Supporting Information

Interaction of the Dihydropyridine/Pyridinium Redox Pair Fixed into a V-Shaped Conformation

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General procedures.

All experiments with moisture- or air-sensitive compounds were conducted in anhydrous solvents under nitrogen atmosphere in well-dried glassware. Anhydrous dichloromethane, toluene, ethanol were purchased from Kanto Chemical Co., Inc. and used without further purification. Column chromatography were performed on a silica gel (Silica gel 60N, Kanto Chemical Co., Inc.) or alumina (Alminium oxide 90, Merck).

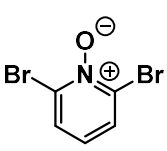
UV-vis absorption spectra were measured on a JASCO V-570 spectrometer. ^{1}H and ^{13}C NMR spectra were obtained on a Varian Mercury plus (300 MHz), JEOL RESONANCE ECS-400 (400 MHz), and JEOL RESONANCE ECA-500 (500 MHz) spectrometers. NOESY spectra were obtained on a Bruker AVANCE (700 MHz) spectrometer. The chemical shift was recorded by using tetramethylsilane (0.00 ppm) as an internal standard for ^{1}H NMR spectra.

Data collection for X-ray crystal analysis for **1** was performed on a Rigaku VariMax with RAPID II diffractomete (Mo-Kα, λ = 0.71075 Å). CCDC 1949498 (**1**) contains the supplementary crystallographic data. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. The structure was conducted by direct methods (SHELXL-2016/6 and SIR2014) using Yadokari-XG 2009.[S1]

Cyclic voltammetric measurements were made with a BAS ALS-612D electrochemical analyzer. Cyclic voltammograms were recorded with a glassy carbon working electrode (BAS, 3.0 mm diameter) and a Pt wire counter electrode. A nonaqueous $Ag/AgNO_3$ electrode was used as a reference electrode and all the potentials were calibrated with ferrocene/ferrocinium couple as an internal reference. The measurement was carried out under argon atmosphere at room temperature with 0.1 M *n*-Bu_4NPF_6 as supporting electrolyte.

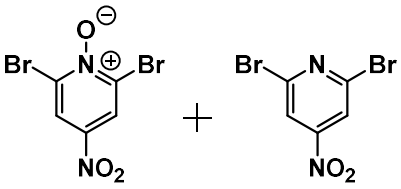
Computational Details.

Geometrical optimizations and energy calculations of all of the possible structures were performed with the Gaussian 09 program[S2] at the CAM-B3LYP/6-31G** functional with Grimme's D3 empirical dispersion. Ground state optimizations had no imaginary frequencies. The Cartesian coordinates of the optimized geometry of **1** are reported in Table S2.

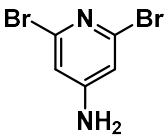


2, 6-Dibromopyridine-*N*-oxide (4). Trifluoroacetic acid (50 mL) and 30% hydrogen peroxide were added to 2,6-dibromopyridine (10.1 g, 42.3 mmol) placed under nitrogen atmosphere, and the mixture was refluxed overnight with stirring. The resulting mixture turned orange and was quenched with water after cooling. The solution was neutralized by $NaHCO_3$ and extracted with

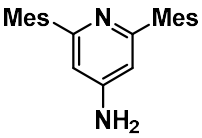
dichloromethane three times. The extract was washed with brine and dried over anhydrous Na_2SO_4 and concentrated in vacuo. The precipitated solid was washed with dichloromethane/hexane to afford **4** as a white solid (7.86 g, 74%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.64 (d, 2H, J = 8.1 Hz), 6.92 (t, 1H , J = 8.1 Hz).



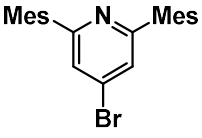
2,6-Dibromo-4-nitropyridine-1-oxide (5) & 2, 6-Dibromo-4-nitropyridine (5'). The pyridine *N*-oxide **4** (4.00 g, 15.8 mmol) was dissolved in conc. sulfuric acid (12 mL), and then white fuming nitric acid (6 mL) was added dropwise to the solution in an ice bath. The resulting mixture was heated at 90 °C for 5 hours. After cooling to room temperature, the reaction mixture was poured into ice water. The precipitated white solid was collected and dried under reduced pressure. A part of the *N*-oxide group was eliminated during the reaction. Therefore, the crude white solid containing **5** and **5'** was used for the next reaction without purification (3.87 g, **5**: 78%, **5'**: 5%): **5**, ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 8.49 (s, 2H); **5'**, ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 8.18 (s, 2H).



4-Amino-2, 6-dibromopyridine (6). The crude mixture of **5** and **5'** (5.04 g) was dissolved in acetic acid (100 mL). The iron powder (5.13 g, 91.9 mmol) was added to the acetic acid solution and heated to 100 °C for 2 hours. After cooling down to room temperature, ethyl acetate was added and the resulting mixture was filtered using Celite. The filtrate was extracted three times with ethyl acetate. The combined organic layers were washed with $NaHCO_3$ and brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to provide **6** as a white solid (3.86 g, 91%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 6.67 (s, 2H), 4.30 (s, 2H).

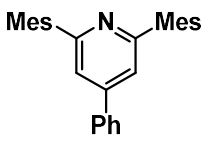


4-Amino-2,6-dimesitylpyridine (7). In a two-necked round flask equipped with a septum and a reflux condenser was placed the bromide **6** (723 mg, 2.87 mmol), mesitylboronic acid (2.38 g, 14.5 mmol), $Pd(PPh_3)_4$ (507 mg, 0.439 mmol), and Na_2CO_3 (3.11 g, 29.3 mmol) under nitrogen atmosphere. To the flask was added dry toluene (12.0 mL), dry ethanol (8.0 mL), and water (4.0 mL). The resulting mixture was refluxed overnight. After cooling and filtering through Celite, the solution was extracted with ethyl acetate three times, and the extract was washed with brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on alumina with dichloromethane as eluent to provide the title compound as a white solid (863 mg, 91%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 6.86 (s, 4H), 6.43 (s, 2H), 4.13 (s, 2H), 2.27 (s, 6H), 2.08 (s, 12H).

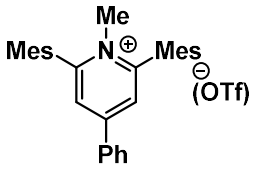


4-Bromo-2,6-dimesitylpyridine (8). The amino pyridine **7** (611 mg, 1.85 mmol) and copper (II) bromide (810 mg, 3.63 mmol) was dissolved in acetonitrile (30 mL) and cooled in an ice bath. To the resulting mixture was added dropwise tert-butyl nitrite (1.8 mL, 23.9 mmol) via syringe. After stirring in an ice bath for 30 min, the reaction mixture was warmed to room temperature and stirred for 3 h. The reaction was then treated with concentrated aqueous ammonia (28%)

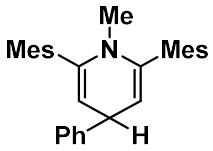
until the solution was basic. The mixture was extracted with dichloromethane three times. The extract was washed with water and brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on alumina (dichloromethane/hexane = 15/85) to afford **8** as a white solid (573 mg, 79%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.37 (s, 2H), 6.89 (s, 4H), 2.29 (s, 6H), 2.05 (s, 12H).



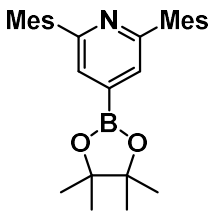
2,6-Dimesityl-4-phenylpyridine (13) In a two-necked round flask equipped with a septum and a reflux condenser was placed the bromide **8** (1.20 g, 3.05 mmol), phenylboronic acid (567 mg, 4.65 mmol), $Pd(PPh_3)_4$ (182 mg, 0.157 mmol), and Na_2CO_3 (972 mg, 9.17 mmol) under nitrogen atmosphere. To the flask was added dry toluene (6.0 mL), dry ethanol (4.0 mL), and water (2.0 mL). The resulting mixture was refluxed overnight. After cooling and filtering through Celite, the solution was extracted with dichloromethane three times, and the extract was washed with water and brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on alumina (dichloromethane/hexane = 1/4) to provide **13** as a white solid (1.11 mg, 93%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.73-7.70 (m, 2H), 7.52-7.43 (m, 3H), 7.45 (s, 2H), 6.93 (s, 4H), 2.31 (s, 6H), 2.10 (s, 12H).



2,6-Dimesityl-1-methyl-4-phenylpyridin-1-ium trifluoromethanesulfonate (2) The pyridine **13** (998 mg, 2.55 mmol) was dissolved in dry dichloroethane (5 mL) and then methyl trifluoromethanesulfonate (1.0 mL, 9.1 mmol) was added to the solution. After the mixture was refluxed overnight with stirring under nitrogen atmosphere, the resulting mixture was quenched with methanol and concentrated in vacuo. The residue was purified by column chromatography on alumina (methanol/ethyl acetate = 5/95) to yield **2** as a white solid (1.31 g, 92%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 8.06 (s, 2H), 7.92-7.88 (m, 2H), 7.68-7.59 (m, 3H), 7.12 (s, 4H), 3.62 (s, 3H), 2.40 (s, 6H), 2.13 (s, 12H).

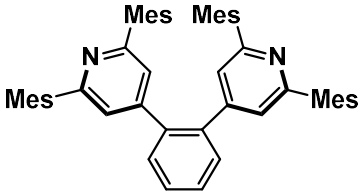


2,6-Dimesityl-1-methyl-4-phenyl-1,4-dihydropyridine (3) The pyridinium trifluoromethanesulfonate salt **2** (1.0 g, 0.38 mmol) was placed under a nitrogen atmosphere and dissolved in dry methanol (50 mL). To this solution, sodium borohydride (1.2 g, 32 mmol) was added, and the resulting mixture was refluxed overnight with stirring. After the solvent was evaporated, the residue was redissolved in ethyl acetate, washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude product was recrystallized from methanol to afford **3** as a yellow solid (670 mg, 95%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.44 (dd, 2H, J =7.8 Hz, 0.9 Hz), 7.34 (t, 2H, J = 7.8 Hz), 7.18 (m, 2H), 6.86 (s, 2H), 6.83 (s, 2H), 4.55 (t, 1H, J = 3.9 Hz), 4.34 (d, 2H, J = 3.9 Hz), 2.37 (s, 6H), 2.33 (s, 6H), 2.26 (s, 6H), 2.22 (s, 3H).

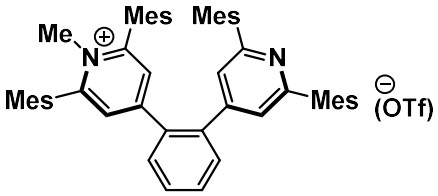


2,6-Dimesityl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (9) To a suspension of the bromide **8** (400 mg, 1.01 mmol) in the solvent mixture of dry diethyl ether (16 mL) and dry THF (8 mL) under nitrogen atmosphere at −78 °C, *n*-BuLi (0.8 mL, 1.5 M in hexane) was added dropwise with stirring. Then, the color of the reaction suspension was turned to yellow solution. Keeping temperature at −78 °C for 30 min, tributyl borate (0.40

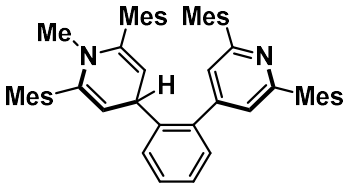
mL, 1.5 mmol) was added and the mixture was stirred for an additional 30 min. The solution was warmed to room temperature and pinacol (180 mg, 1.52 mmol) was added. After stirring for 30 min at 37 °C, the resulting yellow-colored reaction mixture was cooled to room temperature and quenched with acetic acid (86 μL, 1.5 mmol). The precipitated yellow solid was filtered off and the filtrate was concentrated in vacuo. The residue was washed with pentane and dried in vacuo to yield **9** as a white solid (361 mg, 81%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.50 (s, 2H), 6.87 (s, 4H), 2.28 (s, 6H), 2.03 (s, 12H), 1.35 (s, 12H).



1,2-Bis(2,6-dimesitylpyridin-4-yl)benzene (10) In a two-necked round flask equipped with a septum and a reflux condenser was placed the boronic acid **9** (955 mg, 2.16 mmol), $Pd(PPh_3)_4$ (20 mg, 0.035 mmol), Xphos (28 mg, 0.057 mmol), and K_3PO_4 (909 mg, 4.28 mmol) under nitrogen atmosphere. To the flask was added dry DMF (8.0 mL) and *o*-dibromobenzene (86 μL, 0.71 mmol). The resulting mixture was refluxed overnight. After cooling and filtering through Celite, the solution was extracted with dichloromethane three times, and the extract was washed with water and brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography on alumina (dichloromethane/hexane = 7/13) to provide **10** as a white solid (455 mg, 91%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.48 (AA'BB', 2H), 7.38 (AA'BB', 2H), 7.09 (s, 4H), 6.83 (s, 8H), 2.27 (s, 12H), 1.94 (s, 24H).

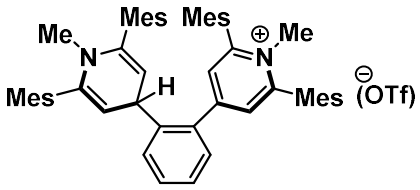


4-(2-(2,6-Dimesitylpyridin-4-yl)phenyl)-2,6-dimesityl-1-methylpyridin-1-ium trifluoromethanesulfonate (11) The bispyridine **10** (498 mg, 0.706 mmol) and 2,6-di-*tert*-butyl-4-methylpyridine (DTBMP) (147 mg, 0.716 mmol) were dissolved in dry dichloromethane (125 mL) and then methyl trifluoromethanesulfonate (80 μL, 0.71 mmol) was added to the solution. The mixture was stirred overnight at room temperature under nitrogen atmosphere, and then the reaction was quenched with methanol and concentrated in vacuo. The residue was purified by column chromatography on alumina (dichloromethane, then methanol/dichloromethane = 5/95) to yield **11** as a white solid (428 mg, 70%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 7.73 (s, 2H), 7.68-7.61 (m, 3H), 7.44-7.42 (m, 1H), 7.09 (s, 2H), 7.04 (s, 4H), 6.88 (s, 4H), 3.63 (s, 3H), 2.36 (s, 6H), 2.29 (s, 6H), 1.97 (s, 12H), 1.94 (s, 12H).

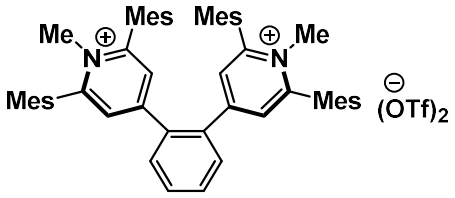


4-(2-(2,6-Dimesityl-1-methyl-1,4-dihydropyridin-4-yl)phenyl)-2,6-dimesitylpyridine (12) The pyridinium trifluoromethanesulfonate salt **11** (310 mg, 0.36 mmol) was placed under a nitrogen atmosphere and dissolved in dry ethanol (30 mL). To this solution, sodium borohydride (409 mg, 10.8 mmol) was added, and the resulting mixture was refluxed overnight with stirring. After the solvent was evaporated, the residue was redissolved in ethyl acetate, washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude product was recrystallized from dichloromethane/hexane to afford **12** as a white solid (226 mg, 88%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 8.03 (d, 1H, J = 7.8 Hz), 7.52 (td, 1H, J = 7.2 Hz, 2.2 Hz), 7.28-7.21 (m, 2H), 7.08 (s, 2H), 6.87 (s,

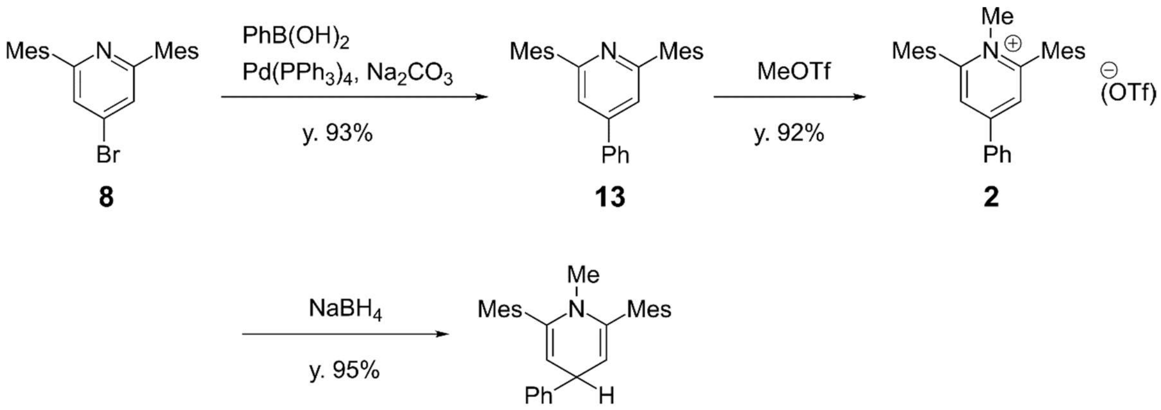
4H), 6.84 (s, 2H), 6.82 (s,2H), 4.81 (t, 1H, J = 3.3 Hz), 4.20 (d, 2H, *J* = 3.3 Hz), 2.32 (s, 6H), 2.28 (s, 12H), 2.25 (s, 6H), 2.21 (s, 3H), 2.07 (s,12H).



4-(2-(2,6-Dimesityl-1-methyl-1,4-dihydropyridin-4-yl)phenyl)-2,6-dimesityl-1-methylpyridin-1-ium trifluoromethanesulfonate (1) The pyridine-dihydropyridine dyad **12** (201 mg, 0.279 mmol) and 2,6-di-*tert*-butyl-4-methylpyridine (DTBMP) (57 mg, 0.28 mmol) were dissolved in dry dichloromethane (5 mL) and then methyl trifluoromethanesulfonate (32 μL, 0.28 mmol) was added to the solution. The mixture was stirred overnight at room temperature under nitrogen atmosphere, and then the reaction was quenched with methanol. The precipitated unreacted pyridine **12** was filtered off, and the filtrate was concentrated in vacuo. The residue was washed with hexane to remove DTBMP, and then dried under vacuum to yield **1** as an orange solid (219 mg, 89%): ^{1}H NMR (300 MHz, chloroform-*d*, 30 °C) δ (ppm) = 8.11 (d, 1H, *J* = 9.0 Hz), 7.70-7.66 (m, 3H), 7.41-7.29 (m, 2H), 7.08 (s, 4H), 6.87 (s, 2H), 6.84 (s, 2H), 4.75 (t, 1H, *J* = 3.3 Hz), 4.14 (d, 2H, *J* = 3.3 Hz), 3.71 (s, 3H), 2.37 (s, 6H), 2.31 (s, 6H), 2.26 (s, 12H), 2.23 (s, 3H), 2.10 (s, 12H); ^{1}H NMR (400 MHz, acetone-d_6, 25 °C) δ (ppm) = 8.25 (s, 2H), 8.20 (dd, 1H, *J* = 7.7 Hz, 1.1 Hz), 7.77 (ddd, 1H, *J* = 7.7 Hz, 7.7 Hz, 1.1 Hz), 7.60 (dd, 1H, *J* = 7.7 Hz, 1.1 Hz), 7.44 (ddd, 1H, *J* = 7.7 Hz, 7.7 Hz, 1.1 Hz), 7.19 (s, 4H), 6.88 (s, 2H), 6.88 (s, 2H), 4.98 (t, 1H, *J* = 3.4 Hz), 4.25 (d, 2H, *J* = 3.4 Hz), 3.81 (s, 3H), 2.38 (s, 6H), 2.34 (s, 6H), 2.29 (s, 6H), 2.24 (s, 3H), 2.23 (s, 6H), 2.19 (s, 12H); ^{1}H NMR (500 MHz, acetonitrile-d_3, 30 °C) δ (ppm) = 8.13 (dd, 1H, *J* = 7.7 Hz, 1.3 Hz), 7.89 (s, 2H), 7.69 (ddd, 1H, *J* = 7.7 Hz, 7.7 Hz, 1.3 Hz), 7.45 (dd, 1H, *J* = 7.7 Hz, 1.3 Hz), 7.39 (ddd, 1H, *J* = 7.7 Hz, 7.7 Hz, 1.3 Hz), 7.14 (s, 4H), 6.88 (s, 2H), 6.87 (s, 2H), 4.81 (t, 1H, *J* = 3.1 Hz), 4.16 (d, 2H, *J* = 3.1 Hz), 3.52 (s, 3H), 2.36 (s, 6H), 2.30 (s, 6H), 2.25 (s, 6H), 2.23 (s, 6H), 2.17 (s, 3H), 2.06 (s, 12H).



4,4'-(1,2-Phenylene)bis(2,6-dimesityl-1-methylpyridin-1-ium) trifluoromethanesulfonate (14) The pyridine **10** (323 mg, 0.458 mmol) was dissolved in dry dichloroethane (40 mL) and then methyl trifluoromethanesulfonate (1.0 mL, 9.1 mmol) was added to the solution. After the mixture was refluxed overnight with stirring under nitrogen atmosphere, the resulting mixture was quenched with methanol and concentrated in vacuo. The residue was purified by column chromatography on alumina (methanol/ethyl acetate = 1/9, then methanol) to yield **14** as a white solid (383 mg, 81%): ^{1}H NMR (300 MHz, chloroform-*d*) δ (ppm) = 8.08 (s, 4H), 7.73 (AA'BB', 2H), 7.58 (AA'BB', 2H), 7.06 (s, 8H), 3.61 (s, 6H), 2.37 (s, 12H), 1.97 (s, 24H); ^{1}H NMR (500 MHz, acetone-d_6) δ (ppm) = 8.42 (s, 4H), 7.92 (AA'BB', 2H), 7.84 (AA'BB', 2H), 7.19 (s, 8H), 3.85 (s, 6H), 2.38 (s, 12H), 2.11 (s, 24H); ^{1}H NMR (500 MHz, acetonitrile-d_3) δ (ppm) = 7.98 (s, 4H), 7.77 (AA'BB', 2H), 7.67 (AA'BB', 2H), 7.14 (s, 8H), 3.53 (s, 6H), 2.37 (s, 12H), 1.93 (s, 24H).



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Scheme S1. Synthetic route to the reference compounds **2** and **3**.

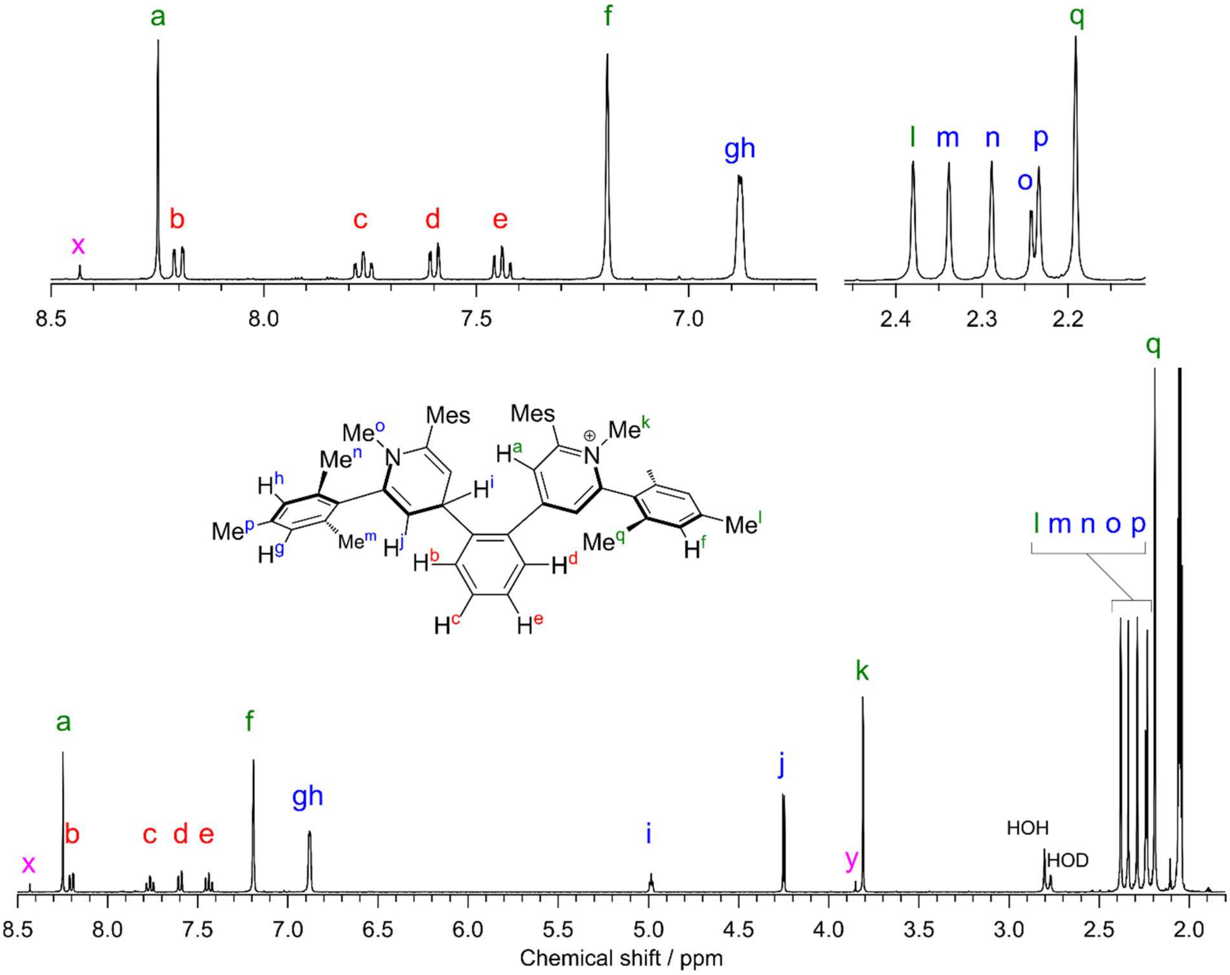


Figure S1. 400 MHz ^{1}H-NMR spectrum of **1** in acetone-d_6. Spectral asignment and conformational analysis were achieved by combining the NOESY experiments.

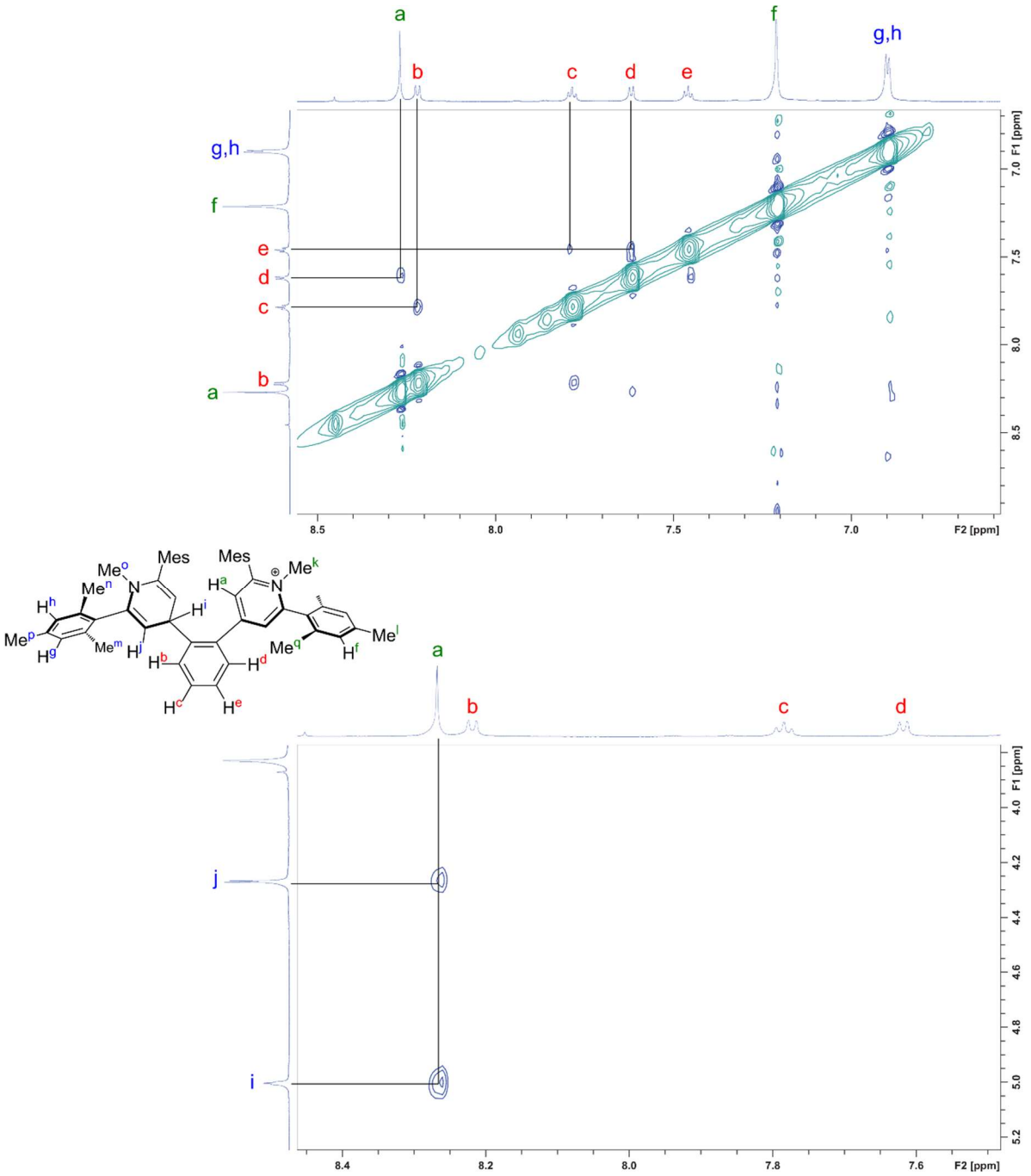


Figure S2. 700 MHz NOESY spectra of **1** in acetone-d_6 at room temperature.

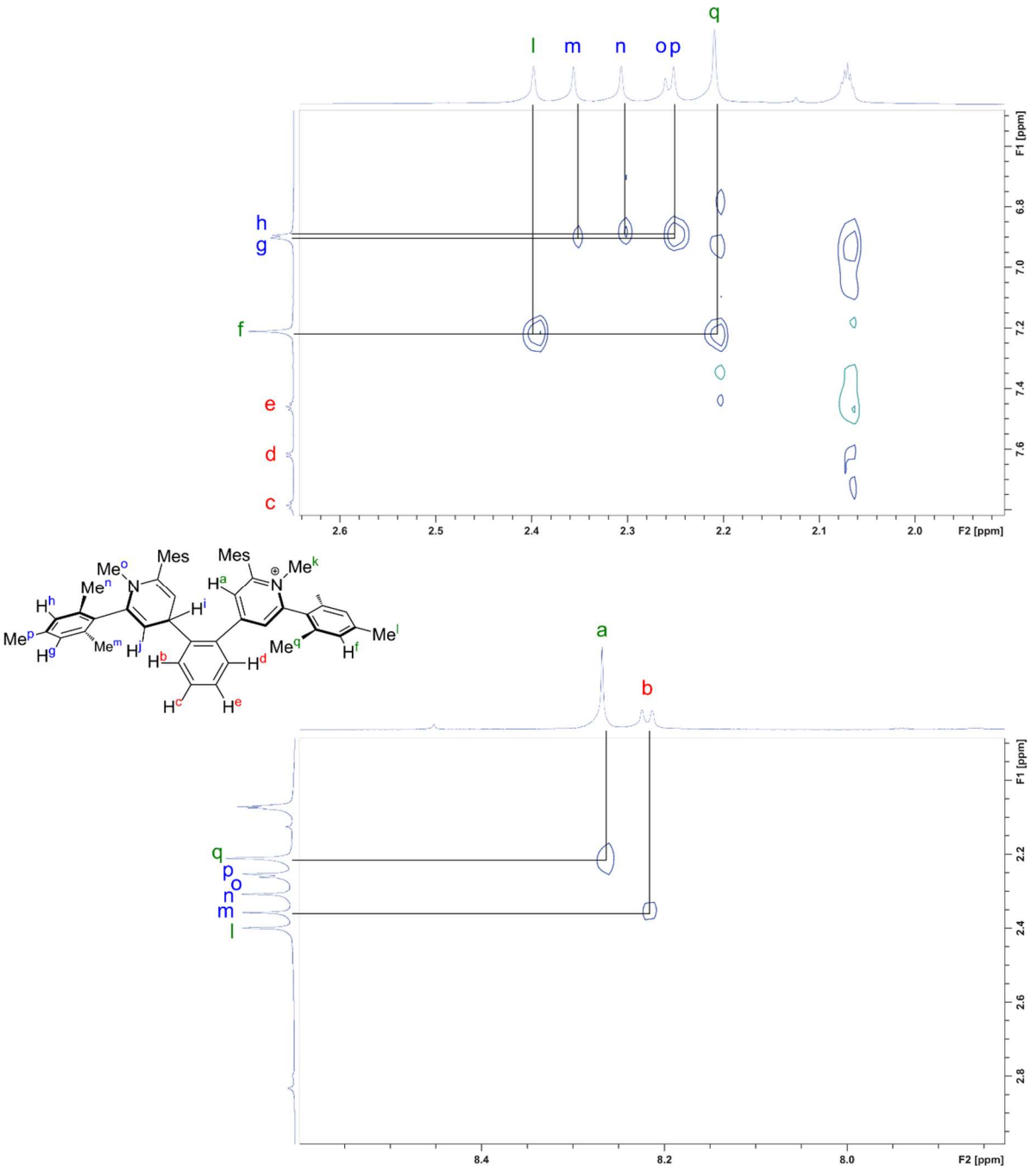


Figure S2. (continued)

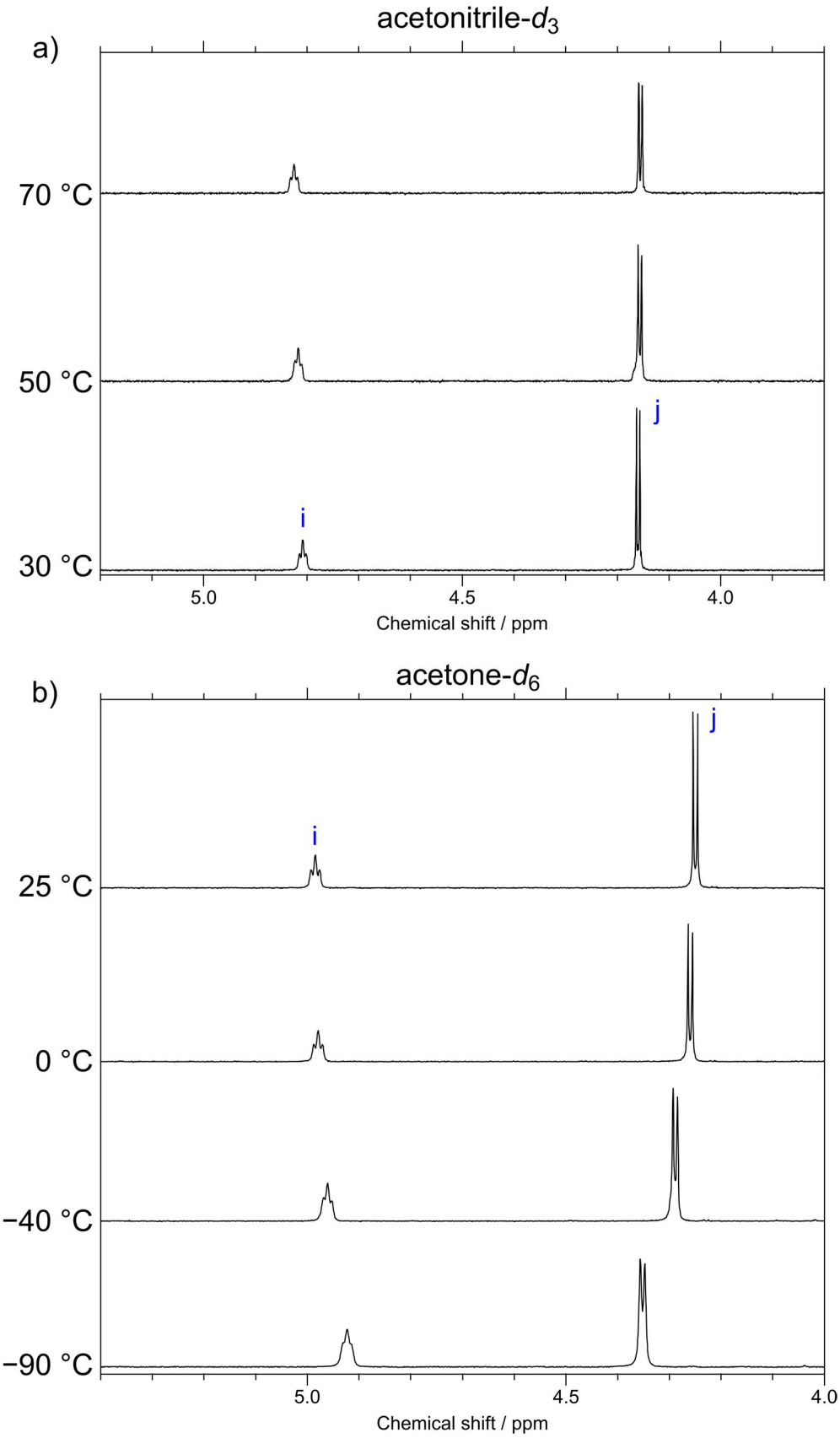


Figure S3. Variable temperature ^{1}H-NMR spectra (methine and vinylene proton region) of **1** in a) acetonitrile-d_3 (500 MHz) and b) acetone-d_6 (400 MHz).

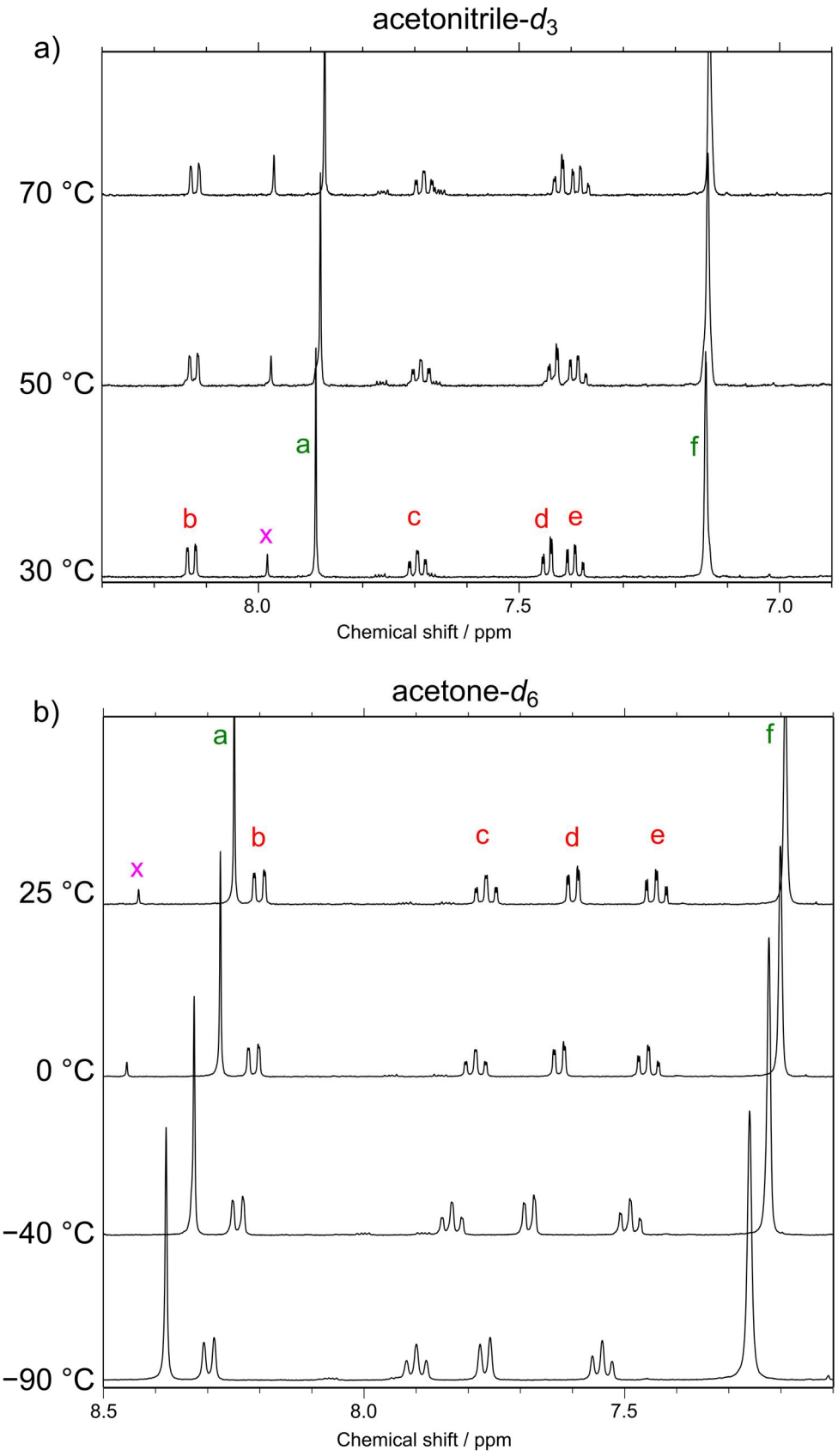


Figure S4. Variable temperature ^{1}H-NMR spectra (aromatic proton region) of **1** in a) acetonitrile-d_3 (500 MHz) and b) acetone-d_6 (400 MHz).

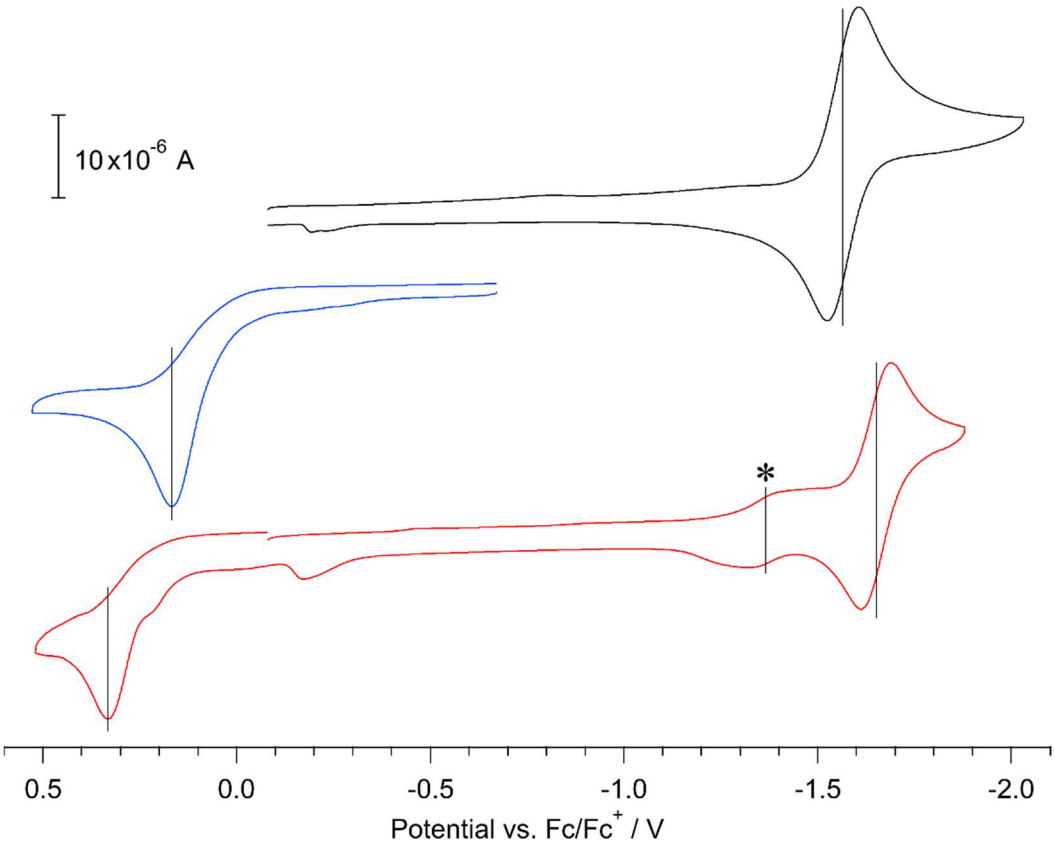
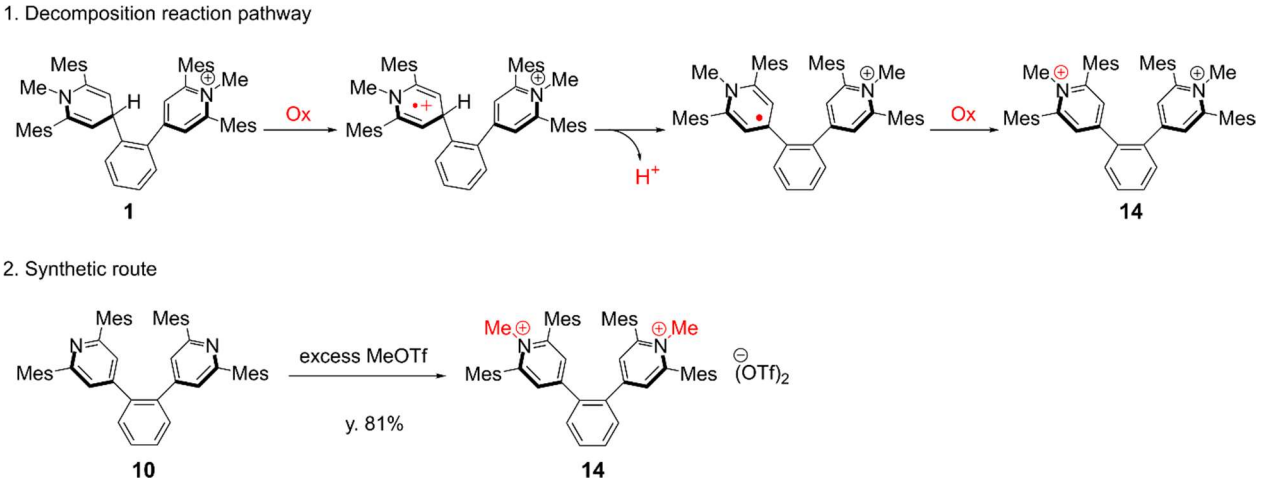


Figure S5. Cyclic voltammograms of **1** (red), **2** (black), and **3** (blue) measured in dichloromethane at a scan rate of 0.1 V/sec. The star symbol in the voltammogram is the redox process derived from the contaminated dication **14**. The Coulomb repulsion between the two pyridinium moieties in **14** is accounted for its higher reduction potential. See ref. 12.

Table S1. Redox potentials (V vs. Fc/Fc^{+}) of **1**, **2**, and **3** in dichloromethane at room temperature.

	E_1 [a]	E_2
1	0.32	−1.66
2	n/a	−1.57
3	0.17	n/a

[a] Oxidation peak potential (irreversible).



Scheme S2. Possible decomposition process and synthetic route of **1**.

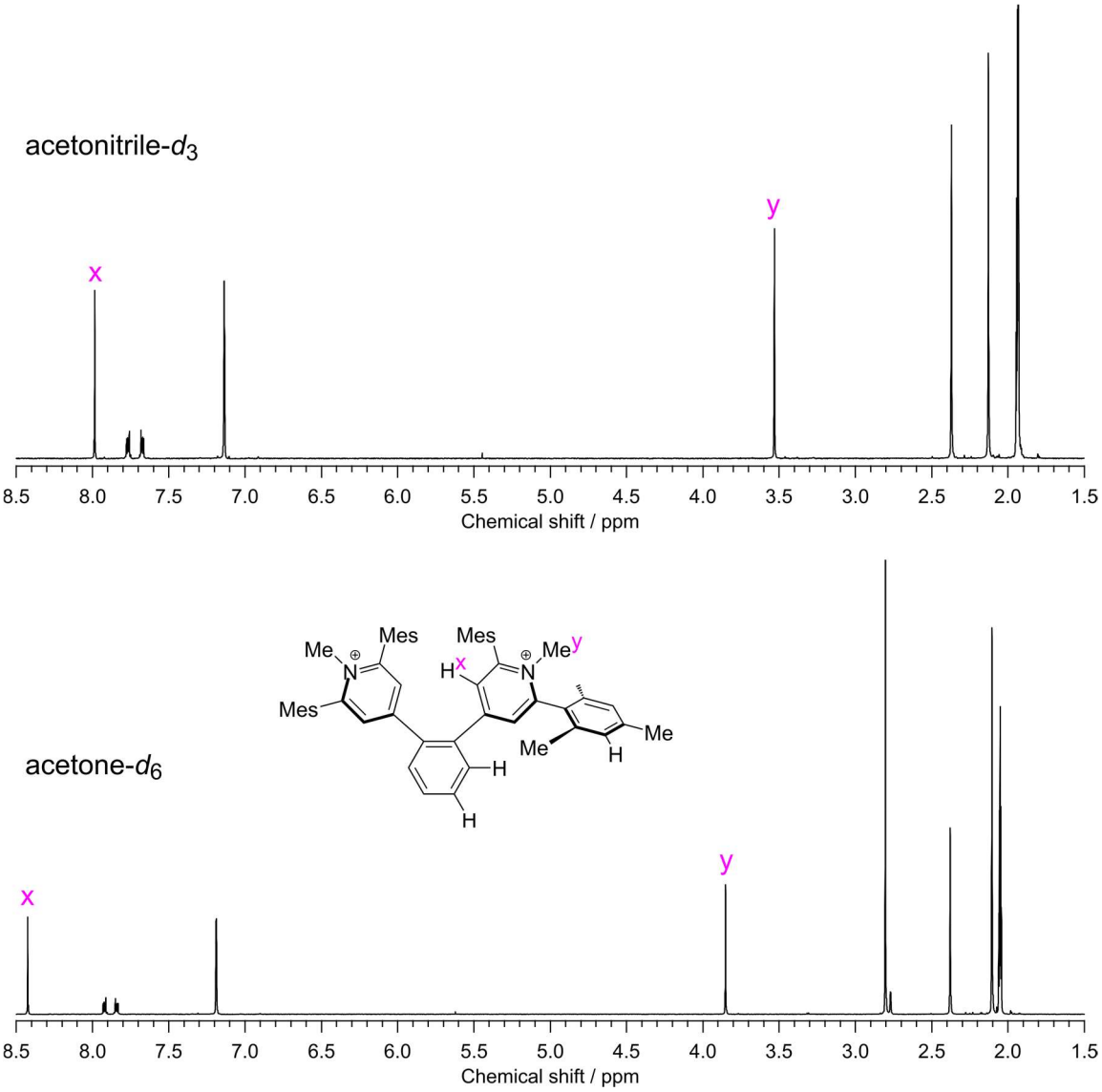


Figure S6. 500 MHz ^{1}H-NMR spectra of the independently synthesized dication **14** in acetonitrile-d_3 and acetone-d_6.

Table S2. Optimized geometries and Hartree-Fock energies of **1** at the CAM-B3LYP-D3/6-31G** level of theory. *E*(RCAM-B3LYP) = −2200.540057 a.u.

C	0.361508	-1.256991	2.037336	H	1.461122	-2.648331	4.944629
C	-1.002084	-1.143811	2.366569	H	2.272612	-1.895476	2.732489
C	-1.463120	-1.601147	3.609047	H	1.202653	1.291108	1.346742
C	-0.587884	-2.134663	4.539057	H	0.089013	-0.737855	-0.008049
C	0.764223	-2.231513	4.225161	H	1.532469	-2.885321	0.037740
C	1.222443	-1.802135	2.988485	H	5.267790	0.973741	-0.662401
N	3.672677	-0.305171	-0.254772	H	5.212868	-0.470266	-1.680977
C	2.932488	0.685129	0.384819	H	5.761812	-0.595919	-0.005897
C	1.674828	0.475257	0.809830	H	5.539117	3.543894	2.937462
C	0.937227	-0.836033	0.685068	H	3.907757	5.101090	-0.693778
C	1.882226	-1.862070	0.118241	H	5.088239	1.352240	3.652737
C	3.118342	-1.589405	-0.320763	H	5.128267	0.219623	2.298966
C	5.053468	-0.091478	-0.671005	H	3.592308	0.602958	3.064161
C	3.586989	2.002141	0.635410	H	5.319735	6.104787	2.465238
C	4.357747	2.171794	1.796575	H	5.087409	6.582746	0.777878
C	4.945291	3.407523	2.037520	H	6.548911	5.720762	1.264454
C	4.795807	4.475084	1.152762	H	2.710658	1.906100	-1.956712
C	4.031753	4.280525	0.007856	H	2.848262	3.645734	-2.258178
C	3.421149	3.057645	-0.266702	H	1.520143	3.014257	-1.282395
C	4.551759	1.029346	2.759012	H	4.746232	-4.004348	-3.930500
C	5.468998	5.792838	1.428109	H	6.193556	-5.056869	-0.047729
C	2.584213	2.895430	-1.509531	H	3.189601	-2.270477	-4.239479
C	3.966735	-2.658906	-0.919912	H	3.358468	-0.931157	-3.096532
C	3.951868	-2.854578	-2.307782	H	2.036456	-2.069518	-2.907260
C	4.751548	-3.852094	-2.854428	H	5.800355	-6.652831	-2.831836
C	5.562048	-4.658141	-2.057066	H	7.236554	-6.021812	-2.025766
C	5.561597	-4.441687	-0.682495	H	6.798500	-5.446944	-3.640676
C	4.774067	-3.452542	-0.098143	H	4.893295	-2.196646	1.661326
C	3.089872	-1.988899	-3.189782	H	5.601084	-3.805985	1.862422
C	6.397793	-5.749581	-2.670106	H	3.845458	-3.595328	1.841055
C	4.784408	-3.252578	1.395452	H	-3.477303	-2.100988	1.691461
N	-3.821072	0.503585	-0.370952	H	-0.847017	1.210933	0.944309
C	-4.125080	-0.643367	0.304662	H	-4.947338	0.185806	-2.116775
C	-3.220215	-1.170127	1.201214	H	-4.334828	1.843817	-1.896591
C	-1.987217	-0.554789	1.439741	H	-5.712039	1.253656	-0.929592
C	-1.754657	0.650290	0.773123	H	-8.642917	-1.254850	1.079819
C	-2.654501	1.170997	-0.132723	H	-6.794081	-3.737860	-1.870963
C	-4.766972	0.982850	-1.397658	H	-5.791723	-0.124680	2.630696
C	-5.426376	-1.306052	0.037925	H	-7.435952	0.389428	2.245986
C	-6.555014	-0.908953	0.768482	H	-6.061507	1.107940	1.407267
C	-7.762294	-1.550575	0.517025	H	-9.803334	-3.284197	0.198425
C	-7.869286	-2.566076	-0.431961	H	-9.066201	-4.232446	-1.101439
C	-6.726825	-2.942432	-1.134631	H	-9.762550	-2.649091	-1.445138
C	-5.497334	-2.329545	-0.915795	H	-3.523197	-3.204303	-1.017346
C	-6.458210	0.171683	1.814878	H	-3.789215	-1.923866	-2.192417
C	-9.194222	-3.222874	-0.706007	H	-4.526855	-3.506726	-2.437166
C	-4.273054	-2.763167	-1.680861	H	-0.274853	3.654597	-3.223581
C	-2.340306	2.439438	-0.837877	H	-3.060338	5.744971	-0.742983
C	-1.357996	2.436075	-1.839988	H	-0.198888	1.286134	-3.240736
C	-1.029583	3.646899	-2.442585	H	-1.304621	0.306254	-2.275242
C	-1.632740	4.844618	-2.067371	H	0.174168	0.946172	-1.553950
C	-2.592818	4.816558	-1.057630	H	-1.904286	6.295281	-3.628945
C	-2.961513	3.631524	-0.432131	H	-0.233475	6.126501	-3.092093
C	-0.640593	1.174376	-2.249214	H	-1.406846	6.990251	-2.086626
C	-1.270780	6.134241	-2.750732	H	-4.957085	3.236789	0.308617
C	-3.999888	3.637274	0.660343	H	-4.188132	4.651888	1.013359
H	-2.515706	-1.502733	3.856545	H	-3.689262	3.037028	1.520227
H	-0.955561	-2.468513	5.502856				

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