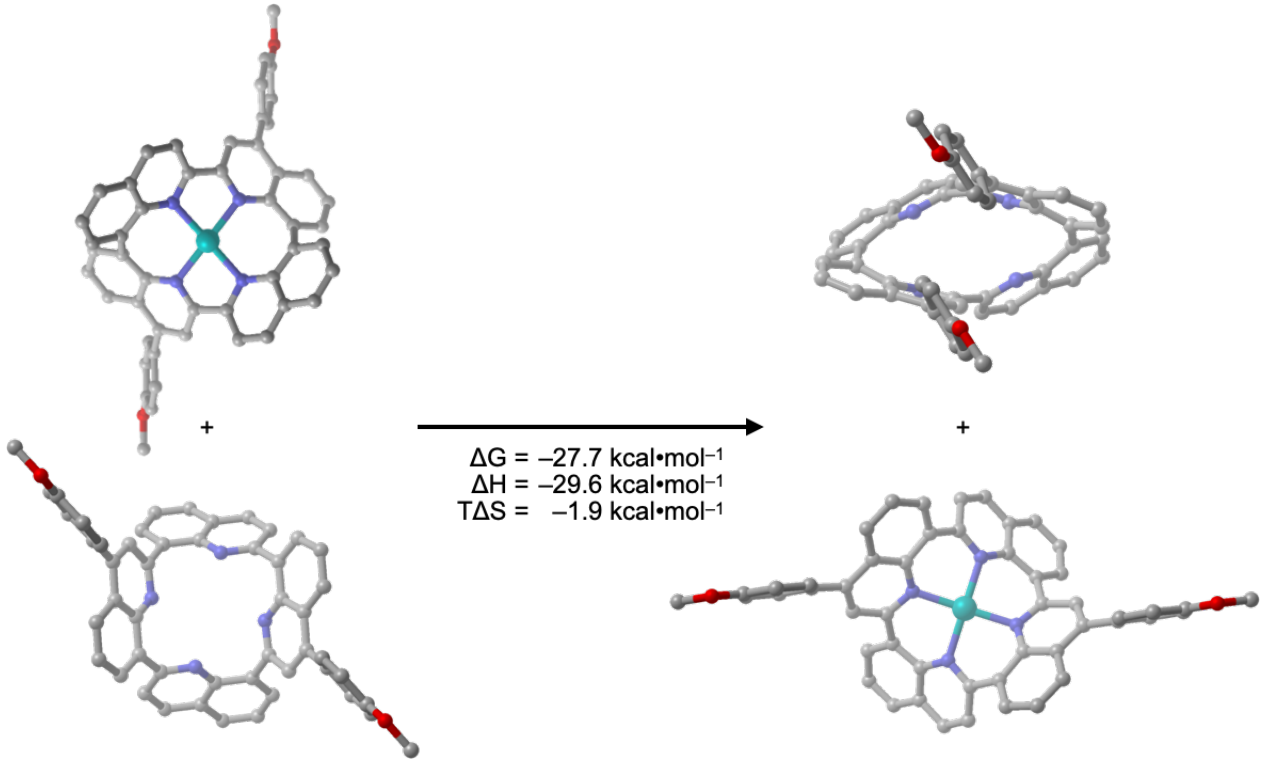


Figure S25. Difference in Gibbs free energy, enthalpy, and entropy within ligand metathesis between ***i*-TEQ 6b**/Pd(II) and **TEQ 7b** to give ***i*-TEQ 6b** and **TEQ 7b**/Pd(II) calculated at the B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(chloroform) level of theory.

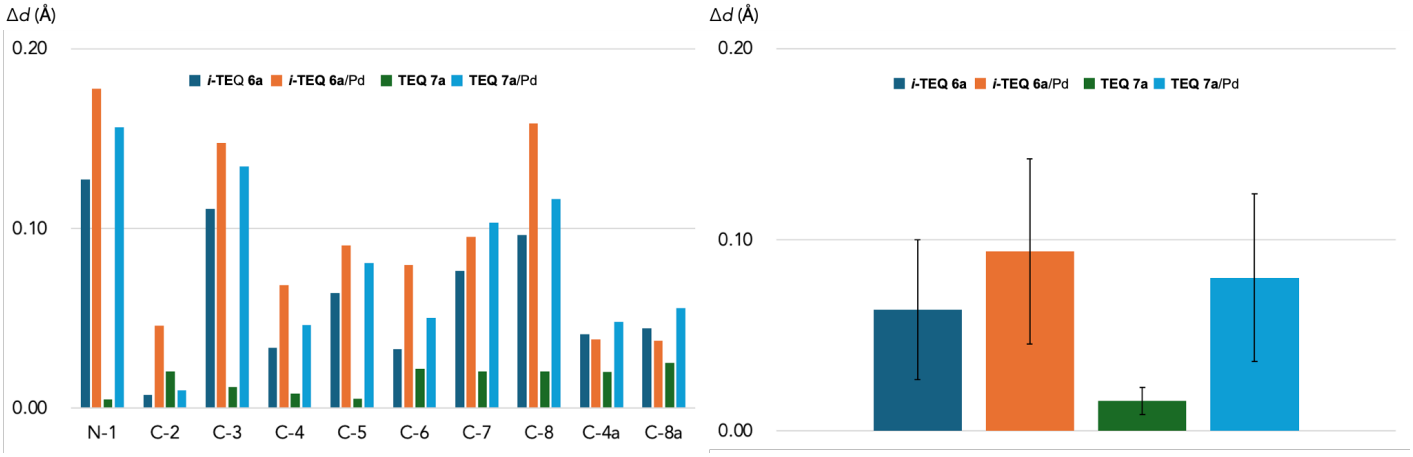


Figure S26. Evaluation of planarity of each quinoline panel for ***i*-TEQ 6a** and **TEQ 7a** in the absence or presence of Pd. Δ*d* shows distances from least square plane (LSP) on the each position (left) and averaged values (right).

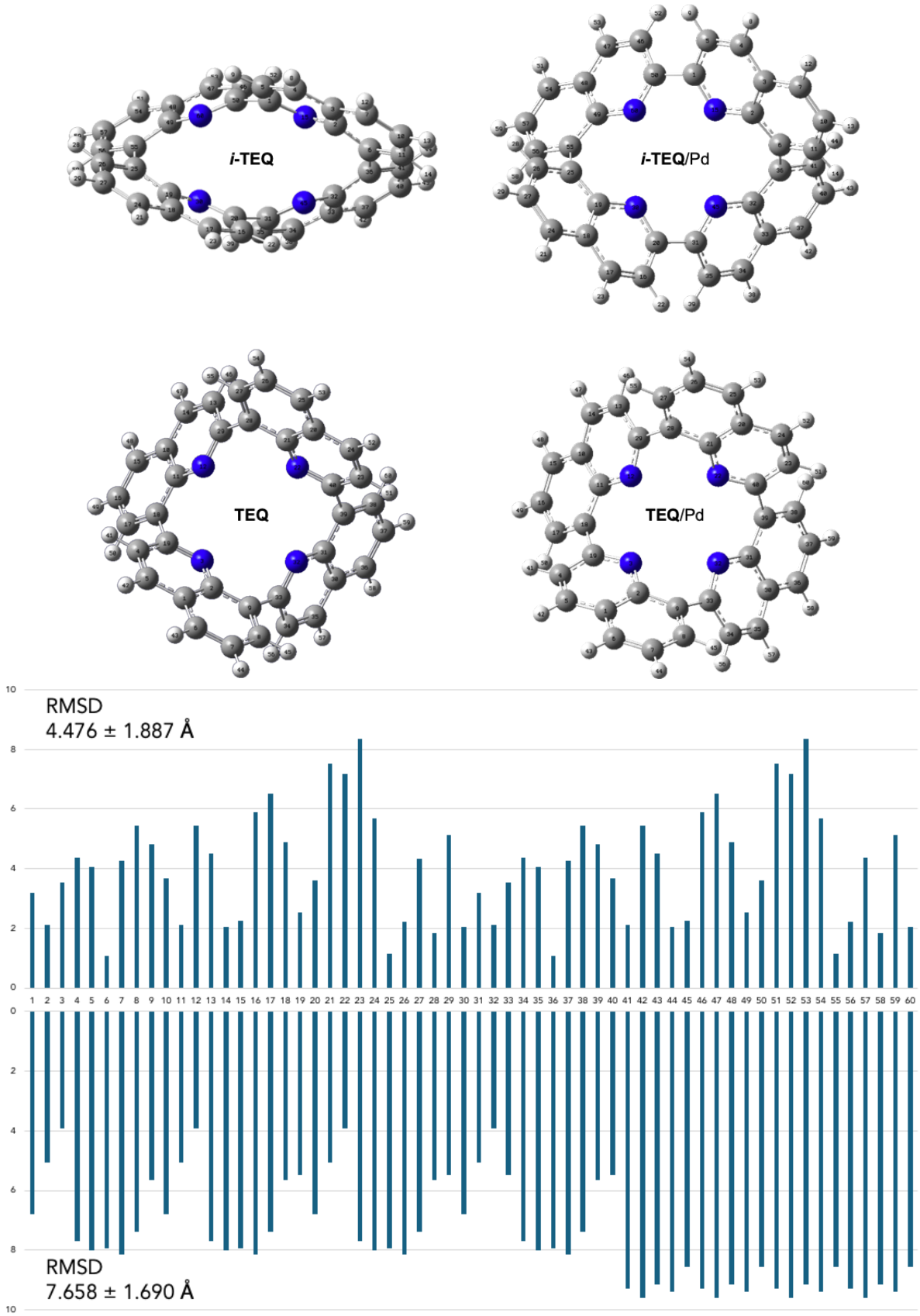


Figure S27. Differences of distance (Δd_i) of ***i*-TEQ 6a** (upper) and **TEQ 7a** (lower) within complexation with Pd(II). RMSD denotes root mean square deviation.

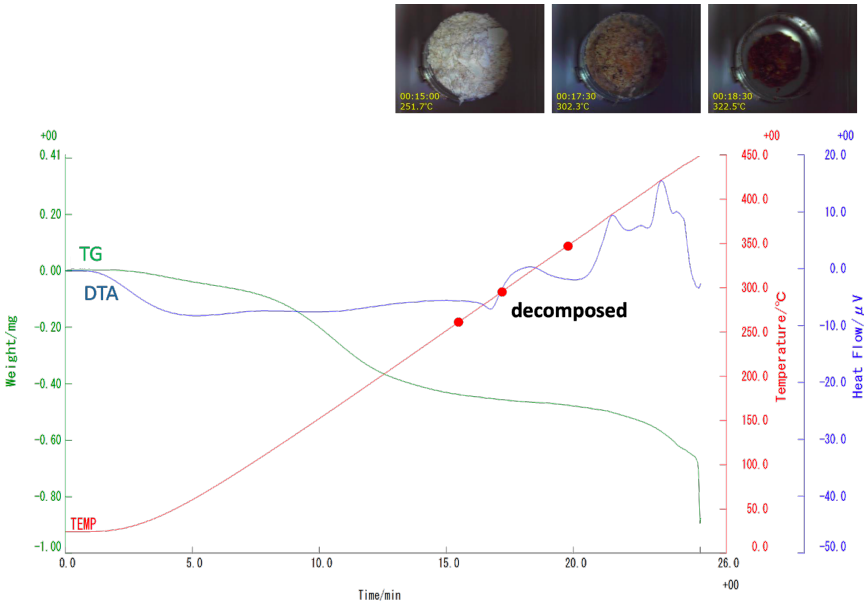


Figure S28. TG-DTA analysis of **TEQ 7b**.

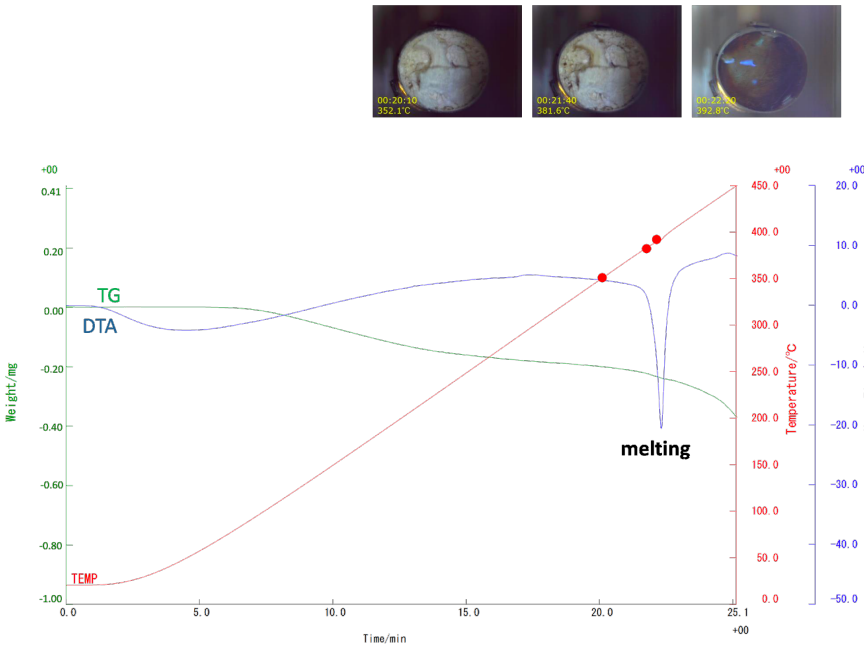


Figure S29. TG-DTA analysis of ***i*-TEQ 6b**.

9. Solid state structures

9-1. Solid state structure of cyclic diamide **5**.

Single crystals of **5** were obtained by slow evaporation from solution in *n*-hexane/CH_2Cl_2 at room temperature. A suitable crystal was selected, and the sample was measured on a Rigaku R-AXIS RAPID II diffractometer using multilayer mirror monochromated Cu-K**α** radiation (**λ** = 1.54184). The data were collected at 93.15 K. Solvent mask was used. Refined structure and crystallographic parameters are summarized in Table S8 and Figure S29. CCDC 2392427 contains the supplementary crystallographic data.

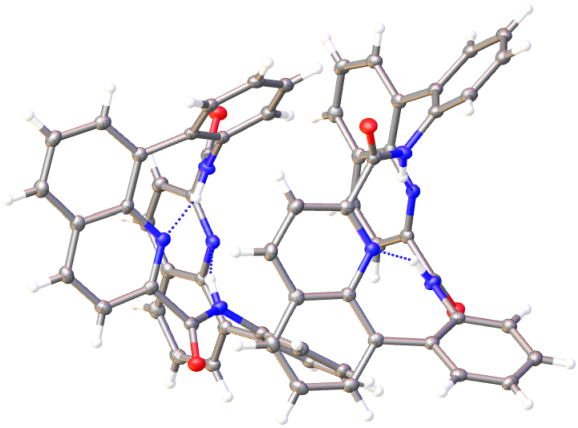


Figure S29. ORTEP diagram of **5**.
Ellipsoids are set at 50% probability.

Table S8.. Selected crystal data of cyclic diamide **5**

Empirical Formula	$C_{32}H_{20}N_4O_2$
Formula Weight	492.54
Crystal Dimensions	0.2 × 0.02 × 0.02 mm
Crystal System	tetragonal
Space group	P-4
Lattice Parameters	
a	14.10340(10) Å
b	14.10340(10) Å
c	11.60890(10) Å
α	90 °
β	90 °
γ	90 °
V	2309.08(4) Å^3
Z value	4
R_1	0.0276
wR_2	0.0679
D_{calc}	1.417 g/cm^3
F_{000}	1024.0

9-2. Solid state structure of ***i*-TEQ 6b**.

Single crystals of ***i*-TEQ 6b** were obtained by slow evaporation from solution in CH_2Cl_2 at –20 °C. A suitable crystal was selected, and the sample was measured on a Rigaku R-AXIS RAPID II diffractometer using multilayer mirror monochromated Cu-K**α** radiation (**λ** = 1.54184). The data were collected at 93.15 K. Refined structure and crystallographic parameters are summarized in Table S9 and Figure S30. CCDC 2392429 contains the supplementary crystallographic data.

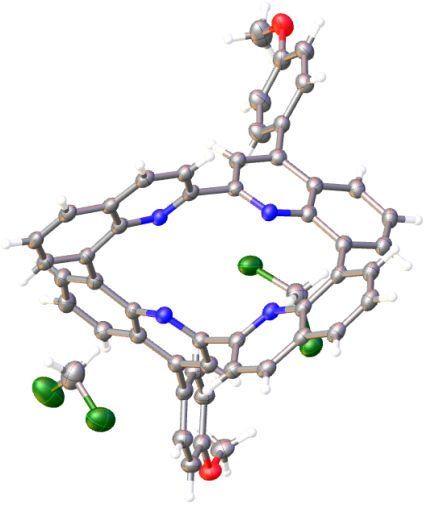


Figure S30. ORTEP diagram of ***i*-TEQ 6b**
Ellipsoids are set at 50% probability.

Table S9. Selected crystal data of ***i*-TEQ 6b**

Empirical Formula	$C_{52}H_{36}Cl_4N_4O_2$
Formula Weight	890.65
Crystal Dimensions	0.2 × 0.05 × 0.05 mm
Crystal System	monoclinic
Space group	C2/c
Lattice Parameters	
a	33.5543(2) Å
b	14.90160 (10) Å
c	18.95070(10) Å
α	90 °
β	91.3870(10) °
γ	90 °
V	9472.82(10) Å^3
Z value	8
R_1	0.0601
wR_2	0.1689
D_{calc}	1.249 g/cm^3
F_{000}	3680.0

9-3. Solid state structure of ***i*-TEQ 6d**

Single crystals of ***i*-TEQ 6d** were obtained by slow evaporation from solution in THF/CH_2Cl_2 at room temperature. A suitable crystal was selected, and the sample was measured on a Rigaku R-AXIS RAPID II diffractometer using multilayer mirror monochromated Cu-K**α** radiation (**λ** = 1.54184). The data were collected at 93.15 K. Refined structure and crystallographic parameters are summarized in Table S10 and Figure S31. CCDC 2392433 contains the supplementary crystallographic data. An alert level B has been found due to the high thermal energy around the Br atom. In the geometry check, the interatomic distances and angles appear to be within acceptable values.

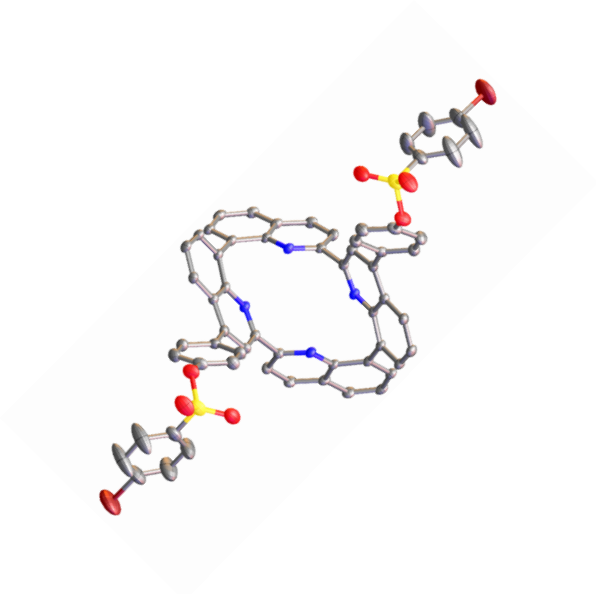


Figure S31. ORTEP diagram of ***i*-TEQ 6d**. Ellipsoids are set at 50% probability.

Table S10. Selected crystal data of ***i*-TEQ 6d**

Empirical Formula	$C_{30}H_{17}BrN_2O_3S$
Formula Weight	565.42
Crystal Dimensions	0.1 × 0.05 × 0.01 mm
Crystal System	orthorhombic
Space group	Pnna
Lattice Parameters	
a	12.36400(10) Å
b	35.4478(2) Å
c	13.14950(10) Å
α	90 °
β	90 °
γ	90 °
V	5763.12(7) Å^3
Z value	8
R_1	0.0887
wR_2	0.2413
D_{calc}	1.303 g/cm^3
F_{000}	2288.0

9-4. Solid state structure of **6b/Pd(BF$_4$)$_2$**

Single crystals of **6b/Pd(BF$_4$)$_2$** were obtained by slow evaporation from solution in $CDCl_3$ at room temperature. A suitable crystal was selected, and the sample was measured on a Rigaku R-AXIS RAPID II diffractometer using multilayer mirror monochromated Cu-K**α** radiation (**λ** = 1.54184). The data were collected at 93.15 K. Refined structure and crystallographic parameters are summarized in Tables S11 and Figure S32. CCDC 2392430 contains the supplementary crystallographic data.

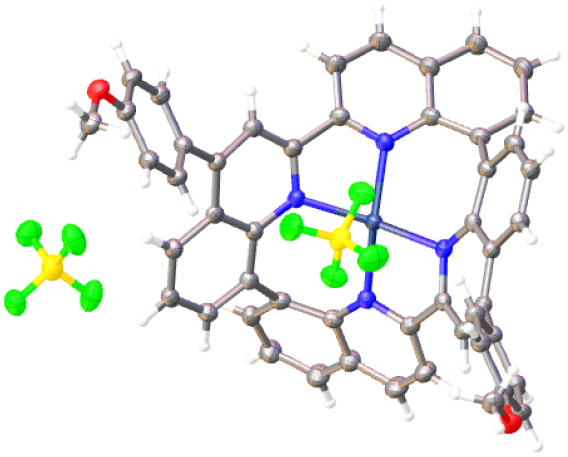


Figure S32. ORTEP diagram of **6b/Pd**.
Ellipsoids are set at 50% probability.

Table S11. Selected crystal data of **6b/Pd(BF$_4$)$_2$**

Empirical Formula	$C_{100}H_{64}B_3F_{12}N_8O_4Pd_2$
Formula Weight	1914.82
Crystal Dimensions	0.08 × 0.08 × 0.02 mm
Crystal System	tetragonal
Space group	P4/ncc
Lattice Parameters	
a	20.05360(10) Å
b	20.05360(10) Å
c	24.3689(2) Å
α	90 °
β	90 °
γ	90 °
V	9799.88(13) Å^3
Z value	4
R_1	0.0408
wR_2	0.1194
D_{calc}	1.298 g/cm^3
F_{000}	3868.0

9-5. Solid state structure of **11**

Single crystals of **11** were obtained by slow evaporation from solution in acetone/Et_2O at room temperature. A suitable crystal was selected, and the sample was measured on a Rigaku R-AXIS RAPID II diffractometer using multilayer mirror monochromated Cu-K**α** radiation (**λ** = 1.54184). The data were collected at 93.15 K. Solvent mask was used. Refined structure and crystallographic parameters are summarized in Table S12 and Figure S33. CCDC 2392428 contains the supplementary crystallographic data.

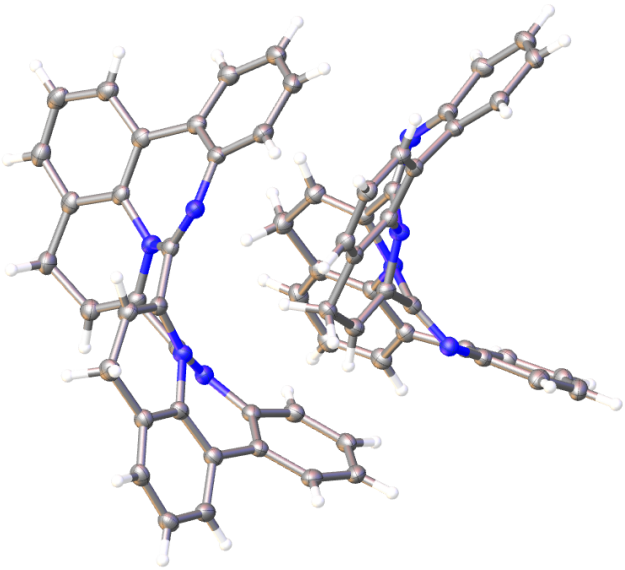


Figure S33. ORTEP diagram of **11**.
Ellipsoids are set at 50% probability.

Table S12. Selected crystal data of **11**

Empirical Formula	$C_{64}H_{40}N_8$
Formula Weight	921.04
Crystal Dimensions	0.3 × 0.1 × 0.05 mm
Crystal System	triclinic
Space group	P-1
Lattice Parameters	
a	11.24280(10)
b	12.05930(10) Å
c	16.9374(2) Å
α	97.1790(10) °
β	90.8250(10) °
γ	103.7300(10) °
V	2210.96(4) Å^3
Z value	2
R_1	0.0393
wR_2	0.0898
D_{calc}	1.383 g/cm^3
F_{000}	960.0

10. References

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11. Optimized coordinates

Table S13. Cartesian coordinates and energies of **TEQ 7a**.

B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.461334 (Hartree/Particle)
Thermal correction to Energy= 0.488270
Thermal correction to Enthalpy= 0.489214
Thermal correction to Gibbs Free Energy= 0.405043
Sum of electronic and zero-point Energies= -1602.567522
Sum of electronic and thermal Energies= -1602.540586
Sum of electronic and thermal Enthalpies= -1602.539642
Sum of electronic and thermal Free Energies= -1602.623813

C	-3.82234100	2.30432200	2.92948200
C	-2.85214800	1.26192600	0.94913200
C	-1.73721300	2.15308500	1.03310800
C	-1.69335600	3.10748600	2.09996600
C	-2.74978900	3.15747500	3.04521500
N	-0.77710800	2.08508900	0.07136000
C	0.24150000	2.92117600	0.13850100
C	0.38430600	3.89542900	1.16715100
C	-0.58033100	3.98434100	2.13923600
C	-0.24176400	-2.92128200	0.13855600
C	1.26218400	2.85158600	-0.94910400
C	-0.38526800	-3.89483900	1.16773600
C	0.57914400	-3.98363700	2.14004600
C	1.69252800	-3.10723000	2.10057300
C	1.73695800	-2.15335300	1.03330300
N	0.77716700	-2.08561300	0.07118900
C	2.74881400	-3.15722800	3.04599400
C	3.82170800	-2.30454000	2.93005200
C	3.87180900	-1.36211600	1.87522100
C	2.85204200	-1.26241900	0.94927300
C	2.15345100	1.73676900	-1.03310100
C	3.10803700	1.69313500	-2.09985000
C	3.15798500	2.74965600	-3.04499700
C	2.30468300	3.82208900	-2.92926700
C	1.36180700	3.87156400	-1.87482200
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C	2.92183700	-0.24186500	-0.13847600
C	3.89625800	-0.38437600	-1.16691600
C	3.98511100	0.58031600	-2.13897900
H	-4.63501000	2.34477300	3.64852300
H	-2.70042800	3.88393500	3.85235900
H	1.25099500	4.54788000	1.16661600
H	-0.50691500	4.71876400	2.93748800
H	-1.25220800	-4.54696100	1.16731400
H	0.50529800	-4.71762100	2.93866300
H	2.69903400	-3.88329600	3.85346600
H	4.63431300	-2.34506200	3.64916400
H	4.72092100	-0.68851600	1.80100600
H	3.88453000	2.70046200	-3.85207700
H	2.34511300	4.63482100	-3.64824200
H	0.68788100	4.72042200	-1.80064400
H	4.54897600	-1.25086800	-1.16629300
H	4.71969000	0.50703400	-2.93710100
C	-3.87201900	1.36155300	1.87493400
H	-4.72094300	0.68770100	1.80078900
C	-2.30348800	-3.82155500	-2.93053600
C	-1.26198100	-2.85180900	-0.94954300
C	-2.15336800	-1.73711300	-1.03341000
C	-3.10745100	-1.69305600	-2.10053500
C	-3.15691100	-2.74920500	-3.04613200
N	-2.08570400	-0.77725800	-0.07138900
C	-2.92168600	0.24143600	-0.13864700
C	-3.89567000	0.38440600	-1.16749300
C	-3.98435100	-0.58007300	-2.13976500
H	-2.34353200	-4.63398400	-3.64987300
H	-3.88317700	-2.69979500	-3.85345100
H	-4.54811800	1.25110000	-1.16699800
H	-4.71861200	-0.50652100	-2.93815200
C	-1.36098800	-3.87136900	-1.87573900
H	-0.68692300	-4.72013000	-1.80171900

Table S14. Cartesian coordinates and energies of **TEQ 7a**.

B3LYP-D3/6-31G(d,p)/IEFPCM($CHCl_3$)
Zero-point correction= 0.461833 (Hartree/Particle)
Thermal correction to Energy= 0.488672
Thermal correction to Enthalpy= 0.489616
Thermal correction to Gibbs Free Energy= 0.405828
Sum of electronic and zero-point Energies= -1602.580635
Sum of electronic and thermal Energies= -1602.553797
Sum of electronic and thermal Enthalpies= -1602.552852

Sum of electronic and thermal Free Energies= -1602.636640
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C -0.05364800 -3.13398900 0.93385900
C -1.31054900 -2.45685600 1.02121500
C -2.21265000 -2.80815900 2.07694700
C -1.85180300 -3.81414800 3.01019600
N -1.62163000 -1.52971500 0.07288900
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C -3.75182300 -1.19517300 1.16068300
C -3.45780700 -2.13157200 2.12035600
C 2.79457000 0.92483400 0.14190300
C -3.13416200 0.05376200 -0.93406400
C 3.75200900 1.19502000 1.16037200
C 3.45813400 2.13120300 2.12029700
C 2.21293100 2.80772600 2.07728200
C 1.31064200 2.45660300 1.02164700
N 1.62155900 1.52963900 0.07309900
C 1.85222100 3.81349800 3.01081800
C 0.64659600 4.46551400 2.89273300
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C 0.05371600 3.13373800 0.93465300
C -2.45691900 1.31063600 -1.02112600
C -2.80813100 2.21299300 -2.07666800
C -3.81410500 1.85241300 -3.01003700
C -4.46620800 0.64684100 -2.89189100
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H -4.16606700 -2.36635700 2.91048000
H 4.69476600 0.65878400 1.16248300
H 4.16654400 2.36586600 2.91032300
H 2.54586300 4.06379700 3.80900800
H 0.36998000 5.24038900 3.60093100
H -1.19658100 4.64697000 1.77026700
H -4.06447400 2.54610700 -3.80816000
H -5.24122700 0.37032300 -3.59997100
H -4.64761900 -1.19638800 -1.76949900
H -0.65875300 4.69456000 -1.16217200
H -2.36620100 4.16658200 -2.90973300
C 0.24624100 -4.12738500 1.84667800
H 1.19676200 -4.64743000 1.76892600
C 4.46592800 -0.64621000 -2.89251200
C 3.13400100 -0.05355500 -0.93446900
C 2.45673300 -1.31040000 -1.02177500
C 2.80787700 -2.21252200 -2.07754400
C 3.81378800 -1.85173900 -3.01090100
N 1.52964800 -1.62141100 -0.07336300
C 0.92475700 -2.79435500 -0.14244200
C 1.19495400 -3.75162600 -1.16106500
C 2.13123700 -3.45765500 -2.12085900
H 5.24091400 -0.36954700 -3.60057000
H 4.06409500 -2.54525500 -3.80919900
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C 4.12732500 0.24626400 -1.84739300
H 4.64746600 1.19673500 -1.76967800

Table S15. Cartesian coordinates and energies of **TEQ 7a**.
M06-2X/6-31G(d,p)/IEFPCM($CHCl_3$)
Zero-point correction= 0.466638 (Hartree/Particle)
Thermal correction to Energy= 0.493285
Thermal correction to Enthalpy= 0.494229
Thermal correction to Gibbs Free Energy= 0.410945
Sum of electronic and zero-point Energies= -1601.873107
Sum of electronic and thermal Energies= -1601.846461
Sum of electronic and thermal Enthalpies= -1601.845517
Sum of electronic and thermal Free Energies= -1601.928801
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C 3.10904000 -0.39819300 0.92512900
C 2.29840000 -1.57171000 1.01330100
C 2.56471200 -2.50958000 2.04864700
C 3.61469000 -2.27012400 2.97139900
N 1.33188400 -1.77042200 0.07539600
C 0.61702200 -2.87104000 0.14233700
C 0.79750500 -3.86443200 1.14605600
C 1.76550100 -3.67880300 2.09286400
C -0.61689700 2.87097700 0.14230800
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C -3.61409300 2.27056900 2.97199600
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C -4.13821700 0.21633900 1.82024100
C -3.10876100 0.39824100 0.92599500
C -1.57218600 -2.29801000 -1.01317400
C -2.51021300 -2.56447100 -2.04835400
C -2.27059900 -3.61420800 -2.97133100
C -1.14770400 -4.39026700 -2.85488600
C -0.21614300 -4.13761100 -1.81966600
N -1.77101400 -1.33169600 -0.07512100
C -2.87176400 -0.61703100 -0.14182300
C -3.86538100 -0.79775300 -1.14525400
C -3.67971900 -1.76563800 -2.09217200
H 5.20086300 -0.96383500 3.55262200
H 3.79499000 -2.99604600 3.75916800
H 0.16563500 -4.74566300 1.14211400
H 1.93864700 -4.41362700 2.87430100
H -0.16537300 4.74581200 1.14162700
H -1.93808700 4.41409700 2.87417800
H -3.79429300 2.99664800 3.75964300
H -5.20018600 0.96439500 3.55368800
H -4.75916100 -0.67132000 1.73831900
H -2.99663400 -3.79464300 -3.75896400
H -0.96384600 -5.19977800 -3.55313600
H 0.67175200 -4.75822600 -1.73781600
H -4.74681300 -0.16616400 -1.14101800
H -4.41470600 -1.93896400 -2.87341500
C 4.13864500 -0.21613000 1.81917100
H 4.75956200 0.67152500 1.73699500
C 1.14696200 4.38999200 -2.85555200
C 0.39814300 3.10806900 -0.92576600
C 1.57191600 2.29778700 -1.01389300

C 2.50971100 2.56426300 -2.04927900
C 2.26985200 3.61396000 -2.97223700
N 1.77096300 1.33146300 -0.07590200
C 2.87178200 0.61693700 -0.14274400
C 3.86521800 0.79771000 -1.14634800
C 3.67926700 1.76551000 -2.09329600
H 0.96292200 5.19948200 -3.55378000
H 2.99570200 3.79439700 -3.76004000
H 4.74671700 0.16621400 -1.14223500
H 4.41409500 1.93887200 -2.87468200
C 0.21567500 4.13737200 -1.82007400
H -0.67218800 4.75800400 -1.73800200

Table S16. Cartesian coordinates and energies of **TEQ 7a**.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.458912 (Hartree/Particle)
Thermal correction to Energy= 0.485914
Thermal correction to Enthalpy= 0.486859
Thermal correction to Gibbs Free Energy= 0.402496
Sum of electronic and zero-point Energies= -1602.956735
Sum of electronic and thermal Energies= -1602.929733
Sum of electronic and thermal Enthalpies= -1602.928789
Sum of electronic and thermal Free Energies= -1603.013151
C -4.05504900 1.65610000 2.97653500
C -2.99188900 0.81188300 0.96081300
C -2.02598100 1.85640200 1.04123000
C -2.09415100 2.77960100 2.12680200
C -3.12242800 2.65391100 3.09023800
N -1.08747000 1.95207000 0.06442800
C -0.19336500 2.91153300 0.13742300
C -0.16620000 3.86502400 1.18867800
C -1.11446500 3.79762500 2.17157300
C 0.19333500 -2.91153600 0.13728300
C 0.81202000 2.99173500 -0.96098800
C 0.16591400 -3.86511000 1.18845700
C 1.11393000 -3.79777800 2.17159800
C 2.09361900 -2.77974200 2.12715200
C 2.02571800 -1.85646300 1.04163000
N 1.08745200 -1.95206200 0.06458700
C 3.12164700 -2.65411500 3.09086100
C 4.05428800 -1.65628600 2.97747100
C 3.98698800 -0.73746100 1.90751700
C 2.99164200 -0.81193400 0.96153500
C 1.85659100 2.02586000 -1.04112900
C 2.77997700 2.09396100 -2.12654600
C 2.65439900 3.12212300 -3.09012000
C 1.65651500 4.05470000 -2.97669600
C 0.73759000 3.98720800 -1.90683900
N 1.95211500 1.08743900 -0.06422900
C 2.91162600 0.19336500 -0.13696600
C 3.86532300 0.16615500 -1.18803400
C 3.79806000 1.11432200 -2.17103300
H -4.84523000 1.56030500 3.71149200
H -3.16270900 3.35923000 3.91320500
H 0.60332900 4.62634900 1.19825800
H -1.12610100 4.51403600 2.98604700
H -0.60361000 -4.62644200 1.19778500
H 1.12536500 -4.51425200 2.98601900
H 3.16172400 -3.35949400 3.91378600
H 4.84427800 -1.56053800 3.71263800
H 4.72228400 0.05639700 1.84147300
H 3.35985900 3.16235200 -3.91296900
H 1.56079900 4.84478900 -3.71176100
H -0.05630300 4.72246300 -1.84076400
H 4.62668700 -0.60333700 -1.19739900
H 4.51462100 1.12591400 -2.98537600
C -3.98748000 0.73735000 1.90653400
H -4.72276400 -0.05649800 1.84024400
C -1.65576800 -4.05452200 -2.97736200
C -0.81177400 -2.99166600 -0.96138600
C -1.85632300 -2.02578500 -1.04173600
C -2.77944000 -2.09382800 -2.12738700
C -2.65362100 -3.12193700 -3.09098500
N -1.95209300 -1.08741900 -0.06480700
C -2.91159300 -0.19334600 -0.13773100
C -3.86502800 -0.16608100 -1.18903400
C -3.79751500 -1.11419100 -2.17207200
H -1.55987000 -4.84457300 -3.71244500
H -3.35887500 -3.16212000 -3.91401300
H -4.62639600 0.60340600 -1.19854300
H -4.51387200 -1.12573900 -2.98659400
C -0.73711200 -3.98709100 -1.90727000
H 0.05676100 -4.72235200 -1.84103300

Table S17. Cartesian coordinates and energies of **TEQ 7a**.
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.459339 (Hartree/Particle)
Thermal correction to Energy= 0.486186
Thermal correction to Enthalpy= 0.487131
Thermal correction to Gibbs Free Energy= 0.403380
Sum of electronic and zero-point Energies= -1602.997733
Sum of electronic and thermal Energies= -1602.970886
Sum of electronic and thermal Enthalpies= -1602.969942
Sum of electronic and thermal Free Energies= -1603.053692
C -4.06318500 1.79175600 2.93208300
C -2.98522900 0.89228100 0.94641000
C -1.99317200 1.91256500 1.03090100
C -2.06121300 2.85501400 2.10045100
C -3.10795100 2.76817700 3.04862500
N -1.03259100 1.97539800 0.07065800
C -0.12710400 2.92753700 0.14025200
C -0.10330300 3.89770900 1.17566400
C -1.06597600 3.85802500 2.14624000
C 0.12705600 -2.92756200 0.14013400
C 0.89242100 2.98502200 -0.94657600
C 0.10295600 -3.89774400 1.17552800
C 1.06538600 -3.85810500 2.14634800
C 2.06066100 -2.85511900 2.10083200
C 1.99291300 -1.91264600 1.03128700
N 1.03258900 -1.97544900 0.07078700
C 3.10715900 -2.76832400 3.04927400
C 4.06243800 -1.79191400 2.93300100
C 4.00049400 -0.85863400 1.87551900
C 2.98499500 -0.89236100 0.94708500
C 1.91277700 1.99301800 -1.03080800
C 2.85540600 2.06101800 -2.10020400
C 2.76865100 3.10765200 -3.04850100
C 1.79213700 4.06282300 -2.93222500
C 0.85872800 4.00065000 -1.87486900
N 1.97549200 1.03252300 -0.07047900

C 2.92769400 0.12707800 -0.13982800
C 3.89806500 0.10326200 -1.17504900
C 3.85849400 1.06584900 -2.14571700
H -4.86912600 1.72525100 3.65333400
H -3.14426700 3.48730000 3.85969600
H 0.67447700 4.65073600 1.18441200
H -1.07932100 4.58658600 2.94971800
H -0.67485000 -4.65074600 1.18406600
H 1.07850700 -4.58668200 2.94981500
H 3.14325900 -3.48746500 3.86033800
H 4.86819700 -1.72544300 3.65445800
H 4.75891300 -0.08711100 1.80425000
H 3.48790800 3.14393900 -3.85945500
H 1.72569000 4.86868000 -3.65357400
H 0.08714500 4.75900700 -1.80357900
H 4.65114800 -0.67446700 -1.18359100
H 4.58720200 1.07917000 -2.94906200
C -4.00096200 0.85851300 1.87458500
H -4.75936100 0.08699000 1.80309200
C -1.79135400 -4.06262100 -2.93295100
C -0.89218300 -2.98498900 -0.94696600
C -1.91252700 -1.99298900 -1.03138500
C -2.85486300 -2.06089800 -2.10104200
C -2.76784700 -3.10745000 -3.04940600
N -1.97549400 -1.03256500 -0.07099800
C -2.92765900 -0.12710000 -0.14054400
C -3.89775000 -0.10319600 -1.17602800
C -3.85793000 -1.06571500 -2.14675300
H -1.72470400 -4.86841300 -3.65435400
H -3.48688300 -3.14367200 -3.86055800
H -4.65081800 0.67454600 -1.18472000
H -4.58641900 -1.07896900 -2.95029900
C -0.85822600 -4.00053200 -1.87534000
H -0.08665000 -4.75888200 -1.80391500

Table S18. Cartesian coordinates and energies of **TEQ 7a** (TS).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.460572 (Hartree/Particle)
Thermal correction to Energy= 0.486429
Thermal correction to Enthalpy= 0.487373
Thermal correction to Gibbs Free Energy= 0.406008
Sum of electronic and zero-point Energies= -1602.478498
Sum of electronic and thermal Energies= -1602.452641
Sum of electronic and thermal Enthalpies= -1602.451697
Sum of electronic and thermal Free Energies= -1602.533062
C -1.79031200 2.45072600 -0.16182600
C -2.84783500 3.29961300 -0.64134400
C -0.56141600 3.22793000 0.21453700
C -4.13965400 2.87415500 -0.53582300
H -2.61401400 4.29133000 -1.00949400
N -1.97688600 1.16328500 0.07022100
C -0.87853000 4.38696800 0.92629500
C 0.81429700 3.03465400 -0.17169300
C -4.39387000 1.56459200 -0.06657100
H -4.97251500 3.52497800 -0.78993000
C -3.26008300 0.68858700 0.06584900
C 0.02125600 5.44336000 1.15462800
H -1.89149600 4.49527100 1.29868200
C 1.66054200 4.19853700 -0.08760700
N 1.31381100 1.81503500 -0.54000400
C -5.70651600 1.13084700 0.23614900
C -3.54795900 -0.70889000 0.23986700
C 1.26471700 5.37910500 0.57936000
H -0.29474100 6.31062500 1.72560900
C 2.93818500 4.10774200 -0.68314200
C 2.59094900 1.72550900 -0.90016800
C -5.91973200 -0.16738000 0.62832000
C -4.84630600 -1.07865300 0.57664900
C -2.64003400 -1.83651900 -0.12560900
H 1.96637700 6.20662900 0.64454300
C 3.39131400 2.90030900 -1.11546700
H 3.56746300 4.99238900 -0.73694700
C 3.37465200 0.45082800 -0.81075800
H -6.90877000 -0.51232200 0.91320000
H -5.04965800 -2.12700800 0.77190700
C -3.25552900 -2.81113500 -0.98014500
N -1.40193400 -1.95697300 0.32090100
H 4.39792800 2.82992000 -1.49949600
C 4.67390600 0.43386800 -1.31807500
C 3.03318400 -0.65292200 0.06665700
C -2.61985500 -3.99438800 -1.21879500
H -4.22687500 -2.60552400 -1.41306400
C -0.72637200 -3.10735400 0.03181800
C 5.70436800 -0.37432100 -0.79659500
H 4.94347900 1.12666600 -2.10658200
C 4.12224400 -1.28354300 0.76511500
N 1.78309200 -1.18333900 0.12007100
C -1.33661300 -4.20632300 -0.66681500
H -3.08112900 -4.77276100 -1.82131000
C 0.62096700 -3.28076900 0.48441800
C 5.45789200 -1.12960800 0.32545300
H 6.69815700 -0.32009900 -1.22946000
C 3.77782700 -2.13793600 1.84315700
C 1.57273000 -2.21822900 0.92276300
C -0.67980600 -5.45262500 -0.80166000
C 1.21338200 -4.53414200 0.35176300
C 2.48488200 -2.56731100 1.96695700
H 4.55826700 -2.49856200 2.50847100
C 0.57063700 -5.62585900 -0.26474500
H -1.18521700 -6.25813600 -1.32804800
H 2.23896400 -4.66169800 0.67982400
H 2.18594400 -3.27055400 2.73647800
H 1.08736500 -6.57708400 -0.34662800
H 6.25374400 -1.65919900 0.84224200
H -6.52490000 1.84252400 0.16417600

Table S19. Cartesian coordinates and energies of **TEQ 7a** (TS).
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.458743 (Hartree/Particle)
Thermal correction to Energy= 0.484505
Thermal correction to Enthalpy= 0.485449
Thermal correction to Gibbs Free Energy= 0.404642
Sum of electronic and zero-point Energies= -1602.910280
Sum of electronic and thermal Energies= -1602.884518
Sum of electronic and thermal Enthalpies= -1602.883573
Sum of electronic and thermal Free Energies= -1602.964381
C -1.91605600 2.38485900 -0.14916600
C -3.01258100 3.17378000 -0.62576600
C -0.73023300 3.21319200 0.24437900
C -4.27300300 2.67147600 -0.54607500

H -2.83773000 4.18179100 -0.97469200
N -2.03222800 1.08928500 0.06350200
C -1.09592500 4.34551000 0.96527100
C 0.64942900 3.07825400 -0.13548100
C -4.45592600 1.34622700 -0.09891600
H -5.13702400 3.27572200 -0.80066200
C -3.28156500 0.53589300 0.03744400
C -0.23620100 5.42409800 1.21881800
H -2.11252700 4.41594000 1.32993000
C 1.45180900 4.26378000 -0.02823300
N 1.19647300 1.88747700 -0.52533700
C -5.74117600 0.83625700 0.18556200
C -3.48825800 -0.87355700 0.19371900
C 1.01008500 5.41369700 0.65613700
H -0.58608600 6.26812200 1.80054200
C 2.73025400 4.23087800 -0.61988900
C 2.46968300 1.85082300 -0.89428900
C -5.88210600 -0.47148700 0.56358000
C -4.76242500 -1.31879000 0.51187800
C -2.51437600 -1.94588900 -0.16316100
H 1.67834200 6.26370000 0.74005000
C 3.22372400 3.05510600 -1.07983500
H 3.32727400 5.13569000 -0.65277200
C 3.29846100 0.60590300 -0.85657500
H -6.84977100 -0.87399900 0.83754400
H -4.91210800 -2.37602300 0.69421700
C -3.05326400 -2.94304600 -1.03441200
N -1.28858900 -2.01339800 0.31675100
H 4.22802100 3.02928000 -1.46928000
C 4.57083100 0.64644200 -1.41500600
C 3.04069600 -0.51026200 0.02773200
C -2.36683900 -4.09906300 -1.23502200
H -4.01332200 -2.78276500 -1.50434300
C -0.55473800 -3.13483500 0.06557800
C 5.65014700 -0.11940500 -0.94106000
H 4.78096900 1.35806200 -2.20167100
C 4.17842200 -1.08047900 0.68696000
N 1.82517600 -1.10677200 0.13127400
C -1.10438900 -4.26019400 -0.62938400
H -2.77633100 -4.89848100 -1.84284600
C 0.78268200 -3.25070300 0.55741300
C 5.48339300 -0.87419600 0.19132600
H 6.61945000 -0.02752300 -1.41539200
C 3.91547000 -1.92920300 1.78740000
C 1.69539600 -2.14100300 0.94879800
C -0.41132400 -5.48785100 -0.70611200
C 1.40734300 -4.48866800 0.48584000
C 2.65626600 -2.41841600 1.96406700
H 4.73308200 -2.23825000 2.42959200
C 0.81544400 -5.61225600 -0.11527600
H -0.87130300 -6.31806000 -1.23064200
H 2.42303700 -4.58426100 0.84521600
H 2.42312600 -3.11452500 2.75889200
H 1.35828400 -6.54922100 -0.14693300
H 6.32083300 -1.36090900 0.67865000
H -6.59694100 1.49832600 0.11181500

Table S20 Cartesian coordinates and energies of ***i*-TEQ 6a**.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.461758 (Hartree/Particle)
Thermal correction to Energy= 0.488345
Thermal correction to Enthalpy= 0.489289
Thermal correction to Gibbs Free Energy= 0.407004
Sum of electronic and zero-point Energies= -1602.576268
Sum of electronic and thermal Energies= -1602.549681
Sum of electronic and thermal Enthalpies= -1602.548737
Sum of electronic and thermal Free Energies= -1602.631022
C 0.54579200 0.50889400 -1.90781200
C 2.66577800 1.02697400 -1.16191000
C 2.57533300 2.35953900 -1.66768400
C 1.34827900 2.74034100 -2.27710800
C 0.31319100 1.84251800 -2.34618000
C 3.79100900 0.65292900 -0.35294000
C 3.67192300 3.24339300 -1.50213300
H 1.23484200 3.75471500 -2.65128200
H -0.66110400 2.11185900 -2.73696900
C 4.78974800 2.83350100 -0.81036900
C 4.83365300 1.55113400 -0.21377400
H 3.60783900 4.24827800 -1.91147000
H 5.62869000 3.51034600 -0.67878800
H 5.68396900 1.27881200 0.40480900
N 1.68685000 0.10836200 -1.38320700
C -0.31317200 1.84254300 2.34614200
C -1.34825900 2.74036700 2.27707200
C -2.57532400 2.35955600 1.66767300
C -2.66577400 1.02698600 1.16191500
C -0.54578200 0.50891100 1.90780300
H -3.60783400 4.24829300 1.91145500
H 0.66113200 2.11189400 2.73690100
H -1.23481300 3.75474700 2.65122600
C -3.67191800 3.24340500 1.50212700
C -3.79100800 0.65293300 0.35295400
C -4.83365500 1.55113600 0.21378700
C -4.78974800 2.83350600 0.81037500
H -5.68397200 1.27880900 -0.40479300
H -5.62869300 3.51034700 0.67880000
N -1.68684700 0.10837300 1.38321600
C 0.54578400 -0.50890700 1.90781100
C 2.66577300 -1.02698000 1.16191600
C 2.57532200 -2.35955600 1.66766600
C 1.34825000 -2.74037300 2.27704100
C 0.31316500 -1.84254400 2.34611400
C 3.79101100 -0.65292300 0.35296000
C 3.67192300 -3.24339900 1.50212800
H 1.23478900 -3.75476100 2.65116800
H -0.66115100 -2.11190800 2.73683700
C 4.78975800 -2.83349000 0.81039000
C 4.83366300 -1.55111900 0.21380200
H 3.60784000 -4.24828900 1.91145100
H 5.62871300 -3.51032200 0.67883000
H 5.68398400 -1.27879100 -0.40477200
N 1.68685300 -0.10836600 1.38323000
C -0.31318200 -1.84254600 -2.34613600
C -1.34827200 -2.74037000 -2.27705600
C -2.57533200 -2.35955300 -1.66765700
C -2.66577200 -1.02698000 -1.16189900
C -0.54578400 -0.50891600 -1.90780500
H -3.60785600 -4.24828200 -1.91144400
H 0.66112000 -2.11190600 -2.73689600
H -1.23482400 -3.75475400 -2.65119900

C -3.67193600 -3.24339200 -1.50211800
C -3.79101000 -0.65291900 -0.35294400
C -4.83366600 -1.55111100 -0.21378700
C -4.78976700 -2.83348200 -0.81037700
H -5.68398800 -1.27877700 0.40478400
H -5.62872300 -3.51031200 -0.67881200
N -1.68684300 -0.10837200 -1.38320500

Table S21 Cartesian coordinates and energies of ***i*-TEQ 6a**.
B3LYP-D3/6-31G(d,p)/IEFPCM($CHCl_3$)
Zero-point correction= 0.461864 (Hartree/Particle)
Thermal correction to Energy= 0.488473
Thermal correction to Enthalpy= 0.489417
Thermal correction to Gibbs Free Energy= 0.406952
Sum of electronic and zero-point Energies= -1602.585271
Sum of electronic and thermal Energies= -1602.558663
Sum of electronic and thermal Enthalpies= -1602.557718
Sum of electronic and thermal Free Energies= -1602.640183
C 0.55152100 -0.50401200 1.97045300
C 2.66059800 -1.01876000 1.18717100
C 2.59238900 -2.34101400 1.72502100
C 1.38634100 -2.71789700 2.37673900
C 0.34607000 -1.82581800 2.45362800
C 3.77370300 -0.65023800 0.35903300
C 3.69151500 -3.22212300 1.55692000
H 1.29295400 -3.72245600 2.78068300
H -0.61002100 -2.09448200 2.88778600
C 4.79425100 -2.81836400 0.83777600
C 4.82030100 -1.54504800 0.22039700
H 3.64121200 -4.21819100 1.98829700
H 5.63586900 -3.49114900 0.70429100
H 5.66313400 -1.27618100 -0.40960800
N 1.67434100 -0.10505800 1.40409300
C -0.34607200 -1.82582600 -2.45362500
C -1.38634300 -2.71790500 -2.37673200
C -2.59238900 -2.34102000 -1.72501300
C -2.66059800 -1.01876400 -1.18716600
C -0.55152000 -0.50402000 -1.97045100
H -3.64121400 -4.21819600 -1.98828500
H 0.61001800 -2.09449200 -2.88778400
H -1.29295800 -3.72246400 -2.78067400
C -3.69151600 -3.22212700 -1.55691000
C -3.77370300 -0.65023900 -0.35903000
C -4.82030100 -1.54504800 -0.22039100
C -4.79425200 -2.81836600 -0.83776600
H -5.66313500 -1.27617900 0.40961300
H -5.63587000 -3.49115000 -0.70428000
N -1.67433900 -0.10506400 -1.40409000
C 0.55152000 0.50400900 -1.97045600
C 2.66059600 1.01876100 -1.18717200
C 2.59238500 2.34101300 -1.72502400
C 1.38633700 2.71789400 -2.37674300
C 0.34606700 1.82581400 -2.45363200
C 3.77370200 0.65024000 -0.35903500
C 3.69151000 3.22212400 -1.55692500
H 1.29295000 3.72245300 -2.78068800
H -0.61002400 2.09447700 -2.88779000
C 4.79424700 2.81836600 -0.83778000
C 4.82029900 1.54505100 -0.22040100
H 3.64120600 4.21819100 -1.98830300
H 5.63586400 3.49115200 -0.70429600
H 5.66313300 1.27618500 0.40960400
N 1.67433900 0.10505700 -1.40409400
C -0.34606700 1.82582400 2.45362500
C -1.38633600 2.71790300 2.37673300
C -2.59238500 2.34102000 1.72501600
C -2.66059500 1.01876500 1.18716900
C -0.55151900 0.50401600 1.97045300
H -3.64120600 4.21819800 1.98828900
H 0.61002500 2.09448800 2.88778200
H -1.29294900 3.72246300 2.78067500
C -3.69151000 3.22212900 1.55691400
C -3.77370200 0.65024200 0.35903400
C -4.82029900 1.54505200 0.22039600
C -4.79424700 2.81836900 0.83777100
H -5.66313300 1.27618400 -0.40960700
H -5.63586400 3.49115500 0.70428500
N -1.67433800 0.10506200 1.40409300

Table S22 Cartesian coordinates and energies of ***i*-TEQ 6a**.
M06-2X/6-31G(d,p)/IEFPCM($CHCl_3$)
Zero-point correction= 0.466492 (Hartree/Particle)
Thermal correction to Energy= 0.492982
Thermal correction to Enthalpy= 0.493926
Thermal correction to Gibbs Free Energy= 0.411532
Sum of electronic and zero-point Energies= -1601.877495
Sum of electronic and thermal Energies= -1601.851005
Sum of electronic and thermal Enthalpies= -1601.850061
Sum of electronic and thermal Free Energies= -1601.932454
C 0.55412000 -0.50182200 1.94463600
C 2.65926400 -1.01521700 1.18167000
C 2.59446000 -2.32326700 1.72737300
C 1.38929400 -2.70229000 2.37842500
C 0.34845000 -1.81868200 2.44080700
C 3.77495400 -0.64944900 0.35956400
C 3.69565400 -3.20340500 1.57173700
H 1.30233700 -3.70400900 2.79022800
H -0.60895500 -2.08227300 2.87484000
C 4.79595500 -2.80538500 0.85695200
C 4.82058500 -1.53633000 0.23025300
H 3.64415700 -4.19442100 2.01350600
H 5.63947100 -3.47614200 0.73234100
H 5.66491100 -1.26834000 -0.39832800
N 1.66986400 -0.10236600 1.38320100
C -0.34845000 -1.81868900 -2.44080100
C -1.38929300 -2.70229700 -2.37841600
C -2.59446000 -2.32327200 -1.72736600
C -2.65926400 -1.01522100 -1.18166800
C -0.55412100 -0.50182700 -1.94463500
H -3.64415700 -4.19442800 -2.01349200
H 0.60895600 -2.08228100 -2.87483300
H -1.30233600 -3.70401800 -2.79021500
C -3.69565400 -3.20341000 -1.57172600
C -3.77495400 -0.64945000 -0.35956200
C -4.82058500 -1.53633100 -0.23024800
C -4.79595400 -2.80538800 -0.85694300
H -5.66491000 -1.26833900 0.39833200
H -5.63947100 -3.47614500 -0.73232900
N -1.66986400 -0.10237000 -1.38320200
C 0.55411800 0.50182300 -1.94463600

C 2.65926300 1.01521700 -1.18167400
C 2.59445900 2.32326700 -1.72737600
C 1.38929200 2.70229100 -2.37842700
C 0.34844800 1.81868300 -2.44080700
C 3.77495300 0.64944900 -0.35956900
C 3.69565400 3.20340400 -1.57174200
H 1.30233500 3.70401000 -2.79022900
H -0.60895800 2.08227400 -2.87483900
C 4.79595500 2.80538400 -0.85695900
C 4.82058600 1.53632900 -0.23025900
H 3.64415700 4.19442100 -2.01351000
H 5.63947200 3.47614000 -0.73234900
H 5.66491200 1.26833900 0.39832000
N 1.66986200 0.10236700 -1.38320300
C -0.34844800 1.81869000 2.44080100
C -1.38929100 2.70229800 2.37841800
C -2.59445900 2.32327200 1.72736900
C -2.65926300 1.01522100 1.18167100
C -0.55411900 0.50182800 1.94463500
H -3.64415600 4.19442800 2.01349600
H 0.60895900 2.08228300 2.87483100
H -1.30233400 3.70401900 2.79021600
C -3.69565300 3.20340900 1.57173100
C -3.77495400 0.64945000 0.35956700
C -4.82058600 1.53633000 0.23025400
C -4.79595500 2.80538700 0.85694900
H -5.66491200 1.26833800 -0.39832500
H -5.63947100 3.47614300 0.73233700
N -1.66986300 0.10237000 1.38320400

Table S23 Cartesian coordinates and energies of ***i*-TEQ 6a**.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.459362 (Hartree/Particle)
Thermal correction to Energy= 0.486017
Thermal correction to Enthalpy= 0.486961
Thermal correction to Gibbs Free Energy= 0.404498
Sum of electronic and zero-point Energies= -1602.963539
Sum of electronic and thermal Energies= -1602.936884
Sum of electronic and thermal Enthalpies= -1602.935939
Sum of electronic and thermal Free Energies= -1603.018402
C 0.54913600 -0.50438800 1.95173800
C 2.65367500 -1.02109300 1.17606600
C 2.57464300 -2.34455900 1.69504200
C 1.36656100 -2.72007600 2.33428400
C 0.33491200 -1.82739900 2.41641900
C 3.76386400 -0.65223100 0.35264600
C 3.66217400 -3.23000000 1.51203600
H 1.26342400 -3.72760800 2.72263300
H -0.62627500 -2.09711100 2.83259200
C 4.76035500 -2.82926100 0.79467100
C 4.79572600 -1.55191000 0.19601000
H 3.60615600 -4.22983400 1.92837500
H 5.59249400 -3.50738200 0.64786300
H 5.63432600 -1.28612900 -0.43705400
N 1.67367700 -0.10876800 1.40206200
C -0.33491200 -1.82740700 -2.41641400
C -1.36656200 -2.72008400 -2.33427600
C -2.57464400 -2.34456500 -1.69503400
C -2.65367500 -1.02109800 -1.17606200
C -0.54913600 -0.50439600 -1.95173500
H -3.60615700 -4.22984000 -1.92836200
H 0.62627400 -2.09712100 -2.83258700
H -1.26342600 -3.72761700 -2.72262200
C -3.66217500 -3.23000500 -1.51202500
C -3.76386300 -0.65223300 -0.35264300
C -4.79572600 -1.55191000 -0.19600500
C -4.76035500 -2.82926300 -0.79466200
H -5.63432600 -1.28612800 0.43705800
H -5.59249500 -3.50738400 -0.64785200
N -1.67367600 -0.10877400 -1.40205900
C 0.54913500 0.50438500 -1.95174100
C 2.65367300 1.02109400 -1.17606800
C 2.57463900 2.34455900 -1.69504500
C 1.36655600 2.72007300 -2.33428800
C 0.33490800 1.82739500 -2.41642200
C 3.76386200 0.65223300 -0.35264900
C 3.66216800 3.23000100 -1.51204000
H 1.26341800 3.72760500 -2.72263600
H -0.62628000 2.09710600 -2.83259300
C 4.76035000 2.82926400 -0.79467600
C 4.79572400 1.55191300 -0.19601400
H 3.60614900 4.22983500 -1.92838000
H 5.59248900 3.50738700 -0.64786900
H 5.63432400 1.28613400 0.43704900
N 1.67367600 0.10876700 -1.40206300
C -0.33490800 1.82740400 2.41641600
C -1.36655700 2.72008200 2.33427900
C -2.57463900 2.34456500 1.69503700
C -2.65367200 1.02109800 1.17606400
C -0.54913400 0.50439200 1.95173800
H -3.60615000 4.22984100 1.92836700
H 0.62627900 2.09711600 2.83258800
H -1.26341900 3.72761400 2.72262500
C -3.66216900 3.23000600 1.51203000
C -3.76386200 0.65223500 0.35264700
C -4.79572400 1.55191400 0.19600900
C -4.76035000 2.82926600 0.79466700
H -5.63432400 1.28613200 -0.43705300
H -5.59248900 3.50738900 0.64785800
N -1.67367400 0.10877200 1.40206100

Table S24 Cartesian coordinates and energies of ***i*-TEQ 6a**.
B3LYP-D3/6-311+G(2d,p)SMD(Et_2O)
Zero-point correction= 0.459375 (Hartree/Particle)
Thermal correction to Energy= 0.486044
Thermal correction to Enthalpy= 0.486988
Thermal correction to Gibbs Free Energy= 0.404445
Sum of electronic and zero-point Energies= -1603.001292
Sum of electronic and thermal Energies= -1602.974623
Sum of electronic and thermal Enthalpies= -1602.973679
Sum of electronic and thermal Free Energies= -1603.056221
C 0.55388600 -0.50056900 2.01615600
C 2.64648800 -1.01509000 1.19977100
C 2.58839800 -2.32885900 1.74799300
C 1.40211700 -2.69945700 2.42916900
C 0.36668800 -1.81128200 2.52283100
C 3.74454400 -0.65061100 0.35762400
C 3.67720600 -3.21266600 1.56010500
H 1.31867700 -3.69821100 2.84378700
H -0.57480700 -2.08004300 2.98361100

C 4.75986700 -2.81767800 0.81606600
C 4.77933700 -1.54800900 0.19975500
H 3.63346600 -4.20491500 1.99567500
H 5.59376800 -3.49305200 0.66495200
H 5.61142700 -1.28627400 -0.44369100
N 1.65866500 -0.10876200 1.42263400
C -0.36669200 -1.81137900 -2.52276400
C -1.40211800 -2.69955400 -2.42906400
C -2.58840600 -2.32892900 -1.74790600
C -2.64651000 -1.01512600 -1.19977100
C -0.55391100 -0.50063300 -2.01618900
H -3.63343800 -4.20501900 -1.99545100
H 0.57481100 -2.08017500 -2.98350700
H -1.31866100 -3.69833700 -2.84360800
C -3.67718800 -3.21274600 -1.55993600
C -3.74453600 -0.65062500 -0.35759600
C -4.77931700 -1.54802800 -0.19965900
C -4.75984200 -2.81773100 -0.81589800
H -5.61139400 -1.28626400 0.44379300
H -5.59372300 -3.49311400 -0.66470900
N -1.65870200 -0.10879900 -1.42271200
C 0.55388300 0.50061700 -2.01613600
C 2.64650600 1.01508400 -1.19976500
C 2.58843700 2.32886000 -1.74797100
C 1.40216200 2.69948600 -2.42914400
C 0.36671600 1.81133100 -2.52281600
C 3.74455600 0.65058000 -0.35762100
C 3.67726100 3.21264400 -1.56007900
H 1.31874200 3.69824200 -2.84376000
H -0.57476700 2.08011000 -2.98361000
C 4.75991800 2.81763200 -0.81604700
C 4.77936500 1.54795800 -0.19974500
H 3.63354000 4.20489800 -1.99564100
H 5.59383200 3.49299100 -0.66493100
H 5.61145000 1.28620300 0.44370100
N 1.65866000 0.10877800 -1.42262800
C -0.36670700 1.81143100 2.52272700
C -1.40214800 2.69958900 2.42902800
C -2.58843500 2.32893600 1.74788700
C -2.64652800 1.01512600 1.19976600
C -0.55390700 0.50068100 2.01614700
H -3.63351000 4.20500600 1.99542800
H 0.57479400 2.08023500 2.98346900
H -1.31870600 3.69837400 2.84356900
C -3.67724200 3.21272700 1.55992400
C -3.74455400 0.65059900 0.35760000
C -4.77935300 1.54797900 0.19966600
C -4.75989500 2.81768500 0.81590100
H -5.61142900 1.28619900 -0.44378000
H -5.59379000 3.49305200 0.66472200
N -1.65870200 0.10881900 1.42269900

Table S25 Cartesian coordinates and energies of ***i*-TEQ 6a** (TS).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.460529 (Hartree/Particle)
Thermal correction to Energy= 0.486410
Thermal correction to Enthalpy= 0.487354
Thermal correction to Gibbs Free Energy= 0.405938
Sum of electronic and zero-point Energies= -1602.477671
Sum of electronic and thermal Energies= -1602.451791
Sum of electronic and thermal Enthalpies= -1602.450846
Sum of electronic and thermal Free Energies= -1602.532262
C 0.56584700 -2.73629300 -0.42770100
C 2.68626800 -1.93273200 -0.02109100
C 3.08644400 -3.16642400 0.60802300
C 2.13484000 -4.20629000 0.67629700
C 0.88618700 -3.99873400 0.16821500
C 3.66378600 -0.89056400 -0.10530200
C 4.38237700 -3.34211400 1.14752500
H 2.40075800 -5.14699500 1.15150000
H 0.12572500 -4.76353000 0.25942900
C 5.29322700 -2.32026400 1.07400600
C 4.92299400 -1.11339900 0.44969900
H 4.63105000 -4.29007800 1.61734600
H 6.29054300 -2.42711500 1.48956300
H 5.64887300 -0.30858700 0.41083700
N 1.43436200 -1.74573200 -0.53388200
C -0.93667600 3.97199000 1.01388400
C -2.15150700 4.30528800 0.49456900
C -2.98569300 3.29326100 -0.02337900
C -2.58447200 1.92425600 0.20103900
C -0.50876800 2.60494200 0.98022500
H -4.38137000 4.68693100 -0.90436800
H -0.27572400 4.75862400 1.34493700
H -2.46452300 5.34387500 0.42645000
C -4.15369400 3.63664300 -0.74261600
C -3.54998900 0.91324700 -0.15395500
C -4.65500100 1.30653100 -0.91099000
C -4.95404900 2.64252600 -1.23958500
H -5.34229600 0.53530600 -1.24068800
H -5.83265800 2.86825900 -1.83581900
N -1.34056400 1.61560100 0.67613900
C 0.98926500 2.42730900 1.01129000
C 2.79131100 1.55283400 -0.15053000
C 3.40277000 2.85142700 -0.22277900
C 2.93324200 3.80558000 0.71375700
C 1.77742500 3.56353000 1.40080000
C 3.54362400 0.46426300 -0.72605400
C 4.44501700 3.12456400 -1.14078700
H 3.49249900 4.72550400 0.86366400
H 1.42761200 4.26272700 2.15009300
C 4.93097800 2.10812200 -1.92769500
C 4.52410700 0.78218500 -1.65687800
H 4.83817500 4.13531800 -1.21120000
H 5.69324700 2.29615000 -2.67742000
H 5.06317000 -0.03448500 -2.12765000
N 1.55217500 1.39959200 0.39398300
C -1.54943300 -3.78439300 -1.22701100
C -2.86766400 -3.95087400 -0.90841600
C -3.54924800 -2.91684600 -0.22074900
C -2.88656000 -1.64066600 -0.14172000
C -0.88742000 -2.60142400 -0.76916000
H -5.26425700 -4.11738400 0.32545900
H -0.98748500 -4.56372200 -1.73032100
H -3.39061900 -4.87687600 -1.13359600
C -4.81726400 -3.12774500 0.37084800
C -3.67997200 -0.51772300 0.28181400
C -4.88628500 -0.79325700 0.92070100
C -5.43902800 -2.08812400 1.01662400

H -5.46272100 0.04292100 1.30333600
H -6.38357300 -2.23285500 1.53185800
N -1.55002200 -1.52628700 -0.37779900

Table S26 Cartesian coordinates and energies of ***i*-TEQ 6a** (TS).
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.458593 (Hartree/Particle)
Thermal correction to Energy= 0.484439
Thermal correction to Enthalpy= 0.485383
Thermal correction to Gibbs Free Energy= 0.404384
Sum of electronic and zero-point Energies= -1602.909603
Sum of electronic and thermal Energies= -1602.883757
Sum of electronic and thermal Enthalpies= -1602.882813
Sum of electronic and thermal Free Energies= -1602.963811
C -0.53505200 -2.79853800 0.80516100
C -2.57203400 -1.97018300 0.09149300
C -3.00105800 -3.27947800 -0.31885600
C -2.18532600 -4.37017700 0.03384000
C -0.97521000 -4.14115500 0.60906200
C -3.48961100 -0.89238700 -0.12207500
C -4.18869000 -3.48028500 -1.05353300
H -2.51131200 -5.37882700 -0.19472500
H -0.32822600 -4.97593300 0.82491100
C -4.97207400 -2.40794600 -1.37432100
C -4.62637700 -1.13886700 -0.87910600
H -4.45224000 -4.48669700 -1.35932100
H -5.87318200 -2.52724700 -1.96377000
H -5.29940700 -0.31330400 -1.07389300
N -1.33460900 -1.76114500 0.62406800
C 0.97510800 4.14126600 -0.60756100
C 2.18521000 4.37013200 -0.03224100
C 3.00111700 3.27934000 0.31977000
C 2.57218500 1.97020100 -0.09116200
C 0.53518000 2.79870000 -0.80452800
H 4.45236500 4.48618200 1.36058400
H 0.32794400 4.97604400 -0.82290300
H 2.51106100 5.37869400 0.19690300
C 4.18885100 3.47989300 1.05435700
C 3.48978400 0.89234900 0.12193200
C 4.62668000 1.13857000 0.87884500
C 4.97239300 2.40747500 1.37449700
H 5.29976300 0.31295200 1.07321800
H 5.87360500 2.52659300 1.96382400
N 1.33481400 1.76129700 -0.62391100
C -0.95111000 2.63834600 -0.94276200
C -2.80148100 1.62661900 0.00054400
C -3.46994400 2.89037000 0.09172500
C -2.94895100 3.93488000 -0.70480900
C -1.72215600 3.79303900 -1.27817300
C -3.51500400 0.47947200 0.48431200
C -4.59899400 3.06107900 0.92198300
H -3.51850700 4.85009500 -0.82386400
H -1.31129700 4.57787900 -1.89695000
C -5.09145200 1.98693900 1.61387800
C -4.58336400 0.70212200 1.33527800
H -5.04952400 4.04376700 1.00703600
H -5.92344800 2.09773900 2.29887500
H -5.10539100 -0.15772900 1.73839100
N -1.52490700 1.55170900 -0.46121600
C 1.72246000 -3.79295100 1.27799400
C 2.94900500 -3.93483100 0.70410800
C 3.46974900 -2.89030700 -0.09256600
C 2.80141300 -1.62652200 -0.00098200
C 0.95130400 -2.63822600 0.94290700
H 5.04891500 -4.04370700 -1.00858700
H 1.31190600 -4.57777800 1.89698200
H 3.51856400 -4.85007700 0.82290300
C 4.59850100 -3.06099100 -0.92323400
C 3.51490400 -0.47936200 -0.48477800
C 4.58298600 -0.70195700 -1.33610100
C 5.09084800 -1.98677900 -1.61509800
H 5.10498900 0.15791800 -1.73919600
H 5.92261900 -2.09754500 -2.30037400
N 1.52499800 -1.55159200 0.46122600

Table S27 Cartesian coordinates and energies of ***i*-TEQ 6a** (Int).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.460696 (Hartree/Particle)
Thermal correction to Energy= 0.487419
Thermal correction to Enthalpy= 0.488363
Thermal correction to Gibbs Free Energy= 0.403724
Sum of electronic and zero-point Energies= -1602.477966
Sum of electronic and thermal Energies= -1602.451243
Sum of electronic and thermal Enthalpies= -1602.450299
Sum of electronic and thermal Free Energies= -1602.534938
C 0.52352200 -2.64406400 0.65098300
C 2.66166700 -1.94327200 0.12570900
C 3.02157800 -3.25749600 -0.35105900
C 2.05921300 -4.28235400 -0.24352200
C 0.82371100 -3.98636100 0.24915100
C 3.67402500 -0.92648100 0.05029300
C 4.28409800 -3.53415300 -0.92554400
H 2.30282500 -5.28477800 -0.58584000
H 0.05532000 -4.74701100 0.27343200
C 5.20836300 -2.53055300 -1.04378700
C 4.89089200 -1.25054300 -0.55298100
H 4.49126000 -4.54197800 -1.27551500
H 6.17679100 -2.70707500 -1.50158800
H 5.63195700 -0.46631900 -0.65753600
N 1.41725500 -1.66757600 0.62196600
C -0.82372300 3.98637400 -0.24926600
C -2.05923100 4.28238200 0.24337800
C -3.02158700 3.25751400 0.35096800
C -2.66166300 1.94327200 -0.12573000
C -0.52351600 2.64405600 -0.65101700
H -4.49127600 4.54203300 1.27535700
H -0.05533700 4.74702900 -0.27358200
H -2.30286000 5.28482500 0.58562800
C -4.28410300 3.53419000 0.92544600
C -3.67400500 0.92647900 -0.05027400
C -4.89087400 1.25055500 0.55300800
C -5.20835300 2.53057900 1.04375800
H -5.63192500 0.46632300 0.65759900
H -6.17677600 2.70710800 1.50157000
N -1.41723800 1.66756100 -0.62196800
C 0.94493800 2.44299400 -0.90771500
C 2.88123500 1.56334800 -0.00935000
C 3.52497200 2.84686400 -0.09700900

C 2.92614500 3.79365700 -0.96532500
C 1.66040200 3.56945800 -1.42996200
C 3.66555600 0.48689700 0.54509000
C 4.69429700 3.13604800 0.64674600
H 3.46626700 4.70286800 -1.21694500
H 1.16473900 4.28027400 -2.08223100
C 5.24625100 2.15772600 1.43738900
C 4.76087800 0.83595900 1.32777200
H 5.12038400 4.13462600 0.59707700
H 6.10390800 2.36593300 2.06952400
H 5.32092200 0.03747700 1.80479700
N 1.57362000 1.41508400 -0.36159600
C -1.66037800 -3.56947400 1.42998000
C -2.92614200 -3.79366600 0.96538000
C -3.52498400 -2.84687500 0.09708900
C -2.88123800 -1.56336200 0.00940600
C -0.94493100 -2.44301500 0.90773300
H -5.12041800 -4.13462500 -0.59698000
H -1.16469500 -4.28031400 2.08220500
H -3.46624800 -4.70288600 1.21700500
C -4.69432200 -3.13605200 -0.64666000
C -3.66556000 -0.48691000 -0.54504700
C -4.76088000 -0.83596800 -1.32772000
C -5.24626600 -2.15774000 -1.43731100
H -5.32093000 -0.03749300 -1.80474900
H -6.10392700 -2.36594700 -2.06944200
N -1.57362200 -1.41509100 0.36163000

Table S28 Cartesian coordinates and energies of ***i*-TEQ 6a** (Int).
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.458601 (Hartree/Particle)
Thermal correction to Energy= 0.484445
Thermal correction to Enthalpy= 0.485390
Thermal correction to Gibbs Free Energy= 0.404394
Sum of electronic and zero-point Energies= -1602.909595
Sum of electronic and thermal Energies= -1602.883750
Sum of electronic and thermal Enthalpies= -1602.882806
Sum of electronic and thermal Free Energies= -1602.963802
C 0.53570000 -2.79837300 0.80469400
C 2.57259700 -1.96975900 0.09142300
C 3.00168600 -3.27888700 -0.31933000
C 2.18587700 -4.36970400 0.03279400
C 0.97580000 -4.14087200 0.60822400
C 3.49015100 -0.89191000 -0.12173400
C 4.18953900 -3.47940300 -1.05384900
H 2.51163900 -5.37823100 -0.19655100
H 0.32864400 -4.97571100 0.82335900
C 4.97290000 -2.40689900 -1.37417100
C 4.62700900 -1.13799400 -0.87864000
H 4.45329200 -4.48569100 -1.35983500
H 5.87414800 -2.52588600 -1.96346100
H 5.30002600 -0.31233900 -1.07311800
N 1.33505700 -1.76099800 0.62384300
C -0.97579600 4.14086200 -0.60828400
C -2.18587300 4.36970400 -0.03285600
C -3.00167700 3.27889200 0.31929400
C -2.57258900 1.96975700 -0.09143900
C -0.53569400 2.79836100 -0.80472200
H -4.45327800 4.48571200 1.35978800
H -0.32864200 4.97569900 -0.82344000
H -2.51163600 5.37823500 0.19646800
C -4.18952600 3.47942000 1.05381700
C -3.49014300 0.89191200 0.12173800
C -4.62699500 1.13800700 0.87864900
C -4.97288200 2.40692100 1.37416300
H -5.30001200 0.31235600 1.07314300
H -5.87412600 2.52591600 1.96345800
N -1.33504900 1.76098800 -0.62385400
C 0.95047300 2.63778500 -0.94263400
C 2.80086500 1.62661800 0.00114600
C 3.46898700 2.89061300 0.09199000
C 2.94794400 3.93470600 -0.70500800
C 1.72137000 3.79241500 -1.27854000
C 3.51489400 0.47986600 0.48480400
C 4.59786500 3.06198200 0.92231200
H 3.51747500 4.84986700 -0.82452100
H 1.31082500 4.57697800 -1.89791800
C 5.09069400 1.98809900 1.61436000
C 4.58324600 0.70308500 1.33569100
H 5.04810700 4.04481700 1.00710700
H 5.92259500 2.09932100 2.29939500
H 5.10577600 -0.15651800 1.73866900
N 1.52425000 1.55133400 -0.46062300
C -1.72136500 -3.79241500 1.27855200
C -2.94795000 -3.93470400 0.70504300
C -3.46900000 -2.89061300 -0.09195400
C -2.80086800 -1.62662200 -0.00113200
C -0.95046500 -2.63779400 0.94261900
H -5.04814300 -4.04481600 -1.00703400
H -1.31081500 -4.57697400 1.89793100
H -3.51748500 -4.84985800 0.82457600
C -4.59789300 -3.06198300 -0.92225500
C -3.51489900 -0.47986900 -0.48478800
C -4.58326600 -0.70309000 -1.33565600
C -5.09072600 -1.98810300 -1.61430500
H -5.10579800 0.15651300 -1.73863200
H -5.92263900 -2.09932600 -2.29932500
N -1.52424500 -1.55134100 0.46061400

Table S29 Cartesian coordinates and energies of biphenyl.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.181890 (Hartree/Particle)
Thermal correction to Energy= 0.190732
Thermal correction to Enthalpy= 0.191676
Thermal correction to Gibbs Free Energy= 0.147410
Sum of electronic and zero-point Energies= -463.155340
Sum of electronic and thermal Energies= -463.146498
Sum of electronic and thermal Enthalpies= -463.145553
Sum of electronic and thermal Free Energies= -463.189820
C -0.74228800 0.00000000 0.00000000
C -1.46361200 -1.13546700 -0.40522100
C -2.85754000 -1.13608200 -0.40435900
C -3.56099200 0.00000000 0.00000000
C -2.85754000 1.13608200 0.40435900
C -1.46361200 1.13546700 0.40522200
C 0.74228800 0.00000000 0.00000000
C 1.46361200 -1.13546700 0.40522100
C 2.85754000 -1.13608200 0.40435900
C 3.56099200 0.00000000 0.00000000

C 2.85754000 1.13608200 -0.40435900
C 1.46361200 1.13546600 -0.40522200
H -0.92478800 -2.01402000 -0.74739600
H -3.39512300 -2.02242100 -0.72908600
H -4.64699200 0.00000000 -0.00000100
H -3.39512300 2.02242200 0.72908700
H -0.92478900 2.01402000 0.74739800
H 0.92478800 -2.01402100 0.74739500
H 3.39512300 -2.02242100 0.72908700
H 4.64699200 0.00000000 0.00000100
H 3.39512300 2.02242100 -0.72908800
H 0.92478900 2.01402000 -0.74739800

Table S30 Cartesian coordinates and energies of biphenyl.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.180938 (Hartree/Particle)
Thermal correction to Energy= 0.189823
Thermal correction to Enthalpy= 0.190767
Thermal correction to Gibbs Free Energy= 0.147012
Sum of electronic and zero-point Energies= -463.269709
Sum of electronic and thermal Energies= -463.260825
Sum of electronic and thermal Enthalpies= -463.259880
Sum of electronic and thermal Free Energies= -463.303635
C 0.00000000 0.74117500 0.00000000
C -0.42245700 1.46021500 1.12451400
C -0.42300500 2.84992500 1.12486400
C 0.00000000 3.55136000 0.00000000
C 0.42300500 2.84992500 -1.12486400
C 0.42245700 1.46021500 -1.12451400
C 0.00000000 -0.74117500 0.00000000
C 0.42245700 -1.46021500 1.12451400
C 0.42300500 -2.84992500 1.12486400
C 0.00000000 -3.55136000 0.00000000
C -0.42300500 -2.84992500 -1.12486400
C -0.42245700 -1.46021500 -1.12451400
H -0.77604200 0.92419600 1.99728600
H -0.76268700 3.38632200 2.00314900
H 0.00000000 4.63477100 0.00000000
H 0.76268700 3.38632100 -2.00314900
H 0.77604200 0.92419600 -1.99728600
H 0.77604200 -0.92419600 1.99728600
H 0.76268700 -3.38632200 2.00314900
H 0.00000000 -4.63477100 0.00000000
H -0.76268700 -3.38632100 -2.00314900
H -0.77604200 -0.92419600 -1.99728600

Table S31 Cartesian coordinates and energies of 2,8-diphenylquinoline.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.297680 (Hartree/Particle)
Thermal correction to Energy= 0.313763
Thermal correction to Enthalpy= 0.314707
Thermal correction to Gibbs Free Energy= 0.252764
Sum of electronic and zero-point Energies= -863.804364
Sum of electronic and thermal Energies= -863.788281
Sum of electronic and thermal Enthalpies= -863.787337
Sum of electronic and thermal Free Energies= -863.849280
C 3.26462500 -1.33005400 0.09212900
C 2.12051500 -0.54587500 0.07482000
C 0.84561100 -1.20973300 0.02686900
C 0.79998500 -2.64161900 -0.00120500
C 2.00056300 -3.39198700 0.02079300
C 3.21235500 -2.74146500 0.06522200
H 4.23224200 -0.84103300 0.15025000
C -0.48307900 -3.24246300 -0.06790300
H 1.94758400 -4.47735700 0.00368600
H 4.13806000 -3.30850700 0.08909400
C -1.61029200 -2.46233000 -0.09588700
C -1.47429100 -1.04248500 -0.05480100
H -0.55813700 -4.32624900 -0.10789400
H -2.58873800 -2.92087200 -0.17519100
N -0.28511100 -0.46101400 -0.00619700
C 2.23822000 0.93526100 0.08430200
C 1.44991100 1.74078200 0.92458500
C 3.18702900 1.56216000 -0.74025200
C 1.61257300 3.12438200 0.93889000
H 0.70972500 1.27538500 1.56312600
C 3.34712800 2.94750500 -0.72727400
H 3.78643300 0.95702800 -1.41421400
C 2.56017500 3.73467400 0.11367900
H 0.99745000 3.72839300 1.59986600
H 4.08131300 3.41065900 -1.38032300
H 2.68114100 4.81404400 0.12446600
C -2.65455800 -0.13740800 -0.08055900
C -3.95164600 -0.59247600 0.20656200
C -2.47401200 1.22339000 -0.38642100
C -5.03716700 0.28222600 0.17878900
H -4.12157100 -1.62907800 0.47870900
C -3.55923100 2.09402600 -0.41621400
H -1.47063400 1.57714100 -0.59495100
C -4.84667900 1.62797000 -0.13650800
H -6.03160700 -0.08836800 0.40998200
H -3.40104000 3.14056500 -0.66051200
H -5.69284500 2.30847000 -0.16041000

Table S32. Cartesian coordinates and energies of 2,8-diphenylquinoline.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.296104 (Hartree/Particle)
Thermal correction to Energy= 0.312250
Thermal correction to Enthalpy= 0.313194
Thermal correction to Gibbs Free Energy= 0.251040
Sum of electronic and zero-point Energies= -864.014195
Sum of electronic and thermal Energies= -863.998049
Sum of electronic and thermal Enthalpies= -863.997104
Sum of electronic and thermal Free Energies= -864.059259
C 3.26200800 -1.32253600 0.07525500
C 2.12175700 -0.54278700 0.06846900
C 0.85007500 -1.20236500 0.02439500
C 0.80355500 -2.62928100 -0.00595300
C 2.00118100 -3.37752400 0.00820500
C 3.20925800 -2.73018900 0.04606600
H 4.22826300 -0.83487200 0.12504700
C -0.47579400 -3.22895500 -0.06870700
H 1.94945400 -4.46052300 -0.01096100
H 4.13262500 -3.29660900 0.06250500
C -1.59793900 -2.45078700 -0.09286400
C -1.46253900 -1.03438100 -0.05477100
H -0.55210500 -4.31023500 -0.10953400
H -2.57534600 -2.90683300 -0.16798100

N -0.27865600 -0.45479200 -0.00742400
C 2.23634800 0.93631400 0.09012700
C 1.50219700 1.71945700 0.98875400
C 3.12108500 1.57887900 -0.78262700
C 1.65819600 3.09897900 1.01738800
H 0.80773700 1.24105000 1.66493500
C 3.27149400 2.96128000 -0.75954400
H 3.68035600 0.98978700 -1.50012200
C 2.54114300 3.72682800 0.14248100
H 1.08629900 3.68720800 1.72554600
H 3.95504600 3.43927100 -1.45147600
H 2.65613200 4.80413200 0.16278700
C -2.64607800 -0.13696100 -0.08448900
C -3.92264300 -0.58138700 0.27835500
C -2.48991100 1.20087000 -0.47103800
C -5.01179400 0.28203200 0.25013300
H -4.07262000 -1.60086300 0.61059300
C -3.57893600 2.05992900 -0.50430600
H -1.50225400 1.55066600 -0.74039300
C -4.84556000 1.60488200 -0.14520200
H -5.99049700 -0.07900600 0.54333600
H -3.44008300 3.08950600 -0.81268200
H -5.69503700 2.27707800 -0.17039800

Table S33 Cartesian coordinates and energies of 2-phenyl-pyridine.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.169929 (Hartree/Particle)
Thermal correction to Energy= 0.178694
Thermal correction to Enthalpy= 0.179638
Thermal correction to Gibbs Free Energy= 0.135233
Sum of electronic and zero-point Energies= -479.203605
Sum of electronic and thermal Energies= -479.194840
Sum of electronic and thermal Enthalpies= -479.193896
Sum of electronic and thermal Free Energies= -479.238301
C -0.76264500 0.02666400 -0.00064400
C -2.70161600 -1.19783000 -0.23999500
C -3.51704600 -0.08568800 -0.02550000
C -2.89518700 1.13548200 0.23035900
C -1.50522100 1.19424100 0.24967200
C 0.72449100 0.02448900 -0.00513200
C 1.41890200 -1.17676100 0.21429400
C 2.81104900 -1.20080700 0.22640700
C 3.53853400 -0.02780500 0.01155700
C 2.86009600 1.16937200 -0.22162000
C 1.46637300 1.19525400 -0.23083300
H -3.14457100 -2.17413300 -0.43030100
H -4.59773600 -0.17974300 -0.04969200
H -3.48320500 2.02832700 0.42256500
H -1.00314700 2.12721200 0.47906100
H 0.84608300 -2.08322900 0.37314100
H 3.33082600 -2.13776700 0.40497500
H 4.62442600 -0.04764300 0.01971200
H 3.41593000 2.08422600 -0.40560500
H 0.95760600 2.13027800 -0.44321100
N -1.36751300 -1.15531400 -0.23172000

Table S34 Cartesian coordinates and energies of 2-phenyl-pyridine.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.169031 (Hartree/Particle)
Thermal correction to Energy= 0.177819
Thermal correction to Enthalpy= 0.178763
Thermal correction to Gibbs Free Energy= 0.134336
Sum of electronic and zero-point Energies= -479.323891
Sum of electronic and thermal Energies= -479.315103
Sum of electronic and thermal Enthalpies= -479.314158
Sum of electronic and thermal Free Energies= -479.358586
C -0.76107900 0.02058400 -0.00255300
C -2.70126300 -1.18198700 -0.28516500
C -3.50689700 -0.07858400 -0.02521900
C -2.88156400 1.12525500 0.27483100
C -1.49628600 1.17702000 0.29155400
C 0.72358200 0.01818800 -0.00604400
C 1.42000100 -1.16753300 0.25510000
C 2.80814200 -1.18558800 0.26830200
C 3.52869400 -0.02236600 0.01085000
C 2.84791900 1.15941400 -0.26297200
C 1.45830600 1.17960800 -0.27004300
H -3.14768100 -2.14528100 -0.51418800
H -4.58566600 -0.16663200 -0.05028500
H -3.46433700 2.01012600 0.50257100
H -0.98980800 2.09674800 0.55196500
H 0.85605300 -2.07075800 0.44584200
H 3.33063700 -2.11107000 0.48015700
H 4.61209100 -0.03811800 0.01814100
H 3.39929300 2.06664200 -0.48009300
H 0.94622800 2.10319100 -0.51053900
N -1.37059100 -1.14413000 -0.27648900

Table S35 Cartesian coordinates and energies of 2-phenyl-8-(2-pyridyl)quinoline.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.285790 (Hartree/Particle)
Thermal correction to Energy= 0.301748
Thermal correction to Enthalpy= 0.302692
Thermal correction to Gibbs Free Energy= 0.240979
Sum of electronic and zero-point Energies= -879.852953
Sum of electronic and thermal Energies= -879.836996
Sum of electronic and thermal Enthalpies= -879.836051
Sum of electronic and thermal Free Energies= -879.897764
C -3.21691600 -1.36434900 0.03029300
C -2.08687300 -0.55892200 0.04886500
C -0.79824500 -1.19631800 0.02043000
C -0.72839900 -2.62923700 -0.00250200
C -1.91446300 -3.40109400 0.00085500
C -3.13882700 -2.77230100 0.01216300
H -4.18607200 -0.87888800 0.02733300
C 0.56267900 -3.21381400 -0.04878400
H -1.84039100 -4.48537700 -0.01077500
H -4.05459100 -3.35565400 0.01071500
C 1.68096300 -2.42077600 -0.06922700
C 1.52326500 -1.00423800 -0.04191900
H 0.65055900 -4.29682700 -0.08278500
H 2.66755600 -2.86375800 -0.13702500
N 0.32666100 -0.43677200 -0.00675000
C 2.69301600 -0.08688100 -0.07097800
C 3.97431700 -0.50426800 0.32334900
C 5.05262900 0.37921700 0.29246800
H 4.13209900 -1.51561600 0.68418300

C 3.59812900 2.12331000 -0.52368600
C 4.87016800 1.69505700 -0.13456300
H 6.03460600 0.03991600 0.60903600
H 3.44758800 3.14577500 -0.85813400
H 5.71096300 2.38199900 -0.16143000
C -2.27638900 0.92024700 0.07646900
C -1.37575300 1.80256100 0.70021300
C -3.67205400 2.67332400 -0.47735900
C -1.66019600 3.16517800 0.70894300
H -0.47285300 1.41863800 1.15224000
C -2.82959000 3.62184500 0.10365400
H -4.60026700 2.98196600 -0.95589900
H -0.97555200 3.85937400 1.18796700
H -3.08746000 4.67587600 0.08386400
H 1.52880600 1.56762400 -0.78798800
C 2.51983000 1.24391300 -0.49008700
N -3.41505200 1.36394800 -0.49509000

Table S36 Cartesian coordinates and energies of 2-phenyl-8-(2-pyridyl)quinoline.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.284233 (Hartree/Particle)
Thermal correction to Energy= 0.300254
Thermal correction to Enthalpy= 0.301199
Thermal correction to Gibbs Free Energy= 0.239247
Sum of electronic and zero-point Energies= -880.068572
Sum of electronic and thermal Energies= -880.052552
Sum of electronic and thermal Enthalpies= -880.051607
Sum of electronic and thermal Free Energies= -880.113559
C -3.22733000 -1.34122700 0.02487800
C -2.09600500 -0.54872700 0.04667400
C -0.81464000 -1.18845000 0.02095400
C -0.75164400 -2.61624200 -0.00232100
C -1.93956000 -3.37854100 -0.00198600
C -3.15666500 -2.74618600 0.00691900
H -4.19389300 -0.85485900 0.02117500
C 0.53312200 -3.20506300 -0.04783200
H -1.87342300 -4.46092100 -0.01468600
H -4.07300200 -3.32401200 0.00282700
C 1.64930300 -2.41827000 -0.06768600
C 1.49905000 -1.00404500 -0.04493400
H 0.61807800 -4.28593200 -0.08137500
H 2.63234800 -2.86402200 -0.13159900
N 0.31023800 -0.43328900 -0.00972400
C 2.67578600 -0.09870400 -0.07962700
C 3.93833900 -0.51205200 0.36017300
C 5.02276800 0.35711500 0.32731900
H 4.07741900 -1.50986100 0.75717500
C 3.61318300 2.07693800 -0.58916900
C 4.86577500 1.65351900 -0.15105000
H 5.99030700 0.02186300 0.68172200
H 3.48276500 3.08492400 -0.96519300
H 5.71190400 2.32970200 -0.18051700
C -2.26369700 0.92925100 0.08189900
C -1.42773600 1.76642600 0.83241600
C -3.53587800 2.72717800 -0.58376900
C -1.68008700 3.12942400 0.85278000
H -0.59739400 1.34886700 1.37997700
C -2.75273600 3.63062800 0.12518300
H -4.38692700 3.07309600 -1.16317900
H -1.04623100 3.79103100 1.43165700
H -2.98180000 4.68888300 0.10758400
H 1.55196000 1.53702100 -0.88483900
C 2.52839100 1.21244400 -0.55042200
N -3.30888900 1.41496300 -0.60786500

Table S37 Cartesian coordinates and energies of 8-phenyl-2-(2-pyridyl)quinoline.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.285930 (Hartree/Particle)
Thermal correction to Energy= 0.301830
Thermal correction to Enthalpy= 0.302774
Thermal correction to Gibbs Free Energy= 0.241423
Sum of electronic and zero-point Energies= -879.855740
Sum of electronic and thermal Energies= -879.839841
Sum of electronic and thermal Enthalpies= -879.838896
Sum of electronic and thermal Free Energies= -879.900247
C -3.21913200 -1.42060400 -0.05672700
C -2.10483700 -0.59530500 -0.05249900
C -0.80534200 -1.20971600 -0.03476300
C -0.70151700 -2.63955800 -0.03718100
C -1.87442000 -3.43310800 -0.04781000
C -3.11108600 -2.82919500 -0.05257600
H -4.20539700 -0.96762000 -0.08782000
C 0.60463300 -3.19587600 -0.02197300
H -1.78048400 -4.51577100 -0.05325600
H -4.01434000 -3.43175000 -0.06485200
C 1.70330100 -2.37606300 0.00257900
C 1.49945800 -0.96738800 0.02128100
H 0.71791000 -4.27710800 -0.02777100
H 2.71558000 -2.75968400 0.01436200
N 0.29628900 -0.41787800 0.00494800
C 2.66074300 -0.03552500 0.06392800
C 2.45923900 1.35358200 0.11024900
C 3.57162400 2.18720200 0.14591100
H 1.44720600 1.74061200 0.11866900
C 4.94364800 0.22596100 0.08962100
C 4.84581600 1.61748700 0.13541300
H 3.44753800 3.26566500 0.18283100
H 5.91943900 -0.25650100 0.08061800
H 5.74105300 2.23029300 0.16274000
C -2.27446800 0.88051400 -0.05084400
C -1.54630500 1.71168700 -0.91979700
C -3.21162500 1.47448800 0.80959000
C -1.75362600 3.08935400 -0.92537900
H -0.82070300 1.26928200 -1.59133600
C -3.41645100 2.85426200 0.80584700
H -3.76608800 0.84838900 1.50257700
C -2.68774400 3.66755600 -0.06215700
H -1.18675200 3.71376100 -1.61024600
H -4.14043000 3.29280700 1.48663700
H -2.84442900 4.74233200 -0.06608400
N 3.88634500 -0.58972700 0.05457400

Table S38 Cartesian coordinates and energies of 8-phenyl-2-(2-pyridyl)quinoline.
B3LYP-D3/6-311+G(2d,p)
Zero-point correction= 0.284265 (Hartree/Particle)
Thermal correction to Energy= 0.300262
Thermal correction to Enthalpy= 0.301206

Thermal correction to Gibbs Free Energy= 0.239385
Sum of electronic and zero-point Energies= -880.071197
Sum of electronic and thermal Energies= -880.055200
Sum of electronic and thermal Enthalpies= -880.054256
Sum of electronic and thermal Free Energies= -880.116077
C -3.22008500 -1.40514100 -0.03929400
C -2.10632300 -0.58905100 -0.04422000
C -0.81297200 -1.20524100 -0.03344900
C -0.71470500 -2.63034200 -0.03758400
C -1.88780000 -3.41693200 -0.04150200
C -3.11770800 -2.81060300 -0.03687700
H -4.20293500 -0.94950900 -0.06013700
C 0.58540900 -3.18977300 -0.02873400
H -1.79993300 -4.49770000 -0.04808400
H -4.02121700 -3.40844300 -0.04256200
C 1.68264800 -2.37660000 -0.00621100
C 1.48719200 -0.97016300 0.01782600
H 0.69606200 -4.26887000 -0.03689200
H 2.68944000 -2.76815400 0.00068900
N 0.28988200 -0.42026500 0.00476500
C 2.65228600 -0.04405100 0.06365000
C 2.45851300 1.34062200 0.13735800
C 3.56901300 2.16827200 0.17580300
H 1.45138800 1.73270800 0.16512300
C 4.93189600 0.21269300 0.06803500
C 4.83730300 1.59829500 0.14008800
H 3.44805300 3.24363900 0.23439300
H 5.90355100 -0.27125700 0.03902900
H 5.73224600 2.20722600 0.16839300
C -2.26613400 0.88572900 -0.05079300
C -1.59123100 1.69182000 -0.97513700
C -3.13351200 1.49952700 0.85837200
C -1.78602700 3.06658200 -0.99181700
H -0.91554400 1.23330000 -1.68406300
C -3.32252500 2.87756000 0.84758900
H -3.64826200 0.89165900 1.59330100
C -2.64997600 3.66646800 -0.07879100
H -1.26228700 3.67294200 -1.72176600
H -3.99168300 3.33394800 1.56757500
H -2.79622800 4.74008000 -0.09001200
N 3.87380000 -0.59539300 0.03082800

Table S39. Cartesian coordinates and energies of ***i*-TEQ 6a•H$^+$**.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.475666 (Hartree/Particle)
Thermal correction to Energy= 0.502509
Thermal correction to Enthalpy= 0.503453
Thermal correction to Gibbs Free Energy= 0.419805
Sum of electronic and zero-point Energies= -1602.978857
Sum of electronic and thermal Energies= -1602.952014
Sum of electronic and thermal Enthalpies= -1602.951070
Sum of electronic and thermal Free Energies= -1603.034718
C -0.53086600 2.30710300 -0.31661900
C -2.62438500 1.45389200 -0.85308200
C -2.80350100 2.42199800 -1.88959000
C -1.75971500 3.36190700 -2.09054600
C -0.64040400 3.32678900 -1.29348800
C -3.67752300 0.53563000 -0.54600000
C -3.99583300 2.42022000 -2.65497500
H -1.86421300 4.11060300 -2.87075400
H 0.16321200 4.04500900 -1.40898700
C -4.98158600 1.49919800 -2.38564500
C -4.82450200 0.57536500 -1.32956100
H -4.11738600 3.15209700 -3.44798000
H -5.89333200 1.48259400 -2.97325600
H -5.62583000 -0.12910000 -1.13042100
N -1.47396100 1.39614300 -0.12345000
C 0.69925700 -2.96099100 -1.81473500
C 1.78439900 -2.80591800 -2.64300000
C 2.82694000 -1.91861900 -2.27936800
C 2.70756100 -1.21443900 -1.03370300
C 0.67663200 -2.20481600 -0.61465200
H 4.04069600 -2.26391300 -4.03972600
H -0.12074200 -3.62494800 -2.06710600
H 1.85246400 -3.35380800 -3.57847900
C 3.96801100 -1.72633600 -3.09890200
C 3.75883600 -0.32932800 -0.62720300
C 4.85408200 -0.18269500 -1.46242600
C 4.96284000 -0.87015200 -2.69288800
H 5.64909900 0.49332900 -1.16402700
H 5.83931000 -0.71421200 -3.31355500
N 1.62575000 -1.38354200 -0.22106800
C -0.52919600 -2.32805600 0.26045400
C -2.64016700 -1.37029200 0.88452700
C -2.86261700 -2.44516000 1.79792900
C -1.89451500 -3.47715600 1.86519000
C -0.77318200 -3.45419900 1.06375200
C -3.65853200 -0.40756100 0.61509300
C -4.05079600 -2.46892400 2.56919100
H -2.05977000 -4.30444800 2.54934700
H -0.04454400 -4.25505000 1.07510600
C -4.98461500 -1.47462300 2.40041100
C -4.79432800 -0.47978800 1.41758400
H -4.20761200 -3.27774700 3.27531200
H -5.89243800 -1.46665800 2.99394700
H -5.57696600 0.25547400 1.26438400
N -1.42971700 -1.33957400 0.23019000
C 0.61434600 2.90651800 1.83700100
C 1.67745100 2.76280000 2.69354500
C 2.75765800 1.91788500 2.33372000
C 2.69071000 1.25794800 1.06407000
C 0.65344200 2.21592900 0.59706100
H 3.91396500 2.22424600 4.13891800
H -0.23944600 3.52665700 2.08828700
H 1.69935600 3.27836200 3.64968600
C 3.87627400 1.71327900 3.18105400
C 3.75013300 0.37674300 0.68000800
C 4.82289200 0.21120800 1.54093200
C 4.89248100 0.87600300 2.78622400
H 5.62480600 -0.46300100 1.25612100
H 5.75075900 0.71253600 3.42994100
N 1.64775000 1.44768000 0.20664100
H -1.16623500 -0.40113700 -0.14112900

Table S40. Cartesian coordinates and energies of ***i*-TEQ 6a•H$^+$**.
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.473214 (Hartree/Particle)
Thermal correction to Energy= 0.500173

Thermal correction to Enthalpy= 0.501117
Thermal correction to Gibbs Free Energy= 0.417433
Sum of electronic and zero-point Energies= -1603.438818
Sum of electronic and thermal Energies= -1603.411859
Sum of electronic and thermal Enthalpies= -1603.410915
Sum of electronic and thermal Free Energies= -1603.494599
C -0.55506000 0.46379700 2.05613600
C -2.64826800 0.97739900 1.24417300
C -2.61280800 2.26826600 1.84769900
C -1.43943100 2.62825000 2.55416100
C -0.39278400 1.74995800 2.62539200
C -3.74824100 0.62661600 0.40049200
C -3.71508200 3.14245700 1.69527500
H -1.37621300 3.60870800 3.01307000
H 0.53552400 2.00848800 3.11799100
C -4.79372800 2.76001100 0.94017100
C -4.79796900 1.51240000 0.28087100
H -3.68675700 4.11564900 2.17247300
H -5.63915200 3.42659800 0.81889000
H -5.63343200 1.25753700 -0.36061600
N -1.64275200 0.07991200 1.42710900
C 0.36571800 1.86142800 -2.58161800
C 1.42944500 2.72201700 -2.45656300
C 2.60367600 2.34170000 -1.76702200
C 2.65747400 1.04296500 -1.20026000
C 0.47944000 0.56198700 -2.07865600
H 3.67216900 4.19997100 -2.01837400
H -0.55302000 2.15295200 -3.06929000
H 1.37045200 3.72114500 -2.87232200
C 3.70330400 3.21006600 -1.58019800
C 3.73323500 0.63391700 -0.37120600
C 4.78010400 1.52354500 -0.22684800
C 4.77843600 2.79344900 -0.83908700
H 5.61330400 1.24629100 0.40706200
H 5.62442800 3.45226800 -0.68895600
N 1.60489000 0.20494400 -1.45910500
C -0.61500400 -0.44508300 -2.09951600
C -2.67207300 -0.98478700 -1.23234800
C -2.63173700 -2.27250500 -1.84871100
C -1.48048300 -2.60784500 -2.59766500
C -0.44535100 -1.71445500 -2.69625800
C -3.74953900 -0.65258300 -0.35201600
C -3.71371400 -3.16673500 -1.66719600
H -1.41997400 -3.58032900 -3.07255600
H 0.46297300 -1.95328500 -3.23524700
C -4.77040400 -2.80443500 -0.87368200
C -4.77574600 -1.55988400 -0.20578500
H -3.68544200 -4.13649800 -2.15054600
H -5.59933300 -3.48629600 -0.72632100
H -5.59391200 -1.32639400 0.46513300
N -1.68590700 -0.07563700 -1.43642300
C 0.44060900 -1.79996800 2.64963100
C 1.48839100 -2.67525500 2.55700600
C 2.63973300 -2.32117600 1.81060600
C 2.65193800 -1.03397100 1.20029800
C 0.56712300 -0.52362100 2.04877200
H 3.73311100 -4.15983800 2.10847900
H -0.46878100 -2.05604100 3.17713600
H 1.44388200 -3.64893000 3.03170200
C 3.74118000 -3.18840400 1.62735100
C 3.73586600 -0.67245400 0.33831600
C 4.78401200 -1.55681000 0.18266500
C 4.79662400 -2.80487800 0.83786800
H 5.60659100 -1.29407800 -0.47190300
H 5.63886300 -3.47025800 0.69302100
N 1.63725200 -0.14600800 1.38233200
H 1.64701800 -0.73242000 -1.06973200

Table S41. Cartesian coordinates and energies of ***i*-TEQ 6a•H^+** (TS1-1).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.474758 (Hartree/Particle)
Thermal correction to Energy= 0.500494
Thermal correction to Enthalpy= 0.501438
Thermal correction to Gibbs Free Energy= 0.421127
Sum of electronic and zero-point Energies= -1602.905375
Sum of electronic and thermal Energies= -1602.879640
Sum of electronic and thermal Enthalpies= -1602.878696
Sum of electronic and thermal Free Energies= -1602.959007
C 0.77419100 -1.84413700 1.39981200
C 2.74670700 -1.39702200 0.27949400
C 3.38553800 -2.47506300 0.98723900
C 2.74897600 -2.93456500 2.16887500
C 1.44099400 -2.59931300 2.40579600
C 3.49644600 -0.74935900 -0.78265700
C 4.51980900 -3.12436200 0.44593600
H 3.27686900 -3.62251900 2.82335700
H 0.89501000 -3.00021300 3.25334500
C 4.95946700 -2.74201100 -0.79990200
C 4.46344500 -1.55826300 -1.38269300
H 4.96665400 -3.95896300 0.97754300
H 5.74099400 -3.29585600 -1.30927900
H 4.92901000 -1.23525400 -2.30608900
N 1.42758000 -1.15044400 0.47853700
C -1.46575200 3.79077700 0.35953300
C -2.82233600 3.91614300 0.45444700
C -3.65336200 2.77940600 0.37284300
C -3.04457500 1.51212900 0.09572700
C -0.86283200 2.51034800 0.26699700
H -5.46890700 3.88432600 0.74532500
H -0.83689900 4.66783100 0.36565000
H -3.27609500 4.89434800 0.58264300
C -5.05220000 2.90619300 0.52850700
C -3.88723700 0.39276300 -0.17232900
C -5.25577400 0.56804100 0.06370500
C -5.84492100 1.79216400 0.42033200
H -5.90013400 -0.29593400 -0.04671400
H -6.91640600 1.84812600 0.57814700
N -1.65732000 1.43692000 0.10056800
C 0.61747700 2.46687900 0.35328600
C 2.65548400 1.73438400 -0.46298200
C 3.23823700 3.02048700 -0.14325800
C 2.51601300 3.86711200 0.72771500
C 1.22128000 3.56723700 1.03548400
C 3.54322600 0.72658100 -1.01970100
C 4.48428800 3.42609100 -0.66535700
H 2.99881100 4.75282600 1.12993500
H 0.66372700 4.17227500 1.73909300
C 5.18298900 2.54562800 -1.45179400
C 4.74213000 1.21448800 -1.54876900

H 4.86269500 4.41800600 -0.43880000
H 6.12679500 2.82698000 -1.90695800
H 5.45272000 0.51932100 -1.97255300
N 1.31690100 1.54332300 -0.29296600
C -0.86071300 -3.60952500 1.00007700
C -1.83894000 -4.10844100 0.18569600
C -2.66817200 -3.21517400 -0.52981800
C -2.53560900 -1.81937600 -0.23166400
C -0.63032600 -2.20062400 1.03053700
H -3.64370800 -4.72890000 -1.72486400
H -0.17806000 -4.27521000 1.51146400
H -1.96104000 -5.17921000 0.05055100
C -3.59469300 -3.66791000 -1.49909100
C -3.53191300 -0.93383900 -0.75002500
C -4.38403600 -1.41420300 -1.74181400
C -4.39654600 -2.76225600 -2.15032600
H -5.08891000 -0.72834100 -2.20007800
H -5.07602400 -3.07986600 -2.93379300
N -1.47959200 -1.33464400 0.49180000
H -1.26064900 0.46168500 0.13733800

Table S42. Cartesian coordinates and energies of ***i*-TEQ 6a•H$^+$** (TS1-1).
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.472223 (Hartree/Particle)
Thermal correction to Energy= 0.498066
Thermal correction to Enthalpy= 0.499010
Thermal correction to Gibbs Free Energy= 0.418293
Sum of electronic and zero-point Energies= -1603.359768
Sum of electronic and thermal Energies= -1603.333925
Sum of electronic and thermal Enthalpies= -1603.332981
Sum of electronic and thermal Free Energies= -1603.413698
C 0.77397800 -1.87110400 1.38752100
C 2.74054600 -1.40291400 0.27042700
C 3.38229100 -2.47930400 0.96714200
C 2.75180300 -2.94819700 2.14399900
C 1.44789700 -2.62353000 2.38472300
C 3.48742000 -0.74364100 -0.78289800
C 4.50883600 -3.12443000 0.41444500
H 3.28163700 -3.63982000 2.78952300
H 0.90701200 -3.03652900 3.22659500
C 4.93881800 -2.73397500 -0.82742700
C 4.44578900 -1.54550400 -1.39429600
H 4.95857500 -3.96065800 0.93679600
H 5.71479400 -3.28379900 -1.34571700
H 4.91628900 -1.20966600 -2.30788500
N 1.42263300 -1.17091800 0.47422600
C -1.47845000 3.80286400 0.29847400
C -2.83089700 3.92017200 0.40434900
C -3.65166300 2.78112600 0.35371700
C -3.04272700 1.51796400 0.08769700
C -0.87476600 2.53079700 0.21525200
H -5.46239700 3.87651900 0.74214500
H -0.85998600 4.68483000 0.29476200
H -3.28895900 4.89464400 0.52752600
C -5.04445500 2.89889400 0.53686100
C -3.87939600 0.39189600 -0.14530100
C -5.23740100 0.55772500 0.11762500
C -5.82523900 1.78011500 0.46936900
H -5.87973100 -0.30752700 0.02811000
H -6.89136800 1.82859000 0.65109700
N -1.66057300 1.45450100 0.07136000
C 0.60715900 2.48827200 0.30831300
C 2.65882800 1.74458500 -0.45520200
C 3.24105500 3.01729400 -0.11340900
C 2.50158200 3.87011600 0.72899000
C 1.20084200 3.58280200 0.99708100
C 3.54899400 0.73562000 -0.99569800
C 4.50447300 3.41127400 -0.59370900
H 2.97614500 4.75478200 1.13785400
H 0.62827900 4.20151800 1.67131000
C 5.21517000 2.53359000 -1.36266100
C 4.76368600 1.21214200 -1.48500700
H 4.88453600 4.39582900 -0.34799700
H 6.17357200 2.80705800 -1.78644500
H 5.47532300 0.51495000 -1.89726900
N 1.31621300 1.56600600 -0.31871800
C -0.86745300 -3.62592800 0.99130000
C -1.84625000 -4.11179800 0.17757500
C -2.66962000 -3.21222500 -0.52835500
C -2.53553700 -1.82299000 -0.21965100
C -0.63219900 -2.22287200 1.02747200
H -3.64267700 -4.71065400 -1.73574300
H -0.19343700 -4.29968700 1.49929800
H -1.97368900 -5.17891300 0.03532900
C -3.59311800 -3.65376400 -1.50059100
C -3.52823200 -0.93279300 -0.72725200
C -4.37831300 -1.40213800 -1.71816500
C -4.39077900 -2.74298600 -2.13894800
H -5.08688600 -0.71633500 -2.16512600
H -5.06971400 -3.05061300 -2.92431700
N -1.47688700 -1.35260300 0.50245200
H -1.25305100 0.49364500 0.10233300

Table S43. Cartesian coordinates and energies of ***i*-TEQ 6a•H$^+$** (TS1-2).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.475027 (Hartree/Particle)
Thermal correction to Energy= 0.500881
Thermal correction to Enthalpy= 0.501826
Thermal correction to Gibbs Free Energy= 0.420346
Sum of electronic and zero-point Energies= -1602.898221
Sum of electronic and thermal Energies= -1602.872367
Sum of electronic and thermal Enthalpies= -1602.871423
Sum of electronic and thermal Free Energies= -1602.952903
C 0.67988300 -1.91654200 1.57051500
C 2.68399700 -1.39690200 0.36699600
C 3.28597600 -2.56128300 0.94698200
C 2.69360400 -3.08949300 2.12071500
C 1.40472800 -2.75669300 2.44620200
C 3.38209600 -0.70581400 -0.68316100
C 4.36164900 -3.21024800 0.30169300
H 3.22863600 -3.84519000 2.68842300
H 0.87992800 -3.25267600 3.25333500
C 4.72651100 -2.77076500 -0.95021100
C 4.24026300 -1.53682600 -1.41771800
H 4.80597000 -4.08896500 0.75659400
H 5.43890000 -3.32521300 -1.55131100
H 4.62425600 -1.16619800 -2.36070700
N 1.38319300 -1.11389000 0.73689700

C -1.59749500 3.86509500 0.50621200
C -2.95184200 3.90656200 0.65728900
C -3.70493000 2.72753500 0.48982300
C -2.99890200 1.54670900 0.06192700
C -0.95042600 2.61558600 0.23767500
H -5.58010300 3.65465200 1.02923900
H -1.04663100 4.79039300 0.56598500
H -3.45842500 4.83921500 0.88808200
C -5.10558400 2.73897700 0.68873800
C -3.80032800 0.40085100 -0.26479000
C -5.17385400 0.45864600 -0.03793400
C -5.83365200 1.60300600 0.44982500
H -5.76592900 -0.42747500 -0.23843400
H -6.90602600 1.57802000 0.61272700
N -1.63572100 1.51529400 -0.03901100
C 0.55327700 2.62623900 0.24404600
C 2.63899400 1.82121400 -0.42476600
C 3.22264100 3.12815900 -0.25716700
C 2.45987100 4.09429700 0.42771500
C 1.16037000 3.82545200 0.72883700
C 3.53371800 0.76849100 -0.84591000
C 4.52759400 3.44441400 -0.69349300
H 2.91802300 5.03749800 0.71034300
H 0.59770000 4.53718500 1.31134800
C 5.31034800 2.46011900 -1.23583700
C 4.82568700 1.14401400 -1.23921100
H 4.89273700 4.45943000 -0.56949600
H 6.31969600 2.66176100 -1.57750800
H 5.54288400 0.37426000 -1.48770000
N 1.29753400 1.61308800 -0.21774700
C -0.95768600 -3.66572700 1.14312400
C -1.86239100 -4.12387600 0.22044200
C -2.57366500 -3.20463500 -0.58125300
C -2.45537300 -1.80834300 -0.24403200
C -0.71755100 -2.25707100 1.19529100
H -3.41543500 -4.67784900 -1.92642300
H -0.36228800 -4.36429800 1.71581200
H -2.00474300 -5.18989100 0.06880700
C -3.37121200 -3.62272400 -1.67406800
C -3.36103600 -0.88720500 -0.86757800
C -4.07817200 -1.33733500 -1.96780900
C -4.05773100 -2.68263500 -2.40193300
H -4.72240200 -0.63429100 -2.48540500
H -4.63908300 -2.97135300 -3.27150200
N -1.48529200 -1.36939800 0.59767500
H 0.89806600 -0.35217600 0.22004400

Table S44. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$.

B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.489877 (Hartree/Particle)
Thermal correction to Energy= 0.516730
Thermal correction to Enthalpy= 0.517674
Thermal correction to Gibbs Free Energy= 0.434778
Sum of electronic and zero-point Energies= -1603.290497
Sum of electronic and thermal Energies= -1603.263644
Sum of electronic and thermal Enthalpies= -1603.262700
Sum of electronic and thermal Free Energies= -1603.345596
C -0.60305100 -2.41917000 0.36138000
C -2.68849900 -1.38625600 0.94978500
C -2.91851800 -2.40263200 1.92933100
C -1.97841500 -3.45374100 2.03541500
C -0.86191900 -3.49471200 1.22433600
C -3.68283900 -0.41629100 0.64854800
C -4.09071100 -2.35090400 2.72378500
H -2.15189400 -4.24266800 2.76141600
H -0.14765300 -4.30659600 1.28165600
C -5.00111400 -1.34166000 2.51792900
C -4.80440400 -0.41017300 1.47547700
H -4.25530800 -3.11501700 3.47623900
H -5.89620100 -1.27524800 3.12665800
H -5.57132600 0.33572200 1.29564200
N -1.49068600 -1.42056900 0.27215800
C 0.86161800 3.49457400 1.22472200
C 1.97819100 3.45365700 2.03570700
C 2.91845400 2.40272900 1.92937000
C 2.68847900 1.38641800 0.94974100
C 0.60294400 2.41922100 0.36148500
H 4.25532100 3.11506100 3.47625300
H 0.14719300 4.30630200 1.28222700
H 2.15161100 4.24250200 2.76181000
C 4.09069300 2.35100400 2.72374900
C 3.68281700 0.41648000 0.64843700
C 4.80444100 0.41037500 1.47530000
C 5.00114500 1.34182700 2.51777300
H 5.57137400 -0.33549100 1.29539700
H 5.89625400 1.27545000 3.12647800
N 1.49068900 1.42074400 0.27207800
C -0.63900700 2.37856700 -0.45869900
C -2.68259200 1.39798200 -0.91839000
C -2.94698900 2.36375300 -1.94817500
C -1.99035700 3.38494000 -2.15678500
C -0.85609300 3.42955100 -1.37970500
C -3.70547600 0.46010800 -0.56333900
C -4.14951200 2.29871700 -2.69578200
H -2.16996000 4.13746400 -2.91873800
H -0.12229200 4.21950200 -1.49272800
C -5.08092400 1.33152000 -2.40489400
C -4.86491400 0.44190400 -1.32929100
H -4.32273200 3.02387900 -3.48472200
H -6.00082000 1.26221500 -2.97525100
H -5.64061200 -0.27838400 -1.09037000
N -1.49027700 1.38251000 -0.24923800
C 0.85633800 -3.42983300 -1.37917000
C 1.99063400 -3.38532100 -2.15621400
C 2.94712800 -2.36395000 -1.94784900
C 2.68256400 -1.39792100 -0.91835600
C 0.63901900 -2.37855200 -0.45856800
H 4.32301500 -3.02438200 -3.48414100
H 0.12266100 -4.21993200 -1.49199300
H 2.17038500 -4.13805500 -2.91792300
C 4.14967800 -2.29900500 -2.69542700
C 3.70539300 -0.45996000 -0.56341400
C 4.86487700 -0.44184400 -1.32934400
C 5.08098600 -1.33162700 -2.40475900
H 5.64051500 0.27852700 -1.09047300
H 6.00087500 -1.26234500 -2.97513600
N 1.49015000 -1.38231200 -0.24936200
H -1.23807500 -0.54807300 -0.21309800
H 1.23813800 0.54830400 -0.21332600

Table S45. Cartesian coordinates and energies of ***i*-TEQ 6a•2H$^+$**.
B3LYP-D3/6-311G+(2d,p)/SMD(Et_2O)
Zero-point correction= 0.488002 (Hartree/Particle)
Thermal correction to Energy= 0.514953
Thermal correction to Enthalpy= 0.515897
Thermal correction to Gibbs Free Energy= 0.432633
Sum of electronic and zero-point Energies= -1603.849663
Sum of electronic and thermal Energies= -1603.822712
Sum of electronic and thermal Enthalpies= -1603.821768
Sum of electronic and thermal Free Energies= -1603.905032
C 0.54777000 2.40385500 0.44879400
C 2.64295100 1.36048100 0.95910400
C 2.80518200 2.24375100 2.06315200
C 1.81841400 3.22412900 2.29357800
C 0.71263500 3.32538700 1.48205900
C 3.65029900 0.42689200 0.60951900
C 3.95641100 2.13119600 2.87482800
H 1.94565800 3.90730000 3.12533200
H -0.04734700 4.07619900 1.64475600
C 4.90420600 1.19079700 2.57481300
C 4.75340900 0.36523300 1.44437800
H 4.06993000 2.80013100 3.71886900
H 5.78862200 1.08656000 3.19025600
H 5.53703900 -0.34478300 1.21137400
N 1.48976900 1.48594100 0.22956400
C -0.71260100 -3.32546700 1.48190600
C -1.81836100 -3.22425400 2.29345500
C -2.80513500 -2.24386400 2.06310500
C -2.64292300 -1.36052300 0.95910900
C -0.54775300 -2.40387100 0.44869600
H -4.06985700 -2.80035800 3.71880200
H 0.04738200 -4.07629300 1.64453900
H -1.94558900 -3.90747400 3.12517200
C -3.95635300 -2.13136600 2.87480400
C -3.65028200 -0.42691900 0.60959300
C -4.75337700 -0.36531600 1.44447600
C -4.90415500 -1.19095300 2.57486000
H -5.53701500 0.34471000 1.21152900
H -5.78856400 -1.08675900 3.19032300
N -1.48975200 -1.48593700 0.22954500
C 0.65806400 -2.37823300 -0.42908600
C 2.65316300 -1.35752000 -0.95181200
C 2.84850300 -2.23978400 -2.05931100
C 1.88205800 -3.24534700 -2.27941200
C 0.79365600 -3.33869500 -1.45195200
C 3.66119400 -0.39760000 -0.63324000
C 3.99411800 -2.10216500 -2.87606500
H 2.01498100 -3.94047800 -3.10041700
H 0.04253100 -4.10661400 -1.58361100
C 4.92311100 -1.13773100 -2.58948100
C 4.76205100 -0.30598200 -1.46342400
H 4.12370000 -2.77217200 -3.71791300
H 5.80127700 -1.02003400 -3.21192000
H 5.53362100 0.41964800 -1.23657400
N 1.53329200 -1.42617500 -0.18062200
C -0.79367900 3.33876100 -1.45178700
C -1.88210500 3.24545300 -2.27922000
C -2.84855200 2.23989100 -2.05913100
C -2.65318300 1.35757300 -0.95168000
C -0.65806700 2.37825900 -0.42896300
H -4.12380200 2.77237300 -3.71766300
H -0.04255300 4.10668200 -1.58343400
H -2.01504700 3.94061900 -3.10019300
C -3.99419600 2.10232200 -2.87585300
C -3.66120900 0.39764000 -0.63312300
C -4.76209300 0.30607300 -1.46327700
C -4.92318600 1.13788100 -2.58928500
H -5.53365900 -0.41956600 -1.23644200
H -5.80137600 1.02022200 -3.21169800
N -1.53328900 1.42619000 -0.18052000
H 1.30690900 0.78646500 -0.48582800
H -1.30689400 -0.78640400 -0.48579300

Table S46. Cartesian coordinates and energies of ***i*-TEQ 6a•2H$^+$** (TS1-2).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.484491 (Hartree/Particle)
Thermal correction to Energy= 0.510780
Thermal correction to Enthalpy= 0.511724
Thermal correction to Gibbs Free Energy= 0.430466
Sum of electronic and zero-point Energies= -1603.282702
Sum of electronic and thermal Energies= -1603.256413
Sum of electronic and thermal Enthalpies= -1603.255468
Sum of electronic and thermal Free Energies= -1603.336726
C 0.62423100 2.22886100 -0.45730800
C 2.73919200 1.31885400 -0.95317000
C 2.97007600 2.33090300 -1.94172800
C 1.97874900 3.32019600 -2.11492400
C 0.84498000 3.31220800 -1.32927500
C 3.78900900 0.42889300 -0.57715100
C 4.18480200 2.33984300 -2.67153200
H 2.13027400 4.10453100 -2.85050800
H 0.10131000 4.09610900 -1.40731700
C 5.14628400 1.39871500 -2.39166700
C 4.95400400 0.47853500 -1.33770500
H 4.34156500 3.09797000 -3.43182100
H 6.07567200 1.37817400 -2.95030000
H 5.75718500 -0.21207100 -1.10437700
N 1.51680300 1.24132200 -0.32853900
C -0.78086900 -3.30794700 -1.34260400
C -1.92093300 -3.34751700 -2.11135800
C -2.94217300 -2.38677200 -1.91415100
C -2.72603200 -1.38533600 -0.91323000
C -0.61442900 -2.23561600 -0.43355500
H -4.29816300 -3.16331400 -3.41360600
H -0.00307900 -4.05555300 -1.44745400
H -2.05731700 -4.12368300 -2.85857000
C -4.15558400 -2.40928700 -2.64588100
C -3.78929900 -0.48981300 -0.56893200
C -4.95521000 -0.55252700 -1.32474400
C -5.13485200 -1.48499600 -2.36922300
H -5.76282300 0.13869500 -1.10705500
H -6.06268700 -1.48049100 -2.93075600
N -1.53051200 -1.29498900 -0.25389900
C 0.61790200 -2.22635800 0.41217200
C 2.71180000 -1.33042200 0.97565700
C 2.92452100 -2.35071400 1.95453200
C 1.93077500 -3.34849700 2.08775600

C 0.82141300 -3.32719200 1.27411000
C 3.77519000 -0.44099900 0.63605400
C 4.12218300 -2.36440500 2.71194200
H 2.06763300 -4.14364000 2.81466100
H 0.07431600 -4.11065700 1.31846800
C 5.09214400 -1.42114400 2.46711700
C 4.92635100 -0.49378700 1.41669800
H 4.26175200 -3.13035300 3.46806800
H 6.00735600 -1.40758000 3.04873800
H 5.73595400 0.19675200 1.20504700
N 1.50818100 -1.23800500 0.31755600
C -0.82671700 3.37131300 1.22378600
C -1.96760400 3.40462100 2.00324300
C -2.96423700 2.41148600 1.87776100
C -2.75380000 1.36562900 0.92296800
C -0.61001700 2.27274800 0.37651200
H -4.31565900 3.22061800 3.36475700
H -0.07521800 4.14817600 1.29056000
H -2.11447600 4.21240300 2.71416100
C -4.16278100 2.43444100 2.63292700
C -3.78139700 0.42995600 0.61011400
C -4.92384400 0.49412900 1.40550200
C -5.11055400 1.46237700 2.41699700
H -5.71548300 -0.22638100 1.23052800
H -6.02604200 1.44929600 2.99837300
N -1.53985700 1.31785900 0.28073400
H 1.31812600 0.06529100 0.00496500
H -1.32212700 0.36015300 -0.11377200

Table S47. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (TS1-3).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.484346 (Hartree/Particle)
Thermal correction to Energy= 0.511150
Thermal correction to Enthalpy= 0.512094
Thermal correction to Gibbs Free Energy= 0.428867
Sum of electronic and zero-point Energies= -1603.235167
Sum of electronic and thermal Energies= -1603.208363
Sum of electronic and thermal Enthalpies= -1603.207419
Sum of electronic and thermal Free Energies= -1603.290646
C 0.57954400 -2.93486600 0.40780300
C 2.47180000 -1.55136200 0.94083500
C 2.79468400 -2.40979800 2.03352400
C 2.02027500 -3.58491900 2.20953800
C 0.94109400 -3.86555900 1.39125300
C 3.25718600 -0.42786600 0.60423800
C 3.88394200 -2.05814700 2.86898200
H 2.27436800 -4.26188500 3.01998100
H 0.32405800 -4.74275100 1.54202800
C 4.60592400 -0.91695200 2.60005600
C 4.30806300 -0.12887700 1.46410700
H 4.13741100 -2.69697200 3.70863100
H 5.43634000 -0.63280000 3.23709800
H 4.93919000 0.72418600 1.23649600
N 1.36451800 -1.86648200 0.20566500
C -1.12534600 4.00527600 1.15359300
C -2.16340700 3.69625700 2.00681100
C -2.78797400 2.42664200 1.95394900
C -2.34200700 1.47056300 0.96787100
C -0.62234800 2.94946500 0.38261000
H -4.18601800 2.83221500 3.55602400
H -0.64791600 4.97757600 1.15075900
H -2.52604800 4.43094600 2.71947400
C -3.88629600 2.11834200 2.79544400
C -3.18712000 0.36372200 0.65404300
C -4.25456300 0.11738600 1.51028200
C -4.57309900 0.94376400 2.61105400
H -4.90501600 -0.72223600 1.28710200
H -5.41101200 0.68545400 3.24941000
N -1.16155200 1.73106400 0.31900500
C 0.66097200 2.94376200 -0.34362300
C 2.34862700 1.43813600 -0.98564400
C 2.79282800 2.39259400 -1.96634500
C 2.19402600 3.67887700 -1.98683300
C 1.18544400 3.99772700 -1.10548000
C 3.18324000 0.31313700 -0.70419200
C 3.86650400 2.07037400 -2.83353500
H 2.55520300 4.41483100 -2.69900300
H 0.72973300 4.97986800 -1.07813800
C 4.53504600 0.87815100 -2.68490100
C 4.22831500 0.04857500 -1.58668600
H 4.16411100 2.78767300 -3.59190200
H 5.35115500 0.61264300 -3.34770400
H 4.87040600 -0.80254300 -1.38184800
N 1.17946900 1.71229000 -0.31095800
C -1.05384900 -3.91613100 -1.27852600
C -2.11304900 -3.64573400 -2.11799500
C -2.82303300 -2.42536600 -1.99484700
C -2.43194700 -1.52790000 -0.94251300
C -0.67276000 -2.89745600 -0.37775400
H -4.18492000 -2.74605900 -3.65095200
H -0.49192600 -4.84098500 -1.34624300
H -2.41074400 -4.36041800 -2.87941100
C -3.90636800 -2.07859700 -2.84138600
C -3.23464900 -0.38784700 -0.64644500
C -4.28684000 -0.09722200 -1.49958800
C -4.59846100 -0.91212700 -2.61605400
H -4.91689500 0.76085100 -1.28698600
H -5.42490500 -0.63242100 -3.26074800
N -1.31811300 -1.75088400 -0.20449100
H 1.06192300 -1.21006600 -0.50878500
H 0.04486400 1.14483100 -0.00171300

Table S48. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (Int1-2).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.488192 (Hartree/Particle)
Thermal correction to Energy= 0.514791
Thermal correction to Enthalpy= 0.515735
Thermal correction to Gibbs Free Energy= 0.433775
Sum of electronic and zero-point Energies= -1603.281482
Sum of electronic and thermal Energies= -1603.254883
Sum of electronic and thermal Enthalpies= -1603.253938
Sum of electronic and thermal Free Energies= -1603.335899
C 0.62103300 -2.30648900 0.40881800
C 2.74803000 -1.35537500 0.92878600
C 2.98282000 -2.38833800 1.89538600
C 2.00841300 -3.39848100 2.03673400
C 0.86500800 -3.39522300 1.25928800
C 3.76579400 -0.41809600 0.59104600

C 4.18666900 -2.38587900 2.64255600
H 2.17351300 -4.19652200 2.75455700
H 0.13112500 -4.18809100 1.33391100
C 5.12093800 -1.40636600 2.40505900
C 4.91537200 -0.45831000 1.37795800
H 4.35435100 -3.16068600 3.38317000
H 6.04080200 -1.37342000 2.97872700
H 5.69867900 0.26561800 1.18122200
N 1.52553400 -1.32427900 0.29979000
C -0.80514200 3.35534900 1.31433500
C -1.92834500 3.37392000 2.10622700
C -2.92676100 2.38409500 1.93654300
C -2.70312800 1.38239800 0.93863500
C -0.61845700 2.27354500 0.41954800
H -4.27299000 3.13788500 3.45524600
H -0.04583800 4.12480300 1.39303500
H -2.07170500 4.15394900 2.84811700
C -4.12873300 2.38433700 2.68728000
C -3.76142000 0.47877400 0.60473500
C -4.91918100 0.52033800 1.37501800
C -5.09679700 1.44328900 2.42730000
H -5.72136500 -0.17824900 1.16016700
H -6.01539700 1.42274900 3.00339000
N -1.51142100 1.30327200 0.26769500
C 0.61875800 2.27342600 -0.42014500
C 2.70350100 1.38207600 -0.93870100
C 2.92745700 2.38368900 -1.93663300
C 1.92908100 3.37347600 -2.10669400
C 0.80561600 3.35500400 -1.31511900
C 3.76160800 0.47833500 -0.60446700
C 4.12965100 2.38378000 -2.68702600
H 2.07266500 4.15345100 -2.84860300
H 0.04643500 4.12455500 -1.39409000
C 5.09759100 1.44272000 -2.42664500
C 4.91964900 0.51984300 -1.37434900
H 4.27423600 3.13726300 -3.45498900
H 6.01635300 1.42210500 -3.00248900
H 5.72174300 -0.17873900 -1.15913500
N 1.51169100 1.30317700 -0.26789500
C -0.86556100 -3.39494700 -1.25993300
C -2.00918700 -3.39810300 -2.03704500
C -2.98349500 -2.38795800 -1.89532500
C -2.74834700 -1.35495600 -0.92882100
C -0.62131000 -2.30630400 -0.40944200
H -4.35557300 -3.16035300 -3.38262700
H -0.13180700 -4.18790900 -1.33479100
H -2.17458300 -4.19612400 -2.75482100
C -4.18758000 -2.38551800 -2.64211500
C -3.76603700 -0.41767700 -0.59075500
C -4.91585500 -0.45797100 -1.37727300
C -5.12175700 -1.40601400 -2.40430900
H -5.69915700 0.26590900 -1.18035700
H -6.04181200 -1.37309300 -2.97767800
N -1.52567700 -1.32395000 -0.30017900
H 1.29508300 -0.36072500 -0.09432800
H -1.29502800 -0.36026900 0.09375500

Table S49. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (Int1-3).
B3LYP-D3/6-31G(d,p)

Zero-point correction= 0.489687 (Hartree/Particle)
Thermal correction to Energy= 0.516622
Thermal correction to Enthalpy= 0.517566
Thermal correction to Gibbs Free Energy= 0.434552
Sum of electronic and zero-point Energies= -1603.265709
Sum of electronic and thermal Energies= -1603.238774
Sum of electronic and thermal Enthalpies= -1603.237830
Sum of electronic and thermal Free Energies= -1603.320844
C -0.49224400 0.42881000 -2.06985600
C -2.69455000 0.98639100 -1.24107800
C -2.60399800 2.27201200 -1.84384700
C -1.39865000 2.61064700 -2.52052400
C -0.33938200 1.73015500 -2.58139700
C -3.77310200 0.64133300 -0.38024300
C -3.69049500 3.16838600 -1.69096800
H -1.31259900 3.59497000 -2.97163800
H 0.60466400 1.99253700 -3.04129800
C -4.78389500 2.80442600 -0.93236300
C -4.80792200 1.56368600 -0.26032600
H -3.64146400 4.14355500 -2.16458000
H -5.61756700 3.48785300 -0.81425300
H -5.64246700 1.32877000 0.39295000
N -1.65501600 0.10669600 -1.47556300
C 0.39953600 1.90408400 2.55295400
C 1.45360900 2.78191600 2.41751200
C 2.61994000 2.38776100 1.71467300
C 2.65751900 1.05863400 1.17016900
C 0.58116700 0.59423400 2.04528800
H 3.70904200 4.24648200 1.95700500
H -0.50534700 2.18142200 3.08469900
H 1.39933200 3.78042900 2.84109200
C 3.72806800 3.25153800 1.52302500
C 3.75697300 0.65977900 0.33966900
C 4.81073800 1.54152200 0.18272800
C 4.80877500 2.82286700 0.78696000
H 5.64890700 1.25605300 -0.44524100
H 5.66052600 3.47826900 0.63838800
N 1.66247600 0.16871900 1.41784400
C -0.49224500 -0.42881100 2.06985700
C -2.69455100 -0.98639100 1.24107900
C -2.60399700 -2.27201300 1.84384600
C -1.39864900 -2.61064900 2.52052100
C -0.33938200 -1.73015600 2.58139500
C -3.77310200 -0.64133300 0.38024400
C -3.69049400 -3.16838800 1.69096600
H -1.31259700 -3.59497300 2.97163400
H 0.60466500 -1.99253900 3.04129500
C -4.78389500 -2.80442700 0.93236200
C -4.80792200 -1.56368700 0.26032600
H -3.64146200 -4.14355700 2.16457700
H -5.61756600 -3.48785300 0.81425200
H -5.64246700 -1.32877000 -0.39295000
N -1.65501700 -0.10669600 1.47556600
C 0.39953800 -1.90408300 -2.55295600
C 1.45361100 -2.78191400 -2.41751400
C 2.61994200 -2.38775900 -1.71467400
C 2.65752000 -1.05863400 -1.17016800
C 0.58116700 -0.59423400 -2.04528700
H 3.70904500 -4.24648000 -1.95700800
H -0.50534500 -2.18142000 -3.08470200

H 1.39933600 -3.78042700 -2.84109600
C 3.72807000 -3.25153700 -1.52302600
C 3.75697300 -0.65977900 -0.33966600
C 4.81073800 -1.54152200 -0.18272600
C 4.80877600 -2.82286600 -0.78696000
H 5.64890700 -1.25605400 0.44524300
H 5.66052700 -3.47826800 -0.63838800
N 1.66247500 -0.16871900 -1.41784200
H -1.74781200 -0.84486500 -1.13076500
H -1.74781400 0.84486500 1.13076700

Table S50. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (TS2-2).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.487711 (Hartree/Particle)
Thermal correction to Energy= 0.513321
Thermal correction to Enthalpy= 0.514266
Thermal correction to Gibbs Free Energy= 0.434370
Sum of electronic and zero-point Energies= -1603.212912
Sum of electronic and thermal Energies= -1603.187301
Sum of electronic and thermal Enthalpies= -1603.186357
Sum of electronic and thermal Free Energies= -1603.266252
C -0.77110800 -1.93775900 -1.18397700
C -2.90826800 -1.44052300 -0.23854800
C -3.44220200 -2.60374800 -0.89769400
C -2.69426800 -3.14404900 -1.96525800
C -1.36602400 -2.81039600 -2.11511400
C -3.72812100 -0.70778400 0.68799200
C -4.62976800 -3.20393400 -0.42641400
H -3.14191100 -3.90514000 -2.59759900
H -0.74028100 -3.32032300 -2.83787200
C -5.17947400 -2.71653900 0.73760100
C -4.73186500 -1.49145100 1.27029100
H -5.03291600 -4.07312000 -0.93424100
H -6.00659400 -3.22865800 1.21712900
H -5.25572200 -1.10716100 2.13673700
N -1.57229000 -1.17044500 -0.41158800
C 1.38655900 3.69168200 0.19658300
C 2.71731700 3.94399500 0.01600600
C 3.59064000 2.87131400 -0.25377000
C 3.05670100 1.54404800 -0.13354000
C 0.88070100 2.37372100 -0.01365900
H 5.29785800 4.12045400 -0.69549000
H 0.70978800 4.49666100 0.44749500
H 3.10724700 4.95577700 0.07394500
C 4.94856300 3.09877700 -0.58456900
C 4.00570800 0.47041900 -0.09032700
C 5.31720800 0.73705900 -0.48361200
C 5.78849900 2.03089100 -0.77529300
H 6.01842300 -0.08820100 -0.54514100
H 6.81770400 2.17301700 -1.08544400
N 1.69585700 1.32071700 -0.09118000
C -0.60882200 2.35070500 -0.21613800
C -2.78163300 1.72322200 0.36652500
C -3.25767700 3.04135000 0.03399100
C -2.40086300 3.87995400 -0.70581600
C -1.09539800 3.51624000 -0.87373100
C -3.76804000 0.77427000 0.83242500
C -4.54791400 3.49149200 0.39763000
H -2.78013600 4.81301000 -1.11146300
H -0.42010500 4.13897400 -1.44505100
C -5.39742100 2.63472200 1.04669200
C -5.02011000 1.28969900 1.18693000
H -4.84197300 4.50704700 0.15233900
H -6.38564500 2.94974000 1.36238000
H -5.80090300 0.61458800 1.50750800
N -1.43872600 1.42573000 0.28121700
C 0.82197000 -3.64348800 -0.54389300
C 1.92122200 -4.08209000 0.15716400
C 2.88685700 -3.16848700 0.60909500
C 2.73795000 -1.78814100 0.23576600
C 0.61650400 -2.26138800 -0.74672400
H 4.06428800 -4.63876800 1.67086500
H 0.05993400 -4.34683400 -0.84610100
H 2.03381900 -5.13740400 0.38677700
C 3.98335400 -3.59216500 1.39726000
C 3.79350000 -0.87548500 0.50541500
C 4.80810800 -1.33638600 1.35009000
C 4.90654700 -2.66478200 1.80916300
H 5.57389900 -0.63344900 1.65645100
H 5.73166900 -2.94730000 2.45371100
N 1.56509400 -1.38756800 -0.37716400
H -1.21775900 -0.31274100 0.10043700
H 1.42618800 -0.31899100 -0.40761700

Table S51. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (TS3-1).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.489157 (Hartree/Particle)
Thermal correction to Energy= 0.514898
Thermal correction to Enthalpy= 0.515842
Thermal correction to Gibbs Free Energy= 0.435484
Sum of electronic and zero-point Energies= -1603.220944
Sum of electronic and thermal Energies= -1603.195203
Sum of electronic and thermal Enthalpies= -1603.194259
Sum of electronic and thermal Free Energies= -1603.274617
C -0.78728500 -1.95214700 -1.34365000
C -2.85921000 -1.40855600 -0.25926500
C -3.45728300 -2.54309100 -0.89992100
C -2.78987600 -3.08470800 -2.02342200
C -1.46883800 -2.78171700 -2.25748800
C -3.58959000 -0.68566400 0.74330500
C -4.61862000 -3.13457600 -0.35498500
H -3.29842400 -3.82397500 -2.63538500
H -0.90817000 -3.28581500 -3.03506700
C -5.06974200 -2.67097500 0.85985100
C -4.56104600 -1.46699300 1.38330300
H -5.07270800 -3.98551700 -0.85083400
H -5.86535700 -3.18305800 1.38972700
H -5.01037000 -1.09587600 2.29620300
N -1.52828000 -1.17174700 -0.52707200
C 1.50623300 3.78969100 -0.16702600
C 2.86523200 3.93114300 -0.28511700
C 3.70079900 2.79905400 -0.32709700
C 3.10103900 1.51571200 -0.11040000
C 0.91114500 2.50630000 -0.19007200
H 5.51406400 3.91275700 -0.70199500
H 0.88053000 4.66495100 -0.08176600
H 3.30775600 4.92107300 -0.34348800
C 5.09454000 2.92664000 -0.53289300

C 3.94021400 0.38372800 0.08077200
C 5.29770300 0.55987700 -0.20716500
C 5.87802200 1.80023500 -0.53183400
H 5.94449900 -0.30855900 -0.15865100
H 6.94135800 1.85771500 -0.73634000
N 1.71752000 1.43206400 -0.10325400
C -0.57334900 2.46828100 -0.32201800
C -2.67795000 1.77286800 0.38971400
C -3.20617800 3.08464700 0.08611700
C -2.42357200 3.93983800 -0.71331700
C -1.12055100 3.61507300 -0.96116600
C -3.61807400 0.79956800 0.91108200
C -4.47277200 3.51453800 0.54179100
H -2.85589400 4.85692000 -1.10160800
H -0.50810200 4.24545000 -1.59138600
C -5.25067400 2.64349100 1.25640900
C -4.84361500 1.30214000 1.35887700
H -4.80364700 4.52325100 0.31663000
H -6.21603100 2.94043000 1.65092400
H -5.59333200 0.61717100 1.72786500
N -1.33693400 1.51884800 0.23215700
C 0.85010100 -3.67397200 -0.89928000
C 1.86619800 -4.14047000 -0.10709100
C 2.71448000 -3.22583400 0.54574300
C 2.56203900 -1.83067300 0.22486200
C 0.61760100 -2.27054400 -0.96004200
H 3.74956100 -4.72304100 1.71468400
H 0.16671900 -4.37038600 -1.36409700
H 2.00285000 -5.20668300 0.04588000
C 3.68662600 -3.66577600 1.47767500
C 3.58984900 -0.93862300 0.67270700
C 4.48202400 -1.40830200 1.63405000
C 4.51466100 -2.74848500 2.07232000
H 5.21041300 -0.71819700 2.04595600
H 5.23245900 -3.04863000 2.82773300
N 1.45964400 -1.37456000 -0.45415500
H -1.08410400 -0.41467600 0.01900600
H 1.34056900 0.46214500 -0.17968500

Table S52. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (TS3-1).
B3LYP-D3/6-311+G(2d,p)/SMD(Et_2O)
Zero-point correction= 0.487429 (Hartree/Particle)
Thermal correction to Energy= 0.513073
Thermal correction to Enthalpy= 0.514017
Thermal correction to Gibbs Free Energy= 0.434650
Sum of electronic and zero-point Energies= -1603.778519
Sum of electronic and thermal Energies= -1603.752875
Sum of electronic and thermal Enthalpies= -1603.751931
Sum of electronic and thermal Free Energies= -1603.831298
C -0.77353900 -1.93254000 -1.42097000
C -2.76925200 -1.42267400 -0.20868200
C -3.37991000 -2.57071900 -0.79333500
C -2.78327600 -3.10343300 -1.95513300
C -1.49703000 -2.77333800 -2.28354900
C -3.46428000 -0.70426000 0.81807300
C -4.47720600 -3.18750500 -0.15991700
H -3.31280600 -3.86288900 -2.51864800
H -0.98380200 -3.27298200 -3.09244700
C -4.86016500 -2.72093000 1.07092300
C -4.36599200 -1.49094600 1.53360800
H -4.93452200 -4.05675300 -0.61543500
H -5.60345800 -3.24526400 1.65769500
H -4.78664400 -1.09715900 2.44842100
N -1.46949000 -1.15996500 -0.56744000
C 1.48685200 3.82820700 -0.26421200
C 2.84420100 3.94865000 -0.32940700
C 3.66475500 2.81242700 -0.27409200
C 3.04931500 1.54604400 -0.04088400
C 0.88441400 2.55639700 -0.21487700
H 5.48816900 3.90735300 -0.60246400
H 0.87354700 4.71311600 -0.26420600
H 3.30142400 4.92611100 -0.42810100
C 5.06211200 2.92831100 -0.42268800
C 3.87225400 0.41452600 0.19168100
C 5.23659700 0.57826300 -0.03522300
C 5.83606500 1.80518300 -0.35353300
H 5.87482000 -0.29011200 0.05235000
H 6.90607000 1.85170200 -0.50982500
N 1.66990300 1.48227500 -0.05657600
C -0.59569100 2.50829700 -0.33937400
C -2.67383700 1.77132500 0.37378600
C -3.24363800 3.04654900 0.02647300
C -2.47780200 3.91325600 -0.77034500
C -1.16785100 3.62798600 -0.99450900
C -3.57030000 0.77987500 0.91702100
C -4.53354500 3.42918500 0.44428400
H -2.93358600 4.80862700 -1.17615800
H -0.56847100 4.26996200 -1.62048000
C -5.28643600 2.54549200 1.16101200
C -4.82325000 1.23270200 1.32194000
H -4.90177600 4.41445000 0.18489200
H -6.27243800 2.80870600 1.52219400
H -5.53904400 0.52312900 1.70692100
N -1.33073700 1.55861000 0.23228400
C 0.95596400 -3.61047300 -1.17349100
C 1.94641700 -4.09720000 -0.37150500
C 2.70755700 -3.20986200 0.40754600
C 2.52452200 -1.80774500 0.17578000
C 0.65032200 -2.22502500 -1.10935400
H 3.70303900 -4.74177600 1.55417600
H 0.33766400 -4.29058200 -1.73715500
H 2.12723300 -5.16343300 -0.30210000
C 3.62092000 -3.67576300 1.37916300
C 3.49643800 -0.91957400 0.73244300
C 4.32842100 -1.41579800 1.72424400
C 4.36447400 -2.77432300 2.08819800
H 5.01746500 -0.73723900 2.21086600
H 5.03144500 -3.09810700 2.87700100
N 1.43933000 -1.34568500 -0.51288100
H -0.98355100 -0.42558000 -0.03488900
H 1.26458100 0.52867800 -0.08688400

Table S53. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (Int2-2).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.488006 (Hartree/Particle)
Thermal correction to Energy= 0.514513
Thermal correction to Enthalpy= 0.515457
Thermal correction to Gibbs Free Energy= 0.431447

Sum of electronic and zero-point Energies= -1603.212710
Sum of electronic and thermal Energies= -1603.186203
Sum of electronic and thermal Enthalpies= -1603.185259
Sum of electronic and thermal Free Energies= -1603.269268
C 0.79809200 -2.03821600 1.01420700
C 2.93348800 -1.50699700 0.08738800
C 3.43862900 -2.76111400 0.57689600
C 2.70044600 -3.38902000 1.60093600
C 1.39747300 -3.01243100 1.84039500
C 3.79204000 -0.67087000 -0.70165800
C 4.60577600 -3.32491800 0.01469700
H 3.13409200 -4.22982300 2.13445100
H 0.78221400 -3.56053400 2.54344000
C 5.18781200 -2.68364500 -1.05510200
C 4.79309200 -1.36963600 -1.38337200
H 4.97851500 -4.27175800 0.38978200
H 6.00690500 -3.14217500 -1.59839800
H 5.35570800 -0.84675000 -2.14842900
N 1.60541600 -1.21919700 0.30315000
C -1.31384300 3.58177600 -0.75572500
C -2.63022300 3.90597000 -0.57909800
C -3.50911100 2.93714700 -0.05005900
C -3.02084400 1.59074700 0.03939000
C -0.83919500 2.31765000 -0.29673500
H -5.13944000 4.31112000 0.30804000
H -0.61302200 4.30634400 -1.15041600
H -2.99853800 4.90132900 -0.80896400
C -4.82215100 3.27438200 0.35964000
C -3.99963900 0.56466700 0.25109200
C -5.24937200 0.94983700 0.73641600
C -5.65315400 2.29443000 0.84340600
H -5.96243300 0.17783400 1.00594900
H -6.63595600 2.53316000 1.23420900
N -1.67115200 1.31514600 -0.01649000
C 0.62754800 2.34554100 0.03400700
C 2.86383200 1.73858500 -0.21442200
C 3.28553800 3.04136200 0.23116400
C 2.31222200 3.90675600 0.76697100
C 0.99537000 3.55448500 0.69033100
C 3.89749500 0.80671700 -0.58025700
C 4.63594800 3.45938200 0.16870500
H 2.61562800 4.84871400 1.21363400
H 0.22836200 4.20406000 1.09053600
C 5.59055600 2.59370400 -0.29515200
C 5.21508800 1.27809500 -0.61014500
H 4.89210600 4.46085200 0.49959300
H 6.63349900 2.88371600 -0.35678800
H 6.01779700 0.58217200 -0.81510600
N 1.52474000 1.42371300 -0.32198800
C -0.86708600 -3.67259100 0.39102600
C -2.05980600 -4.08264600 -0.15365100
C -3.07227000 -3.15221600 -0.42657800
C -2.84531500 -1.77308300 -0.07878300
C -0.62237200 -2.30313100 0.63308900
H -4.41056600 -4.61649200 -1.28362200
H -0.08010900 -4.39288900 0.55507400
H -2.21559100 -5.12980500 -0.39464500
C -4.28074700 -3.56919300 -1.03262700
C -3.90807500 -0.83837600 -0.23318000
C -5.04571000 -1.30116400 -0.90640000
C -5.24569900 -2.63540100 -1.30608100
H -5.82539800 -0.58481800 -1.13432600
H -6.16557500 -2.91096200 -1.80998300
N -1.59619400 -1.40530100 0.39620700
H 1.27528000 -0.31539600 -0.14539200
H -1.42815300 -0.34793200 0.42083000

Table S54. Cartesian coordinates and energies of ***i*-TEQ 6a•**$2H^+$ (TS3-3).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.488551 (Hartree/Particle)
Thermal correction to Energy= 0.514768
Thermal correction to Enthalpy= 0.515712
Thermal correction to Gibbs Free Energy= 0.434353
Sum of electronic and zero-point Energies= -1603.202325
Sum of electronic and thermal Energies= -1603.176109
Sum of electronic and thermal Enthalpies= -1603.175164
Sum of electronic and thermal Free Energies= -1603.256524
C -0.51555000 -2.87975000 -0.97027300
C -2.61677100 -1.83732200 -0.36460800
C -3.24362600 -3.11700300 -0.53620200
C -2.52889900 -4.14241100 -1.20577000
C -1.18475200 -4.02407100 -1.44490300
C -3.39240900 -0.74703700 0.14035400
C -4.52742600 -3.37575800 -0.00487000
H -3.05074700 -5.05967000 -1.46217200
H -0.61794300 -4.83109900 -1.88955800
C -5.14624800 -2.40738000 0.74606300
C -4.58813800 -1.11797900 0.77758100
H -4.97507900 -4.35248000 -0.15618300
H -6.08780300 -2.59847900 1.24841700
H -5.15571400 -0.33583800 1.26936500
N -1.25299800 -1.80299500 -0.61245500
C 1.40730300 4.16189300 0.13875500
C 2.50315100 4.16900900 -0.68649500
C 3.14243200 2.95340800 -1.00864600
C 2.67869400 1.75411400 -0.35051300
C 0.90250100 2.90159000 0.56370400
H 4.52448600 3.81505600 -2.43341400
H 0.89080400 5.08542800 0.36320600
H 2.87043300 5.09842300 -1.11091000
C 4.21660500 2.90368500 -1.93057000
C 3.47311400 0.57306800 -0.48004100
C 4.50827900 0.57172000 -1.40041800
C 4.85486300 1.71133300 -2.16455400
H 5.11005000 -0.32583700 -1.50204400
H 5.66814100 1.64871900 -2.87965100
N 1.51718300 1.74228700 0.36053400
C -0.51548100 2.87975700 0.97023900
C -2.61673100 1.83738000 0.36458000
C -3.24354600 3.11708500 0.53614200
C -2.52879600 4.14247400 1.20571600
C -1.18466100 4.02408500 1.44488900
C -3.39241700 0.74709400 -0.14029300
C -4.52735600 3.37585400 0.00484500
H -3.05061900 5.05975300 1.46210200
H -0.61784100 4.83108300 1.88958300
C -5.14625000 2.40744800 -0.74599500
C -4.58817400 1.11803300 -0.77747400
H -4.97496400 4.35260400 0.15611000

H -6.08783000 2.59854200 -1.24830200
H -5.15578900 0.33588400 -1.26919900
N -1.25295200 1.80301900 0.61241000
C 1.40725500 -4.16191700 -0.13889600
C 2.50307700 -4.16906200 0.68638700
C 3.14232900 -2.95347000 1.00862500
C 2.67862500 -1.75415300 0.35050500
C 0.90244200 -2.90159700 -0.56377800
H 4.52427400 -3.81515800 2.43347500
H 0.89078500 -5.08544900 -0.36342800
H 2.87035800 -5.09849300 1.11076600
C 4.21643200 -2.90377300 1.93063200
C 3.47305900 -0.57312000 0.48009600
C 4.50815900 -0.57180200 1.40054600
C 4.85467300 -1.71142800 2.16469500
H 5.10994300 0.32574000 1.50221900
H 5.66788800 -1.64882900 2.87986500
N 1.51712100 -1.74229900 -0.36055500
H -0.68295500 -1.01205800 -0.31815200
H -0.68292600 1.01209800 0.31802800

Table S55. Cartesian coordinates and energies of ***i*-TEQ 6a•**$4H^+$.
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.515079 (Hartree/Particle)
Thermal correction to Energy= 0.542594
Thermal correction to Enthalpy= 0.543538
Thermal correction to Gibbs Free Energy= 0.459330
Sum of electronic and zero-point Energies= -1603.535197
Sum of electronic and thermal Energies= -1603.507682
Sum of electronic and thermal Enthalpies= -1603.506738
Sum of electronic and thermal Free Energies= -1603.590946
C 0.57924500 -2.39782400 0.47368800
C 2.71132700 -1.35841700 0.96406300
C 2.80356000 -2.15166200 2.16167400
C 1.75835100 -3.04927400 2.45935700
C 0.63355700 -3.15428500 1.63821900
C 3.71437600 -0.40931500 0.62777900
C 3.94300900 -2.00890800 2.99980100
H 1.82839800 -3.66688900 3.35148500
H -0.17604900 -3.83363100 1.88111900
C 4.92579100 -1.10446900 2.66600500
C 4.80081100 -0.31340400 1.49995100
H 4.02244900 -2.61618300 3.89644700
H 5.80160200 -0.98594000 3.29602200
H 5.58498600 0.40373200 1.27426600
N 1.60530600 -1.56419200 0.16362800
C -0.63304700 3.15525700 1.63609400
C -1.75787600 3.05104800 2.45722800
C -2.80338300 2.15360600 2.15999900
C -2.71129400 1.35958200 0.96291000
C -0.57904900 2.39829100 0.47184000
H -4.02227900 2.61945300 3.89441800
H 0.17671200 3.83455000 1.87861600
H -1.82778100 3.66915900 3.34902400
C -3.94292400 2.01166200 2.99811300
C -3.71433700 0.41029300 0.62730000
C -4.80088800 0.31518200 1.49944300
C -4.92590700 1.10725500 2.66479900
H -5.58505200 -0.40214200 1.27431600
H -5.80187400 0.98948000 3.29474600
N -1.60531200 1.56483200 0.16220300
C 0.57933100 2.39803600 -0.47333300
C 2.71140300 1.35889700 -0.96402800
C 2.80324300 2.15187500 -2.16181000
C 1.75781000 3.04929400 -2.45943700
C 0.63315200 3.15417200 -1.63814300
C 3.71438700 0.40965300 -0.62803100
C 3.94241000 2.00888800 -3.00026800
H 1.82760000 3.66674900 -3.35169600
H -0.17665700 3.83327700 -1.88101700
C 4.92515800 1.10431400 -2.66672300
C 4.80042800 0.31328600 -1.50060000
H 4.02159800 2.61591200 -3.89710600
H 5.80072900 0.98560700 -3.29704300
H 5.58437800 -0.40420700 -1.27526400
N 1.60562400 1.56482400 -0.16323500
C -0.63349100 -3.15612100 -1.63507200
C -1.75824100 -3.05188300 -2.45637800
C -2.80340000 -2.15388800 -2.15971100
C -2.71117300 -1.35936700 -0.96294400
C -0.57914700 -2.39836100 -0.47140200
H -4.02220100 -2.62014700 -3.89406900
H 0.17603600 -3.83584100 -1.87719500
H -1.82825400 -3.67040100 -3.34788500
C -3.94286300 -2.01202300 -2.99798900
C -3.71424000 -0.40995800 -0.62764000
C -4.80069600 -0.31498300 -1.49989400
C -4.92570100 -1.10732900 -2.66508900
H -5.58484500 0.40242600 -1.27497900
H -5.80159800 -0.98956500 -3.29513300
N -1.60517500 -1.56430000 -0.16228900
H -1.60450000 1.11836600 -0.75137200
H -1.60410500 -1.11738300 0.75105300
H 1.60508100 1.11911600 0.75071600
H 1.60435500 -1.11836400 -0.75025100

Table S56. Cartesian coordinates and energies of ***i*-TEQ 6a•**$4H^+$ (TS).
B3LYP-D3/6-31G(d,p)
zero-point correction= 0.512759 (Hartree/Particle)
Thermal correction to Energy= 0.539879
Thermal correction to Enthalpy= 0.540823
Thermal correction to Gibbs Free Energy= 0.457299
Sum of electronic and zero-point Energies= -1603.435298
Sum of electronic and thermal Energies= -1603.408179
Sum of electronic and thermal Enthalpies= -1603.407235
Sum of electronic and thermal Free Energies= -1603.490758
C -0.70243200 2.22487800 1.25471100
C -2.87486000 1.45222000 0.47234400
C -3.46771600 2.45228100 1.33341000
C -2.66620100 3.06950700 2.31431000
C -1.27790300 2.97072200 2.27570100
C -3.67388700 0.74492700 -0.49545000
C -4.78002900 2.92243800 1.07418200
H -3.13488400 3.73853500 3.03198300
H -0.65396500 3.56987400 2.92972800
C -5.35390600 2.55799000 -0.11999600
C -4.79623100 1.50441700 -0.87544400
H -5.24847300 3.63314000 1.74759000

H -6.27123800 3.02375600 -0.46555600
H -5.33329200 1.24058600 -1.77765100
N -1.49342000 1.40714600 0.49624700
C 1.63925100 -3.90174000 0.13557600
C 2.97158700 -3.93872800 0.51149100
C 3.71124400 -2.75703900 0.67543200
C 3.11373500 -1.51730000 0.24519800
C 0.98137800 -2.67421900 -0.03413200
H 5.45419100 -3.73587400 1.50965300
H 1.10527100 -4.83176400 0.00708800
H 3.44644900 -4.89732300 0.70447100
C 5.03068800 -2.78647600 1.19639700
C 3.91638600 -0.34212600 0.19551800
C 5.18702100 -0.42817900 0.77875600
C 5.73903800 -1.61505700 1.30608200
H 5.79896000 0.46869600 0.79650100
H 6.73326400 -1.59891000 1.74063800
N 1.75778300 -1.54852600 -0.07122600
C -0.50984700 -2.68015400 -0.01799700
C -2.73511500 -1.79062000 -0.57619600
C -3.25664300 -3.12704600 -0.37226000
C -2.44755700 -4.07122600 0.27519200
C -1.11446300 -3.81678600 0.53265100
C -3.65532700 -0.72871200 -0.88694100
C -4.55990500 -3.49211700 -0.77997300
H -2.87730000 -5.02627900 0.56705800
H -0.53860200 -4.53485800 1.09647700
C -5.33470600 -2.53974300 -1.38986800
C -4.90218700 -1.20478000 -1.35254900
H -4.91412400 -4.50417700 -0.61024200
H -6.31812800 -2.77196100 -1.78497400
H -5.66379200 -0.49273900 -1.63033800
N -1.33167700 -1.68706100 -0.49471000
C 0.70868700 3.85190300 0.06638100
C 1.78439800 4.13867600 -0.77082000
C 2.74719100 3.15989700 -1.06911000
C 2.68288000 1.89150900 -0.38438400
C 0.60870600 2.59239100 0.64886800
H 3.82469600 4.37050700 -2.50964900
H -0.08042100 4.57778200 0.22305500
H 1.85785500 5.11901100 -1.23517900
C 3.78311300 3.40836200 -2.00829000
C 3.67865900 0.91147600 -0.59694800
C 4.64611500 1.20423400 -1.56730500
C 4.70480100 2.42422900 -2.27429000
H 5.40191400 0.45431600 -1.77995100
H 5.49147100 2.58084300 -3.00527900
N 1.60274800 1.68147300 0.46306700
H 1.33982600 -0.67032700 -0.34988000
H 1.65616700 0.90023800 1.11280100
H -0.92394900 -0.97601400 -1.09046700
H -1.05572200 0.97165800 -0.30301000

Table S57. Cartesian coordinates and energies of ***i*-TEQ 6a•**$4H^+$ (Int).
B3LYP-D3/6-31G(d,p)
Zero-point correction= 0.513140 (Hartree/Particle)
Thermal correction to Energy= 0.540946
Thermal correction to Enthalpy= 0.541890
Thermal correction to Gibbs Free Energy= 0.456091
Sum of electronic and zero-point Energies= -1603.447262
Sum of electronic and thermal Energies= -1603.419455
Sum of electronic and thermal Enthalpies= -1603.418511
Sum of electronic and thermal Free Energies= -1603.504311
C 1.05046000 -2.75402300 0.95698900
C 2.94649000 -1.57643900 -0.00774000
C 3.66325500 -2.82265300 -0.03915300
C 3.15805200 -3.89056900 0.73084600
C 1.87572400 -3.84807100 1.25504300
C 3.55136800 -0.39639100 -0.53759200
C 4.84238400 -2.94456700 -0.82018200
H 3.76035600 -4.78681000 0.85819700
H 1.47718200 -4.70011400 1.79221300
C 5.26281500 -1.87192100 -1.57066000
C 4.65231500 -0.61041400 -1.37311400
H 5.37702100 -3.88953700 -0.83338000
H 6.11783500 -1.95493500 -2.23372900
H 5.12163800 0.25743300 -1.82807500
N 1.65036500 -1.62464700 0.47860600
C -1.87599100 3.84749500 -1.25588900
C -3.15808800 3.89018200 -0.73116300
C -3.66298100 2.82250700 0.03938400
C -2.94624600 1.57627700 0.00803600
C -1.05056100 2.75359200 -0.95773400
H -5.37639500 3.88962600 0.83409600
H -1.47775300 4.69937800 -1.79352300
H -3.76043900 4.78638600 -0.85853900
C -4.84168200 2.94469900 0.82100200
C -3.55093100 0.39638800 0.53853900
C -4.65120600 0.61080100 1.37489000
C -5.26156400 1.87238000 1.57227200
H -5.12015000 -0.25685700 1.83059900
H -6.11617500 1.95566100 2.23584100
N -1.65028000 1.62436600 -0.47880700
C 0.41212000 2.96022500 -0.78837700
C 2.58398100 2.07082400 -0.12019900
C 2.95023000 3.38865300 0.35073800
C 2.08114700 4.46033000 0.10552800
C 0.81702400 4.24516600 -0.42193900
C 3.49490100 0.99790900 0.05537900
C 4.16579000 3.61006000 1.04825400
H 2.37547900 5.46540900 0.39630200
H 0.11838200 5.06899600 -0.45492400
C 4.99360300 2.54830100 1.30906300
C 4.65012700 1.27870500 0.80454000
H 4.41056300 4.61513800 1.37781500
H 5.91571800 2.67505000 1.86680700
H 5.33984700 0.46218200 0.99172900
N 1.32370400 1.93800900 -0.70432000
C -0.81686100 -4.24522000 0.41949200
C -2.08109400 -4.46015200 -0.10773600
C -2.95054900 -3.38844500 -0.35158800
C -2.58421400 -2.07087900 0.12000000
C -0.41213800 -2.96050900 0.78705400
H -4.41134300 -4.61448200 -1.37853300
H -0.11801100 -5.06891200 0.45164600
H -2.37536200 -5.46502700 -0.39928300
C -4.16655900 -3.60960000 -1.04838200
C -3.49526500 -0.99788700 -0.05449600
C -4.65104400 -1.27845000 -0.80287800

C -4.99481700 -2.54783600 -1.30774700
H -5.34093600 -0.46190500 -0.98930400
H -5.91740500 -2.67438400 -1.86474900
N -1.32381900 -1.93835000 0.70388500
H -1.08865700 0.79531400 -0.34219600
H -1.16070300 -1.09202800 1.24326200
H 1.16065300 1.09136300 -1.24319800
H 1.08890400 -0.79540000 0.34249500

Table S58. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).
B3LYP-D3/6-31G(d,p)-SDD(Pd)
Zero-point correction= 0.467475 (Hartree/Particle)
Thermal correction to Energy= 0.494880
Thermal correction to Enthalpy= 0.495824
Thermal correction to Gibbs Free Energy= 0.412318
Sum of electronic and zero-point Energies= -1730.051660
Sum of electronic and thermal Energies= -1730.024256
Sum of electronic and thermal Enthalpies= -1730.023311
Sum of electronic and thermal Free Energies= -1730.106817
C 0.64681600 2.75092900 0.34579300
C 2.54126100 1.48097200 0.90976900
C 2.94280100 2.49930600 1.84230000
C 2.19097300 3.69489000 1.90117300
C 1.08872900 3.85654800 1.09348800
C 3.43959700 0.41654700 0.62063800
C 4.10124200 2.31367100 2.63837600
H 2.50099200 4.48530900 2.57820200
H 0.50917600 4.77182300 1.09882100
C 4.87012400 1.18723800 2.47232900
C 4.56034900 0.28073000 1.43541800
H 4.37264900 3.07931100 3.35839400
H 5.75041300 1.02122200 3.08382300
H 5.24695200 -0.53559800 1.23520400
N 1.31943200 1.58920600 0.28571500
C -1.08883000 -3.85649200 1.09334600
C -2.19098400 -3.69479400 1.90117200
C -2.94272800 -2.49919300 1.84237100
C -2.54126400 -1.48087800 0.90978100
C -0.64692100 -2.75090200 0.34566400
H -4.37230300 -3.07912300 3.35875200
H -0.50932300 -4.77179900 1.09860700
H -2.50088800 -4.48516300 2.57830900
C -4.10107200 -2.31351600 2.63863300
C -3.43972300 -0.41652600 0.62066400
C -4.56038200 -0.28073300 1.43551300
C -4.86998900 -1.18715700 2.47260400
H -5.24713500 0.53547500 1.23533800
H -5.75023700 -1.02109500 3.08413900
N -1.31949000 -1.58908200 0.28566500
C 0.64675500 -2.75100900 -0.34530500
C 2.54103200 -1.48110800 -0.90978400
C 2.94252700 -2.49963300 -1.84214000
C 2.19084900 -3.69527000 -1.90058400
C 1.08867000 -3.85676200 -1.09270400
C 3.43939800 -0.41657800 -0.62105300
C 4.10077700 -2.31398600 -2.63857000
H 2.50072200 -4.48583000 -2.57751300
H 0.50921000 -4.77209700 -1.09771300
C 4.86945600 -1.18739300 -2.47305700
C 4.55983500 -0.28069600 -1.43620100
H 4.37203200 -3.07976500 -3.35849700
H 5.74955900 -1.02130900 -3.08480000
H 5.24642600 0.53572600 -1.23633400
N 1.31934500 -1.58917400 -0.28557900
C -1.08867800 3.85671100 -1.09277900
C -2.19071200 3.69510900 -1.90079200
C -2.94242600 2.49946100 -1.84232100
C -2.54113000 1.48106300 -0.90977800
C -0.64686400 2.75098200 -0.34521100
H -4.37165600 3.07947200 -3.35900700
H -0.50915800 4.77200800 -1.09785900
H -2.50055100 4.48557200 -2.57785000
C -4.10054500 2.31379300 -2.63892000
C -3.43958300 0.41662100 -0.62099400
C -4.55997300 0.28079100 -1.43619200
C -4.86937400 1.18731500 -2.47326800
H -5.24671600 -0.53549700 -1.23630000
H -5.74941000 1.02119900 -3.08509500
N -1.31948000 1.58921600 -0.28542900
Pd 0.00001100 -0.00002900 0.00005400

Table S59. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.465965 (Hartree/Particle)
Thermal correction to Energy= 0.493715
Thermal correction to Enthalpy= 0.494659
Thermal correction to Gibbs Free Energy= 0.409817
Sum of electronic and zero-point Energies= -1730.196840
Sum of electronic and thermal Energies= -1730.169090
Sum of electronic and thermal Enthalpies= -1730.168146
Sum of electronic and thermal Free Energies= -1730.252988
C 0.64643900 -2.75163900 -0.34529700
C 2.53873100 -1.48367400 -0.90831800
C 2.93965100 -2.50131300 -1.83978300
C 2.18586900 -3.69608300 -1.90217900
C 1.08314400 -3.85669600 -1.09648700
C 3.43474200 -0.41635500 -0.62082100
C 4.09735000 -2.31365700 -2.63610000
H 2.49431400 -4.48425800 -2.58171100
H 0.49673100 -4.76739500 -1.10380900
C 4.86434400 -1.18610700 -2.47050900
C 4.55426600 -0.27813500 -1.43512100
H 4.36797300 -3.07889800 -3.35623500
H 5.74447100 -1.01935500 -3.08159900
H 5.23916600 0.53916700 -1.23478400
N 1.31996600 -1.59258600 -0.28194200
C -1.08318200 3.85667700 -1.09660100
C -2.18591600 3.69604000 -1.90227000
C -2.93967300 2.50125300 -1.83985500
C -2.53873000 1.48363600 -0.90837500
C -0.64643500 2.75162900 -0.34541900
H -4.36801100 3.07878500 -3.35631200
H -0.49679000 4.76738800 -1.10392800
H -2.49439800 4.48420600 -2.58179500
C -4.09737200 2.31356400 -2.63616300
C -3.43473100 0.41632100 -0.62083900
C -4.55425400 0.27806300 -1.43513700
C -4.86434500 1.18600300 -2.47054900

H -5.23914100 -0.53924300 -1.23477700
H -5.74446800 1.01922200 -3.08163600
N -1.31994900 1.59257200 -0.28203100
C 0.64643800 2.75164000 0.34530100
C 2.53873500 1.48367400 0.90830600
C 2.93966100 2.50131000 1.83977000
C 2.18589100 3.69609300 1.90215600
C 1.08316800 3.85670900 1.09646800
C 3.43474200 0.41636100 0.62079600
C 4.09736000 2.31365100 2.63608200
H 2.49435600 4.48427200 2.58167500
H 0.49677000 4.76741600 1.10376800
C 4.86435300 1.18609900 2.47048400
C 4.55427300 0.27813500 1.43509200
H 4.36798700 3.07888600 3.35622000
H 5.74448100 1.01934500 3.08157000
H 5.23916800 -0.53916800 1.23474900
N 1.31996000 1.59259000 0.28194000
C -1.08312400 -3.85664500 1.09669800
C -2.18586400 -3.69600100 1.90236100
C -2.93965500 -2.50124000 1.83989000
C -2.53872600 -1.48364000 0.90838500
C -0.64641400 -2.75162100 0.34546100
H -4.36801200 -3.07877400 3.35632900
H -0.49669600 -4.76733200 1.10407800
H -2.49431800 -4.48414200 2.58192800
C -4.09737600 -2.31356300 2.63616800
C -3.43474100 -0.41634900 0.62081200
C -4.55429000 -0.27810500 1.43507800
C -4.86438100 -1.18603100 2.47050200
H -5.23919500 0.53917600 1.23468500
H -5.74452700 -1.01926300 3.08156000
N -1.31994300 -1.59257400 0.28204300
Pd 0.00000400 -0.00000200 0.00000100

Table S60. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).
B3LYP-D3BJ/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.467012 (Hartree/Particle)
Thermal correction to Energy= 0.494610
Thermal correction to Enthalpy= 0.495554
Thermal correction to Gibbs Free Energy= 0.411431
Sum of electronic and zero-point Energies= -1730.312863
Sum of electronic and thermal Energies= -1730.285265
Sum of electronic and thermal Enthalpies= -1730.284321
Sum of electronic and thermal Free Energies= -1730.368444
C 0.64773500 -2.75689200 -0.34013700
C 2.53168700 -1.48198200 -0.90809800
C 2.93960300 -2.50079400 -1.83325100
C 2.19822400 -3.70267700 -1.88428100
C 1.09795400 -3.86552100 -1.07656000
C 3.42260100 -0.41307900 -0.62140300
C 4.09564700 -2.30952500 -2.62934300
H 2.51648800 -4.49467300 -2.55408500
H 0.52450700 -4.78357100 -1.07031700
C 4.85672400 -1.17800500 -2.46679900
C 4.54268800 -0.27087600 -1.43294300
H 4.36945600 -3.07602200 -3.34621900
H 5.73620300 -1.00871700 -3.07745300
H 5.22331000 0.54873000 -1.23011700
N 1.31406000 -1.59374600 -0.28324800
C -1.09797000 3.86548800 -1.07670300
C -2.19824700 3.70261100 -1.88440800
C -2.93961400 2.50072300 -1.83333900
C -2.53168300 1.48194200 -0.90815700
C -0.64773000 2.75688300 -0.34025800
H -4.36947700 3.07589800 -3.34631600
H -0.52454000 4.78354800 -1.07049000
H -2.51652700 4.49458600 -2.55422900
C -4.09566200 2.30942400 -2.62941800
C -3.42259700 0.41305000 -0.62141400
C -4.54268700 0.27081600 -1.43294400
C -4.85673300 1.17790600 -2.46683200
H -5.22330700 -0.54878300 -1.23008500
H -5.73621400 1.00859100 -3.07747600
N -1.31404600 1.59373200 -0.28333100
C 0.64772700 2.75689200 0.34018900
C 2.53169600 1.48197500 0.90808800
C 2.93962600 2.50077100 1.83325400
C 2.19824300 3.70264900 1.88432200
C 1.09795800 3.86550700 1.07662500
C 3.42261400 0.41308800 0.62134900
C 4.09569100 2.30949900 2.62931400
H 2.51651700 4.49463200 2.55413700
H 0.52451300 4.78355800 1.07041200
C 4.85678100 1.17799500 2.46672100
C 4.54272800 0.27088500 1.43285400
H 4.36950700 3.07598500 3.34620000
H 5.73628000 1.00870400 3.07734600
H 5.22335500 -0.54870700 1.22999300
N 1.31405400 1.59374700 0.28326700
C -1.09794200 -3.86545800 1.07680200
C -2.19823200 -3.70257400 1.88448600
C -2.93962200 -2.50070200 1.83336300
C -2.53169200 -1.48194000 0.90816000
C -0.64771900 -2.75687200 0.34031800
H -4.36951200 -3.07586500 3.34632000
H -0.52448400 -4.78350100 1.07062700
H -2.51650600 -4.49452800 2.55433500
C -4.09569400 -2.30940500 2.62940700
C -3.42261400 -0.41306900 0.62137100
C -4.54273500 -0.27084100 1.43286200
C -4.85679100 -1.17791300 2.46676200
H -5.22336700 0.54873700 1.22996400
H -5.73629600 -1.00860400 3.07737200
N -1.31404800 -1.59373000 0.28334900
Pd 0.00000400 0.00000300 0.00000200

Table S61. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).
CAM-B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.473557 (Hartree/Particle)
Thermal correction to Energy= 0.500543
Thermal correction to Enthalpy= 0.501487
Thermal correction to Gibbs Free Energy= 0.418785
Sum of electronic and zero-point Energies= -1729.195889
Sum of electronic and thermal Energies= -1729.168904
Sum of electronic and thermal Enthalpies= -1729.167960
Sum of electronic and thermal Free Energies= -1729.250662
C 0.64516500 -2.73218200 -0.34839900

C 2.52928000 -1.47673400 -0.90810200
C 2.92269100 -2.48409700 -1.83535000
C 2.16759400 -3.67326800 -1.90361500
C 1.07028500 -3.83343300 -1.10174600
C 3.42546200 -0.41419500 -0.62086000
C 4.07815400 -2.30020200 -2.63125400
H 2.47480500 -4.45821600 -2.58666000
H 0.47809700 -4.73971800 -1.11182500
C 4.84516500 -1.18270100 -2.46519100
C 4.53807600 -0.27833300 -1.42906500
H 4.34219600 -3.06402200 -3.35434600
H 5.72582000 -1.01791700 -3.07469800
H 5.22687200 0.53414500 -1.22551800
N 1.31449000 -1.58235200 -0.28032600
C -1.07029800 3.83339400 -1.10187300
C -2.16761200 3.67320300 -1.90373100
C -2.92270100 2.48402900 -1.83543200
C -2.52928000 1.47669400 -0.90815800
C -0.64516700 2.73216600 -0.34850000
H -4.34220800 3.06390300 -3.35444500
H -0.47811200 4.73968000 -1.11198300
H -2.47483200 4.45813400 -2.58679200
C -4.07816300 2.30010400 -2.63133200
C -3.42546100 0.41416000 -0.62088200
C -4.53807300 0.27826800 -1.42908300
C -4.84516600 1.18260300 -2.46523800
H -5.22686700 -0.53420400 -1.22550700
H -5.72581900 1.01779500 -3.07474100
N -1.31448600 1.58233300 -0.28039600
C 0.64516400 2.73220000 0.34825900
C 2.52924100 1.47676000 0.90810700
C 2.92263200 2.48417200 1.83531000
C 2.16756500 3.67336600 1.90345500
C 1.07028500 3.83349600 1.10153500
C 3.42542000 0.41418300 0.62097500
C 4.07803900 2.30028200 2.63130300
H 2.47476800 4.45836700 2.58644300
H 0.47812400 4.73980100 1.11153300
C 4.84501000 1.18273600 2.46537100
C 4.53796400 0.27832200 1.42926900
H 4.34205700 3.06413300 3.35437000
H 5.72561000 1.01794800 3.07495800
H 5.22674900 -0.53418800 1.22580800
N 1.31447700 1.58235500 0.28028300
C -1.07028000 -3.83345100 1.10169800
C -2.16755000 -3.67328300 1.90362100
C -2.92262100 -2.48409100 1.83542600
C -2.52924000 -1.47672500 0.90817000
C -0.64516600 -2.73218800 0.34836600
H -4.34203900 -3.06398300 3.35451800
H -0.47811600 -4.73975400 1.11172800
H -2.47474600 -4.45824800 2.58665400
C -4.07802500 -2.30016700 2.63141200
C -3.42542200 -0.41416700 0.62098700
C -4.53796800 -0.27827100 1.42927500
C -4.84500600 -1.18263600 2.46542100
H -5.22675500 0.53422600 1.22577500
H -5.72560800 -1.01782700 3.07499700
N -1.31448200 -1.58235100 0.28033700
Pd 0.00000100 -0.00000100 -0.00001000

Table S62. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).

ωB97XD/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.472604 (Hartree/Particle)
Thermal correction to Energy= 0.499748
Thermal correction to Enthalpy= 0.500692
Thermal correction to Gibbs Free Energy= 0.417653
Sum of electronic and zero-point Energies= -1729.577422
Sum of electronic and thermal Energies= -1729.550278
Sum of electronic and thermal Enthalpies= -1729.549333
Sum of electronic and thermal Free Energies= -1729.632373
C 0.64554800 -2.73994600 -0.35013200
C 2.52647700 -1.47870700 -0.91145600
C 2.92011400 -2.48101300 -1.84441000
C 2.16720400 -3.67330500 -1.91409500
C 1.07129500 -3.83903500 -1.10835800
C 3.41777500 -0.41096500 -0.62366800
C 4.07212300 -2.28696400 -2.64563800
H 2.47262600 -4.45553100 -2.60124500
H 0.48157400 -4.74725700 -1.12161300
C 4.83308100 -1.16304200 -2.47947800
C 4.52624800 -0.26342800 -1.43757600
H 4.33878800 -3.04599100 -3.37305800
H 5.70929700 -0.99061300 -3.09326500
H 5.21093600 0.55344400 -1.23472600
N 1.31431400 -1.58915900 -0.27911300
C -1.07130100 3.83899300 -1.10850400
C -2.16721600 3.67323500 -1.91422700
C -2.92012200 2.48094400 -1.84449800
C -2.52647700 1.47867000 -0.91151400
C -0.64554500 2.73993000 -0.35024500
H -4.33880600 3.04586900 -3.37315500
H -0.48158000 4.74721400 -1.12179300
H -2.47264500 4.45543700 -2.60140100
C -4.07213500 2.28686500 -2.64571300
C -3.41777400 0.41093800 -0.62368100
C -4.52624900 0.26336900 -1.43758100
C -4.83308900 1.16294700 -2.47951200
H -5.21093600 -0.55349700 -1.23469700
H -5.70930800 0.99049600 -3.09328900
N -1.31431000 1.58914500 -0.27918500
C 0.64555100 2.73995600 0.35004500
C 2.52645600 1.47872200 0.91145800
C 2.92007900 2.48105500 1.84438800
C 2.16718500 3.67336100 1.91400400
C 1.07129700 3.83907300 1.10823200
C 3.41775100 0.41095900 0.62373100
C 4.07205500 2.28700800 2.64566600
H 2.47260200 4.45561400 2.60112500
H 0.48159500 4.74730700 1.12143600
C 4.83299100 1.16306100 2.47957900
C 4.52618400 0.26342200 1.43769100
H 4.33870700 3.04605300 3.37307200
H 5.70917600 0.99063200 3.09341200
H 5.21086600 -0.55346900 1.23489000
N 1.31431000 1.58916200 0.27908200
C -1.07129500 -3.83903000 1.10839100
C -2.16718200 -3.67328600 1.91415600
C -2.92007500 -2.48098100 1.84449500

C -2.52645200 -1.47868600 0.91152500
C -0.64554700 -2.73994300 0.35016200
H -4.33870300 -3.04591900 3.37320000
H -0.48159100 -4.74726300 1.12162900
H -2.47260100 -4.45551100 2.60130800
C -4.07205100 -2.28690300 2.64576400
C -3.41774900 -0.41093700 0.62375100
C -4.52618300 -0.26336700 1.43770400
C -4.83298900 -1.16296400 2.47962900
H -5.21086600 0.55351300 1.23486800
H -5.70917500 -0.99051200 3.09345300
N -1.31430500 -1.58915200 0.27915500
Pd 0.00000200 0.00000000 -0.00000500

Table S63. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).
M06-2X/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.470871 (Hartree/Particle)
Thermal correction to Energy= 0.498437
Thermal correction to Enthalpy= 0.499382
Thermal correction to Gibbs Free Energy= 0.415075
Sum of electronic and zero-point Energies= -1729.341289
Sum of electronic and thermal Energies= -1729.313723
Sum of electronic and thermal Enthalpies= -1729.312778
Sum of electronic and thermal Free Energies= -1729.397085
C 0.65280200 -2.75609900 -0.34040800
C 2.54533100 -1.50692100 -0.88858100
C 2.95072000 -2.52416300 -1.80269500
C 2.19477700 -3.71610200 -1.86977900
C 1.08338200 -3.86826500 -1.08241900
C 3.43055600 -0.42616600 -0.61497900
C 4.11116700 -2.34518400 -2.59561700
H 2.51145400 -4.50566200 -2.54401000
H 0.48521700 -4.77129100 -1.09479500
C 4.86856400 -1.21654100 -2.44312300
C 4.54738800 -0.29595500 -1.42169400
H 4.38323800 -3.11901300 -3.30556300
H 5.75101200 -1.05304700 -3.05036500
H 5.22798500 0.52700100 -1.22835800
N 1.33045500 -1.61267100 -0.26464200
C -1.08339700 3.86823100 -1.08255100
C -2.19479600 3.71604000 -1.86989900
C -2.95072900 2.52409600 -1.80278100
C -2.54533200 1.50688500 -0.88863500
C -0.65280300 2.75608700 -0.34051500
H -4.38325000 3.11888800 -3.30566900
H -0.48523900 4.77126100 -1.09495400
H -2.51148500 4.50557900 -2.54414900
C -4.11117400 2.34508300 -2.59569700
C -3.43055400 0.42613700 -0.61499400
C -4.54738500 0.29589400 -1.42170400
C -4.86856400 1.21644100 -2.44316600
H -5.22797900 -0.52705800 -1.22833700
H -5.75101100 1.05292100 -3.05040500
N -1.33045100 1.61266000 -0.26471000
C 0.65280400 2.75610100 0.34039600
C 2.54533100 1.50692100 0.88857500
C 2.95072300 2.52416800 1.80268300
C 2.19478800 3.71611400 1.86975200
C 1.08339500 3.86827500 1.08239000
C 3.43055300 0.42616300 0.61498000
C 4.11116600 2.34518700 2.59561000
H 2.51147300 4.50568100 2.54397000
H 0.48523800 4.77130600 1.09475400
C 4.86855700 1.21653900 2.44312600
C 4.54738200 0.29595000 1.42170000
H 4.38323900 3.11901900 3.30555200
H 5.75100200 1.05304300 3.05037400
H 5.22797600 -0.52701000 1.22836800
N 1.33045200 1.61267000 0.26463800
C -1.08338100 -3.86822600 1.08256400
C -2.19477500 -3.71603500 1.86991800
C -2.95071600 -2.52409600 1.80279400
C -2.54532800 -1.50688800 0.88864200
C -0.65279900 -2.75608600 0.34051600
H -4.38323400 -3.11889000 3.30568400
H -0.48521600 -4.77125200 1.09497200
H -2.51145500 -4.50556900 2.54417800
C -4.11116200 -2.34508700 2.59571100
C -3.43055300 -0.42614300 0.61500000
C -4.54738500 -0.29590300 1.42171000
C -4.86855900 -1.21645000 2.44317400
H -5.22798300 0.52704500 1.22834200
H -5.75100700 -1.05293300 3.05041200
N -1.33045000 -1.61266100 0.26470900
Pd 0.00000000 0.00000000 0.00000000

Table S64. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II).
B3LYP-D3/6-311+G(2d,p)-SDD(Pd)/SMD(Et_2O)
Zero-point correction= 0.465660 (Hartree/Particle)
Thermal correction to Energy= 0.493141
Thermal correction to Enthalpy= 0.494085
Thermal correction to Gibbs Free Energy= 0.410270
Sum of electronic and zero-point Energies= -1730.635726
Sum of electronic and thermal Energies= -1730.608245
Sum of electronic and thermal Enthalpies= -1730.607301
Sum of electronic and thermal Free Energies= -1730.691116
C 0.64823900 2.74783400 0.34134600
C 2.52660300 1.47519900 0.91087400
C 2.92960800 2.48686300 1.83845300
C 2.19254600 3.68691700 1.88599100
C 1.10034200 3.85205600 1.07746000
C 3.41685600 0.40980300 0.62343100
C 4.07611900 2.28905400 2.64030500
H 2.50775800 4.47576100 2.55830000
H 0.53081100 4.76992500 1.07297200
C 4.83071700 1.15914900 2.47977500
C 4.52503600 0.26066600 1.44070800
H 4.34812300 3.05150700 3.35997200
H 5.70259500 0.98263600 3.09664800
H 5.20847000 -0.55500500 1.24044800
N 1.31166800 1.58863700 0.28695200
C -1.10038500 -3.85210700 1.07735700
C -2.19259100 -3.68698000 1.88588100
C -2.92963300 -2.48691900 1.83837500
C -2.52662800 -1.47522800 0.91083600
C -0.64825300 -2.74784800 0.34129700
H -4.34810800 -3.05158300 3.35991600
H -0.53086400 -4.76998100 1.07283600

H -2.50781600 -4.47584300 2.55816100
C -4.07613000 -2.28910300 2.64026800
C -3.41686100 -0.40979500 0.62343700
C -4.52498200 -0.26062800 1.44078500
C -4.83066600 -1.15915900 2.47982600
H -5.20840900 0.55506900 1.24061600
H -5.70250500 -0.98259700 3.09674200
N -1.31166300 -1.58865200 0.28695100
C 0.64739100 -2.74807800 -0.34048100
C 2.52585300 -1.47593300 -0.91081100
C 2.92821800 -2.48771200 -1.83852000
C 2.19095300 -3.68767200 -1.88557200
C 1.09907100 -3.85254600 -1.07655200
C 3.41645000 -0.41071600 -0.62381700
C 4.07437000 -2.29010600 -2.64096400
H 2.50570400 -4.47665000 -2.55793300
H 0.52943600 -4.77033600 -1.07176500
C 4.82921700 -1.16032100 -2.48087300
C 4.52423900 -0.26176200 -1.44165200
H 4.34584600 -3.05263900 -3.36075000
H 5.70081000 -0.98395600 -3.09819300
H 5.20792300 0.55378100 -1.24173900
N 1.31109100 -1.58908300 -0.28641700
C -1.09904200 3.85254400 -1.07655600
C -2.19088200 3.68766500 -1.88560600
C -2.92817400 2.48770900 -1.83855000
C -2.52583900 1.47591900 -0.91083700
C -0.64737200 2.74806500 -0.34048600
H -4.34584700 3.05273500 -3.36072400
H -0.52937100 4.77031400 -1.07170200
H -2.50566100 4.47663100 -2.55797300
C -4.07434800 2.29019500 -2.64095800
C -3.41646300 0.41073700 -0.62380200
C -4.52426100 0.26185100 -1.44165800
C -4.82924400 1.16042500 -2.48084200
H -5.20798300 -0.55368200 -1.24181400
H -5.70086800 0.98411100 -3.09813000
N -1.31106400 1.58907300 -0.28645200
Pd -0.00001500 -0.00000600 0.00021000

Table S65. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).
B3LYP-D3/6-31G(d,p)-SDD(Pd)
Zero-point correction= 0.466887 (Hartree/Particle)
Thermal correction to Energy= 0.493486
Thermal correction to Enthalpy= 0.494430
Thermal correction to Gibbs Free Energy= 0.412481
Sum of electronic and zero-point Energies= -1729.998327
Sum of electronic and thermal Energies= -1729.971728
Sum of electronic and thermal Enthalpies= -1729.970784
Sum of electronic and thermal Free Energies= -1730.052734
C 0.53132000 2.79731400 -0.36910200
C 2.50080600 1.82848800 0.54890000
C 2.94912600 3.18158100 0.84194600
C 2.20716300 4.29100800 0.39233200
C 1.01961300 4.10868000 -0.25639900
C 3.41184300 0.73449400 0.84158400
C 4.12967100 3.45466000 1.56555400
H 2.58528900 5.28987100 0.58587700
H 0.42470100 4.95181600 -0.57842600
C 4.92589600 2.41108100 1.94179600
C 4.58540900 1.12320200 1.51438500
H 4.39325300 4.48524000 1.77921600
H 5.85158600 2.56668600 2.48466400
H 5.36144000 0.39614800 1.67842400
N 1.23122500 1.70497300 0.01003000
C -1.12938300 -3.88243800 -0.64625600
C -1.97152100 -4.14896200 0.40962600
C -2.52777300 -3.09182400 1.16962900
C -2.30882900 -1.75451200 0.70597300
C -0.71676300 -2.54511600 -0.84192400
H -3.43600300 -4.31880900 2.70597000
H -0.67058000 -4.68399800 -1.21110600
H -2.19377600 -5.17535900 0.68670000
C -3.29974700 -3.30617000 2.33972800
C -3.12974900 -0.70028500 1.20631100
C -3.81930600 -0.95103900 2.38835400
C -3.85519700 -2.22920900 2.99213600
H -4.41916600 -0.15447700 2.81764300
H -4.40509100 -2.36745800 3.91678200
N -1.31069700 -1.52510600 -0.20828600
C 0.60973500 -2.26722500 -1.41266600
C 2.67485500 -1.39974500 -0.65117200
C 3.32321500 -2.43035500 -1.43923300
C 2.58004100 -3.12363900 -2.41981500
C 1.20704700 -3.08663700 -2.37829000
C 3.45498700 -0.69738800 0.35439700
C 4.61023800 -2.91077500 -1.10238000
H 3.09640200 -3.79646400 -3.09767900
H 0.59640800 -3.73120200 -2.99984800
C 5.11126100 -2.54933000 0.12107000
C 4.51138100 -1.49204500 0.82961900
H 5.09086600 -3.65400300 -1.72954400
H 5.98889500 -3.03250000 0.53657500
H 4.96305600 -1.25784900 1.78203200
N 1.30935500 -1.32734700 -0.72292300
C -1.53373100 3.56616400 -1.56582700
C -2.88074300 3.42534300 -1.78018900
C -3.59447000 2.38977600 -1.14076500
C -2.87203300 1.42534500 -0.34494800
C -0.87822200 2.62128700 -0.75488800
H -5.50568200 3.05718700 -1.89465800
H -0.97679800 4.36842600 -2.03179200
H -3.41414500 4.12110500 -2.42065400
C -5.00137600 2.31808200 -1.28031000
C -3.61467800 0.41232800 0.33525800
C -5.00024400 0.40012700 0.15732900
C -5.69931900 1.33158200 -0.63299700
H -5.57128800 -0.38472500 0.64020800
H -6.77740000 1.25589300 -0.72421200
N -1.50539100 1.55212100 -0.22917700
Pd -0.04601200 0.08062800 -0.10231000

Table S66. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.467536 (Hartree/Particle)
Thermal correction to Energy= 0.494042
Thermal correction to Enthalpy= 0.494986
Thermal correction to Gibbs Free Energy= 0.413290

Sum of electronic and zero-point Energies= -1730.141569
Sum of electronic and thermal Energies= -1730.115063
Sum of electronic and thermal Enthalpies= -1730.114119
Sum of electronic and thermal Free Energies= -1730.195815
C 0.53065200 2.80066800 -0.36817100
C 2.49938500 1.82985700 0.54375500
C 2.95241700 3.18091700 0.83216700
C 2.21152600 4.29159500 0.38355800
C 1.02213400 4.11119200 -0.26037300
C 3.40480500 0.73177400 0.84176200
C 4.13350800 3.45120000 1.55545500
H 2.59181300 5.28930900 0.57554500
H 0.42871200 4.95459900 -0.58207300
C 4.92029400 2.40435000 1.94169900
C 4.57432400 1.11534900 1.52228500
H 4.40154800 4.48160500 1.76307400
H 5.84410000 2.55534900 2.48856900
H 5.34305300 0.38447100 1.69987900
N 1.22986800 1.70870100 0.00906300
C -1.12486100 -3.87764100 -0.65094200
C -1.95750500 -4.14647600 0.41058700
C -2.51346800 -3.09010100 1.17263800
C -2.30115100 -1.75414800 0.70738800
C -0.71892400 -2.53842300 -0.84983700
H -3.40845400 -4.31648000 2.71545400
H -0.66473400 -4.67663100 -1.21757900
H -2.17249700 -5.17266300 0.69119300
C -3.27947500 -3.30410200 2.34661500
C -3.12280200 -0.70139000 1.20940100
C -3.80960700 -0.95037700 2.39222800
C -3.83861900 -2.22800800 2.99712000
H -4.41388400 -0.15595600 2.81876300
H -4.38821900 -2.36679000 3.92161000
N -1.31126400 -1.52131400 -0.21305000
C 0.60493200 -2.25850000 -1.42505100
C 2.66808200 -1.39809900 -0.65855100
C 3.31518700 -2.42985100 -1.44334500
C 2.57339100 -3.12089400 -2.42694500
C 1.20116100 -3.07935300 -2.38988000
C 3.44516200 -0.69982900 0.35313800
C 4.59728100 -2.91731000 -1.09856200
H 3.08877400 -3.79813300 -3.10021900
H 0.59089100 -3.72534400 -3.00945600
C 5.09548600 -2.55561900 0.12561200
C 4.49818500 -1.49567900 0.83160200
H 5.07417200 -3.66610100 -1.72141000
H 5.97022900 -3.04003900 0.54506900
H 4.95196100 -1.26071800 1.78236100
N 1.30443900 -1.31980100 -0.73682200
C -1.53873200 3.57140100 -1.55615600
C -2.88369300 3.42502800 -1.77360100
C -3.59410400 2.38571000 -1.13636200
C -2.87001500 1.42597100 -0.33958900
C -0.88098500 2.62659300 -0.74637900
H -5.50464200 3.04553500 -1.89289000
H -0.98607200 4.37774600 -2.01877400
H -3.41829400 4.11662400 -2.41681300
C -4.99996700 2.30649900 -1.27963900
C -3.60985300 0.40842400 0.33728500
C -4.99373000 0.38590400 0.15472600
C -5.69439200 1.31467300 -0.63693800
H -5.56003600 -0.40326800 0.63573700
H -6.77135300 1.23210700 -0.73239800
N -1.50522600 1.55771100 -0.21932500
Pd -0.04604300 0.08347600 -0.09862900

Table S67. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).
B3LYP-D3BJ/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.468226 (Hartree/Particle)
Thermal correction to Energy= 0.494647
Thermal correction to Enthalpy= 0.495591
Thermal correction to Gibbs Free Energy= 0.414432
Sum of electronic and zero-point Energies= -1730.258808
Sum of electronic and thermal Energies= -1730.232386
Sum of electronic and thermal Enthalpies= -1730.231442
Sum of electronic and thermal Free Energies= -1730.312602
C 0.52857900 2.80123600 -0.39563900
C 2.48967100 1.83335700 0.53073100
C 2.95595500 3.18477300 0.78722300
C 2.22943600 4.29123300 0.30809700
C 1.03433200 4.10773900 -0.32387700
C 3.37933100 0.73469900 0.86131600
C 4.13162200 3.45886500 1.51588200
H 2.62356600 5.28769300 0.47408600
H 0.44569700 4.94640100 -0.66419600
C 4.89437400 2.41231700 1.94802500
C 4.53857000 1.11765900 1.55732200
H 4.41028000 4.49122300 1.69572900
H 5.80988700 2.56495800 2.50750800
H 5.29224500 0.38028800 1.76614200
N 1.22177700 1.71223800 -0.00137500
C -1.12873200 -3.86252500 -0.73454300
C -1.95641100 -4.15102700 0.32516000
C -2.49967700 -3.10982900 1.11581300
C -2.28486100 -1.76549000 0.67915000
C -0.71594500 -2.52218100 -0.90432800
H -3.38844500 -4.36543000 2.63671500
H -0.67593900 -4.64972900 -1.32262200
H -2.17529900 -5.18182400 0.58360700
C -3.25588000 -3.34595500 2.29076400
C -3.09446400 -0.72043400 1.21206900
C -3.77059600 -0.99177100 2.39554000
C -3.80181900 -2.28192700 2.97085500
H -4.36593300 -0.20355200 2.84449300
H -4.34364100 -2.43852700 3.89664900
N -1.30286700 -1.51758900 -0.24319700
C 0.61404800 -2.23879600 -1.45831100
C 2.66272200 -1.39240700 -0.64074900
C 3.32224900 -2.42629600 -1.40968000
C 2.60108100 -3.11149900 -2.41166500
C 1.22909600 -3.05987000 -2.41014000
C 3.41905900 -0.69878900 0.38721500
C 4.59071300 -2.92232600 -1.03215700
H 3.12931300 -3.79181200 -3.07096700
H 0.62982400 -3.70092400 -3.04454800
C 5.06189700 -2.56247500 0.20304400
C 4.45683800 -1.49673700 0.89188300
H 5.07618100 -3.67512700 -1.64279500
H 5.92322500 -3.05151800 0.64327700

H 4.89227900 -1.25650800 1.84933600
N 1.30324300 -1.30797100 -0.74974200
C -1.55931800 3.58053200 -1.53816800
C -2.90854700 3.43781600 -1.72661700
C -3.60540700 2.39433500 -1.08317600
C -2.86680800 1.42657100 -0.31159000
C -0.88687000 2.62997000 -0.74933800
H -5.52688700 3.06677000 -1.79229700
H -1.01402600 4.38864800 -2.00552700
H -3.45829700 4.13468000 -2.34997700
C -5.01325400 2.32051700 -1.19604700
C -3.59337700 0.40378400 0.36886600
C -4.98063200 0.38717900 0.21813200
C -5.69614500 1.32552900 -0.54696000
H -5.53548400 -0.40671700 0.70339400
H -6.77481200 1.24673100 -0.61883900
N -1.50188500 1.55863700 -0.21659100
Pd -0.04653400 0.08631300 -0.10385800

Table S68. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).
CAM-B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.474561 (Hartree/Particle)
Thermal correction to Energy= 0.500493
Thermal correction to Enthalpy= 0.501437
Thermal correction to Gibbs Free Energy= 0.421459
Sum of electronic and zero-point Energies= -1729.138777
Sum of electronic and thermal Energies= -1729.112845
Sum of electronic and thermal Enthalpies= -1729.111901
Sum of electronic and thermal Free Energies= -1729.191879
C 0.52920300 2.78302600 -0.35048600
C 2.48906800 1.82203600 0.55381700
C 2.92435000 3.16148000 0.86031000
C 2.17658500 4.27142000 0.43413400
C 0.99876900 4.09306100 -0.21836100
C 3.40409400 0.73347700 0.83177500
C 4.10607400 3.43684700 1.57596700
H 2.54912500 5.26710500 0.64724800
H 0.39581000 4.93326200 -0.52931500
C 4.90937000 2.40199600 1.92822800
C 4.57229000 1.11816100 1.49130400
H 4.35751500 4.46722900 1.80038400
H 5.83872600 2.55439100 2.46357500
H 5.35393600 0.39720700 1.64469200
N 1.22431000 1.69697600 0.01358200
C -1.11049300 -3.86895000 -0.59230600
C -1.94207500 -4.12354800 0.46510700
C -2.50732800 -3.05980600 1.20192400
C -2.29922000 -1.74093300 0.72305100
C -0.71804100 -2.53472200 -0.80886200
H -3.40070800 -4.26945400 2.75443500
H -0.64222600 -4.67266000 -1.14447000
H -2.15391900 -5.14494300 0.76307600
C -3.27900700 -3.26196400 2.37190700
C -3.12372500 -0.68688600 1.20656200
C -3.81641500 -0.92041200 2.37743700
C -3.84439800 -2.18723800 3.00047400
H -4.43209300 -0.12530100 2.78437300
H -4.40145600 -2.31538800 3.92114400
N -1.30691900 -1.51602300 -0.19342000
C 0.60326100 -2.25787600 -1.39651300
C 2.66342400 -1.39414200 -0.66767400
C 3.29682300 -2.41484500 -1.45446100
C 2.54715900 -3.11595700 -2.41725400
C 1.18126700 -3.08202300 -2.36017000
C 3.45000600 -0.69777200 0.33123000
C 4.58579100 -2.89761500 -1.13380600
H 3.05687700 -3.79416000 -3.09318700
H 0.56406600 -3.73461100 -2.96454500
C 5.10093900 -2.53604600 0.07226500
C 4.50996500 -1.47776600 0.78527300
H 5.05171800 -3.64529200 -1.76502000
H 5.98848900 -3.00950400 0.47496100
H 4.98584900 -1.23652000 1.72216100
N 1.30023200 -1.32205400 -0.72296400
C -1.51858700 3.54395400 -1.56880100
C -2.85443800 3.39505800 -1.80065400
C -3.56814800 2.36101400 -1.16652400
C -2.85990400 1.41690000 -0.35949000
C -0.87799500 2.60549200 -0.74789800
H -5.46424200 3.01270900 -1.95619300
H -0.95777800 4.34626700 -2.02730400
H -3.38386200 4.08112200 -2.45321000
C -4.96917700 2.27965500 -1.32927700
C -3.60477000 0.40835800 0.31575300
C -4.97647500 0.38060800 0.11700500
C -5.66762000 1.29836000 -0.69160400
H -5.54733900 -0.40310800 0.60025000
H -6.74247500 1.21355300 -0.79959600
N -1.49966000 1.54718100 -0.22344100
Pd -0.04577200 0.08089400 -0.09643600

Table S69. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).
ωB97XD/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.473622 (Hartree/Particle)
Thermal correction to Energy= 0.499735
Thermal correction to Enthalpy= 0.500680
Thermal correction to Gibbs Free Energy= 0.420300
Sum of electronic and zero-point Energies= -1729.519736
Sum of electronic and thermal Energies= -1729.493623
Sum of electronic and thermal Enthalpies= -1729.492678
Sum of electronic and thermal Free Energies= -1729.573058
C 0.53096700 2.78646600 -0.35286300
C 2.48854300 1.82389900 0.55665500
C 2.92409400 3.16301100 0.86555000
C 2.17755900 4.27499000 0.43743800
C 1.00002500 4.09741900 -0.21950900
C 3.40091800 0.73184700 0.83689100
C 4.10405500 3.43615100 1.58802300
H 2.54894200 5.27082600 0.65259400
H 0.39803100 4.93876000 -0.53120900
C 4.90367300 2.39796700 1.94469200
C 4.56712900 1.11378800 1.50356700
H 4.35730900 4.46576200 1.81483700
H 5.83016900 2.54787100 2.48555700
H 5.34864600 0.39219700 1.66072400
N 1.22501500 1.69992300 0.01319900
C -1.11103800 -3.87547300 -0.58412000
C -1.94197600 -4.12707400 0.47680200

C -2.50684500 -3.05978200 1.21171000
C -2.29895700 -1.74223400 0.72753000
C -0.71970000 -2.54079900 -0.80524400
H -3.40005100 -4.26176000 2.77344500
H -0.64381200 -4.68150100 -1.13460000
H -2.15202900 -5.14806400 0.77783700
C -3.27645700 -3.25626500 2.38582600
C -3.11977400 -0.68320600 1.20981200
C -3.80997400 -0.91073800 2.38489200
C -3.83746500 -2.17624200 3.01307900
H -4.42254800 -0.11258400 2.79189000
H -4.39138200 -2.30007800 3.93625000
N -1.30812800 -1.52013800 -0.19160400
C 0.60101500 -2.26173100 -1.39815800
C 2.66233600 -1.39358900 -0.67424200
C 3.29641500 -2.40944900 -1.46708400
C 2.54482600 -3.11006300 -2.43081400
C 1.17736900 -3.08195700 -2.36756900
C 3.44836600 -0.69936800 0.32846700
C 4.58885000 -2.89059400 -1.15096500
H 3.05398100 -3.78334300 -3.11228000
H 0.56063900 -3.73350000 -2.97403600
C 5.10219000 -2.53628400 0.05969400
C 4.50911300 -1.48209900 0.77961100
H 5.05744300 -3.63249600 -1.78718600
H 5.98984900 -3.01114500 0.46043100
H 4.98357800 -1.24822100 1.72002900
N 1.29803700 -1.32566200 -0.72424300
C -1.51556300 3.54068500 -1.58385900
C -2.85311300 3.39074100 -1.81592700
C -3.56826900 2.35992100 -1.17460800
C -2.85974400 1.42019300 -0.36219000
C -0.87714300 2.60738000 -0.75395200
H -5.46787900 3.00479300 -1.96739500
H -0.95347200 4.33744000 -2.05159800
H -3.38066200 4.07201200 -2.47526800
C -4.97053700 2.27477500 -1.33840700
C -3.60261500 0.40970300 0.31464700
C -4.97508900 0.37630400 0.11355100
C -5.66785700 1.29181700 -0.69826300
H -5.54400600 -0.40887200 0.59837800
H -6.74240200 1.20446100 -0.80713200
N -1.50012100 1.55297000 -0.22195700
Pd -0.04621600 0.07993800 -0.09397800

Table S70. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).
M06-2X/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.471945 (Hartree/Particle)
Thermal correction to Energy= 0.498432
Thermal correction to Enthalpy= 0.499376
Thermal correction to Gibbs Free Energy= 0.417963
Sum of electronic and zero-point Energies= -1729.284206
Sum of electronic and thermal Energies= -1729.257719
Sum of electronic and thermal Enthalpies= -1729.256775
Sum of electronic and thermal Free Energies= -1729.338188
C 0.55204400 2.78200400 -0.24346900
C 2.52882000 1.79854400 0.59409200
C 2.93134300 3.12375700 1.00144000
C 2.14548400 4.24727100 0.68270400
C 0.97826400 4.09441800 0.00152500
C 3.48254700 0.71389800 0.76108000
C 4.12759300 3.38485900 1.70056500
H 2.49231000 5.22871900 0.98830000
H 0.34885600 4.93599700 -0.25162200
C 4.99199500 2.35761200 1.90774300
C 4.67860700 1.10185200 1.37394900
H 4.34428000 4.40104300 2.01029900
H 5.94565900 2.49949900 2.40130500
H 5.50471300 0.41662600 1.41568600
N 1.26358400 1.68739500 0.05207100
C -1.09751600 -3.93068900 -0.23628200
C -1.97823200 -4.09390600 0.80192800
C -2.60670700 -2.97081900 1.38908200
C -2.37813400 -1.69699600 0.80162700
C -0.72686300 -2.61325900 -0.57617200
H -3.60043700 -4.05066200 2.97665500
H -0.58491000 -4.77246200 -0.68378100
H -2.18789800 -5.08329600 1.19658500
C -3.45999500 -3.07864800 2.51605000
C -3.23249300 -0.60763700 1.13988500
C -4.01705100 -0.75117500 2.26892300
C -4.08503800 -1.96028700 2.99939000
H -4.66610800 0.07050200 2.55533300
H -4.71160200 -2.01415600 3.88192500
N -1.34694600 -1.54837400 -0.08635000
C 0.58057400 -2.37691000 -1.21991000
C 2.67380800 -1.43500900 -0.71760200
C 3.25774300 -2.45048400 -1.55397200
C 2.43816800 -3.22439300 -2.39947700
C 1.08510800 -3.24335800 -2.19191100
C 3.53611400 -0.70066200 0.19543000
C 4.59802100 -2.87229500 -1.38828300
H 2.90552200 -3.90638900 -3.10224500
H 0.42754600 -3.93765500 -2.70086200
C 5.22688100 -2.48021600 -0.24604300
C 4.66545800 -1.44861000 0.53113600
H 5.01718700 -3.60640600 -2.06700700
H 6.17045600 -2.91412800 0.06262600
H 5.21558400 -1.21347100 1.42742600
N 1.30957000 -1.40494100 -0.64232900
C -1.41303000 3.57279300 -1.57380200
C -2.72694600 3.41941700 -1.91687400
C -3.48665000 2.37428300 -1.35057100
C -2.84469500 1.43884800 -0.47893600
C -0.83920600 2.61957200 -0.71374600
H -5.31076900 2.99429100 -2.32067800
H -0.81089300 4.37523200 -1.97953800
H -3.20643300 4.10514000 -2.60775700
C -4.86682000 2.27127900 -1.64446100
C -3.63800700 0.43256200 0.14684500
C -4.98613800 0.38263000 -0.17769900
C -5.60833700 1.28007500 -1.06743500
H -5.59130800 -0.39647200 0.27258000
H -6.66656700 1.17786300 -1.27671800
N -1.50159200 1.56933100 -0.23249500
Pd -0.04408200 0.06096500 -0.05511500

Table S71. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS1).

B3LYP-D3/6-311+G(2d,p)-SDD(Pd)/SMD(Et_2O)
Zero-point correction= 0.465134 (Hartree/Particle)
Thermal correction to Energy= 0.491600
Thermal correction to Enthalpy= 0.492544
Thermal correction to Gibbs Free Energy= 0.411175
Sum of electronic and zero-point Energies= -1730.584121
Sum of electronic and thermal Energies= -1730.557655
Sum of electronic and thermal Enthalpies= -1730.556711
Sum of electronic and thermal Free Energies= -1730.638080
C 0.54167600 2.79219900 -0.38073900
C 2.50281600 1.82410400 0.52870900
C 2.96961800 3.17050800 0.78600400
C 2.23824700 4.27596500 0.32396700
C 1.04466400 4.09556000 -0.29959600
C 3.39681100 0.72676400 0.84540900
C 4.15512300 3.44126300 1.49273100
H 2.63384700 5.27059400 0.48977200
H 0.46160500 4.93783300 -0.63817600
C 4.93017800 2.39941900 1.89547600
C 4.56919600 1.10878700 1.51044700
H 4.43193600 4.47215900 1.67422200
H 5.85796400 2.55361600 2.43106700
H 5.32871800 0.37460200 1.70146800
N 1.23358000 1.70506400 0.00423600
C -1.16555300 -3.84405900 -0.74665400
C -2.00592400 -4.13116800 0.29559000
C -2.53965900 -3.09426600 1.09010400
C -2.30333600 -1.75258200 0.67078200
C -0.72733000 -2.51323000 -0.89267500
H -3.44231200 -4.35458800 2.59150900
H -0.72725500 -4.63291400 -1.34016700
H -2.24409600 -5.15984700 0.53880800
C -3.29798300 -3.33394500 2.25871900
C -3.10694200 -0.70838900 1.20956800
C -3.77652700 -0.98268800 2.38969800
C -3.82249500 -2.27428900 2.95104100
H -4.36003500 -0.19469400 2.85001300
H -4.35764000 -2.43218200 3.87874800
N -1.30718600 -1.50989700 -0.23305400
C 0.60857000 -2.24318800 -1.43482400
C 2.65597800 -1.40940800 -0.62601300
C 3.30722500 -2.44685300 -1.38918800
C 2.58343700 -3.12711600 -2.38629600
C 1.21796300 -3.06472600 -2.38441600
C 3.42079300 -0.71343900 0.39003400
C 4.56660900 -2.95140800 -1.00682700
H 3.10603200 -3.81067100 -3.04433700
H 0.61376400 -3.70514700 -3.01271300
C 5.03885000 -2.58858400 0.22138900
C 4.44839300 -1.51217500 0.89877500
H 5.04463500 -3.71203800 -1.61091300
H 5.89204200 -3.08467800 0.66613500
H 4.88684300 -1.26631300 1.85149200
N 1.30045000 -1.31833800 -0.72958300
C -1.53110800 3.56030500 -1.54784300
C -2.87552800 3.43084700 -1.73715200
C -3.58385700 2.40795200 -1.08139600
C -2.85866000 1.44207600 -0.30183000
C -0.87248200 2.62089000 -0.74101100
H -5.49388200 3.09837800 -1.79158100
H -0.97560000 4.35166100 -2.02791600
H -3.41414700 4.12439900 -2.37174800
C -4.98920800 2.35110100 -1.19124600
C -3.59528500 0.42780100 0.37630600
C -4.97807900 0.42802300 0.22523800
C -5.68021900 1.37196000 -0.53824400
H -5.54706000 -0.35671700 0.70523600
H -6.75857800 1.30722900 -0.60697100
N -1.49537300 1.56422800 -0.20065700
Pd -0.04288900 0.08756200 -0.10575600

Table S72. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (EQ2).
B3LYP-D3/6-31G(d,p)-SDD(Pd)
Zero-point correction= 0.467034 (Hartree/Particle)
Thermal correction to Energy= 0.494488
Thermal correction to Enthalpy= 0.495432
Thermal correction to Gibbs Free Energy= 0.410241
Sum of electronic and zero-point Energies= -1730.003536
Sum of electronic and thermal Energies= -1729.976082
Sum of electronic and thermal Enthalpies= -1729.975138
Sum of electronic and thermal Free Energies= -1730.060328
C 0.57206500 2.86711400 0.27877100
C 2.66992400 1.81100700 0.37171900
C 3.27370900 3.11691200 0.56435000
C 2.45344100 4.23680100 0.79262000
C 1.10019700 4.11550300 0.65277700
C 3.56886400 0.69662000 0.29390200
C 4.67336300 3.32247100 0.50891300
H 2.90775400 5.19236100 1.03528000
H 0.44292000 4.96200400 0.79872000
C 5.49655700 2.27257300 0.20998400
C 4.93072700 0.99125400 0.11597800
H 5.05936100 4.32549800 0.65941600
H 6.56482800 2.40455100 0.07851600
H 5.60146700 0.16769300 -0.09450900
N 1.29406800 1.72716800 0.23244200
C -1.35502900 -3.80999800 -0.93025200
C -2.25144800 -4.09176300 0.07054000
C -2.76041700 -3.04969900 0.87811900
C -2.44427000 -1.70520900 0.49641300
C -0.82154900 -2.49881300 -1.00770800
H -3.80893600 -4.31078000 2.28904500
H -0.93926500 -4.60678900 -1.53111400
H -2.55942600 -5.11569200 0.26084600
C -3.61145900 -3.28715000 1.98669800
C -3.27125900 -0.65793700 0.98748400
C -4.06623400 -0.92799800 2.09551600
C -4.18076200 -2.22360300 2.64830500
H -4.68401500 -0.12969800 2.49512700
H -4.80261600 -2.38240100 3.52261000
N -1.37850100 -1.47057900 -0.34778700
C 0.57963900 -2.34528700 -1.41483800
C 2.57489000 -1.65053400 -0.38994500
C 3.15705300 -2.91834900 -0.76199200
C 2.52729800 -3.66434700 -1.78230300
C 1.23594600 -3.36469900 -2.13332800
C 3.37146800 -0.77747100 0.42197100
C 4.28343100 -3.43094800 -0.07372800
H 3.03233800 -4.52830700 -2.20388600

H 0.68126600 -3.98230300 -2.82930800
C 4.77857200 -2.73358200 1.00039300
C 4.34484000 -1.40621000 1.20377600
H 4.68768500 -4.39482900 -0.36570700
H 5.56001100 -3.14698000 1.62858400
H 4.86511000 -0.80781400 1.94423600
N 1.26505900 -1.40436200 -0.71846700
C -1.42473800 3.95154700 -0.71862300
C -2.71331100 3.86872300 -1.17714400
C -3.46277600 2.69944000 -0.93925900
C -2.82866900 1.59035400 -0.27027700
C -0.83485700 2.81382900 -0.12847200
H -5.26071900 3.49037700 -1.83661100
H -0.84153800 4.84883600 -0.87271400
H -3.17185900 4.70311400 -1.69899400
C -4.82740700 2.64382500 -1.31343900
C -3.64615500 0.50385100 0.13754000
C -4.98809100 0.50544800 -0.24607500
C -5.58111800 1.54520900 -0.98649100
H -5.60521200 -0.33729700 0.04598100
H -6.62794500 1.48141400 -1.26275000
N -1.47844000 1.64562400 0.01700500
Pd -0.04676400 0.10062600 -0.10861900

Table S73. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (EQ2).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.467784 (Hartree/Particle)
Thermal correction to Energy= 0.495077
Thermal correction to Enthalpy= 0.496021
Thermal correction to Gibbs Free Energy= 0.411971
Sum of electronic and zero-point Energies= -1730.146887
Sum of electronic and thermal Energies= -1730.119594
Sum of electronic and thermal Enthalpies= -1730.118650
Sum of electronic and thermal Free Energies= -1730.202700
C 0.83040300 2.82277600 -0.11625700
C 2.82455300 1.60271100 -0.24634200
C 3.46599000 2.71830200 -0.89463000
C 2.72017700 3.89077000 -1.12806200
C 1.42668800 3.96768700 -0.68642800
C 3.63722200 0.50983300 0.15616200
C 4.83388500 2.66635600 -1.25541200
H 3.18540100 4.73058600 -1.63392000
H 0.84577100 4.86612500 -0.83853600
C 5.58318800 1.56348800 -0.93409100
C 4.98256500 0.51495500 -0.21309300
H 5.27051700 3.51907100 -1.76487400
H 6.63253800 1.50161700 -1.19986900
H 5.59499300 -0.33211000 0.07424800
N 1.47274800 1.65463200 0.02623500
C -1.25104100 -3.36965200 -2.12512600
C -2.52838600 -3.68228800 -1.73893700
C -3.14324200 -2.93214100 -0.71284500
C -2.56508100 -1.65788700 -0.36585000
C -0.58795700 -2.33974900 -1.42699200
H -4.64875800 -4.41698600 -0.26753100
H -0.70688000 -3.98910200 -2.82649200
H -3.03122400 -4.55788400 -2.13726900
C -4.25169000 -3.44463600 0.00377900
C -3.35535400 -0.77980300 0.44516600
C -4.31617400 -1.39892900 1.24751200
C -4.73967400 -2.73339400 1.07179700
H -4.83758000 -0.78816300 1.97639600
H -5.51194900 -3.14108800 1.71432400
N -1.26602800 -1.40187900 -0.72195200
C 0.82051300 -2.48606200 -1.04292700
C 2.44051100 -1.71000700 0.46935400
C 2.76877800 -3.05794600 0.82221700
C 2.26957800 -4.08785800 -0.00684000
C 1.36712700 -3.79340200 -0.99686300
C 3.25756700 -0.66559500 0.98493600
C 3.61645700 -3.31060200 1.92972900
H 2.58783700 -5.11194800 0.16065600
H 0.95665000 -4.58099800 -1.61234900
C 4.17210500 -2.25621200 2.61629300
C 4.04864700 -0.95034100 2.09109500
H 3.81952400 -4.33878100 2.21093300
H 4.79199300 -2.42705800 3.48937900
H 4.65936300 -0.15569700 2.50737700
N 1.37306000 -1.46656600 -0.36703000
C -1.11985700 4.12155400 0.63211400
C -2.47459300 4.23904600 0.74980200
C -3.28670000 3.11300300 0.52256100
C -2.67392400 1.81008300 0.35300700
C -0.58162200 2.87244700 0.27322200
H -5.07875700 4.31113600 0.58209700
H -0.46907000 4.97211200 0.77925700
H -2.93567300 5.19507800 0.97479400
C -4.68689200 3.30804000 0.45065400
C -3.56470300 0.68886700 0.28707300
C -4.92744700 0.96740900 0.09915200
C -5.50080300 2.24714500 0.16539300
H -5.59075600 0.13381700 -0.09400800
H -6.56951900 2.36812800 0.02839700
N -1.29781300 1.73051000 0.22739100
Pd 0.04341100 0.10472800 -0.11211800

Table S74. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (EQ2).
B3LYP-D3BJ/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.468447 (Hartree/Particle)
Thermal correction to Energy= 0.495640
Thermal correction to Enthalpy= 0.496585
Thermal correction to Gibbs Free Energy= 0.413145
Sum of electronic and zero-point Energies= -1730.263954
Sum of electronic and thermal Energies= -1730.236761
Sum of electronic and thermal Enthalpies= -1730.235817
Sum of electronic and thermal Free Energies= -1730.319256
C 0.83635300 2.82833700 -0.22031800
C 2.83114300 1.59810100 -0.14311500
C 3.53335600 2.70824300 -0.73551200
C 2.81196900 3.86613700 -1.08360500
C 1.47998100 3.94872900 -0.78294800
C 3.60048700 0.49804900 0.32314600
C 4.93198700 2.66795800 -0.94197200
H 3.32708700 4.69082600 -1.56391500
H 0.91454600 4.83631400 -1.02509700
C 5.64975700 1.57382900 -0.53507400
C 4.97775200 0.51490100 0.09983500
H 5.41253200 3.52247500 -1.40599700

H 6.72241300 1.51902000 -0.68119700
H 5.55564000 -0.34040600 0.42838700
N 1.46409300 1.66575700 0.01472000
C -1.31138500 -3.27165000 -2.22161600
C -2.54963800 -3.62171300 -1.74902900
C -3.10315800 -2.91128300 -0.66072300
C -2.53160600 -1.63185200 -0.33304200
C -0.61805300 -2.24723600 -1.54458600
H -4.52937900 -4.44052600 -0.11854800
H -0.80781200 -3.86365000 -2.97483800
H -3.06167800 -4.49902400 -2.13038600
C -4.13564500 -3.46233600 0.13467200
C -3.27165900 -0.78399500 0.55287500
C -4.14857000 -1.43768700 1.41863900
C -4.54973400 -2.78009500 1.25234000
H -4.62815000 -0.84977300 2.19322600
H -5.25551100 -3.21886100 1.94808700
N -1.26834900 -1.34381700 -0.77284800
C 0.80423200 -2.39607900 -1.22029100
C 2.38226600 -1.72848700 0.38825900
C 2.70665700 -3.09815300 0.64157900
C 2.25427200 -4.05732200 -0.29282500
C 1.37088700 -3.69353700 -1.27673600
C 3.15125600 -0.72340800 1.04045600
C 3.48779100 -3.43866300 1.77289700
H 2.58319100 -5.08716400 -0.20076900
H 0.98005900 -4.42994900 -1.96386400
C 3.97235100 -2.44291400 2.58852400
C 3.86341000 -1.09721800 2.17306000
H 3.68682300 -4.48568800 1.97499100
H 4.53160100 -2.68351300 3.48539700
H 4.43078900 -0.33687600 2.69957500
N 1.34801400 -1.42684100 -0.46584200
C -1.15095200 4.17191300 0.31855600
C -2.50242400 4.27550800 0.47205800
C -3.29568300 3.11617300 0.42178000
C -2.66509200 1.81518300 0.33308200
C -0.59165900 2.90070500 0.09990900
H -5.10124500 4.28546400 0.51400200
H -0.51825900 5.04594000 0.35404400
H -2.97879800 5.24020000 0.60837600
C -4.70007500 3.27999900 0.45128800
C -3.53141800 0.67608900 0.40348800
C -4.91218000 0.91507300 0.33321100
C -5.50975300 2.18351700 0.35512300
H -5.56733600 0.05763200 0.25760600
H -6.58898700 2.27278100 0.31194300
N -1.29361300 1.75154100 0.16779500
Pd 0.03778600 0.12933500 -0.13734900

Table S75. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (EQ2).
CAM-B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.474644 (Hartree/Particle)
Thermal correction to Energy= 0.501426
Thermal correction to Enthalpy= 0.502370
Thermal correction to Gibbs Free Energy= 0.419521
Sum of electronic and zero-point Energies= -1729.144189
Sum of electronic and thermal Energies= -1729.117408
Sum of electronic and thermal Enthalpies= -1729.116464
Sum of electronic and thermal Free Energies= -1729.199313
C 0.83476700 2.78755000 -0.14765600
C 2.81761300 1.58017200 -0.28662800
C 3.43626000 2.67134300 -0.96970900
C 2.68290000 3.83072400 -1.22548200
C 1.40410900 3.91592200 -0.76226200
C 3.63718800 0.50347100 0.12943800
C 4.79626500 2.61742500 -1.34880700
H 3.13658800 4.65509200 -1.76486800
H 0.81114700 4.80414100 -0.92508300
C 5.55261500 1.53418500 -1.00983000
C 4.96828200 0.50411500 -0.25440800
H 5.21925500 3.45729600 -1.88888600
H 6.59812600 1.47116400 -1.28713700
H 5.58920600 -0.33034100 0.04921800
N 1.47427800 1.63235500 0.01085000
C -1.21333900 -3.35296100 -2.12196100
C -2.50735400 -3.64241400 -1.79840300
C -3.15015700 -2.89051700 -0.79792400
C -2.57242200 -1.64120100 -0.41139700
C -0.57562400 -2.33756400 -1.39552000
H -4.68161900 -4.36799000 -0.43465900
H -0.64577900 -3.97788200 -2.79861000
H -3.00750200 -4.50711400 -2.22222000
C -4.28566500 -3.40617400 -0.12960300
C -3.37128700 -0.77600600 0.40127600
C -4.34892300 -1.40257600 1.15940100
C -4.78728300 -2.72366600 0.93842300
H -4.87997900 -0.80772000 1.89320800
H -5.58044000 -3.13579500 1.55068900
N -1.25836700 -1.40172500 -0.71250100
C 0.82342200 -2.49267300 -0.97111500
C 2.43746500 -1.69525200 0.51474500
C 2.74921400 -3.02352000 0.90551100
C 2.23461900 -4.07294500 0.11816400
C 1.34172900 -3.80211500 -0.87857800
C 3.26508700 -0.64650200 0.99292100
C 3.60121000 -3.25218700 2.01248100
H 2.53981100 -5.09359900 0.32273700
H 0.91910500 -4.60298100 -1.46688400
C 4.17436800 -2.19100100 2.65566200
C 4.06188400 -0.90362300 2.08977500
H 3.78793400 -4.27309800 2.32749600
H 4.80179500 -2.34150900 3.52618400
H 4.68980900 -0.10552500 2.47114500
N 1.37226800 -1.46615500 -0.32563600
C -1.07495400 4.08917100 0.66483500
C -2.41818200 4.21273100 0.82852700
C -3.24194100 3.09964200 0.60201000
C -2.65435400 1.80504400 0.38839900
C -0.56774700 2.84335500 0.27642500
H -5.01049500 4.32228200 0.72442100
H -0.40869600 4.92942800 0.79945700
H -2.86721900 5.16577200 1.08551500
C -4.63740700 3.31780200 0.55854400
C -3.55885100 0.70047200 0.29721700
C -4.90900500 1.00447200 0.13002400
C -5.46478800 2.28560400 0.24796000
H -5.58720700 0.19040700 -0.08751600
H -6.53251700 2.42445000 0.12754000

N -1.28470800 1.71400200 0.23210700
Pd 0.04578400 0.09722500 -0.10544000

Table S76. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (EQ2).
ωB97XD/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.473827 (Hartree/Particle)
Thermal correction to Energy= 0.500745
Thermal correction to Enthalpy= 0.501689
Thermal correction to Gibbs Free Energy= 0.418744
Sum of electronic and zero-point Energies= -1729.525821
Sum of electronic and thermal Energies= -1729.498903
Sum of electronic and thermal Enthalpies= -1729.497959
Sum of electronic and thermal Free Energies= -1729.580903
C 0.83599200 2.79607100 -0.13111900
C 2.81617500 1.58630000 -0.28771200
C 3.43357400 2.67844300 -0.97070500
C 2.68120300 3.84297600 -1.21468600
C 1.40411600 3.92849800 -0.74151100
C 3.63412100 0.50337000 0.11829000
C 4.79132500 2.61860700 -1.36250500
H 3.13224600 4.66933900 -1.75360700
H 0.81120300 4.81862000 -0.89758500
C 5.54488300 1.52691600 -1.03719700
C 4.96228000 0.49597100 -0.27930600
H 5.21525100 3.45887100 -1.90150900
H 6.58708600 1.45931400 -1.32548100
H 5.58144400 -0.34343300 0.01684300
N 1.47495100 1.63883300 0.01909400
C -1.21373200 -3.36269400 -2.12182100
C -2.50784400 -3.65306000 -1.79245400
C -3.14830700 -2.89846900 -0.79018700
C -2.57008800 -1.64690400 -0.41123600
C -0.57437000 -2.34521300 -1.39762300
H -4.68067100 -4.37466000 -0.41333700
H -0.64953000 -3.98678300 -2.80266500
H -3.00841100 -4.51860000 -2.21424900
C -4.28279500 -3.41137600 -0.11479600
C -3.36656800 -0.77646600 0.39926500
C -4.34437100 -1.39791900 1.16334500
C -4.78139200 -2.72234400 0.95268200
H -4.87583400 -0.79603800 1.89209600
H -5.57282900 -3.13116100 1.56932200
N -1.25600300 -1.40769500 -0.71535700
C 0.82637000 -2.50016800 -0.97182000
C 2.43939100 -1.69758400 0.51309200
C 2.75123900 -3.02427700 0.91034800
C 2.23718400 -4.07798400 0.12566600
C 1.34438200 -3.81031800 -0.87433500
C 3.26386500 -0.64382800 0.98825100
C 3.60252700 -3.24629500 2.02107500
H 2.54089000 -5.09840500 0.33393600
H 0.92271300 -4.61393500 -1.46047100
C 4.17228200 -2.17926200 2.66147500
C 4.05987200 -0.89360800 2.08893500
H 3.79148800 -4.26514000 2.34206300
H 4.79776500 -2.32497400 3.53421600
H 4.68500000 -0.09212300 2.46916000
N 1.37487400 -1.47115100 -0.32928600
C -1.07859000 4.09214900 0.68818600
C -2.42522500 4.21469100 0.83948600
C -3.24663000 3.10109300 0.59723300
C -2.65487300 1.80793800 0.38565700
C -0.56837100 2.84849500 0.29369600
H -5.02170600 4.31921900 0.70404400
H -0.41346900 4.93166900 0.83645800
H -2.87671800 5.16642100 1.09754000
C -4.64352200 3.31639300 0.53827200
C -3.55606100 0.70052000 0.28471600
C -4.90611500 1.00040600 0.10224700
C -5.46579100 2.28193700 0.21385900
H -5.57984600 0.18262700 -0.11951700
H -6.53222200 2.41901900 0.08118900
N -1.28410800 1.71815200 0.23850700
Pd 0.04742000 0.09685100 -0.10434200

Table S77. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (EQ2).
M06-2X/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.472500 (Hartree/Particle)
Thermal correction to Energy= 0.499690
Thermal correction to Enthalpy= 0.500634
Thermal correction to Gibbs Free Energy= 0.416248
Sum of electronic and zero-point Energies= -1729.292234
Sum of electronic and thermal Energies= -1729.265044
Sum of electronic and thermal Enthalpies= -1729.264099
Sum of electronic and thermal Free Energies= -1729.348485
C 0.82979200 2.73009600 0.37230300
C 2.67625200 1.63782800 -0.52024500
C 3.08839500 2.83328000 -1.17670600
C 2.37568500 4.02079800 -0.91079200
C 1.30101600 3.98824500 -0.06761800
C 3.56890200 0.53819700 -0.51134500
C 4.22619500 2.83378900 -2.01938900
H 2.69274200 4.95028700 -1.37302200
H 0.74012700 4.88560500 0.15085500
C 4.97875100 1.69798900 -2.14633600
C 4.67408500 0.57964800 -1.34290600
H 4.49306200 3.75109100 -2.53350900
H 5.84781100 1.67429800 -2.79323200
H 5.35512600 -0.26533800 -1.33560100
N 1.46468300 1.58970200 0.13233900
C -1.08836500 -3.79607900 -1.51295700
C -2.43939800 -3.97167600 -1.45561400
C -3.22501300 -3.01796500 -0.78071800
C -2.64565600 -1.74967000 -0.43649700
C -0.55065600 -2.66399600 -0.87896200
H -4.91898600 -4.34927300 -0.67503700
H -0.42983400 -4.54051200 -1.94177200
H -2.90829400 -4.87060600 -1.84277000
C -4.54153000 -3.37077500 -0.39869400
C -3.54232500 -0.74627100 0.05863900
C -4.75581500 -1.20713100 0.56367500
C -5.25800400 -2.50906400 0.37746300
H -5.38975000 -0.49233800 1.07478900
H -6.22634600 -2.77613300 0.78309200
N -1.27913000 -1.60711200 -0.49497400
C 0.82983600 -2.72979100 -0.37356300
C 2.67579600 -1.63792000 0.52055200
C 3.08758200 -2.83366000 1.17670100

C 2.37520200 -4.02109900 0.90955500
C 1.30102500 -3.98816000 0.06576300
C 3.56844900 -0.53828400 0.51263900
C 4.22478400 -2.83446600 2.02020400
H 2.69210000 -4.95086100 1.37133400
H 0.74042000 -4.88547600 -0.15360900
C 4.97713000 -1.69864300 2.14823200
C 4.67300900 -0.58000100 1.34500600
H 4.49135700 -3.75197700 2.53411600
H 5.84571500 -1.67515400 2.79577300
H 5.35405500 0.26498600 1.33845300
N 1.46457600 -1.58950200 -0.13266100
C -1.08825700 3.79692300 1.51129600
C -2.43932500 3.97237200 1.45447500
C -3.22515800 3.01823100 0.78045100
C -2.64580600 1.74987000 0.43643800
C -0.55071500 2.66454600 0.87769200
H -4.91939600 4.34923500 0.67526500
H -0.42960200 4.54159800 1.93949300
H -2.90813100 4.87142600 1.84145400
C -4.54197800 3.37066600 0.39912200
C -3.54260200 0.74618000 -0.05788300
C -4.75655800 1.20660100 -0.56221100
C -5.25887200 2.50849900 -0.37612900
H -5.39069400 0.49152300 -1.07268200
H -6.22755100 2.77522600 -0.78117600
N -1.27923400 1.60744500 0.49440800
Pd 0.06271100 0.00008800 -0.00012700

Table S78. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS2).
B3LYP-D3/6-31G(d,p)-SDD(Pd)
Zero-point correction= 0.466810 (Hartree/Particle)
Thermal correction to Energy= 0.493432
Thermal correction to Enthalpy= 0.494377
Thermal correction to Gibbs Free Energy= 0.411994
Sum of electronic and zero-point Energies= -1730.001727
Sum of electronic and thermal Energies= -1729.975104
Sum of electronic and thermal Enthalpies= -1729.974160
Sum of electronic and thermal Free Energies= -1730.056543
C 0.73743300 2.90786900 -0.18544500
C 2.75557800 1.72150000 0.15490800
C 3.49599300 2.93680100 -0.10864300
C 2.79472500 4.11706700 -0.40823100
C 1.42921400 4.11284300 -0.42159500
C 3.51502500 0.56900600 0.53386600
C 4.90935600 2.98900400 -0.06160100
H 3.34641900 5.02935400 -0.61237600
H 0.90384700 5.03129000 -0.62695500
C 5.61897000 1.86132300 0.24805500
C 4.91219300 0.68213600 0.53371300
H 5.40368200 3.93080300 -0.27708600
H 6.70309000 1.86206200 0.27487400
H 5.49291300 -0.20624000 0.74909900
N 1.37450700 1.74264000 0.06095100
C -1.43977300 -3.35940000 -1.99873600
C -2.48187800 -3.80366500 -1.22377600
C -2.89266000 -3.05267000 -0.09749400
C -2.42230100 -1.69988500 -0.00390400
C -0.73554200 -2.20934600 -1.56665800
H -4.03382900 -4.62399200 0.85857200
H -1.05936100 -3.96480500 -2.81093500
H -2.94437200 -4.76597900 -1.42253900
C -3.71021800 -3.59030700 0.92681900
C -3.09484100 -0.81518900 0.89700600
C -3.77367500 -1.41590200 1.95406900
C -4.03209200 -2.80486500 2.00981600
H -4.21818000 -0.77541800 2.70957400
H -4.57771900 -3.21531600 2.85253800
N -1.30508200 -1.33231200 -0.70911500
C 0.73562200 -2.20948200 -1.56642600
C 2.42212600 -1.70000300 -0.00338200
C 2.89224800 -3.05289900 -0.09652500
C 2.48150300 -3.80412500 -1.22267200
C 1.43970100 -3.35982800 -1.99801200
C 3.09473900 -0.81517700 0.89731200
C 3.70962800 -3.59038500 0.92800000
H 2.94382200 -4.76660000 -1.42106100
H 1.05935900 -3.96537300 -2.81013700
C 4.03167300 -2.80464800 2.01074100
C 3.77351700 -1.41566800 1.95454400
H 4.03304700 -4.62415200 0.86008500
H 4.57724400 -3.21492500 2.85358400
H 4.21814200 -0.77500400 2.70982700
N 1.30508900 -1.33239300 -0.70891500
C -1.42886700 4.11306300 -0.42093600
C -2.79436500 4.11744700 -0.40727300
C -3.49571100 2.93717600 -0.10790300
C -2.75540200 1.72170100 0.15521200
C -0.73718000 2.90794600 -0.18523800
H -5.40326700 3.93152100 -0.27573000
H -0.90343000 5.03151000 -0.62610400
H -3.34599700 5.02986200 -0.61101300
C -4.90905000 2.98957700 -0.06062400
C -3.51495600 0.56917900 0.53392800
C -4.91212900 0.68252200 0.53392200
C -5.61878000 1.86189600 0.24873600
H -5.49296800 -0.20583300 0.74904700
H -6.70289700 1.86277900 0.27567400
N -1.37433200 1.74273200 0.06105700
Pd 0.00000500 0.17135100 -0.18652600

Table S79. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS2).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.466635 (Hartree/Particle)
Thermal correction to Energy= 0.493333
Thermal correction to Enthalpy= 0.494277
Thermal correction to Gibbs Free Energy= 0.411584
Sum of electronic and zero-point Energies= -1730.145968
Sum of electronic and thermal Energies= -1730.119270
Sum of electronic and thermal Enthalpies= -1730.118326
Sum of electronic and thermal Free Energies= -1730.201019
C 0.71840600 2.90293200 -0.23324400
C 2.73317600 1.73631500 0.18041900
C 3.46838300 2.95721900 -0.06580600
C 2.76904400 4.12346400 -0.42093800
C 1.40591200 4.10621300 -0.48756200
C 3.49254300 0.58790100 0.57897900
C 4.87720400 3.02880600 0.04121400

H 3.32151100 5.03463200 -0.62521700
H 0.87918700 5.01140200 -0.74207200
C 5.58705100 1.91157000 0.38457900
C 4.88678500 0.72042800 0.63255400
H 5.36516900 3.97665400 -0.15977100
H 6.66878200 1.92619500 0.45639100
H 5.47206100 -0.16217700 0.85637800
N 1.35658900 1.74824100 0.05211100
C -1.42099800 -3.38099100 -1.97377300
C -2.44513800 -3.83123300 -1.17951800
C -2.85753900 -3.07040800 -0.06065300
C -2.40449800 -1.71228700 0.01327400
C -0.73177700 -2.21328200 -1.56592600
H -3.96348800 -4.64624700 0.92437400
H -1.03880500 -3.99396100 -2.77868400
H -2.89017300 -4.80541900 -1.35602400
C -3.65624300 -3.60717500 0.97868900
C -3.07507800 -0.82589800 0.91506400
C -3.73534600 -1.42308500 1.98501800
C -3.97778200 -2.81391500 2.05544900
H -4.18048400 -0.78038000 2.73772700
H -4.51137800 -3.22139600 2.90692400
N -1.30181600 -1.33862900 -0.70868600
C 0.73920700 -2.18804200 -1.59362200
C 2.42949400 -1.68191000 -0.03537000
C 2.92108600 -3.02293500 -0.16434100
C 2.51609700 -3.75502100 -1.30490400
C 1.45814100 -3.31470100 -2.05955700
C 3.08339100 -0.81129100 0.89537600
C 3.74095500 -3.57683100 0.84899000
H 2.99124300 -4.70574200 -1.52560600
H 1.07818100 -3.91075600 -2.87835800
C 4.03790600 -2.81934200 1.95808800
C 3.75538900 -1.43430500 1.94359300
H 4.07811600 -4.60338700 0.75164900
H 4.58230600 -3.24527400 2.79345700
H 4.18084700 -0.81192600 2.72426100
N 1.30523600 -1.31830000 -0.72690700
C -1.45444300 4.09328900 -0.49294300
C -2.81907500 4.09105800 -0.45832900
C -3.51026800 2.91319200 -0.12598800
C -2.76203600 1.70621300 0.14451200
C -0.75572600 2.89605200 -0.23935100
H -5.42239500 3.89701600 -0.27832200
H -0.93470900 5.01000600 -0.71837500
H -3.37967400 4.99593400 -0.66772900
C -4.92254200 2.96017800 -0.05507900
C -3.50903400 0.55306100 0.54853700
C -4.90561000 0.66053300 0.57300900
C -5.62063800 1.83427900 0.28525800
H -5.47897000 -0.22703900 0.80858300
H -6.70395200 1.83030100 0.33076200
N -1.38427300 1.73436800 0.03561200
Pd -0.00612800 0.17068500 -0.19129200

Table S80. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS2).
B3LYP-D3BJ/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.467581 (Hartree/Particle)
Thermal correction to Energy= 0.494089
Thermal correction to Enthalpy= 0.495034
Thermal correction to Gibbs Free Energy= 0.413471
Sum of electronic and zero-point Energies= -1730.263555
Sum of electronic and thermal Energies= -1730.237046
Sum of electronic and thermal Enthalpies= -1730.236102
Sum of electronic and thermal Free Energies= -1730.317665
C 0.71860900 2.89514000 -0.26888700
C 2.72496900 1.73161200 0.18256100
C 3.46224200 2.94993100 -0.06362800
C 2.76995100 4.11003100 -0.44944400
C 1.40814100 4.09259800 -0.53677700
C 3.47663700 0.58691700 0.60052500
C 4.86698300 3.02560600 0.07522400
H 3.32785200 5.01617200 -0.65838400
H 0.88219700 4.99161000 -0.81270600
C 5.57038100 1.91435000 0.44872500
C 4.86811400 0.72337500 0.68715900
H 5.35602500 3.97255600 -0.12508100
H 6.64938000 1.93298000 0.54906400
H 5.44754100 -0.15757000 0.92913200
N 1.35237200 1.74462800 0.03851200
C -1.41957300 -3.36828900 -1.98970700
C -2.44279800 -3.81980200 -1.19552000
C -2.85204700 -3.06320500 -0.07331300
C -2.39664800 -1.70706400 0.00761300
C -0.73117000 -2.20183600 -1.58094300
H -3.95645200 -4.64267900 0.90417500
H -1.03544500 -3.97978300 -2.79435100
H -2.88816900 -4.79318500 -1.37308700
C -3.64696300 -3.60507300 0.96508700
C -3.05698200 -0.82618200 0.92074200
C -3.71273500 -1.43009200 1.98924800
C -3.96007900 -2.81956500 2.04943500
H -4.15026000 -0.79134000 2.74910400
H -4.49037100 -3.23183900 2.90020800
N -1.29857700 -1.33230400 -0.71757900
C 0.73810200 -2.17738400 -1.60754800
C 2.41996700 -1.67799200 -0.03820400
C 2.91183400 -3.01773700 -0.17117800
C 2.51044500 -3.74653600 -1.31451400
C 1.45559700 -3.30425300 -2.07184200
C 3.06442800 -0.81269800 0.90245700
C 3.72584100 -3.57613400 0.84316700
H 2.98481800 -4.69745700 -1.53403200
H 1.07504400 -3.89895300 -2.89091500
C 4.01475800 -2.82511700 1.95826400
C 3.72999500 -1.44152500 1.95076500
H 4.06347500 -4.60172700 0.74202200
H 4.55418800 -3.25519900 2.79426800
H 4.14829800 -0.82244600 2.73712900
N 1.30151400 -1.31274900 -0.73495400
C -1.45196100 4.08120700 -0.54108100
C -2.81565700 4.08079900 -0.48260700
C -3.50090700 2.90976800 -0.11763800
C -2.75156400 1.70418400 0.15029800
C -0.75254000 2.88902000 -0.27402800
H -5.40947300 3.89940800 -0.23374600
H -0.93172300 4.99087400 -0.79135900
H -3.38102100 4.98123900 -0.69633900
C -4.90978800 2.96232500 -0.01402800

C -3.49226200 0.55482300 0.57125300
C -4.88688500 0.66728100 0.62666400
C -5.60344900 1.84229100 0.35224100
H -5.45539600 -0.21894300 0.87571400
H -6.68491400 1.84271900 0.42437300
N -1.37770100 1.73216800 0.02455000
Pd -0.00579900 0.17036300 -0.19374200

Table S81. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS2).
CAM-B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.473598 (Hartree/Particle)
Thermal correction to Energy= 0.499763
Thermal correction to Enthalpy= 0.500707
Thermal correction to Gibbs Free Energy= 0.419412
Sum of electronic and zero-point Energies= -1729.142660
Sum of electronic and thermal Energies= -1729.116494
Sum of electronic and thermal Enthalpies= -1729.115550
Sum of electronic and thermal Free Energies= -1729.196845
C 0.71913600 2.88455900 -0.24168600
C 2.72232300 1.73050900 0.18350600
C 3.45034600 2.94129600 -0.06065400
C 2.75548500 4.10323500 -0.42287300
C 1.39902300 4.08501200 -0.49728400
C 3.48046300 0.58751200 0.58508900
C 4.85590200 3.01846700 0.05144300
H 3.30992300 5.01270500 -0.62635300
H 0.87268400 4.98741400 -0.75808100
C 5.56373900 1.91059300 0.39708000
C 4.86449600 0.72094900 0.64210600
H 5.33967500 3.96772700 -0.14953600
H 6.64422200 1.92729800 0.47502100
H 5.45031700 -0.15949000 0.86959400
N 1.34905300 1.73856100 0.04858700
C -1.41229200 -3.36243800 -1.96667400
C -2.43380300 -3.81187700 -1.17873700
C -2.84894400 -3.05272600 -0.06581200
C -2.39913300 -1.70713800 0.01215900
C -0.73370100 -2.19713700 -1.55834700
H -3.94993300 -4.63349000 0.91247700
H -1.02508600 -3.97567200 -2.76790000
H -2.87654500 -4.78650600 -1.35522200
C -3.64680600 -3.59406200 0.97057000
C -3.06396400 -0.82666600 0.91788300
C -3.72149400 -1.42153900 1.97724200
C -3.96428900 -2.81123800 2.04430800
H -4.17387600 -0.78157300 2.72707300
H -4.49948900 -3.21993800 2.89323600
N -1.29521600 -1.33187800 -0.70325300
C 0.74191000 -2.17050000 -1.58726200
C 2.42489300 -1.67570300 -0.03754100
C 2.91380300 -3.00351400 -0.17196500
C 2.50736800 -3.73237400 -1.30817500
C 1.45211300 -3.29256400 -2.05639400
C 3.07229800 -0.81189700 0.89808300
C 3.73335300 -3.56247600 0.83771500
H 2.98150100 -4.68255900 -1.53072500
H 1.06884200 -3.88683500 -2.87395000
C 4.02541000 -2.81669200 1.94447200
C 3.74146800 -1.43303100 1.93521500
H 4.06763700 -4.58881400 0.73530400
H 4.57166300 -3.24434400 2.77678100
H 4.17349400 -0.81376400 2.71391200
N 1.29872200 -1.31112800 -0.72149500
C -1.44858500 4.07172600 -0.50371800
C -2.80676000 4.07013900 -0.46170300
C -3.49343800 2.89640100 -0.12222900
C -2.75206300 1.69983300 0.14672700
C -0.75728500 2.87747700 -0.24822300
H -5.39874600 3.88610200 -0.27163300
H -0.92915800 4.98576100 -0.73575200
H -3.36954000 4.97315000 -0.67054000
C -4.90273000 2.94822800 -0.04744400
C -3.49758800 0.55189600 0.55354300
C -4.88420900 0.65957600 0.58016300
C -5.59872600 1.83130500 0.29439700
H -5.45775400 -0.22620200 0.81884100
H -6.68105700 1.82864500 0.34440800
N -1.37749100 1.72447600 0.03203900
Pd -0.00631700 0.17085500 -0.18973900

Table S82. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS2).
ωB97XD/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.472932 (Hartree/Particle)
Thermal correction to Energy= 0.499286
Thermal correction to Enthalpy= 0.500230
Thermal correction to Gibbs Free Energy= 0.418311
Sum of electronic and zero-point Energies= -1729.523882
Sum of electronic and thermal Energies= -1729.497528
Sum of electronic and thermal Enthalpies= -1729.496583
Sum of electronic and thermal Free Energies= -1729.578502
C 0.72028600 2.89896000 -0.20348400
C 2.72572200 1.73477100 0.17792000
C 3.45593300 2.94388000 -0.06864100
C 2.75883300 4.11655400 -0.39560900
C 1.39957800 4.10388100 -0.44479100
C 3.48448200 0.58551300 0.56087000
C 4.86607400 3.00936600 0.00739200
H 3.31258700 5.02776100 -0.59347400
H 0.87278400 5.01342100 -0.68028000
C 5.57503200 1.89121300 0.32361100
C 4.87181600 0.70574300 0.58427400
H 5.35233000 3.95678500 -0.19800100
H 6.65737800 1.89825100 0.37126600
H 5.45422800 -0.18109700 0.79966900
N 1.34997800 1.74671900 0.06289300
C -1.41356200 -3.37366100 -1.96191800
C -2.43257200 -3.82268200 -1.16780900
C -2.84594500 -3.05834500 -0.05588900
C -2.39801500 -1.71134400 0.01263600
C -0.73423700 -2.20588000 -1.55820000
H -3.94749700 -4.63305900 0.93638900
H -1.03096600 -3.98865100 -2.76449500
H -2.87387600 -4.79872500 -1.34056300
C -3.64420600 -3.59305000 0.98568700
C -3.06431600 -0.82417400 0.91104700
C -3.72552500 -1.41006200 1.97453600
C -3.96397300 -2.80087500 2.05410000
H -4.18250500 -0.76301700 2.71611400

H -4.49980500 -3.20352100 2.90553800
N -1.29453000 -1.33708500 -0.70558800
C 0.74333000 -2.18043200 -1.58552400
C 2.42289400 -1.68119900 -0.03344400
C 2.90778300 -3.01191900 -0.15455300
C 2.50358800 -3.74790000 -1.28877400
C 1.45299800 -3.30779300 -2.04612700
C 3.07205100 -0.80931500 0.89365100
C 3.72562500 -3.56346400 0.86269800
H 2.97484400 -4.70122700 -1.50432600
H 1.07463700 -3.90487700 -2.86437000
C 4.02114000 -2.80556100 1.96242200
C 3.74439400 -1.41954500 1.93657000
H 4.05802000 -4.59166300 0.77165200
H 4.56712100 -3.22595100 2.79862700
H 4.18315300 -0.79111600 2.70479200
N 1.29856600 -1.31702400 -0.72251800
C -1.44886000 4.09136100 -0.44775500
C -2.80916000 4.08427900 -0.43320700
C -3.49736200 2.90012900 -0.12879200
C -2.75449600 1.70461100 0.14135700
C -0.75798200 2.89213400 -0.20920000
H -5.40760700 3.87882400 -0.30964500
H -0.92954000 5.01289600 -0.65037300
H -3.37115100 4.98896500 -0.63729000
C -4.90978300 2.94181300 -0.08457300
C -3.50061700 0.55050700 0.53042100
C -4.88948100 0.64667900 0.52866700
C -5.60644200 1.81542700 0.23117300
H -5.46024700 -0.24464400 0.75730000
H -6.68954200 1.80533600 0.25738500
N -1.37784600 1.73272100 0.04524500
Pd -0.00603600 0.17239700 -0.18914300

Table S83. Cartesian coordinates and energies of ***i*-TEQ 6a**/Pd(II) (TS2).
M06-2X/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.471383 (Hartree/Particle)
Thermal correction to Energy= 0.498062
Thermal correction to Enthalpy= 0.499007
Thermal correction to Gibbs Free Energy= 0.416408
Sum of electronic and zero-point Energies= -1729.288965
Sum of electronic and thermal Energies= -1729.262286
Sum of electronic and thermal Enthalpies= -1729.261342
Sum of electronic and thermal Free Energies= -1729.343940
C 0.72247300 2.93294400 0.08760000
C 2.74970900 1.75737500 0.11857700
C 3.45682700 2.97788800 -0.13592400
C 2.73975800 4.18277800 -0.19187000
C 1.38814500 4.16964600 -0.03992100
C 3.54490400 0.59348500 0.34157200
C 4.85932900 3.02446500 -0.30919700
H 3.27440400 5.11372000 -0.34840000
H 0.85405500 5.10337300 -0.06667700
C 5.58760500 1.87679900 -0.21174400
C 4.91749500 0.69005900 0.13048800
H 5.32021900 3.98360200 -0.51981100
H 6.66050300 1.86725400 -0.36162200
H 5.50945800 -0.21081300 0.24082400
N 1.36986800 1.76433300 0.16007200
C -1.39919000 -3.53451000 -1.75624600
C -2.43763200 -3.93572400 -0.96333200
C -2.89886100 -3.08906900 0.06753200
C -2.44966500 -1.73900500 0.05305800
C -0.73803800 -2.33079800 -1.41925400
H -4.06926100 -4.58230300 1.10154100
H -0.99167900 -4.19931500 -2.50425900
H -2.87100300 -4.92414800 -1.07936200
C -3.77527800 -3.53824000 1.08654500
C -3.18049000 -0.78658800 0.82109600
C -3.95816000 -1.27532900 1.85437800
C -4.20043400 -2.65606500 2.04260600
H -4.49234000 -0.56227600 2.47465300
H -4.81665800 -2.98464400 2.87110400
N -1.31663200 -1.40902400 -0.64259300
C 0.74058900 -2.30487900 -1.45440700
C 2.47026000 -1.71402600 -0.00323200
C 2.95669000 -3.05086300 -0.05302200
C 2.50725400 -3.86293100 -1.11700300
C 1.43546600 -3.46473600 -1.86618000
C 3.18137600 -0.77733200 0.80435300
C 3.84757700 -3.52374400 0.94265500
H 2.97334600 -4.82808200 -1.28835400
H 1.03457000 -4.10359300 -2.64066200
C 4.24132600 -2.67799000 1.94391000
C 3.96238200 -1.29683500 1.82004700
H 4.17138300 -4.55847400 0.90793500
H 4.86180300 -3.02861500 2.76009600
H 4.47674100 -0.60154500 2.47599200
N 1.31581200 -1.39102200 -0.66428600
C -1.43844200 4.15606200 -0.04851400
C -2.78583300 4.15270300 -0.23730600
C -3.48885700 2.93818900 -0.20389800
C -2.77299800 1.72996400 0.07799900
C -0.75888100 2.92649600 0.08081600
H -5.35717100 3.91118100 -0.64343500
H -0.91668500 5.09711400 -0.04418500
H -3.32840100 5.07761300 -0.40327200
C -4.88683800 2.96102900 -0.41436800
C -3.55658600 0.56001100 0.30256900
C -4.92372100 0.63059400 0.05416900
C -5.60019000 1.80272900 -0.32542100
H -5.50552500 -0.27646800 0.17070600
H -6.66852900 1.77623600 -0.50324600
N -1.39465300 1.75214400 0.14365800
Pd -0.00640000 0.14973600 -0.14896300

Table S84. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
B3LYP-D3/6-31G(d,p)-SDD(Pd)
Zero-point correction= 0.468415 (Hartree/Particle)
Thermal correction to Energy= 0.495528
Thermal correction to Enthalpy= 0.496472
Thermal correction to Gibbs Free Energy= 0.414032
Sum of electronic and zero-point Energies= -1730.089062
Sum of electronic and thermal Energies= -1730.061949
Sum of electronic and thermal Enthalpies= -1730.061005
Sum of electronic and thermal Free Energies= -1730.143444
C -1.25107100 -3.65094000 -1.74306300
C -0.41242200 -2.74130700 -1.02971600

N -0.96052700 -1.82737300 -0.15234200
C -3.09047800 -2.91520200 -0.36745000
C -2.61751600 -3.71046000 -1.38038200
C -0.69589800 -4.49228000 -2.73975600
C 0.66070200 -4.48557800 -2.97490400
C 1.50285100 -3.70389800 -2.15979100
C 0.99865600 -2.84710700 -1.18692200
C -3.65155300 1.25096800 1.74263800
C -2.74162900 0.41238400 1.02962000
N -1.82742800 0.96042200 0.15243700
C -2.91555400 3.09027500 0.36704200
C -3.71107200 2.61739200 1.37981200
C -4.49301000 0.69573700 2.73916600
C -4.48612200 -0.66084100 2.97452100
C -3.70418500 -1.50298300 2.15968100
C -2.84731300 -0.99873800 1.18690200
C -2.24299900 -1.93784200 0.21653100
C 1.25113400 3.65126100 -1.74278000
C 0.41244400 2.74147900 -1.02959200
N 0.96048300 1.82735200 -0.15239300
C 3.09052600 2.91508400 -0.36740800
C 2.61758700 3.71058800 -1.38016500
C 0.69591500 4.49275700 -2.73926100
C -0.66069800 4.48596500 -2.97448400
C -1.50283800 3.70407600 -2.15965700
C -0.99868200 2.84718400 -1.18679800
C -1.93791600 2.24287700 -0.21657300
C 3.65136500 -1.25111600 1.74276200
C 2.74161800 -0.41242500 1.02962200
N 1.82750500 -0.96041900 0.15230000
C 1.93781800 -2.24293800 -0.21659600
C 2.91529800 -3.09041500 0.36715200
C 3.71073900 -2.61753300 1.37996900
C 4.49284400 -0.69592600 2.73929800
C 4.48608200 0.66068300 2.97446700
C 3.70423900 1.50286600 2.15957500
C 2.84734500 0.99866200 1.18679000
C 2.24301400 1.93771400 0.21646900
H -4.12834800 -2.96126200 -0.06349200
H -3.27920800 -4.39916200 -1.89735200
H -1.35500200 -5.15283100 -3.29456500
H 1.09242100 -5.11773900 -3.74295000
H 2.57804700 -3.78315200 -2.28678900
H -2.96161900 4.12812600 0.06302300
H -4.39993200 3.27912100 1.89651400
H -5.15386500 1.35475600 3.29371900
H -5.11839000 -1.09245800 3.74253800
H -3.78323300 -2.57819200 2.28669600
H 4.12843200 2.96099400 -0.06354600
H 3.27930700 4.39929400 -1.89709300
H 1.35489100 5.15356100 -3.29392400
H -1.09234300 5.11831100 -3.74242600
H -2.57802800 3.78316300 -2.28682500
H 2.96134700 -4.12827000 0.06313500
H 4.39952000 -3.27927500 1.89677500
H 5.15362100 -1.35492500 3.29395900
H 5.11841500 1.09237400 3.74239200
H 3.78344200 2.57805900 2.28663200
Pd 0.00010800 -0.00006300 0.00050500

Table S85. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.468979 (Hartree/Particle)
Thermal correction to Energy= 0.496077
Thermal correction to Enthalpy= 0.497021
Thermal correction to Gibbs Free Energy= 0.414530
Sum of electronic and zero-point Energies= -1730.231408
Sum of electronic and thermal Energies= -1730.204310
Sum of electronic and thermal Enthalpies= -1730.203366
Sum of electronic and thermal Free Energies= -1730.285857
C -1.63787500 -3.64427400 2.15848400
C -1.10251900 -2.80747700 1.18619500
C 0.31107800 -2.75600800 1.02556200
C 1.11571100 -3.69611600 1.73716500
C 0.53076900 -4.51569500 2.73440700
C -0.82393400 -4.45769000 2.97089700
H -2.71482900 -3.68389300 2.28507700
C 2.47886800 -3.80612400 1.37490300
H 1.16666500 -5.19954800 3.28709700
H -1.27869800 -5.07398400 3.73811900
C 2.97963400 -3.02859900 0.36286500
C 2.16756900 -2.02042800 -0.21898500
H 4.01401000 -3.11280800 0.05696400
C 2.80754900 -1.10249800 -1.18606500
C 2.75607500 0.31109600 -1.02540500
C 3.64441000 -1.63783500 -2.15830900
C 3.69624000 1.11574000 -1.73691800
C 4.45788400 -0.82387800 -2.97064900
H 3.68403100 -2.71478600 -2.28492500
C 2.02041700 2.16755900 0.21913700
C 3.80622900 2.47888900 -1.37461700
C 4.51588300 0.53081800 -2.73412000
H 5.07422700 -1.27862800 -3.73784000
C 3.02863300 2.97963400 -0.36262300
H 4.51873200 3.11458400 -1.89075700
H 5.19977900 1.16672300 -3.28674500
H 3.11282600 4.01400100 -0.05668700
C 1.10243000 2.80751700 1.18617800
C -0.31115500 2.75604700 1.02543800
C 1.63771300 3.64435200 2.15847400
C -1.11583800 3.69619500 1.73693300
C 0.82371400 4.45780600 2.97079000
H 2.71465800 3.68396800 2.28515300
C -2.16755600 2.02041900 -0.21921500
C -0.53096900 4.51581300 2.73418800
H 1.27842100 5.07412700 3.73802500
H -1.16690400 5.19969200 3.28679800
C -2.80746600 1.10245200 -1.18630900
C -2.75600100 -0.31113600 -1.02559600
C -3.64425500 1.63775500 -2.15863400
C -3.69610600 -1.11580700 -1.73716000
C -4.45766700 0.82377000 -2.97100700
H -3.68387100 2.71470300 -2.28528900
C -2.02043100 -2.16755800 0.21905800
C -3.80611700 -2.47894500 -1.37482400
C -4.51567700 -0.53092000 -2.73444100
H -5.07395300 1.27849200 -3.73826100
C -3.02859800 -2.97965500 -0.36275300
H -4.51857700 -3.11466000 -1.89100000

H -5.19952600 -1.16684500 -3.28710100
H -3.11280900 -4.01401400 -0.05679400
N 0.89096500 -1.86310800 0.14844800
N 1.86311800 0.89096500 -0.14833900
N -0.89097900 1.86311300 0.14831800
N -1.86310800 -0.89097400 -0.14844500
C -2.47896900 3.80619000 1.37456800
C -2.97966300 3.02861600 0.36253100
H -4.01401700 3.11280800 0.05655000
H 3.11455500 -4.51858600 1.89111100
H -3.11469200 4.51867700 1.89069600
Pd -0.00000100 -0.00000300 -0.00002000

Table S86. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
B3LYP-D3BJ/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.469702 (Hartree/Particle)
Thermal correction to Energy= 0.496732
Thermal correction to Enthalpy= 0.497676
Thermal correction to Gibbs Free Energy= 0.415387
Sum of electronic and zero-point Energies= -1730.349599
Sum of electronic and thermal Energies= -1730.322569
Sum of electronic and thermal Enthalpies= -1730.321625
Sum of electronic and thermal Free Energies= -1730.403914
C 1.60857000 3.64075300 2.17218200
C 1.08270800 2.80016100 1.19895700
C -0.32772500 2.74714700 1.02543300
C -1.13986700 3.68845400 1.72450600
C -0.56573200 4.50999300 2.72527200
C 0.78633900 4.45383600 2.97516600
H 2.68417300 3.68251600 2.30558400
C -2.49798400 3.79844700 1.34561000
H -1.20775700 5.19420900 3.26948300
H 1.23273400 5.07251800 3.74485900
C -2.98671000 3.01780000 0.33071300
C -2.16882600 2.00741500 -0.23654300
H -4.01654700 3.09903400 0.01073500
C -2.80027100 1.08268700 -1.19882400
C -2.74725000 -0.32774100 -1.02527600
C -3.64095700 1.60853100 -2.17197800
C -3.68863300 -1.13989600 -1.72423000
C -4.45412000 0.78628500 -2.97486500
H -3.68272900 2.68413200 -2.30539900
C -2.00740700 -2.16880300 0.23668800
C -3.79859900 -2.49800000 -1.34527900
C -4.51026400 -0.56578000 -2.72493000
H -5.07287600 1.23266500 -3.74450800
C -3.01785600 -2.98669800 -0.33044000
H -4.51355200 -3.13823800 -1.85152600
H -5.19454000 -1.20781300 -3.26905700
H -3.09907500 -4.01651900 -0.01040800
C -1.08261700 -2.80020500 1.19893600
C 0.32780200 -2.74718700 1.02530500
C -1.60840600 -3.64083100 2.17217100
C 1.13999600 -3.68852500 1.72427800
C -0.78611500 -4.45394100 2.97506500
H -2.68399900 -3.68259200 2.30565800
C 2.16880800 -2.00740800 -0.23678100
C 0.56593600 -4.51009600 2.72506100
H -1.23245100 -5.07264600 3.74477400
H 1.20800100 -5.19433100 3.26920100
C 2.80018100 -1.08264300 -1.19907600
C 2.74717300 0.32777900 -1.02547000
C 3.64079600 -1.60845100 -2.17231100
C 3.68850100 1.13996000 -1.72446700
C 4.45389900 -0.78617400 -2.97522800
H 3.68256300 -2.68404700 -2.30577300
C 2.00742400 2.16879500 0.23661400
C 3.79849600 2.49805000 -1.34547400
C 4.51005900 0.56588200 -2.72525000
H 5.07259700 -1.23252500 -3.74493400
C 3.01783200 2.98671100 -0.33055700
H 4.51341200 3.13830700 -1.85175000
H 5.19429100 1.20793600 -3.26940700
H 3.09907300 4.01652200 -0.01049700
N -0.89702500 1.85372100 0.14439200
N -1.85374000 -0.89702000 -0.14431100
N 0.89703700 -1.85372800 0.14425600
N 1.85372800 0.89702600 -0.14441800
C 2.49808400 -3.79850500 1.34527400
C 2.98673500 -3.01781500 0.33037300
H 4.01654800 -3.09903400 0.01031400
H -3.13821200 4.51334100 1.85195400
H 3.13834900 -4.51341900 1.85154100
Pd 0.00000000 0.00000200 -0.00008700

Table S87. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
CAM-B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.475858 (Hartree/Particle)
Thermal correction to Energy= 0.502447
Thermal correction to Enthalpy= 0.503391
Thermal correction to Gibbs Free Energy= 0.421897
Sum of electronic and zero-point Energies= -1729.233280
Sum of electronic and thermal Energies= -1729.206692
Sum of electronic and thermal Enthalpies= -1729.205748
Sum of electronic and thermal Free Energies= -1729.287241
C 1.61333400 3.62033300 2.16348900
C 1.08515800 2.79192700 1.19368100
C -0.32284200 2.73988200 1.02568100
C -1.12595900 3.66892500 1.72969400
C -0.54945400 4.48553900 2.72992700
C 0.79616400 4.42918800 2.97322000
H 2.68949100 3.66460900 2.29171200
C -2.48496500 3.77740600 1.36240800
H -1.19020500 5.16466300 3.28166100
H 1.24620900 5.04462300 3.74285000
C -2.97658500 3.00465800 0.35178000
C -2.15929700 2.00348700 -0.22384800
H -4.00882600 3.08481800 0.03979900
C -2.79203400 1.08513800 -1.19355200
C -2.73998200 -0.32285800 -1.02552700
C -3.62053400 1.61329500 -2.16329000
C -3.66910400 -1.12598800 -1.72941900
C -4.42947200 0.79610900 -2.97292200
H -3.66481900 2.68944900 -2.29153300
C -2.00348000 -2.15927500 0.22399300
C -3.77755800 -2.48498200 -1.36207900
C -4.48581000 -0.54950300 -2.72958800
H -5.04498000 1.24613900 -3.74250200

C -3.00471600 -2.97657300 -0.35150800
H -4.48900800 -3.12283500 -1.87589600
H -5.16499600 -1.19026200 -3.28123700
H -3.08486200 -4.00879900 -0.03947300
C -1.08506800 -2.79197000 1.19366300
C 0.32291900 -2.73992100 1.02555700
C -1.61317100 -3.62041400 2.16347800
C 1.12608800 -3.66900000 1.72946500
C -0.79594100 -4.42930200 2.97311500
H -2.68931800 -3.66468900 2.29178600
C 2.15928300 -2.00347800 -0.22408000
C 0.54965700 -4.48565000 2.72971300
H -1.24592800 -5.04476300 3.74275900
H 1.19044800 -5.16479800 3.28137100
C 2.79194700 -1.08509300 -1.19379800
C 2.73990700 0.32289700 -1.02571900
C 3.62037700 -1.61321600 -2.16361500
C 3.66897000 1.12605400 -1.72965800
C 4.42925300 -0.79600100 -2.97327900
H 3.66465700 -2.68936600 -2.29189800
C 2.00349400 2.15927100 0.22391500
C 3.77744900 2.48503600 -1.36228100
C 4.48560400 0.54960400 -2.72990700
H 5.04470600 -1.24600300 -3.74292100
C 3.00468400 2.97659100 -0.35163300
H 4.48885700 3.12290900 -1.87613200
H 5.16474500 1.19038400 -3.28158800
H 3.08484900 4.00880800 -0.03957300
N -0.89322100 1.84752600 0.14626100
N -1.84754200 -0.89321600 -0.14618100
N 0.89323500 -1.84753100 0.14613100
N 1.84753100 0.89322400 -0.14628800
C 2.48506600 -3.77746600 1.36207500
C 2.97661300 -3.00467300 0.35144500
H 4.00883000 -3.08481700 0.03938400
H -3.12280900 4.48879400 1.87632200
H 3.12294700 -4.48887900 1.87591000
Pd 0.00000100 0.00000300 -0.00008300

Table S88. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
ωB97XD/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.474823 (Hartree/Particle)
Thermal correction to Energy= 0.501624
Thermal correction to Enthalpy= 0.502568
Thermal correction to Gibbs Free Energy= 0.420535
Sum of electronic and zero-point Energies= -1729.613919
Sum of electronic and thermal Energies= -1729.587118
Sum of electronic and thermal Enthalpies= -1729.586174
Sum of electronic and thermal Free Energies= -1729.668208
C -1.62977400 -3.61212000 2.16669200
C -1.09648700 -2.78860800 1.19382900
C 0.31292900 -2.74443600 1.02609100
C 1.11289700 -3.67491500 1.73346800
C 0.53137500 -4.48764500 2.73616500
C -0.81557400 -4.42348600 2.97910700
H -2.70658300 -3.65035600 2.29598700
C 2.47374700 -3.78695600 1.36873100
H 1.16778400 -5.16904100 3.29049400
H -1.26865400 -5.03467100 3.75035300
C 2.96944700 -3.01529800 0.35668600
C 2.15387200 -2.01352000 -0.22138900
H 4.00291100 -3.09682800 0.04743400
C 2.78872300 -1.09646800 -1.19370200
C 2.74454600 0.31294400 -1.02593700
C 3.61234000 -1.62973600 -2.16648800
C 3.67511300 1.11292400 -1.73318200
C 4.42379800 -0.81551900 -2.97879400
H 3.65058600 -2.70654200 -2.29580300
C 2.01351400 2.15384500 0.22153100
C 3.78712900 2.47376000 -1.36838300
C 4.48794600 0.53142300 -2.73580700
H 5.03506400 -1.26858500 -3.74998600
C 3.01536700 2.96943100 -0.35640200
H 4.49803900 3.11047200 -1.88456100
H 5.16941000 1.16784000 -3.29004300
H 3.09688600 4.00287700 -0.04708800
C 1.09639700 2.78864900 1.19381200
C -0.31300700 2.74447400 1.02596900
C 1.62961100 3.61220200 2.16668200
C -1.11302500 3.67499200 1.73323900
C 0.81535100 4.42360300 2.97900100
H 2.70641000 3.65043800 2.29606100
C -2.15385800 2.01351000 -0.22161900
C -0.53157800 4.48776100 2.73594800
H 1.26837400 5.03481600 3.75026000
H -1.16802600 5.16918200 3.29020000
C -2.78863800 1.09642300 -1.19394500
C -2.74447200 -0.31298400 -1.02612900
C -3.61218500 1.62965600 -2.16681000
C -3.67497900 -1.11299100 -1.73342200
C -4.42358200 0.81541100 -2.97914900
H -3.65042700 2.70645800 -2.29616300
C -2.01352700 -2.15384200 0.22145100
C -3.78701700 -2.47381700 -1.36858900
C -4.48774000 -0.53152400 -2.73612600
H -5.03479200 1.26844900 -3.75040000
C -3.01533200 -2.96945100 -0.35653200
H -4.49788300 -3.11054800 -1.88480300
H -5.16915900 -1.16796100 -3.29039400
H -3.09686600 -4.00289000 -0.04719500
N 0.88620700 -1.85576300 0.14518800
N 1.85578200 0.88620000 -0.14511700
N -0.88622100 1.85576700 0.14506000
N -1.85577100 -0.88620800 -0.14522500
C -2.47384800 3.78701900 1.36839700
C -2.96947500 3.01531500 0.35635200
H -4.00291700 3.09682900 0.04701900
H 3.11044900 -4.49779500 1.88501700
H -3.11058600 4.49788500 1.88460300
Pd -0.00000100 -0.00000300 -0.00010500

Table S89. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
M06-2X/6-31G(d,p)-SDD(Pd)/IEFPCM(Et_2O)
Zero-point correction= 0.473073 (Hartree/Particle)
Thermal correction to Energy= 0.500086
Thermal correction to Enthalpy= 0.501030
Thermal correction to Gibbs Free Energy= 0.418843
Sum of electronic and zero-point Energies= -1729.378182

Sum of electronic and thermal Energies= -1729.351169
Sum of electronic and thermal Enthalpies= -1729.350225
Sum of electronic and thermal Free Energies= -1729.432412
C 1.62696800 3.66075400 2.12782000
C 1.09249000 2.81952400 1.16971200
C -0.31971100 2.77513600 1.00310200
C -1.11569000 3.71892300 1.70113200
C -0.53201800 4.54838800 2.68912800
C 0.81586200 4.48749700 2.93002600
H 2.70456700 3.69717400 2.25402800
C -2.48102800 3.82391500 1.34695400
H -1.16944800 5.23796600 3.23229500
H 1.27245300 5.11046700 3.68957900
C -2.98701800 3.03251900 0.35542700
C -2.17093300 2.02155600 -0.21480500
H -4.02401100 3.10305600 0.05491400
C -2.81970600 1.09247600 -1.16958900
C -2.77531700 -0.31972000 -1.00295500
C -3.66110500 1.62693800 -2.12755800
C -3.71924400 -1.11571200 -1.70077300
C -4.48800200 0.81581600 -2.92959200
H -3.69754400 2.70453500 -2.25378300
C -2.02155500 -2.17087800 0.21492300
C -3.82420100 -2.48102800 -1.34649700
C -4.54887700 -0.53205700 -2.68863800
H -5.11110600 1.27239300 -3.68904200
C -3.03264600 -2.98697300 -0.35507100
H -4.54492600 -3.11109700 -1.85819000
H -5.23857100 -1.16949000 -3.23165300
H -3.10317800 -4.02393600 -0.05445200
C -1.09240200 -2.81956200 1.16969100
C 0.31978700 -2.77517600 1.00297800
C -1.62681300 -3.66082400 2.12780800
C 1.11581300 -3.71900000 1.70090500
C -0.81565200 -4.48760700 2.92991800
H -2.70440200 -3.69723900 2.25410100
C 2.17092400 -2.02155000 -0.21503100
C 0.53220900 -4.54850200 2.68891000
H -1.27218800 -5.11060200 3.68948200
H 1.16967200 -5.23810800 3.23200000
C 2.81962800 -1.09243300 -1.16982600
C 2.77524900 0.31975700 -1.00313800
C 3.66094900 -1.62686000 -2.12788300
C 3.71911300 1.11577700 -1.70101000
C 4.48777200 -0.81570500 -2.92996200
H 3.69738300 -2.70445100 -2.25414900
C 2.02157500 2.17087500 0.21485500
C 3.82409400 2.48108300 -1.34669900
C 4.54866200 0.53216000 -2.68896800
H 5.11081000 -1.27225200 -3.68948500
C 3.03261900 2.98699200 -0.35519100
H 4.54477400 3.11117100 -1.85843000
H 5.23830200 1.16961500 -3.23202600
H 3.10316800 4.02394700 -0.05454900
N -0.89879900 1.87822000 0.13593900
N -1.87824900 -0.89877900 -0.13594100
N 0.89881700 -1.87822600 0.13581200
N 1.87824700 0.89878600 -0.13603500
C 2.48112600 -3.82398000 1.34662400
C 2.98704700 -3.03254000 0.35509800
H 4.02401800 -3.10306400 0.05450400
H -3.11108600 4.54452100 1.85882600
H 3.11121900 -4.54461200 1.85841900
Pd 0.00000400 0.00000300 -0.00025600

Table S90. Cartesian coordinates and energies of **TEQ 7a**/Pd(II).
B3LYP-D3/6-311+G(2d,p)-SDD(Pd)/SMD(Et_2O)
Zero-point correction= 0.464778 (Hartree/Particle)
Thermal correction to Energy= 0.492239
Thermal correction to Enthalpy= 0.493183
Thermal correction to Gibbs Free Energy= 0.409314
Sum of electronic and zero-point Energies= -1730.673357
Sum of electronic and thermal Energies= -1730.645896
Sum of electronic and thermal Enthalpies= -1730.644952
Sum of electronic and thermal Free Energies= -1730.728820
C -3.68469700 -1.11317200 1.72553700
C -2.74300000 -0.30906300 1.02712700
N -1.85597700 -0.88654900 0.14930500
C -3.04252700 -2.95459500 0.32281600
C -3.81081200 -2.46360700 1.33870200
C -4.49200500 -0.53862000 2.73210200
C -4.42116700 0.80663000 2.98666700
C -3.61169900 1.62366000 2.18158500
C -2.78695000 1.09933500 1.20132300
C 1.11322100 -3.68284500 -1.72650500
C 0.30911700 -2.74193800 -1.02696400
N 0.88673600 -1.85573600 -0.14829800
C 2.95504300 -3.04162200 -0.32389800
C 2.46381000 -3.80905300 -1.34027900
C 0.53863700 -4.48935200 -2.73369500
C -0.80662900 -4.41845800 -2.98806600
C -1.62362900 -3.60976800 -2.18220200
C -1.09930700 -2.78595500 -1.20114400
C -2.02265800 -2.14973300 -0.23830000
C 3.68479800 1.11320600 1.72531200
C 2.74306100 0.30908100 1.02697100
N 1.85597800 0.88655100 0.14919800
C 3.04252000 2.95461000 0.32261800
C 3.81087100 2.46363900 1.33846100
C 4.49218300 0.53866700 2.73182100
C 4.42136500 -0.80658100 2.98640800
C 3.61184300 -1.62362400 2.18139800
C 2.78702700 -1.09931700 1.20117900
C 2.15017300 -2.02252000 0.23856500
C -1.11332200 3.68281200 -1.72650400
C -0.30917600 2.74191900 -1.02699100
N -0.88674200 1.85573200 -0.14827600
C -2.15016000 2.02251800 0.23864900
C -2.95506400 3.04161000 -0.32378200
C -2.46388800 3.80902500 -1.34020300
C -0.53879200 4.48930100 -2.73374000
C 0.80646200 4.41840500 -2.98817600
C 1.62350700 3.60973200 -2.18234000
C 1.09923600 2.78593300 -1.20124300
C 2.02262900 2.14973200 -0.23843200
H -3.14473200 -3.97986300 -0.00095800
H -4.53120000 -3.09733500 1.84229700
H -5.17713400 -1.17619800 3.27764500
H -5.02600600 1.25443700 3.76447900

H -3.64814300 2.69694000 2.32041800
H 3.98053200 -3.14376100 -0.00081000
H 3.09752500 -4.52874800 -1.84487600
H 1.17625300 -5.17384100 -3.27999500
H -1.25443100 -5.02255600 -3.76645800
H -2.69690500 -3.64605600 -2.32109900
H 3.14469600 3.97987700 -0.00117000
H 4.53128200 3.09737900 1.84200900
H 5.17734800 1.17624900 3.27731100
H 5.02626400 -1.25437300 3.76418300
H 3.64829800 -2.69690100 2.32024600
H -3.98053300 3.14375800 -0.00063100
H -3.09763200 4.52871300 -1.84477400
H -1.17643600 5.17378400 -3.28001600
H 1.25422600 5.02249600 -3.76659500
H 2.69677700 3.64602500 -2.32129100
Pd -0.00000300 0.00000100 0.00212900

Table S91. Cartesian coordinates and energies of **TEQ 7a**/Pd(II) (TS).
B3LYP-D3/6-31G(d,p)-SDD(Pd)
Zero-point correction= 0.466647 (Hartree/Particle)
Thermal correction to Energy= 0.493286
Thermal correction to Enthalpy= 0.494231
Thermal correction to Gibbs Free Energy= 0.412470
Sum of electronic and zero-point Energies= -1730.023244
Sum of electronic and thermal Energies= -1729.996604
Sum of electronic and thermal Enthalpies= -1729.995660
Sum of electronic and thermal Free Energies= -1730.077421
C 2.25736400 3.66360500 -0.46012600
C 1.78766900 2.41911000 0.06766000
N 0.53905100 1.96194100 -0.28070600
C 0.34586200 3.69733400 -1.91663500
C 1.56566000 4.20205400 -1.57012100
C 3.36835400 4.32533800 0.10764400
C 4.01395700 3.76264600 1.18429200
C 3.67153900 2.46109800 1.57919500
C 2.63294300 1.72182500 0.99714900
C -3.66373400 2.25726900 0.45989700
C -2.41915500 1.78762800 -0.06775300
N -1.96196900 0.53903400 0.28071200
C -3.69750500 0.34585200 1.91651600
C -4.20226400 1.56559000 1.56987200
C -4.32538000 3.36834400 -0.10781100
C -3.76244700 4.01423500 -1.18415400
C -2.46086200 3.67183000 -1.57892600
C -1.72177800 2.63296700 -0.99711700
C -0.25027300 2.68397900 -1.11496200
C -2.25739500 -3.66359400 -0.46000500
C -1.78766300 -2.41913300 0.06783200
N -0.53900400 -1.96203200 -0.28045200
C -0.34594300 -3.69726100 -1.91658300
C -1.56573700 -4.20198700 -1.57005500
C -3.36849300 -4.32524200 0.10764900
C -4.01427200 -3.76243200 1.18412600
C -3.67182600 -2.46088700 1.57902400
C -2.63298200 -1.72177400 0.99722200
C -2.68404800 -0.25026700 1.11496200
C 3.66385000 -2.25728000 0.45979900
C 2.41922400 -1.78766700 -0.06776200
N 1.96206300 -0.53904300 0.28065800
C 2.68418700 0.25031100 1.11481600
C 3.69784700 -0.34570500 1.91619400
C 4.20257100 -1.56546500 1.56958900
C 4.32539000 -3.36846600 -0.10781000
C 3.76232700 -4.01450100 -1.18399400
C 2.46073500 -3.67206500 -1.57871500
C 1.72176000 -2.63307800 -0.99699100
C 0.25025500 -2.68402400 -1.11481300
H -0.19775300 4.13322400 -2.74189400
H 1.98989100 5.04426300 -2.10837500
H 3.67824900 5.28218000 -0.30073500
H 4.83307000 4.27421400 1.67693900
H 4.30701700 2.00500800 2.32466700
H -4.13338800 -0.19773000 2.74180300
H -5.04452500 1.98982800 2.10804000
H -5.28231100 3.67813800 0.30044000
H -4.27385900 4.83354000 -1.67664400
H -2.00456500 4.30756200 -2.32405200
H 0.19760600 -4.13301700 -2.74196000
H -1.99002900 -5.04411800 -2.10838500
H -3.67837100 -5.28209300 -0.30072300
H -4.83354100 -4.27389500 1.67662200
H -4.30750200 -2.00464500 2.32423500
H 4.13391900 0.19795500 2.74132400
H 5.04494900 -1.98961400 2.10764200
H 5.28233400 -3.67825400 0.30041400
H 4.27363300 -4.83393700 -1.67637400
H 2.00432500 -4.30788100 -2.32370000
Pd 0.00003100 -0.00002500 0.00010000

Table S92. Cartesian coordinates and energies of ***i*-TEQ 6a**/Cu(II).
B3LYP-D3/6-31G(d,p)-SDD(Cu)
Zero-point correction= 0.467041 (Hartree/Particle)
Thermal correction to Energy= 0.494646
Thermal correction to Enthalpy= 0.495590
Thermal correction to Gibbs Free Energy= 0.411113
Sum of electronic and zero-point Energies= -1799.478075
Sum of electronic and thermal Energies= -1799.450470
Sum of electronic and thermal Enthalpies= -1799.449526
Sum of electronic and thermal Free Energies= -1799.534004
C 0.63425400 2.67866500 0.37373400
C 2.52856600 1.42935400 0.95096300
C 2.89406300 2.42586500 1.92023900
C 2.11454500 3.60368000 1.99753300
C 1.03072200 3.77170600 1.16451100
C 3.45716600 0.40079000 0.63054300
C 4.05228100 2.24609500 2.71792400
H 2.39380600 4.38004800 2.70385700
H 0.43624800 4.67747900 1.17665100
C 4.85830100 1.15215900 2.51108600
C 4.58137300 0.27285100 1.44154400
H 4.29792400 2.99205400 3.46729300
H 5.74226000 0.99286500 3.11913400
H 5.29305500 -0.51553000 1.21796600
N 1.32053900 1.53113200 0.30172400
C -1.03065000 -3.77192900 1.16425100
C -2.11464200 -3.60402000 1.99711100
C -2.89417400 -2.42621300 1.91988200

C -2.52850800 -1.42949200 0.95082200
C -0.63403900 -2.67874000 0.37378100
H -4.29825200 -2.99278100 3.46658400
H -0.43621900 -4.67773200 1.17633300
H -2.39399300 -4.38050500 2.70327400
C -4.05254500 -2.24666100 2.71739500
C -3.45711700 -0.40095100 0.63039800
C -4.58145300 -0.27319500 1.44130200
C -4.85858000 -1.15271100 2.51062100
H -5.29302000 0.51531600 1.21780700
H -5.74268300 -0.99354600 3.11850000
N -1.32031100 -1.53114500 0.30194700
C 0.63401800 -2.67874900 -0.37341500
C 2.52829800 -1.42953900 -0.95105700
C 2.89354500 -2.42612000 -1.92036900
C 2.11398700 -3.60393500 -1.99739400
C 1.03033900 -3.77190200 -1.16414300
C 3.45701600 -0.40103100 -0.63081700
C 4.05161000 -2.24642000 -2.71829200
H 2.39307500 -4.38034900 -2.70373700
H 0.43590300 -4.67770300 -1.17602900
C 4.85771100 -1.15250300 -2.51164600
C 4.58106000 -0.27316200 -1.44207200
H 4.29705000 -2.99239400 -3.46771000
H 5.74156600 -0.99325600 -3.11986700
H 5.29284400 0.51516800 -1.21865300
N 1.32036600 -1.53124800 -0.30165900
C -1.03030100 3.77219700 -1.16374800
C -2.11416000 3.60444500 -1.99677400
C -2.89370200 2.42661200 -1.91987500
C -2.52823600 1.42978800 -0.95086500
C -0.63380900 2.67882300 -0.37340200
H -4.29739000 2.99329900 -3.46689000
H -0.43582200 4.67796700 -1.17559100
H -2.39341600 4.38101800 -2.70287800
C -4.05187000 2.24711700 -2.71770400
C -3.45690800 0.40119300 -0.63076200
C -4.58103400 0.27348300 -1.44197100
C -4.85790000 1.15310100 -2.51127900
H -5.29266900 -0.51504100 -1.21874000
H -5.74182500 0.99393400 -3.11941800
N -1.32012200 1.53131200 -0.30183700
Cu 0.00009900 -0.00015700 0.00043300

Table S93. Cartesian coordinates and energies of ***i*-TEQ 6a**/Cu(II).
B3LYP-D3/6-311+G(2d,p)-SDD(Cu)/SMD(Et_2O)
Zero-point correction= 0.465576 (Hartree/Particle)
Thermal correction to Energy= 0.492973
Thermal correction to Enthalpy= 0.493917
Thermal correction to Gibbs Free Energy= 0.409779
Sum of electronic and zero-point Energies= -1800.072882
Sum of electronic and thermal Energies= -1800.045485
Sum of electronic and thermal Enthalpies= -1800.044541
Sum of electronic and thermal Free Energies= -1800.128679
C 0.63543200 2.67363600 -0.37066700
C 2.51415300 1.42432700 -0.95306600
C 2.87867100 2.41215800 -1.92037000
C 2.11172600 3.59396300 -1.98817200
C 1.03884500 3.76522000 -1.15387600
C 3.43699500 0.39599700 -0.63281500
C 4.02516800 2.22042500 -2.72371100
H 2.39479400 4.36865300 -2.69078800
H 0.45667200 4.67600500 -1.15411200
C 4.82008300 1.12496600 -2.51931600
C 4.54909100 0.25531600 -1.44623700
H 4.26896600 2.96090200 -3.47583100
H 5.69589700 0.95510400 -3.13259200
H 5.25759800 -0.53259400 -1.22351900
N 1.31455700 1.53071800 -0.30244900
C -1.03888100 -3.76530700 -1.15353500
C -2.11176600 -3.59413400 -1.98784200
C -2.87870100 -2.41231700 -1.92015500
C -2.51416300 -1.42438600 -0.95296000
C -0.63544900 -2.67364200 -0.37045000
H -4.26902400 -2.96121700 -3.47553400
H -0.45670600 -4.67609200 -1.15369200
H -2.39484200 -4.36889700 -2.69037400
C -4.02520900 -2.22066100 -2.72349800
C -3.43700800 -0.39603300 -0.63278700
C -4.54910600 -0.25541900 -1.44621900
C -4.82010900 -1.12517200 -2.51921300
H -5.25760800 0.53251700 -1.22358000
H -5.69592300 -0.95536300 -3.13250400
N -1.31455900 -1.53070100 -0.30235300
C 0.63538800 -2.67360000 0.37084700
C 2.51417600 -1.42433200 0.95308200
C 2.87869600 -2.41212100 1.92043300
C 2.11168300 -3.59387000 1.98838200
C 1.03874900 -3.76512800 1.15415700
C 3.43704000 -0.39605200 0.63273200
C 4.02526200 -2.22041100 2.72367900
H 2.39474200 -4.36851800 2.69104800
H 0.45652100 -4.67587800 1.15448800
C 4.82023800 -1.12502300 2.51915200
C 4.54921000 -0.25540300 1.44605600
H 4.26906200 -2.96085700 3.47583000
H 5.69611400 -0.95518700 3.13234700
H 5.25773900 0.53246300 1.22325400
N 1.31456400 -1.53071300 0.30251600
C -1.03877200 3.76523000 1.15384400
C -2.11169300 3.59403300 1.98809700
C -2.87869200 2.41227000 1.92025200
C -2.51416800 1.42440300 0.95298000
C -0.63540100 2.67363400 0.37063400
H -4.26905200 2.96112700 3.47561000
H -0.45654800 4.67598400 1.15409800
H -2.39475000 4.36873900 2.69070000
C -4.02525300 2.22062100 2.72351800
C -3.43704400 0.39611000 0.63270400
C -4.54920300 0.25551400 1.44605400
C -4.82022300 1.12521100 2.51908900
H -5.25773100 -0.53237400 1.22332700
H -5.69609000 0.95541800 3.13230900
N -1.31455600 1.53072700 0.30240600
Cu 0.00005300 -0.00001100 -0.00021200

Table S94. Cartesian coordinates and energies of ***i*-TEQ 6a**/Cu(II) (TS1).
B3LYP-D3/6-31G(d,p)-SDD(Cu)

Zero-point correction= 0.466552 (Hartree/Particle)
Thermal correction to Energy= 0.493385
Thermal correction to Enthalpy= 0.494329
Thermal correction to Gibbs Free Energy= 0.410689
Sum of electronic and zero-point Energies= -1799.424566
Sum of electronic and thermal Energies= -1799.397734
Sum of electronic and thermal Enthalpies= -1799.396790
Sum of electronic and thermal Free Energies= -1799.480429
C 0.51799100 2.71593900 0.04148900
C 2.55190600 1.71634400 0.68473200
C 2.91742900 2.98770500 1.28859900
C 2.02220300 4.07606000 1.26066600
C 0.85383900 3.97561400 0.55626800
C 3.58704600 0.71465700 0.53685500
C 4.21240100 3.24885700 1.79318100
H 2.30545400 5.00675900 1.74241300
H 0.17349000 4.81065200 0.44714200
C 5.21069900 2.35987000 1.51080500
C 4.88644800 1.18107400 0.82917600
H 4.40949400 4.19646400 2.28362300
H 6.24640700 2.57145500 1.75316700
H 5.73206000 0.60533100 0.48849400
N 1.26474500 1.60493400 0.18002500
C -1.07862800 -3.85754700 0.28578000
C -1.96877000 -3.89238600 1.33649500
C -2.66450900 -2.72085100 1.72023000
C -2.45383200 -1.53604900 0.94169100
C -0.74868700 -2.59610000 -0.25459300
H -3.73868100 -3.59357400 3.38606800
H -0.54445200 -4.74373700 -0.03379600
H -2.15155200 -4.81940000 1.87234800
C -3.60990100 -2.70415600 2.77720700
C -3.39687900 -0.47658000 1.02331600
C -4.30184700 -0.50126400 2.07925200
C -4.36776900 -1.57604600 2.99457700
H -5.02056300 0.30760000 2.16747800
H -5.08025100 -1.53930700 3.81160500
N -1.38666900 -1.47480500 0.07614500
C 0.50495500 -2.43025300 -1.00737900
C 2.63661600 -1.46427800 -0.77622800
C 3.14530400 -2.54180900 -1.60542300
C 2.24519400 -3.37300600 -2.30616300
C 0.91751600 -3.37239900 -1.95544400
C 3.59147600 -0.68986900 -0.00534100
C 4.50369300 -2.94041700 -1.56429200
H 2.63523700 -4.10230000 -3.00969500
H 0.21500600 -4.10102400 -2.34285100
C 5.26810600 -2.46547000 -0.53273900
C 4.77846800 -1.40390900 0.24687900
H 4.85606200 -3.71660100 -2.23539800
H 6.24686900 -2.87928200 -0.31554700
H 5.40049500 -1.09913900 1.07596200
N 1.27518400 -1.40665400 -0.57776200
C -1.25597600 3.56088700 -1.51209600
C -2.48510900 3.37176500 -2.09678400
C -3.30179800 2.29246300 -1.68863100
C -2.79116800 1.37051800 -0.70752800
C -0.79247500 2.58040100 -0.61411700
H -4.97332900 2.84957800 -2.94222100
H -0.62750400 4.40534800 -1.76741100
H -2.85526000 4.06571200 -2.84568700
C -4.62182800 2.15639200 -2.18445000
C -3.67908300 0.42187900 -0.13123700
C -4.97324200 0.34489200 -0.64318100
C -5.44256700 1.17831400 -1.67830600
H -5.65153300 -0.38972300 -0.22203900
H -6.45722400 1.06037200 -2.04301500
N -1.48602800 1.48902100 -0.28176900
Cu -0.04462700 0.04654700 -0.03126500

Table S95. Cartesian coordinates and energies of ***i*-TEQ 6a**/Cu(II) (EQ2).
B3LYP-D3/6-31G(d,p)-SDD(Cu)
Zero-point correction= 0.466559 (Hartree/Particle)
Thermal correction to Energy= 0.494280
Thermal correction to Enthalpy= 0.495224
Thermal correction to Gibbs Free Energy= 0.408207
Sum of electronic and zero-point Energies= -1799.425139
Sum of electronic and thermal Energies= -1799.397418
Sum of electronic and thermal Enthalpies= -1799.396474
Sum of electronic and thermal Free Energies= -1799.483491
C -0.49760500 2.71338900 0.42381000
C -2.61805000 1.72929600 0.60466800
C -3.10236400 2.99322000 1.13265000
C -2.19155900 4.01983600 1.45025400
C -0.88929800 3.90774500 1.04488700
C -3.60884200 0.73698400 0.27306600
C -4.48155500 3.30086300 1.22752100
H -2.55350600 4.92470200 1.92863200
H -0.17484100 4.71087600 1.17657600
C -5.38551700 2.45375900 0.64916400
C -4.92710000 1.22184000 0.15923000
H -4.78074300 4.25044900 1.65909700
H -6.43627500 2.70974600 0.56872200
H -5.65775600 0.59081000 -0.32887600
N -1.26562200 1.61036600 0.32958900
C 1.17813900 -3.87659800 0.18336500
C 2.11194700 -3.91821500 1.19263600
C 2.81253200 -2.74498400 1.55546600
C 2.54902700 -1.55122800 0.80538500
C 0.80680000 -2.61186800 -0.32732000
H 3.98319700 -3.64221400 3.13946100
H 0.64115300 -4.76585500 -0.12048000
H 2.32881500 -4.85070400 1.70568900
C 3.82008800 -2.74334800 2.55309200
C 3.49574700 -0.49638500 0.85093000
C 4.47312600 -0.53785300 1.83961800
C 4.59796500 -1.62316200 2.73474900
H 5.19630000 0.27027200 1.88874200
H 5.36397000 -1.60012000 3.50231000
N 1.43677800 -1.48245900 -0.00684800
C -0.48729300 -2.48470800 -1.01259100
C -2.62609400 -1.59518200 -0.65679900
C -3.16423700 -2.78527100 -1.28762500
C -2.30347900 -3.62852800 -2.02096300
C -0.94742700 -3.50634600 -1.85475100
C -3.56007300 -0.73739300 0.03058000
C -4.49337600 -3.21899800 -1.05886200
H -2.72373600 -4.44262000 -2.60380400
H -0.24829600 -4.21850600 -2.27714100

C -5.22228300 -2.59224500 -0.08337500
C -4.73743900 -1.38353300 0.44733700
H -4.85761300 -4.10434100 -1.56968200
H -6.17708500 -2.98273100 0.25136800
H -5.35096200 -0.88810600 1.18971600
N -1.25618600 -1.46012800 -0.58409300
C 1.26071600 3.78153300 -0.97311500
C 2.42104400 3.65774000 -1.69825500
C 3.22057200 2.50265200 -1.54907300
C 2.76688500 1.46503000 -0.66227200
C 0.81987600 2.67030500 -0.22415700
H 4.78708400 3.18053100 -2.87653100
H 0.64866300 4.67241800 -1.03470300
H 2.74939100 4.45380700 -2.36002400
C 4.48136700 2.39942400 -2.18751900
C 3.68361100 0.45490400 -0.27620400
C 4.92071500 0.40819500 -0.91460700
C 5.30999500 1.34287700 -1.89559200
H 5.61928400 -0.37203700 -0.63029400
H 6.27925000 1.24833100 -2.37310700
N 1.49545400 1.52460700 -0.12852200
Cu 0.05418500 0.04021100 -0.03305200

Table S96. Cartesian coordinates and energies of ***i*-TEQ 6a**/Cu(II) (TS2).
B3LYP-D3/6-31G(d,p)-SDD(Cu)
Zero-point correction= 0.466156 (Hartree/Particle)
Thermal correction to Energy= 0.492994
Thermal correction to Enthalpy= 0.493938
Thermal correction to Gibbs Free Energy= 0.410495
Sum of electronic and zero-point Energies= -1799.419728
Sum of electronic and thermal Energies= -1799.392889
Sum of electronic and thermal Enthalpies= -1799.391945
Sum of electronic and thermal Free Energies= -1799.475388
C 0.74066500 2.80694500 -0.41393800
C 2.73915900 1.70419700 0.19199000
C 3.47512700 2.91789800 -0.08830100
C 2.78903500 4.02867400 -0.61128000
C 1.43286600 3.98116600 -0.77299100
C 3.48444000 0.58549800 0.69035900
C 4.86609400 3.03128900 0.14337600
H 3.34390400 4.92682800 -0.86442900
H 0.91611000 4.84792400 -1.15288200
C 5.55713000 1.95866800 0.63746900
C 4.86334300 0.76075900 0.87283900
H 5.36011400 3.97039200 -0.08428300
H 6.62564400 2.00676500 0.81659300
H 5.45101500 -0.09642700 1.17576900
N 1.36977800 1.69346800 0.00558800
C -1.44538400 -3.20286100 -2.12412900
C -2.49300600 -3.68232700 -1.37489500
C -2.89920700 -2.99728000 -0.20573800
C -2.42180300 -1.65324400 -0.03678300
C -0.74057300 -2.08355100 -1.62241000
H -4.02956900 -4.62509800 0.66824000
H -1.06794800 -3.76551500 -2.96797300
H -2.95815400 -4.63121600 -1.62587400
C -3.69749600 -3.59995300 0.79733700
C -3.07068600 -0.82570800 0.93925100
C -3.70696100 -1.50296000 1.97835000
C -3.97818500 -2.88971000 1.94197600
H -4.10495900 -0.92197400 2.80446000
H -4.49655400 -3.35539600 2.77312400
N -1.30504700 -1.25711900 -0.72254400
C 0.74064000 -2.08337800 -1.62258700
C 2.42200000 -1.65303500 -0.03710900
C 2.89963600 -2.99694100 -0.20640700
C 2.49347800 -3.68179400 -1.37570300
C 1.44565200 -3.20239900 -2.12468800
C 3.07076000 -0.82560700 0.93910200
C 3.69806200 -3.59970800 0.79649700
H 2.95883700 -4.63050300 -1.62696900
H 1.06825100 -3.76490200 -2.96865000
C 3.97862600 -2.88969400 1.94131400
C 3.70714700 -1.50300600 1.97804100
H 4.03031300 -4.62476400 0.66715700
H 4.49707900 -3.35549800 2.77234400
H 4.10502200 -0.92215900 2.80430600
N 1.30509000 -1.25698800 -0.72267000
C -1.43315300 3.98120000 -0.77276800
C -2.78937500 4.02850300 -0.61143200
C -3.47546300 2.91757400 -0.08877600
C -2.73938400 1.70399100 0.19172200
C -0.74091500 2.80694200 -0.41390600
H -5.36062500 3.96976100 -0.08528100
H -0.91639000 4.84817500 -1.15215100
H -3.34428800 4.92662700 -0.86459300
C -4.86649900 3.03076700 0.14259900
C -3.48457000 0.58527400 0.69018500
C -4.86351400 0.76036500 0.87247900
C -5.55745200 1.95811700 0.63674500
H -5.45108400 -0.09684000 1.17556000
H -6.62600300 2.00608100 0.81568300
N -1.36998900 1.69338700 0.00545900
Cu -0.00003200 0.17691300 -0.14854200

Table S97. Cartesian coordinates and energies of ***i*-TEQ 6a**/Cu(II) (TS2).
B3LYP-D3/6-311+G(2d,p)-SDD(Cu)/SMD(Et_2O)
Zero-point correction= 0.462609 (Hartree/Particle)
Thermal correction to Energy= 0.489556
Thermal correction to Enthalpy= 0.490501
Thermal correction to Gibbs Free Energy= 0.407653
Sum of electronic and zero-point Energies= -1800.018915
Sum of electronic and thermal Energies= -1799.991969
Sum of electronic and thermal Enthalpies= -1799.991024
Sum of electronic and thermal Free Energies= -1800.073872
C 0.72941300 2.79588500 -0.41104800
C 2.72222100 1.71233400 0.21352700
C 3.44855700 2.92447100 -0.06242500
C 2.76360300 4.02335600 -0.59997700
C 1.41724200 3.96540500 -0.78081100
C 3.47081100 0.59636000 0.71026300
C 4.83061800 3.04907000 0.18482000
H 3.31726700 4.92001000 -0.85115000
H 0.90345900 4.82050600 -1.18381500
C 5.51981900 1.98793900 0.68960500
C 4.83873400 0.78612400 0.91369500
H 5.31615500 3.98978200 -0.04296900
H 6.58338900 2.04405100 0.88341300

H 5.43237200 -0.06211300 1.22078100
N 1.35959100 1.69750800 0.02225400
C -1.42308800 -3.22187800 -2.07149200
C -2.46131400 -3.70182500 -1.32198500
C -2.88011200 -3.00470500 -0.17032200
C -2.41375500 -1.66249800 -0.01544800
C -0.73797300 -2.08686600 -1.59093500
H -3.98915300 -4.62852600 0.72205100
H -1.03319800 -3.79378500 -2.89997900
H -2.91012200 -4.65965200 -1.55663600
C -3.67005800 -3.60005400 0.83792500
C -3.07091600 -0.83013900 0.94613600
C -3.70394900 -1.49450400 1.98578900
C -3.95963000 -2.87968800 1.96652500
H -4.11728500 -0.90901200 2.79748800
H -4.47578200 -3.33805900 2.80032300
N -1.30566400 -1.26570400 -0.70021900
C 0.74012400 -2.05596900 -1.62452200
C 2.43492000 -1.63351000 -0.06911900
C 2.93053000 -2.95765300 -0.27834800
C 2.52031400 -3.61749300 -1.45538200
C 1.45564800 -3.14168200 -2.16969000
C 3.07632100 -0.82481800 0.92396000
C 3.73346200 -3.57607400 0.70494600
H 2.99739100 -4.54910200 -1.73550200
H 1.07201400 -3.68747700 -3.01887600
C 4.00112100 -2.89712200 1.86460300
C 3.71533300 -1.51973700 1.94036400
H 4.07476300 -4.59192600 0.54901200
H 4.52125200 -3.37878700 2.68263900
H 4.10796400 -0.96172700 2.78133100
N 1.30639400 -1.24403800 -0.72329600
C -1.44385100 3.95431700 -0.80026800
C -2.79588400 3.99444400 -0.66050300
C -3.48121200 2.88812100 -0.13887600
C -2.74571600 1.68981400 0.16941000
C -0.75233600 2.78948000 -0.42313600
H -5.36330100 3.92683700 -0.17715000
H -0.92768000 4.82481600 -1.16515700
H -3.35313200 4.88540500 -0.92398900
C -4.87006400 2.99658400 0.07565100
C -3.48706300 0.57578900 0.67881200
C -4.86087300 0.74900900 0.85310700
C -5.55477500 1.93492500 0.58573800
H -5.44681900 -0.09977100 1.17405800
H -6.62271400 1.97982700 0.75688100
N -1.38010200 1.68678800 0.00205400
Cu -0.00571400 0.16908800 -0.09040800

Table S98. Cartesian coordinates and energies of ***i*-TEQ 6a**/Co(II).
B3LYP-D3/6-31G(d,p)-SDD(Co)
Zero-point correction= 0.467894 (Hartree/Particle)
Thermal correction to Energy= 0.495144
Thermal correction to Enthalpy= 0.496088
Thermal correction to Gibbs Free Energy= 0.412446
Sum of electronic and zero-point Energies= -1747.995743
Sum of electronic and thermal Energies= -1747.968493
Sum of electronic and thermal Enthalpies= -1747.967549
Sum of electronic and thermal Free Energies= -1748.051192

C -0.62863700 -2.66118700 0.37605800
C -2.50582300 -1.40166000 0.96678800
C -2.87193900 -2.39842500 1.93576600
C -2.10239400 -3.58256700 2.00675400
C -1.03153500 -3.75633500 1.15942500
C -3.44522100 -0.38904800 0.63591700
C -4.03000200 -2.21783100 2.73393700
H -2.38281900 -4.35894000 2.71248000
H -0.44696900 -4.66851000 1.15660500
C -4.84249500 -1.12976200 2.52146700
C -4.57231400 -0.26019300 1.44289200
H -4.27216500 -2.96210900 3.48608600
H -5.72687500 -0.97129600 3.12907300
H -5.29010600 0.51927700 1.20795000
N -1.29082600 -1.49508800 0.32189800
C 1.03159100 3.75649900 1.15917300
C 2.10255000 3.58279800 2.00639900
C 2.87203300 2.39862800 1.93550900
C 2.50579700 1.40174900 0.96667000
C 0.62860000 2.66130700 0.37595700
H 4.27231200 2.96239900 3.48574500
H 0.44708200 4.66870800 1.15634900
H 2.38303300 4.35925700 2.71200700
C 4.03008600 2.21804400 2.73369200
C 3.44514100 0.38903300 0.63589600
C 4.57222200 0.26021300 1.44287700
C 4.84246300 1.12986600 2.52138500
H 5.29003700 -0.51926500 1.20802500
H 5.72682800 0.97141600 3.12901400
N 1.29078700 1.49516900 0.32186100
C -0.62875000 2.66123600 -0.37602800
C -2.50584700 1.40157100 -0.96679100
C -2.87207300 2.39837100 -1.93569900
C -2.10265500 3.58259200 -2.00659700
C -1.03180000 3.75639600 -1.15928000
C -3.44520700 0.38889500 -0.63593900
C -4.03010900 2.21771200 -2.73388600
H -2.38316300 4.35900500 -2.71224700
H -0.44736000 4.66865100 -1.15643900
C -4.84250500 1.12956100 -2.52148700
C -4.57228500 0.25998700 -1.44293200
H -4.27233500 2.96200000 -3.48600500
H -5.72685700 0.97106800 -3.12912900
H -5.29003900 -0.51952200 -1.20800900
N -1.29082600 1.49505400 -0.32193400
C 1.03154800 -3.75635800 -1.15935900
C 2.10252800 -3.58268100 -2.00656600
C 2.87209600 -2.39856700 -1.93557300
C 2.50588700 -1.40170000 -0.96672200
C 0.62864200 -2.66119000 -0.37604800
H 4.27248000 -2.96237400 -3.48571900
H 0.44694100 -4.66850500 -1.15662800
H 2.38302000 -4.35911600 -2.71219900
C 4.03022400 -2.21803100 -2.73366400
C 3.44524400 -0.38901600 -0.63591800
C 4.57240000 -0.26022900 -1.44278400
C 4.84267800 -1.12990300 -2.52125300
H 5.29021300 0.51922400 -1.20781100
H 5.72709200 -0.97151000 -3.12882500
N 1.29086100 -1.49509800 -0.32188700

Co -0.00004300 0.00004500 -0.00000400

Table S99. Cartesian coordinates and energies of ***i*-TEQ 6a**/Co(II).
B3LYP-D3/6-311+G(2d,p)-SDD(Co)/SMD(Et_2O)
Zero-point correction= 0.466292 (Hartree/Particle)
Thermal correction to Energy= 0.493323
Thermal correction to Enthalpy= 0.494267
Thermal correction to Gibbs Free Energy= 0.411267
Sum of electronic and zero-point Energies= -1748.591409
Sum of electronic and thermal Energies= -1748.564378
Sum of electronic and thermal Enthalpies= -1748.563434
Sum of electronic and thermal Free Energies= -1748.646434
C -0.63217900 -2.66920100 0.36832300
C -2.49554300 -1.40920700 0.95806000
C -2.86516600 -2.39943100 1.92152500
C -2.10980700 -3.58828900 1.98424700
C -1.04499400 -3.76334800 1.14209000
C -3.42341400 -0.38900000 0.63501800
C -4.01124100 -2.20606900 2.72531400
H -2.39734000 -4.36334000 2.68448900
H -0.46927400 -4.67800000 1.13221400
C -4.80693200 -1.11103100 2.52199700
C -4.53711100 -0.24566200 1.44605500
H -4.25531900 -2.94785200 3.47602700
H -5.68235200 -0.94099300 3.13573100
H -5.24665900 0.53960600 1.21743200
N -1.28872800 -1.50966800 0.31159300
C 1.04499000 3.76341900 1.14186600
C 2.10981100 3.58841800 1.98402500
C 2.86517000 2.39955600 1.92137600
C 2.49553700 1.40926500 0.95798400
C 0.63216900 2.66922100 0.36817600
H 4.25534100 2.94809000 3.47582000
H 0.46926600 4.67806800 1.13194300
H 2.39734700 4.36351700 2.68421200
C 4.01125300 2.20625200 2.72516600
C 3.42340700 0.38903700 0.63500200
C 4.53711100 0.24575600 1.44603800
C 4.80694300 1.11119900 2.52191900
H 5.24666000 -0.53952500 1.21746300
H 5.68236900 0.94120600 3.13565400
N 1.28871700 1.50968200 0.31151900
C -0.63217700 2.66919900 -0.36833100
C -2.49554300 1.40920700 -0.95806400
C -2.86516700 2.39943000 -1.92152900
C -2.10980600 3.58828600 -1.98425500
C -1.04499100 3.76334500 -1.14210000
C -3.42341500 0.38900100 -0.63501900
C -4.01124300 2.20606800 -2.72531600
H -2.39733900 4.36333600 -2.68449800
H -0.46927000 4.67799600 -1.13222700
C -4.80693600 1.11103100 -2.52199600
C -4.53711400 0.24566300 -1.44605300
H -4.25532200 2.94785100 -3.47602900
H -5.68235700 0.94099400 -3.13572800
H -5.24666200 -0.53960400 -1.21742900
N -1.28872800 1.50966600 -0.31159800
C 1.04498900 -3.76341700 -1.14187700
C 2.10981200 -3.58841200 -1.98403200
C 2.86517300 -2.39955300 -1.92137500
C 2.49553900 -1.40926500 -0.95797900
C 0.63216800 -2.66922100 -0.36818300
H 4.25534900 -2.94808300 -3.47581700
H 0.46926500 -4.67806500 -1.13195800
H 2.39735000 -4.36350900 -2.68422200
C 4.01126000 -2.20624700 -2.72515900
C 3.42340900 -0.38904100 -0.63498900
C 4.53711800 -0.24576000 -1.44602000
C 4.80695200 -1.11119800 -2.52190300
H 5.24666800 0.53951900 -1.21743900
H 5.68238200 -0.94120400 -3.13563400
N 1.28871600 -1.50968300 -0.31151900
Co -0.00000500 0.00000000 0.00000200

Table S100. Cartesian coordinates and energies of ***i*-TEQ 6a**/Co(II) (TS).
B3LYP-D3/6-31G(d,p)-SDD(Co)
Zero-point correction= 0.467170 (Hartree/Particle)
Thermal correction to Energy= 0.493474
Thermal correction to Enthalpy= 0.494418
Thermal correction to Gibbs Free Energy= 0.413005
Sum of electronic and zero-point Energies= -1747.944872
Sum of electronic and thermal Energies= -1747.918567
Sum of electronic and thermal Enthalpies= -1747.917623
Sum of electronic and thermal Free Energies= -1747.999036
C 0.73744900 2.00927700 -1.66608800
C 2.39061300 1.62097400 -0.03772700
C 2.88992500 2.94864200 -0.26321800
C 2.50835100 3.59103500 -1.46527500
C 1.45869300 3.09965600 -2.20334200
C 3.00240100 0.83488800 0.99691000
C 3.67186200 3.58967300 0.72852600
H 2.99061300 4.52220600 -1.74803700
H 1.09108000 3.63488900 -3.06943700
C 3.90003900 2.93894600 1.91981200
C 3.60240800 1.56206100 2.02496500
H 4.02388900 4.60171300 0.55663700
H 4.39492400 3.44291200 2.74292200
H 3.95016400 1.02734500 2.90303900
N 1.27688100 1.20862900 -0.72073700
C -1.44764500 -3.86424800 -1.02244500
C -2.78445100 -3.94131900 -0.74560200
C -3.42427000 -2.88690700 -0.06635100
C -2.68587800 -1.67471900 0.21397100
C -0.73708000 -2.72196300 -0.60793500
H -5.27635900 -3.98570900 0.09012800
H -0.95076700 -4.68774800 -1.51255600
H -3.35570500 -4.82374800 -1.01685300
C -4.77513700 -3.05088300 0.31948800
C -3.39920500 -0.59026600 0.82576800
C -4.73916900 -0.81980400 1.16627000
C -5.42106200 -2.03037700 0.96386500
H -5.31717700 0.00555700 1.56105300
H -6.45720800 -2.12177200 1.27074600
N -1.33580100 -1.63585800 -0.07577100
C 0.73692000 -2.72193700 -0.60805500
C 2.68568800 -1.67484100 0.21411000
C 3.42401500 -2.88707700 -0.06617100
C 2.78427700 -3.94128300 -0.74582200

C 1.44751200 -3.86409800 -1.02284800
C 3.39902500 -0.59045500 0.82604900
C 4.77474900 -3.05126400 0.32003800
H 3.35553600 -4.82367700 -1.01717800
H 0.95068000 -4.68744000 -1.51327300
C 5.42061500 -2.03089700 0.96469400
C 4.73885600 -0.82021700 1.16691500
H 5.27591100 -3.98614200 0.09075600
H 6.45664900 -2.12246600 1.27190100
H 5.31690200 0.00505000 1.56184200
N 1.33564200 -1.63590200 -0.07572400
C -1.45841300 3.10014100 -2.20289000
C -2.50785300 3.59163200 -1.46458500
C -2.88948800 2.94904500 -0.26265100
C -2.39046700 1.62121200 -0.03751000
C -0.73739400 2.00944700 -1.66597100
H -4.02312400 4.60212800 0.55763300
H -1.09074000 3.63551000 -3.06887400
H -2.98987400 4.52301400 -1.74705700
C -3.67129500 3.58997500 0.72926100
C -3.00237900 0.83498700 0.99692500
C -3.60229700 1.56199300 2.02515300
C -3.89966300 2.93896200 1.92035500
H -3.95016200 1.02710700 2.90308100
H -4.39449100 3.44279900 2.74357800
N -1.27687700 1.20875900 -0.72069800
Co -0.00004400 -0.17151400 -0.20078000

Table S101. Cartesian coordinates and energies of ***i*-TEQ 6a**/Co(II) (TS).
B3LYP-D3/6-311+G(2d,p)-SDD(Co)/SMD(Et_2O)
Zero-point correction= 0.464572 (Hartree/Particle)
Thermal correction to Energy= 0.490938
Thermal correction to Enthalpy= 0.491882
Thermal correction to Gibbs Free Energy= 0.410259
Sum of electronic and zero-point Energies= -1748.543398
Sum of electronic and thermal Energies= -1748.517031
Sum of electronic and thermal Enthalpies= -1748.516087
Sum of electronic and thermal Free Energies= -1748.597710
C -0.73327100 -2.03325100 -1.61496900
C -2.37263700 -1.64661800 0.01032700
C -2.85026100 -2.97998700 -0.18384100
C -2.45952800 -3.64350100 -1.36538800
C -1.43069400 -3.14857800 -2.11765900
C -3.00098100 -0.84530200 1.01701100
C -3.61775100 -3.60679600 0.82197300
H -2.92010800 -4.59055800 -1.61973000
H -1.05444000 -3.69558700 -2.96947700
C -3.86401500 -2.92916400 1.98733300
C -3.59597700 -1.54855500 2.05540600
H -3.94690500 -4.62829800 0.67729600
H -4.35393500 -3.41765900 2.81986300
H -3.96585300 -0.99928000 2.91202900
N -1.27225200 -1.23430800 -0.67884200
C 1.42620500 3.84336600 -1.04442900
C 2.74691000 3.93961900 -0.73185700
C 3.37771300 2.90715200 -0.02048400
C 2.65363400 1.69122200 0.24584100
C 0.71637300 2.71015100 -0.61629400
H 5.19484400 4.03784300 0.18620900
H 0.93982500 4.64529200 -1.57417900
H 3.31734000 4.82117600 -0.99796000
C 4.70663000 3.09720900 0.40885800
C 3.37133100 0.61250500 0.86097600
C 4.68513500 0.87316600 1.25305100
C 5.34249400 2.09649200 1.08128700
H 5.27008800 0.06281000 1.66121900
H 6.36133000 2.20781600 1.42968100
N 1.31459100 1.64325000 -0.06204000
C -0.75709200 2.70342300 -0.62466900
C -2.70021500 1.65103200 0.18254500
C -3.44359300 2.84519400 -0.12526900
C -2.80459200 3.90063200 -0.79396000
C -1.46943300 3.83737800 -1.04689500
C -3.40825300 0.57021600 0.80329800
C -4.79805100 2.99880500 0.23328700
H -3.38136400 4.77405100 -1.07281700
H -0.97538600 4.66823900 -1.52159500
C -5.43994700 1.98430600 0.87806400
C -4.74999600 0.79038300 1.11694900
H -5.29965700 3.92514100 -0.01781600
H -6.48054600 2.06622100 1.16490100
H -5.32393900 -0.02908300 1.52217800
N -1.35199400 1.62524900 -0.08976300
C 1.46996700 -3.03950700 -2.25042800
C 2.55808100 -3.50750800 -1.56811200
C 2.95223000 -2.88736600 -0.36408100
C 2.41632700 -1.59112000 -0.08362600
C 0.73559900 -1.99212900 -1.66234800
H 4.13849000 -4.53167900 0.37699100
H 1.08674600 -3.56458100 -3.11322700
H 3.06296000 -4.41034700 -1.89034400
C 3.76111400 -3.53952100 0.59117400
C 3.01764200 -0.82807600 0.97129200
C 3.63421400 -1.57672500 1.96486900
C 3.97211300 -2.93312100 1.80195200
H 3.96715200 -1.07412800 2.86375100
H 4.48225700 -3.45345900 2.60237200
N 1.28029700 -1.19743500 -0.72420600
Co -0.00733100 0.17319300 -0.18453600

Table S102. Cartesian coordinates and energies of ***i*-TEQ 6b**.
B3LYP-D3/6-31G(d,p)/IEFPCM($CHCl_3$)
Zero-point correction= 0.689212 (Hartree/Particle)
Thermal correction to Energy= 0.730411
Thermal correction to Enthalpy= 0.731356
Thermal correction to Gibbs Free Energy= 0.615983
Sum of electronic and zero-point Energies= -2293.572453
Sum of electronic and thermal Energies= -2293.531254
Sum of electronic and thermal Enthalpies= -2293.530310
Sum of electronic and thermal Free Energies= -2293.645682
C -2.43811100 -0.58046300 1.88803000
C -3.00317500 -2.67744400 1.10066400
C -4.32843900 -2.57559000 1.62260600
C -4.67544200 -1.36186100 2.27888200
C -3.75833400 -0.34349100 2.36335400
C -2.65361300 -3.78640000 0.25619200
C -5.23683400 -3.64765900 1.42695900
H -5.68031800 -1.24221500 2.67515500
H -4.00733100 0.62066900 2.79075500

C -4.85441800 -4.74965200 0.69367400
C -3.57526100 -4.80420000 0.08884700
H -6.23715400 -3.57720100 1.84555500
H -5.55009500 -5.56866200 0.53824200
H -3.32450100 -5.64387900 -0.55281100
N -2.06747800 -1.71879900 1.33405500
C -3.75833300 0.34350500 -2.36335100
C -4.67543500 1.36188000 -2.27888000
C -4.32842400 2.57560800 -1.62260500
C -3.00316000 2.67745500 -1.10066300
C -2.43810800 0.58047000 -1.88802800
H -6.23713400 3.57722900 -1.84555500
H -4.00733500 -0.62065400 -2.79075000
H -5.68031100 1.24224000 -2.67515300
C -5.23681300 3.64768200 -1.42695900
C -2.65359200 3.78640900 -0.25619100
C -3.57523400 4.80421400 -0.08884700
C -4.85439100 4.74967300 -0.69367500
H -3.32447000 5.64389200 0.55281100
H -5.55006400 5.56868700 -0.53824300
N -2.06746700 1.71880500 -1.33405400
C -1.40689800 -0.49827600 -1.85415500
C -0.90527000 -2.63314900 -1.15454300
C 0.47113400 -2.49712300 -1.51775600
C 0.90770300 -1.20523900 -1.97431000
C -0.04169100 -0.20999000 -2.10119600
C -1.33211900 -3.79314800 -0.42090200
C 1.32129300 -3.62847900 -1.38723200
H 0.24673500 0.80138900 -2.36143800
C 0.85252400 -4.79183800 -0.81665900
C -0.45694700 -4.85483400 -0.28672800
H 2.34535400 -3.56808700 -1.73715000
H 1.50796600 -5.65253500 -0.72461300
H -0.76939800 -5.73321000 0.27059700
N -1.82989600 -1.67207600 -1.42359200
C -0.04168700 0.20998400 2.10119500
C 0.90771000 1.20522900 1.97431000
C 0.47114700 2.49711500 1.51775800
C -0.90525700 2.63314800 1.15454700
C -1.40689300 0.49827700 1.85415800
H 2.34537500 3.56806500 1.73714400
H 0.24673500 -0.80139600 2.36143700
C 1.32131400 3.62846500 1.38723000
C -1.33209900 3.79314900 0.42090500
C -0.45692000 4.85483000 0.28672900
C 0.85255100 4.79182600 0.81665800
H -0.76936700 5.73320700 -0.27059700
H 1.50799900 5.65251900 0.72461000
N -1.82988700 1.67207900 1.42359700
C 2.33323500 -0.89365500 -2.24099300
C 2.71144700 -0.23291100 -3.41713300
C 3.33574200 -1.17887000 -1.29426800
C 4.03828000 0.12368300 -3.66344600
H 1.95527200 -0.00137300 -4.16134200
C 4.65848000 -0.83042200 -1.52447400
H 3.06680500 -1.64807600 -0.35402700
C 5.02174800 -0.17677700 -2.71174800
H 4.28929800 0.62680200 -4.58900100
H 5.42589200 -1.03443900 -0.78596400
C 2.33324200 0.89364300 2.24099300
C 2.71145200 0.23288300 3.41712400
C 3.33575100 1.17887700 1.29427600
C 4.03828600 -0.12371000 3.66343600
H 1.95527600 0.00133100 4.16132700
C 4.65848900 0.83043100 1.52448200
H 3.06681600 1.64810000 0.35404300
C 5.02175600 0.17676900 2.71174600
H 4.28930300 -0.62684200 4.58898400
H 5.42590400 1.03446400 0.78597800
O 6.34484200 0.12634100 -2.83731300
O 6.34485000 -0.12634600 2.83731200
C 6.77233500 -0.80891600 4.01314200
C 6.77232800 0.80889600 -4.01315200
H 6.57865100 0.21612700 -4.91554900
H 6.28301300 1.78567800 -4.11144000
H 7.84733300 0.95405200 -3.90184700
H 7.84734200 -0.95406200 3.90184100
H 6.57864900 -0.21616100 4.91554700
H 6.28302600 -1.78570300 4.11141300

Table S103. Cartesian coordinates and energies of **TEQ 7b**.
B3LYP-D3/6-31G(d,p)/IEFPCM($CHCl_3$)
Zero-point correction= 0.689079 (Hartree/Particle)
Thermal correction to Energy= 0.730683
Thermal correction to Enthalpy= 0.731628
Thermal correction to Gibbs Free Energy= 0.613438
Sum of electronic and zero-point Energies= -2293.563148
Sum of electronic and thermal Energies= -2293.521543
Sum of electronic and thermal Enthalpies= -2293.520599
Sum of electronic and thermal Free Energies= -2293.638789
C -2.27797000 1.35085700 3.99242700
C -1.20216500 -0.55877700 2.93719700
C -2.09646300 -0.44500000 1.82548400
C -3.04816700 0.62919900 1.80270300
C -3.12153100 1.50856100 2.91645700
N -2.03352600 -1.40407600 0.85942100
C -2.88747200 -1.32782000 -0.14542100
C -3.83272600 -0.28074700 -0.28384000
C -3.91948300 0.71819500 0.66681400
C 2.88762200 -1.32788500 0.14553700
C -2.86132900 -2.41657300 -1.16811000
C 3.83275600 -0.28070200 0.28389800
C 3.91951800 0.71810000 -0.66690300
C 3.04828500 0.62889900 -1.80283800
C 2.09666000 -0.44536600 -1.82552400
N 2.03375900 -1.40433900 -0.85936000
C 3.12163200 1.50812400 -2.91669900
C 2.27813400 1.35020800 -3.99268700
C 1.31373300 0.31797600 -3.99817100
C 1.20238200 -0.55933300 -2.93723600
C -1.79091000 -2.50531900 -2.11190500
C -1.80580300 -3.56449600 -3.07633800
C -2.87162200 -4.50101200 -3.08065800
C -3.89885200 -4.38356400 -2.17301300
C -3.89297500 -3.33394400 -1.22313900
N -0.81253400 -1.55829700 -2.08055400
C 0.16475700 -1.63113500 -2.96753100
C 0.24102300 -2.64868600 -3.96056600
C -0.73957900 -3.60798500 -4.00982300
H -2.35089700 2.02080800 4.84357000

H -3.86812000 2.29392500 2.92405100
H -4.46654800 -0.25285700 -1.16360400
H 4.46650800 -0.25261800 1.16370700
H 3.86816500 2.29354100 -2.92436200
H 2.35104500 2.02004800 -4.84392000
H 0.64248500 0.21454900 -4.84594000
H -2.86562700 -5.30203000 -3.81501400
H -4.71891100 -5.09493700 -2.17758800
H -4.71021000 -3.25421100 -0.51196200
H 1.07201500 -2.65259200 -4.65756300
H -0.71324100 -4.39892000 -4.75472700
C -1.31351700 0.31867800 3.99801000
H -0.64223300 0.21538500 4.84576700
C 3.89878400 -4.38350400 2.17345100
C 2.86145600 -2.41652300 1.16835100
C 1.79105200 -2.50504000 2.11217800
C 1.80585100 -3.56409500 3.07674200
C 2.87157600 -4.50071900 3.08115100
N 0.81275700 -1.55793000 2.08069300
C -0.16456000 -1.63059600 2.96765300
C -0.24091700 -2.64801700 3.96081700
C 0.73961600 -3.60737800 4.01022500
H 4.71876300 -5.09496800 2.17808900
H 2.86552000 -5.30164100 3.81561100
H -1.07192400 -2.65177200 4.65779700
H 0.71321100 -4.39820900 4.75523700
C 3.89299300 -3.33400700 1.22343600
H 4.71020700 -3.25446600 0.51221500
C -4.89213100 1.82350900 0.48279600
C -6.22822200 1.54800500 0.16483300
C -4.49803400 3.17331400 0.55975600
C -7.15417400 2.56825900 -0.05881700
H -6.55716000 0.51476600 0.10526900
C -5.40506900 4.19845800 0.33385300
H -3.46307500 3.41608500 0.77845000
C -6.74288800 3.90462800 0.02550600
H -8.18031000 2.31162300 -0.29096300
H -5.09991800 5.23847500 0.38175800
C 4.89206200 1.82352700 -0.48295900
C 6.22816500 1.54818000 -0.16491600
C 4.49783000 3.17328400 -0.56007900
C 7.15400700 2.56855100 0.05866300
H 6.55719100 0.51497700 -0.10523900
C 5.40475700 4.19854200 -0.33424400
H 3.46285600 3.41592000 -0.77884900
C 6.74258600 3.90486600 -0.02580000
H 8.18017400 2.31206100 0.29083700
H 5.09951300 5.23852500 -0.38227400
O 7.55295400 4.98196400 0.17320200
C 8.91955200 4.74726200 0.50354100
H 9.37259100 5.73188200 0.62301900
H 9.01591600 4.18768000 1.44200100
H 9.43901800 4.20419700 -0.29546300
O -7.55335700 4.98162900 -0.17359900
C -8.91994200 4.74676900 -0.50387200
H -9.37307800 5.73133500 -0.62344000
H -9.01628900 4.18706900 -1.44226200
H -9.43933400 4.20374700 0.29521500

Table S104. Cartesian coordinates and energies of ***i*-TEQ 6b**/Pd(II).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM($CHCl_3$)
Zero-point correction= 0.695065 (Hartree/Particle)
Thermal correction to Energy= 0.737122
Thermal correction to Enthalpy= 0.738066
Thermal correction to Gibbs Free Energy= 0.621061
Sum of electronic and zero-point Energies= -2421.175886
Sum of electronic and thermal Energies= -2421.133830
Sum of electronic and thermal Enthalpies= -2421.132886
Sum of electronic and thermal Free Energies= -2421.249891
C 2.17341000 1.51147700 1.80418800
C 0.19126900 2.11072200 2.91136200
C 0.92692800 3.04372400 3.71754000
C 2.33571600 3.07750600 3.59522200
C 2.96926300 2.25509000 2.69402400
C -1.17389400 1.85094400 3.22191300
C 0.24114200 3.87393700 4.63956200
H 2.90720300 3.75100500 4.22603600
H 4.04725800 2.24201800 2.59254700
C -1.11681200 3.74055600 4.79826100
C -1.79843600 2.70115300 4.12864900
H 0.80811900 4.59745400 5.21619900
H -1.66013600 4.38056200 5.48469400
H -2.84271100 2.52475100 4.36429800
N 0.83488400 1.46307300 1.88421300
C -2.96930100 2.25330900 -2.69549500
C -2.33575000 3.07507200 -3.59728800
C -0.92697100 3.04111200 -3.71966900
C -0.19131600 2.10866600 -2.91284800
C -2.17344700 1.51023700 -1.80521400
H -0.80816700 4.59367700 -5.21952800
H -4.04728900 2.24035600 -2.59393200
H -2.90722000 3.74819700 -4.22852000
C -0.24119400 3.87058900 -4.64235200
C 1.17382400 1.84859500 -3.22325300
C 1.79837000 2.69812400 -4.13063100
C 1.11675000 3.73703700 -4.80100600
H 2.84263700 2.52153700 -4.36617300
H 1.66006300 4.37651300 -5.48794200
N -0.83492600 1.46178400 -1.88521100
C -2.74461600 0.81809100 -0.64383100
C -2.46190800 0.26592100 1.61076100
C -3.53104500 -0.69303800 1.51907800
C -4.24371700 -0.82630600 0.27859600
C -3.89778400 0.03771900 -0.75298000
C -1.92605900 0.60213700 2.88498400
C -3.91530500 -1.40477900 2.68322800
H -4.41884000 -0.00232400 -1.70148200
C -3.27785400 -1.18282100 3.88135100
C -2.31448300 -0.16287600 3.98059600
H -4.74306200 -2.09968500 2.62831900
H -3.56651700 -1.73662100 4.76801500
H -1.90068200 0.07764000 4.95423000
N -2.00553000 0.89503100 0.47517900
C 3.89780300 0.03834900 0.75294800
C 4.24381500 -0.82637400 -0.27801700
C 3.53107000 -0.69405700 -1.51856900
C 2.46189700 0.26479900 -1.61093200
C 2.74458800 0.81857100 0.64326600

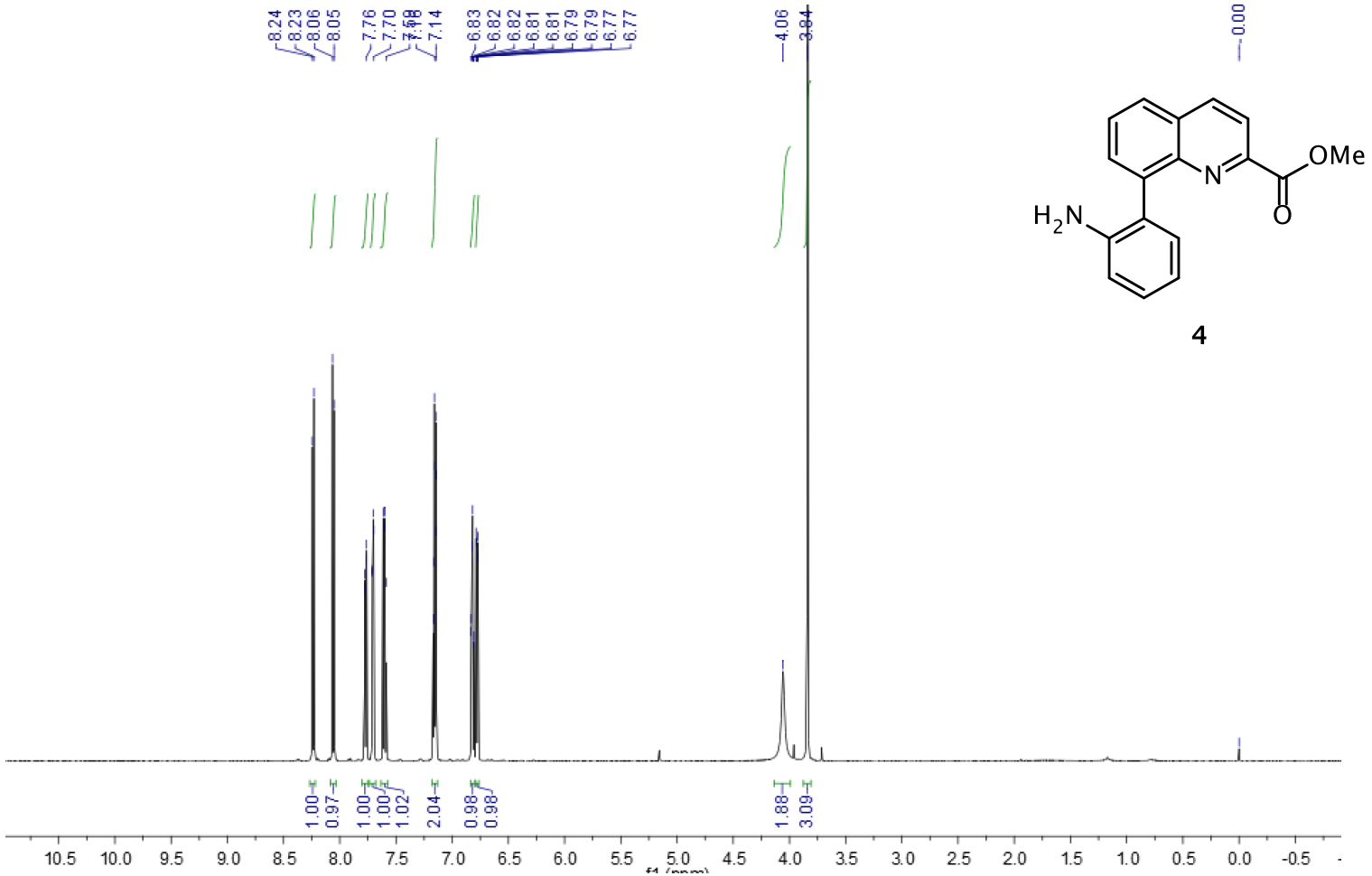
H 4.74306400 -2.10152300 -2.62680900
H 4.41883500 -0.00101600 1.70149100
C 3.91528100 -1.40668300 -2.68219100
C 1.92597500 0.60002500 -2.88539000
C 2.31437000 -0.16582500 -3.98043700
C 3.27776000 -1.18567500 -3.88045400
H 1.90051600 0.07392500 -4.95423900
H 3.56637800 -1.74016900 -4.76670000
N 2.00549400 0.89471100 -0.47579200
Pd -0.00000300 1.16862600 -0.00041400
C 5.31084500 -1.81646200 -0.05604700
C 6.51252600 -1.42861900 0.55967300
C 5.13950200 -3.17817900 -0.38632800
C 7.52756700 -2.34644000 0.81414400
H 6.67258300 -0.38463400 0.81263600
C 6.13312200 -4.10393300 -0.11851900
H 4.20459000 -3.51491800 -0.82239300
C 7.34193200 -3.69698500 0.47617100
H 8.45014300 -2.00546800 1.26665500
H 5.99918200 -5.15428700 -0.35300100
C -5.31075000 -1.81654600 0.05734500
C -6.51246500 -1.42907000 -0.55852800
C -5.13936800 -3.17805300 0.38845700
C -7.52753800 -2.34704800 -0.81233900
H -6.67252600 -0.38524200 -0.81212800
C -6.13301400 -4.10396700 0.12129900
H -4.20442000 -3.51452200 0.82466500
C -7.34187600 -3.69738000 -0.47353100
H -8.45016300 -2.00634300 -1.26495600
H -5.99905300 -5.15417500 0.35642200
O -8.25120300 -4.67563900 -0.67846700
O 8.25124800 -4.67509900 0.68177900
C -9.50552100 -4.33643100 -1.27563000
H -10.06596500 -5.26894500 -1.33814200
H -10.05777200 -3.61912600 -0.65785100
H -9.36815900 -3.92497600 -2.28206100
C 9.50569100 -4.33542600 1.27843000
H 10.06603800 -5.26793900 1.34179000
H 10.05792400 -3.61881800 0.65982500
H 9.36853300 -3.92292700 2.28445800

Table S105. Cartesian coordinates and energies of **TEQ 7b**/Pd(II).
B3LYP-D3/6-31G(d,p)-SDD(Pd)/IEFPCM($CHCl_3$)
Zero-point correction= 0.696075 (Hartree/Particle)
Thermal correction to Energy= 0.737942
Thermal correction to Enthalpy= 0.738886
Thermal correction to Gibbs Free Energy= 0.622040
Sum of electronic and zero-point Energies= -2421.213079
Sum of electronic and thermal Energies= -2421.171212
Sum of electronic and thermal Enthalpies= -2421.170268
Sum of electronic and thermal Free Energies= -2421.287114
C -1.65215600 -3.79146800 -0.86593400
C -1.38823600 -2.72199600 -0.01811300
C -2.26538900 -1.60051800 -0.01827800
C -3.47398300 -1.65917800 -0.78107600
C -3.70272800 -2.78028600 -1.61779000
C -2.78683000 -3.80690900 -1.69317800
H -0.98118200 -4.64431600 -0.86916000
C -4.45009900 -0.62162900 -0.59287600
H -4.63034900 -2.84212900 -2.17222200
H -2.96850400 -4.65690000 -2.34129500
C -4.19605300 0.31358200 0.39810800
C -2.94504900 0.37633300 1.04247700
H -4.91340600 1.10053200 0.59048700
C -2.70250400 1.51709000 1.95411500
C -1.59617100 2.39576600 1.78009900
C -3.68289400 1.84546300 2.88183200
C -1.61268900 3.65988600 2.44296300
C -3.62153600 3.03104000 3.64082000
H -4.52796500 1.17715500 3.01236900
C 0.31583700 2.99859000 0.54651100
C -0.63113700 4.61057400 2.07549000
C -2.62050100 3.94408100 3.39794700
H -4.39262400 3.23825200 4.37435300
C 0.27719100 4.30774900 1.09432200
H -0.61721900 5.58081500 2.56229100
H -2.59827700 4.89925500 3.91264200
H 1.02051100 5.02954400 0.78256800
C 1.39047800 2.69306900 -0.42363300
C 2.26789000 1.58433600 -0.25581600
C 1.65605200 3.62505300 -1.42018500
C 3.47751200 1.52889600 -1.01734900
C 2.79293300 3.51886500 -2.23755600
H 0.98567000 4.46832300 -1.55088500
C 2.94574500 -0.21325100 1.08764200
C 3.70848500 2.51477100 -2.00943000
H 2.97618900 4.26394400 -3.00358600
H 4.63758800 2.49501700 -2.56432500
C 2.70281500 -1.20455700 2.15997100
C 1.59539200 -2.09811800 2.11997700
C 3.68375800 -1.39187300 3.12555800
C 1.61029600 -3.24803800 2.96559700
C 3.62072100 -2.44953700 4.05450900
H 4.53052000 -0.71363700 3.15310700
C -0.31523100 -2.87918400 0.98846600
C 0.62795500 -4.24221000 2.74472100
C 2.61778400 -3.38668200 3.95254200
H 4.39204400 -2.54578700 4.81038000
C -0.27855700 -4.09069900 1.72750400
H 0.61297300 -5.12788100 3.37229500
H 2.59412200 -4.25347400 4.60515600
H -1.02188300 -4.85110900 1.52764800
N -1.97873600 -0.51190100 0.77881900
N -0.56010400 2.06341000 0.93199600
N 1.98005000 0.62626600 0.69396700
N 0.56022600 -1.89663500 1.23065000
C 4.45248400 0.52969800 -0.67665700
C 4.19714500 -0.24747300 0.44228700
H 4.91382000 -0.99716900 0.75070200
Pd 0.00023400 0.06961400 0.89819100
C 5.68802400 0.30986800 -1.44711100
C 6.91458300 0.14007800 -0.78397000
C 5.67040500 0.19698500 -2.85418200
C 8.09174500 -0.10738500 -1.48440200
H 6.95709900 0.23459400 0.29686200
C 6.83115700 -0.06753800 -3.56049400
H 4.73090600 0.28100700 -3.39082800
C 8.05619600 -0.21546500 -2.88421700
H 9.02174200 -0.20876300 -0.93942700

H 6.81960400 -0.17351900 -4.63981100
C -5.68695900 -0.52254200 -1.38621400
C -6.91438900 -0.26518900 -0.75351600
C -5.67073400 -0.61791000 -2.79458800
C -8.09348800 -0.13112700 -1.48108000
H -6.95594900 -0.20078500 0.32963500
C -6.83347500 -0.46697800 -3.53052900
H -4.73116900 -0.77478300 -3.31450400
C -8.05923300 -0.22956200 -2.88157900
H -9.02390500 0.04312100 -0.95566800
H -6.82304400 -0.52040300 -4.61376900
O 9.13055900 -0.46020300 -3.66702600
C 10.40805700 -0.63595400 -3.04935200
H 11.10843100 -0.82037900 -3.86367000
H 10.71321100 0.26383300 -2.50319800
H 10.40487300 -1.49502900 -2.36870200
O -9.13578000 -0.10974500 -3.68995000
C -10.41477000 0.13981900 -3.10155800
H -11.11730800 0.19786400 -3.93264800
H -10.70976400 -0.67552500 -2.43130300
H -10.42085500 1.08766500 -2.55125500

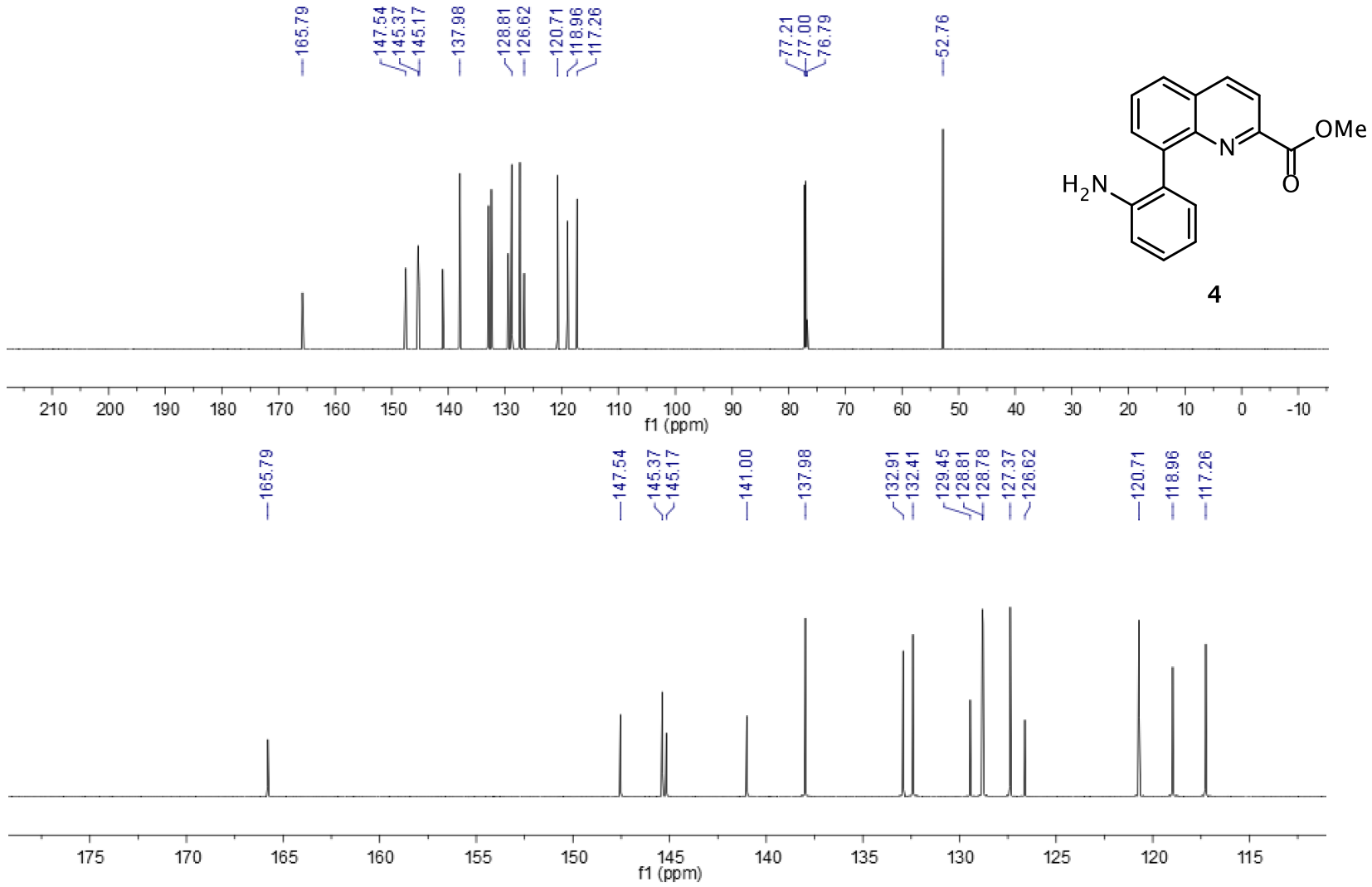
12. Spectra

^{1}H NMR (600 MHz, $CDCl_3$)

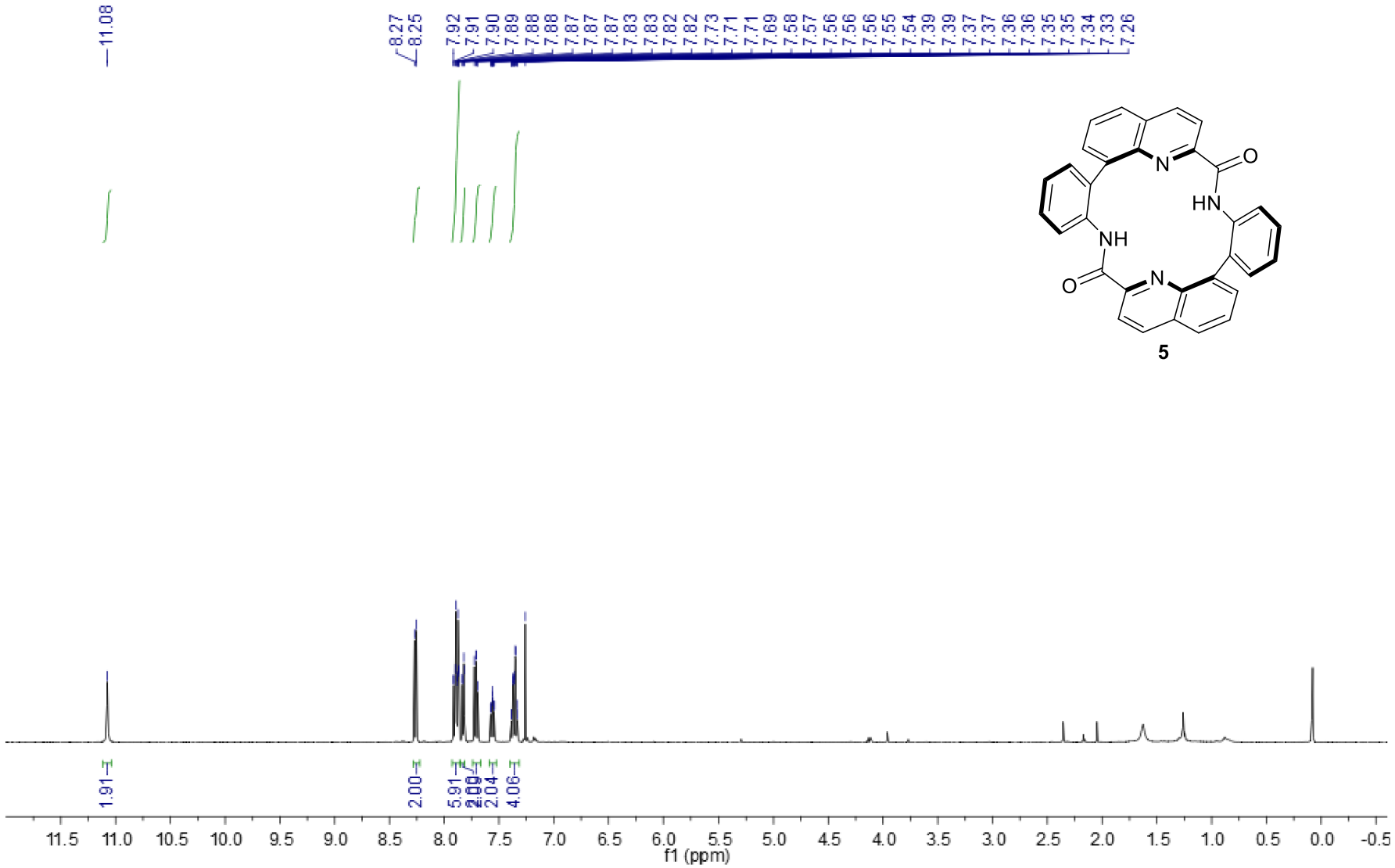


4

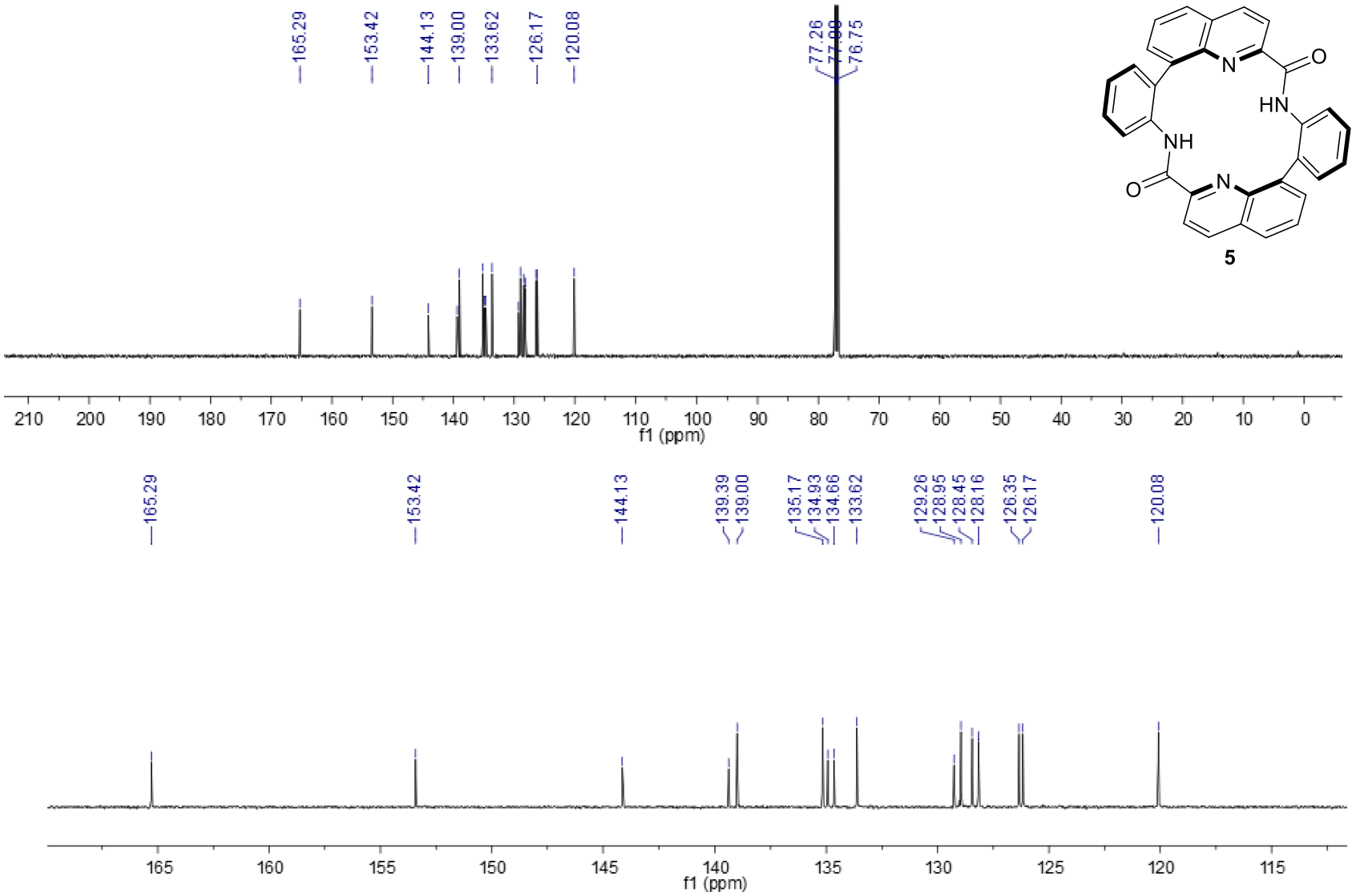
^{13}C NMR (151 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)

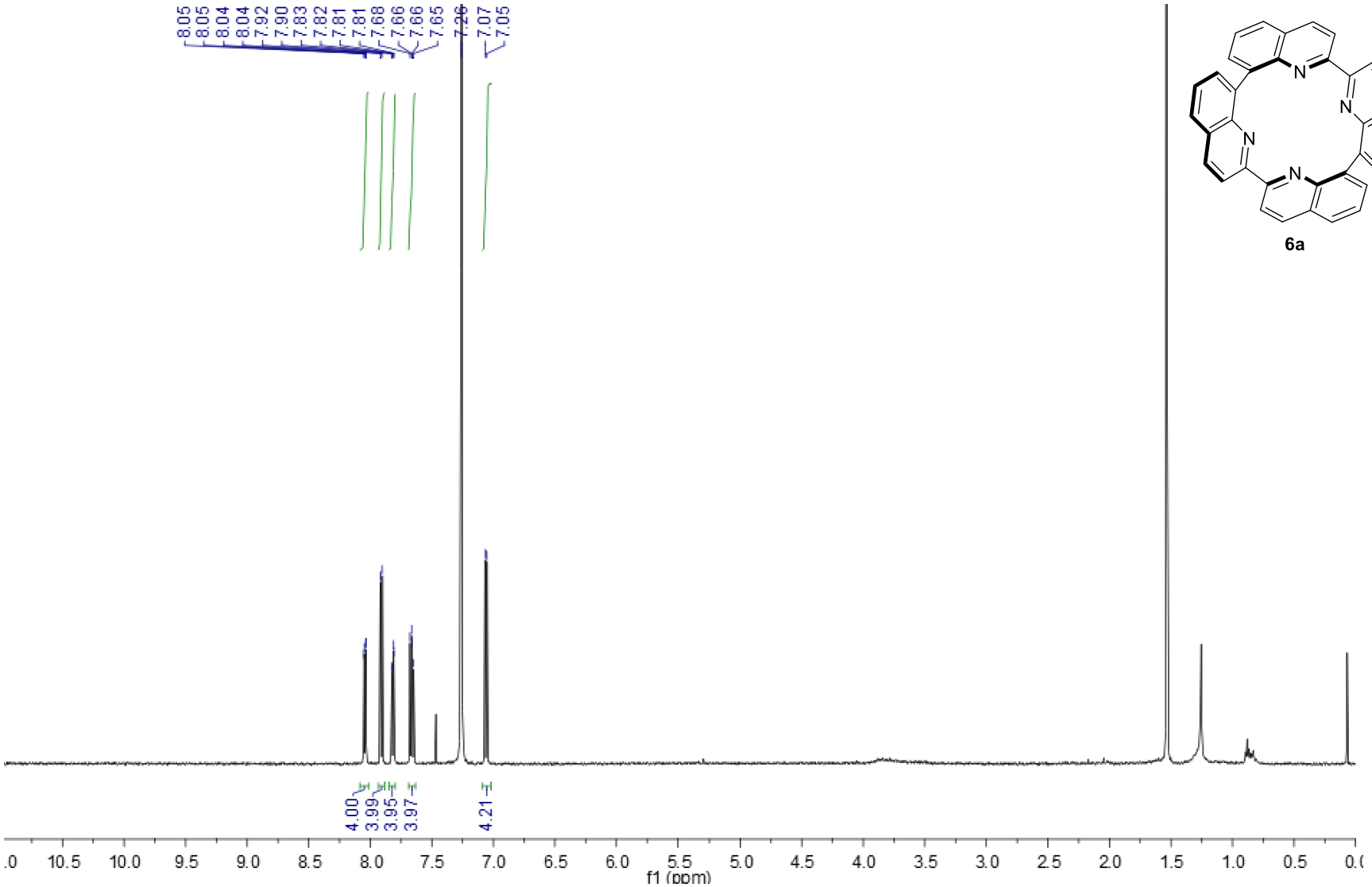


^{13}C NMR (162 MHz, $CDCl_3$)



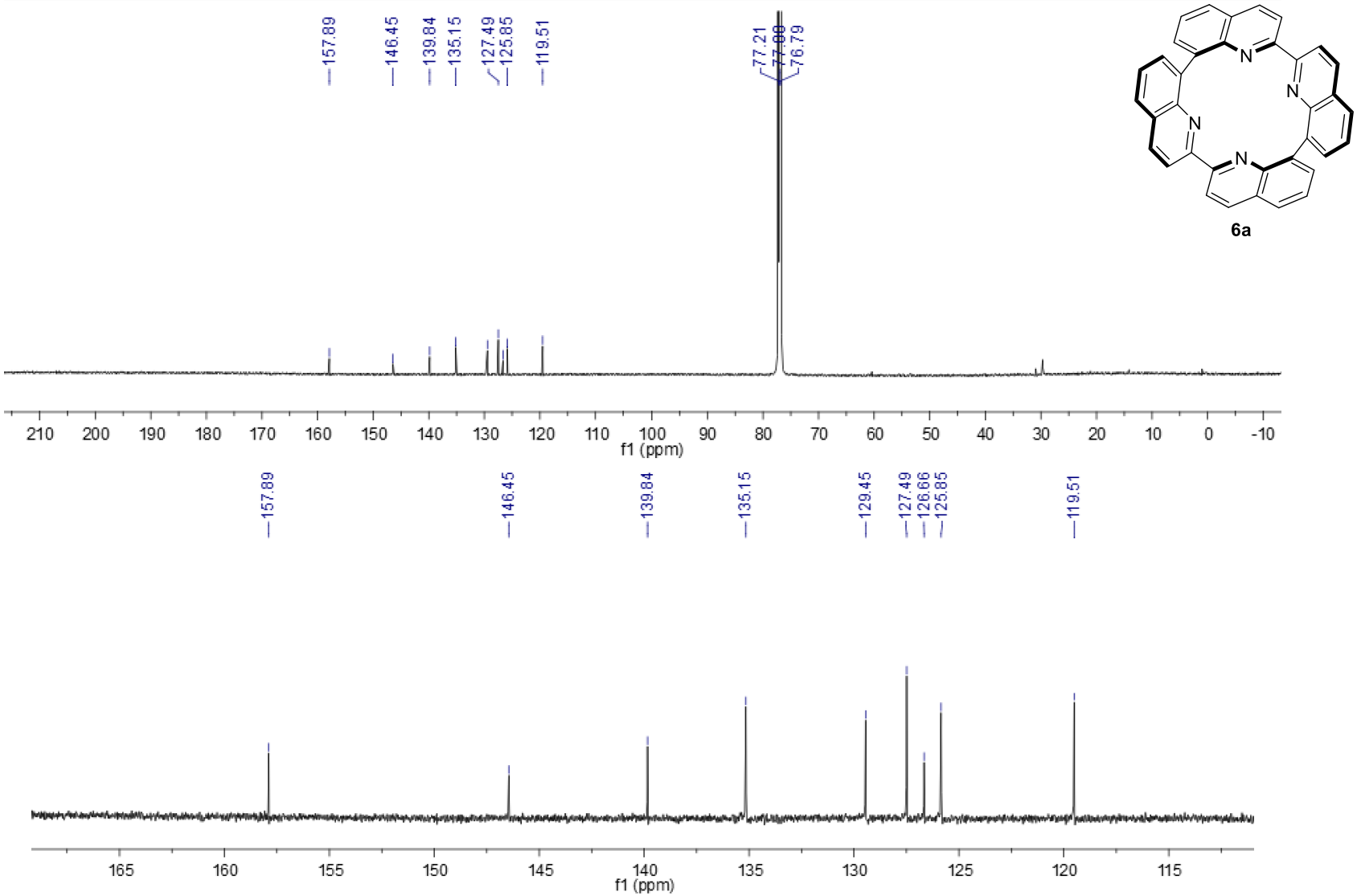
5

^{1}H NMR (500 MHz, $CDCl_3$)



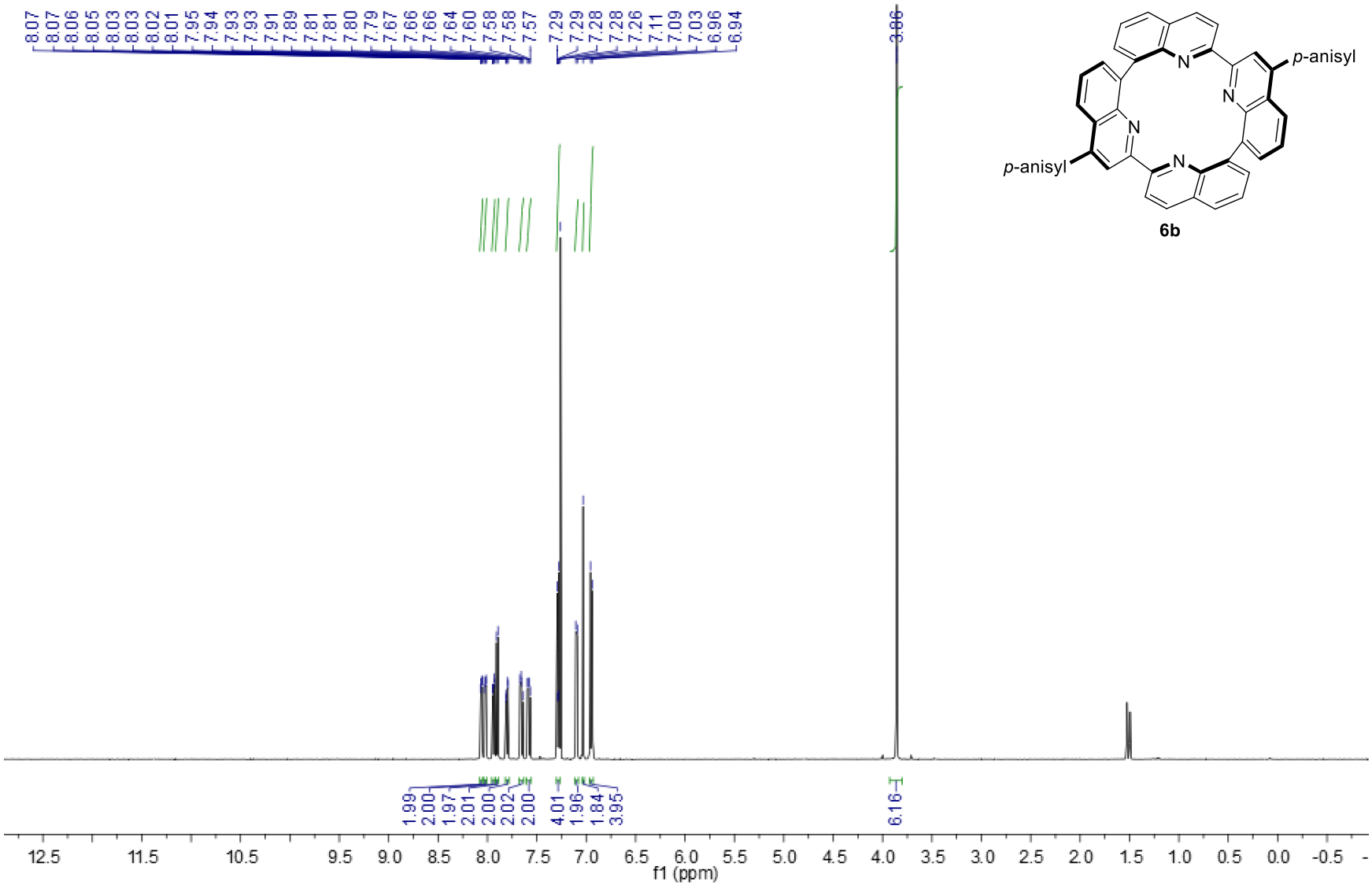
6a

^{13}C NMR (151 MHz, $CDCl_3$)



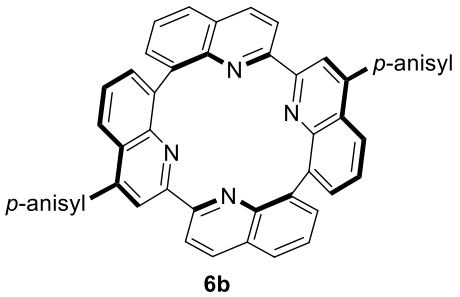
6a

^{1}H NMR (500 MHz, $CDCl_3$)

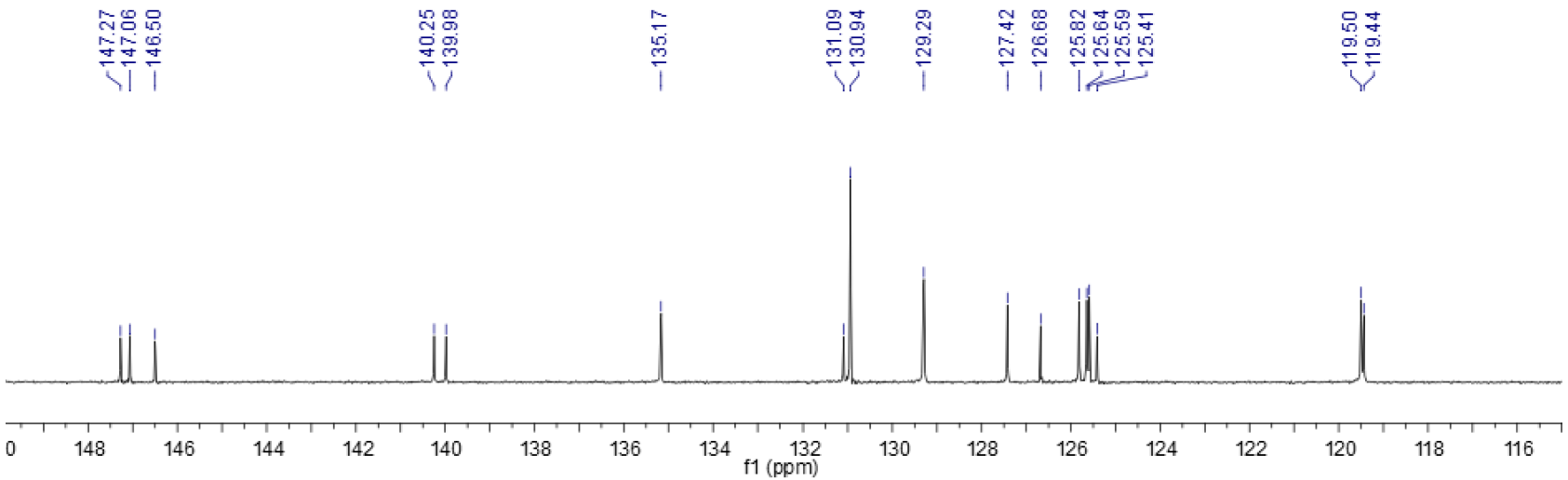


6b

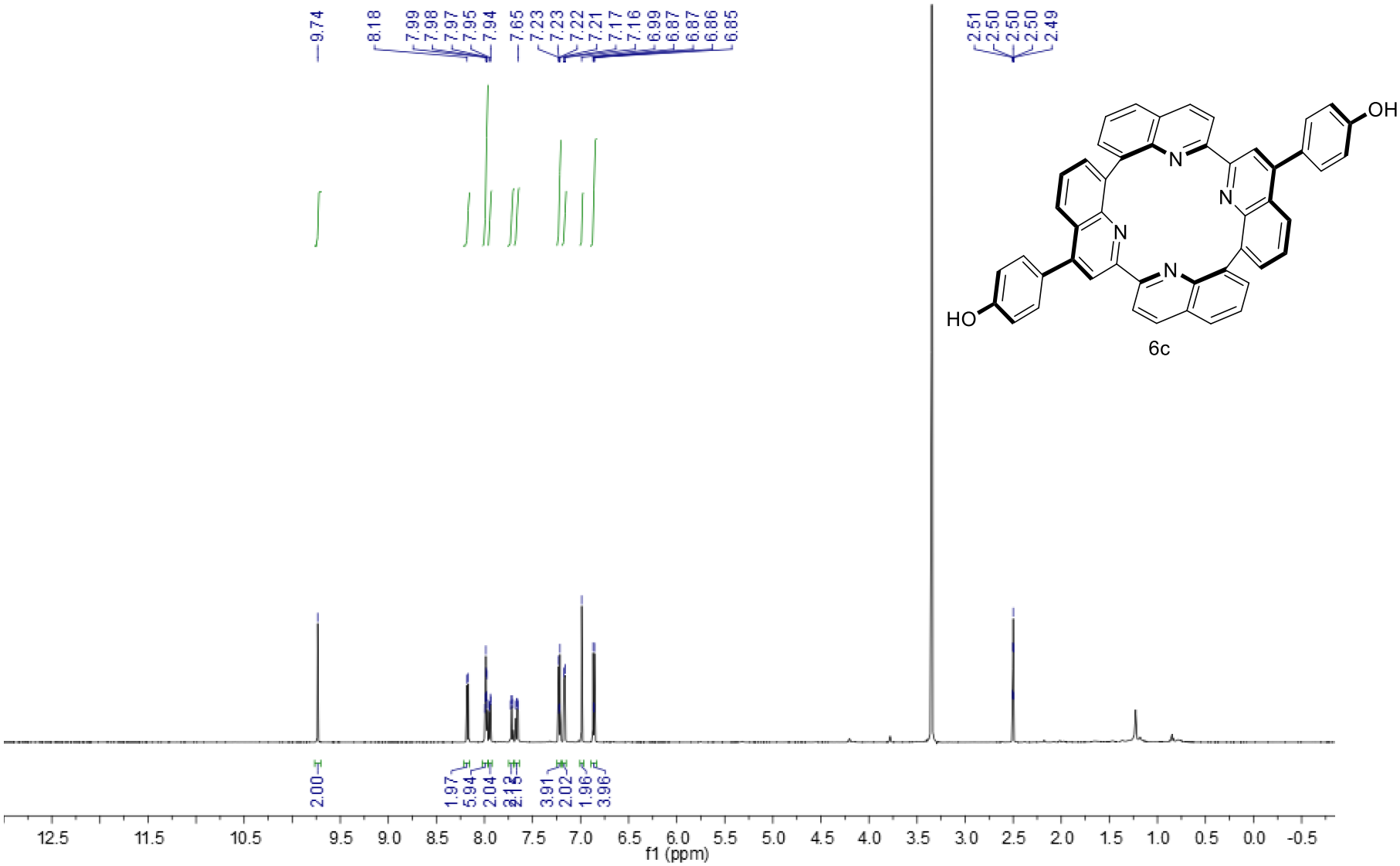
^{13}C NMR (151 MHz, $CDCl_3$)



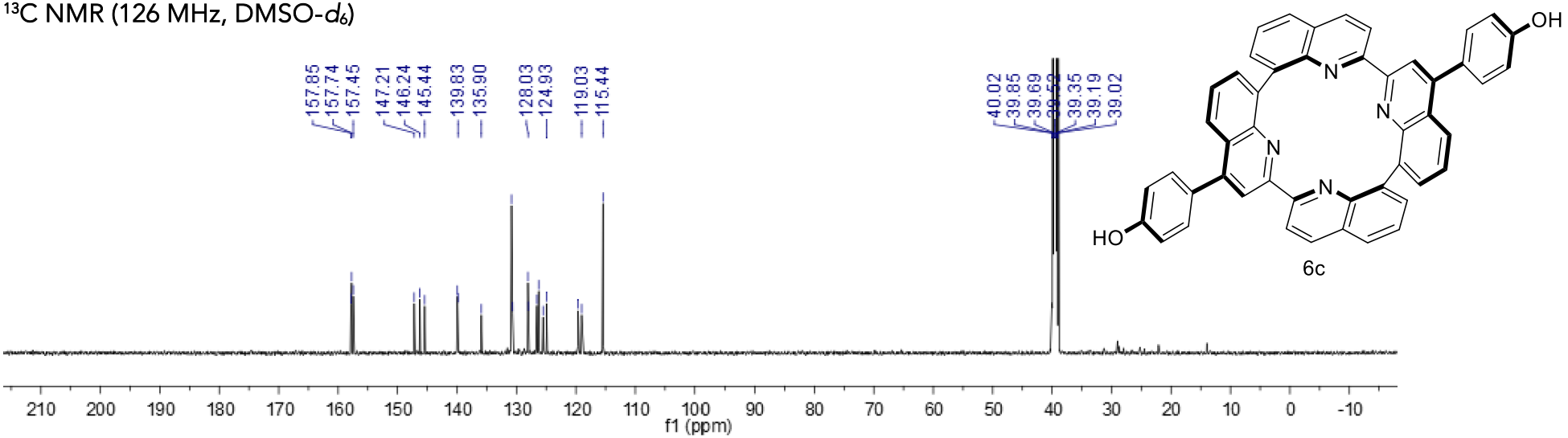
6b

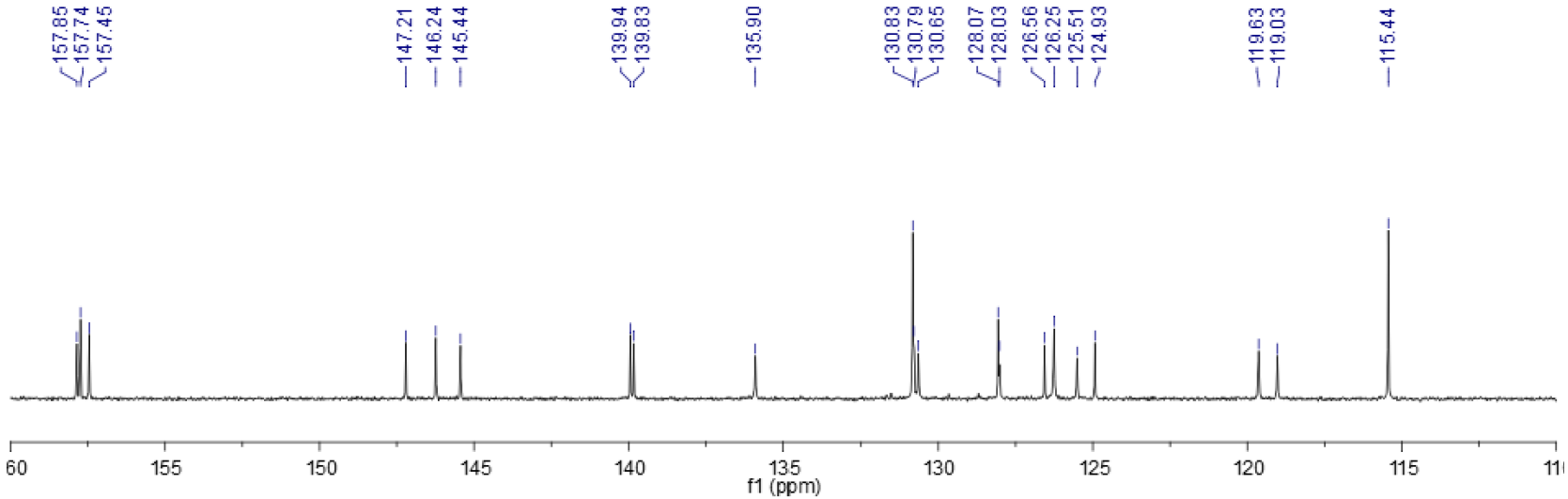


^{1}H NMR (600 MHz, DMSO-d_6)

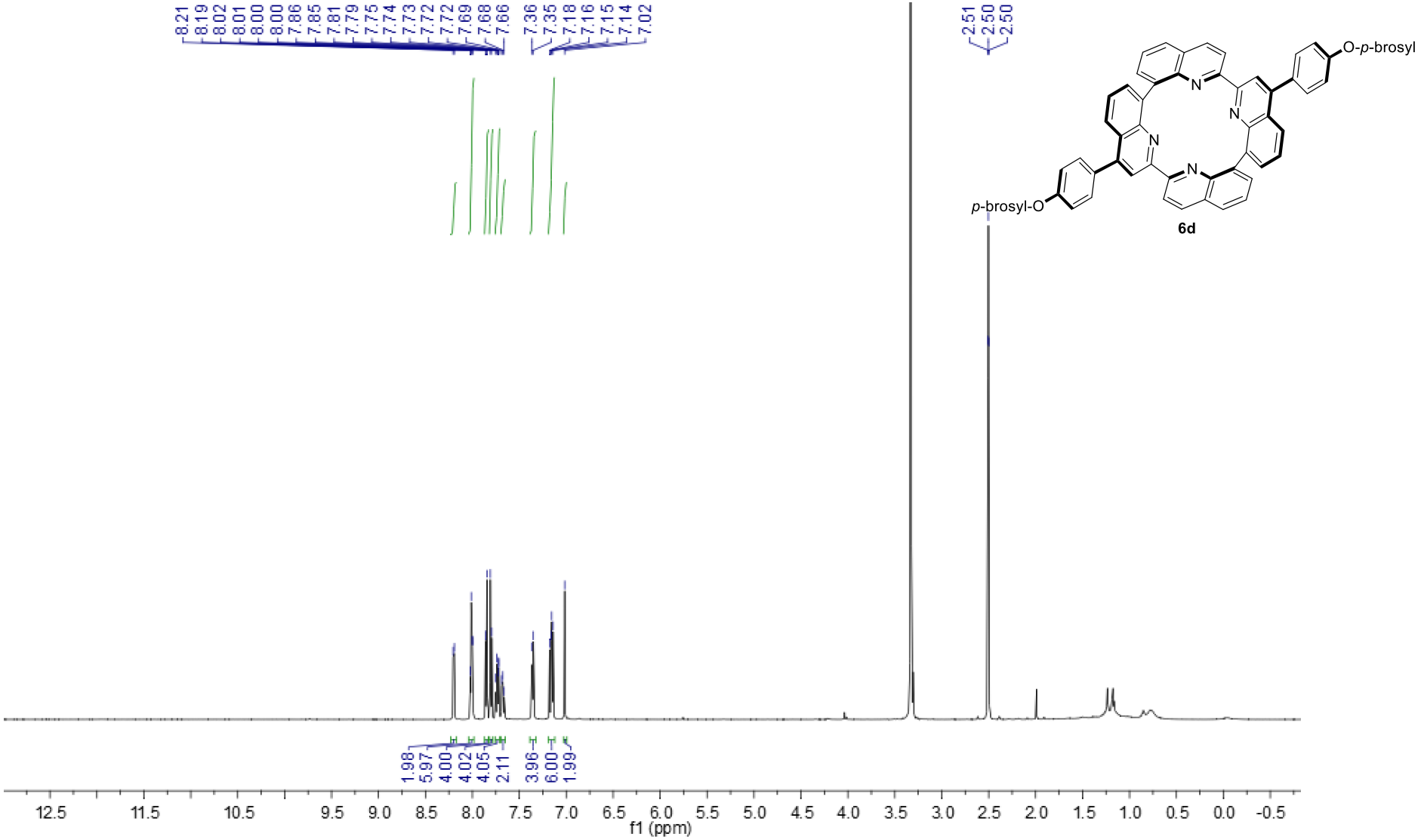


^{13}C NMR (126 MHz, DMSO-d_6)

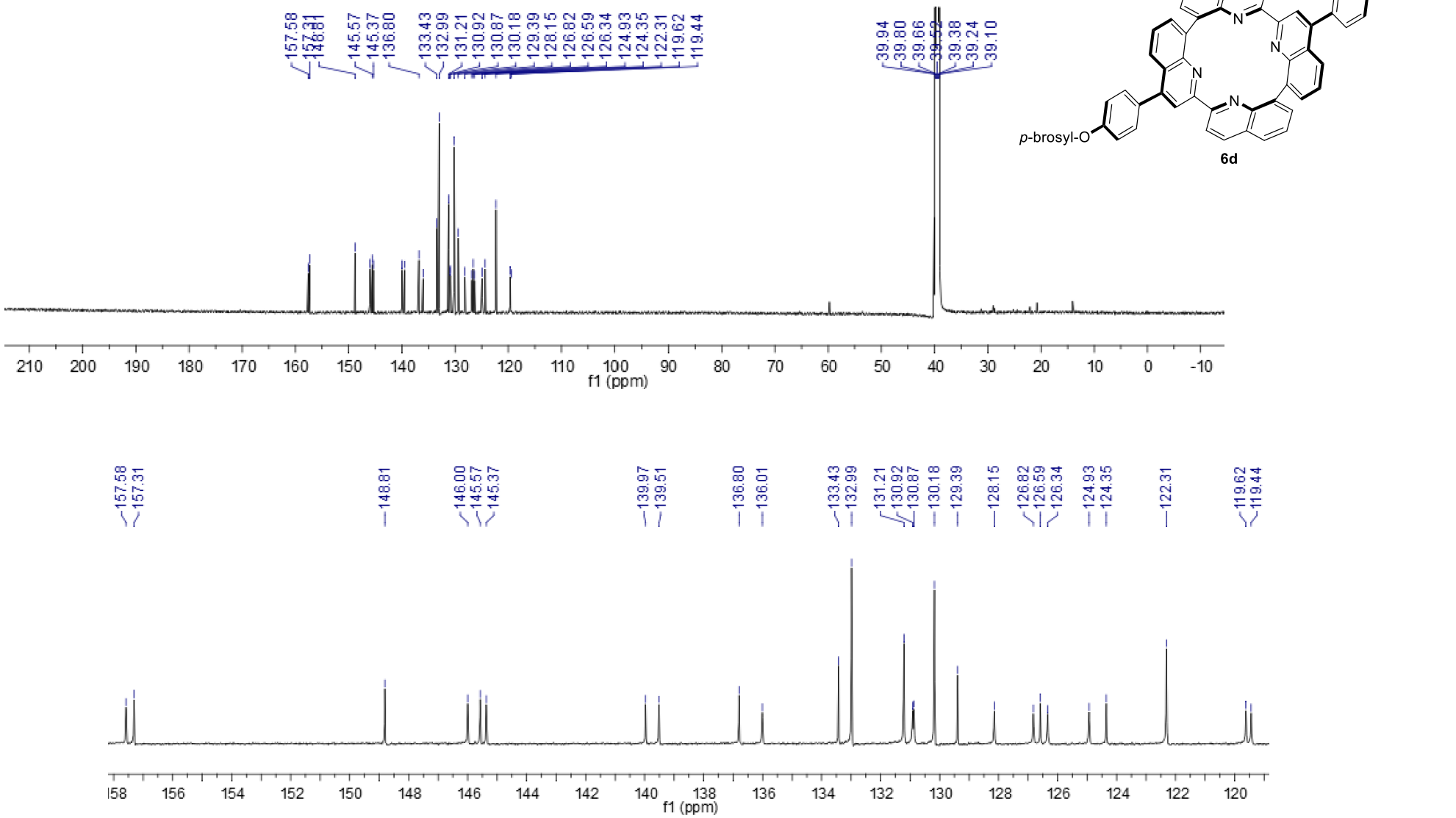




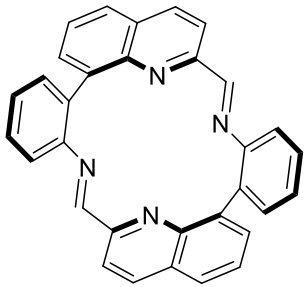
^{1}H NMR (600 MHz, DMSO-d_6)



^{13}C NMR (151 MHz, $CDCl_3$)

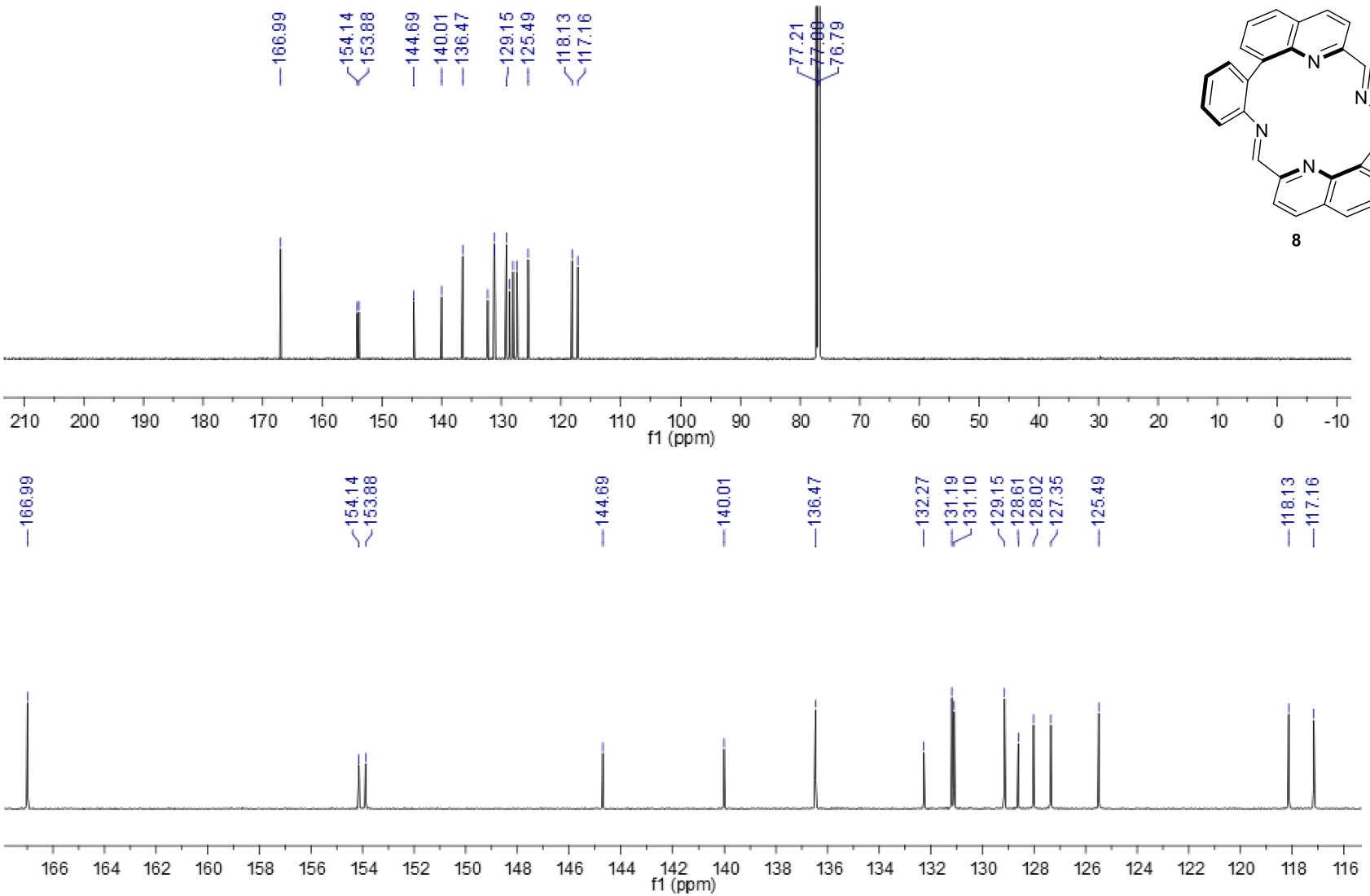


^{1}H NMR (600 MHz, $CDCl_3$)



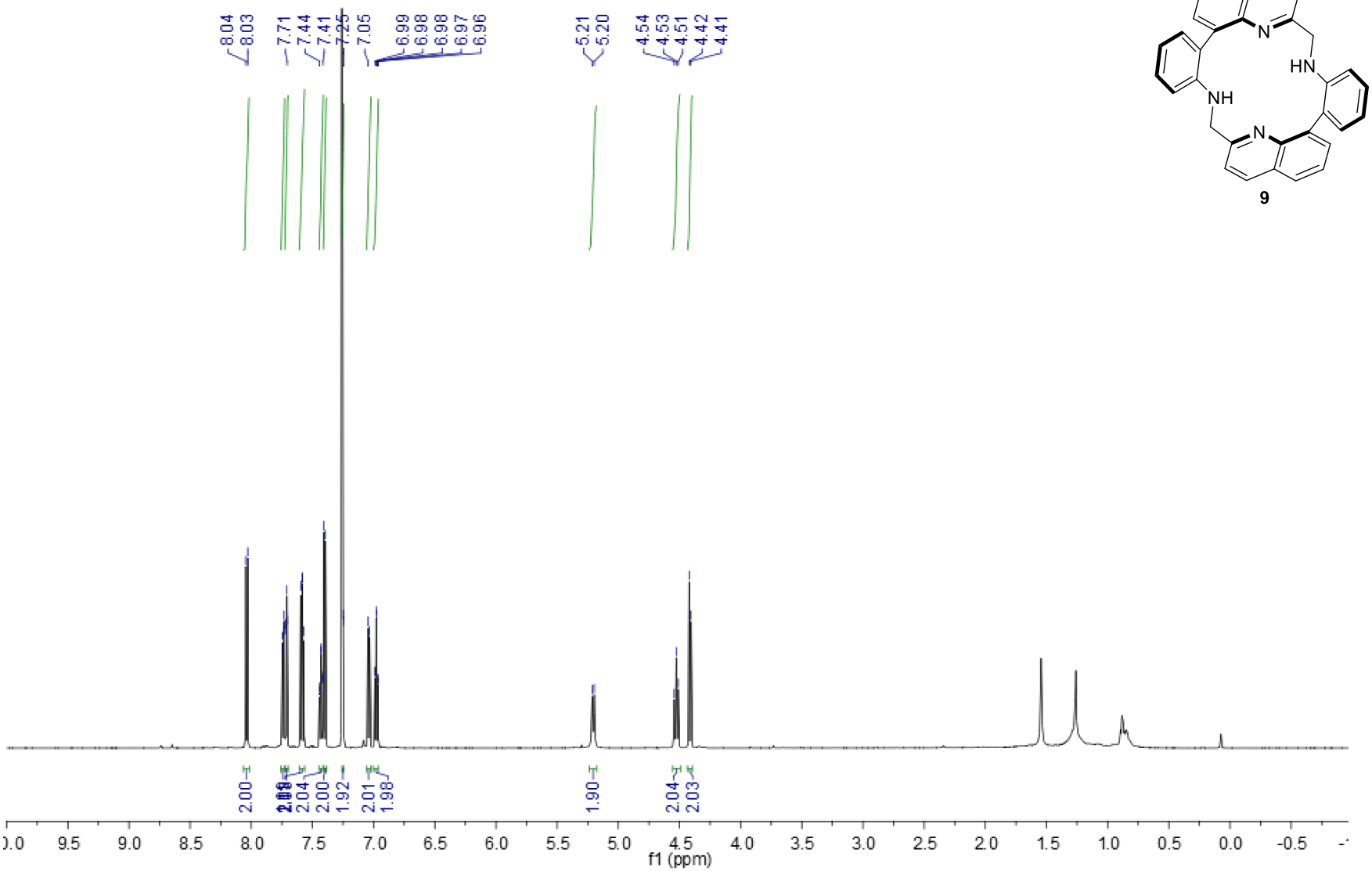
8

^{13}C NMR (151 MHz, $CDCl_3$)



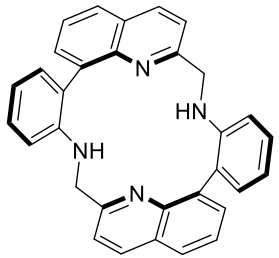
8

^{1}H NMR (600 MHz, $CDCl_3$)



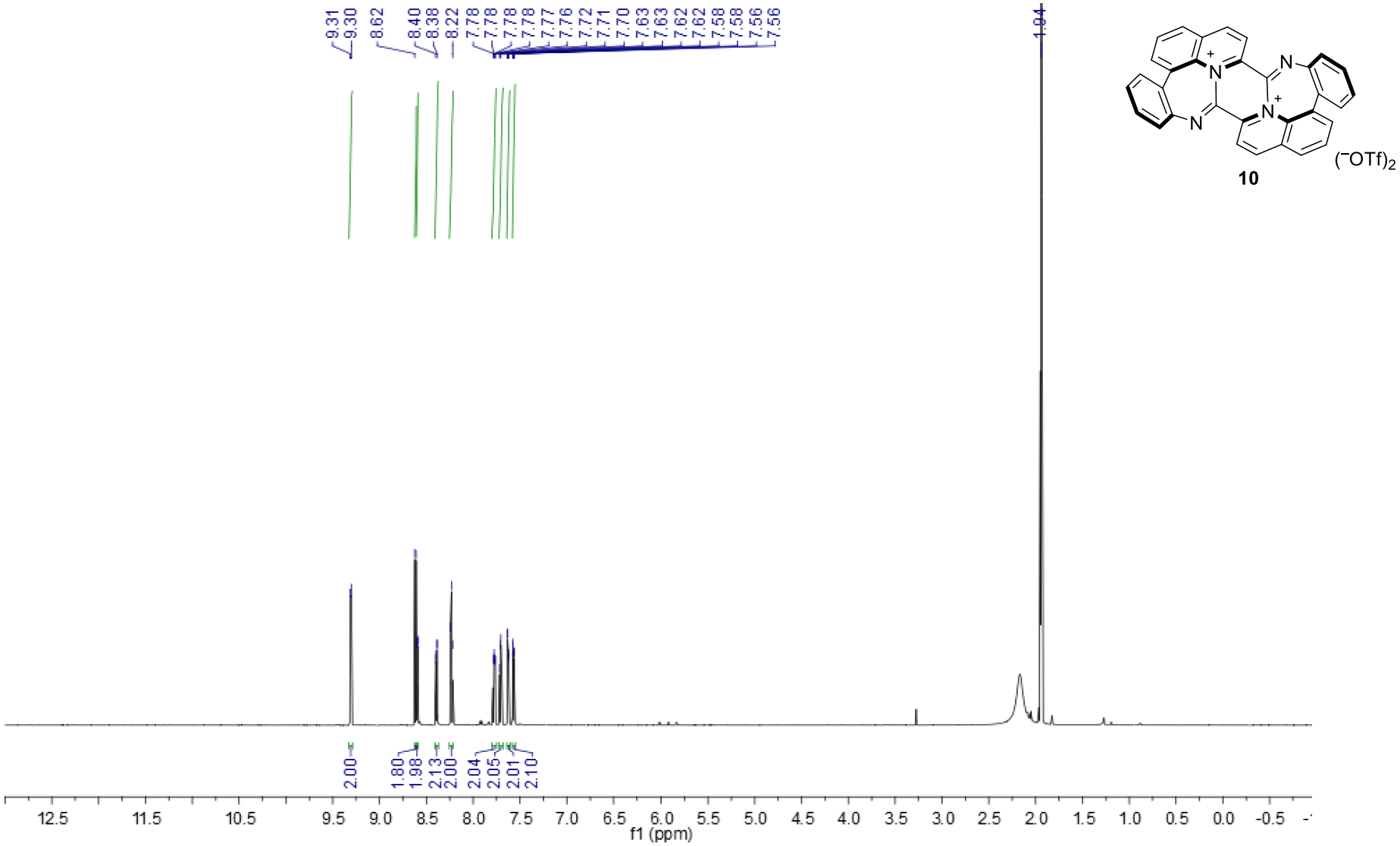
9

^{13}C NMR (126 MHz, $CDCl_3$)



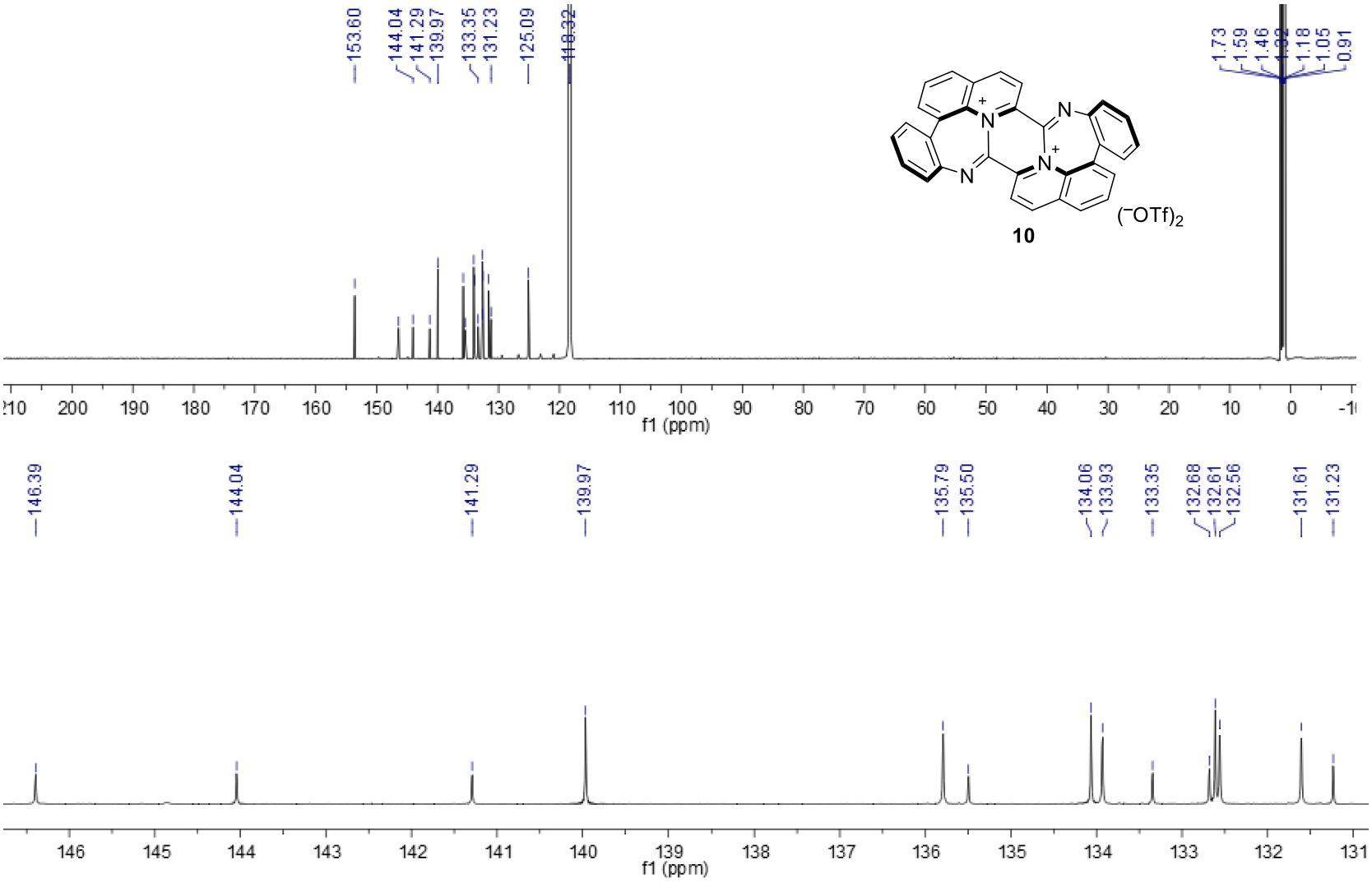
9

^{1}H NMR (600 MHz, CD_3CN)

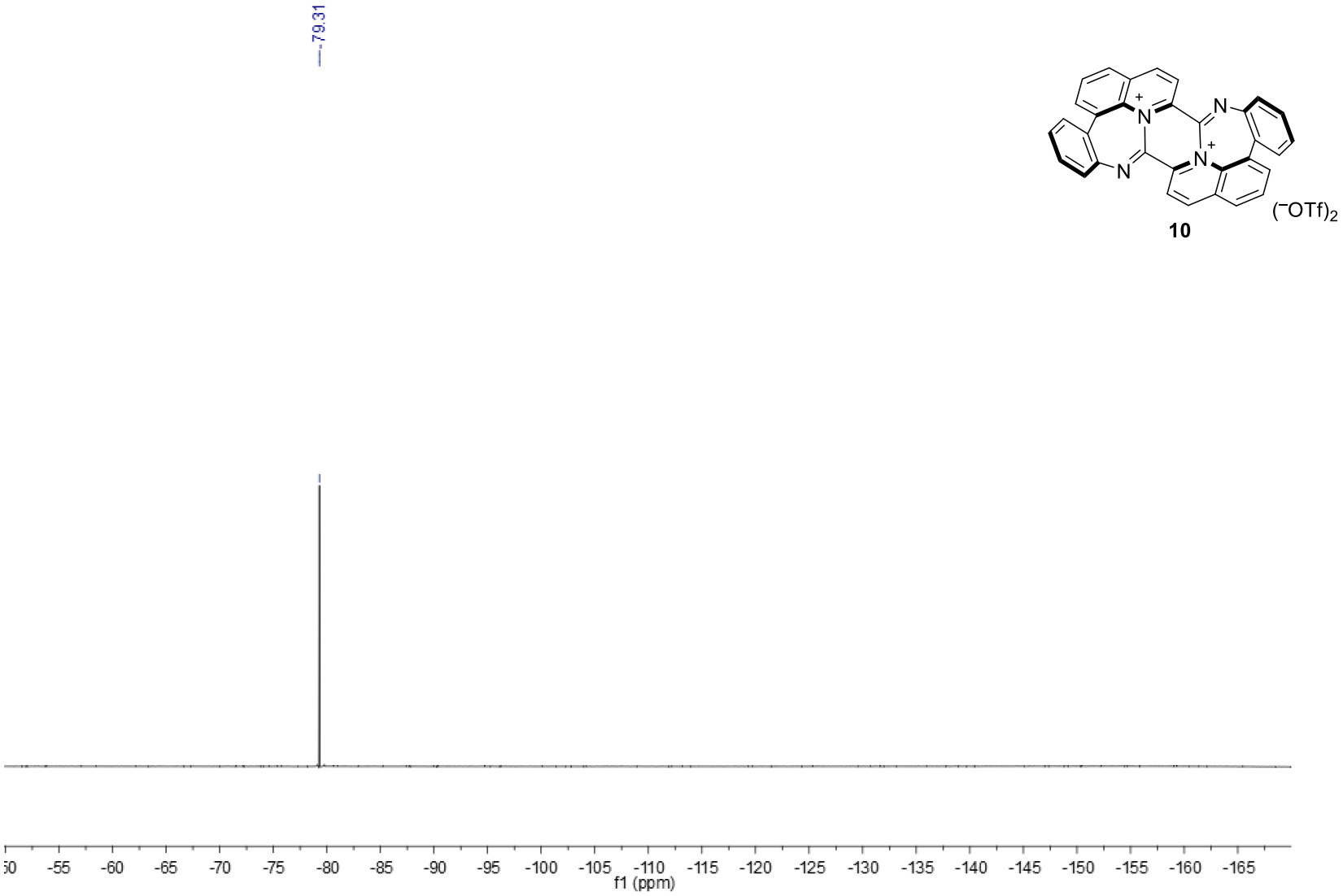


10

^{13}C NMR (151 MHz, CD_3CN)

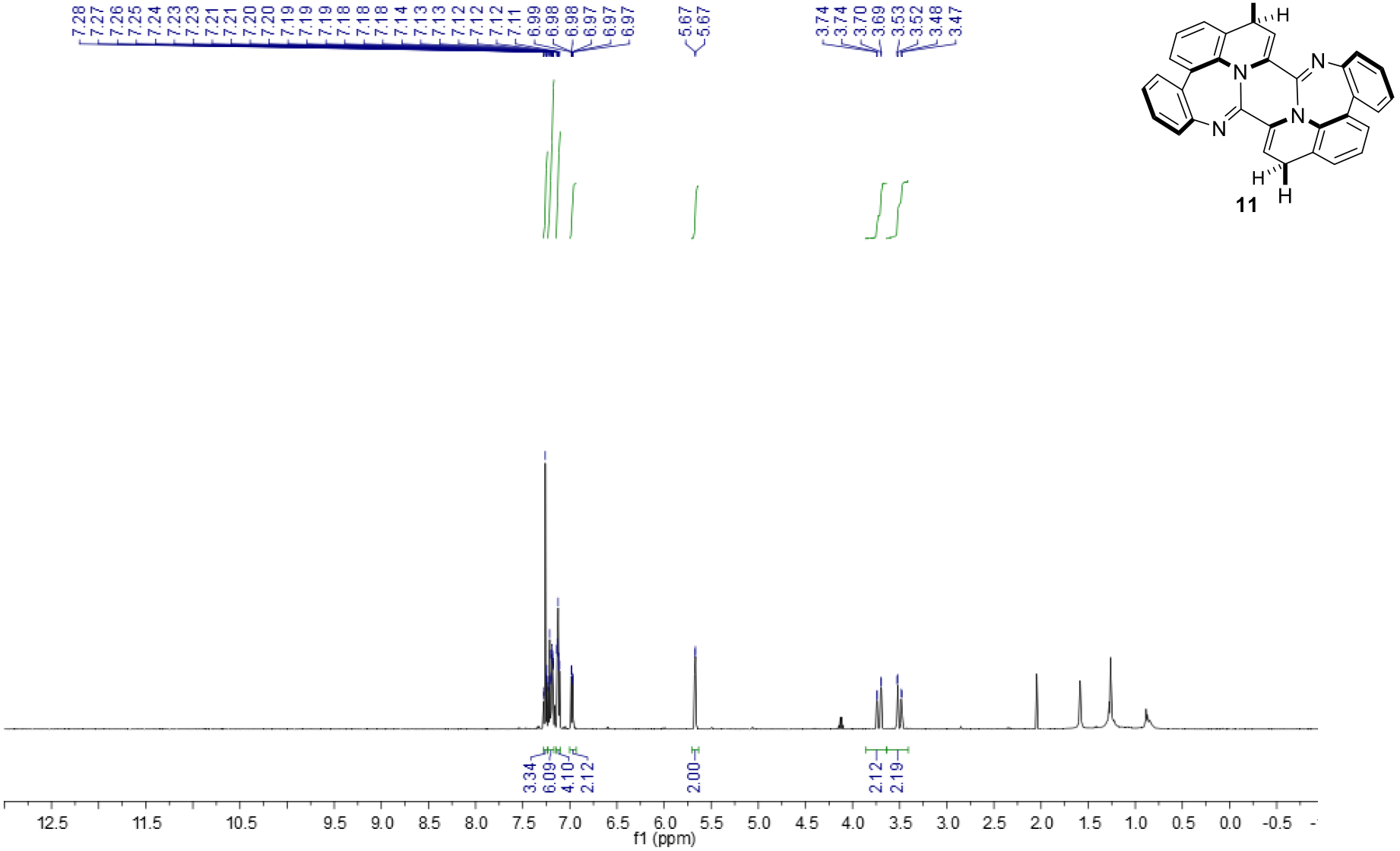


^{19}F NMR (471 MHz, CD_3CN)



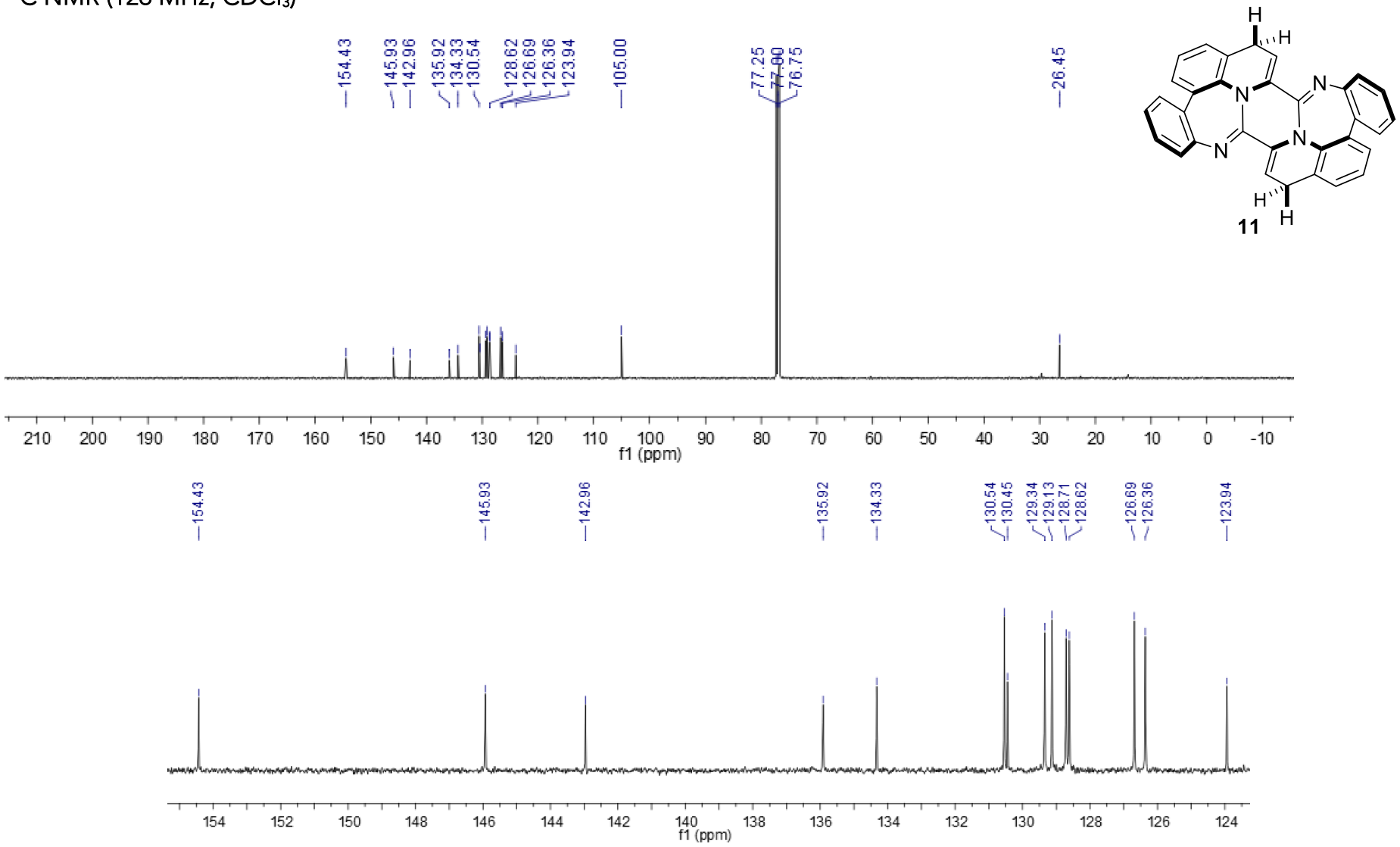
10

^{1}H NMR (500 MHz, $CDCl_3$)



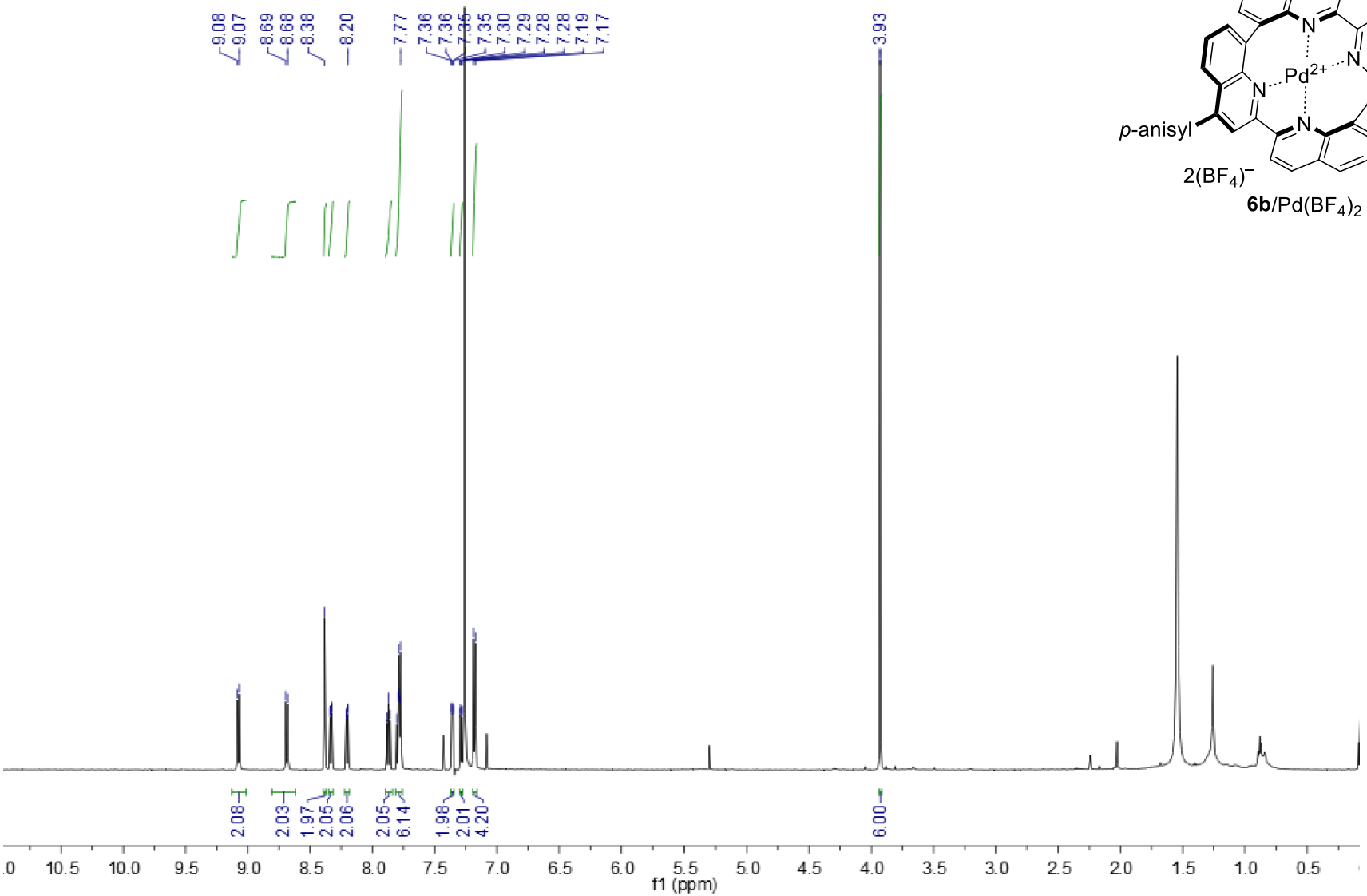
11

^{13}C NMR (126 MHz, $CDCl_3$)



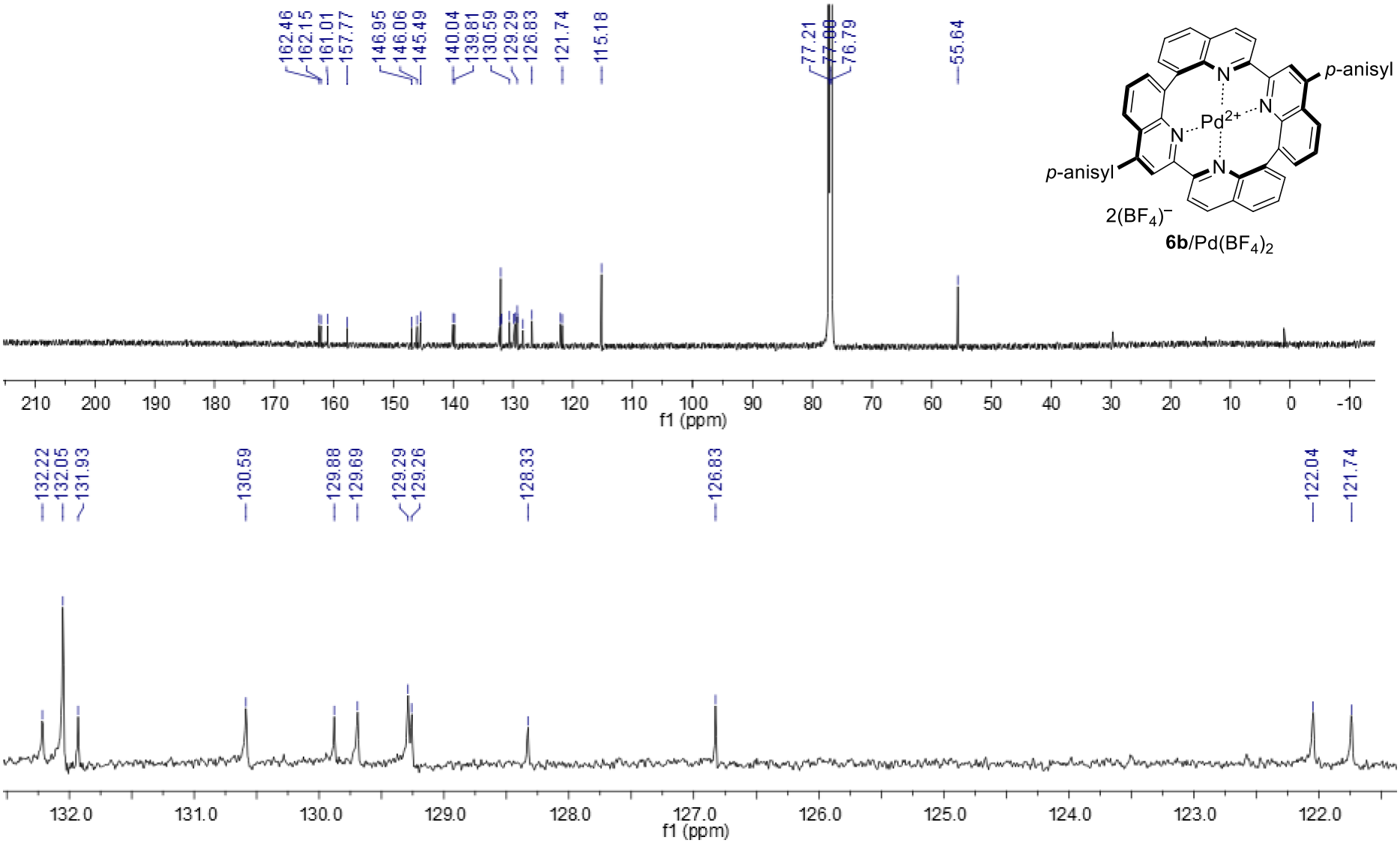
11

^{1}H NMR (600 MHz, $CDCl_3$)



6b/$Pd(BF_4)_2$

^{13}C NMR (151 MHz, $CDCl_3$)



^{19}F NMR (471 MHz, $CDCl_3$)