Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Photoinduced Generation of Carbocations Enabled by the Promotion of Aromaticity

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1. General Methods

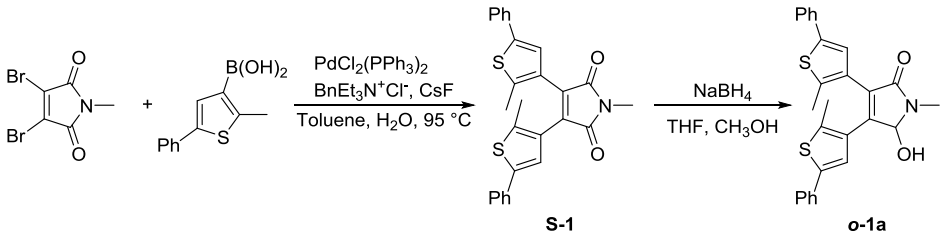
^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker Biospin avance III spectrometer. Deuterated reagents for characterization and *in situ* reactions were purchased from Sigma-Aldrich Chemical Co. and Cambridge Isotope Laboratories, Inc. (purity ≥ 99.9%). The chemical shifts (δ) for ^{1}H NMR spectra, given in ppm, are referenced to the residual proton signal of the deuterated solvent. Mass spectra were recorded on a Bruker IMPACT-II or ThermoScientificLCQ Fleet spectrometer. Crystallographic data was collected on a Mercury single crystal diffractometer. The structures were solved with direct methods by using OlexSys or SHELXS-97 and refined with the full-matrix least-squares technique based on F2. The UV-Vis spectra were recorded on a Perkin-Elmer Lambda 365 spectrometer.

Irradiation experiments*:* The UV and visible light irradiation experiments were carried out on a CEL−HXF300 xenon lamp with bandpass filters at 313 ± 10 and 650 ± 10 nm, respectively. The light intensity was adjusted to tune the time.

Computations*:* Density functional theory (DFT) calculations were performed by using Gaussian 09 packages. The method and basis set of M06-2X-D3/def2-TZVP with an ultrafine integration grid were utilized for the optimization and frequency analysis. The polarizable continuum model (PCM) was included for acetonitrile. By frequency analysis the number of imaginary frequencies for minima and transition state is 0 and 1, respectively. Eletrostatic potential map and NPA charge were generated by G09 and shown by VMD (version: 1.90).[S1] The anisotropy of the current induced density (ACID) calculations[S2] was carried out by ACID packages (version: 2.0) and the visualization of ACID was presented by POV-Ray (version: 3.7) with isosurface = 0.05. The nucleus-independent chemical shift (NICS) calculation was conducted at M06-2X/def2-TZVP level.

2. Synthesis and Characterization

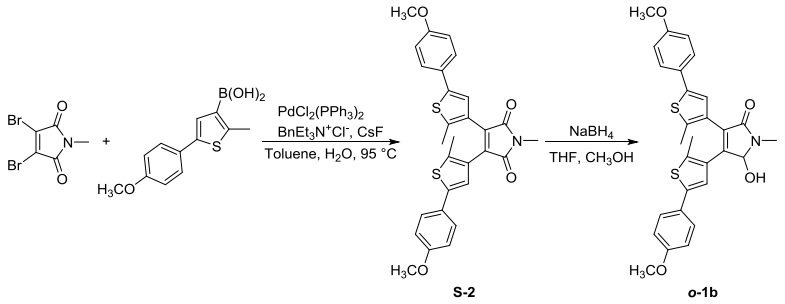
Scheme S1. Synthesis of ***o*-1a**



S-1: (2-Methyl-5-phenylthiophen-3-yl)boronic acid (prepared according to the literature procedure,[S3] 1.40 g, 6.74 mmol), 2,3-dibromo-*N*-methylmaleimide (prepared according to the literature procedure,[S4] 0.60 g, 2.25 mmol), cesium fluoride (1.37 g, 8.99 mmol), $PdCl_2(PPh_3)_2$ (0.08 g, 0.11 mmol), $BnEt_3N^+Cl^-$ (0.03 g, 0.11 mmol) were dissolved in a mixture of toluene (15 mL) and water (15 mL). The flask was degassed with nitrogen for 3 times. The reaction mixture was refluxed at 95 ℃ for 15 h, quenched with 50 mL of saturated aqueous sodium chloride solution, and extracted with ethyl acetate (3 × 50 mL). The organic layers were dried over Na_2SO_4, evaporated, and then purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:50 to 1:30) to give the product **S-1** (0.63 g, 62%) as a green solid. MP: 188.7-189.3 ℃. ^{1}H NMR (CD_3CN): δ = 7.56-7.54 (m, 4H), 7.38-7.34 (m, 4H), 7.29-7.26 (m, 4H), 3.04 (s, 3H), 2.02 (s, 6H). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 170.9, 141.4, 141.2, 133.7, 133.1, 129.0, 127.8, 127.7, 125.6, 124.2, 24.0, 16.4. ESI-HRMS: m/z calcd for $C_{27}H_{22}NO_2S_2$ $[M + H]^+$: 456.1092; found: 456.1086.

***o*-1a**: **S-1** (0.63 g, 1.39 mmol) was dissolved in a mixture of THF (25 mL) and methanol (10 mL), and the solution was stirred for 5 min. $NaBH_4$ (0.05 g, 1.39 mmol) was then added, and the reaction mixture was stirred for 30 min. The reaction mixture was quenched with 2 M HCl (20 mL) and extracted with ethyl acetate (3 × 40 mL). The organic layers were dried over Na_2SO_4, evaporated, and then purified by silica gel column chromatography (ethyl acetate/petroleum ether, 1:3) to give the product ***o*-1a** (0.58 g, 91%) as a white solid. MP: 210.7-211.3 ℃. ^{1}H NMR (CD_3CN): δ = 7.58 (d, *J* = 7.2 Hz, 4H), 7.43-7.37 (m, 4H), 7.34-7.28 (m, 3H), 7.25 (s, 1H), 5.72 (s, 1H), 4.23 (s, 1H), 3.03 (s, 3H), 2.10 (s, 3H), 2.05 (s, 3H). $^{13}C\{^1H\}$ NMR (CD_3CN): δ = 169.0, 146.4, 141.3, 140.7, 139.6, 138.7, 134.2, 133.8, 130.6, 129.4, 129.1, 128.9, 127.7, 127.3, 125.6, 125.5, 124.7, 123.1, 84.7, 77.4, 26.8, 14.85, 14.77. ESI-HRMS: m/z calcd for $C_{27}H_{24}NO_2S_2$ $[M + H]^+$: 458.1248; found: 458.1252.

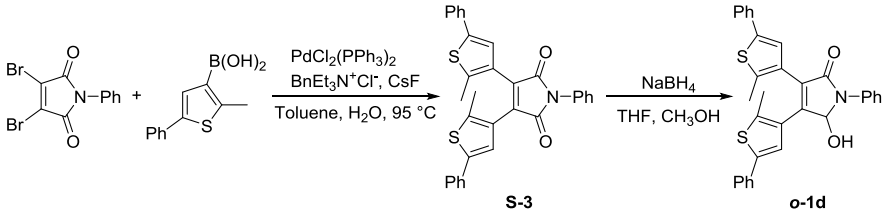
Scheme S2. Synthesis of ***o*-1b**



S-2: Following the procedure of **S-1** with 2,3-dibromo-*N*-methylmaleimide (0.60 g, 2.25 mmol) and (5-(4-methoxyphenyl)-2-methylthiophen-3-yl)boronic acid (prepared according to the literature procedure,[S5] 1.40 g, 6.74 mmol) and purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:40 to 1:20), compound **S-2** was obtained (0.64 g, 55%) as a red solid. MP: 167.3-168.0 ℃. ^{1}H NMR ($CDCl_3$): δ = 7.48-7.44 (m, 4H), 7.17 (s, 2H), 6.91-6.87 (m, 4H), 3.82 (s, 6H), 3.15 (s, 3H), 1.99 (s, 6H). ^{13}C{^{1}H} NMR (CD_3CN): δ = 170.8, 159.5, 140.7, 139.7, 133.8, 128.2, 126.7, 126.3, 123.4, 114.5, 55.1, 23.7, 14.0. ESI-HRMS: m/z calcd for $C_{29}H_{25}NNaO_4S_2$ [M + Na]$^{+}$: 538.1123; found: 538.1116.

***o*-1b**: Following the procedure of ***o*-1a** with **S-2** (0.64 g, 1.24 mmol) and $NaBH_4$ (0.05 g, 1.24 mmol) and purified by silica gel column chromatography (ethyl acetate/petroleum ether, 1:5) compound ***o*-1b** was obtained (0.61 g, 90%) as a white solid. MP: 192.9-193.4 ℃. ^{1}H NMR (CD_3CN): δ = 7.38 (d, *J* = 8.4 Hz, 4H), 7.08 (s, 1H) 6.99 (s, 1H) 6.86-6.82 (m, 4H), 5.59 (d, *J* = 9.6 Hz, 1H), 4.06 (d, *J* = 9.6 Hz, 1H), 3.71 (d, *J* = 2.8 Hz, 6H), 2.91 (s, 3H), 1.97 (s, 3H), 1.92 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 169.1, 159.3, 159.0, 146.4, 141.2, 140.5, 138.7, 137.6, 130.4, 129.3, 129.0, 127.2, 126.85, 126.83, 126.6, 123.7, 122.0, 114.4, 114.3, 84.7, 77.3, 55.4, 26.8, 14.8, 14.7. ESI-HRMS: m/z calcd for $C_{29}H_{27}NNaO_4S_2$ [M + Na]$^{+}$: 540.1279; found: 540.1276.

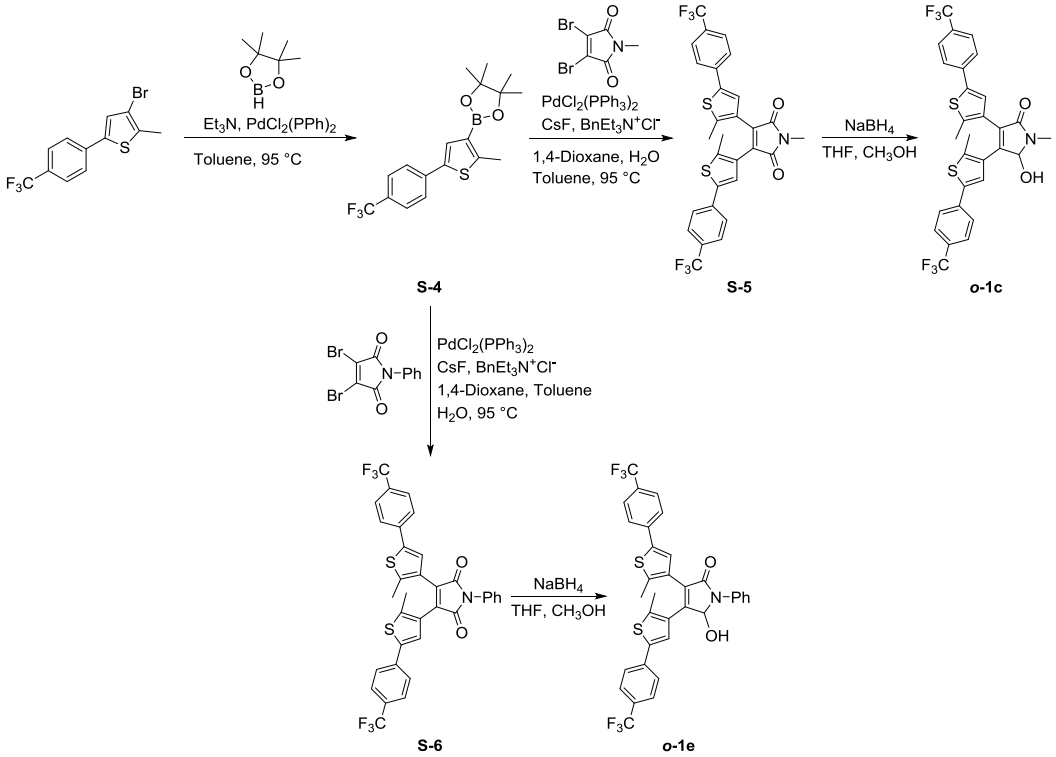
Scheme S3. Synthesis of ***o*-1d**



S-3: Following the procedure of **S-1** with (2-methyl-5-phenylthiophen-3-yl)boronic acid (1.40 g, 6.74 mmol) and 3,4-dibromo-1-phenyl-pyrrole-2,5-dione (prepared according to the literature procedure,[S6] 0.74 g, 2.25 mmol) and purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:50 to 1:30), compound **S-3** was obtained (0.52 g, 45%) as a green solid. MP: 179.1-179.8 ℃. ^{1}H NMR (CD_3CN): δ = 7.63-7.56 (m, 6H), 7.50 (t, *J* = 7.2 Hz, 3H), 7.45-7.39 (m, 6H), 7.34 (t, *J* = 7.2 Hz, 2H), 2.13 (s, 6H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 169.7, 141.7, 141.6, 133.7, 133.0, 131.9, 129.2, 129.1, 127.9, 127.8, 127.7, 126.2, 125.7, 124.4, 15.3. ESI-HRMS: m/z calcd for $C_{32}H_{23}NNaO_2S_2$ $[M + Na]^+$: 540.1068; found: 540.1059.

***o*-1d**: Following the procedure of ***o*-1a** with **S-3** (0.52 g, 1.00 mmol) and $NaBH_4$ (0.04 g, 1.00 mmol) and purified by silica gel column chromatography (CH_2Cl_2/petroleum ether 1:3), compound ***o*-1d** was obtained (0.46 g, 89%) as a white solid. MP: 197.3-198.0 ℃. ^{1}H NMR (CD_3CN): δ = 7.8 (d, *J* = 7.6 Hz, 2H), 7.62-7.60 (m, 4H), 7.50 (t, *J* = 8.0 Hz, 2H), 7.46-7.39 (m, 5H), 7.26-7.24 (m, 4H), 6.49 (d, *J* = 10.0 Hz, 1H), 4.46 (d, *J* = 10.0 Hz, 1H), 2.16 (s, 3H), 2.10 (s, 3H). ^{13}C{^{1}H} NMR (CD_3CN): δ = 167.7, 145.9, 141.7, 140.9, 140.4, 139.1, 137.6, 137.2, 134.2, 133.7, 130.1, 129.3, 129.1, 128.9, 127.8, 127.4, 125.64, 125.61, 125.1, 124.8, 123.0, 121.1, 83.5, 77.3, 15.0, 14.9. ESI-HRMS: m/z calcd for $C_{32}H_{25}NNaO_2S_2$ $[M + Na]^+$: 542.1224; found: 542.1225.

Scheme S4. Synthesis of ***o*-1c** and ***o*-1e**



S-4: 3-Bromo-2-methyl-5-(4-(trifluoromethyl)phenyl)thiophene (prepared according to the literature procedure,[S7] 4.0 g, 12.5 mmol), and $PdCl_2(PPh_3)_2$ (0.44 g, 0.62 mmol) were dissolved in toluene (30 mL). The mixture was degassed by bubbling nitrogen through it for 3 times. Pinacolborane (4.86 g, 38.0 mmol) and Et_3N (10.0 mL, 75.0 mmol) was then added, and the flask was degassed with nitrogen for 3 times .The reaction mixture was refluxed for 20 h, quenched with 50 mL of saturated aqueous sodium chloride solution, and extracted with ethyl acetate (3 × 50 mL). The organic layers were dried over Na_2SO_4, evaporated, and then purified by silica gel column chromatography (petroleum ether) to give the product **S-4** (3.9 g, 84%) as a white solid. MP: 177.7-178.5 ℃. ^{1}H NMR (DMSO-d_6): δ = 7.83 (d, J = 8.4 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H), 7.58 (s, 1H), 2.66 (s, 3H), 1.30 (s, 12H). ^{19}F NMR ($CDCl_3$): δ = -62.42. ^{13}C{^{1}H} NMR (CD_3CN): δ = 153.9, 139.1, 137.8, 130.4, 128.7, 128.4, 125.82, 125.78, 125.74, 125.70, 125.60, 125.56, 122.9, 83.5, 24.9, 16.0. ESI-HRMS: m/z calcd for $C_{29}H_{25}NNaO_4S_2$ $[M + Na]^+$: 369.1307; found: 369.1304.

S-5: **S-4** (1.07 g, 2.92 mmol), 2,3-dibromo-*N*-methylmaleimide (0.26 g, 0.97 mmol), cesium fluoride (0.59 g, 3.89 mmol), $PdCl_2(PPh_3)_2$ (0.07g, 0.01 mmol), $BnEt_3N^+Cl^-$ (0.02 g, 0.01 mmol) were dissolved in a mixture of toluene (15 mL), water (15 mL), and 1,4-dioxane (15 mL). The flask was degassed with nitrogen for 3 times .The reaction mixture was refluxed at 95 ℃ for 15 h, quenched with 50 mL of saturated aqueous sodium chloride solution, and extracted with ethyl acetate (3 × 50 mL). The

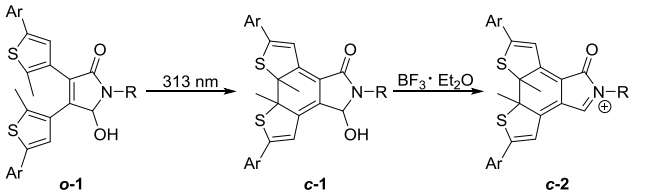
organic layers were dried over Na_2SO_4, evaporated, and then purified by silica gel column chromatography (ethyl acetate/petroleum ether, 1:30) to give the product **S-5** (0.34 g, 58%) as a green solid. MP: 124.9-125.6 ℃. ^{1}H NMR (CD_3CN): δ = 4.77 (d, *J* = 8.4 Hz, 4H), 7.71 (d, *J* = 8.4 Hz, 4H), 7.46 (s, 2H), 3.11 (s, 3H), 2.09 (s, 6H). ^{19}F NMR ($CDCl_3$): δ = -62.56. ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 170.7, 142.6, 139.8, 137.0, 133.1, 129.7, 129.3, 128.1, 126.1, 126.0, 125.7, 24.1, 14.8. ESI-HRMS: m/z calcd for $C_{29}H_{19}F_6NNaO_2S_2$ [M + Na]$^+$: 614.0659; found: 614.0652.

***o*-1c**: Following the procedure of ***o*-1a** with **S-5** (0.20 g, 0.34 mmol) and $NaBH_4$ (0.01 g, 0.34 mmol) and purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:5), compound ***o*-1c** was obtained (0.19 g, 94%) as a white solid. MP: 211.7-212.2 ℃. ^{1}H NMR (CD_3CN): δ = 7.67-7.59 (m, 8H), 7.42 (s, 1H), 7.33 (s, 1H), 5.68 (s, 1H), 4.28 (s, 1H), 2.98 (s, 3H), 2.03 (s, 3H), 1.99 (s, 3H). ^{19}F NMR ($CDCl_3$): δ = -62.51, -62.57. ^{13}C{^{1}H} NMR (CD_3CN): δ = 168.8, 146.3, 141.0, 140.2, 139.8, 139.1, 137.4, 137.0, 130.8, 129.7, 129.1, 128.9, 126.09, 126.05, 125.94, 125.90, 125.55, 125.52, 124.4, 84.8, 77.3, 29.8, 26.8, 14.9, 14.8. ESI-HRMS: m/z calcd for $C_{29}H_{22}F_6NO_2S_2$ [M + H]$^+$: 594.0996; found: 594.0995.

S-6: Following the procedure of **S-5** with 3,4-dibromo-1-phenyl-pyrrole-2,5-dione (0.32 g, 0.97 mmol) and **S-4** (1.07 g, 2.92 mmol) and purified by silica gel column chromatography (ethyl acetate/petroleum ether 1:50 to 1:30), compound **S-6** was obtained (0.22 g, 35%) as a green solid. MP: 110.1-110.9 ℃. ^{1}H NMR ($CDCl_3$): δ = 7.66-7.61 (m, 8H), 7.55-7.48 (m, 6H), 7.44-7.39 (m, 1H), 2.11 (s, 6H). ^{19}F NMR ($CDCl_3$): δ = -62.56. ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 169.3, 143.0, 139.9, 136.9, 132.9, 131.7, 129.2, 128.0, 127.9, 126.04, 125.99, 125.95, 125.7, 125.6, 122.7, 15.3. ESI-HRMS: m/z calcd for $C_{34}H_{22}F_6NO_2S_2$ [M + H]$^+$: 654.0996; found: 654.0986.

***o*-1e**: Following the procedure of ***o*-1a** with **S-6** (0.22 g, 0.33 mmol) and $NaBH_4$ (0.01 g, 0.33 mmol) and purified by silica gel column chromatography (CH_2Cl_2 /petroleum ether 1:3), compound ***o*-1e** was obtained (0.20 g, 92%) as a white solid. MP: 206.4-207.2 ℃. ^{1}H NMR (DMSO-*d*$_6$): δ = 7.84-7.80 (m, 9H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.54 (s, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 6.74 (d, *J* = 10.4 Hz, 1H), 6.68 (d, *J* = 10.0 Hz, 1H), 2.10 (s, 3H), 2.01 (s, 3H). ^{19}F NMR ($CDCl_3$): δ = -62.50, -62.57. ^{13}C{^{1}H} NMR (CD_3CN): δ = 162.2, 140.7, 136.2, 135.1, 145.5, 133.8, 132.0, 131.6, 131.5, 125.1, 124.0, 123.94, 123.87, 120.74, 120.71, 120.67, 120.54, 120.50, 120.46, 120.21, 120.18, 120.0, 119.1, 115.9, 78.2, 71.9, 9.6, 9.5. ESI-HRMS: m/z calcd for $C_{34}H_{23}F_6NNaO_2S_2$ [M + Na]$^+$: 678.0972; found: 678.0963.

Scheme S5. Synthesis of ***c*-2a**, ***c*-2d**, and ***c*-2c**



***c*-2a**: A solution of ***o*-1a** (10.0 mg, 0.021 mmol) in MeCN (1.0 mL) was irradiated at 313 nm for 10 h, and a precipitate formed. The precipitate was filtered, washed with hexane, and dried *in vacuo* to afford ***c*-1a** as a black solid (7.3 mg, 75%). ***c*-1a** (7.3 mg, 0.016 mmol) was dissolved in MeCN (1.0 mL), and then BF_3•Et_2O (2.0 μL, 0.016 mmol) was added. The solution was stored in a desiccator for 3 days, and natural evaporation gave ***c*-2a** as a black solid (8.4 mg, 100%). ^{1}H NMR (CD_3CN): δ = 8.75 (s, 1H), 7.95-7.93 (m, 2H), 7.85-7.83 (m, 2H), 7.77-7.74 (m, 2H), 7.65-7.59 (m, 3H), 7.55-7.51 (m, 3H), 3.51 (s, 3H), 2.01 (s, 3H), 1.94 (s, 3H). ^{13}C{^{1}H} NMR (CD_3CN): δ = 185.6, 177.8, 169.9, 164.9, 162.6, 151.0, 135.6, 133.0, 132.0, 131.8, 130.0, 129.5, 129.1, 128.1, 116.7, 119.6, 115.3, 111.3, 73.9, 69.3, 31.9, 27.2, 27.1. ESI-HRMS: m/z calcd for $C_{27}H_{22}NOS_2^+$ $[M]^+$: 440.1137; found: 440.1137.

***c*-2c**: A solution of ***o*-1c** (2.9 mg, 0.005 mmol) in CD_3CN (0.5 mL) was irradiated at 313 nm for 1.5 h in the NMR tube, and then BF_3•Et_2O (0.63 μL, 0.005 mmol) was added. The solution was illuminated at 313 nm for 20 min, and evaporated to give the product ***c*-2c** (3.3 mg, 100%) as a black solid.^{1}H NMR (CD_3CN): δ = 8.97 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.82 (s, 1H), 7.62 (s, 1H), 3.60 (s, 3H), 2.10 (s, 3H), 2.04(s, 3H). ^{19}F NMR (CD_3CN): δ = 63.61, 63.82, 150.54, 150.60, 151.67, 151.73. ^{13}C{^{1}H} NMR (CD_3CN): δ = 181.6, 177.4, 168.2, 165.2, 162.9, 154.2, 135.9, 135.6, 135.1, 129.9, 129.2, 127.20, 127.16, 126.8, 126.7, 126.1, 126.0, 121.2, 118.4, 117.5, 112.4, 74.2, 70.1, 32.8, 27.6. ESI-HRMS: m/z calcd for $C_{29}H_{20}F_6NOS_2^+$ $[M]^+$: 576.0885; found: 576.0886.

***c*-2d**: Following the procedure of ***c*-2a** with ***o*-1d** (10.0 mg, 0.019 mmol) and BF_3•Et_2O (1.8 μL, 0.015 mmol), compound ***c*-2d** was obtained (7.3 mg, 83%) as a black solid. ^{1}H NMR (CD_3CN): δ = 8.96 (s, 1H), 8.06-8.04 (m, 2H), 7.96 (s, 1H), 7.92-7.84 (m, 3H), 7.72 (t, *J* = 8.0 Hz, 2H), 7.68-7.58 (m, 9H), 2.13 (s, 3H), 2.04 (s, 3H). ^{13}C NMR spectrum of ***c*-2d** was not obtained due to the instability of carbocation. ESI-HRMS: m/z calcd for $C_{32}H_{24}NOS_2^+$ $[M]^+$: 502.1294; found: 502.1291.

^{1}H NMR and ^{13}C NMR Spectra

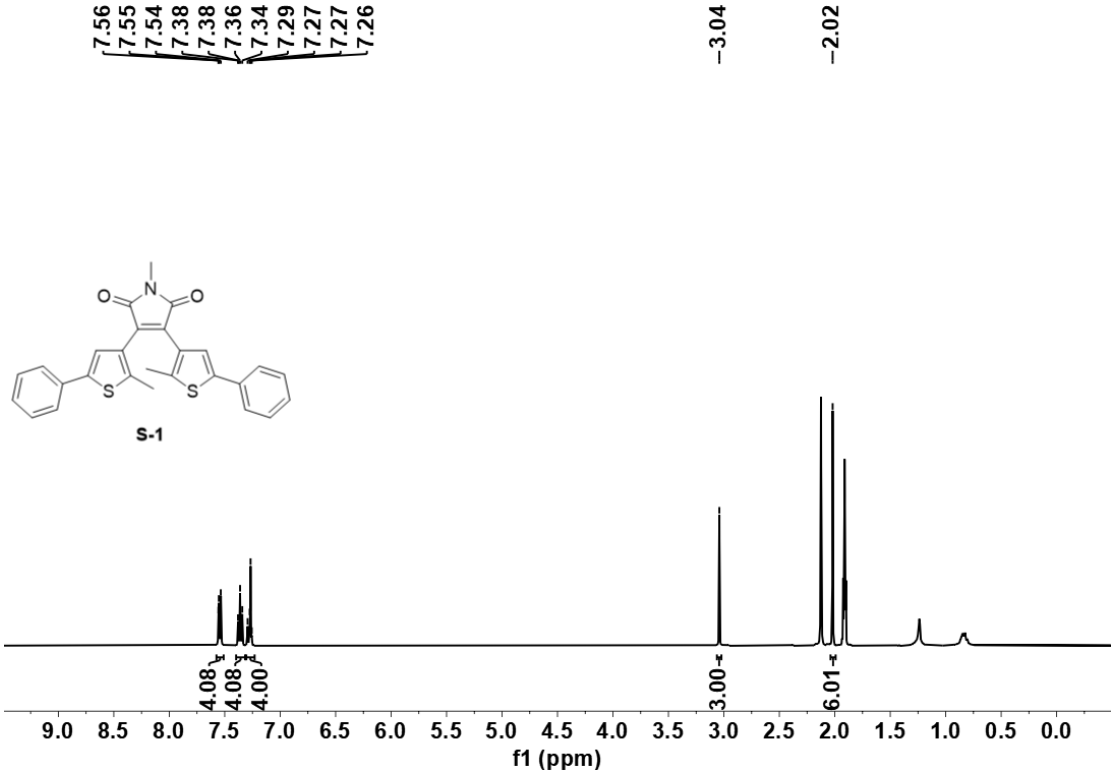


Figure S1. ^{1}H NMR spectrum of **S-1** in CD_3CN.

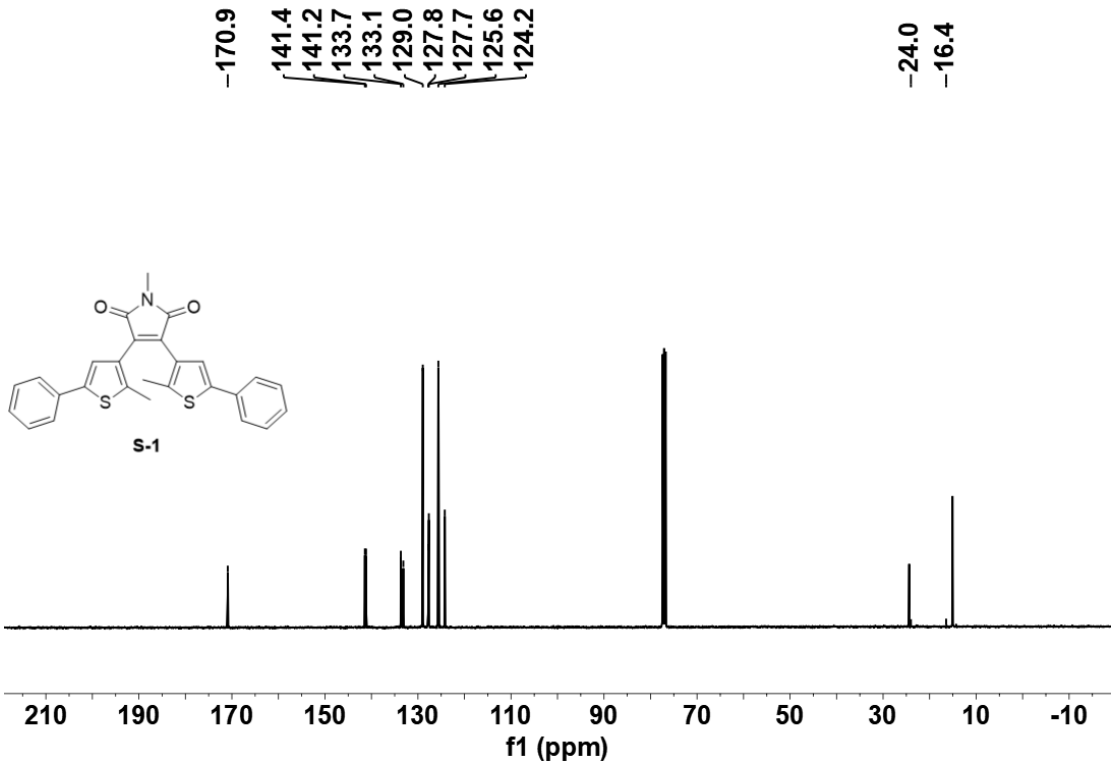


Figure S2. ^{13}C NMR spectrum of **S-1** in $CDCl_3$.

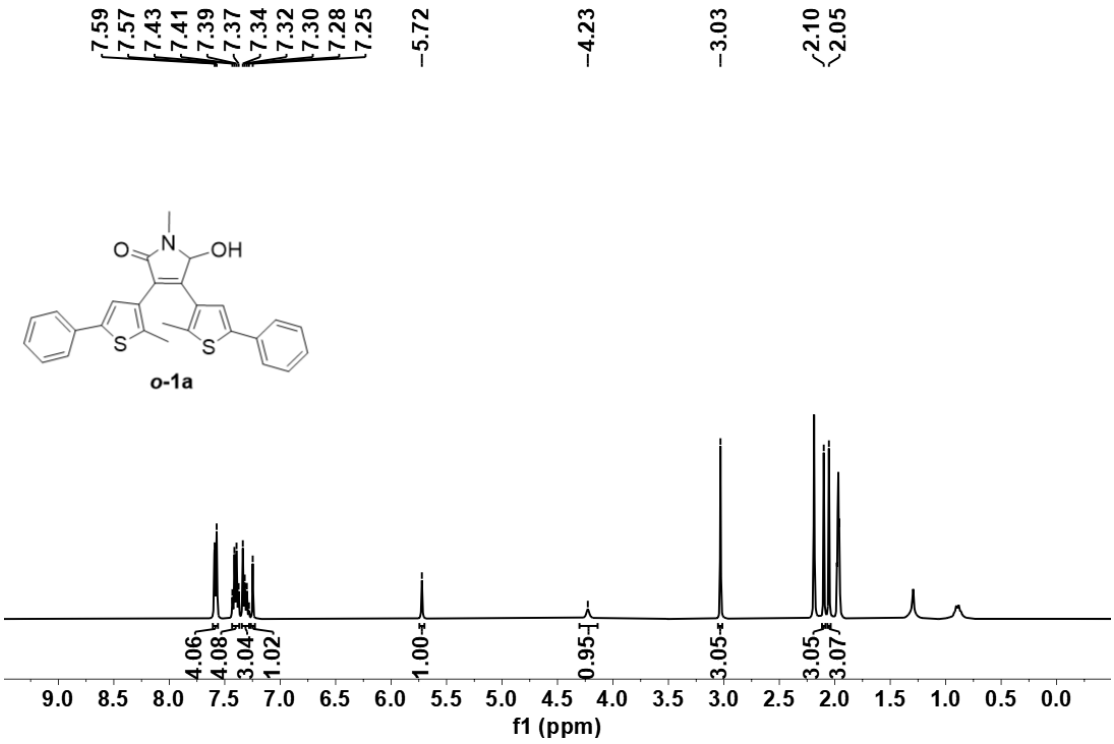


Figure S3. ^{1}H NMR spectrum of ***o*-1a** in CD_3CN.

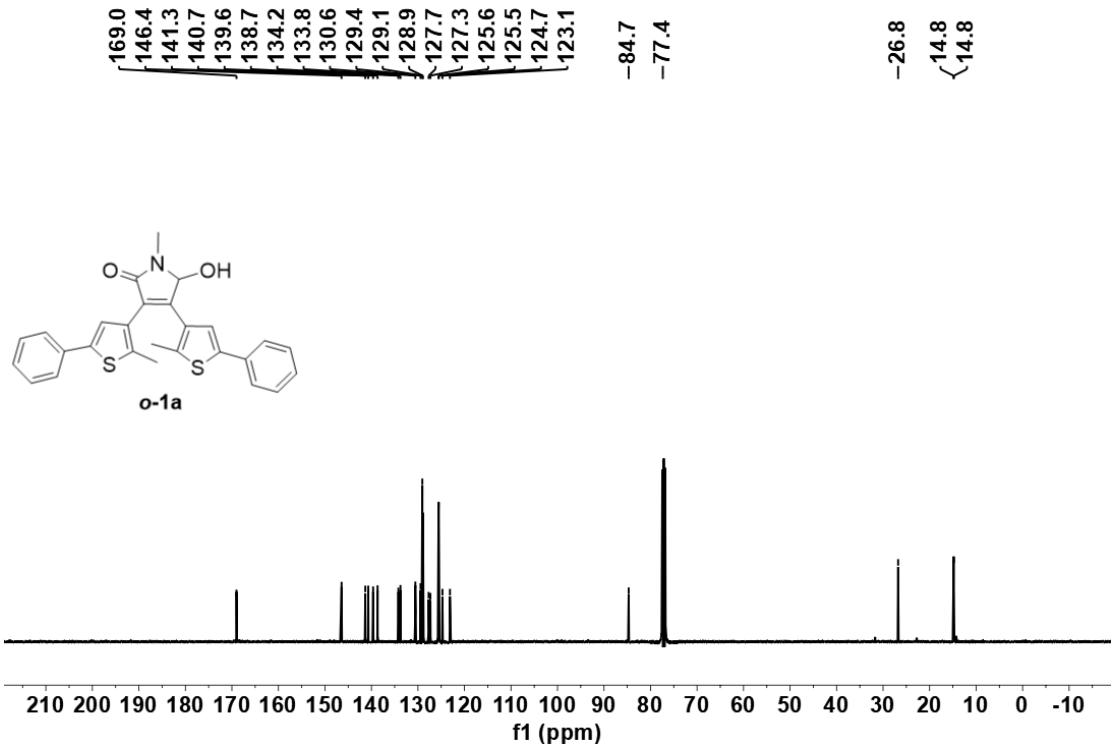


Figure S4. ^{13}C NMR spectrum of ***o*-1a** in $CDCl_3$.

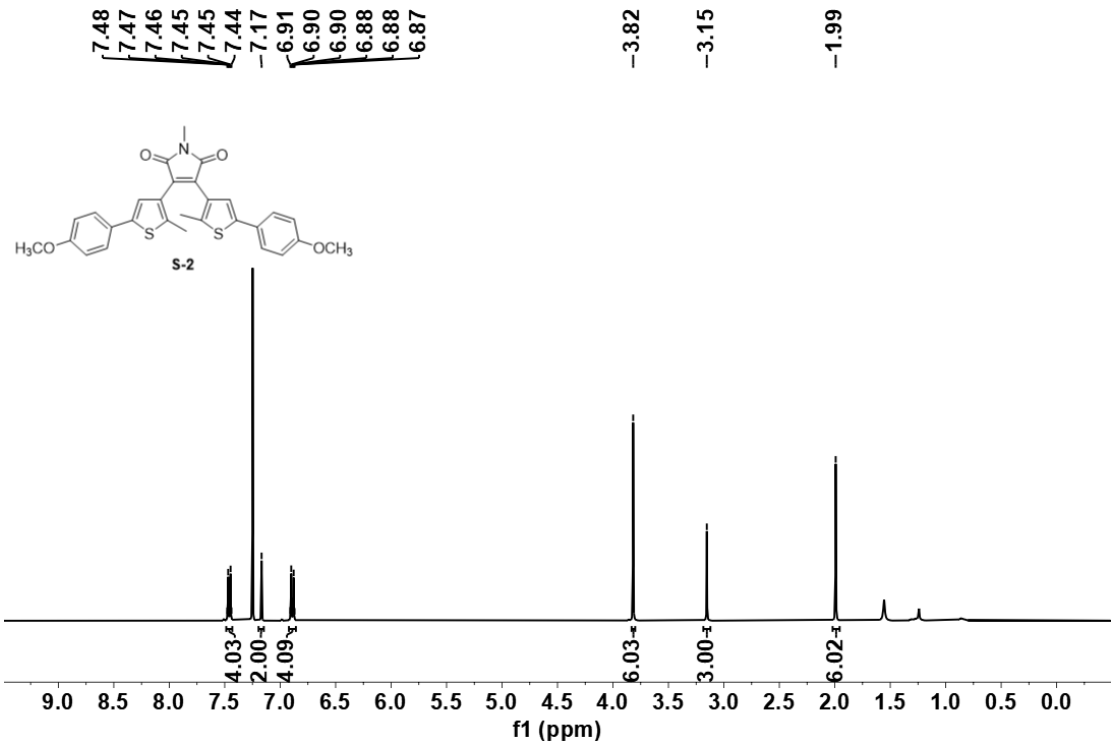


Figure S5. ^{1}H NMR spectrum of **S-2** in $CDCl_3$.

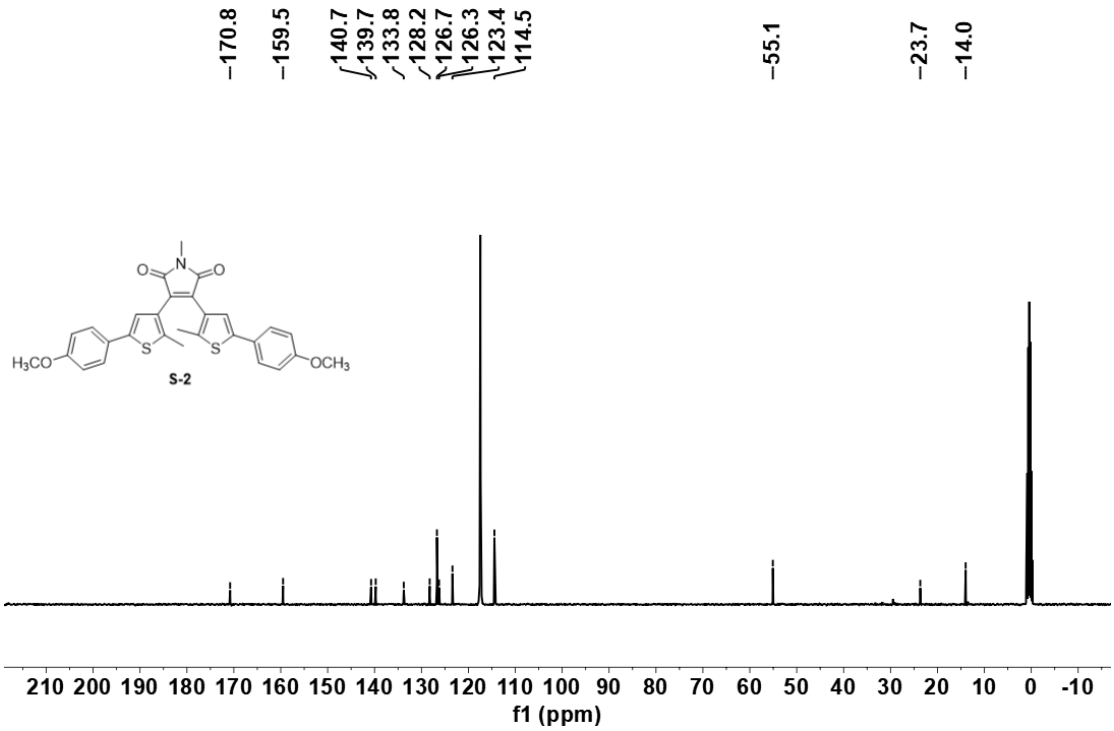


Figure S6. ^{13}C NMR spectrum of **S-2** in CD_3CN.

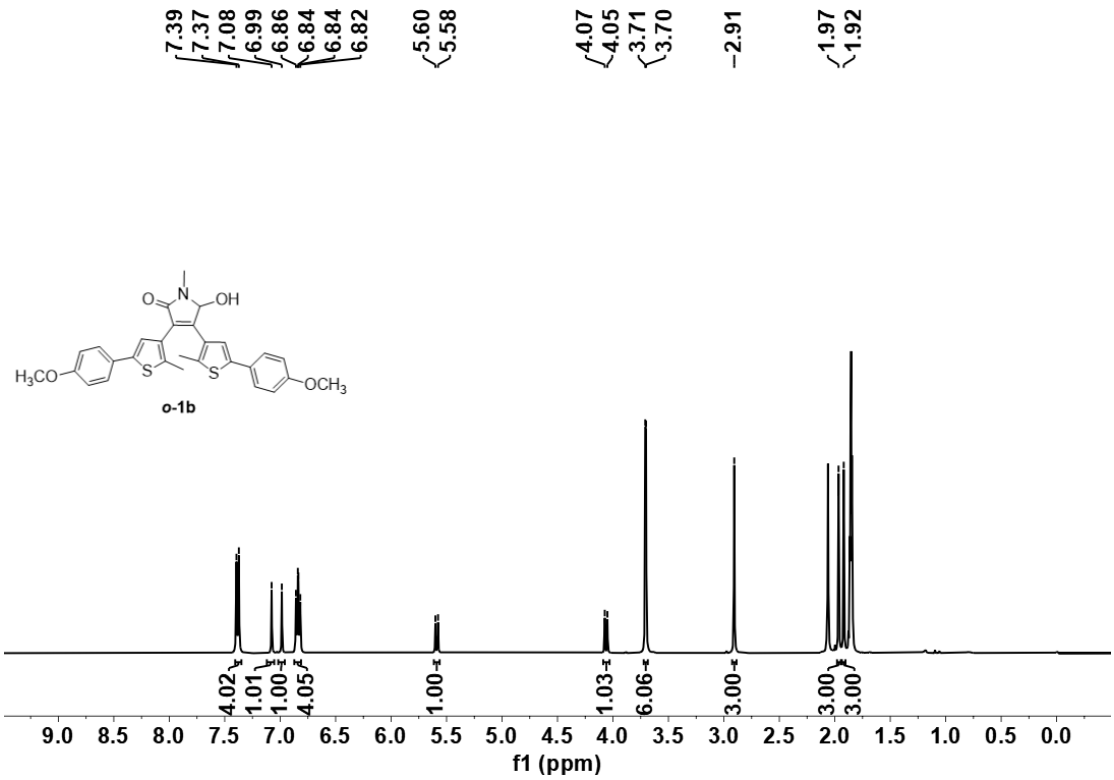


Figure S7. ^{1}H NMR spectrum of ***o*-1b** in CD_3CN.

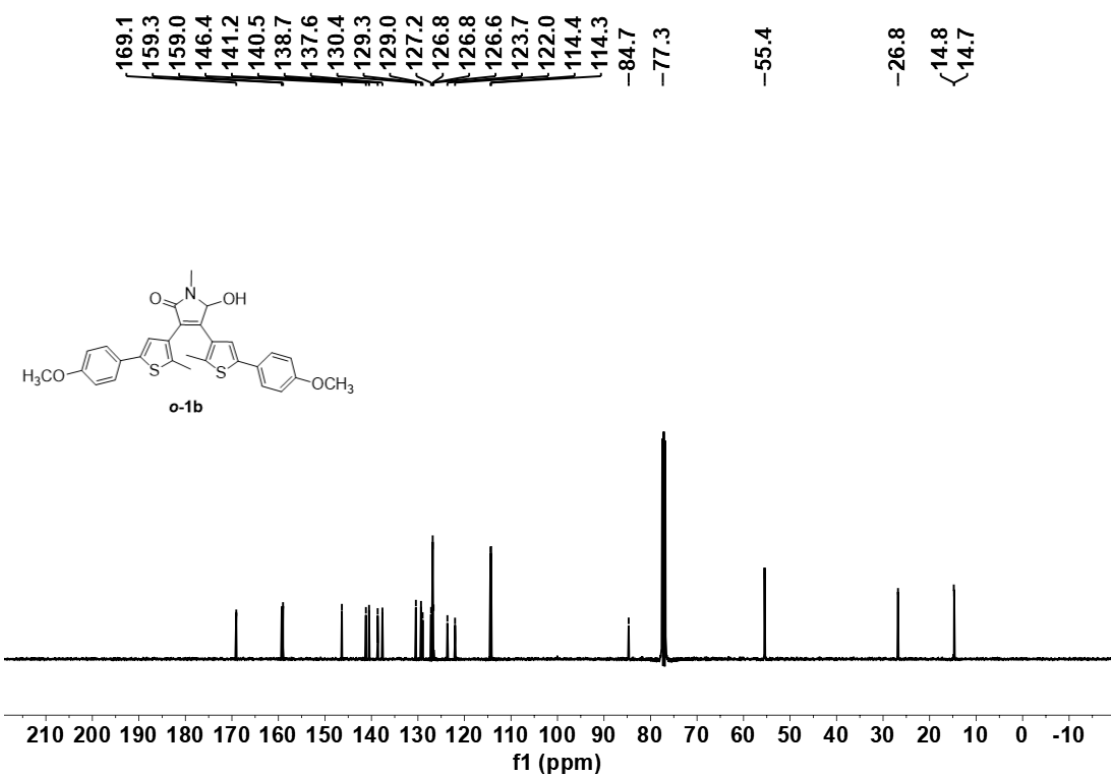


Figure S8. ^{13}C NMR spectrum of ***o*-1b** in $CDCl_3$.

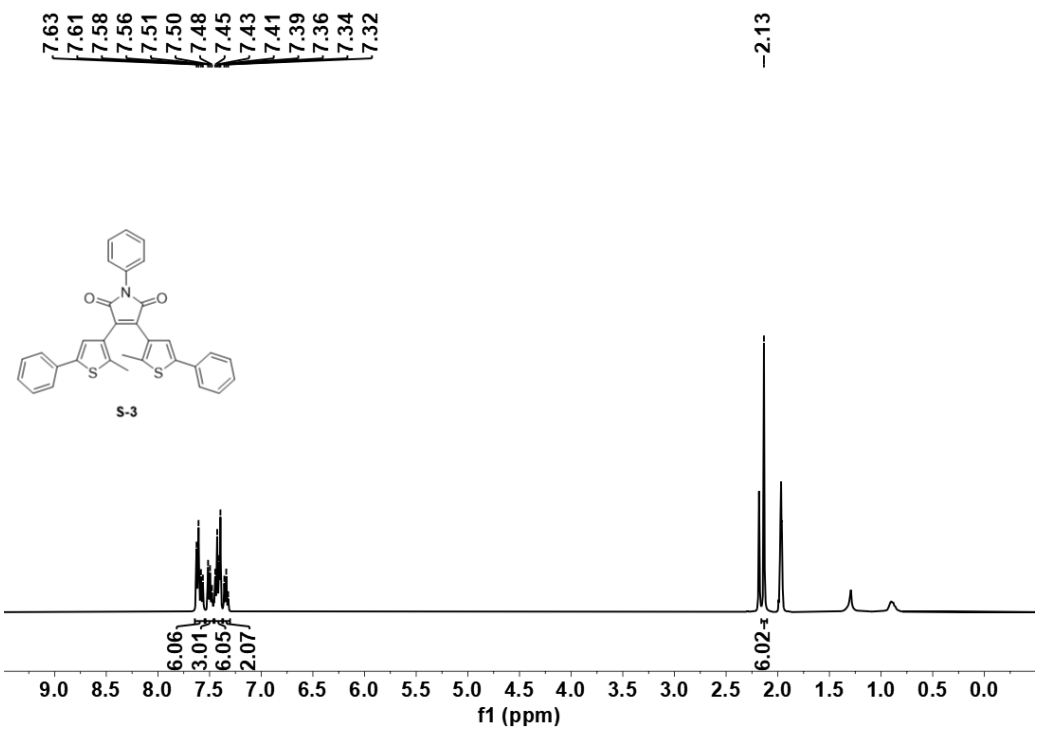


Figure S9. ^{1}H NMR spectrum of **S-3** in CD_3CN.

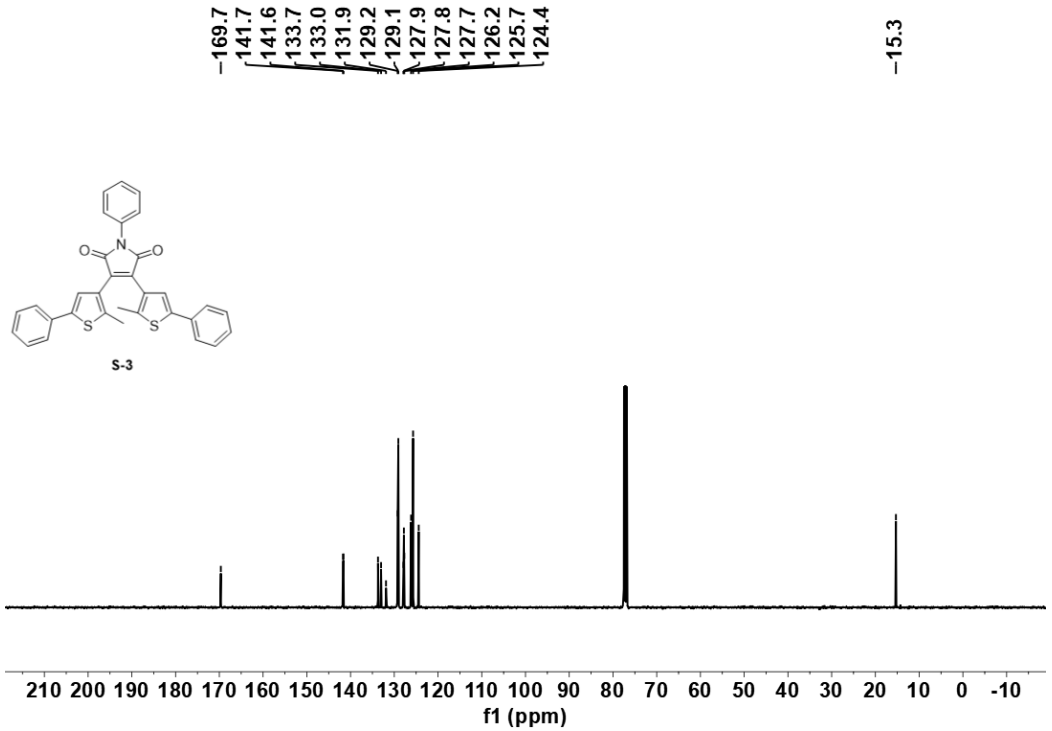


Figure S10. ^{13}C NMR spectrum of **S-3** in $CDCl_3$.

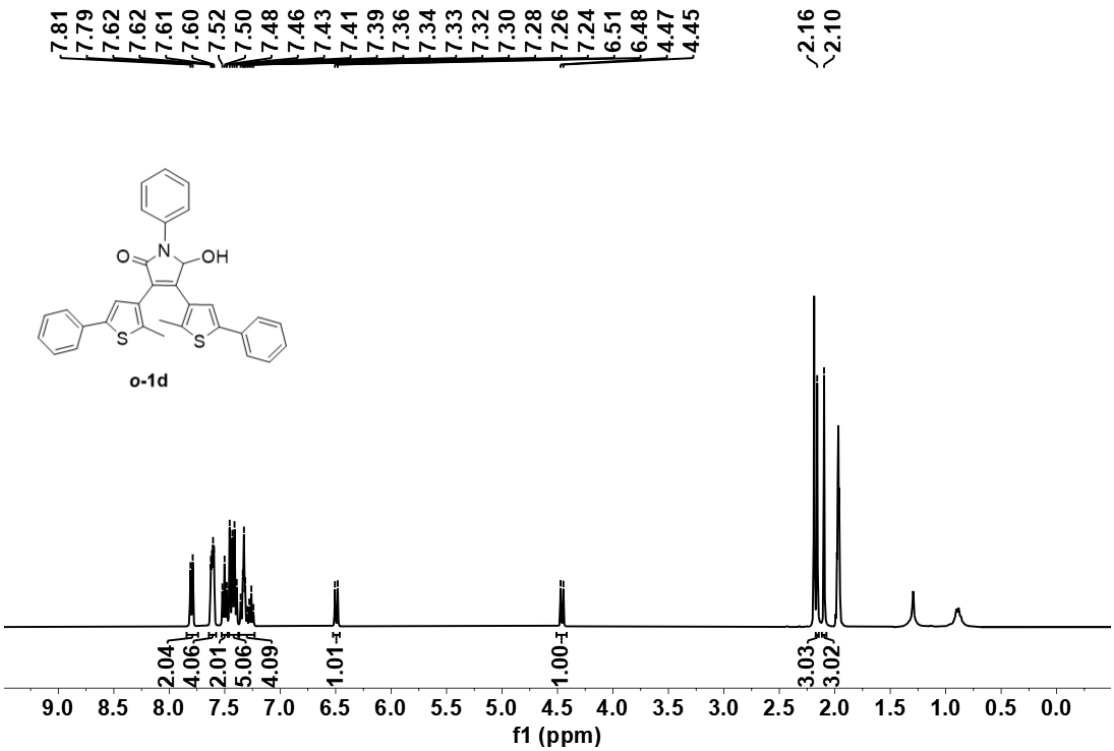


Figure S11. ^{1}H NMR spectrum of ***o*-1d** in CD_3CN.

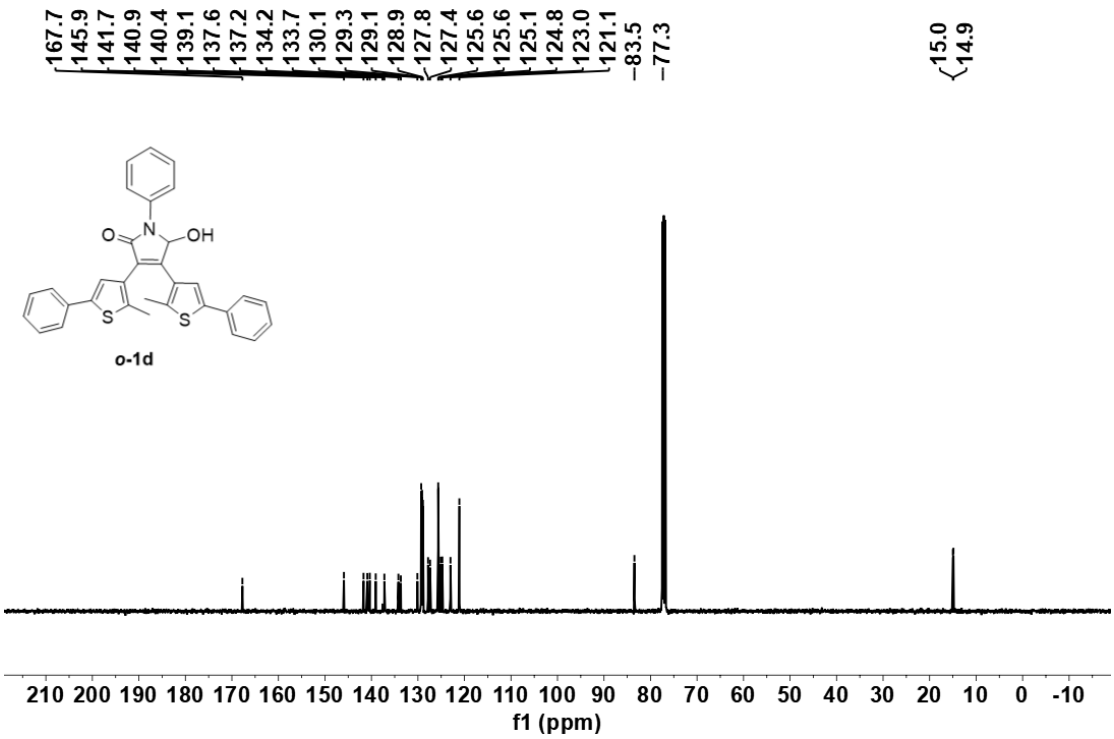


Figure S12. ^{13}C NMR spectrum of ***o*-1d** in $CDCl_3$.

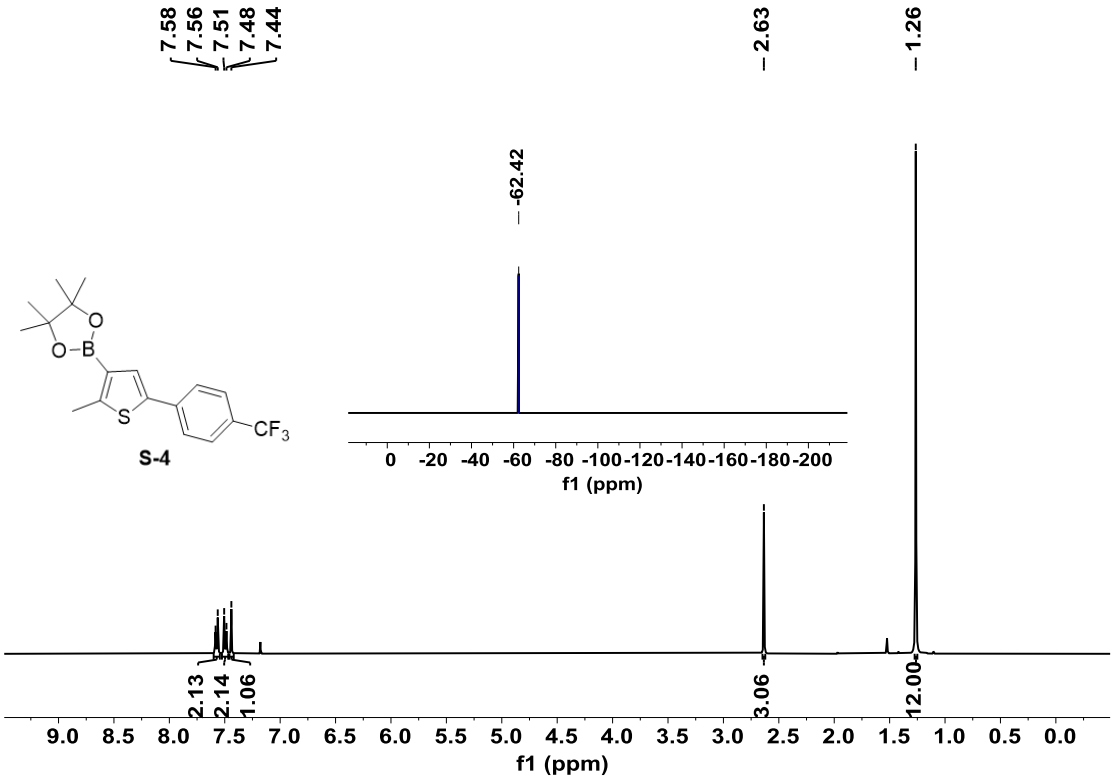


Figure S13. ^{1}H NMR spectrum of **S-4** in $CDCl_3$. Inset: ^{19}F NMR spectrum of **S-4** in $CDCl_3$.

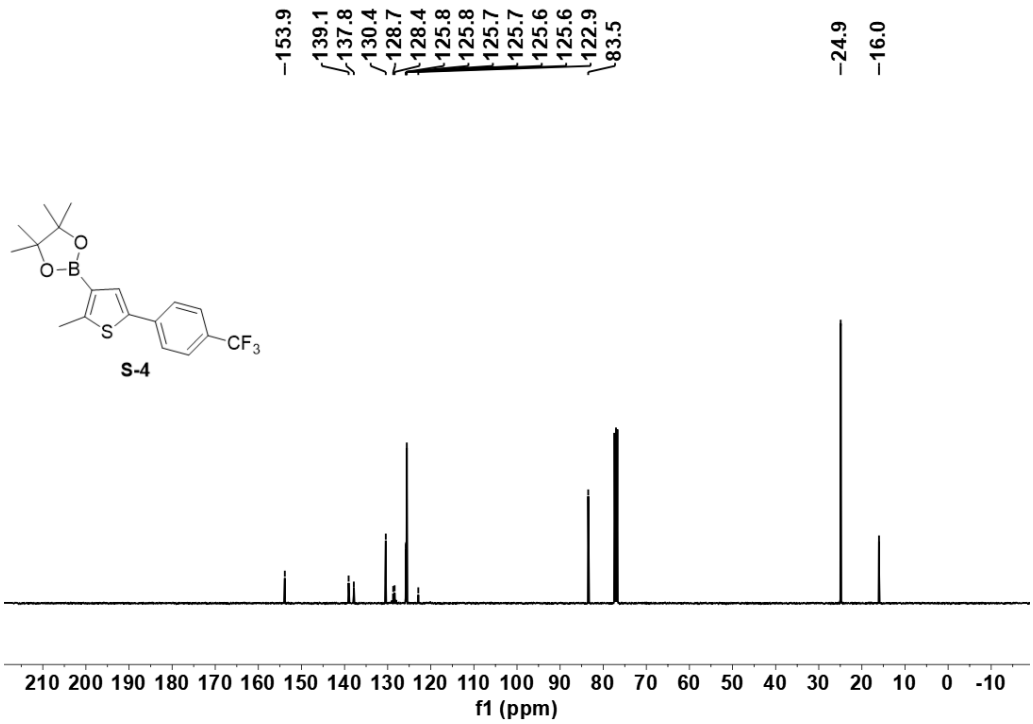


Figure S14. ^{13}C NMR spectrum of **S-4** in $CDCl_3$.

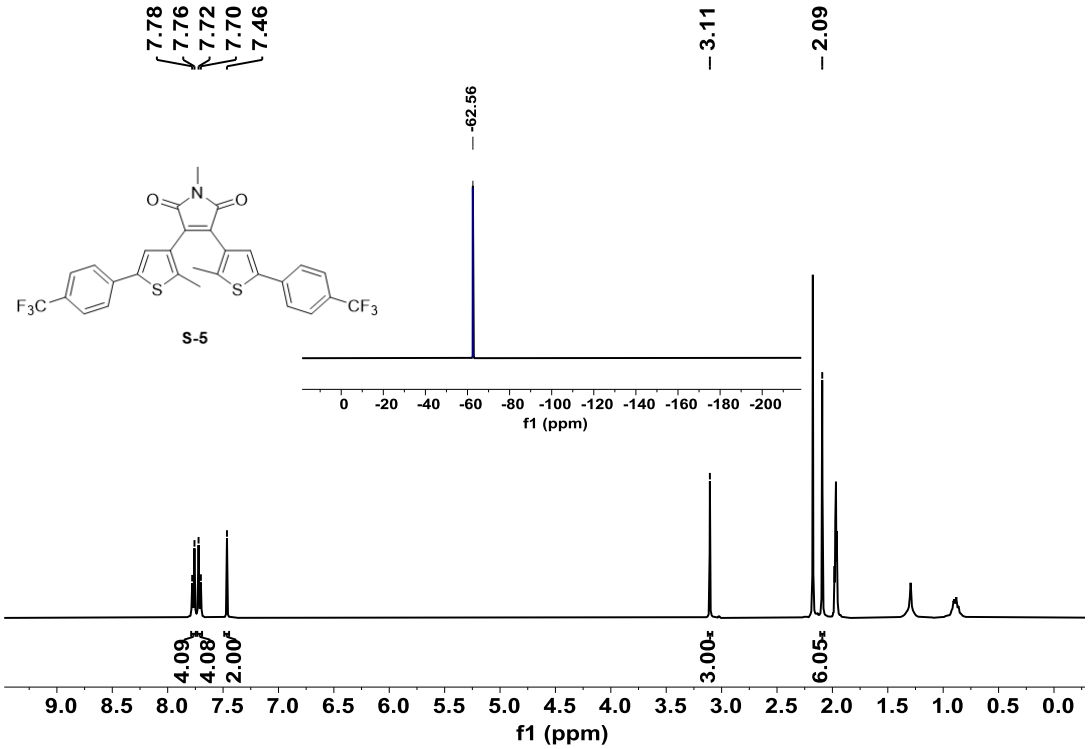


Figure S15. ^{1}H NMR spectrum of **S-5** in CD_3CN. Inset: ^{19}F NMR spectrum of **S-5** in $CDCl_3$.

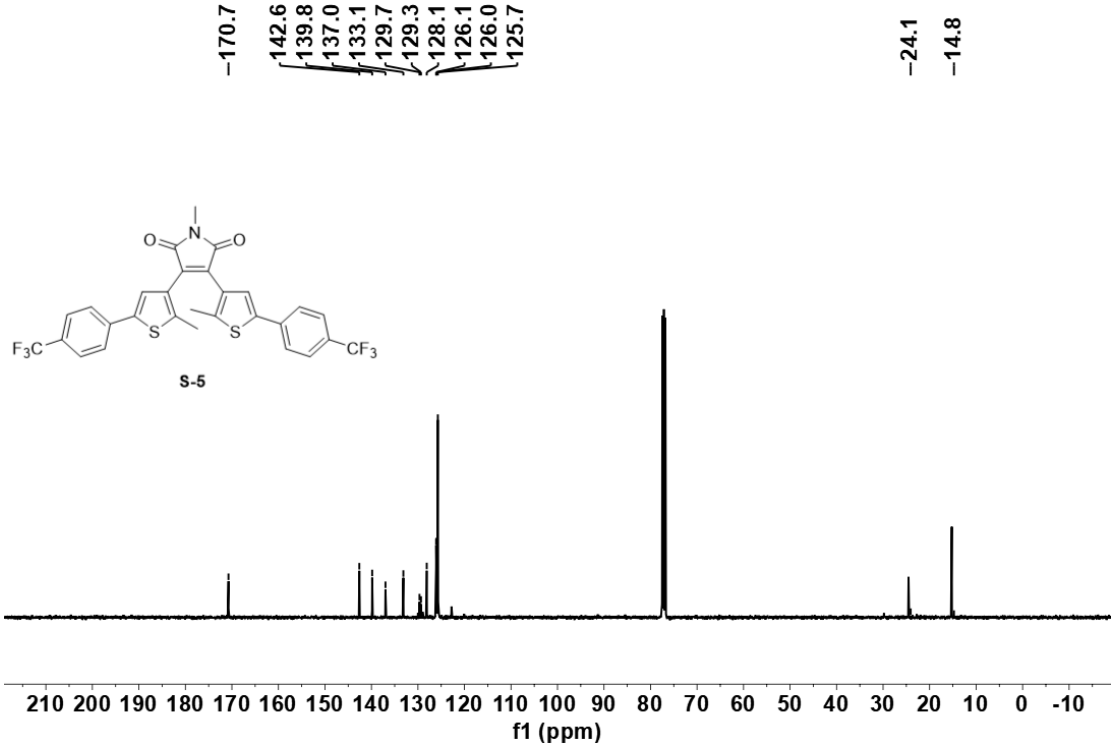


Figure S16. ^{13}C NMR spectrum of **S-5** in $CDCl_3$.

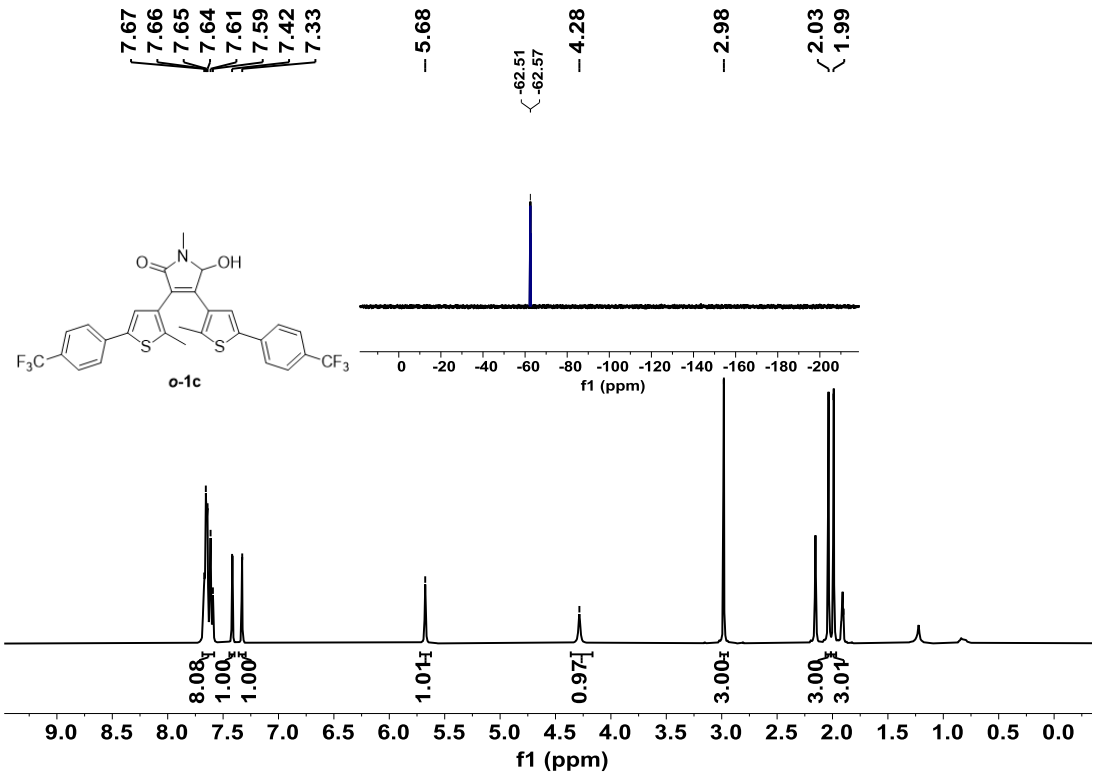


Figure S17. ^{1}H NMR spectrum of ***o*-1c** in CD_3CN. Inset: ^{19}F NMR spectrum of ***o*-1c** in $CDCl_3$.

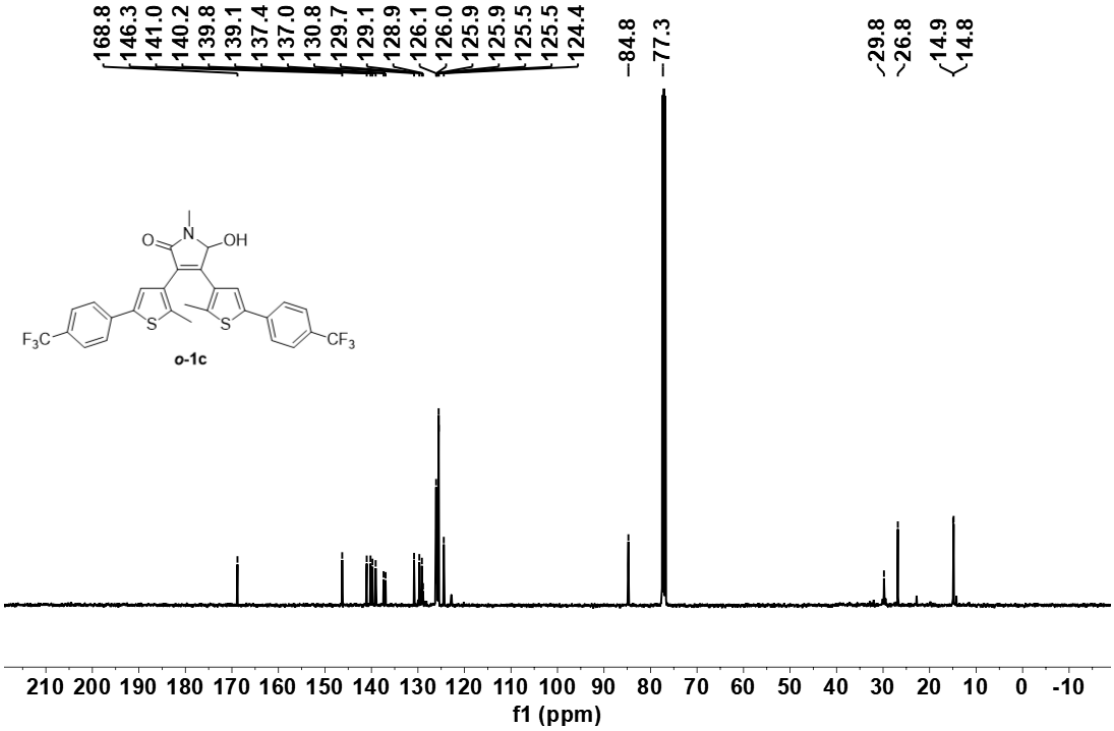


Figure S18. ^{13}C NMR spectrum of ***o*-1c** in $CDCl_3$.

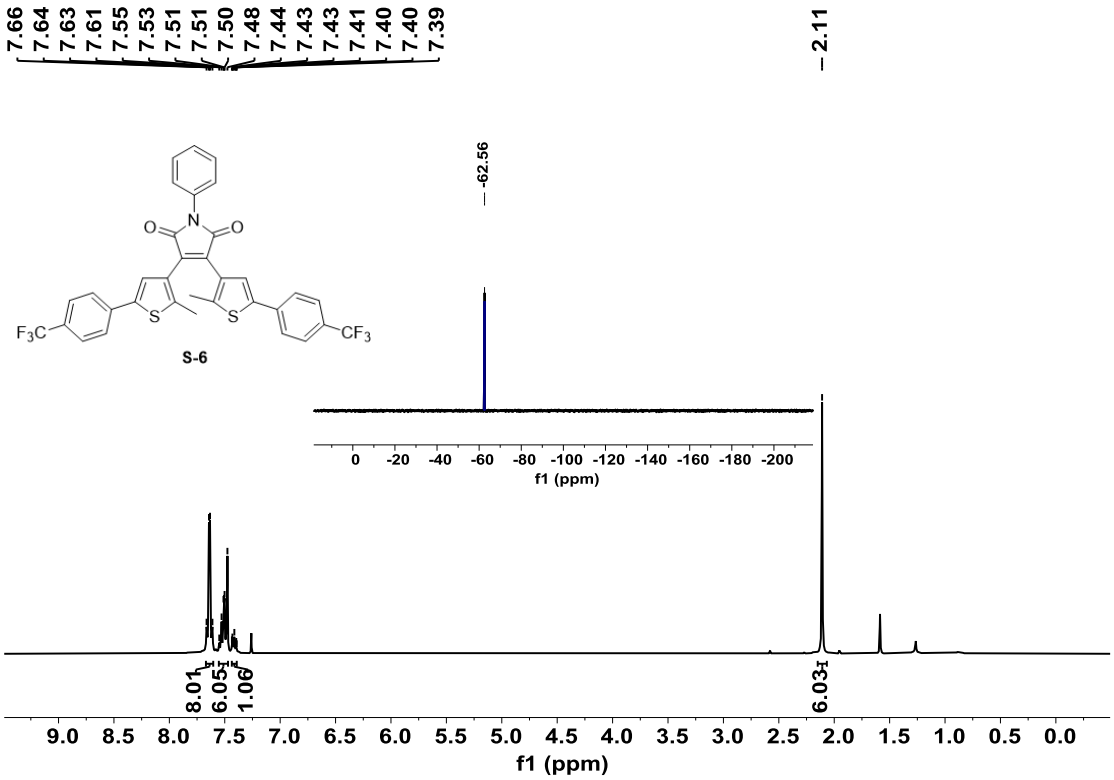


Figure S19. ^{1}H NMR spectrum of **S-6** in $CDCl_3$. Inset: ^{19}F NMR spectrum of **S-6** in $CDCl_3$.

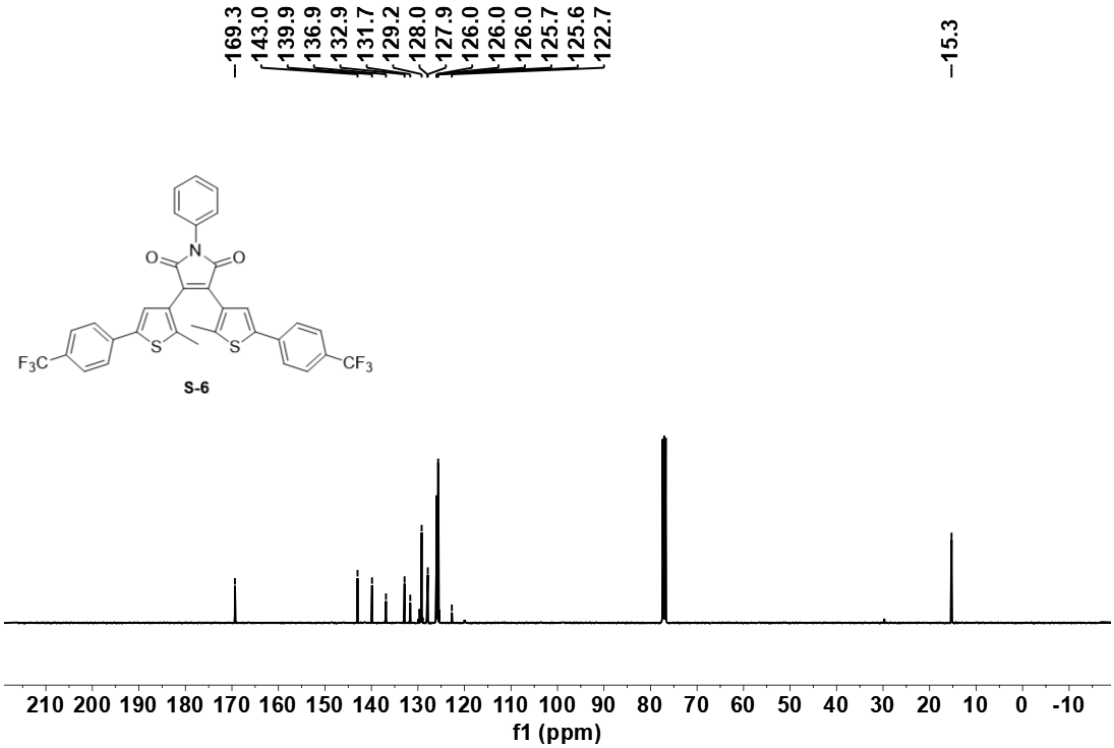


Figure S20. ^{13}C NMR spectrum of **S-6** in $CDCl_3$.

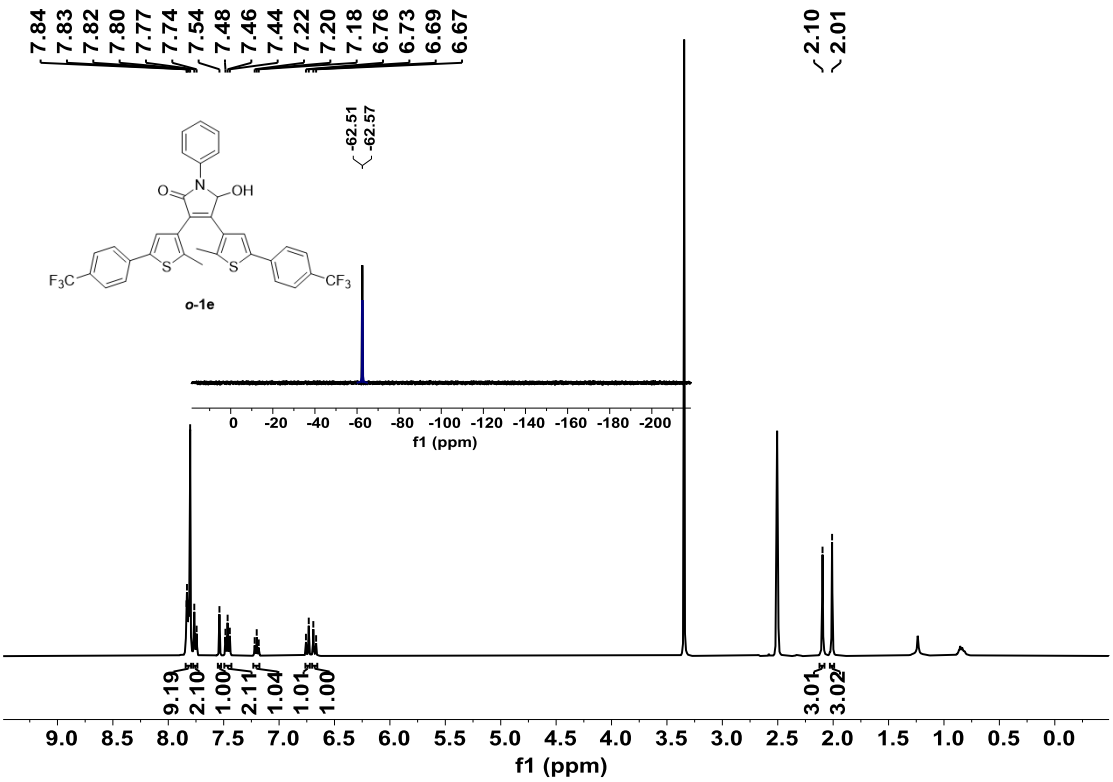


Figure S21. ^{1}H NMR spectrum of ***o*-1e** in CD_3CN. Inset: ^{19}F NMR spectrum of ***o*-1e** in $CDCl_3$.

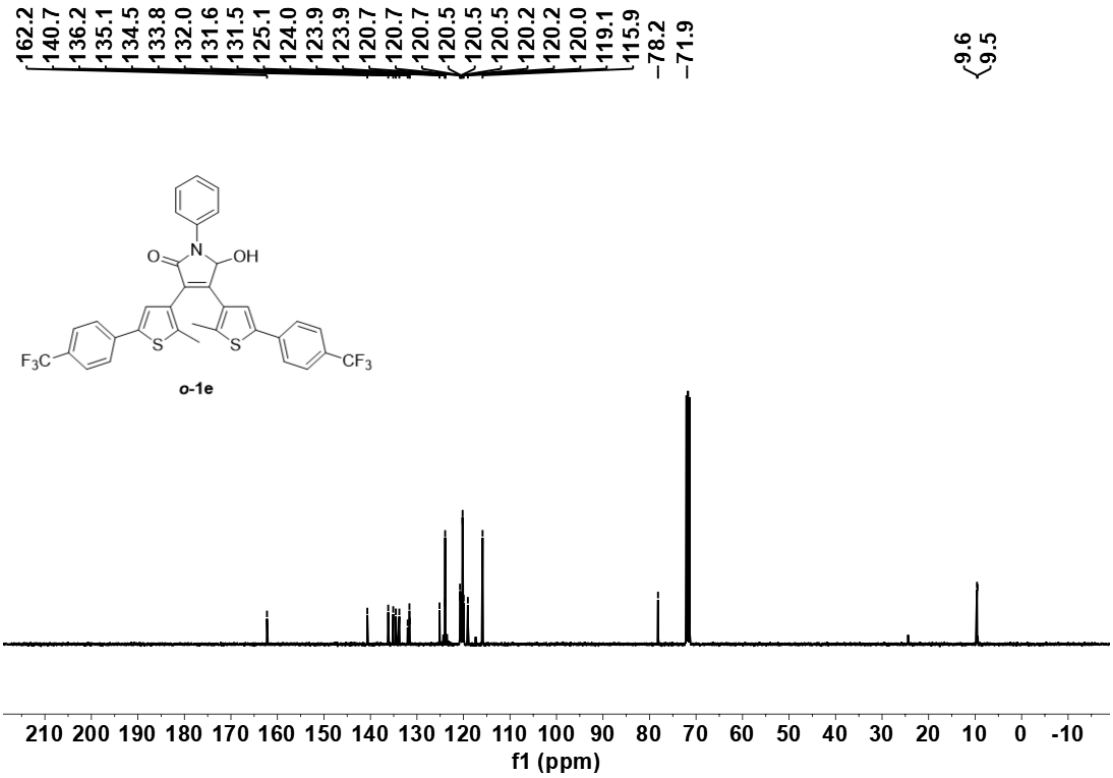


Figure S22. ^{13}C NMR spectrum of ***o*-1e** in $CDCl_3$.

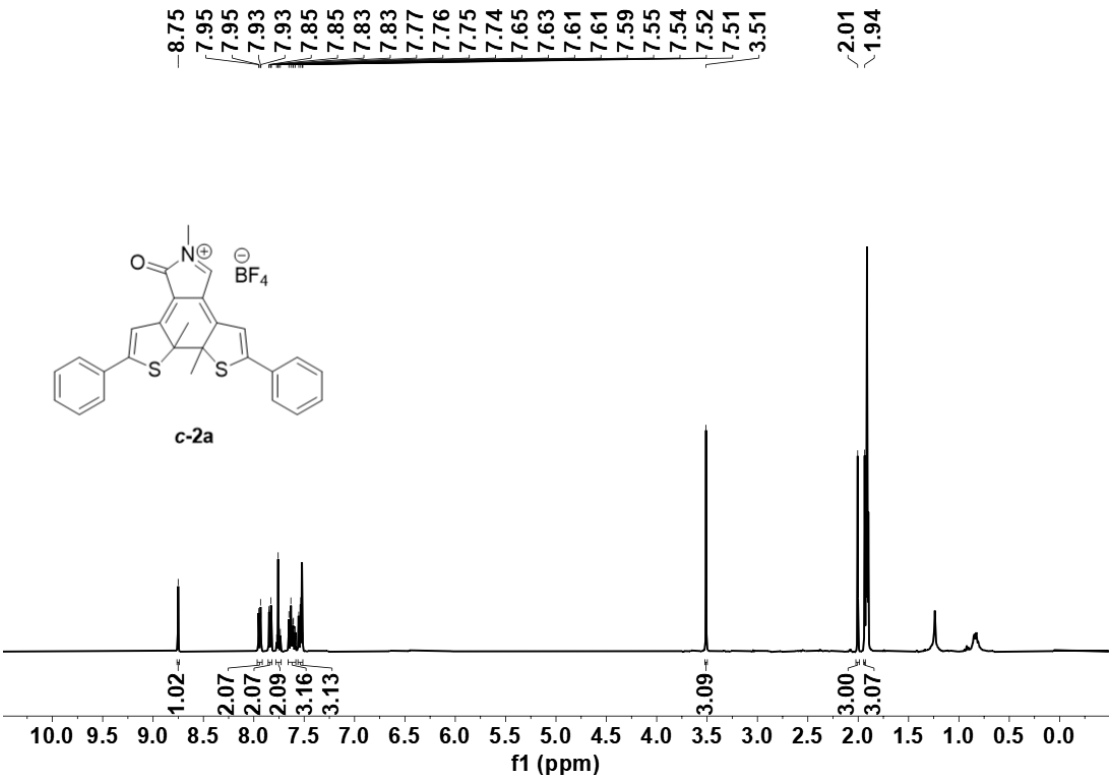


Figure S23. ^{1}H NMR spectrum of ***c*-2a** in CD_3CN.

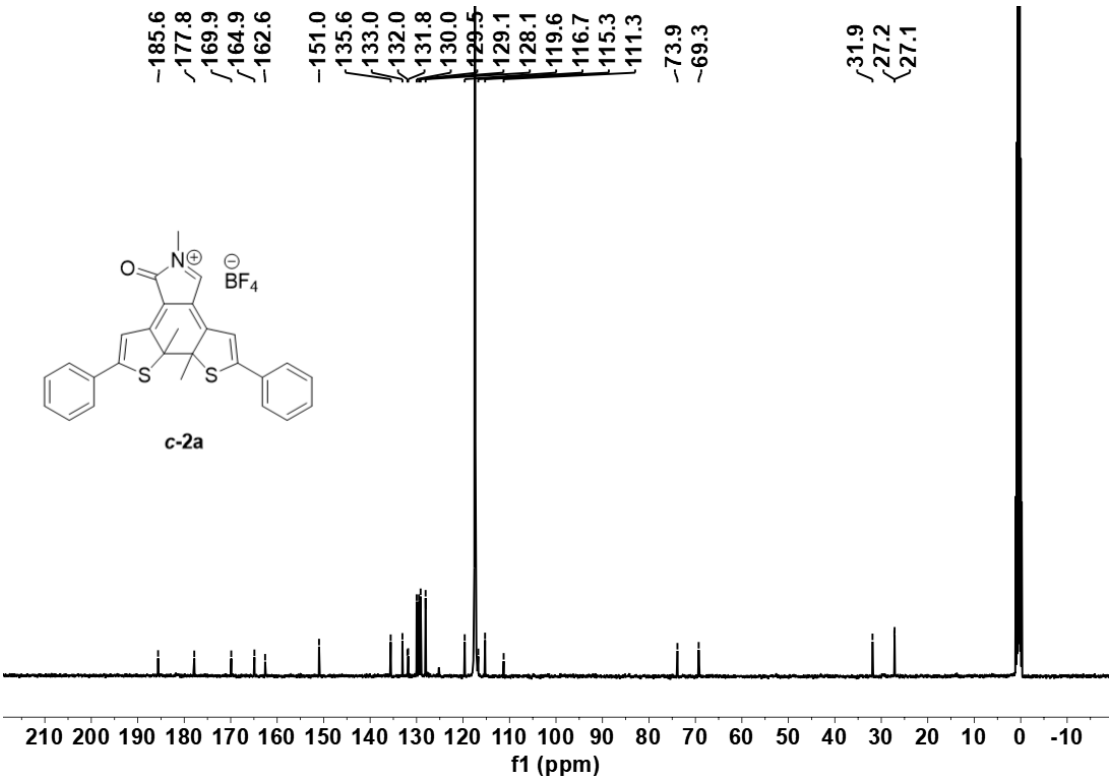


Figure S24. ^{13}C NMR spectrum of ***c*-2a** in CD_3CN.

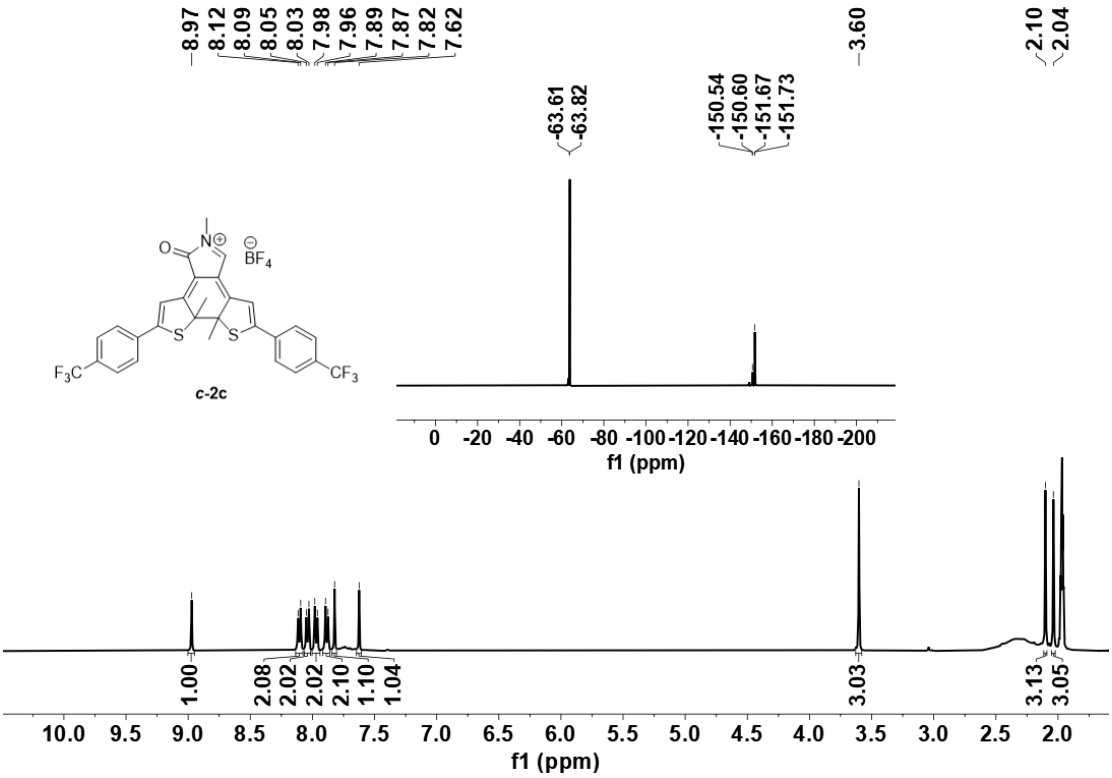


Figure S25. ^{1}H NMR spectrum of ***c*-2c** in CD_3CN. Inset: ^{19}F NMR spectrum of ***c*-2c** in CD_3CN.

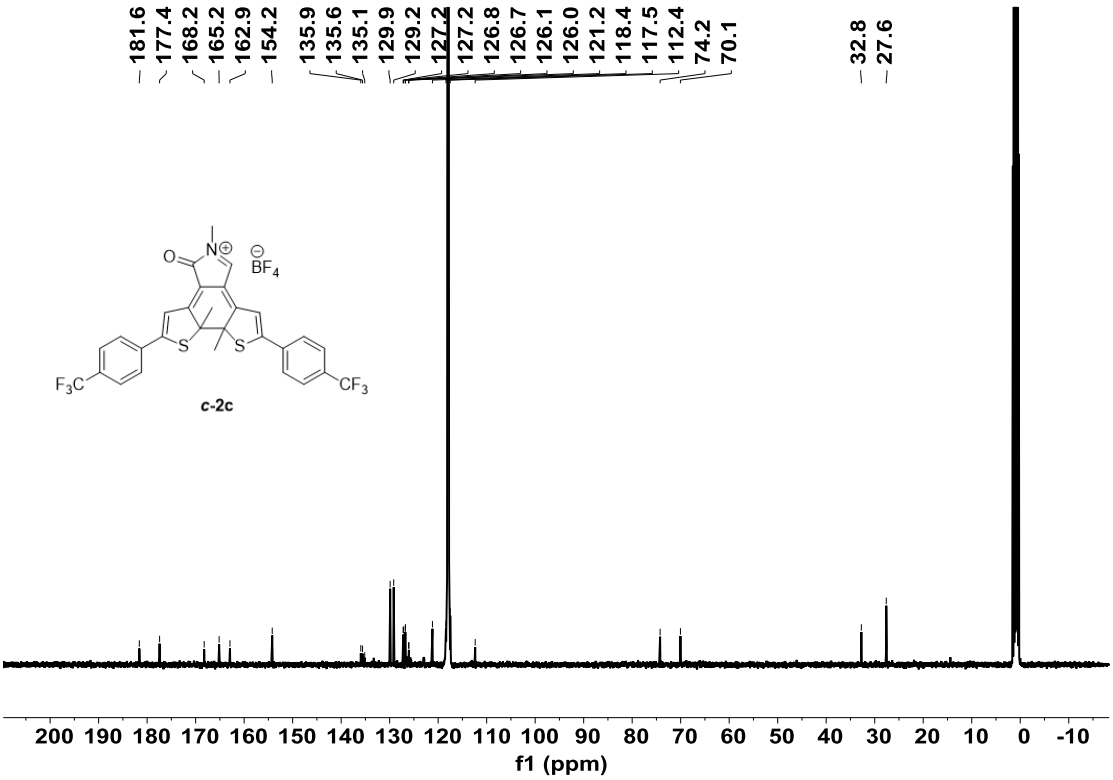


Figure S26. ^{13}C NMR spectrum of ***c*-2c** in CD_3CN.

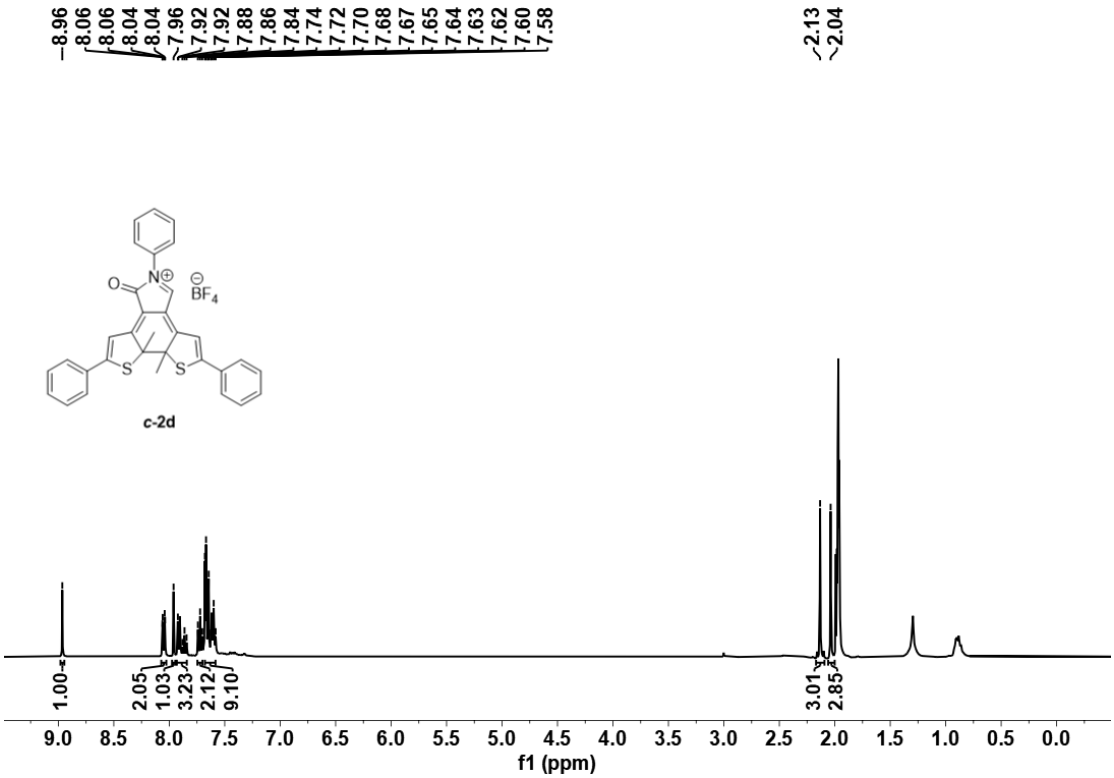


Figure S27. ^{1}H NMR spectrum of ***c*-2d** in CD_3CN.

X-ray Crystallography

Crystals were obtained by slow evaporation after dissolving 3 mg of the compounds in organic solvents (2 mL). Different solutions were chosen with acetonitrile for **S-1** and ***o*-1d** and chloroform for ***o*-1c**. After irradiating the acetonitrile solution of ***o*-1d** at 313 nm for 2 h, the crystal precipitate of ***c*-1d** formed. Notably, due to the sensitivity of ***c*-2a** to water the anhydrous acetonitrile was selected for the crystal preparation in the desiccator.

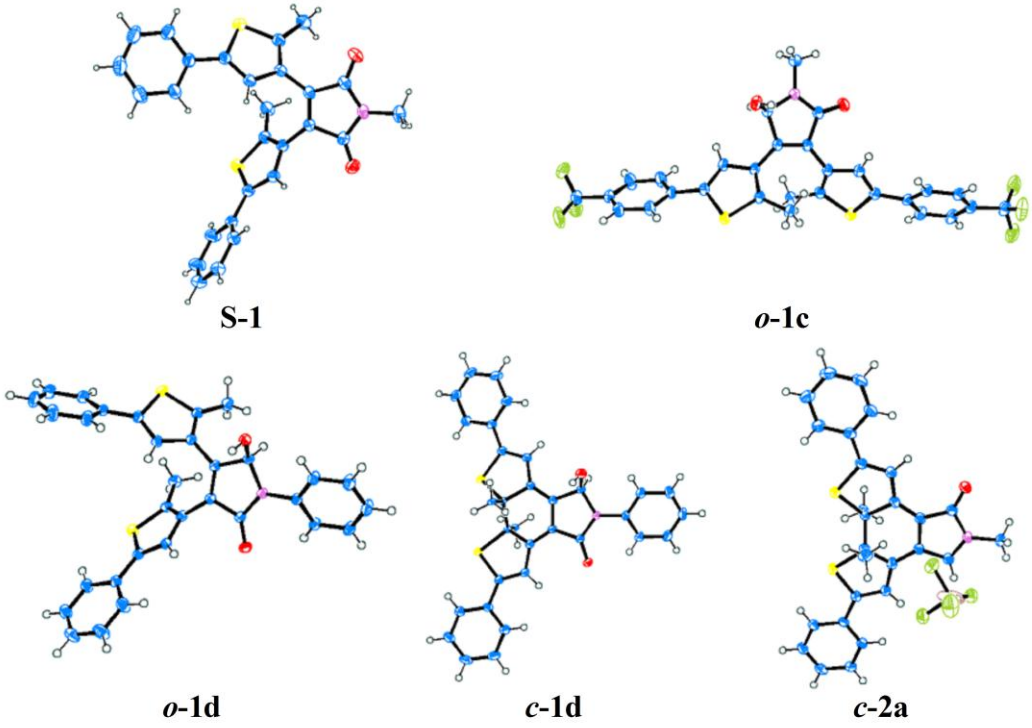


Figure S28. Crystal structures of **S-1**, ***o*-1c**, ***o*-1d**, ***c*-1d**, and ***c*-2a**. The thermal ellipsoids were scaled to the 50% probability level.

Table S1. Summary of crystallographic data.

Compound	**S-1**	***o*-1c**	***o*-1d**	***c*-1d**	***c*-2a**
Formula	$C_{27}H_{21}NO_2S_2$	$C_{29.50}H_{21.50}C_{l1.50}F_6NO_2S_2$	$C_{32}H_{25}NO_2S_2$	$C_{32}H_{25}NO_2S_2$	$C_{27}H_{22}BF_4NOS_2$
Formula weight	455.57	653.27	519.65	519.65	527.38
T/*K*	293(2)	104(2)	100(2)	100(10)	100(2)
Crystallization solvent	acetonitrile	chloroform	acetonitrile	acetonitrile	acetonitrile
Color	green	colorless	colorless	black	black
Crystal system	monoclinic	triclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	*P-1*	$P2_1$	*P*-1	*P*-1
a / Å	11.8816(4)	12.9730(3)	8.9974(2)	8.8947(3)	10.4480(3)
b / Å	18.3769(6)	13.7374(4)	9.5306(17)	13.1617(4)	10.8152(3)
c / Å	11.3381(4)	17.1472(3)	29.6085(5)	13.1668(5)	11.7444(4)
α / °	90.000	95.217(2)	90.000	111.277(3)	102.132(3)
β / °	105.695(4)	99.044(2)	90.837(18)	101.207(3)	100.573(3)
γ / °	90.000	110.871(3)	90.000	107.313(3)	97.621(2)
V/ Å^3	2383.34(14)	2783.90(13)	2538.66(9)	1289.66(8)	1255.02(7)
Z	4	4	4	4	2
D_x / g cm^{-3}	1.270	1.559	1.360	1.336	1.396
μ / mm^{-1}	1.450	2.433	1.407	1.384	1.553
F(000)	952	1332	1088	542	544
θ range / °	3.35 to 51.67	2.27 to 60.35	2.57 to 60.06	3.34 to 55.40	3.42 to 48.71
GOF on F^2	1.031	1.056	1.035	1.046	1.043
R_1 [$I > 2\sigma(I)$]	0.0580	0.0476	0.0362	0.0384	0.0356
wR_2 (all data)	0.1505	0.1291	0.0859	0.1028	0.0904

3. Photoswitching Experiments

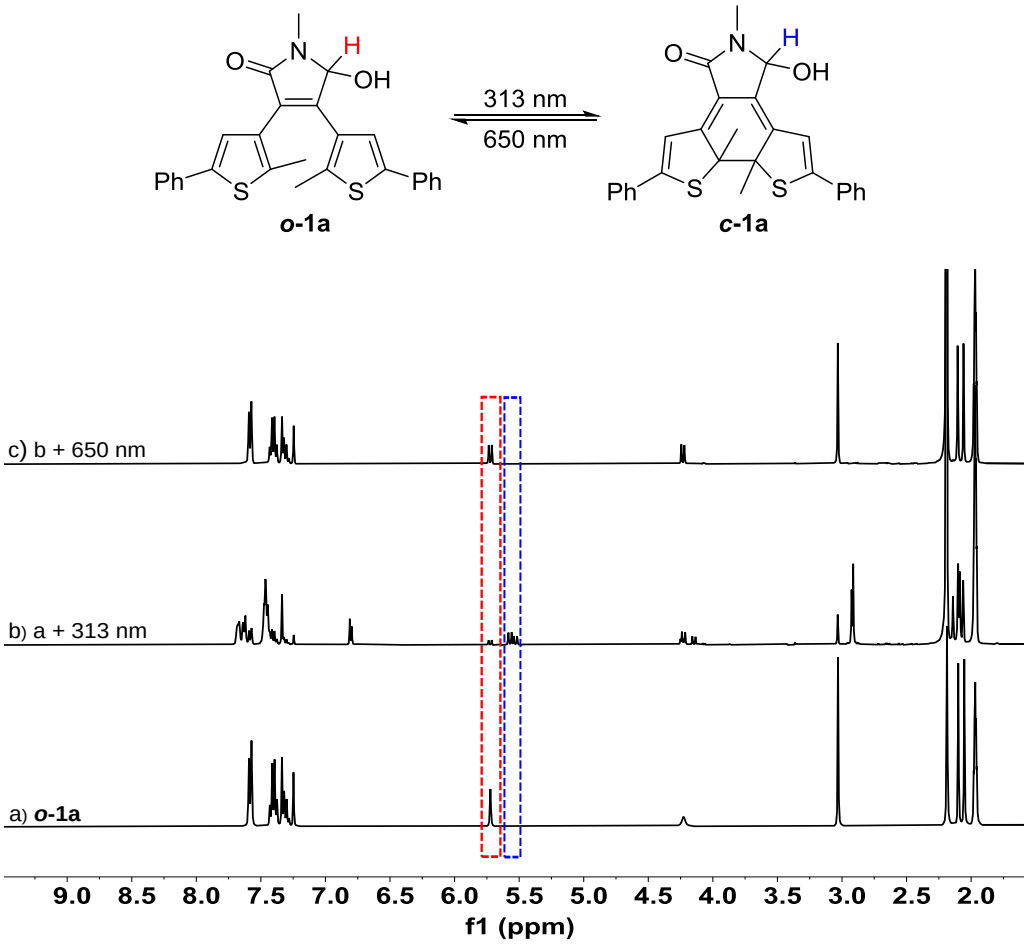


Figure S29. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) Irradiation of ***o*-1a** with UV light (313 nm, 1.5 h). The ratio of ***c*-1a** and ***o*-1a** is 85:5; (c) Further irradiation with visible light (650 nm, 2 h) The ratio of ***o*-1a** and ***c*-1a** is 99:1.

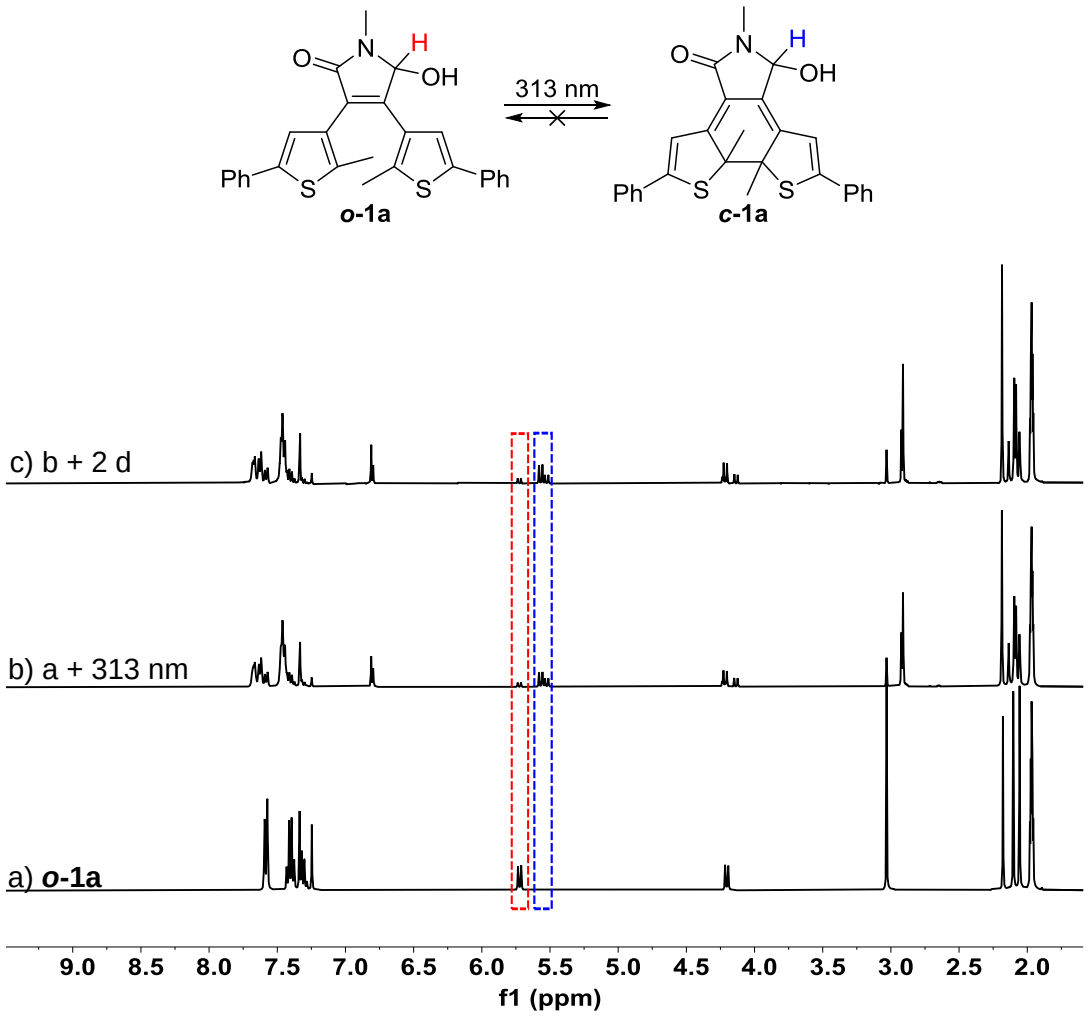


Figure S30. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) Irradiation of ***o*-1a** with UV light (313 nm, 1.5 h). The ratio of ***c*-1a** and ***o*-1a** is 85:5; (c) Panel b at room temperature for 2 days. ***o*-1a** was not observed.

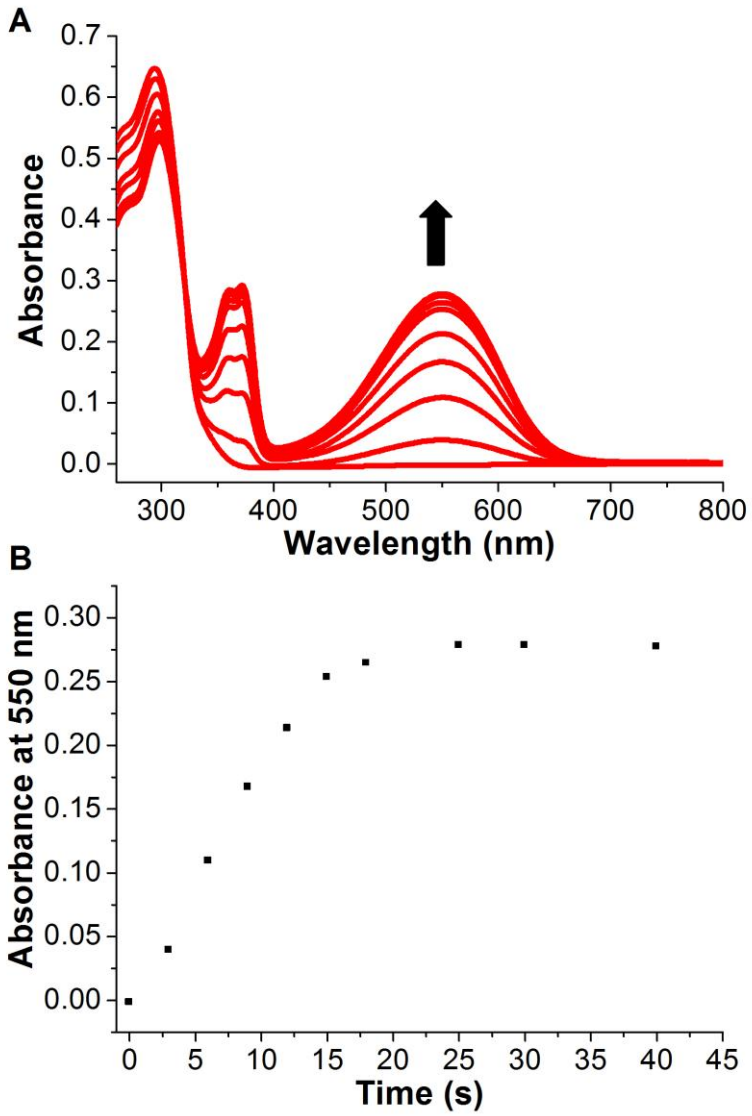


Figure S31. (A) Photocyclization of ***o*-1a** to give ***c*-1a**: changes in absorption spectra upon irradiation of ***o*-1a** (25 μM in MeCN) with 313 nm light after total irradiation of 0, 3, 6, 9, 12, 15, 18, 25, 30, and 40 s. The photostationary state was reached after 25 s. (B) The kinetics profile of the photocyclization of ***o*-1a** to ***c*-1a** with different time.

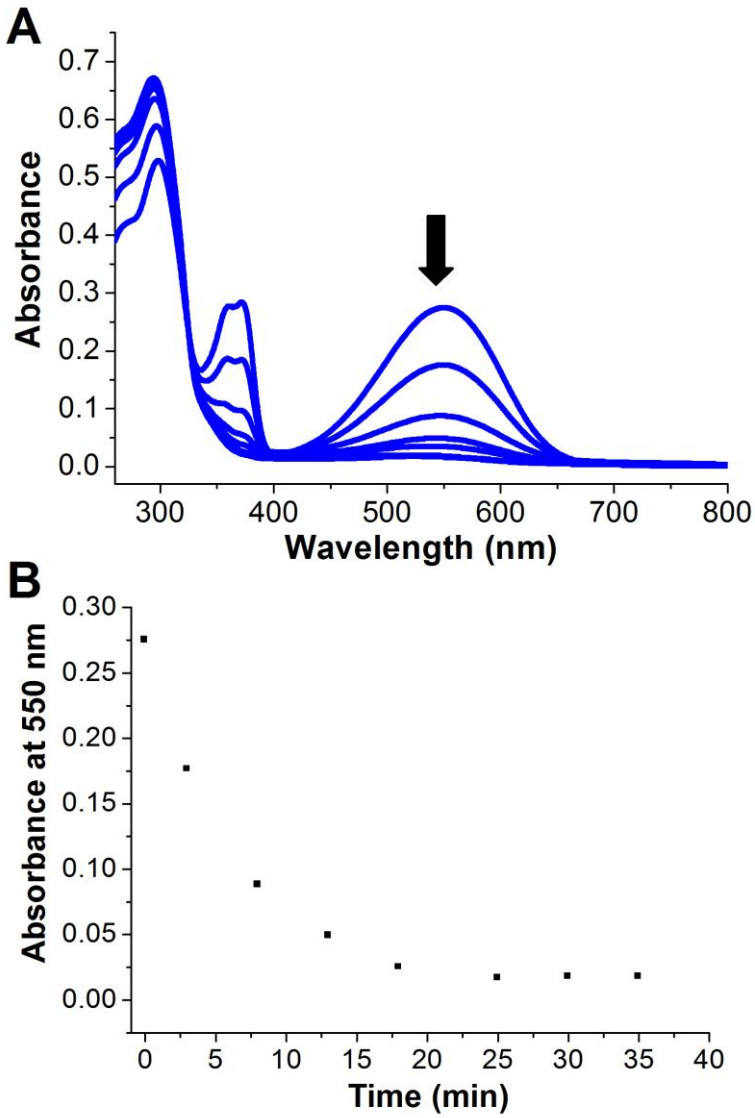


Figure S32. (A) Photocycloreversion of ***c*-1a** to give ***o*-1a**: changes in absorption spectra upon irradiation of ***c*-1a** (25 μM in MeCN) with 650 nm light after total irradiation of 0, 3, 8, 13, 18, 25, 30, and 35 min. The photostationary state was reached after 25 min. (B) The kinetics profile of the photocyclization of ***c*-1a** to ***o*-1a** with different time.

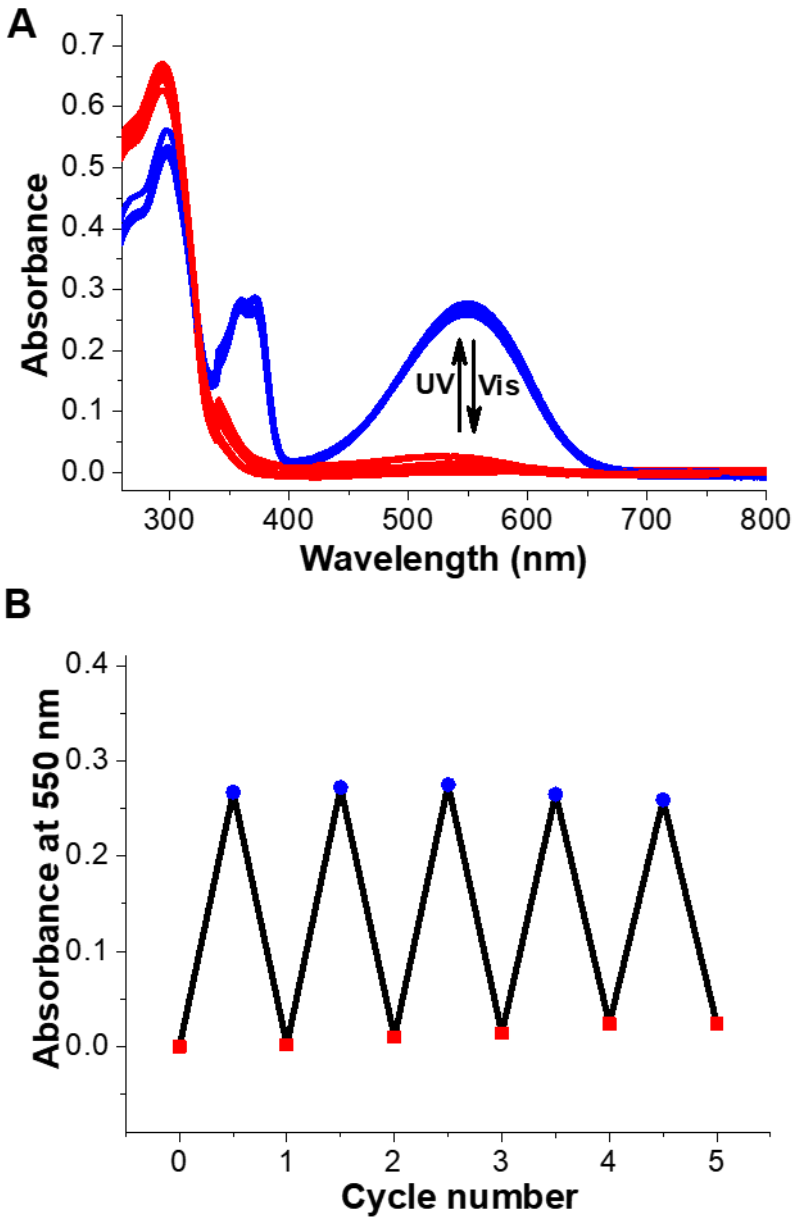


Figure S33. (A) Absorbance spectra of an acetonitrile solution of ***o*-1a** (25 μM, 25 ℃ during repetitive switching cycles consisting of alternating UV (313 nm, 25 s) and visible light irradiation (650 nm, 25 min). (B) Change of absorbance in the visible range (550 nm).

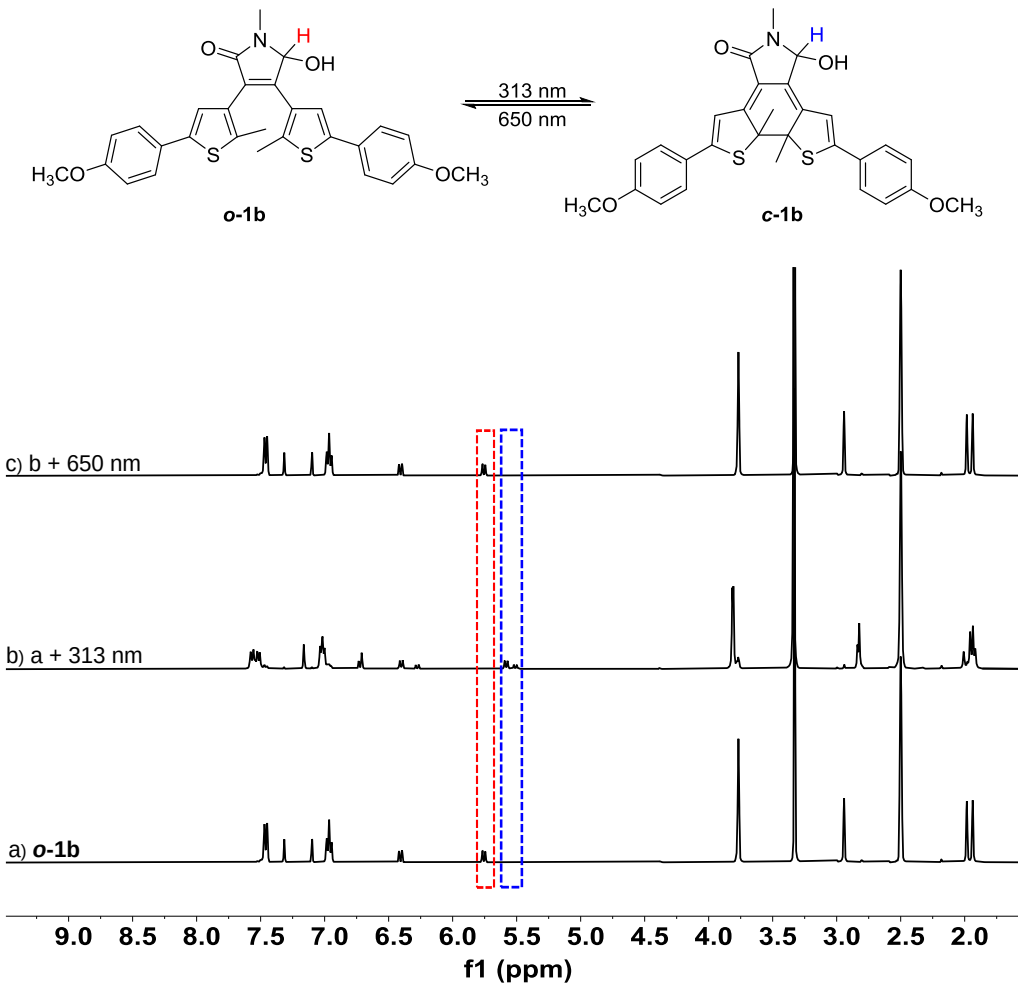


Figure S34. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in DMSO-d_6; (b) Irradiation of ***o*-1b** with UV light (313 nm, 2.5 h). The ratio of ***c*-1b** and ***o*-1b** is 91:9; (c) Further irradiation with visible light (650 nm, 2 h). The ratio of ***o*-1b** and ***c*-1b** is 99:1.

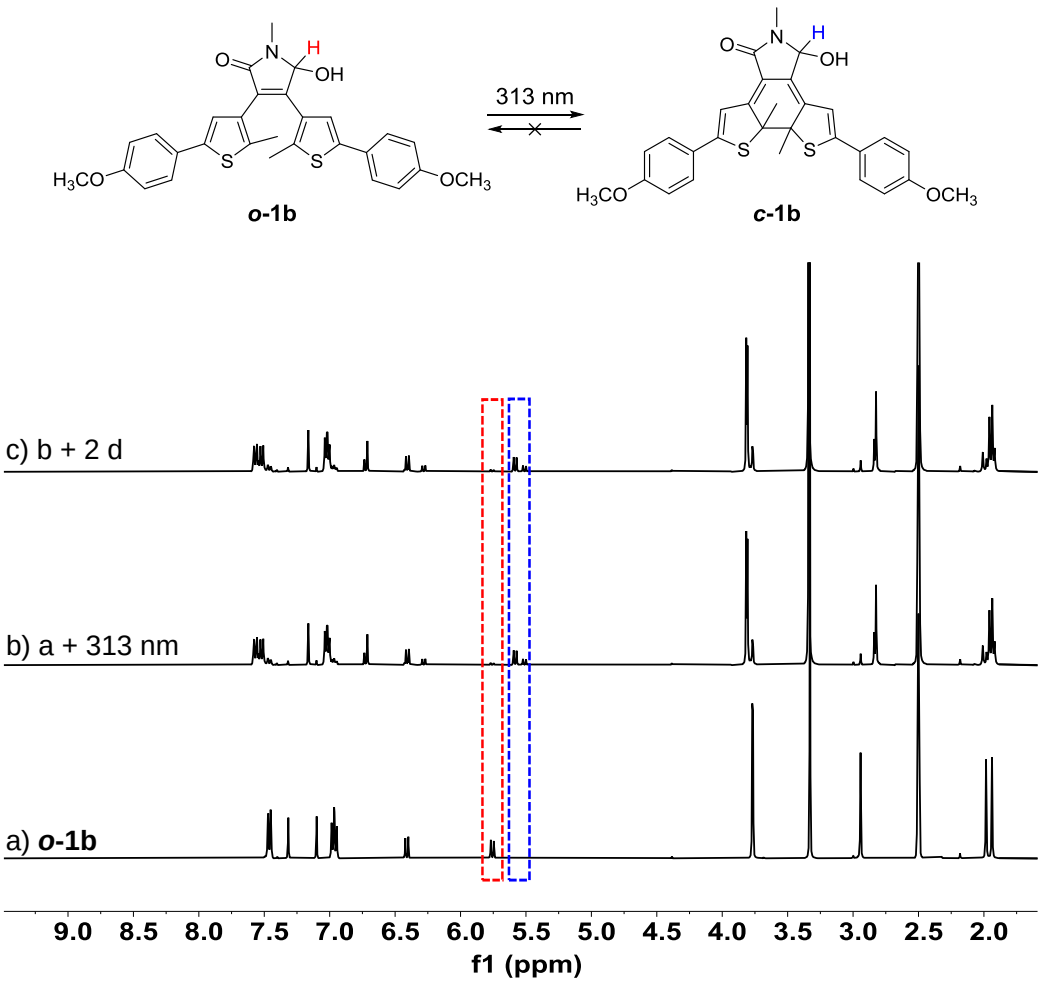


Figure S35. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in DMSO-d_6; (b) Irradiation of ***o*-1b** with UV light (313 nm, 2.5 h). The ratio of ***c*-1b** and ***o*-1b** is 91:9; (c) Panel b at room temperature for 2 days. ***o*-1b** was not observed.

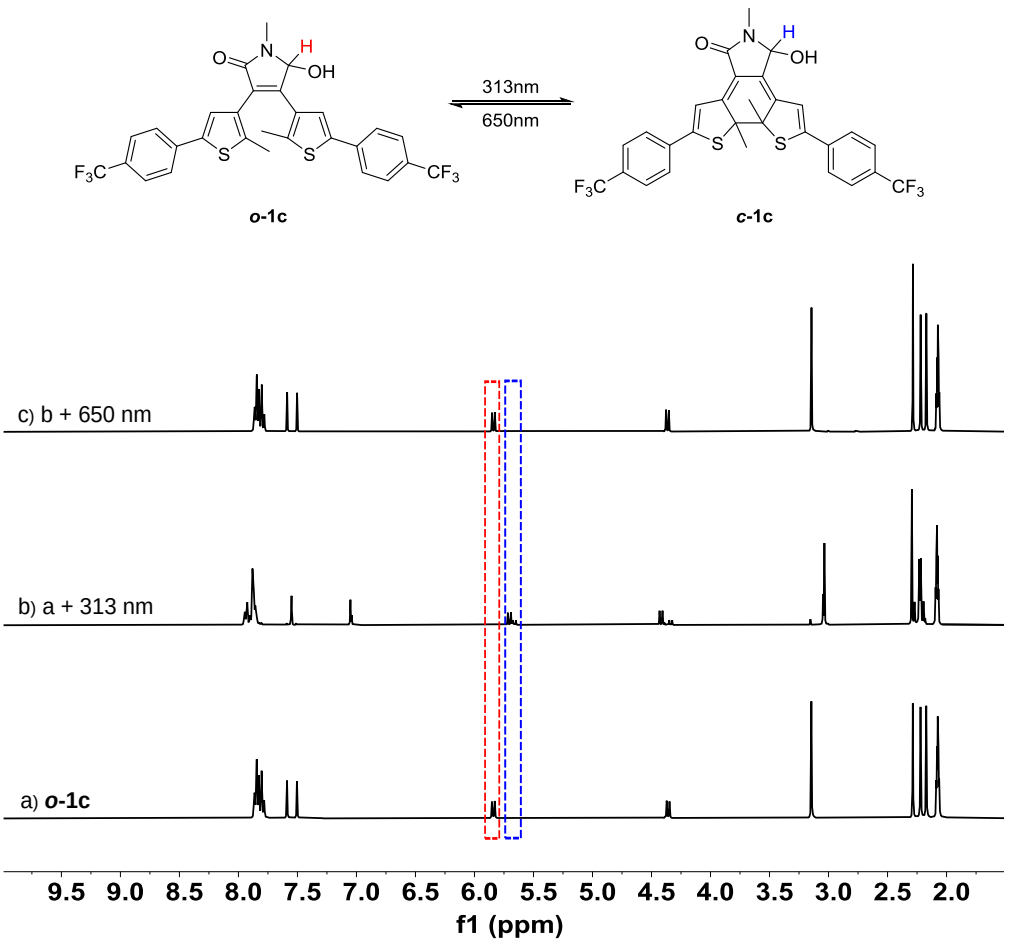


Figure S36. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) Irradiation of ***o*-1c** with UV light (313 nm, 80 min). The ratio of ***c*-1c** and ***o*-1c** is 92:8; (c) Further irradiation with visible light (650 nm, 5 h). The ratio of ***o*-1c** and ***c*-1c** is 99:1.

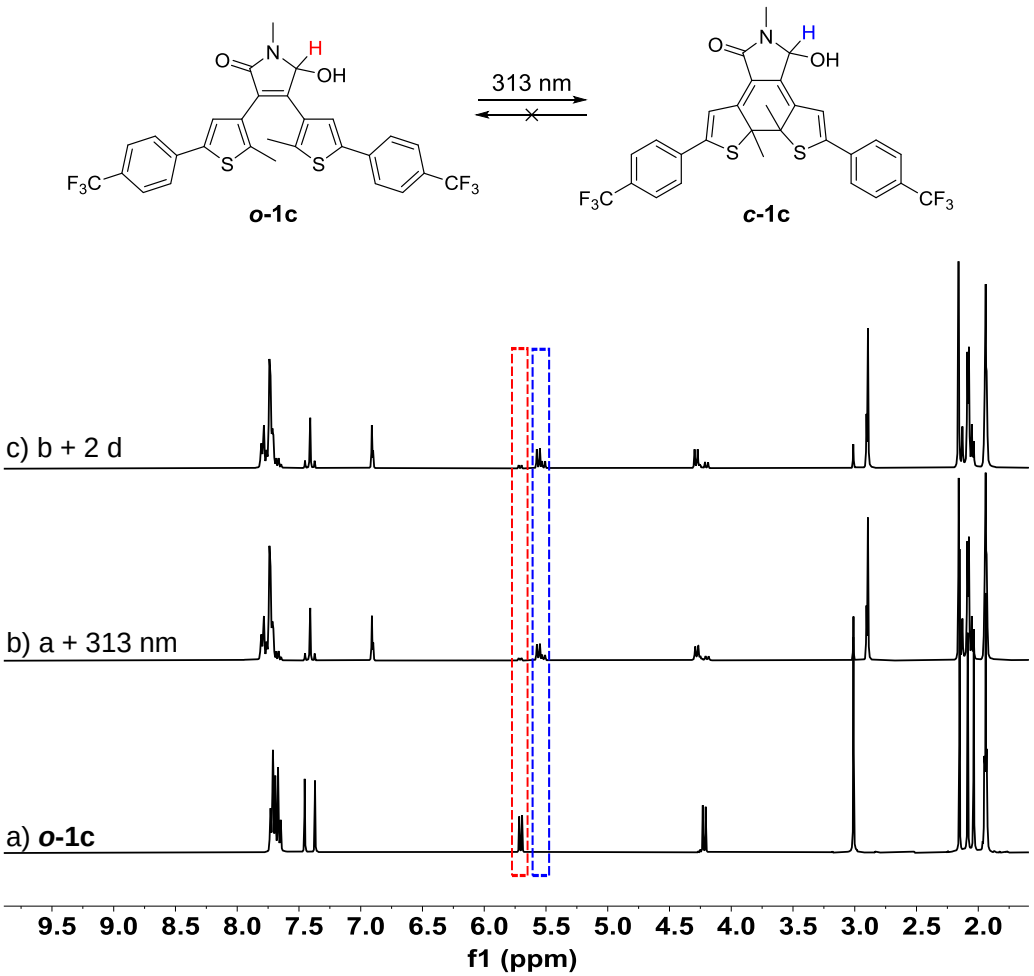


Figure S37. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) Irradiation of ***o*-1c** with UV light (313 nm, 1.5 h). The ratio of ***c*-1c** and ***o*-1c** is 92:8; (c) Panel b at room temperature for 2 days. ***o*-1c** was not observed.

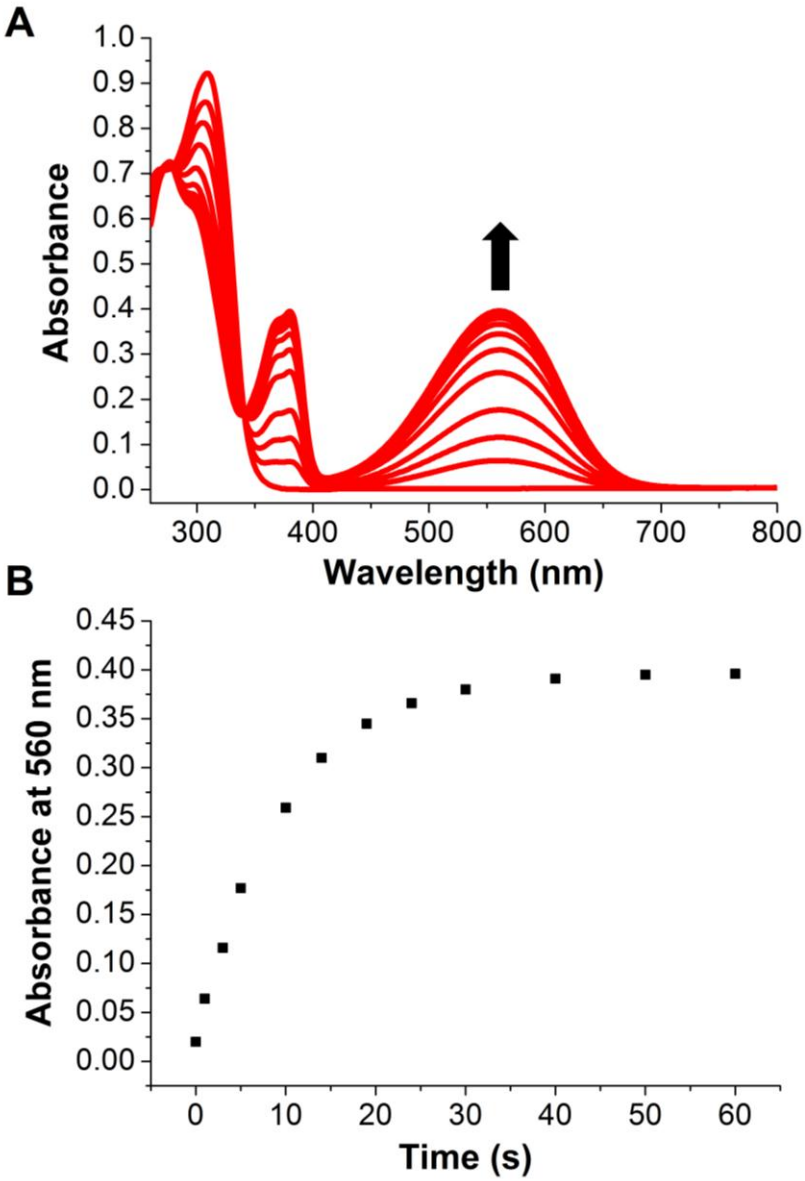


Figure S38. (A) Photocyclization of ***o*-1c** to give ***c*-1c**: changes in absorption spectra upon irradiation of ***o*-1c** (25 μM in MeCN) with 313 nm light after total irradiation of 0, 1, 3, 5, 10, 14, 19, 24, 30, 40, 50 and 60 s. The photostationary state was reached after 40 s. (B) The kinetics profile of the photocyclization of ***o*-1c** to ***c*-1c** with different time.

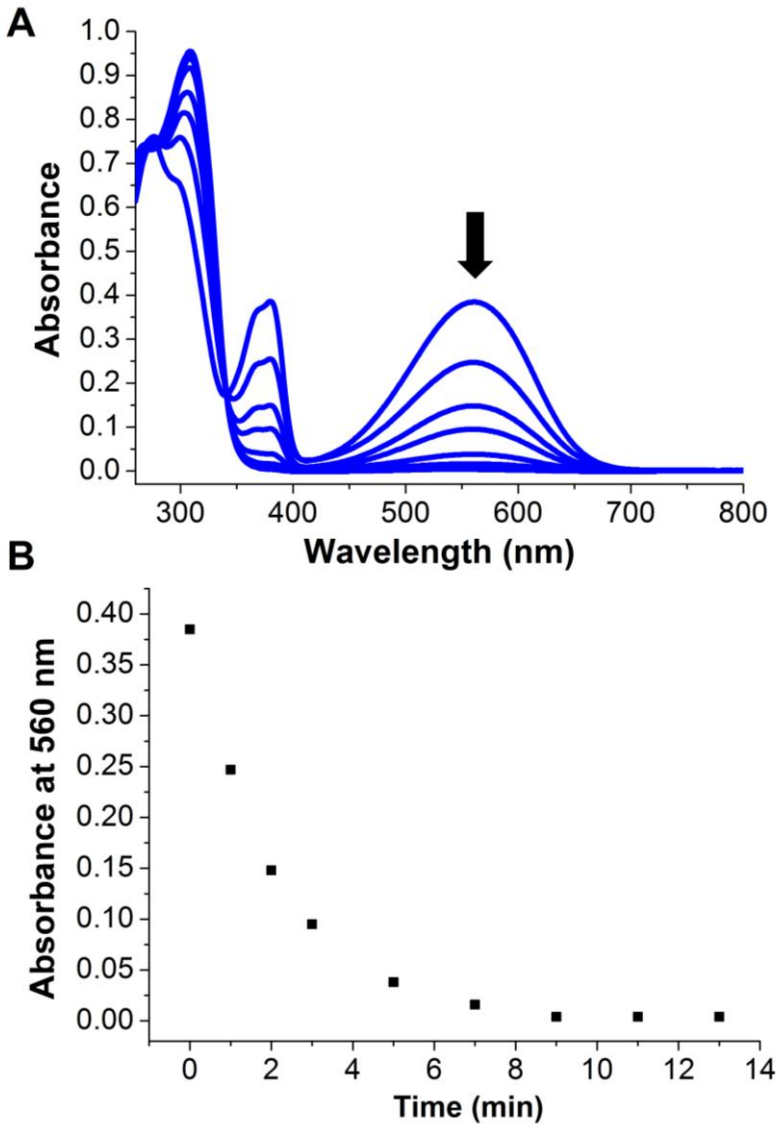


Figure S39. (A) Photocycloreversion of ***c*-1c** to give ***o*-1c**: changes in absorption spectra upon irradiation of ***c*-1c** (25 μM in MeCN) with 650 nm light after total irradiation of 0, 1, 2, 3, 5, 7, 9, 11 and 13 min. The photostationary state was reached after 9 min. (B) The kinetics profile of the photocyclization of ***c*-1c** to ***o*-1c** with different time.

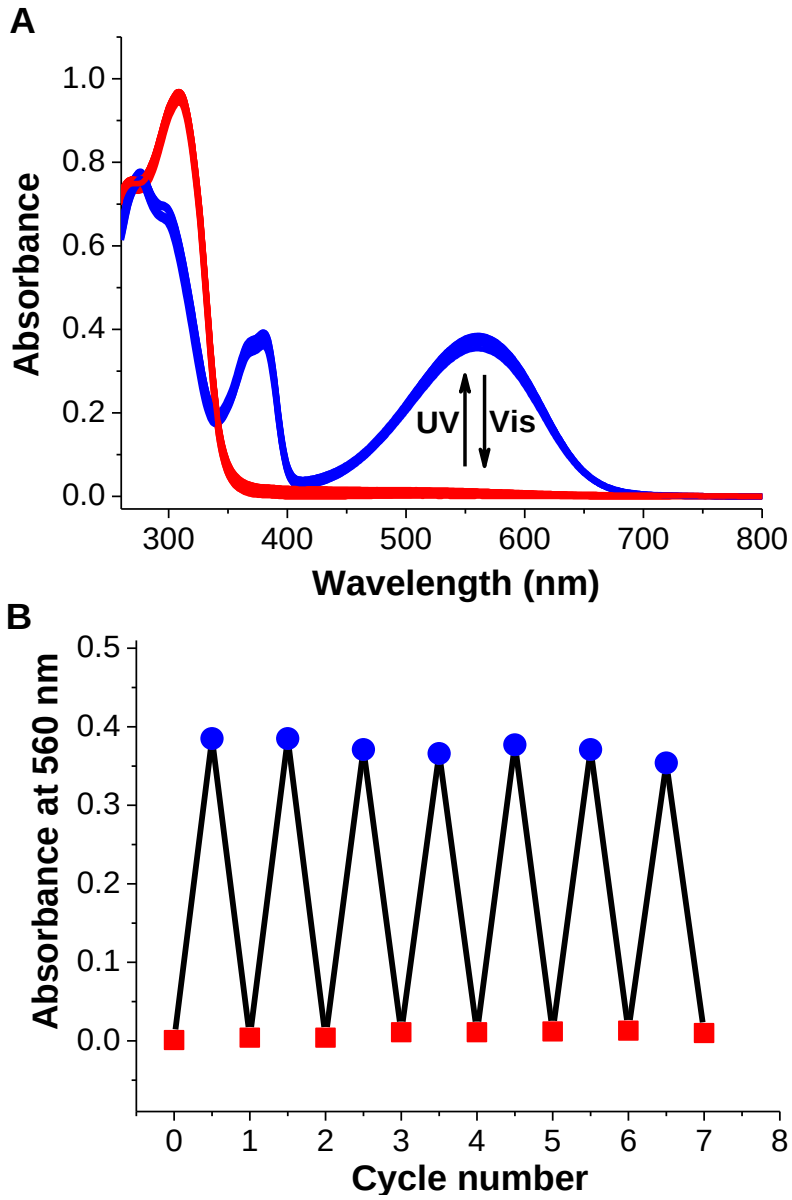


Figure S40. (A) Absorbance spectra of an acetonitrile solution of ***o*-1c** (25 μM, 25 ℃ during repetitive switching cycles consisting of alternating UV (313 nm, 40 s) and visible light irradiation (650 nm, 9 min). (B) Change of absorbance in the visible range (560 nm).

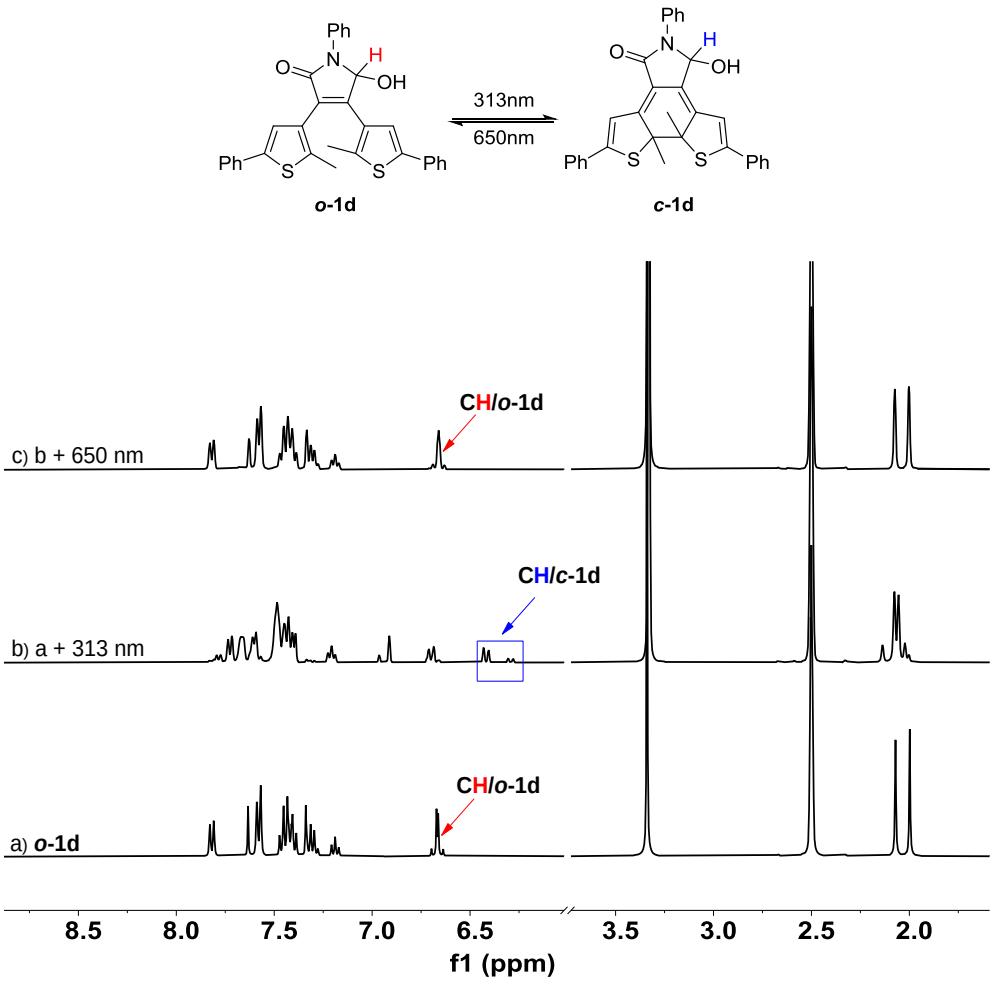


Figure S41. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in DMSO-d_6; (b) Irradiation of ***o*-1d** with UV light (313 nm, 3 h). The ratio of ***c*-1d** and ***o*-1d** is 91:9; (c) Further irradiation with visible light (650 nm, 2 h). The ratio of ***o*-1d** and ***c*-1d** is 99:1.

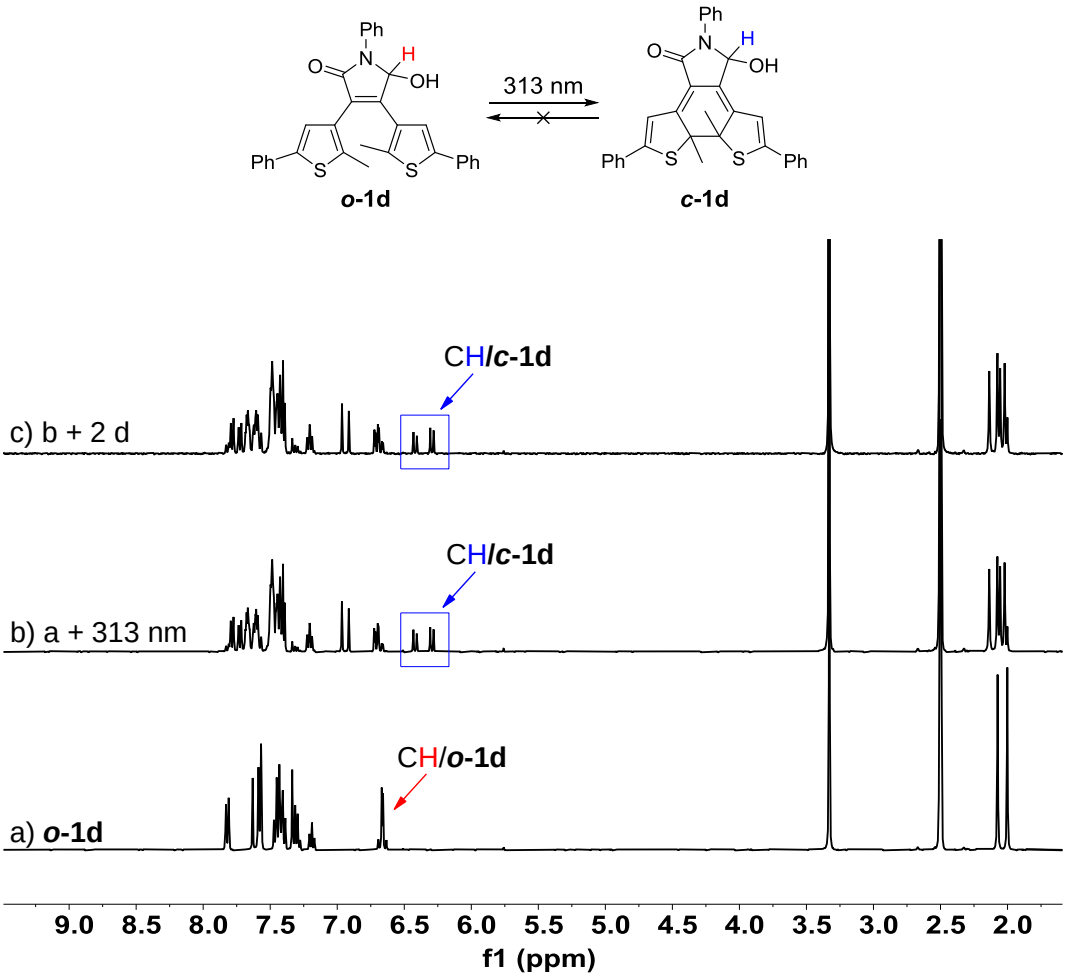


Figure S42. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b) Irradiation of ***o*-1d** with UV light (313 nm, 3 h). The ratio of ***c*-1d** and ***o*-1d** is 91:9; (c) Panel b at room temperature for 2 days. ***o*-1d** was not observed.

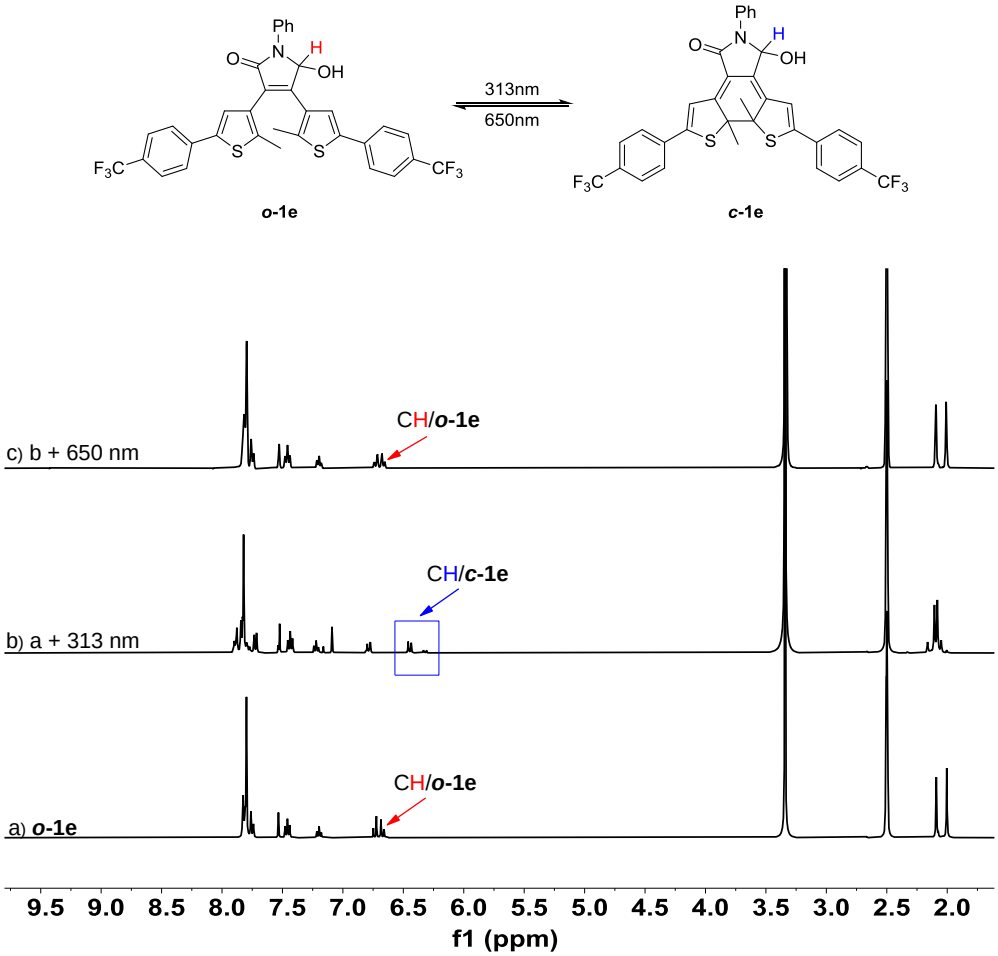


Figure S43. (a) ^{1}H NMR spectrum of ***o*-1e** (5 mM) in DMSO-d_6; (b) Irradiation of ***o*-1e** with UV light (313 nm, 3 h). The ratio of ***c*-1e** and ***o*-1e** is 97:3; (c) Further irradiation with visible light (650 nm, 1.5 h). The ratio of ***o*-1e** and ***c*-1e** is 99:1.

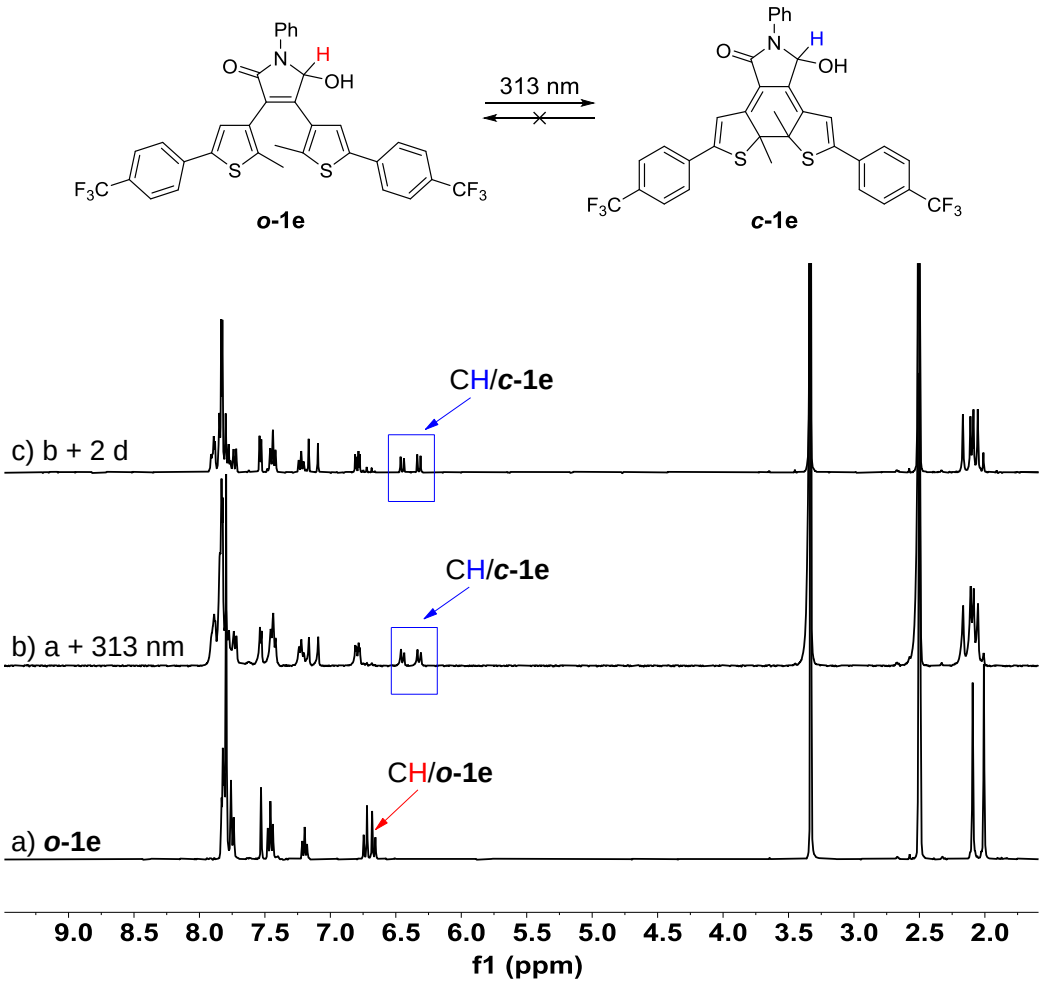


Figure S44. (a) ^{1}H NMR spectrum of ***o*-1e** (5 mM) in CD_3CN; (b) Irradiation of ***o*-1e** with UV light (313 nm, 3 h). The ratio of ***c*-1c** and ***o*-1c** is 97:3; (c) Panel b at room temperature for 2 days. ***o*-1e** was not observed.

4. Generation of Carbocation of *in situ*

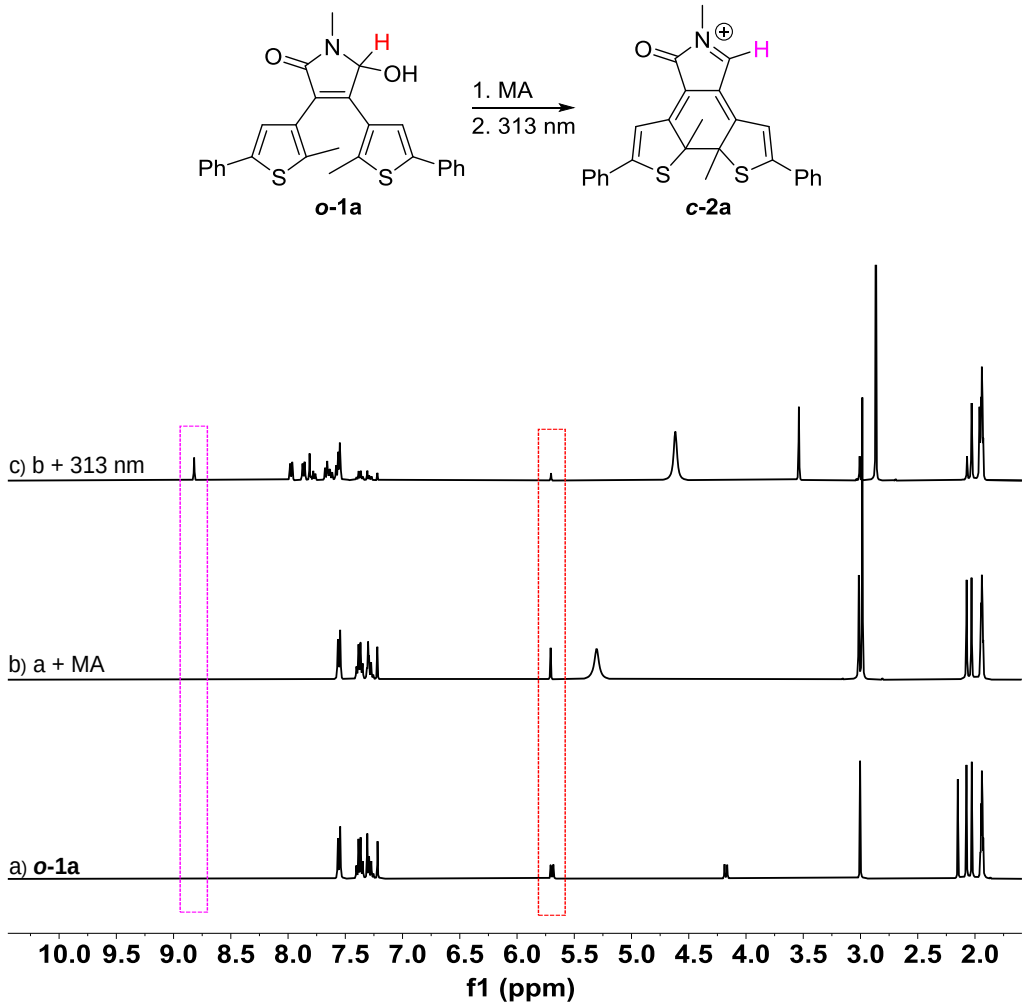


Figure S45. The generation of ***c*-2a** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) No apparent change was detected when MA (4.0 equiv.) was added into panel a; (c) Irradiation of panel b with UV light (313 nm, 1.5 h), with ***c*-2a** (85%) created.

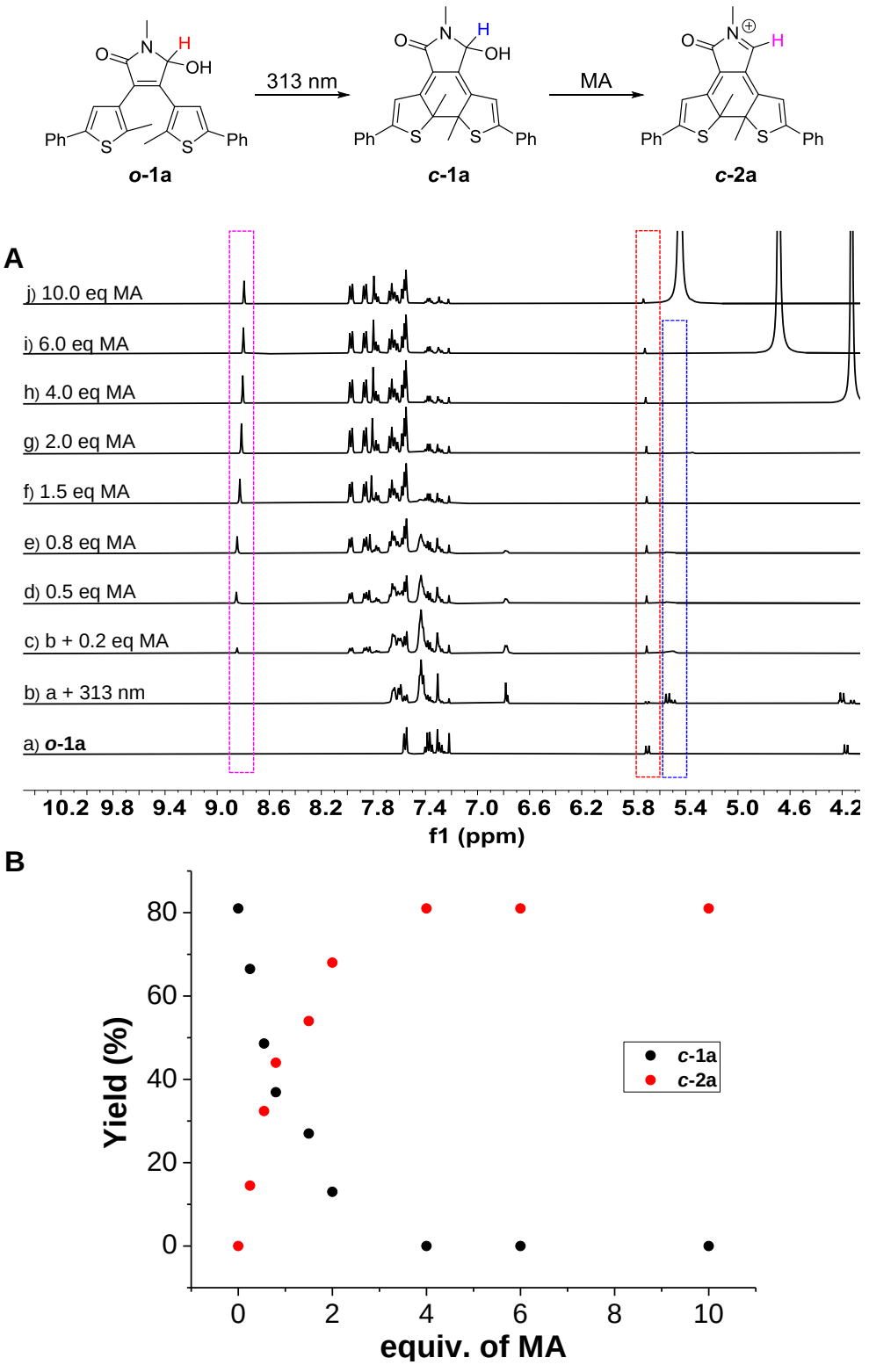


Figure S46. (A) ^{1}H NMR spectra of the titration of MA for the conversion from ***c*-1a** to ***c*-2a**. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) Irradiation of panel a with UV light (313 nm, 1.5 h); (c-j) Titration of MA into panel b, creating ***c*-2a** (85%). (B) Change in the yield of the reaction of ***c*-1a** with different equivalents of MA.

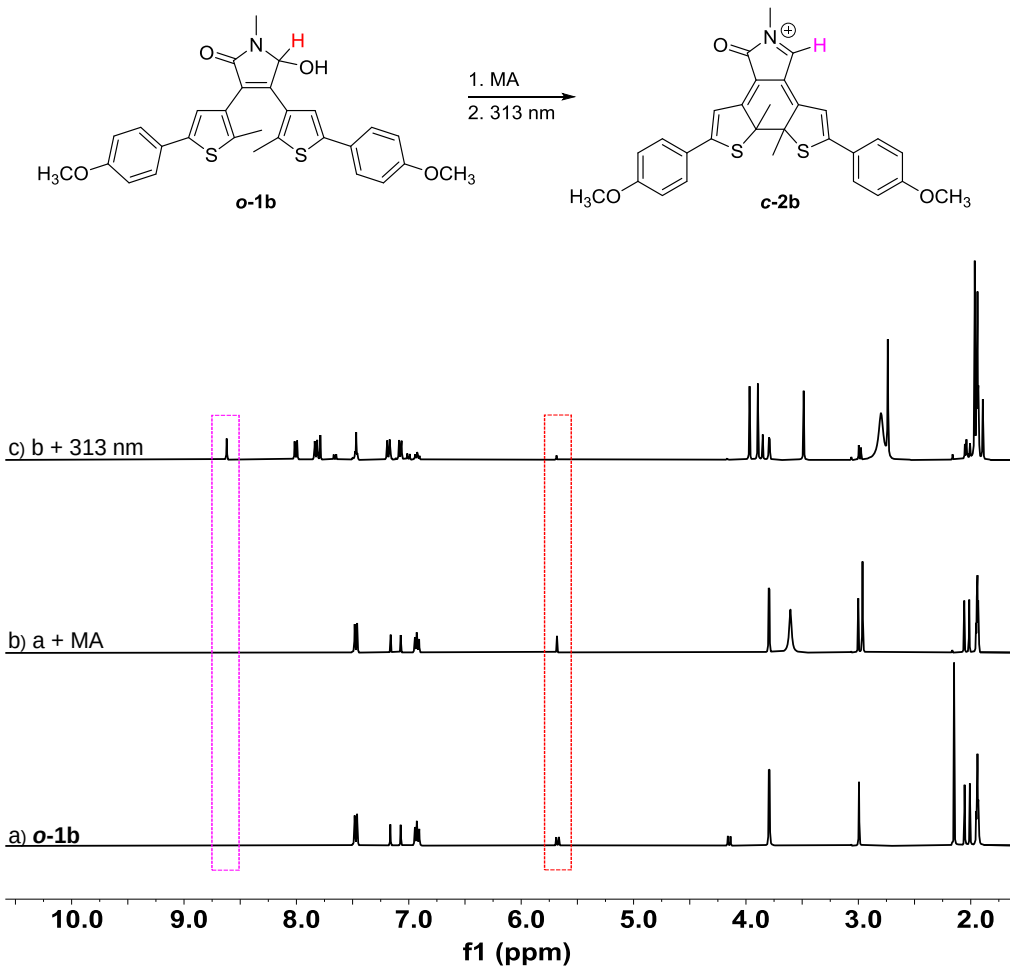


Figure S47. The generation of ***c*-2b** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in CD_3CN; (b) No apparent change was detected when MA (2.0 equiv.) was added into panel a; (c) Irradiation of panel b with UV light (313 nm, 1.5 h), with ***c*-2b** (70%) created.

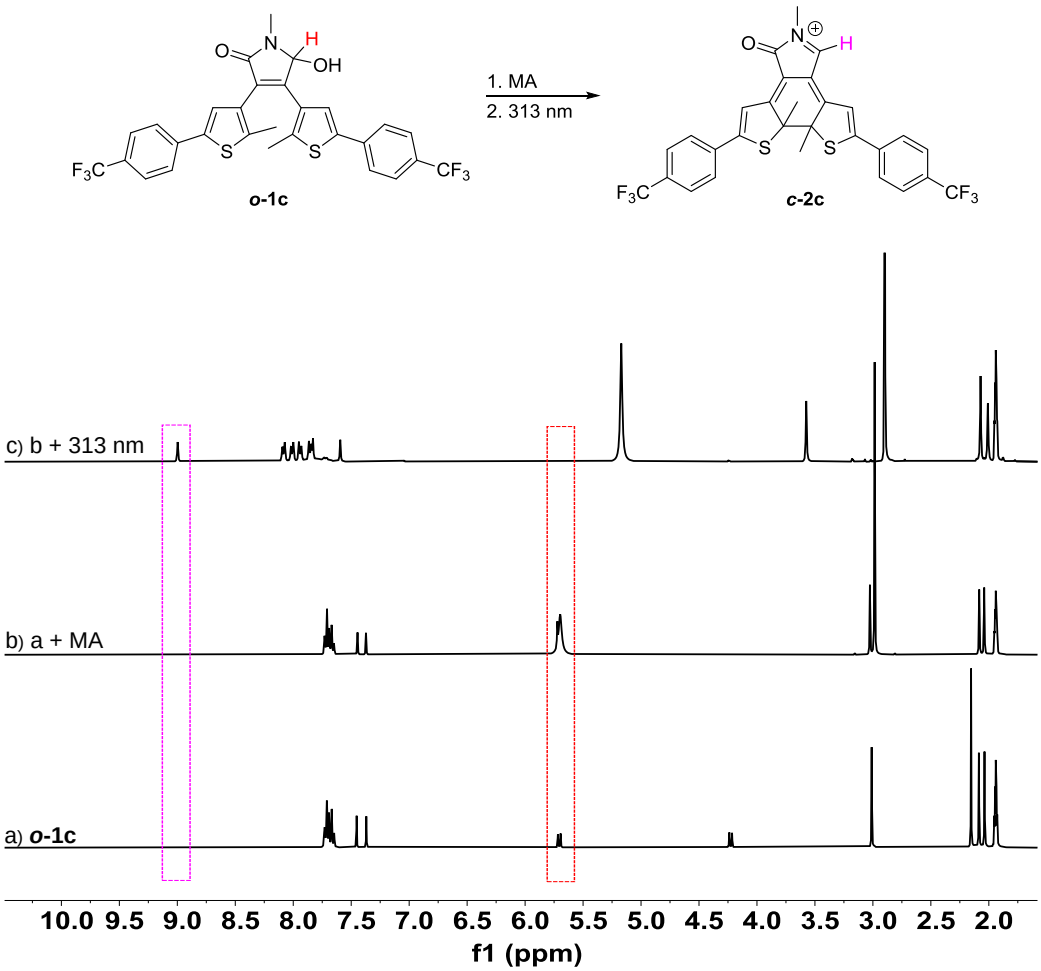


Figure S48. The generation of ***c*-2c** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) No apparent change was detected when MA (7.0 equiv.) was added into panel a; (c) Irradiation of panel b with UV light (313 nm, 1.5 h), with ***c*-2c** (92%) created.

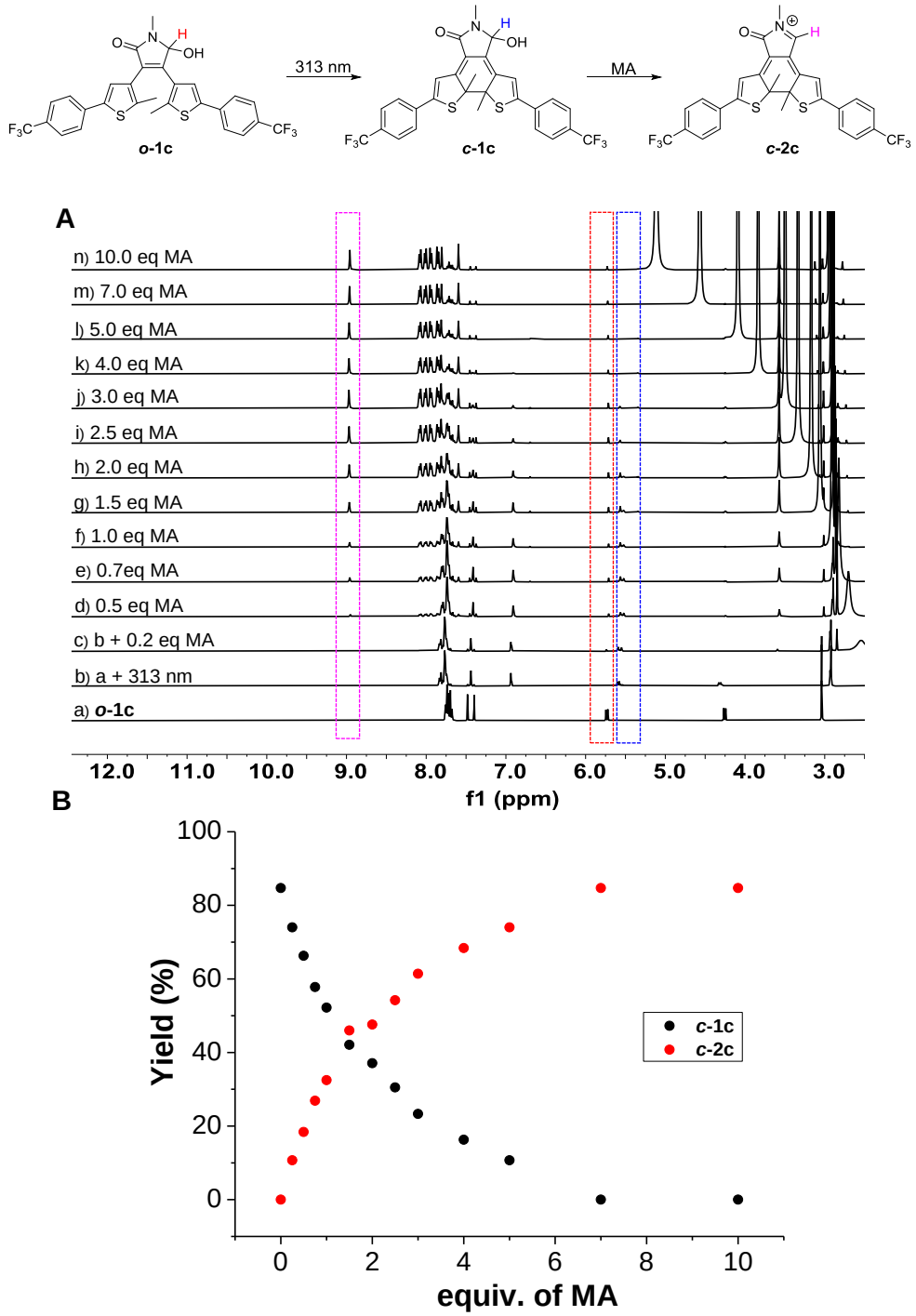


Figure S49. (A) ^{1}H NMR spectra of the titration of MA for the conversion from ***c*-1c** to ***c*-2c**. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) Irradiation of panel a with UV light (313 nm, 1.5 h); (c-j) Titration of MA into panel b, creating ***c*-2c** (92%). (B) Change in the yield of the reaction of ***c*-1c** with different equivalents of MA.

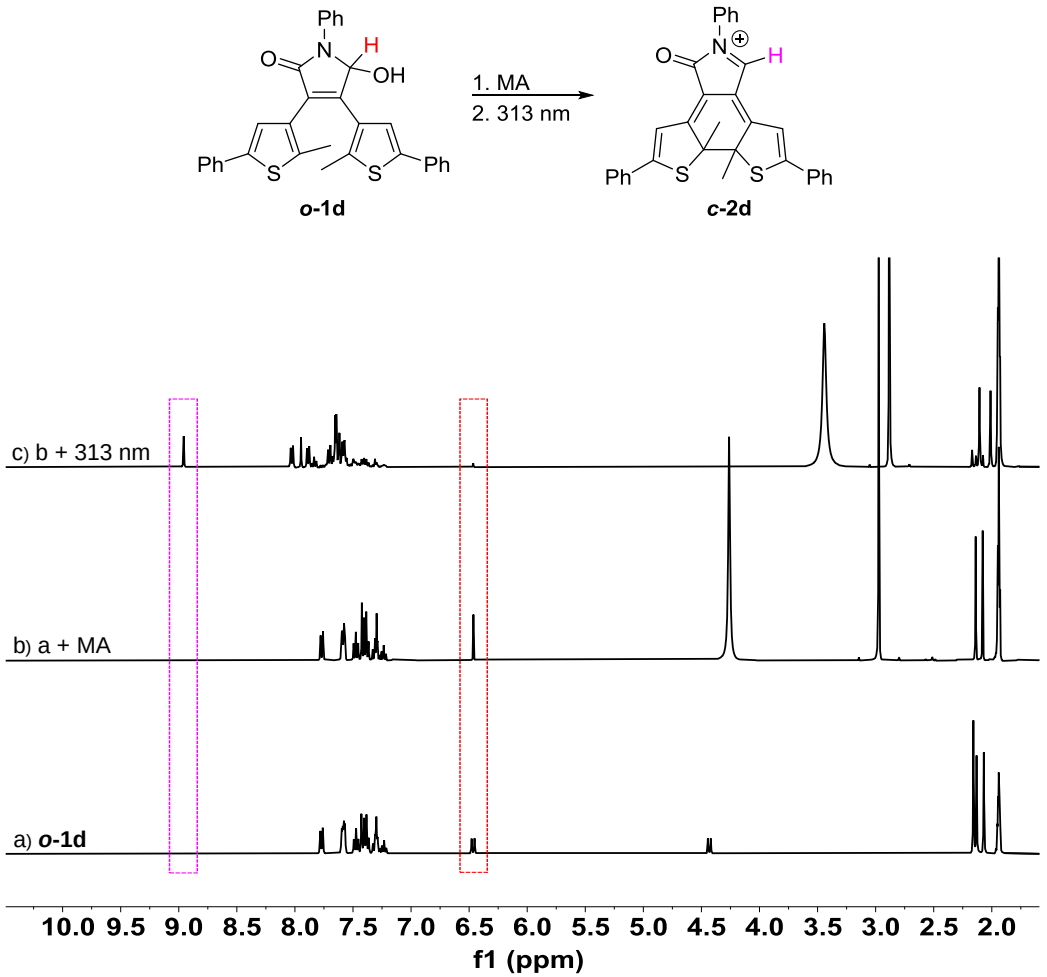


Figure S50. The generation of ***c*-2d** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b) No apparent change was detected when MA (5.0 equiv.) was added into panel a; (c) Irradiation of panel b with UV light (313 nm, 3 h), with ***c*-2d** (93%) created.

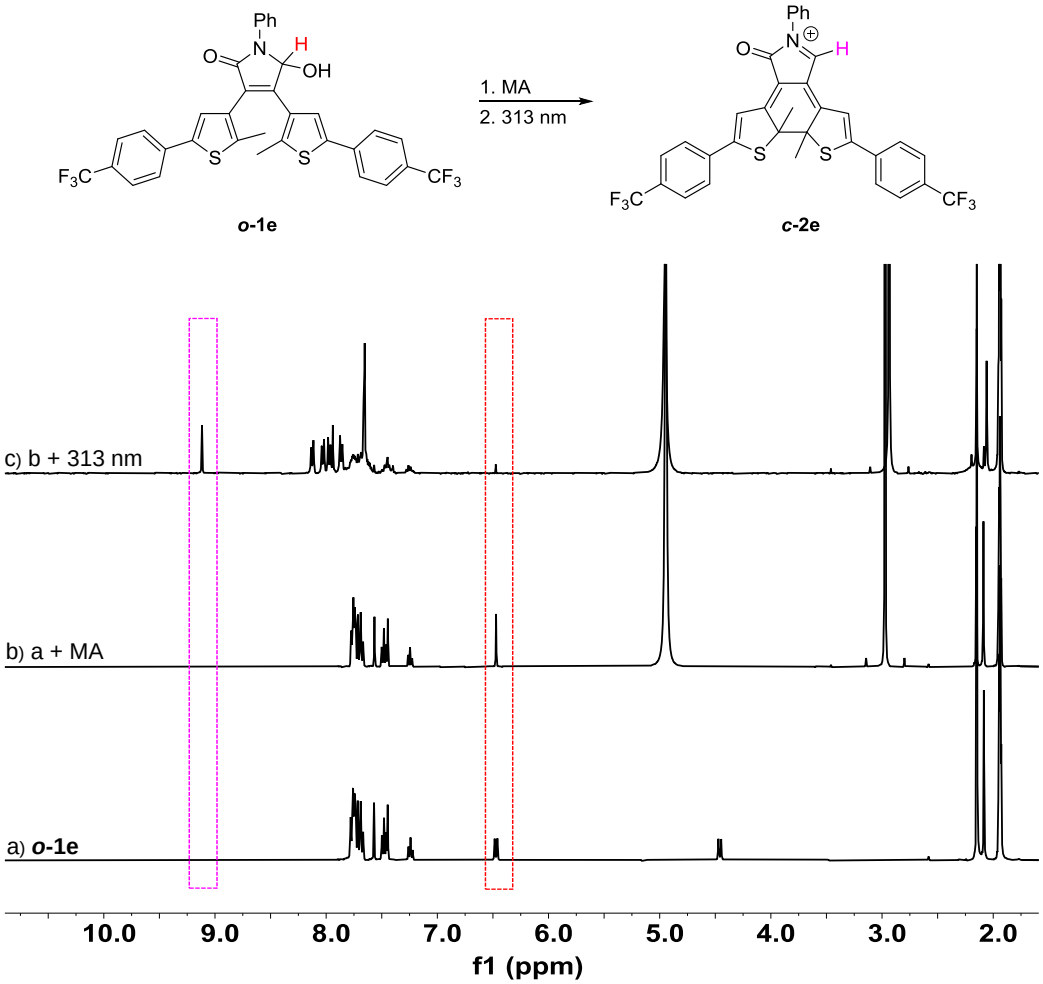


Figure S51. The generation of ***c*-2e** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1e** (5 mM) in CD_3CN; (b) No apparent change was detected when MA (11.0 equiv.) was added into panel a; (c) Irradiation of panel b with UV light (313 nm, 3 h), with ***c*-2e** (93%) created.

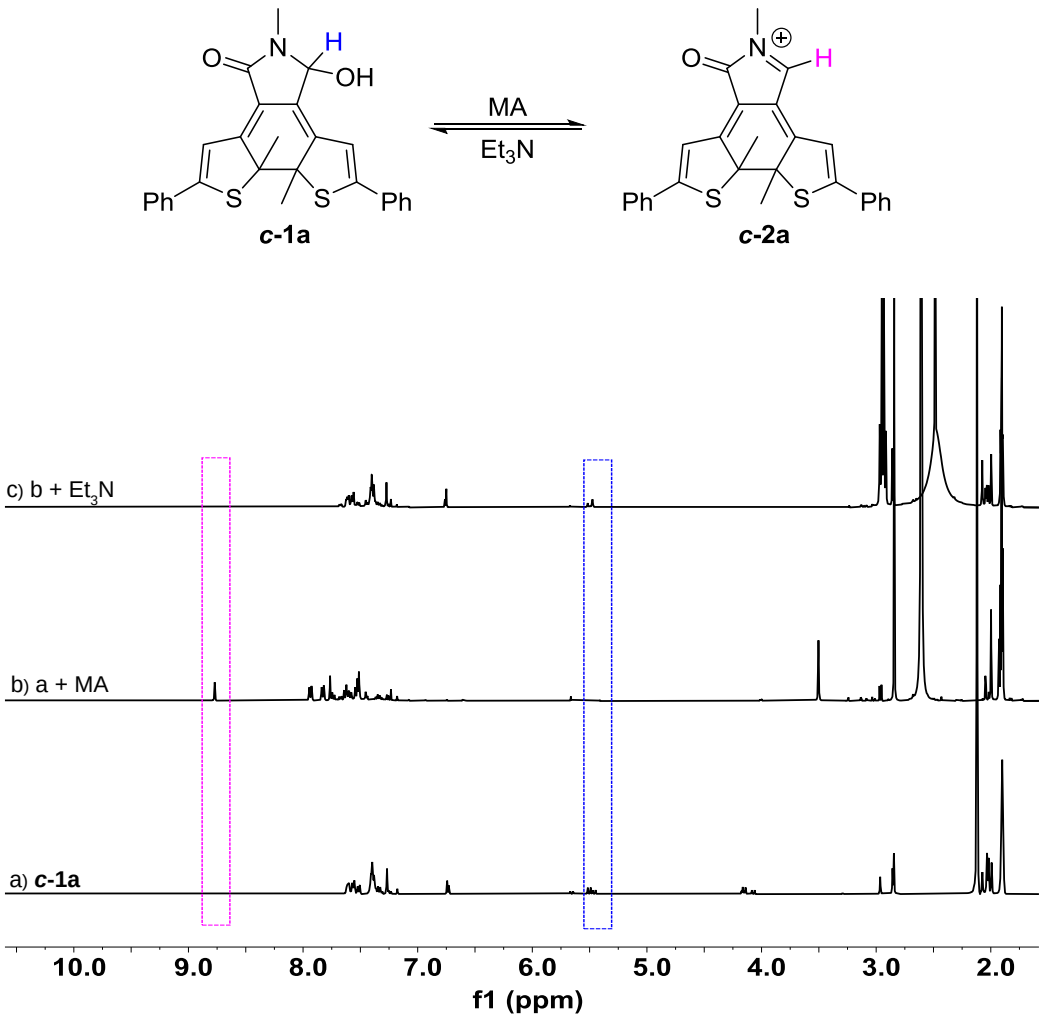


Figure S52. The switching between ***c*-1a** and ***c*-2a**. (a) ^{1}H NMR spectrum of ***c*-1a** (5 mM), created by irradiation of ***o*-1a** at 313 nm for 1.5 h; (b) The addition of MA (4.0 equiv.) into panel a; (c) The addition of Et_3N (4.0 equiv.) into panel b.

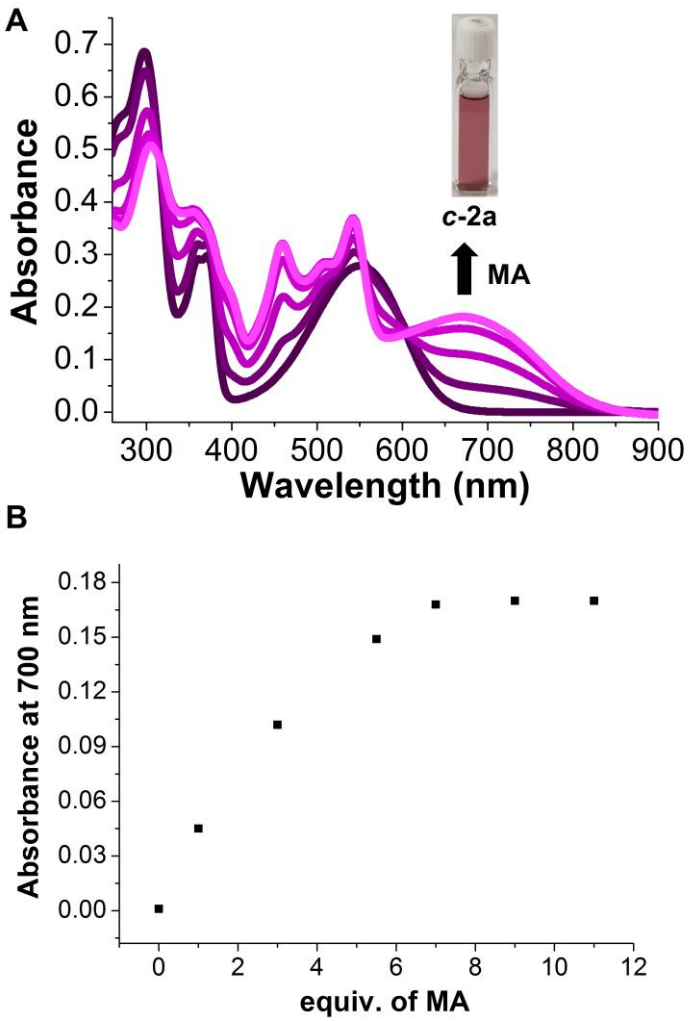


Figure S53. (A) UV-vis spectra of the titration of MA for the switch from ***c*-1a** (25 μM in MeCN) to ***c*-2a**. (B) Change in the absorbance at 700 nm with different equivalents of MA.

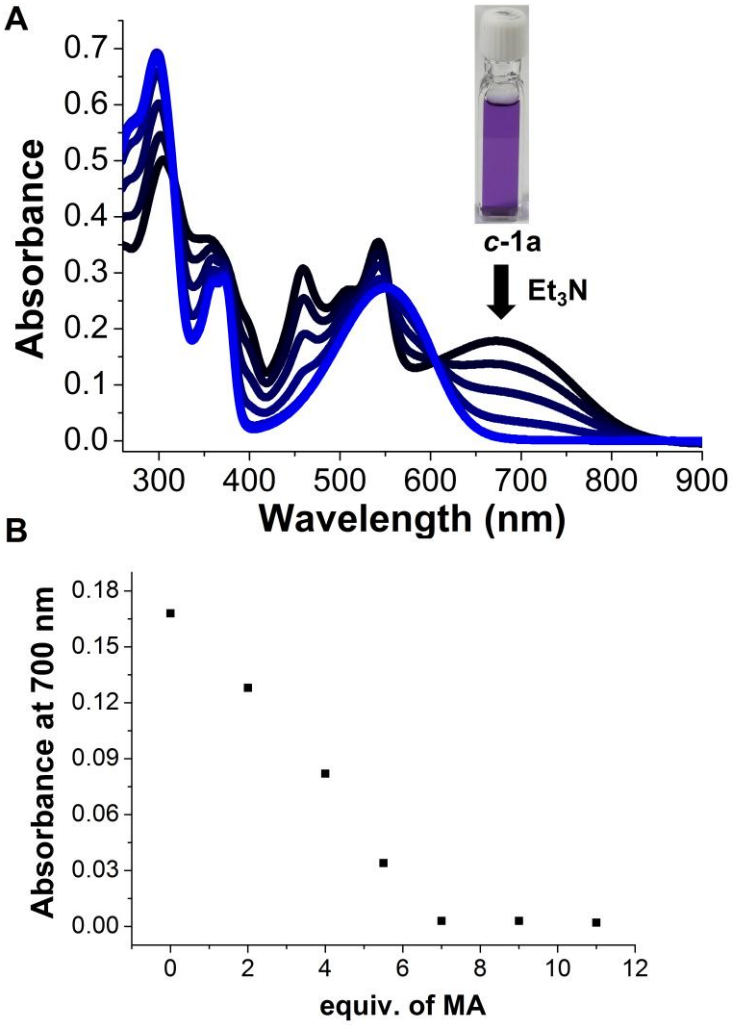


Figure S54. (A) UV-vis spectra of the titration of Et_3N for the switch from ***c*-2a** (25 μM in MeCN) to ***c*-1a**. (B) Change in the absorbance at 700 nm with different equivalents of Et_3N.

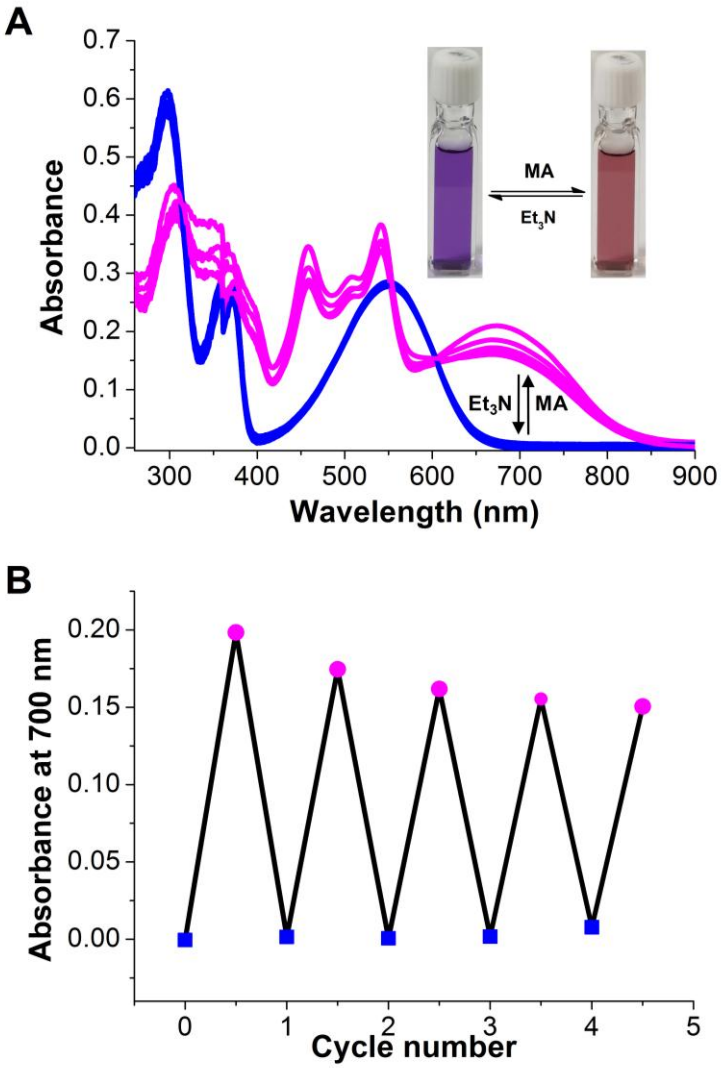


Figure S55. Multiple cycles of switching between ***c*-1a** and ***c*-2a** with consecutive addition of acid/base.

5. The Isolation of Carbocation

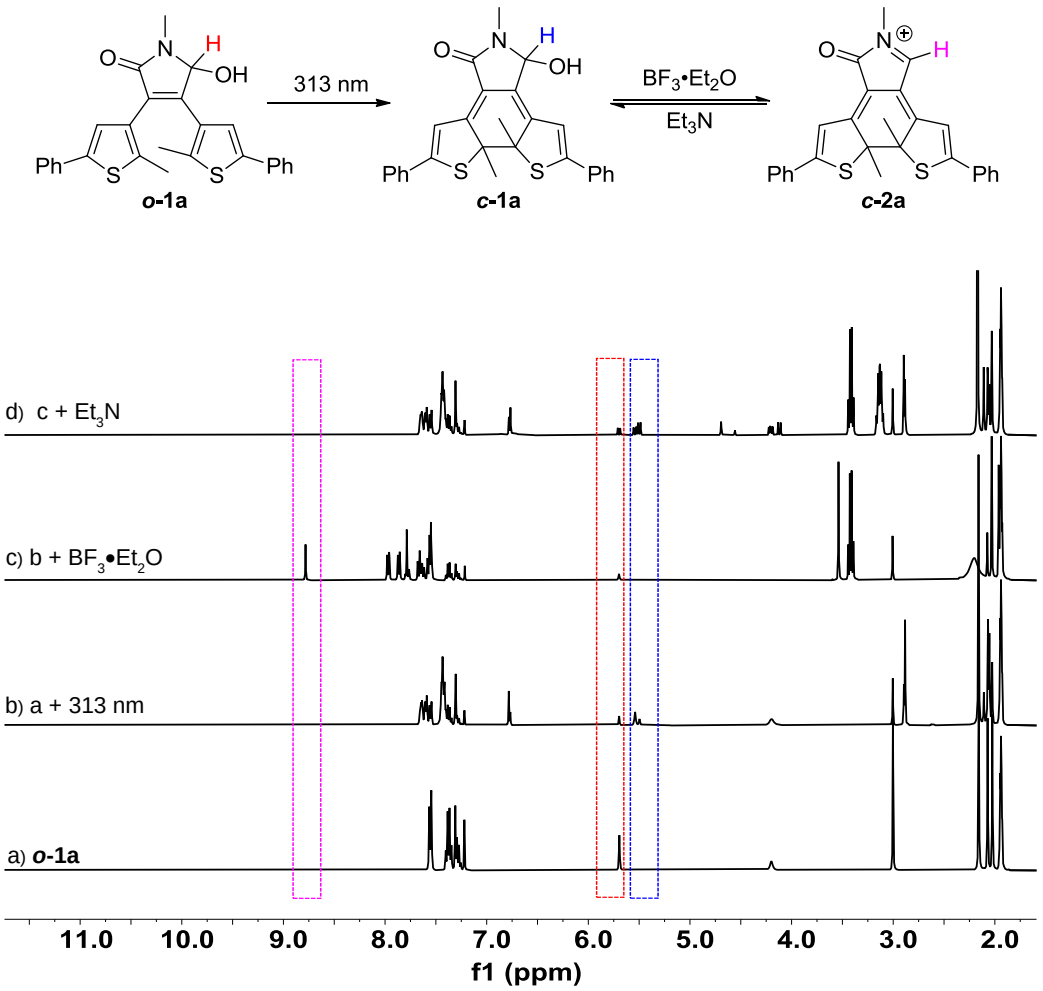


Figure S56. The switching between ***c*-1a** and ***c*-2a**. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) Irradiation of panel a with UV light (313 nm, 1.5 h) to give ***c*-1a**; (c) The addition of BF_3•Et_2O (1.5 equiv.) into panel b to give ***c*-2a**; (d) The addition of Et_3N (1.5 equiv.) into panel c to restore ***c*-1a**.

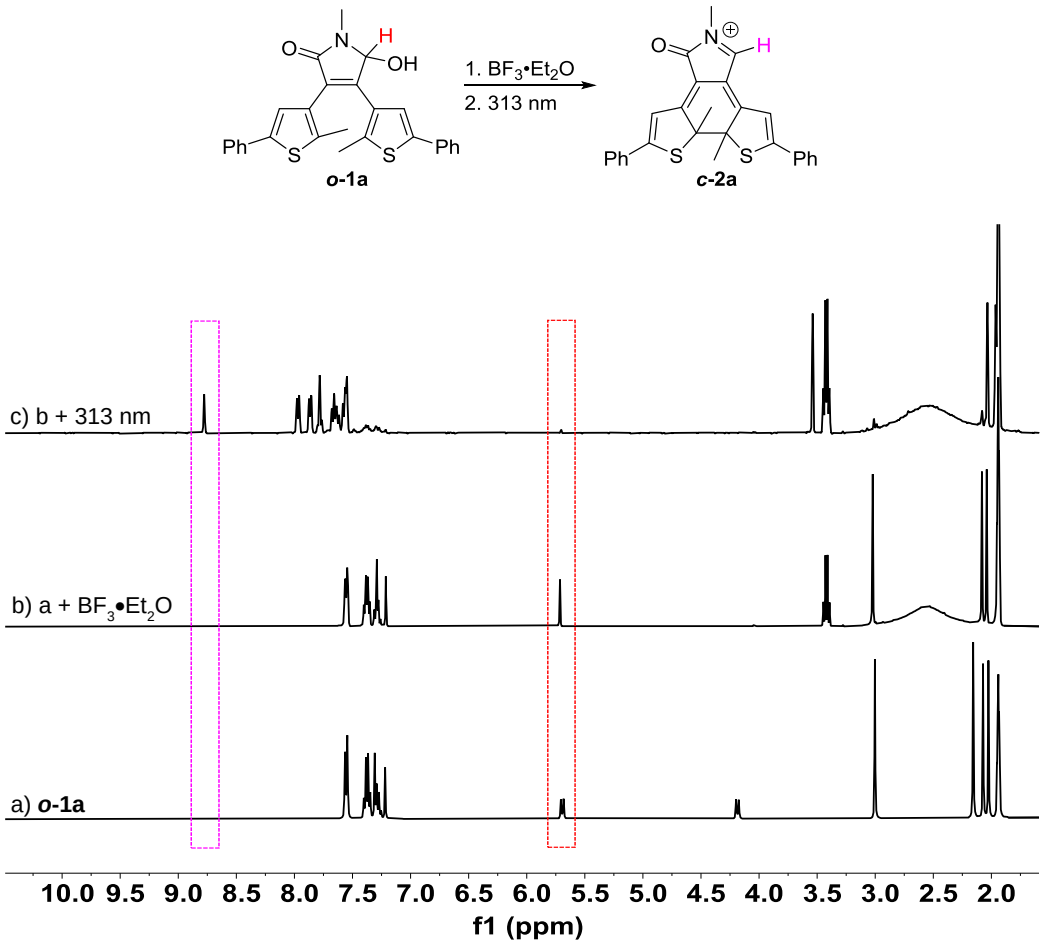


Figure S57. The generation of ***c*-2a** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a; (c) Irradiation of panel b with UV light (313 nm, 1.5 h), with ***c*-2a** (90%) created.

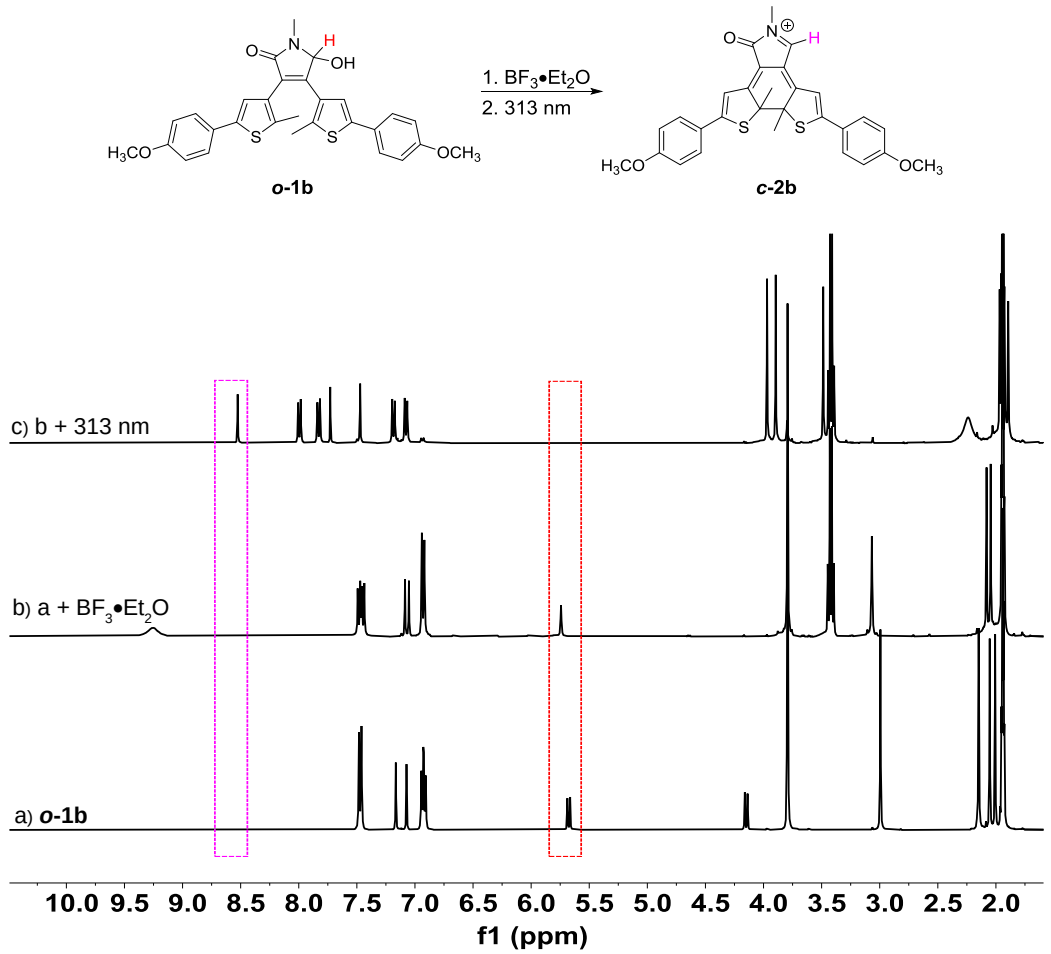


Figure S58. The generation of ***c*-2b** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a; (c) Irradiation of panel b with UV light (313 nm, 2 h), with ***c*-2b** (91%) created.

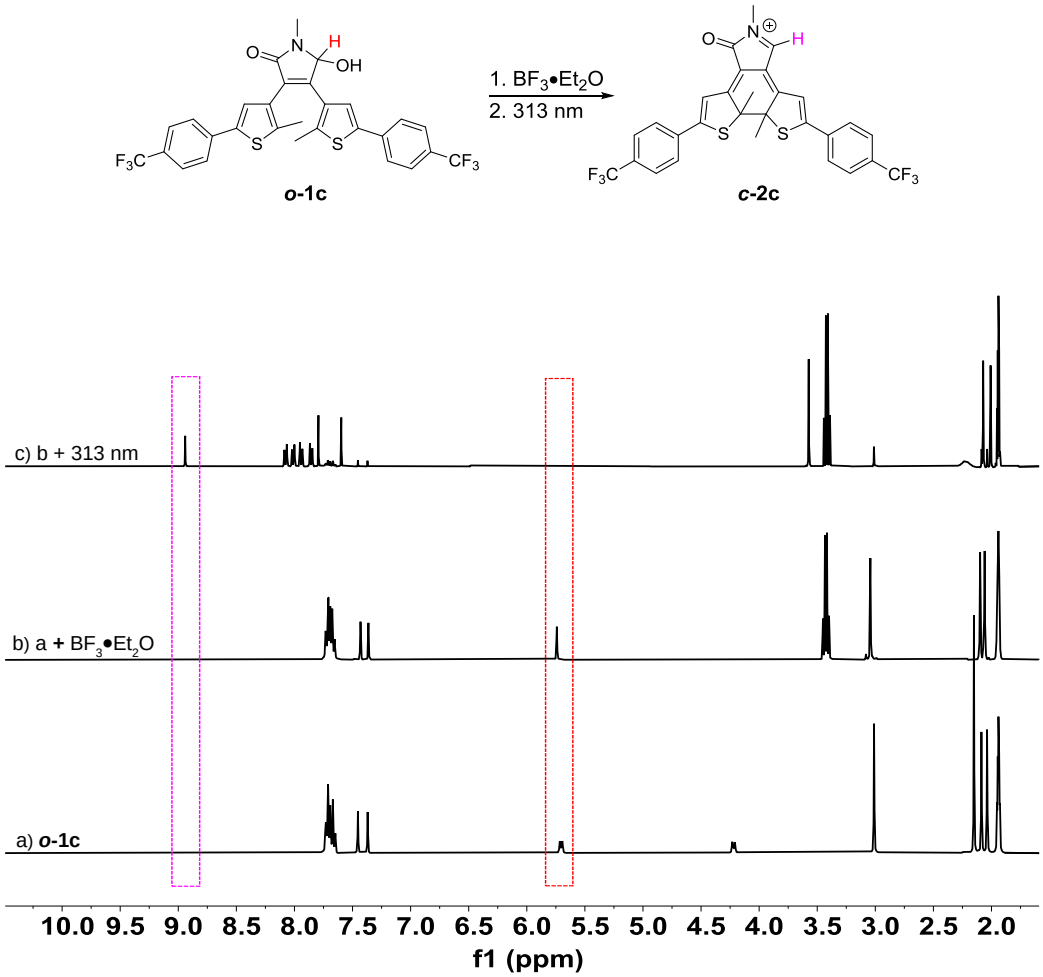


Figure S59. The generation of ***c*-2c** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a; (c) Irradiation of panel b with UV light (313 nm, 1.5 h), with ***c*-2c** (92%) created.

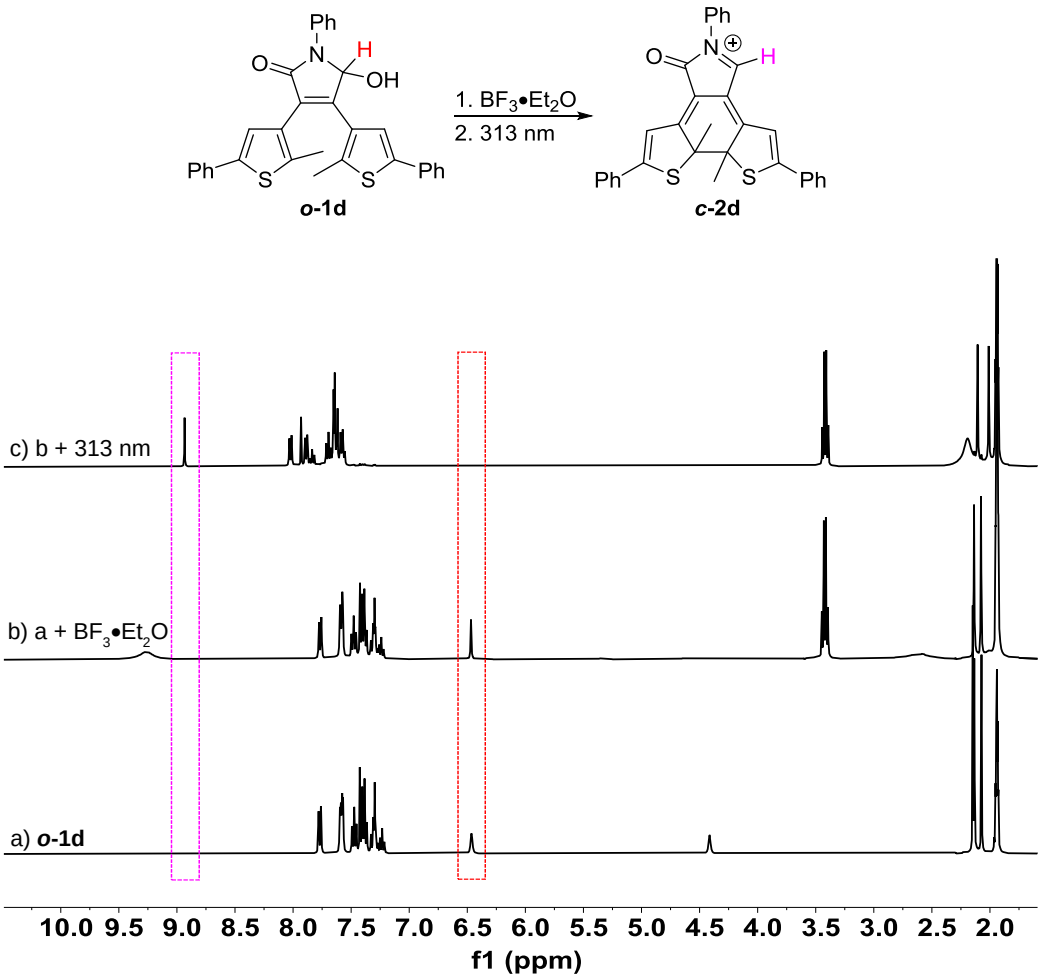


Figure S60. The generation of ***c*-2d** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a; (c) Irradiation of panel b with UV light (313 nm, 3 h), with ***c*-2d** (96%) created.

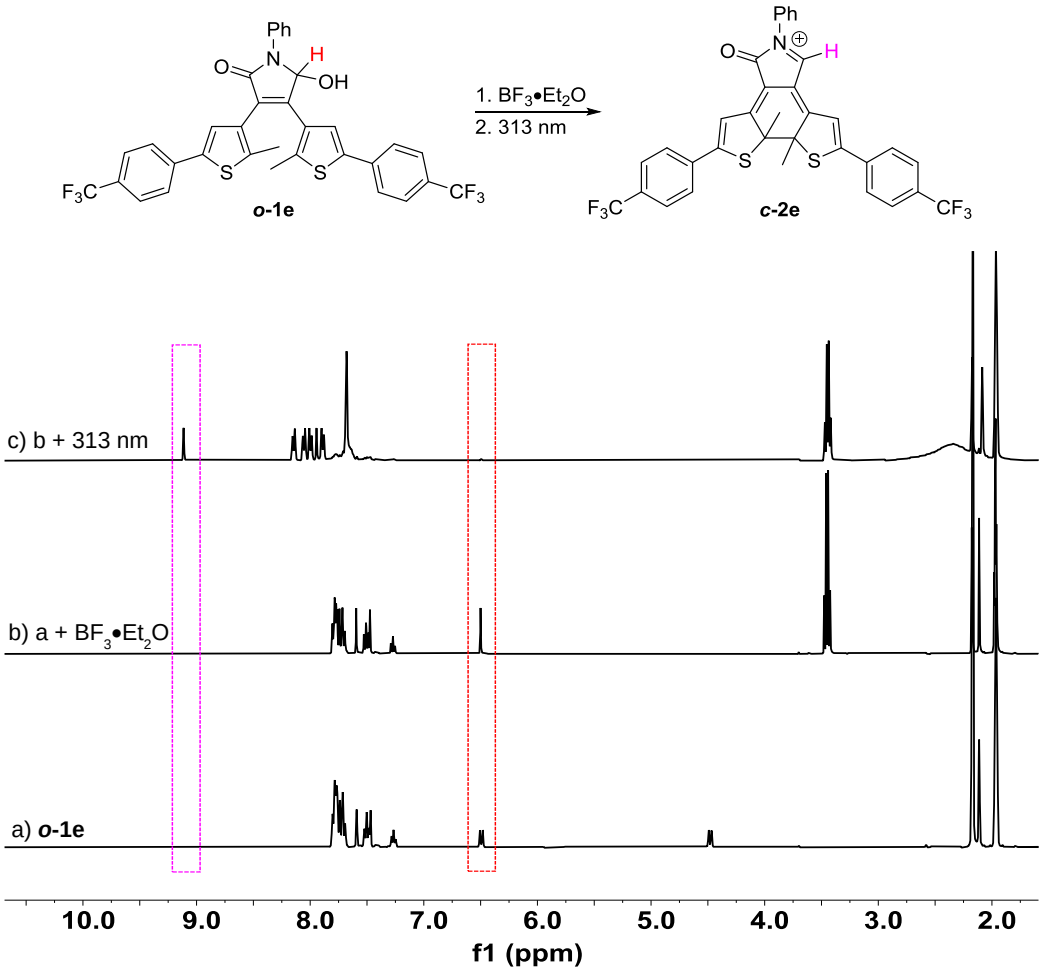
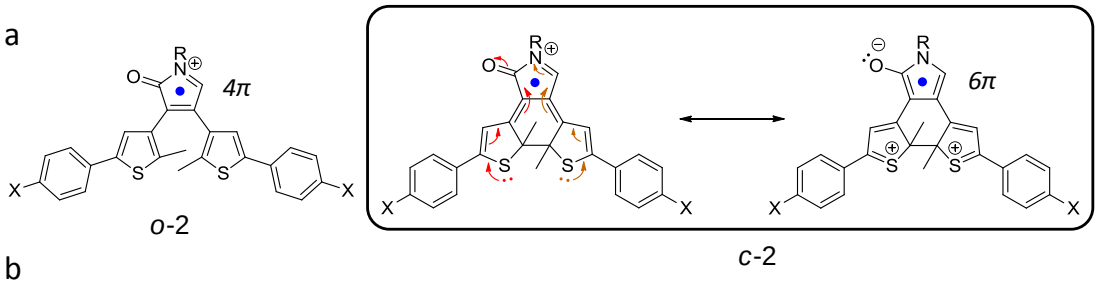


Figure S61. The generation of ***c*-2e** *in situ*. (a) ^{1}H NMR spectrum of ***o*-1e** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a; (c) Irradiation of panel b with UV light (313 nm, 3 h), with ***c*-2e** (97%) created.

6. Computations

a



b

Compound	2a	2b	2c	2d	2e
Substituent	R = Me X = H	R = Me X = OMe	R = Me X = CF_3	R = Ph X = H	R = Ph X = CF_3
o-2	11.6	11.7	11.4	11.6	11.5
c-2	-7.7	-7.7	-7.5	-6.8	-6.6

Figure S62. (a) Representative resonance structures for ***o*-2** and ***c*-2**. (b) The $NICS(1)_{zz}$ values for the *N*-heterocyclic ring with different substituents.

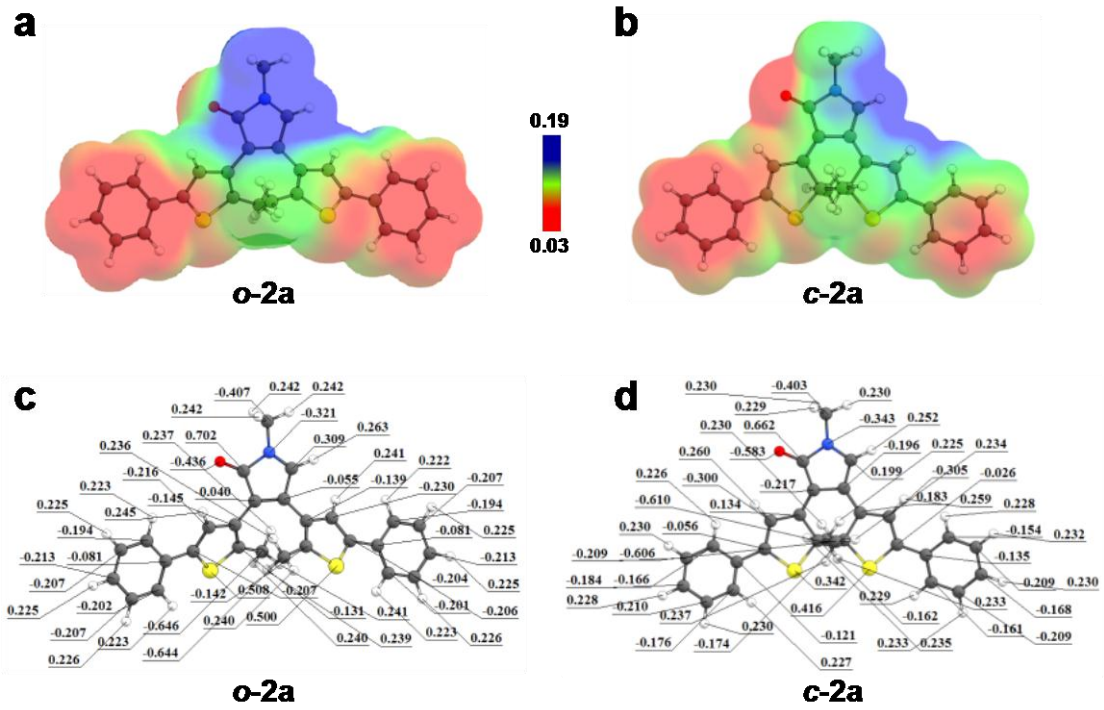


Figure S63. Electrostatic potential (ESP) map (isosurface = 0.001) of ***o*-2a** (a) and ***c*-2a** (b), and NPA charge of ***o*-2a** (c) and ***c*-2a** (d).

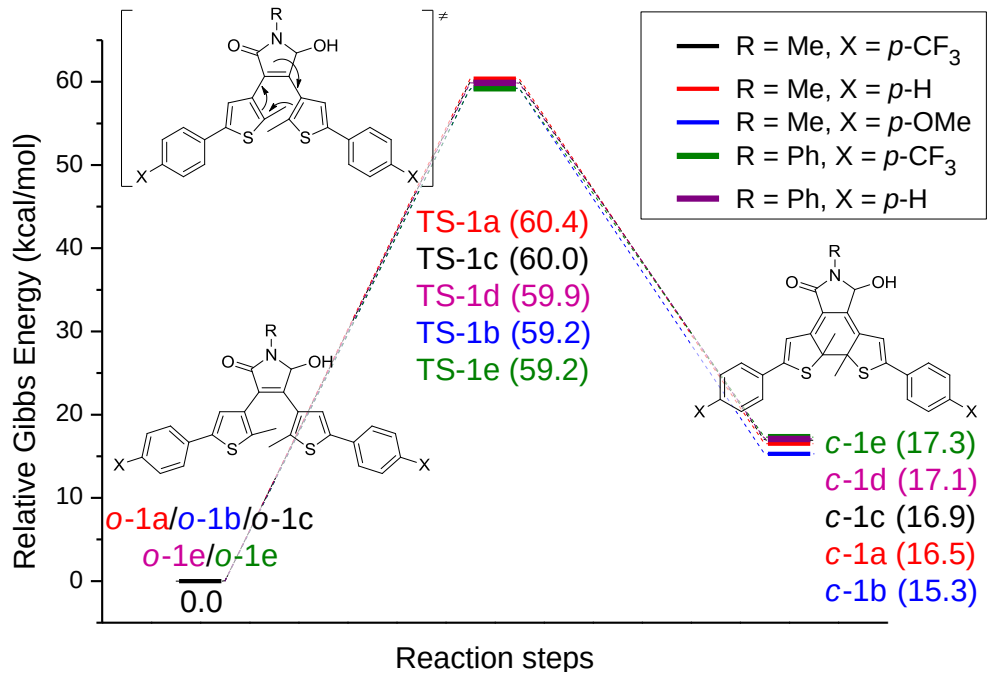


Figure S64. Minimum energy reaction pathways for the thermal conversion between ***o*-1** and ***c*-1** with different substituents.

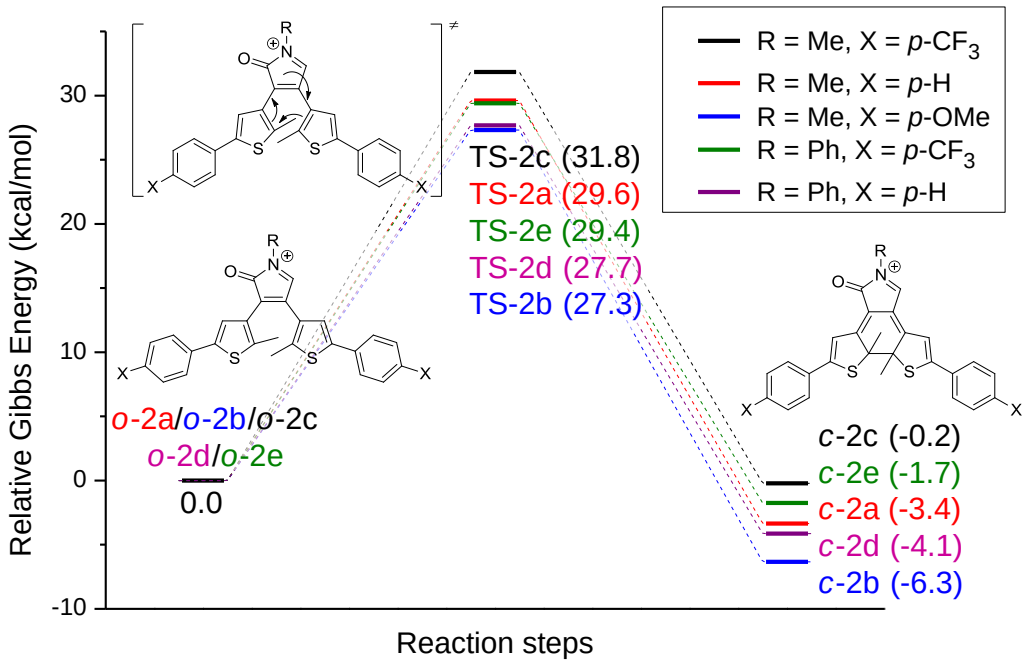


Figure S65. Minimum energy reaction pathways for the thermal conversion between ***o*-2** and ***c*-2** with different substituents.

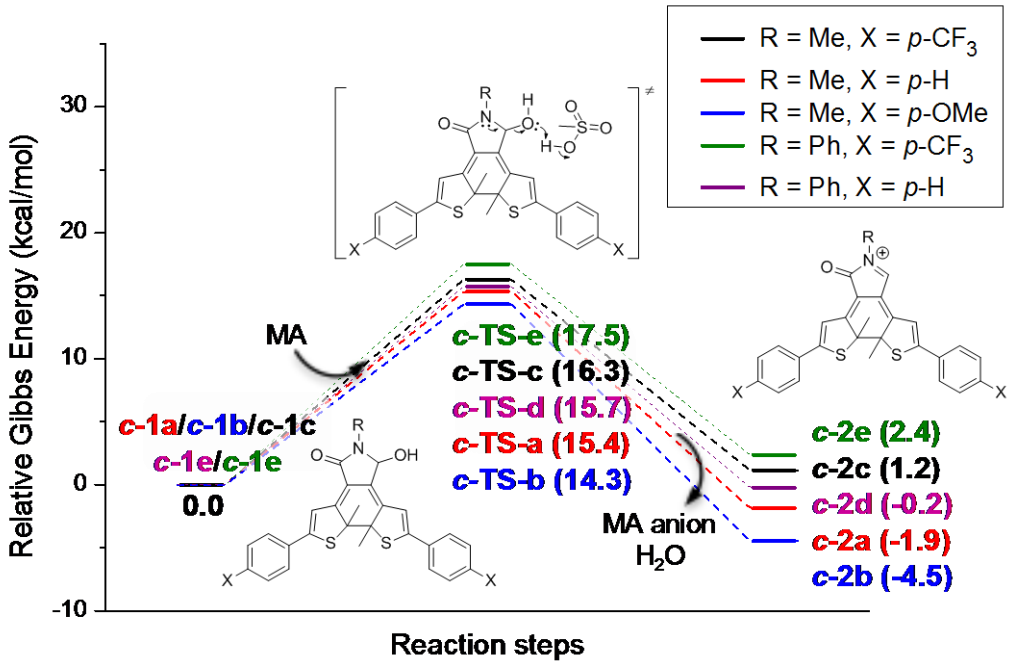


Figure S66. Minimum energy reaction pathways for acid-induced dehydration of ***c*-1** to give ***c*-2** with different substituents.

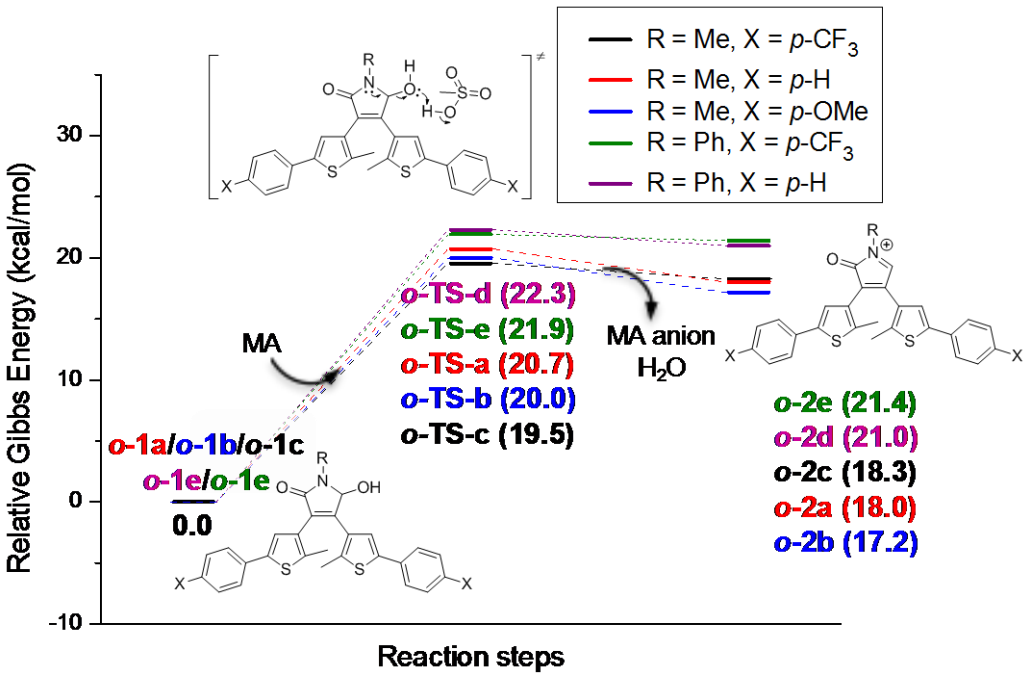


Figure S67. Minimum energy reaction pathways for acid-induced dehydration of ***o*-1** to give ***o*-2** with different substituents.

7. Stability and Switchability of Carbocations

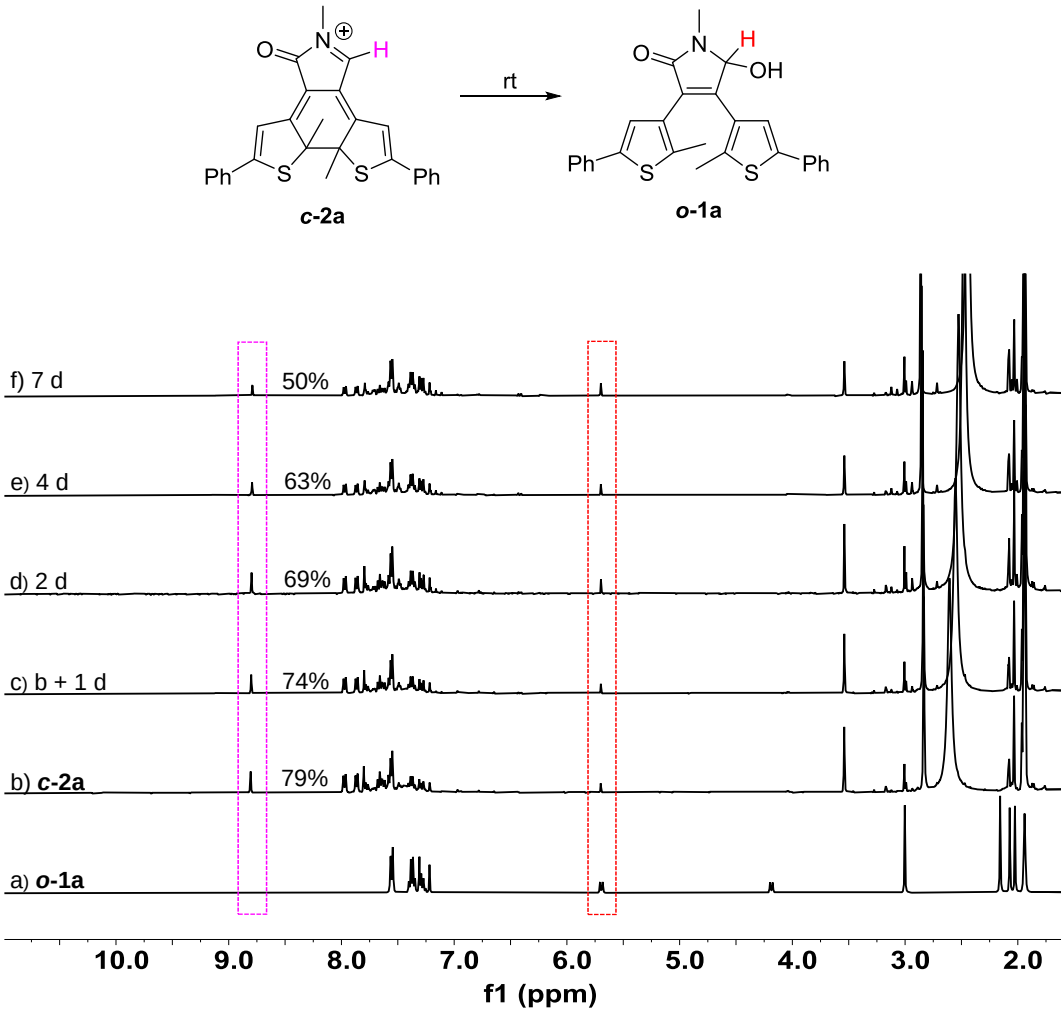


Figure S68. The stability of *in situ* generated ***c*-2a** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) The addition of MA (4.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2a**; (c-f) Panel b at varied time.

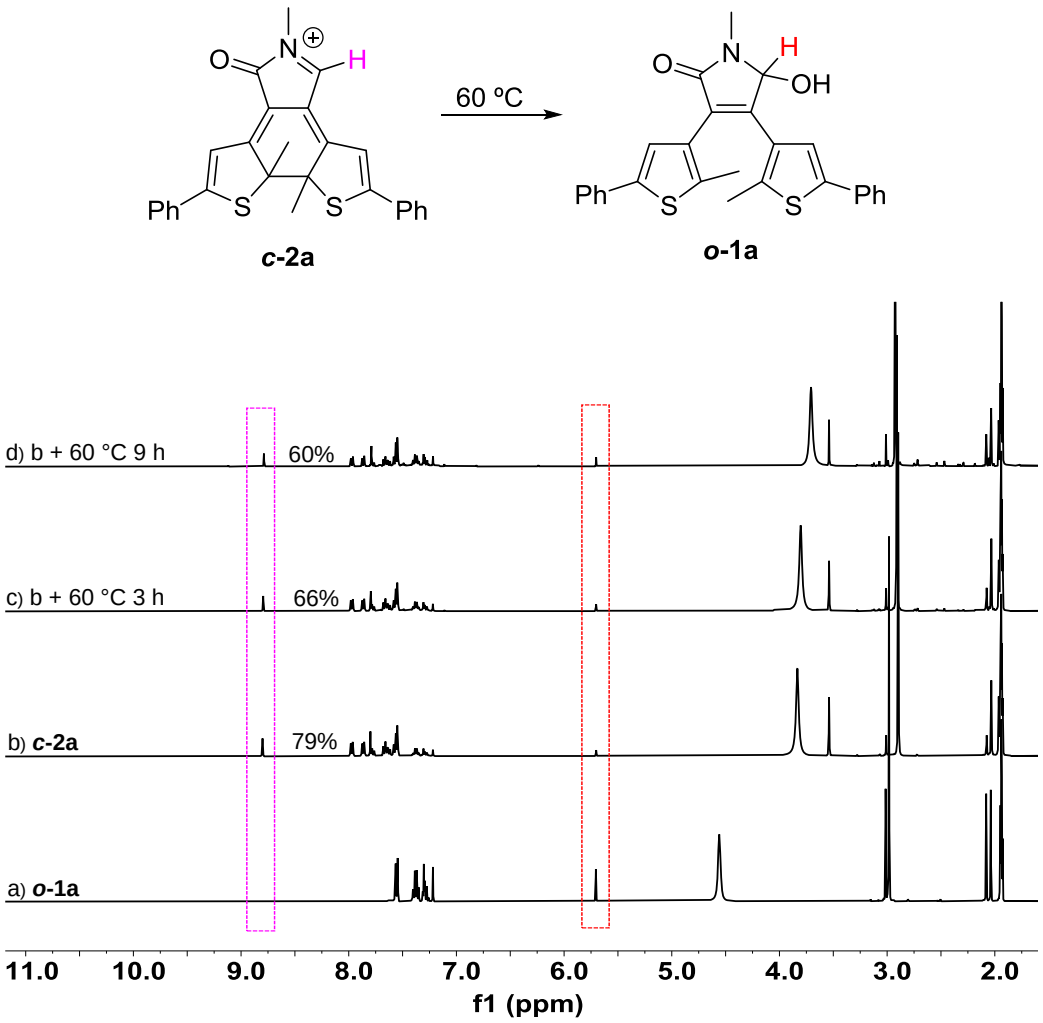


Figure S69. The stability of *in situ* generated ***c*-2a** at 60 ℃. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) The addition of MA (4.0 equiv.) into panel a and then irradiation with UV (313 nm, 1.5 h) to give ***c*-2a**; (c) Heat panel b at 60 ℃ for 3 h; (d) Heat panel b at 60 ℃ for 9 h.

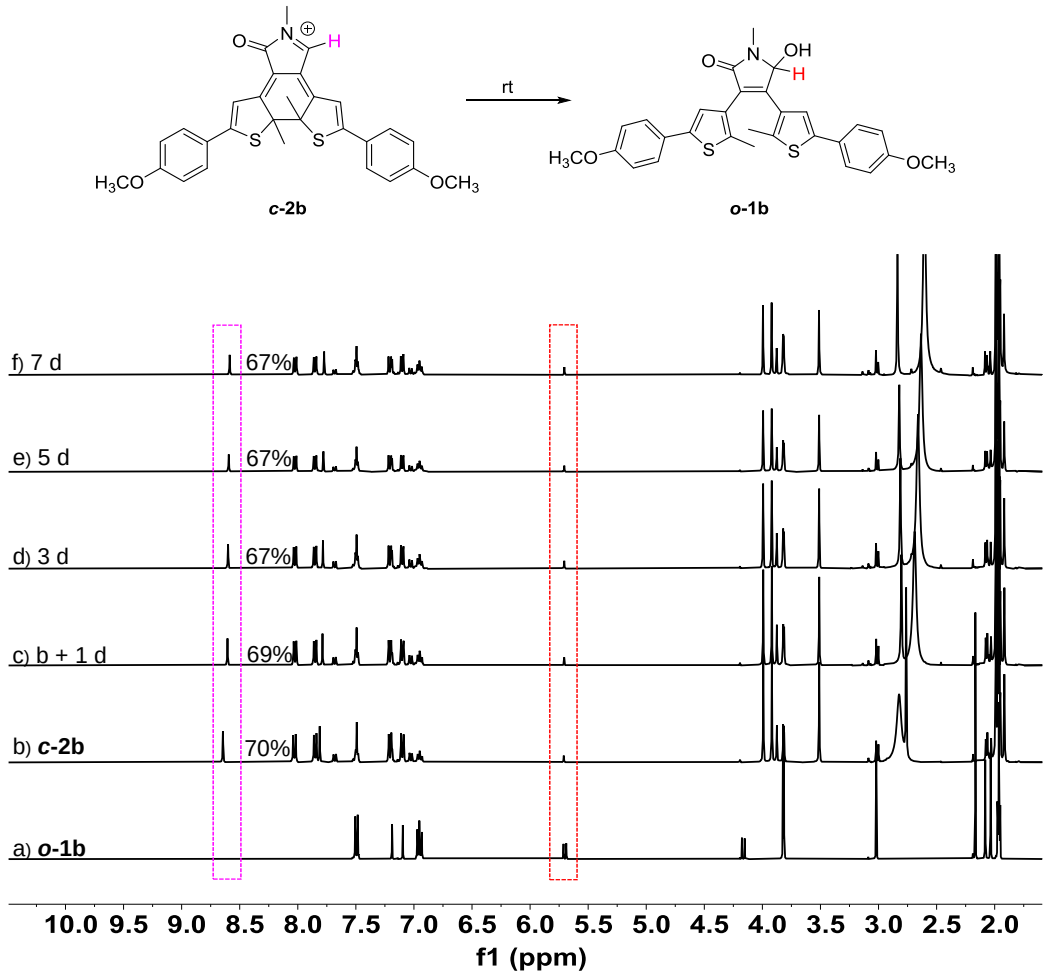


Figure S70. The stability of *in situ* generated ***c*-2b** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in CD_3CN; (b) The addition of MA (2.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2b**; (c-f) Panel b at varied time.

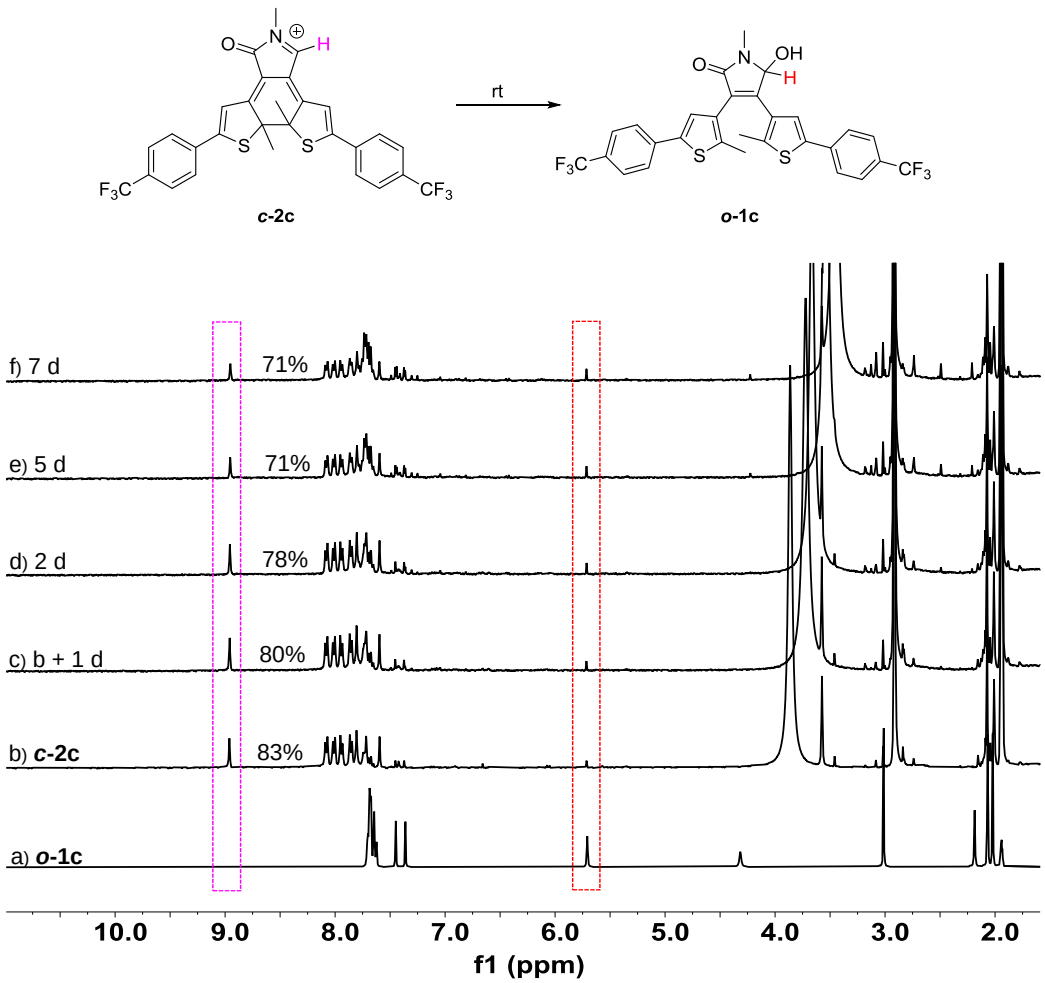


Figure S71. The stability of *in situ* generated ***c*-2c** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) The addition of MA (7.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2c**; (c-f) Panel b at varied time.

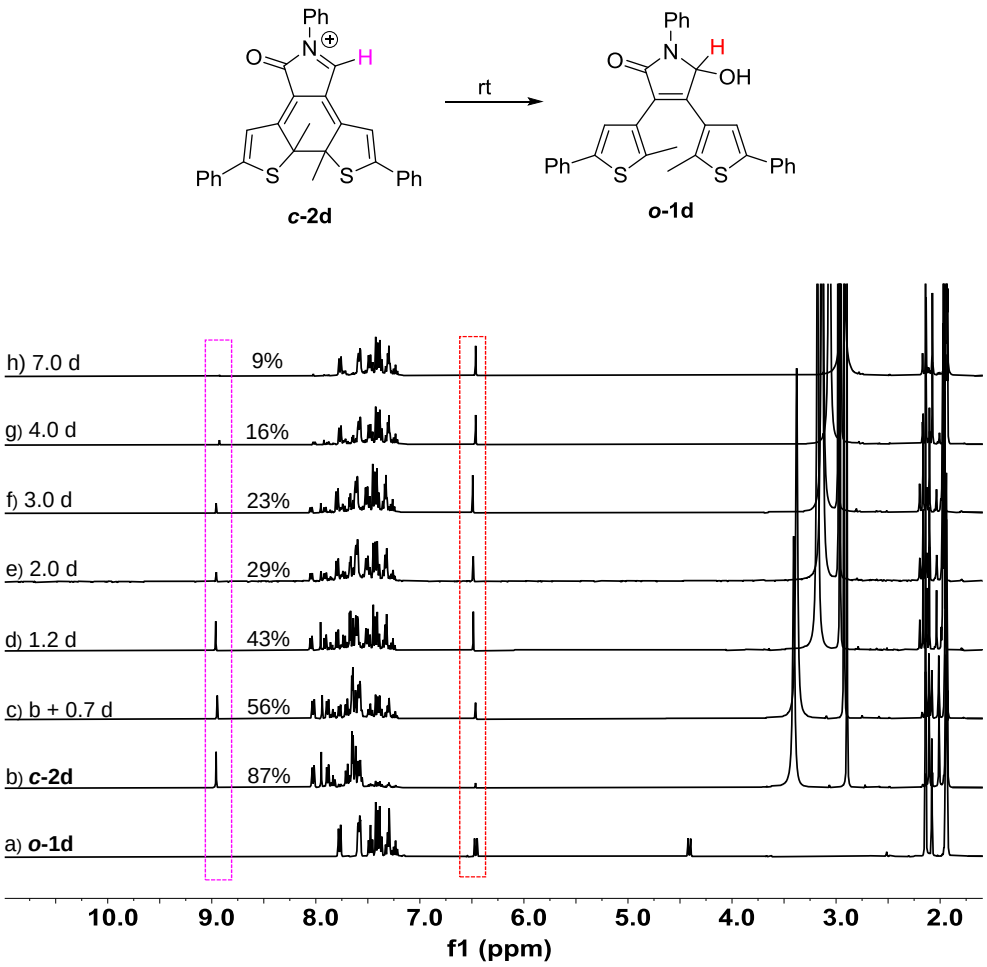


Figure S72. The stability of *in situ* generated ***c*-2d** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b) The addition of MA (5.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2d**; (c-h) Panel b at varied time.

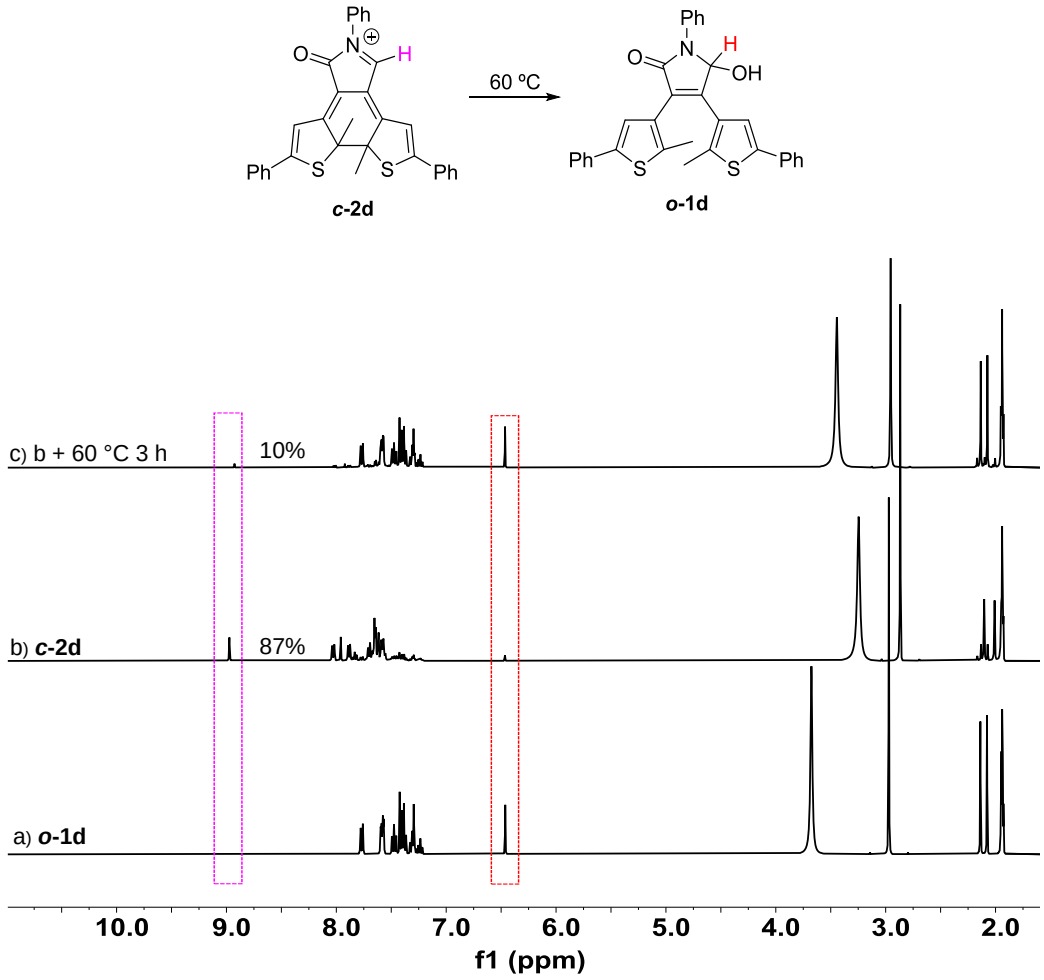


Figure S73. The stability of *in situ* generated ***c*-2d** at 60 ℃. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b) The addition of MA (5.0 equiv.) into panel a and then irradiation with UV (313 nm, 1.5 h) to give ***c*-2d**; (c) Heat panel b at 60 ℃ for 3 h.

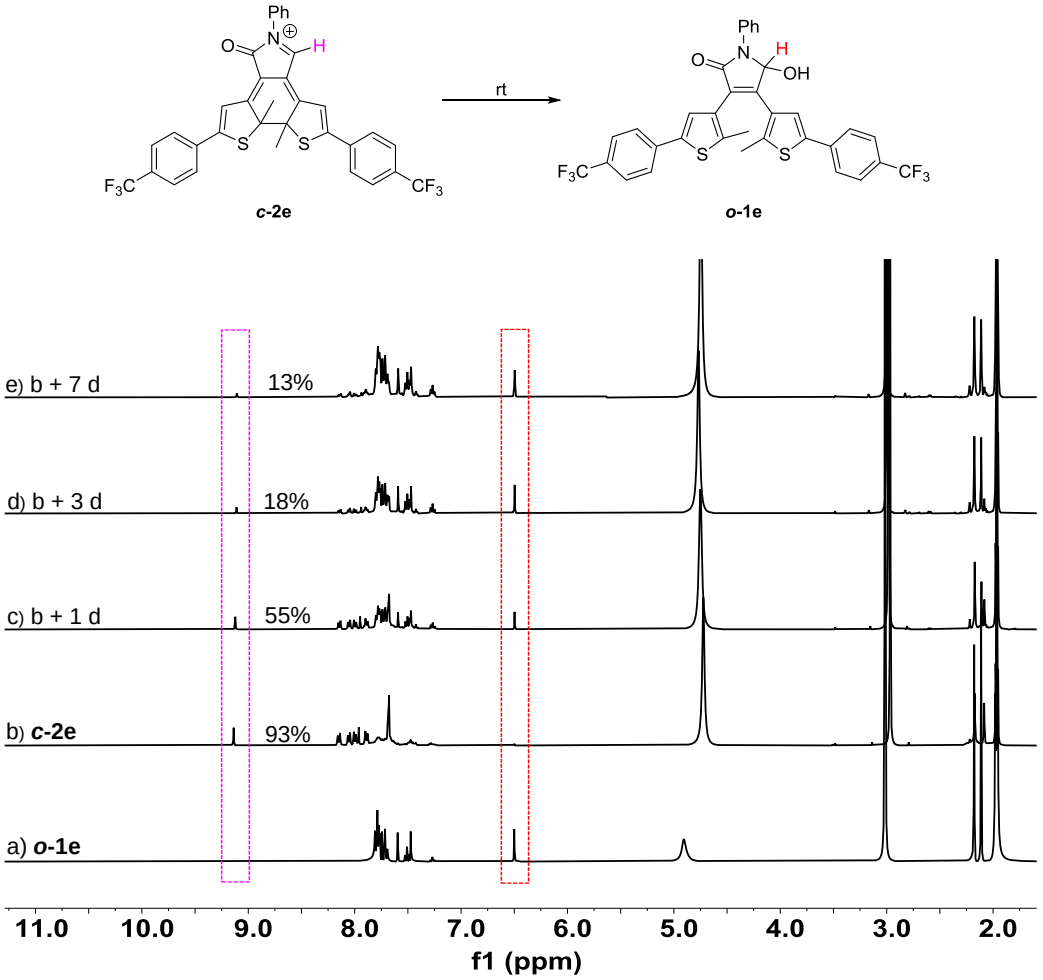


Figure S74. The stability of *in situ* generated ***c*-2e** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1e** (5 mM) in CD_3CN; (b) The addition of MA (11.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2e**; (c-e) Panel b at varied time.

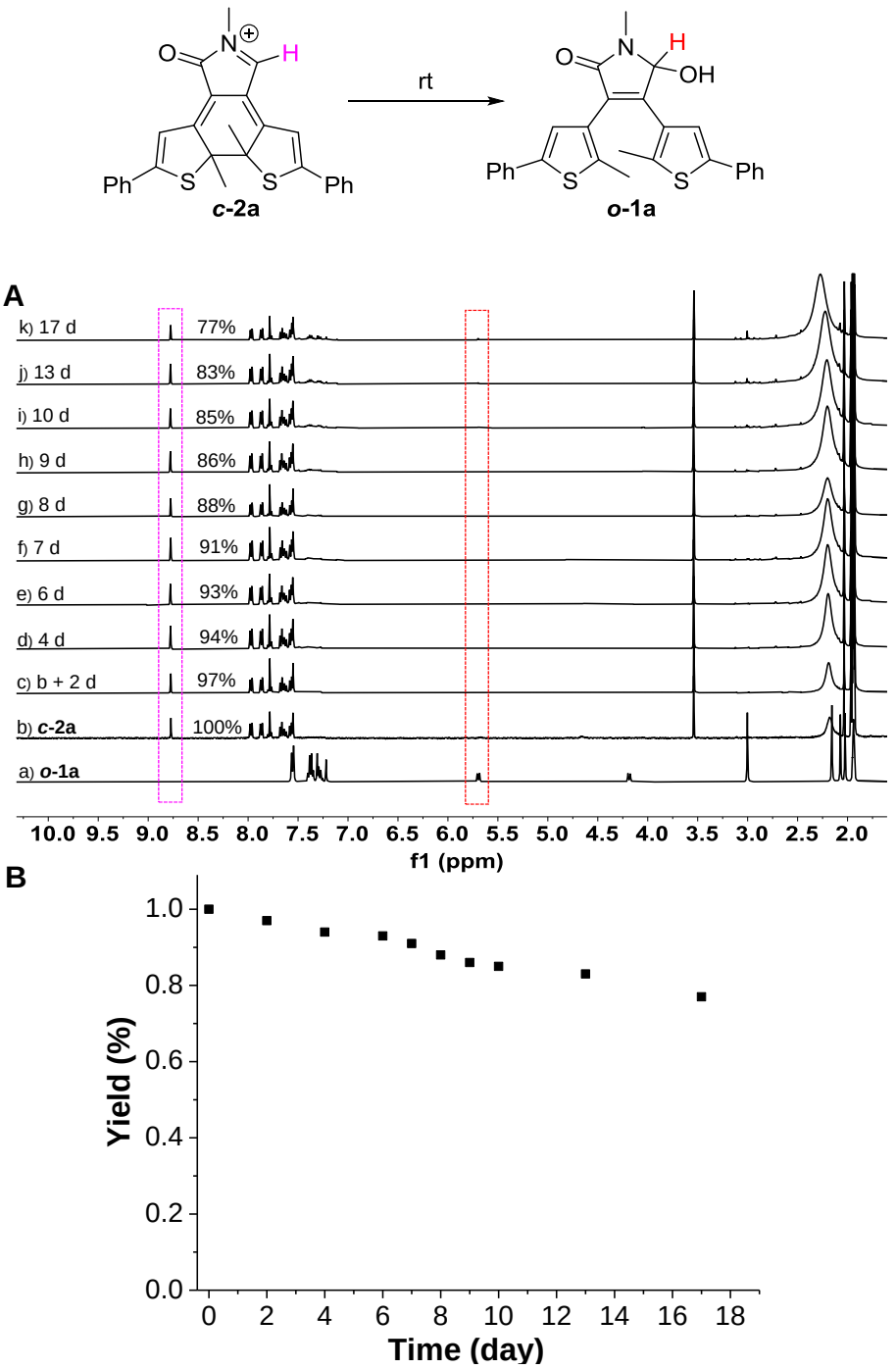


Figure S75. (A) The stability of isolated ***c*-2a** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b-k) Panel b of ***c*-2a** (5 mM in CD_3CN) at varied time. (B) The kinetics profile of ***c*-2a** at varied time.

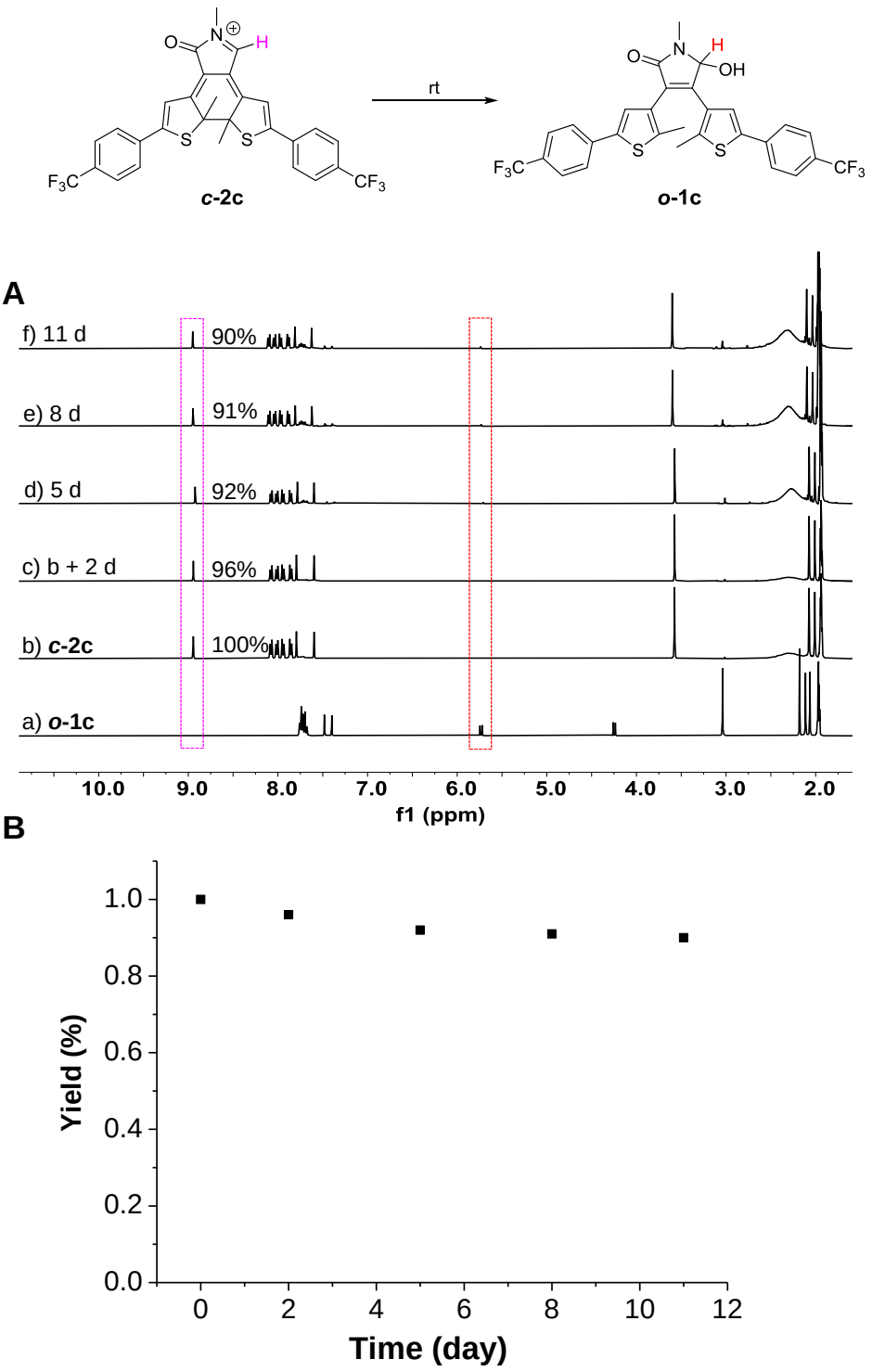


Figure S76. (A) The stability of isolated ***c*-2c** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b-f) Panel b of ***c*-2c** (5 mM in CD_3CN) at varied time. (B) The kinetics profile of ***c*-2c** at varied time.

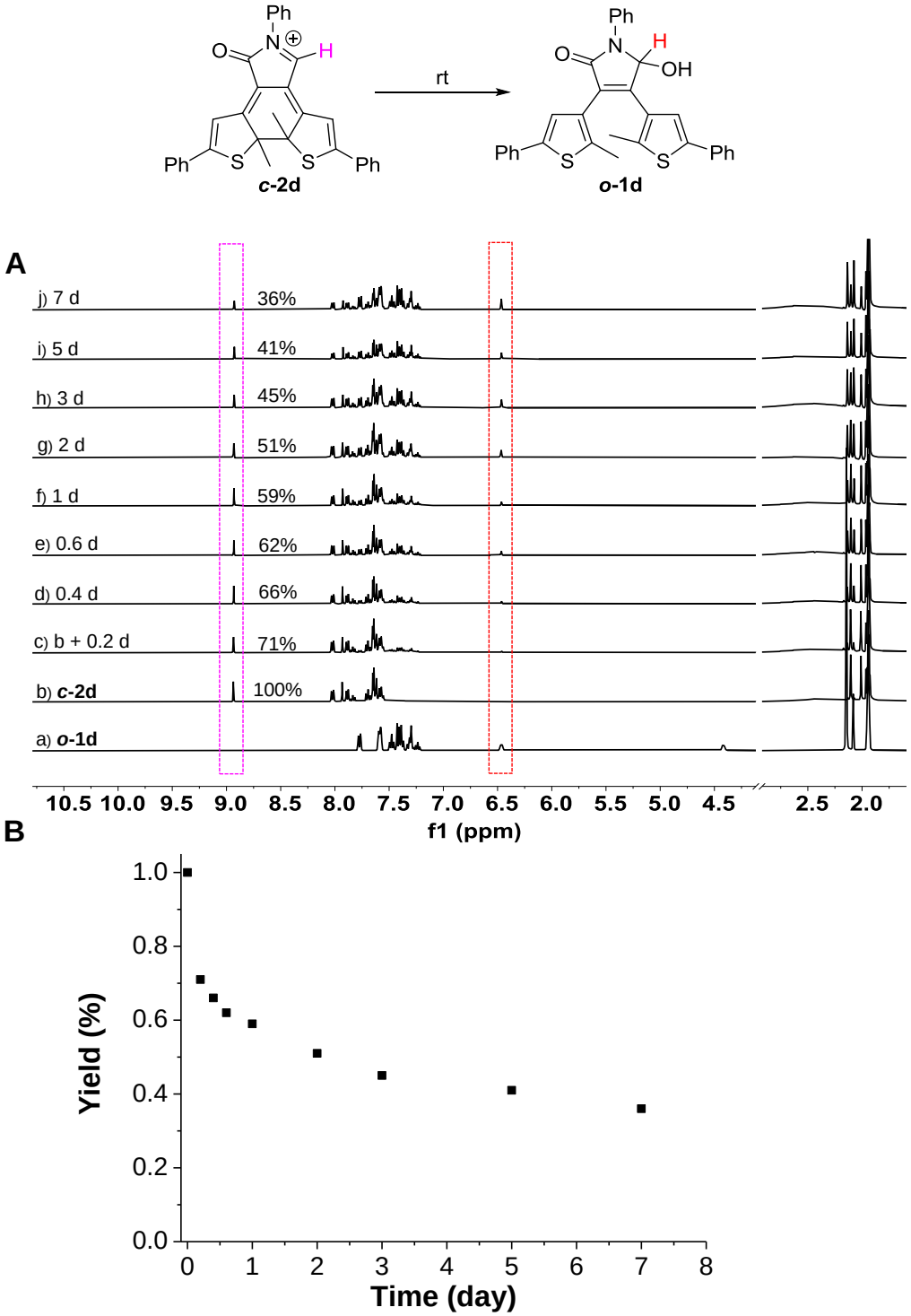


Figure S77. (A) The stability of isolated ***c*-2d** at varied time at room temperature. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b-k) Panel b of ***c*-2d** (5 mM in CD_3CN) at varied time. (B) The kinetics profile of ***c*-2d** at varied time.

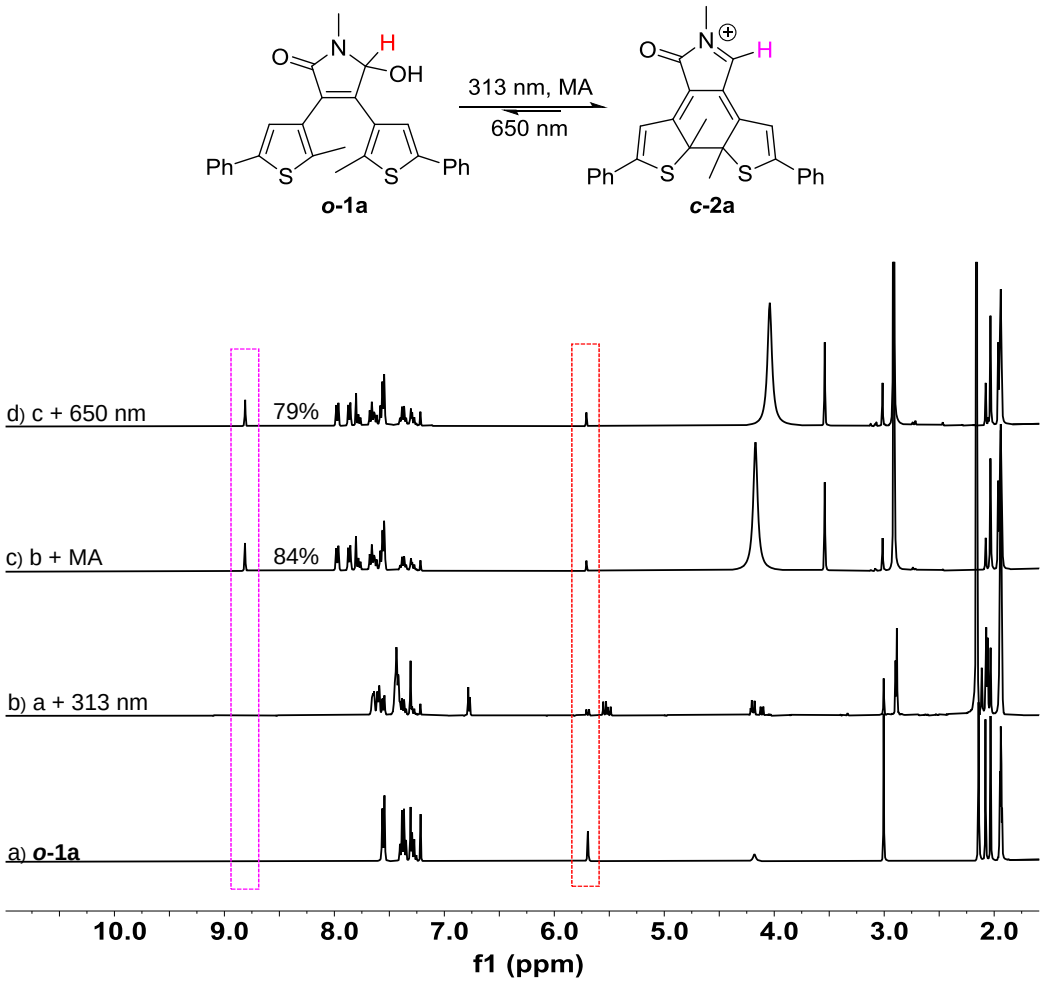


Figure S78. The switchability of *in situ* generated ***c*-2a** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) Irradiation of panel a with UV light (313 nm, 1.5 h) to give ***c*-1a**; (c) The addition of MA (4.0 equiv.) into panel b to give ***c*-2a;** (d) Illumination of panel c at 650 nm for 8 h.

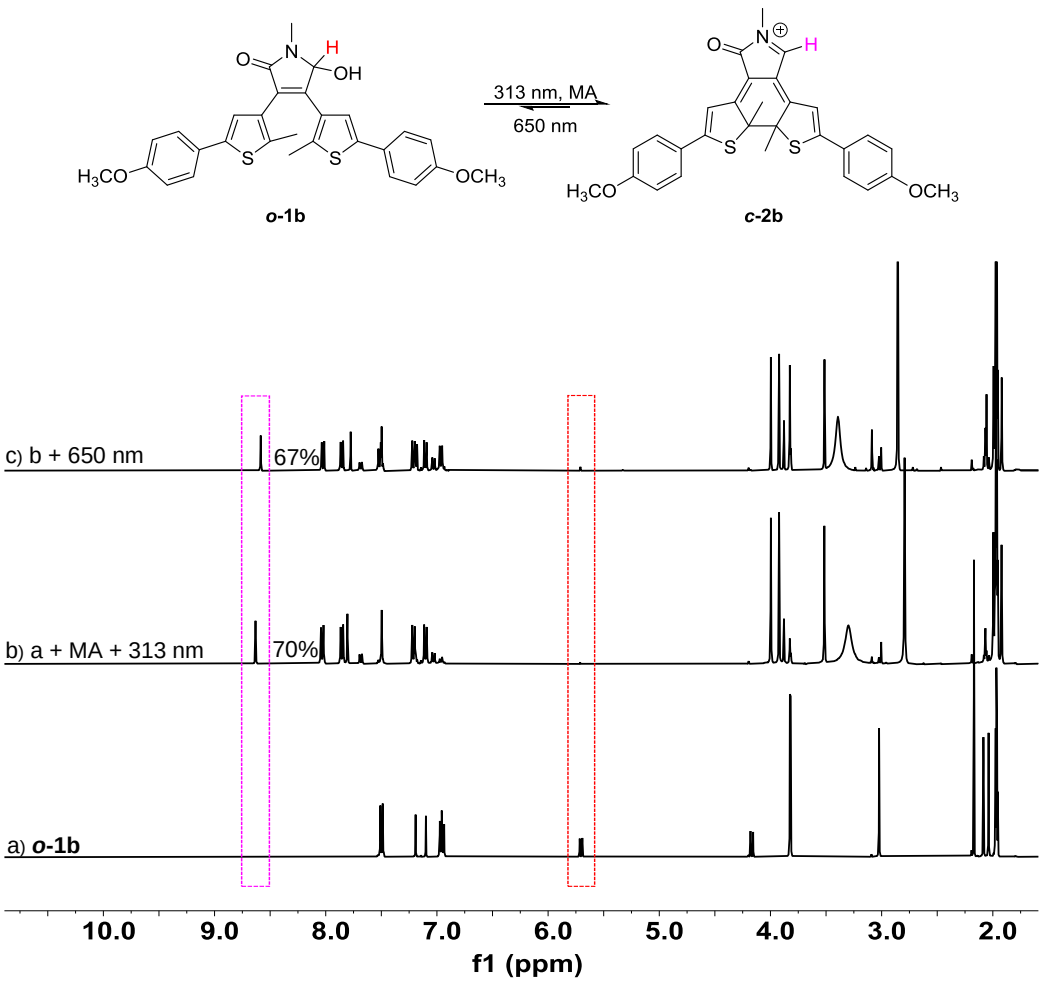


Figure S79. The switchability of *in situ* generated ***c*-2b** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in CD_3CN; (b) The addition of MA (2.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2b**; (c) Illumination of panel b at 650 nm for 4 h.

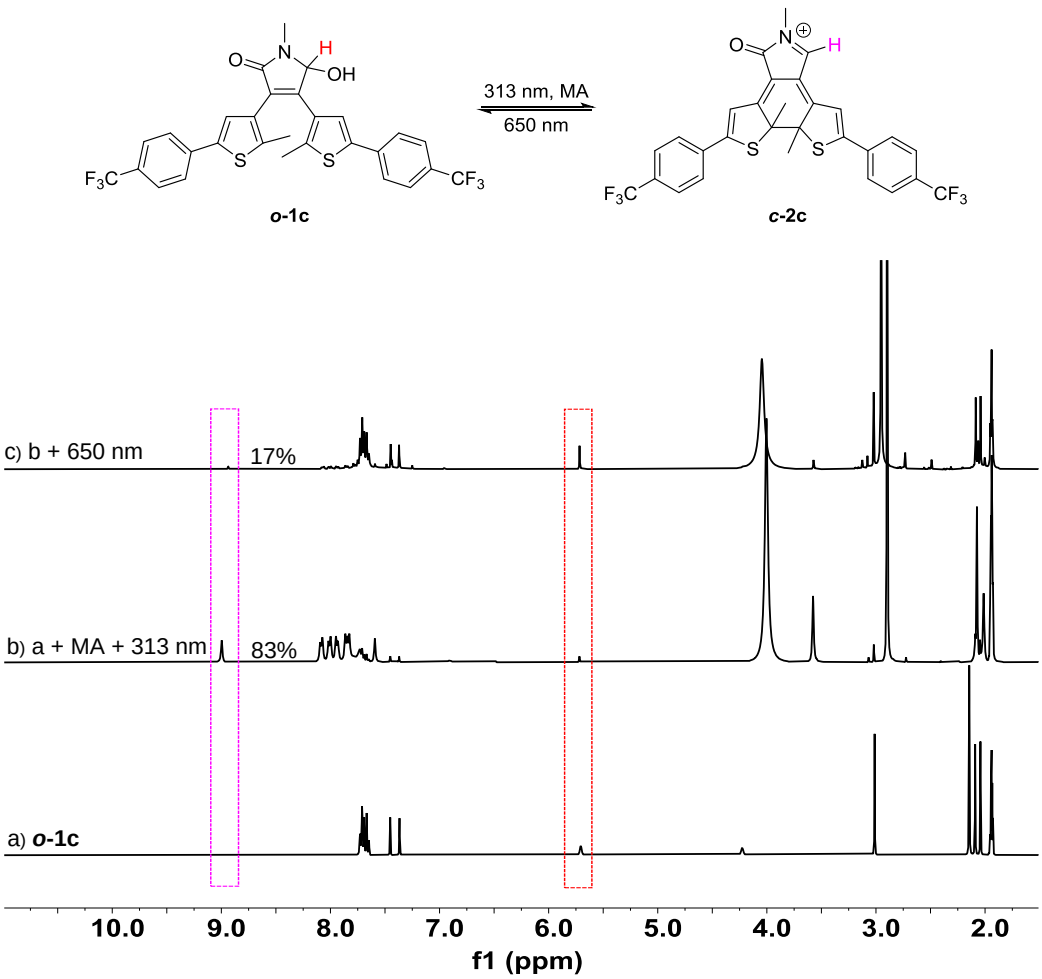


Figure S80. The switchability of *in situ* generated ***c*-2c** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) The addition of MA (7.0 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2c**; (c) Illumination of panel b at 650 nm for 28 h.

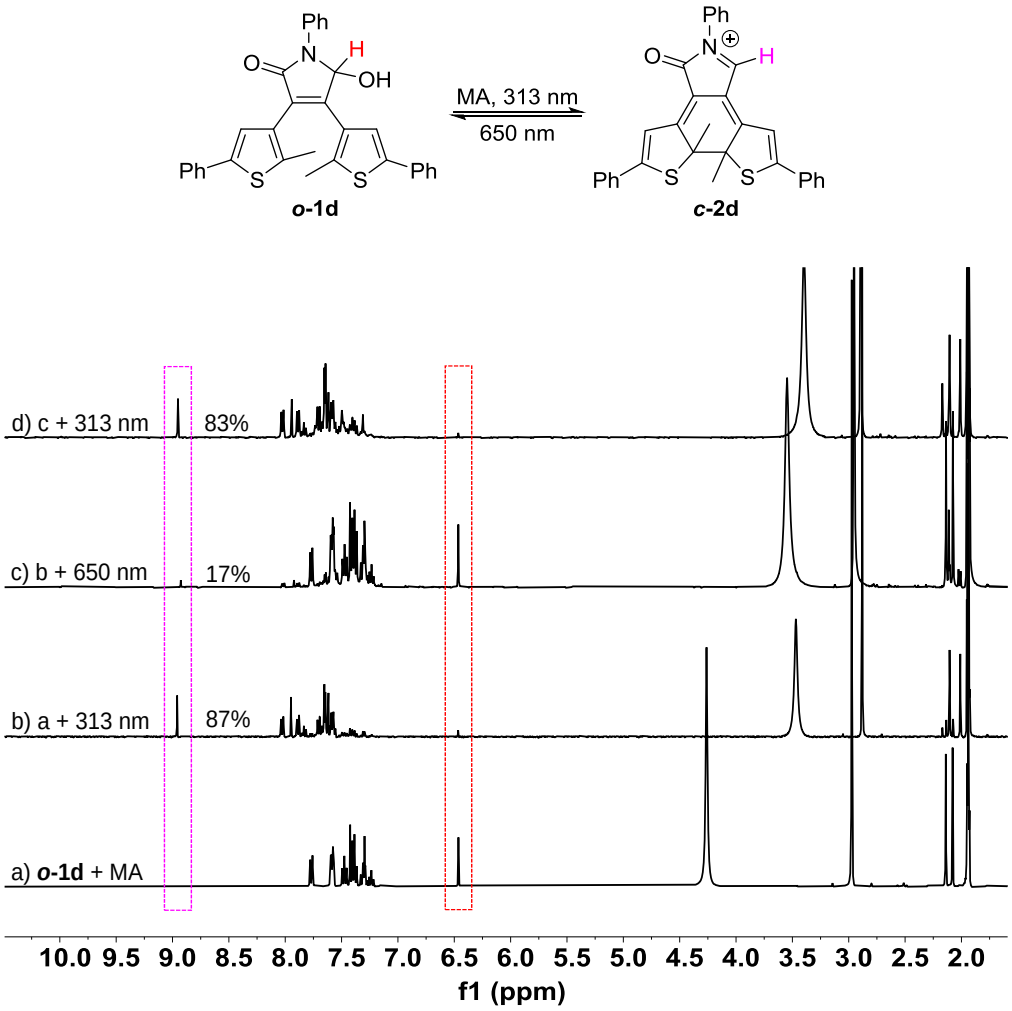


Figure S81. The switchability of *in situ* generated ***c*-2d** under light. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) and MA (5.0 equiv.) in CD_3CN; (b) Irradiation of panel a with UV light (313 nm, 2 h) to give ***c*-2d**; (c) Illumination of panel b at 650 nm for 15 h, with ***o*-2d** generated; (d) Illumination of panel c at 313 nm for 4 h, with ***c*-2d** regenerated.

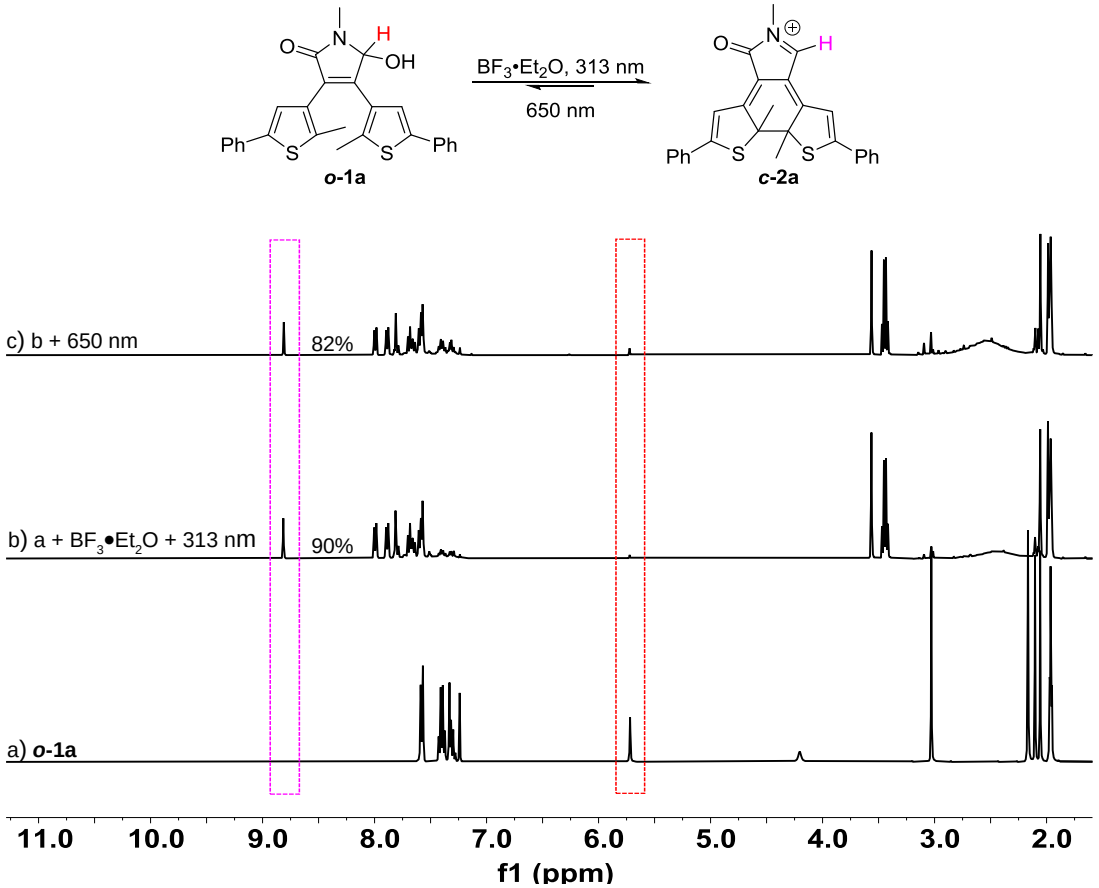


Figure S82. The switchability of *in situ* generated ***c*-2a** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2a**; (c) Illumination of panel c at 650 nm for 8 h.

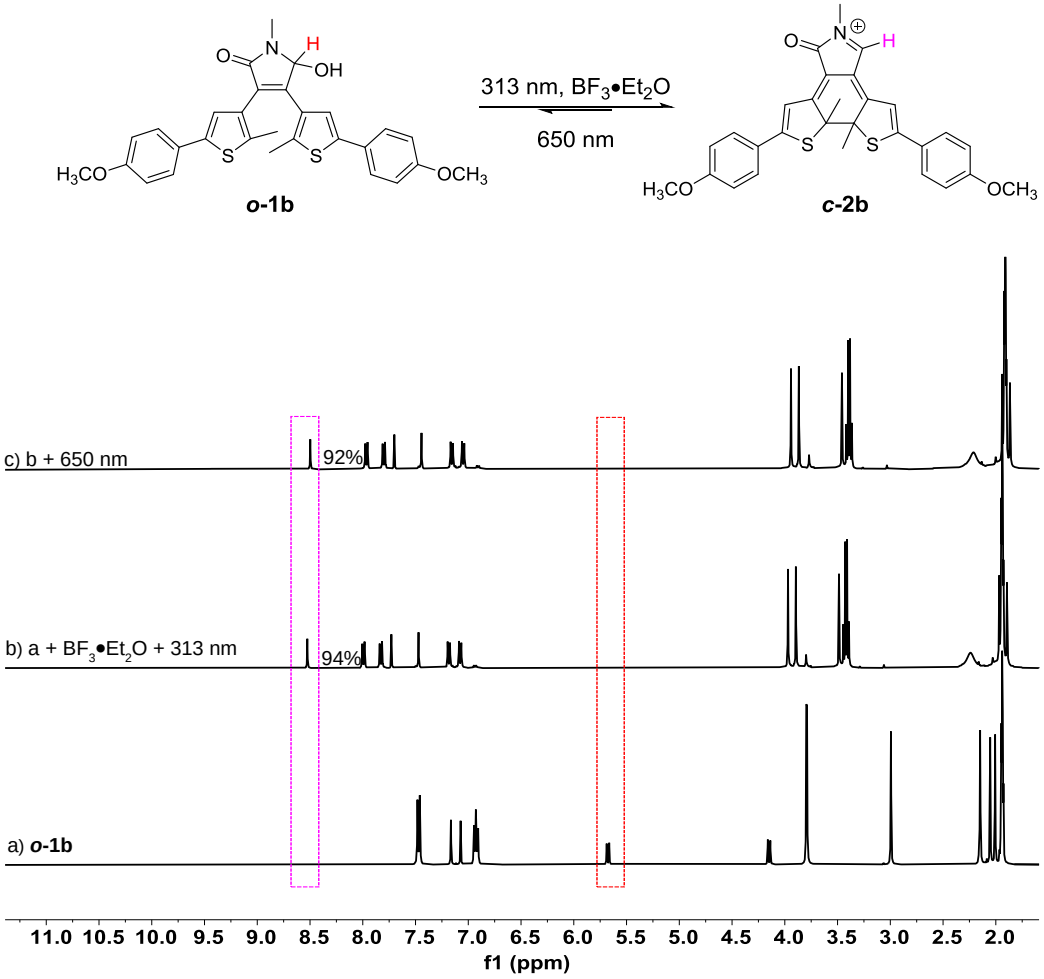


Figure S83. The switchability of *in situ* generated ***c*-2b** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1b** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2b**; (c) Illumination of panel b at 650 nm for 5 h.

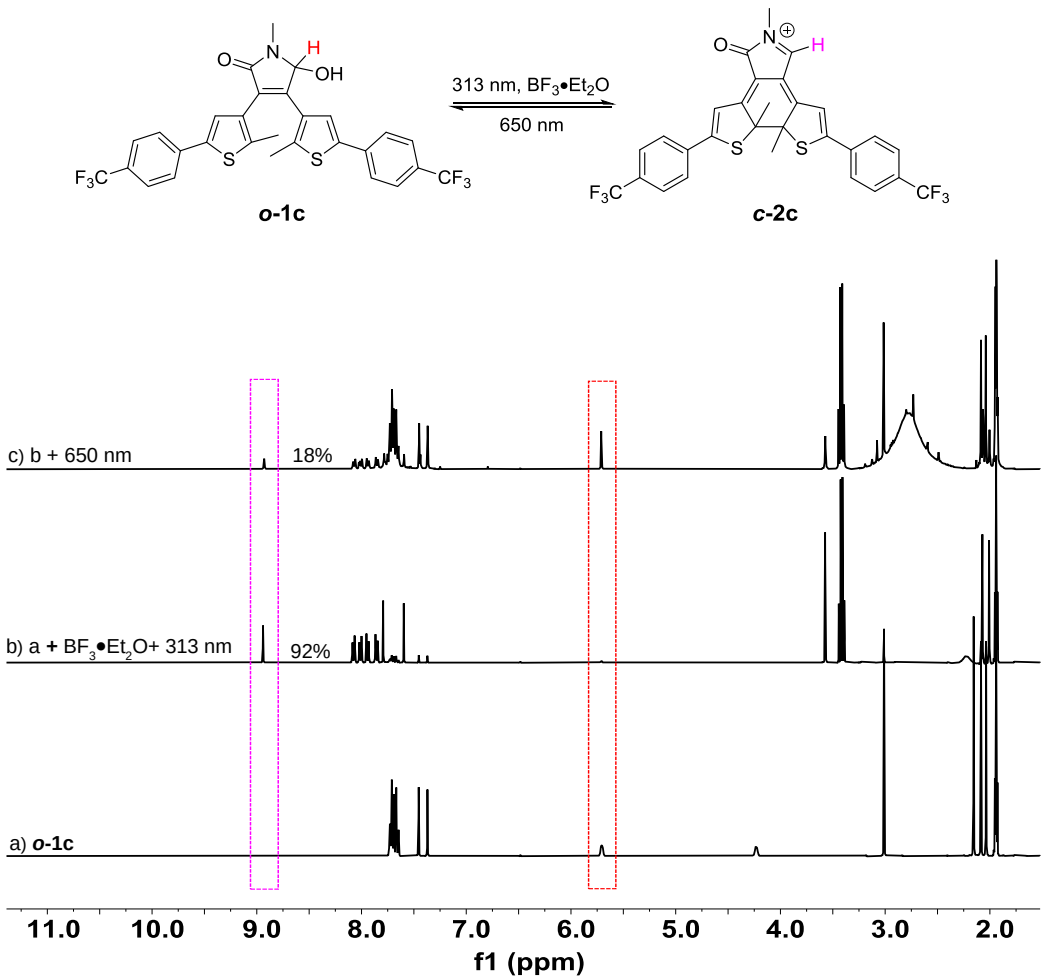


Figure S84. The switchability of *in situ* generated ***c*-2c** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b) The addition of BF_3•Et_2O (1.5 equiv.) into panel a and then irradiation with UV light (313 nm, 1.5 h) to give ***c*-2c**; (c) Illumination of panel b at 650 nm for 28 h.

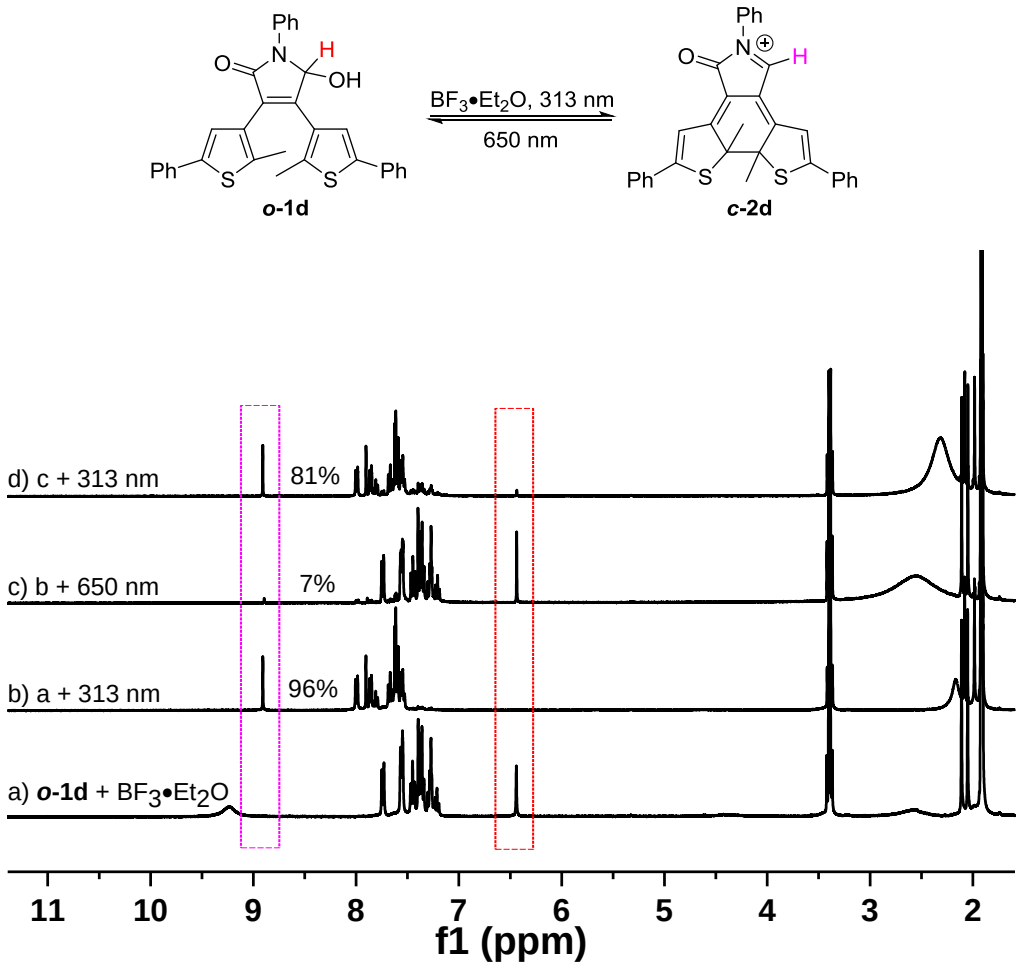


Figure S85. The switchability of *in situ* generated ***c*-2d** under light. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) and BF_3•Et_2O (2.0 equiv.) in CD_3CN; (b) Irradiation with UV light (313 nm, 2 h) to give ***c*-2d**; (c) Illumination of panel b at 650 nm for 20 h to create ***o*-1d**. (d) Illumination of panel c at 313 nm for 4 h.

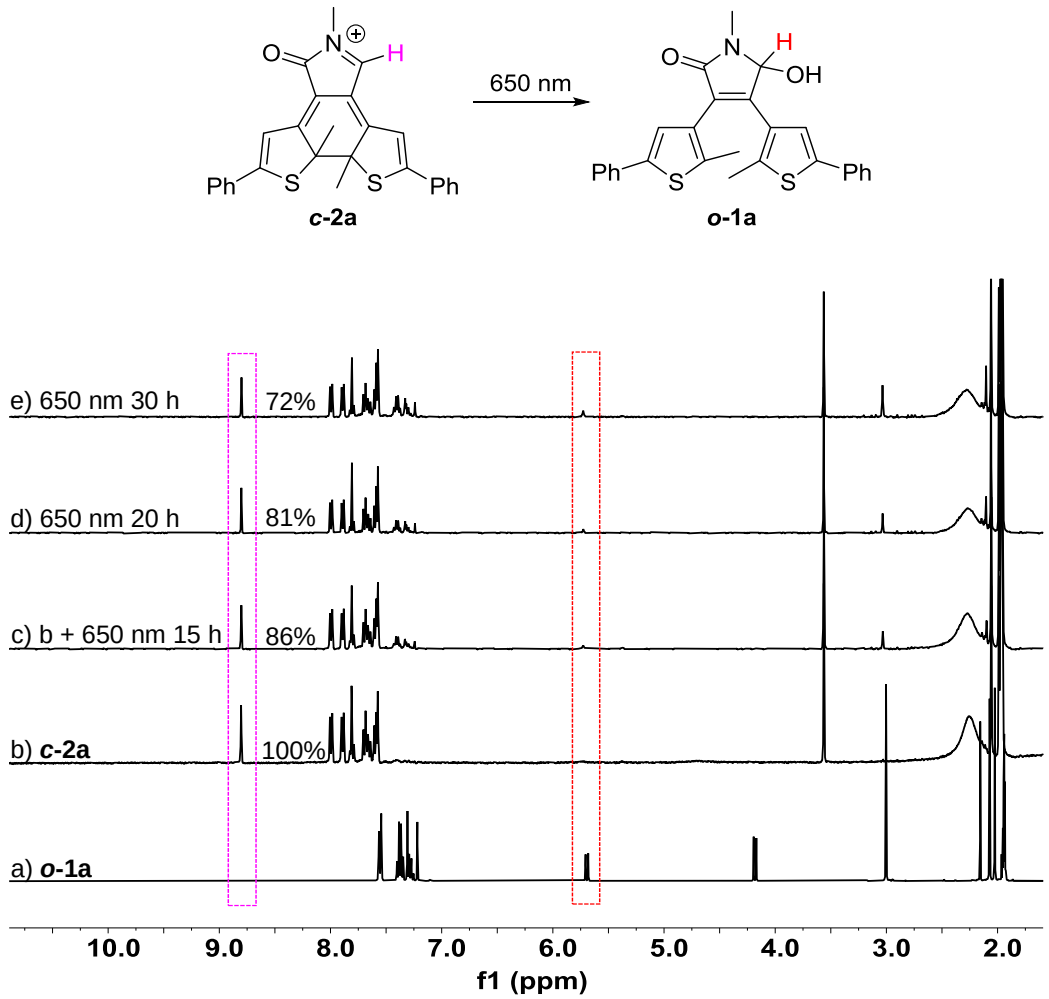


Figure S86. The switchability of isolated ***c*-2a** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1a** (5 mM) in CD_3CN; (b-e) Illumination of panel b at 650 nm at different time.

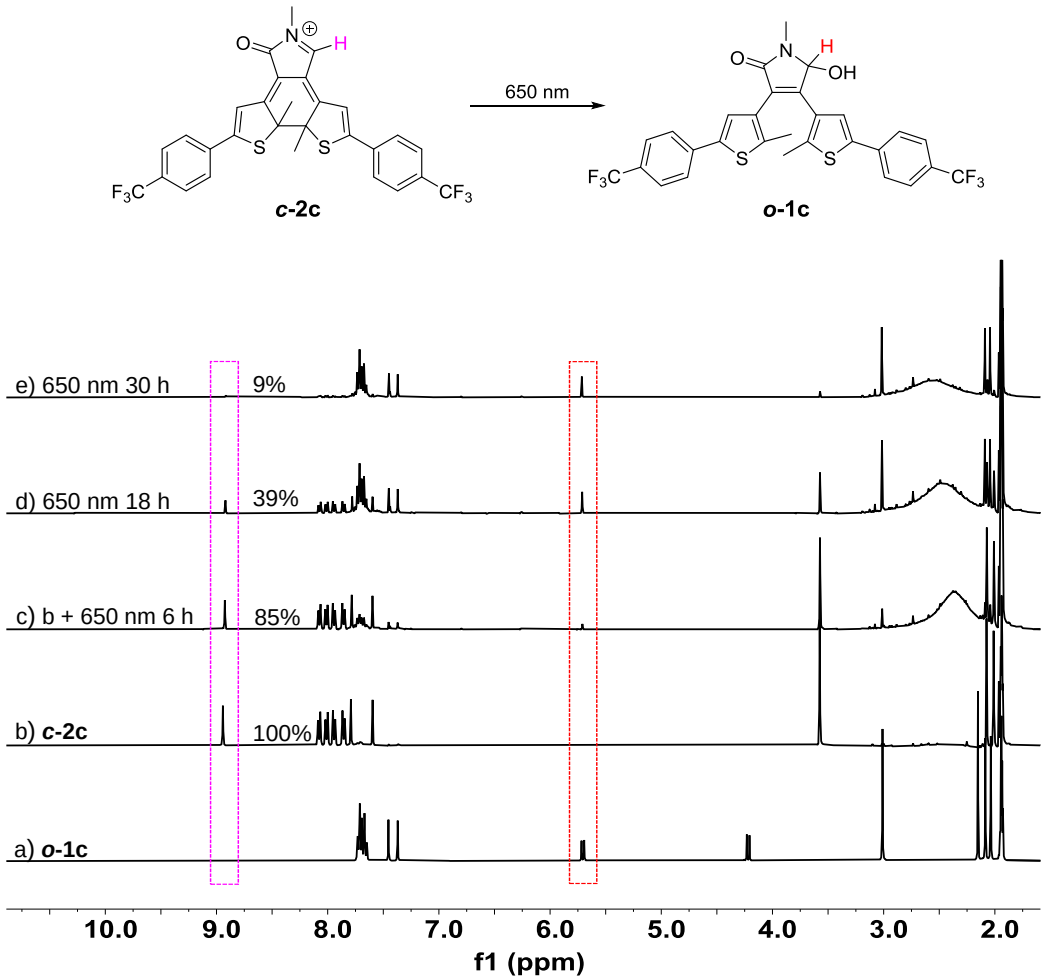


Figure S87. The switchability of isolated ***c*-2c** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1c** (5 mM) in CD_3CN; (b-e) Illumination of panel b at 650 nm at different time.

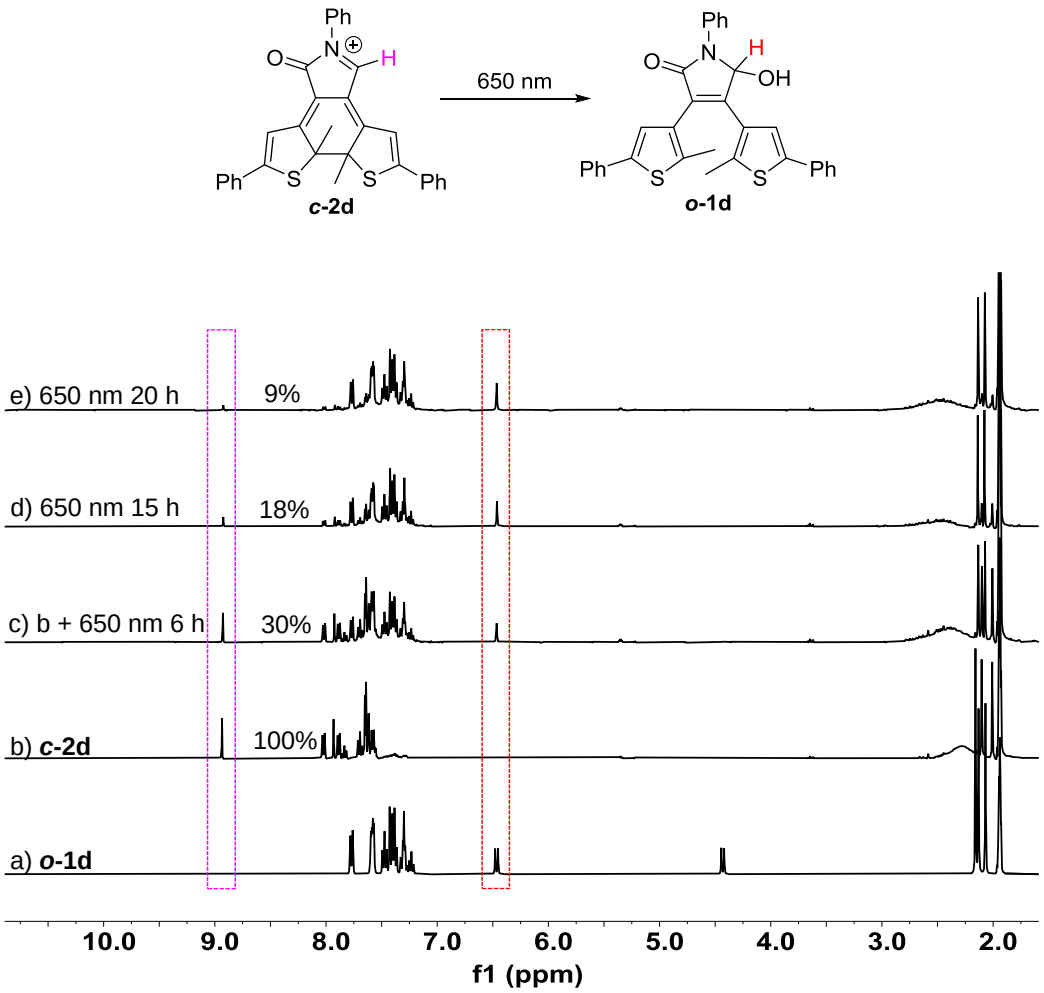
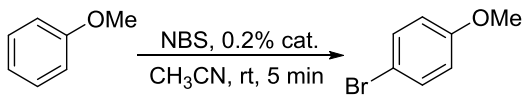


Figure S88. The switchability of isolated ***c*-2d** under visible light illumination. (a) ^{1}H NMR spectrum of ***o*-1d** (5 mM) in CD_3CN; (b-e) Illumination of panel b at 650 nm at different time.

8. Lewis Acid Catalysis

The bromination reactions were carried out with anisole (150 mg, 1.39 mmol), NBS (272 mg, 1.53 mmol), and catalyst ***c*-2a** (0.2%, 1.5 mg, 0.003 mmol) in acetonitrile (8.0 mL) at 25 ^{o}C in the absence of light. The reaction mixture was stirred for 5 min and then evaporated to give the crude product *p*-bromoanisole. A internal standard dibromomethane (1.0 equiv.) was added, and the mixture was dissolved in CD_3CN for ^{1}H NMR analysis to determine the conversion of anisole. For ring-opening polymerization reactions a mixture of cyclohexene oxide (0.5 mL 4.94 mmol) and pre-isolated ***c*-2a** (0.2%, 5.3 mg, 0.01 mmol) was stirred for 5 h and then dried at room temperature for 2 days to afford the polymerized product. For the comparison other catalytic conditions were used by following the similar procedure.

Table S2. Bromination reactions.



entry	cat.	conversoin (%)
1	*c*-2a	97
2	*c*-2c	80
3	*c*-2d	88

Yields were determined by ^{1}H NMR spectrum analysis using dibromomethane as an internal standard.

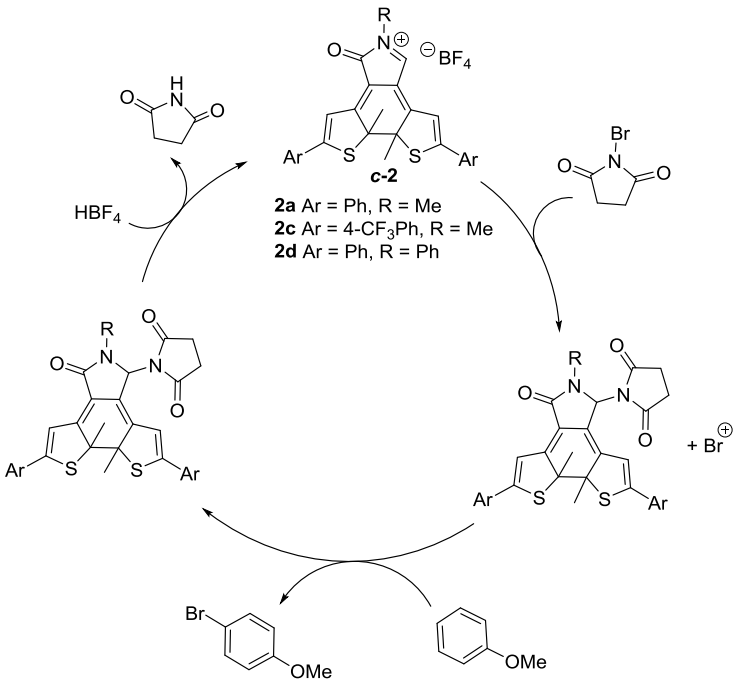


Figure S89. Proposed mechanism of ***c*-2** catalyzed bromination reaction.

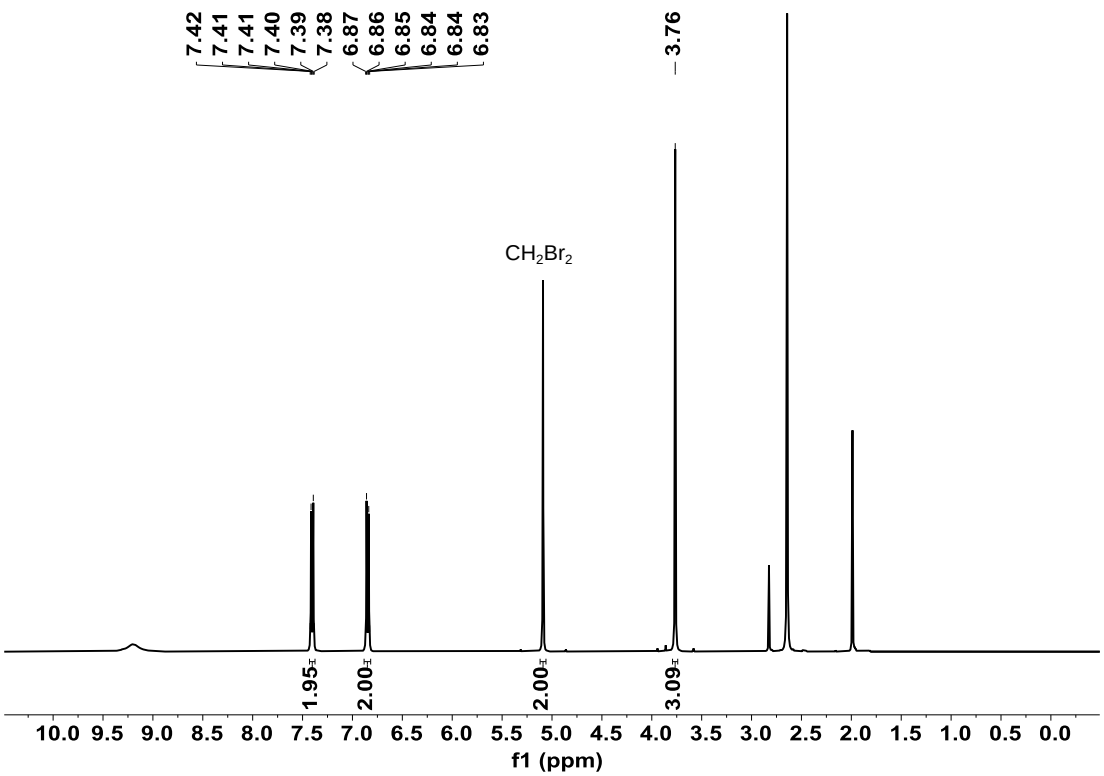


Figure S90. ^{1}H NMR spectrum of *p*-bromoanisole with internal standard dibromomethane in CD_3CN (catalyzed by 0.2% ***c*-2a**).

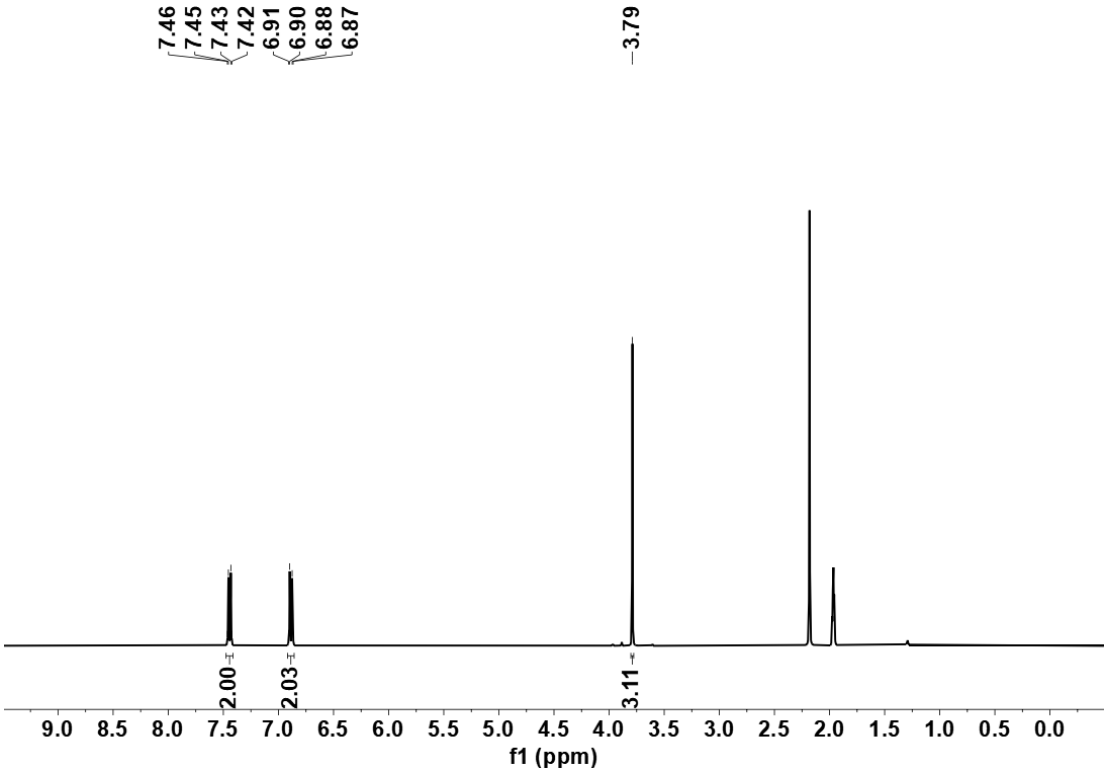


Figure S91. ^{1}H NMR spectrum of isolated *p*-bromoanisole in CD_3CN (catalyzed by 0.2% ***c*-2a**).

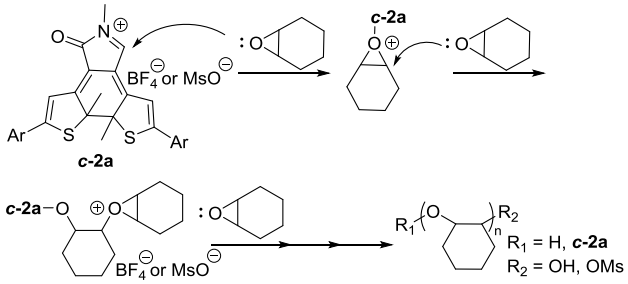


Figure S92. Reaction scheme of ***c*-2a**-catalyzed cationic polymerization of cyclohexene oxide.

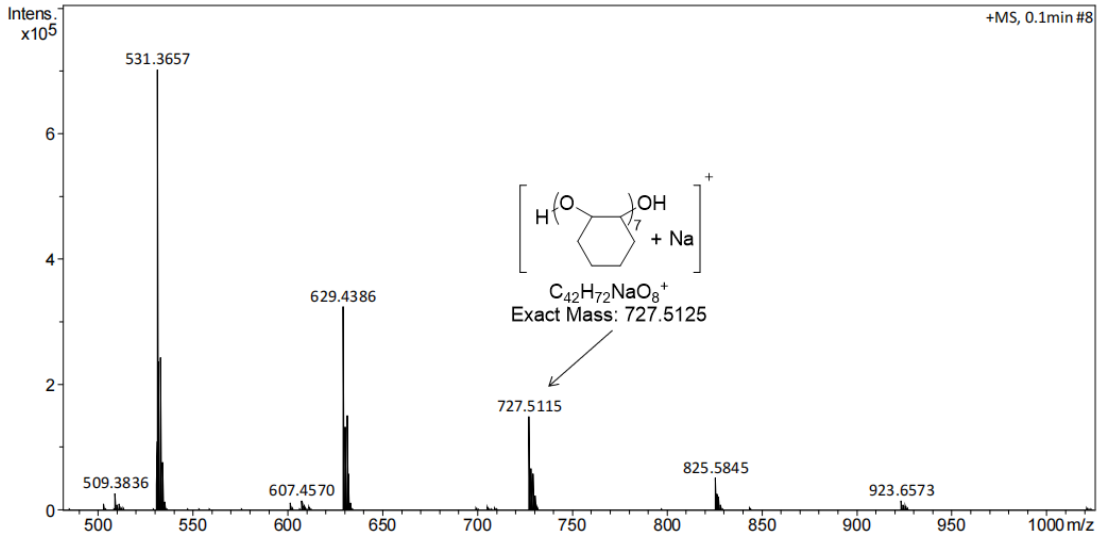


Figure S93. ESI mass spectrum of epoxy polymers catalyzed by isolated ***c*-2a** (0.2%) in MeCN.

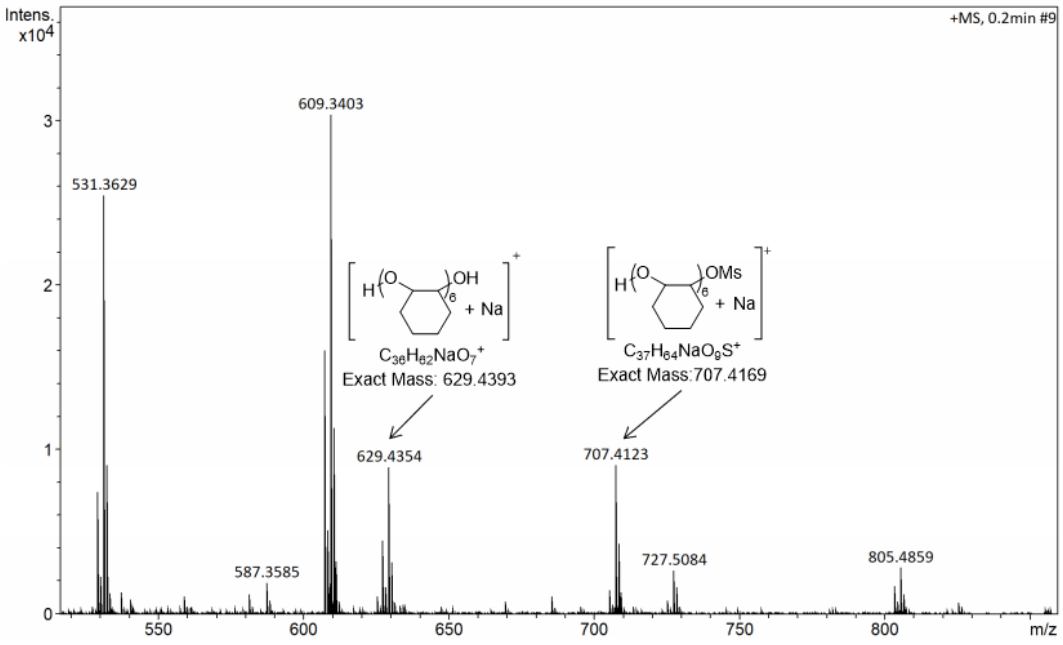


Figure S94. ESI mass spectrum of epoxy polymers catalyzed by MA (0.8%).

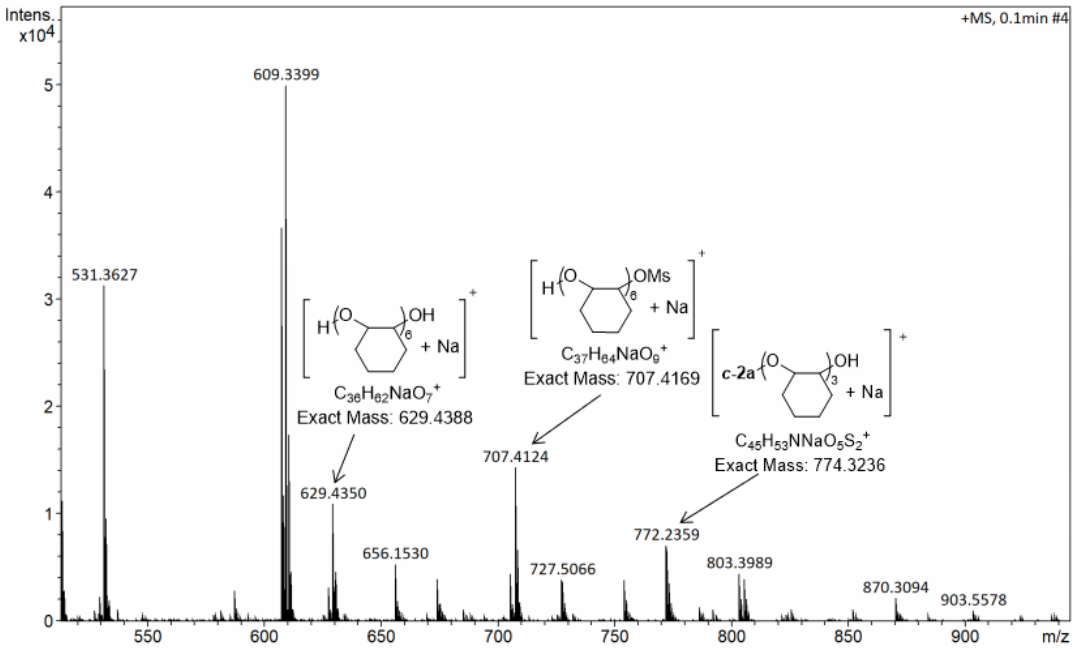


Figure S95. ESI mass spectrum of epoxy polymers catalyzed by *in situ* created ***c*-2a** upon irradiation of a mixture of cyclohexene oxide, ***o*-1a** (0.2%), and MA (0.8%) at 313 nm for 2 h and then waiting in the dark for 5 h.

9. Molecular Coordinates

Molecular coordinates were listed in the order of neutral species (***o*-1** and ***c*-1**), cationic species (***o*-2** and ***c*-2**), TSs for the thermal conversion (**TS1**: ***o*-1** to ***c*-1**; **TS2**: ***o*-2** to ***c*-2)**, TSs for the dehydration (*o*-**TS: *o*-1** to ***o*-2**; ***c*-TS: *c*-1** to ***c*-2**), and other small molecules (acid and water) related to the reactions.

***o*-1a** (acetonitrile)

Imaginary frequency: 0

G = -2043.924677 hartree

S	2.51434100	-1.63421000	1.34539300
S	-2.52196200	-1.70255200	-1.36219400
O	-2.21832400	3.42712200	-0.72133200
O	1.76076800	3.37765700	1.37435800
H	1.16754900	3.12265800	2.09328300
C	1.53925600	0.52199400	0.40819500
C	2.88615500	0.44638400	-0.06191800
H	3.32848400	1.18612400	-0.71536500
C	-1.10804600	3.04412700	-0.39858900
C	-1.54277300	0.50313000	-0.55235300
C	1.19633300	-0.54475400	1.20240900
C	0.64927300	1.62772000	0.07334200
C	3.54419400	-0.67500800	0.34553900
C	-0.64595800	1.62069100	-0.27440500
C	-1.20957900	-0.59704000	-1.30169300
C	-2.87655800	0.44154700	-0.04658000
H	-3.30413700	1.21864900	0.57102700
C	-0.08711300	-0.82151500	1.91443400
H	-0.74346400	-1.45595800	1.31300200
H	-0.61683800	0.11121800	2.10690000
H	0.09355200	-1.32336200	2.86443900
C	1.14885200	3.05902600	0.15468200
H	1.90439500	3.26561400	-0.61005300
C	-3.53576200	-0.70206400	-0.38497400
C	0.06599200	-0.90263200	-2.01619100
H	0.73018600	-1.51127200	-1.39673100
H	0.59213200	0.02196300	-2.25291900
H	-0.12347900	-1.44353900	-2.94285700
C	4.92067900	-1.08456200	0.04155800
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C	5.87781600	-0.12458600	-0.29860000
C	6.60682300	-2.79971200	-0.21490000
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C	7.17686200	-0.50030600	-0.60226500
H	5.60576800	0.92313300	-0.30827800
C	7.54798600	-1.83905500	-0.56097400
H	6.88456300	-3.84518200	-0.18092900
H	7.90519200	0.25680100	-0.86262300
H	8.56377200	-2.13018400	-0.79379200
C	-4.90273900	-1.10343300	-0.03155600
C	-5.28324100	-2.44711400	-0.00997200
C	-5.85427700	-0.13386800	0.29759700
C	-6.57674500	-2.81156100	0.33359600
H	-4.55800100	-3.21564400	-0.24955000
C	-7.14358000	-0.50081700	0.64977500
H	-5.58516700	0.91400400	0.26086900
C	-7.51168800	-1.84094600	0.66858200
H	-6.85186800	-3.85824300	0.34589400
H	-7.86708500	0.26404800	0.90090700
H	-8.51996800	-2.12546200	0.93918500
N	-0.04333800	3.82990800	-0.10058300
C	-0.02253600	5.26685400	-0.22942300
H	-1.04960600	5.61751900	-0.29283800
H	0.45735700	5.70875900	0.64292300
H	0.51727000	5.57375700	-1.12782600

***o*-1b** (acetonitrile)

Imaginary frequency: 0

G = -2272.921327 hartree

S	2.45749200	-1.29928000	1.43398700
S	-2.46622300	-1.34976200	-1.49098300
O	-2.18685200	3.77415800	-0.80584800
O	1.68948100	3.70793500	1.47196600
H	1.06495400	3.44217300	2.15979800
C	1.51781900	0.86116900	0.47188800
C	2.88458000	0.79140500	0.05854600
H	3.35190600	1.53722800	-0.57013400
C	-1.09284500	3.38809300	-0.43445700
C	-1.52066000	0.84841300	-0.62398900
C	1.14225500	-0.21204400	1.24076200
C	0.64173200	1.96834500	0.10659300

C	3.52785700	-0.33166000	0.48440600
C	-0.63684600	1.96371800	-0.29890600
C	-1.15468300	-0.24663300	-1.36407200
C	-2.87590200	0.78418800	-0.17588300
H	-3.32904900	1.55777500	0.42779800
C	-0.17177000	-0.50041700	1.88954200
H	-0.79902600	-1.12776000	1.25054700
H	-0.71221900	0.42874100	2.06940700
H	-0.03389800	-1.01402700	2.84047300
C	1.13611700	3.39906400	0.22188200
H	1.92690000	3.61235000	-0.50434400
C	-3.52112700	-0.35619400	-0.54951100
C	0.15212700	-0.55195500	-2.01973800
H	0.78684100	-1.16307500	-1.37221600
H	0.69004700	0.37256500	-2.22896900
H	0.00529900	-1.08954300	-2.95609000
C	4.91560600	-0.73726700	0.23746400
C	5.30979200	-2.07082700	0.28953400
C	5.88964700	0.22271900	-0.06627700
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H	4.57917300	-2.84042700	0.50878800
C	7.19515600	-0.14261800	-0.31621900
H	5.62090900	1.27112400	-0.09077600
C	7.57438900	-1.48597200	-0.26062300
H	6.88551800	-3.50021400	0.09661600
H	7.94703100	0.60051500	-0.54754700
C	-4.90177400	-0.75882900	-0.26073200
C	-5.29190300	-2.09460700	-0.25911000
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C	-7.54687100	-1.49936500	0.31922800
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H	-7.92183300	0.59437100	0.54268300
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C	-0.01683400	5.60958400	-0.19983000
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H	0.42097100	6.04522100	0.69748000
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O	-8.84373800	-1.75819800	0.61184700
O	8.87764300	-1.74910500	-0.51616900

***o*-1c** (acetonitrile)

Imaginary frequency: 0

G = -2718.115688 hartree

S	2.41550000	-1.14539000	1.49529200
S	-2.41830200	-1.21127300	-1.54217300
O	-2.17815800	3.91557100	-0.85582400
O	1.65720400	3.86966900	1.49357400
H	1.01932200	3.61151200	2.17197300
C	1.50565200	1.01666000	0.50475900
C	2.87883100	0.94230400	0.12313200
H	3.36170500	1.68418500	-0.49822900
C	-1.08940800	3.53603700	-0.46375700
C	-1.50381400	0.99455000	-0.65757100
C	1.11261700	-0.05355400	1.27216400
C	0.63790100	2.12266400	0.11628100
C	3.50709400	-0.18249900	0.56828500
C	-0.63121100	2.11338000	-0.31603400
C	-1.11829700	-0.10269500	-1.38766400
C	-2.86796700	0.92874100	-0.24601500
H	-3.33798000	1.70278200	0.34375400
C	-0.21368400	-0.33134100	1.90008900
H	-0.83226700	-0.95896300	1.25319400
H	-0.75145000	0.60170000	2.06668200
H	-0.09407600	-0.84178000	2.85496200
C	1.12667400	3.55495900	0.23576000
H	1.92968400	3.76680100	-0.47742700
C	-3.49835600	-0.21596200	-0.63437400
C	0.20266400	-0.40115900	-2.01739500
H	0.82844600	-1.00497700	-1.35474600
H	0.73706800	0.52641600	-2.22151300
H	0.07660600	-0.94504700	-2.95288800
C	4.89706100	-0.59234800	0.34587500
C	5.27985600	-1.93190400	0.43193700
C	5.86844200	0.36518500	0.03551000
C	6.59434900	-2.31020600	0.21243200
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C	7.17910400	-0.00871600	-0.19336200
H	5.59768100	1.41132200	-0.01280400
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C	-7.15545100	-0.02057300	0.19063800
H	-5.57747300	1.39300200	-0.05822000
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H	-6.86071500	-3.37589400	-0.19441400
H	-7.89314500	0.73585800	0.42561000
N	-0.04888200	4.32324300	-0.09395100
C	-0.02497800	5.76116700	-0.21273700
H	-1.04634700	6.10787400	-0.34842000
H	0.38869400	6.19990400	0.69439300
H	0.57711300	6.07500600	-1.06801500
C	8.97505700	-1.73089900	-0.31309600
F	9.53488700	-1.05510100	-1.32674100
F	9.12472900	-3.03332000	-0.57833600
F	9.72604600	-1.47098900	0.77187000
C	-8.94964600	-1.73630300	0.39030100
F	-9.48605100	-1.04223800	1.40460200
F	-9.09816600	-3.03375400	0.67978500
F	-9.72325000	-1.49110600	-0.68233600

***o*-1d** (acetonitrile)

Imaginary frequency: 0

G = -2235.609281 hartree

S	2.46122900	-2.52611000	1.32523100
S	-2.56163400	-2.46600800	-1.39832100
O	-2.19874000	2.61109300	-0.65396300
O	1.81771300	2.49356800	1.41375400
H	1.23779900	2.24453600	2.14557600
C	1.52105800	-0.33753500	0.43100400
C	2.86890400	-0.42104900	-0.03518000
H	3.32511600	0.32578800	-0.67068200
C	-1.09308300	2.22903500	-0.33215600
C	-1.55856100	-0.29309000	-0.53360300
C	1.15918000	-1.41661800	1.20037200
C	0.64727900	0.78630200	0.11812200
C	3.50885900	-1.56028500	0.35046400
C	-0.64670900	0.80588600	-0.23021100
C	-1.23765000	-1.37662600	-1.31182700
C	-2.89145000	-0.35366200	-0.02582400
H	-3.31023600	0.41036400	0.61370200
C	-0.13020300	-1.68999100	1.90290200
H	-0.79550300	-2.29816300	1.28445600
H	-0.64505000	-0.75411300	2.11894500
H	0.04062800	-2.21881300	2.83992700
C	1.17839100	2.20073100	0.20795000
H	1.92020400	2.38115200	-0.57421500
C	-3.56290200	-1.48099500	-0.39297200
C	0.03387500	-1.67745100	-2.03548900
H	0.69131200	-2.30954700	-1.43257600
H	0.57030500	-0.75332400	-2.24973300
H	-0.16256800	-2.19222200	-2.97543500
C	4.88065300	-1.98295500	0.04307300
C	5.24521500	-3.33093000	0.05811100
C	5.85175200	-1.02992000	-0.27609500
C	6.54392500	-3.71588600	-0.24019300
H	4.50449900	-4.08675400	0.29052200
C	7.14649800	-1.41764500	-0.58284500
H	5.59415300	0.02143300	-0.26701700
C	7.49914100	-2.76189500	-0.56540400
H	6.80737100	-4.76547000	-0.22480400
H	7.88586900	-0.66585200	-0.82689100
H	8.51160800	-3.06254100	-0.80054800
C	-4.93392400	-1.87647700	-0.04860500
C	-5.32655200	-3.21675900	-0.05299600
C	-5.87678500	-0.90433900	0.29729900
C	-6.62392900	-3.57558800	0.28174900
H	-4.60788500	-3.98717500	-0.30597100
C	-7.17002800	-1.26592700	0.64050900
H	-5.59790800	0.14150200	0.28029400
C	-7.55037200	-2.60272400	0.63350400
H	-6.90876000	-4.61970000	0.27395200
H	-7.88700200	-0.49932100	0.90469000
H	-8.56173300	-2.88291100	0.89702800
N	-0.00603400	3.01506500	-0.02499000
C	0.04825100	4.42364200	-0.05746600
C	1.27815500	5.06399700	-0.21978600
C	-1.10672100	5.19225600	0.10071000
C	1.34534500	6.44867800	-0.24165000
H	2.18798600	4.48985100	-0.31974900

C	-1.02371300	6.57669000	0.07160100
H	-2.05840300	4.70705200	0.24421700
C	0.19655200	7.21505200	-0.10210800
H	2.30748700	6.92755200	-0.36928400
H	-1.92793100	7.15915300	0.19343800
H	0.25286300	8.29515500	-0.12155900

***o*-1e** (acetonitrile)

Imaginary frequency: 0

G = -2909.800241 hartree

S	2.38617800	-1.89512100	1.47772000
S	-2.42680800	-1.88409300	-1.57023000
O	-2.17611900	3.19898100	-0.80500500
O	1.68784300	3.12200600	1.53308900
H	1.05817300	2.86839500	2.22097400
C	1.49339600	0.28955900	0.52458800
C	2.86722000	0.21438700	0.14542800
H	3.35732000	0.96393600	-0.46079100
C	-1.08971400	2.83040900	-0.41059700
C	-1.51143700	0.30281300	-0.64315400
C	1.09073300	-0.79234200	1.27084200
C	0.63244800	1.40629400	0.15475700
C	3.48659500	-0.92244800	0.57161900
C	-0.63472200	1.41206800	-0.28013600
C	-1.12726900	-0.77811300	-1.39758600
C	-2.87340200	0.22734100	-0.22672900
H	-3.34211600	0.98702200	0.38242600
C	-0.23856200	-1.07289800	1.89117100
H	-0.86009100	-1.68402900	1.23147000
H	-0.77048100	-0.13991000	2.07563000
H	-0.12357400	-1.60244800	2.83610100
C	1.13969700	2.82638900	0.28413300
H	1.93331600	3.01755600	-0.44263900
C	-3.50396400	-0.90949100	-0.63686700
C	0.19208800	-1.06228500	-2.03723200
H	0.81925100	-1.68062200	-1.38951700
H	0.72604100	-0.13067000	-2.22312400
H	0.06345700	-1.58560300	-2.98397400
C	4.87475200	-1.33711100	0.34619400
C	5.24944200	-2.67991400	0.41301900
C	5.85230600	-0.38051300	0.05289200
C	6.56246500	-3.06246200	0.19155600
H	4.50723700	-3.43943100	0.62393700
C	7.16133900	-0.75850500	-0.17803200
H	5.58779500	0.66778800	0.01954500
C	7.51528200	-2.10129100	-0.10895600
H	6.83707000	-4.10709300	0.24223600
H	7.90867400	-0.00971900	-0.40675200
C	-4.88746000	-1.32027200	-0.38000600
C	-5.26977600	-2.66139000	-0.44252000
C	-5.85436700	-0.36122200	-0.05955400
C	-6.57856800	-3.03956400	-0.19090900
H	-4.53598500	-3.42299000	-0.67451900
C	-7.15904300	-0.73484300	0.20140400
H	-5.58445900	0.68579900	-0.02909300
C	-7.52032200	-2.07588100	0.13606200
H	-6.85856000	-4.08294900	-0.23880200
H	-7.89756900	0.01617200	0.45060900
N	-0.03473500	3.62755400	-0.03080900
C	8.94801800	-2.48793600	-0.31936200
F	9.50859000	-1.81074400	-1.33175700
F	9.09352400	-3.78988400	-0.58859400
F	9.70085000	-2.23299400	0.76539800
C	-8.94903900	-2.45806500	0.37763100
F	-9.48795800	-1.77471400	1.39770000
F	-9.09205200	-3.75853000	0.65631000
F	-9.72374100	-2.20734500	-0.69288900
C	0.00527800	5.03708900	-0.05688300
C	1.23590200	5.69170300	-0.13328700
C	-1.16678500	5.79169600	0.02277800
C	1.28831700	7.07711000	-0.14803200
H	2.15708100	5.12838900	-0.17198700
C	-1.09805200	7.17707000	0.00197200
H	-2.12040500	5.29527300	0.09959500
C	0.12379300	7.82978900	-0.08618600
H	2.25129500	7.56730500	-0.20865500
H	-2.01515900	7.74884000	0.06260100
H	0.16867700	8.91051100	-0.09975000

***c*-1a** (acetonitrile)

Imaginary frequency: 0

G = -2043.898361 hartree

S	-1.81470700	-1.82567700	0.01978500
S	1.82355100	-1.83221400	0.01536700
O	2.32938000	3.76118700	0.08276600
O	-2.09383700	3.73868400	-0.84214800
H	-1.75289000	3.41380100	-1.68592600
C	-1.42063200	0.81077200	-0.07243500

C	-2.83721200	0.58392700	-0.06729100
H	-3.54998800	1.39602800	-0.03802100
C	1.18181900	3.34487600	0.09353500
C	1.43400100	0.79749200	0.22018000
C	-0.63810800	-0.46941800	-0.37486200
C	-0.71907300	1.94284900	0.09701600
C	-3.18997000	-0.71869400	-0.02336700
C	0.72341900	1.93849900	0.12478500
C	0.65075200	-0.49139800	0.46511600
C	2.84465500	0.57598800	0.17196200
H	3.55037300	1.39315400	0.15030600
C	-0.37423100	-0.49841800	-1.88993200
H	0.07649100	-1.44064500	-2.19400800
H	0.29128100	0.32035700	-2.16931000
H	-1.32043900	-0.37468500	-2.41591900
C	-1.19551600	3.37195200	0.17197600
H	-1.71477700	3.60554800	1.10589600
C	3.19412800	-0.72736900	0.06727900
C	0.39001100	-0.58430600	1.97945500
H	-0.06673200	-1.53660400	2.23965000
H	-0.27065400	0.22445000	2.29501700
H	1.33756100	-0.49061800	2.50898000
C	-4.55106700	-1.26261700	0.02056900
C	-4.78710700	-2.57292100	0.44259000
C	-5.64186200	-0.47270500	-0.35866300
C	-6.07843000	-3.07670700	0.49779900
H	-3.95798100	-3.20216700	0.74268100
C	-6.92947300	-0.97780400	-0.30349600
H	-5.47877100	0.53573800	-0.71533700
C	-7.15355400	-2.28142700	0.12676900
C	4.55442800	-1.26500900	-0.03133300
C	4.78220400	-2.56125800	-0.49936900
C	5.65242500	-0.48228400	0.34213400
C	6.07267300	-3.05852800	-0.60366000
H	3.94726100	-3.18369800	-0.79735300
C	6.93929200	-0.98126200	0.23822300
H	5.49602200	0.51485100	0.73171300
C	7.15484100	-2.27069700	-0.23668600
H	7.77781600	-0.36526400	0.53536700
H	6.23137800	-4.06315800	-0.97277500
H	-6.24290600	-4.09267200	0.83185100
H	-7.76182300	-0.35532700	-0.60469500
H	-8.16072500	-2.67500100	0.16629500
H	8.16168200	-2.65929900	-0.31486600
N	0.05580500	4.11378400	0.10536700
C	0.06826800	5.55404000	0.19116700
H	1.09769800	5.89134500	0.10243400
H	-0.52701400	5.98529200	-0.61297200
H	-0.33942100	5.88393600	1.14928200

***c*-1b** (acetonitrile)

Imaginary frequency: 0

G = -2272.896955 hartree

S	-1.81336800	-1.40219500	-0.00674700
S	1.81873700	-1.41168900	0.07565500
O	2.32970500	4.18300800	0.12041600
O	-2.07193400	4.15655300	-0.90186900
H	-1.71517400	3.81983600	-1.73436200
C	-1.41919200	1.23303000	-0.09882200
C	-2.83463100	1.00542500	-0.11990700
H	-3.54513600	1.81980500	-0.11157200
C	1.18198700	3.76574100	0.10758400
C	1.43159200	1.21932900	0.25067100
C	-0.62979300	-0.04748200	-0.38005600
C	-0.71902900	2.36561400	0.07792400
C	-3.19159200	-0.29769700	-0.07899300
C	0.72258400	2.36081900	0.13551600
C	0.64011900	-0.06572000	0.48872700
C	2.84089600	0.99478000	0.23185700
H	3.54584000	1.81262700	0.22145800
C	-0.33082300	-0.08170300	-1.88831500
H	0.12756300	-1.02474500	-2.17835900
H	0.34056500	0.73641500	-2.15520300
H	-1.26477800	0.03933000	-2.43639100
C	-1.19602100	3.79512600	0.13449200
H	-1.73600400	4.03546400	1.05501400
C	3.19394600	-0.31100800	0.14568000
C	0.34410400	-0.14616200	1.99716700
H	-0.12089800	-1.09547000	2.25394200
H	-0.32188000	0.66629800	2.29118600
H	1.27946500	-0.05063900	2.54763100
C	-4.54729700	-0.84591200	-0.06020500
C	-4.78375500	-2.18668300	0.23374300
C	-5.65647000	-0.03031800	-0.33449100
C	-6.06876000	-2.71259800	0.26810700
H	-3.95363800	-2.84759800	0.45172600
C	-6.93514300	-0.53678300	-0.30531600
H	-5.51298800	1.01187200	-0.58677400

C	-7.15405900	-1.88506000	-0.00141100
C	4.54876600	-0.85466500	0.08074300
C	4.78097700	-2.18890900	-0.24657900
C	5.66199300	-0.04090600	0.34507300
C	6.06532700	-2.71018800	-0.32148800
H	3.94752800	-2.84730000	-0.45931000
C	6.94041900	-0.54317100	0.27611500
H	5.52173600	0.99557700	0.62106500
C	7.15486700	-1.88472200	-0.05994300
H	7.79780300	0.08283000	0.48492700
H	6.19960200	-3.74941400	-0.58204100
H	-6.20582100	-3.75744200	0.50378700
H	-7.78895300	0.09159000	-0.52181400
N	0.05643900	4.53623800	0.09054200
C	0.06838200	5.97654900	0.17153000
H	1.09921200	6.31317100	0.09732400
H	-0.51416400	6.40534400	-0.64323900
H	-0.35366300	6.31078600	1.12200100
O	8.44198800	-2.28668400	-0.10142800
C	8.70474600	-3.64034300	-0.43247000
H	8.25057900	-4.31474800	0.29612300
H	8.33284200	-3.87634200	-1.43142700
H	9.78445600	-3.75239000	-0.40957600
C	-8.70752600	-3.65131500	0.29926000
H	-8.23466900	-4.30994300	-0.43197000
H	-8.35792600	-3.90688200	1.30152100
H	-9.78607200	-3.76623200	0.24936600
O	-8.44177100	-2.29084400	0.00181700

***c*-1c** (acetonitrile)

Imaginary frequency: 0

G = -2718.088723 hartree

S	1.81847900	-1.21876400	-0.01373300
S	-1.82329200	-1.22773700	-0.07057700
O	-2.33117600	4.36335700	-0.11494300
O	2.07316000	4.33925500	0.89748700
H	1.71105400	4.01866400	1.73414500
C	1.41696600	1.41623200	0.09390400
C	2.83395500	1.19333500	0.11574700
H	3.54443100	2.00788300	0.10825100
C	-1.18301300	3.95049200	-0.10566400
C	-1.42790500	1.40289300	-0.25586100
C	0.63164600	0.13211500	0.37132200
C	0.71910800	2.54947000	-0.08129000
C	3.18761900	-0.10842100	0.06731800
C	-0.72182800	2.54375200	-0.13802400
C	-0.64106600	0.11479100	-0.49291700
C	-2.84015400	1.18307900	-0.23829500
H	-3.54481500	2.00144400	-0.22785700
C	0.34113700	0.08943500	1.88122100
H	-0.11183100	-0.85671700	2.16912500
H	-0.33174300	0.90377900	2.15572600
H	1.27731900	0.21152600	2.42514500
C	1.19565600	3.97982600	-0.13617700
H	1.73251000	4.21920400	-1.05846400
C	-3.18934300	-0.12040700	-0.14669100
C	-0.35351700	0.02868200	-2.00282600
H	0.10574100	-0.92329200	-2.25954100
H	0.31427100	0.83760500	-2.30255000
H	-1.29110200	0.12699400	-2.54892300
C	4.55208300	-0.64500000	0.04200300
C	4.79942000	-1.95108800	-0.37985700
C	5.63290000	0.15095700	0.44199500
C	6.09195400	-2.45306400	-0.41751500
H	3.98044800	-2.58513800	-0.69470400
C	6.92030900	-0.34443000	0.40647200
H	5.46204200	1.15688300	0.79973800
C	7.14773000	-1.64816600	-0.02539500
C	-4.55358700	-0.65369200	-0.07605100
C	-4.79348200	-1.94712100	0.38704300
C	-5.64057700	0.13418300	-0.47483900
C	-6.08562600	-2.44497800	0.46515000
H	-3.96917400	-2.57340500	0.70343700
C	-6.92769800	-0.35752100	-0.39947500
H	-5.47504900	1.12997200	-0.86202800
C	-7.14765300	-1.64840500	0.07263600
H	-7.76203000	0.25624500	-0.71441200
H	-6.25852300	-3.44751700	0.83025000
H	6.26985400	-3.46584400	-0.75065400
H	7.74899000	0.27640300	0.72254000
N	-0.05793700	4.71961000	-0.08914200
C	-0.07020200	6.16084900	-0.16296300
H	-1.10081300	6.49682500	-0.08400300
H	0.51494000	6.58464600	0.65237700
H	0.34918100	6.49878300	-1.11308200
C	8.55939500	-2.15420000	-0.05624400
F	9.15477400	-2.04308400	1.14159000
F	9.31867100	-1.45830100	-0.91816900

F	8.63951900	-3.43830600	-0.41556000
C	-8.55945600	-2.15121500	0.14227600
F	-9.16240800	-2.10815700	-1.05619200
F	-9.31197600	-1.40649500	0.96795800
F	-8.63720600	-3.41270200	0.57437900

***c*-1d** (acetonitrile)

Imaginary frequency: 0

G = -2235.582067 hartree

S	1.81456400	-2.68876200	-0.00396200
S	-1.81836000	-2.69976100	-0.04217900
O	-2.34283700	2.86236300	-0.05901200
O	2.13505300	2.86347900	0.81330000
H	1.83174800	2.54355000	1.67319000
C	1.41966800	-0.05257400	0.09802300
C	2.83603700	-0.27896000	0.09567100
H	3.54911100	0.53290100	0.07175300
C	-1.19153100	2.47010100	-0.05678600
C	-1.43403400	-0.06725400	-0.21665400
C	0.63496900	-1.33433600	0.38767800
C	0.71598900	1.07877300	-0.06899800
C	3.18881800	-1.58155500	0.04761100
C	-0.72280800	1.07464400	-0.10755700
C	-0.64529100	-1.35134000	-0.46575800
C	-2.84250100	-0.29152800	-0.17759300
H	-3.55117500	0.52261900	-0.15045400
C	0.35558200	-1.37246800	1.89969500
H	-0.09878000	-2.31628300	2.19333400
H	-0.31192400	-0.55495000	2.17799900
H	1.29653500	-1.25285200	2.43588400
C	1.19673300	2.50159300	-0.15635900
H	1.67271800	2.71163100	-1.11637800
C	-3.18909800	-1.59822100	-0.08890000
C	-0.36925300	-1.42849900	-1.97880900
H	0.09487300	-2.37614000	-2.24272500
H	0.29042200	-0.61381300	-2.28057100
H	-1.31199600	-1.33471700	-2.51672000
C	4.55019700	-2.12469100	0.00651600
C	4.78882600	-3.43165200	-0.42429800
C	5.63849900	-1.33723700	0.39780500
C	6.08061300	-3.93450400	-0.47637600
H	3.96155300	-4.05869100	-0.73400400
C	6.92656000	-1.84148500	0.34577600
H	5.47296800	-0.33170600	0.76151500
C	7.15336300	-3.14168700	-0.09331100
C	-4.54879200	-2.13898100	-0.00516100
C	-4.77748400	-3.43934700	0.45106500
C	-5.64487300	-1.35538800	-0.38235200
C	-6.06759100	-3.94005500	0.53996500
H	-3.94380500	-4.06204000	0.75204500
C	-6.93143900	-1.85807100	-0.29403000
H	-5.48715800	-0.35508500	-0.76312000
C	-7.14806000	-3.15156100	0.16906800
H	-7.76869000	-1.24183300	-0.59413800
H	-6.22752500	-4.94770300	0.90012100
H	6.24735300	-4.94776800	-0.81740500
H	7.75702700	-1.22115900	0.65642900
H	8.16087600	-3.53462100	-0.13038100
H	-8.15467200	-3.54298900	0.23511600
N	-0.05792100	3.26379700	-0.04016100
C	-0.05426500	4.67574800	-0.05135700
C	1.01420900	5.36310900	-0.62891600
C	-1.09330400	5.39845900	0.53753600
C	1.02904900	6.74956300	-0.63560900
H	1.84213100	4.82464300	-1.06705500
C	-1.06751700	6.78520200	0.52008800
H	-1.91225400	4.87481700	1.00404100
C	-0.01250800	7.47004200	-0.06746200
H	1.86497000	7.26613100	-1.08910300
H	-1.88064800	7.33233500	0.97951500
H	0.00222100	8.55172800	-0.07506600

***c*-1e** (acetonitrile)

Imaginary frequency: 0

G = -2909.772670 hartree

S	-1.81673600	-1.97460200	-0.00309800
S	1.81930900	-1.98542100	0.07989100
O	2.34250000	3.57454000	0.09656900
O	-2.12123300	3.57522000	-0.84510400
H	-1.79923700	3.26473600	-1.70175000
C	-1.41687400	0.66089100	-0.10959100
C	-2.83351200	0.43735800	-0.12906300
H	-3.54469900	1.25111200	-0.12003700
C	1.19108000	3.18479800	0.07791100
C	1.42828700	0.64685200	0.24940200
C	-0.62978300	-0.62276900	-0.38382800
C	-0.71694500	1.79318100	0.06508300
C	-3.18605400	-0.86485200	-0.08123300

C	0.72044200	1.78837500	0.12598700
C	0.63800400	-0.63824200	0.48788900
C	2.83850200	0.42537400	0.23416400
H	3.54578800	1.24112800	0.21955300
C	-0.33062400	-0.66689800	-1.89194400
H	0.12530600	-1.61277400	-2.17612000
H	0.34230800	0.14811100	-2.16433000
H	-1.26398400	-0.54706200	-2.44112300
C	-1.19857400	3.21685800	0.13974200
H	-1.68895000	3.42912300	1.09186400
C	3.18501700	-0.88056000	0.15055900
C	0.34209900	-0.71610100	1.99716300
H	-0.12263300	-1.66503300	2.25507300
H	-0.32382400	0.09676700	2.28996300
H	1.27715900	-0.61945400	2.54776000
C	-4.55022100	-1.40204500	-0.05550900
C	-4.79673600	-2.70843600	0.36583100
C	-5.63138100	-0.60633200	-0.45501000
C	-6.08901300	-3.21106600	0.40331700
H	-3.97744900	-3.34219500	0.68045600
C	-6.91851500	-1.10240700	-0.41964200
H	-5.46108200	0.39982600	-0.81235000
C	-7.14516500	-2.40647700	0.01158800
C	4.54874500	-1.41567300	0.08659600
C	4.78898000	-2.70906100	-0.37646700
C	5.63409400	-0.62963900	0.49301700
C	6.08068300	-3.20887800	-0.44679800
H	3.96555200	-3.33335100	-0.69906400
C	6.92087900	-1.12356400	0.42557000
H	5.46748600	0.36583100	0.88055900
C	7.14137700	-2.41435100	-0.04628300
H	7.75417000	-0.51173500	0.74688300
H	6.25441200	-4.21130300	-0.81176700
H	-6.26640800	-4.22408100	0.73598400
H	-7.74753100	-0.48186800	-0.73538800
N	0.05849100	3.97757300	0.04075900
C	-8.55663200	-2.91325800	0.04222300
F	-9.15218200	-2.80121200	-1.15539800
F	-9.31598300	-2.21855400	0.90498100
F	-8.63600400	-4.19773800	0.40027500
C	8.55296700	-2.91928300	-0.10888700
F	9.15512500	-2.86146700	1.08913400
F	9.30619700	-2.18566800	-0.94376000
F	8.62961800	-4.18609300	-0.52510100
C	0.05551600	5.39013800	0.04512600
C	-1.01884900	6.08046200	0.60744800
C	1.10189400	6.10838700	-0.53559500
C	-1.03251700	7.46691900	0.60720100
H	-1.85184800	5.54458100	1.03915700
C	1.07719300	7.49521500	-0.52518300
H	1.92557900	5.58169800	-0.99028800
C	0.01612200	8.18350600	0.04718500
H	-1.87287900	7.98653000	1.04877400
H	1.89588500	8.03951500	-0.97796100
H	0.00226600	9.26522100	0.04943100

***o*-2a** (acetonitrile)

Imaginary frequency: 0

G = -1967.888793 hartree

S	-2.57545100	-1.64336100	-1.27627000
S	2.78985000	-1.50124100	1.36786900
O	-2.17252200	3.48614200	-0.34936500
C	-0.63588500	1.58451900	-0.10534800
C	-1.54711500	0.50353400	-0.38794900
C	1.08804100	3.03754600	0.22049400
C	-1.11057100	3.00516100	-0.15913700
C	0.69702200	1.62363100	0.15369400
C	1.66110200	0.57758100	0.44301300
C	-2.91092000	0.50498500	0.04214900
H	-3.33943900	1.28750200	0.65133000
C	3.00262500	0.60042800	-0.04606800
H	3.38295400	1.36170700	-0.71393900
C	5.13508600	-0.78998300	0.03289600
C	-3.59568800	-0.60568400	-0.34216100
C	-1.22059900	-0.61587900	-1.12990400
C	1.39807500	-0.51585700	1.23826700
C	3.73856600	-0.47302000	0.35483500
C	0.06324700	-0.95762900	-1.80653300
H	-0.11436600	-1.56439100	-2.69280100
H	0.72191700	-1.51943100	-1.13824800
H	0.58968900	-0.05077100	-2.10397300
C	5.60179100	-2.10574300	0.04983700
H	4.92477300	-2.91569100	0.29374800
C	-4.99442500	-0.95393200	-0.06564100
C	0.14203600	-0.87517300	1.95716500
H	0.35828200	-1.43248700	2.86711100
H	-0.50596800	-1.49236600	1.32823000
H	-0.41467000	0.02381200	2.22220400

C	6.02333700	0.23512500	-0.30224900
H	5.68390900	1.26297700	-0.29473100
C	7.34056000	-0.05210800	-0.62278200
H	8.01659500	0.75330500	-0.87860000
C	7.79608500	-1.36502500	-0.60371400
H	8.82604400	-1.58725200	-0.84971400
C	6.92272800	-2.38949300	-0.26322800
H	7.26774400	-3.41501400	-0.24735700
C	-5.92618900	0.05530700	0.19040800
H	-5.61760000	1.09229200	0.15493400
C	-5.42063600	-2.28327500	-0.04915700
H	-4.71039000	-3.08063100	-0.23266300
C	-6.74472900	-2.59605900	0.22006600
H	-7.05805000	-3.63176500	0.23082400
C	-7.24671800	-0.26065000	0.46728500
H	-7.95671700	0.53254600	0.66196600
C	-7.66180500	-1.58698000	0.48234100
H	-8.69433600	-1.83146300	0.69408900
N	0.09102300	3.83081100	0.05203600
C	0.03842800	5.28418400	0.08458600
H	-0.38198300	5.63619300	-0.85424700
H	1.04589700	5.66471100	0.21741700
H	-0.59814300	5.59290400	0.91036600
H	2.08578700	3.40907400	0.42012900

***o*-2b** (acetonitrile)

Imaginary frequency: 0

G = -2196.886780 hartree

S	-2.54069100	-1.33092200	-1.35344500
S	2.71994300	-1.20406300	1.49499400
O	-2.14285100	3.80128500	-0.44711600
C	-0.62912000	1.89226500	-0.12736500
C	-1.53487100	0.81504300	-0.43852400
C	1.08909800	3.33703800	0.25859000
C	-1.09241200	3.31503600	-0.21022100
C	0.69312800	1.92572900	0.18537800
C	1.63914900	0.87669500	0.51927300
C	-2.91497800	0.82670700	-0.06139100
H	-3.36104500	1.61620300	0.52576200
C	2.99933900	0.89002200	0.08207400
H	3.40902900	1.64666700	-0.57332900
C	5.11665000	-0.51539600	0.24408600
C	-3.59163400	-0.28277900	-0.46388700
C	-1.18509400	-0.31118000	-1.15858200
C	1.33810400	-0.21204000	1.30644700
C	3.71373000	-0.18651400	0.51323600
C	0.12317600	-0.66685100	-1.77838500
H	-0.02152000	-1.27776800	-2.66783900
H	0.74916900	-1.22899300	-1.07938400
H	0.66896800	0.23401400	-2.05855000
C	5.58072000	-1.82677300	0.28010500
H	4.89598400	-2.63592900	0.50482200
C	-4.99972300	-0.62382400	-0.24144900
C	0.05218200	-0.56347200	1.97429500
H	0.22816700	-1.11990000	2.89344200
H	-0.57365000	-1.17837700	1.32093200
H	-0.51018300	0.33893900	2.21482400
C	6.03113900	0.49859900	-0.06831700
H	5.70577800	1.53100900	-0.08017300
C	7.34939800	0.20551700	-0.34257200
H	8.05670300	0.98913000	-0.58023000
C	7.80021300	-1.11662600	-0.30454400
C	6.90817500	-2.13655600	0.01286100
H	7.22640600	-3.16789300	0.04801300
C	-5.94145800	0.38678300	-0.00858800
H	-5.63168800	1.42400600	-0.02121100
C	-5.44348000	-1.94264700	-0.24909900
H	-4.73872200	-2.74918100	-0.41335100
C	-6.77729100	-2.26314900	-0.03063700
H	-7.07927200	-3.29991500	-0.04209000
C	-7.26654800	0.08327400	0.21673000
H	-7.99484700	0.86403300	0.39226300
C	-7.69696300	-1.24618800	0.20718100
N	0.10419900	4.13511600	0.04393900
C	0.05845500	5.58872300	0.06581700
H	-0.31340000	5.93822300	-0.89425000
H	1.06010900	5.96483100	0.24610000
H	-0.61602200	5.90575500	0.85764900
H	2.08013800	3.70418100	0.49672700
O	-9.01499700	-1.44703100	0.43314300
O	9.10920600	-1.30775500	-0.58493000
C	-9.49238000	-2.78127700	0.41993500
H	-9.01130300	-3.37624800	1.19899700
H	-10.55923600	-2.72280200	0.61365500
H	-9.32206100	-3.24747500	-0.55274000
C	9.60604800	-2.63453400	-0.55092200
H	9.09585500	-3.26172100	-1.28488200
H	10.66109000	-2.56892500	-0.79937100

H	9.49074500	-3.06966000	0.44394300

***o*-2c** (acetonitrile)

Imaginary frequency: 0

G = -2642.079364 hartree

S	-2.50393600	-1.20854200	-1.42119200
S	2.65267400	-1.11460400	1.54404600
O	-2.12426500	3.92697300	-0.49872800
C	-0.62397900	2.01540300	-0.14271400
C	-1.52277700	0.93862000	-0.48059200
C	1.08542100	3.45620100	0.29877000
C	-1.08210800	3.43919500	-0.23361900
C	0.68668100	2.04392900	0.20796800
C	1.61727400	0.98666800	0.56049200
C	-2.90732000	0.94509100	-0.12795700
H	-3.36645600	1.72996500	0.45541900
C	2.98689400	0.99277300	0.16031700
H	3.42094600	1.75222800	-0.47557000
C	5.08486800	-0.43116700	0.35922400
C	-3.57045900	-0.16635100	-0.54782300
C	-1.15881400	-0.18245400	-1.20211600
C	1.28885900	-0.10654300	1.33260300
C	3.67788800	-0.09497800	0.60121300
C	0.16082300	-0.52872500	-1.80350900
H	0.03221000	-1.12472300	-2.70535700
H	0.77175100	-1.10406400	-1.10228900
H	0.71174500	0.37627000	-2.05868400
C	5.52767100	-1.75386900	0.38910900
H	4.82750500	-2.55620300	0.58455500
C	-4.98081500	-0.51118100	-0.34082900
C	-0.01398600	-0.44829100	1.97257100
H	0.13884900	-1.00590900	2.89500000
H	-0.62901200	-1.05950300	1.30605000
H	-0.57400800	0.45844300	2.20137200
C	6.00628700	0.58394900	0.08458100
H	5.68577300	1.61708600	0.08152500
C	7.33140300	0.28138700	-0.16579100
H	8.03676300	1.07379900	-0.37981400
C	7.75451400	-1.04238400	-0.13512900
C	6.85692200	-2.06058400	0.14707700
H	7.18691900	-3.09006500	0.16697000
C	-5.91990600	0.50098900	-0.11883500
H	-5.60932800	1.53712300	-0.12995000
C	-5.41036700	-1.83832400	-0.35406500
H	-4.69763500	-2.63832700	-0.50975800
C	-6.74384600	-2.15290900	-0.14684600
H	-7.06340700	-3.18577100	-0.15422800
C	-7.24906600	0.19078300	0.09699300
H	-7.96830300	0.98081600	0.27022000
C	-7.65898000	-1.13768200	0.08356800
N	0.10919800	4.25617300	0.06029400
C	0.06531100	5.71012100	0.08506100
H	-0.26620900	6.06318900	-0.88835500
H	1.05914900	6.08380700	0.30811400
H	-0.64123700	6.02431100	0.84950900
H	2.07062200	3.81958300	0.56556300
C	-9.11240200	-1.44998700	0.28015700
F	-9.65343500	-0.71958900	1.26566700
F	-9.32440000	-2.73534700	0.58042100
F	-9.83403600	-1.18680400	-0.82298900
C	9.20418400	-1.34853800	-0.36663500
F	9.72293500	-0.60551000	-1.35422700
F	9.41189600	-2.63005700	-0.68645000
F	9.94840100	-1.09797900	0.72450600

***o*-2d** (acetonitrile)

Imaginary frequency: 0

G = -2159.568394 hartree

S	-2.59353300	-2.48921800	-1.27451800
S	2.73017700	-2.36389500	1.40952300
O	-2.16147600	2.63642700	-0.46013300
C	-0.64119200	0.74151600	-0.14037700
C	-1.55775200	-0.33431700	-0.41520600
C	1.09025600	2.17394000	0.21429500
C	-1.11103800	2.16184500	-0.21307600
C	0.69084600	0.77197300	0.13388700
C	1.63827000	-0.28447900	0.44434700
C	-2.92624800	-0.31397000	0.00013800
H	-3.35475600	0.48237000	0.59101100
C	2.98056000	-0.29189400	-0.04184900
H	3.37393000	0.45108600	-0.72262600
C	5.08918000	-1.71621500	0.06665300
C	-3.61506800	-1.42676000	-0.36897600
C	-1.23251200	-1.47119100	-1.13323600
C	1.35491400	-1.35841200	1.25850200
C	3.69777200	-1.36999700	0.38032400
C	0.05393200	-1.83462200	-1.79303600
H	-0.12193200	-2.45419400	-2.67072500

H	0.70145400	-2.39159400	-1.10995200
H	0.59108400	-0.93758900	-2.10062400
C	5.53219500	-3.03971000	0.10382000
H	4.84027900	-3.83368300	0.35821100
C	-5.01786000	-1.76096000	-0.09622000
C	0.09030700	-1.68433700	1.97846100
H	0.29369000	-2.22710500	2.90007300
H	-0.56419900	-2.30384300	1.35855600
H	-0.45368700	-0.77210000	2.22390200
C	5.99610500	-0.71205900	-0.28167700
H	5.67520700	0.32173800	-0.28958400
C	7.30849700	-1.02758400	-0.59548200
H	7.99932400	-0.23831100	-0.86187000
C	7.74037800	-2.34801400	-0.55644000
H	8.76657400	-2.59209000	-0.79741300
C	6.84834500	-3.35165400	-0.20252400
H	7.17483600	-4.38285700	-0.17097500
C	-5.94477300	-0.74100500	0.13369500
H	-5.62959800	0.29317300	0.07917300
C	-5.45203800	-3.08717800	-0.05566500
H	-4.74561200	-3.89231900	-0.21881200
C	-6.77947500	-3.38647600	0.21233400
H	-7.09921800	-4.41982200	0.24240500
C	-7.26869600	-1.04341200	0.40924800
H	-7.97499400	-0.24226700	0.58373900
C	-7.69176200	-2.36673900	0.44889400
H	-8.72687100	-2.60076400	0.65987300
N	0.10019300	2.98682600	0.03972300
C	0.12096700	4.41253900	0.03381800
C	-0.87363600	5.10779400	0.70817300
C	1.14193900	5.06361300	-0.64523500
C	-0.83129200	6.49310400	0.70374800
H	-1.65185500	4.57768000	1.23816000
C	1.17356400	6.44878300	-0.63206800
H	1.88477400	4.49608200	-1.19049600
C	0.18857300	7.16226300	0.03883800
H	-1.59557000	7.04940800	1.22873700
H	1.96252600	6.96872500	-1.15773700
H	0.21378000	8.24359700	0.04064200
H	2.08542800	2.53697500	0.44059400

***o*-2e** (acetonitrile)

Imaginary frequency: 0

G = -2833.758929 hartree

S	-2.63169500	-1.82921900	-1.56011300
S	2.52399200	-1.94926800	1.41221800
O	2.13642300	3.17903300	0.57537300
C	-1.60393200	0.25583800	-0.53607500
C	-2.97276500	0.24878200	-0.13400400
H	-3.40857400	0.99437600	0.51692700
C	1.10077500	2.70428100	0.27397200
C	1.53724200	0.20753200	0.49977100
C	-1.27161500	-0.82055500	-1.32973500
C	-0.67764100	1.31360600	-0.17108400
C	-3.66003600	-0.83250800	-0.59640800
C	0.63618200	1.28413100	0.17585200
C	1.17536900	-0.92773300	1.20261100
C	2.92383300	0.22575900	0.15387500
H	3.38225300	1.02110500	-0.41556200
C	0.03192900	-1.14457600	-1.97739800
H	0.65179600	-1.76240700	-1.32151900
H	0.58642400	-0.23141700	-2.19387600
H	-0.11942300	-1.68901400	-2.90786200
C	-1.07530800	2.71688000	-0.26926900
H	-2.05836100	3.07822800	-0.54585600
C	3.58962700	-0.88908700	0.55873200
C	-0.14363400	-1.28948500	1.79557100
H	-0.75109600	-1.85402200	1.08263600
H	-0.69848700	-0.39172400	2.06686100
H	-0.01367500	-1.90192000	2.68609100
C	-5.06609100	-1.17841400	-0.36293300
C	-5.50548000	-2.50110600	-0.42782200
C	-5.99039600	-0.17328400	-0.06290400
C	-6.83416600	-2.81735200	-0.19584100
H	-4.80321600	-3.29641000	-0.64346600
C	-7.31519700	-0.48563100	0.17751500
H	-5.67274400	0.86028500	-0.03232000
C	-7.73487900	-1.80911000	0.11154500
H	-7.16145200	-3.84683600	-0.24329200
H	-8.02278600	0.29914100	0.41115300
C	5.00203600	-1.22536700	0.35180500
C	5.43597800	-2.55102100	0.34363600
C	5.93820600	-0.20599300	0.15146800
C	6.77142100	-2.85729000	0.13625700
H	4.72543900	-3.35608400	0.48236200
C	7.26921800	-0.50779400	-0.06441100
H	5.62381800	0.82867100	0.17966900
C	7.68369400	-1.83493500	-0.07257000

H	7.09466800	-3.88896000	0.12685100
H	7.98642600	0.28759300	-0.22079100
N	-0.09676600	3.52925400	-0.04263500
C	-9.18412600	-2.12631700	0.33077400
F	-9.71458800	-1.39481800	1.32053000
F	-9.38522400	-3.41189500	0.63893500
F	-9.92250800	-1.87257400	-0.76356500
C	9.13907900	-2.13795400	-0.26983900
F	9.67697400	-1.39694400	-1.24921400
F	9.35840700	-3.41969600	-0.57984800
F	9.85789500	-1.87905800	0.83598800
C	-0.11671900	4.95520500	-0.03642000
C	-1.16681000	5.60703800	0.59554900
C	0.90917100	5.64868700	-0.66388000
C	-1.19553800	6.99228700	0.58137100
H	-1.93424100	5.04047500	1.10657500
C	0.86843700	7.03399200	-0.66154000
H	1.71045000	5.11731900	-1.15698700
C	-0.18000400	7.70431300	-0.04390000
H	-2.00676900	7.51329300	1.07079100
H	1.65665700	7.58934900	-1.15087100
H	-0.20364100	8.78567700	-0.04679000

***c*-2a** (acetonitrile)

Imaginary frequency: 0

G = -1967.894140 hartree

S	-1.65174000	-1.72810500	-0.09113100
S	1.90819600	-1.61307300	0.22828500
O	-2.32548500	3.93991900	-0.12313500
C	-0.72392000	2.09641700	-0.05179500
C	-1.38344500	0.92147700	-0.20228400
C	1.06338900	3.51459400	0.08747700
C	-1.21820600	3.46368900	-0.05297400
C	0.72428400	2.16333100	0.06000400
C	1.48701300	1.01470000	0.20190600
C	-2.77077800	0.64031300	-0.18667600
H	-3.51789900	1.41857400	-0.14460200
C	2.86268900	0.81841000	0.12184300
H	3.57080300	1.62184900	-0.01479400
C	4.59148000	-1.01860800	-0.01330200
C	-3.05599600	-0.68911400	-0.10689700
C	-0.53175700	-0.32088600	-0.42864500
C	0.71027000	-0.25841200	0.48868700
C	3.22946100	-0.51208600	0.10622100
C	-0.15655400	-0.36377500	-1.92176200
H	-1.06171100	-0.31278900	-2.52492900
H	0.37174200	-1.28500600	-2.15864500
H	0.47702500	0.48819000	-2.17337200
C	4.83226400	-2.33587400	-0.41821700
H	4.00453200	-2.98911700	-0.66565300
C	-4.38881200	-1.28701100	-0.02079200
C	0.34545500	-0.24994100	1.98906100
H	1.24863000	-0.12898300	2.58498700
H	-0.13905300	-1.18472800	2.26236100
H	-0.33075800	0.57786200	2.20140800
C	5.67596500	-0.18516300	0.28447800
H	5.50686500	0.82752600	0.62396900
C	6.97002500	-0.66212500	0.17671300
H	7.80215200	-0.01436500	0.41684000
C	7.19884300	-1.97056900	-0.23339200
H	8.21218300	-2.34007000	-0.31915100
C	6.12863600	-2.80591200	-0.53095700
H	6.30522300	-3.82305500	-0.85302100
C	-5.51285500	-0.55303300	-0.41406400
H	-5.39572900	0.44883500	-0.80473900
C	-4.55997400	-2.59154700	0.44952300
H	-3.70234000	-3.17208400	0.76693500
C	-5.82657800	-3.14634900	0.53503900
H	-5.94650700	-4.15508400	0.90667000
C	-6.77605900	-1.11205100	-0.33089800
H	-7.63774800	-0.53785900	-0.64397100
C	-6.93666800	-2.40845500	0.14557900
H	-7.92552900	-2.84305300	0.20916200
N	-0.03332800	4.26845700	0.02101300
C	-0.10583300	5.71737300	0.04134800
H	0.90166400	6.12039300	0.07546000
H	-0.66781700	6.03903400	0.91612100
H	-0.61586700	6.06223000	-0.85598600
H	2.03998100	3.96562100	0.18713700

***c*-2b** (acetonitrile)

Imaginary frequency: 0

G = -2196.896871 hartree

S	-1.67883200	-1.28257700	-0.12960900
S	1.86099100	-1.21315300	0.30506300
O	-2.29141900	4.38828500	-0.19070300
C	-0.70781700	2.53175400	-0.06817900
C	-1.37845300	1.36257900	-0.23240800

C	1.08877600	3.92428200	0.12759400
C	-1.18680900	3.90391000	-0.08516900
C	0.73683700	2.58308500	0.08736300
C	1.48388900	1.41749500	0.24753000
C	-2.76598600	1.09834300	-0.24967300
H	-3.50000400	1.88949300	-0.22897900
C	2.84968900	1.20313900	0.18971600
H	3.56690100	1.99915000	0.05966200
C	4.55237200	-0.65866100	0.10181800
C	-3.07574300	-0.22954000	-0.17817900
C	-0.53448400	0.11098400	-0.43403800
C	0.67882200	0.16049200	0.52372100
C	3.20797500	-0.13901500	0.19474400
C	-0.11033300	0.06262900	-1.91311300
H	-0.99457400	0.12281000	-2.54576200
H	0.41557900	-0.86457600	-2.13189900
H	0.54067100	0.90724300	-2.14442200
C	4.78918500	-2.01816500	-0.13160600
H	3.95742500	-2.70001100	-0.25955100
C	-4.40930500	-0.80988000	-0.12276600
C	0.26438900	0.18308000	2.00986000
H	1.14897500	0.29465000	2.63478600
H	-0.24215000	-0.74332600	2.27212300
H	-0.40709800	1.02109000	2.19542000
C	5.66262700	0.19440500	0.24732600
H	5.52020100	1.24705000	0.44793500
C	6.94094900	-0.29513700	0.16283400
H	7.79821600	0.35302400	0.28238400
C	7.15906500	-1.65942700	-0.07705000
C	6.07016100	-2.52336500	-0.22523600
H	6.21388100	-3.57629200	-0.41396200
C	-5.54244000	-0.02400400	-0.39136500
H	-5.43072600	1.01738300	-0.66077500
C	-4.60296900	-2.15408400	0.19664000
H	-3.75290500	-2.78857900	0.41615000
C	-5.86933700	-2.71134200	0.25853500
H	-5.97685800	-3.75456900	0.51456700
C	-6.80454400	-0.56375700	-0.33714400
H	-7.67866900	0.03678700	-0.54981000
C	-6.98114000	-1.91399200	-0.00942000
N	-0.00306900	4.69334600	0.02486300
C	-0.05773600	6.14234400	0.04298800
H	0.95404000	6.53286200	0.09598700
H	-0.63151700	6.47535400	0.90603200
H	-0.54467500	6.49497300	-0.86426300
H	2.06475500	4.36652500	0.26283300
C	-8.48303900	-3.71584000	0.34082700
H	-8.11411500	-3.94683400	1.34163000
H	-9.55929500	-3.85305200	0.30734000
H	-8.00585100	-4.37254600	-0.38863000
C	8.72109500	-3.41819000	-0.38478300
H	9.80301100	-3.50028100	-0.40058300
H	8.31560100	-4.03935200	0.41507400
H	8.31290000	-3.73570400	-1.34532300
O	8.43750000	-2.04474300	-0.14749300
O	-8.25120200	-2.35225700	0.01975900

***c*-2c** (acetonitrile)

Imaginary frequency: 0

G = -2642.079702 hartree

S	-1.71023000	-1.08213100	-0.09478300
S	1.85695000	-1.03447300	0.25763000
O	-2.26074600	4.60180200	-0.16605200
C	-0.70380600	2.72227800	-0.05924000
C	-1.38295700	1.56170400	-0.21777900
C	1.11172700	4.10798400	0.09374500
C	-1.16888800	4.10065400	-0.07761300
C	0.74312500	2.75929800	0.07481900
C	1.47832100	1.60219900	0.23784700
C	-2.77830300	1.30989700	-0.22998100
H	-3.51166300	2.10221700	-0.20746700
C	2.85778200	1.38228800	0.19746400
H	3.58502400	2.17294600	0.08826300
C	4.55716900	-0.47771300	0.09021900
C	-3.08752000	-0.01145600	-0.14731200
C	-0.55448000	0.29992300	-0.42506100
C	0.67657400	0.33992500	0.50698400
C	3.19544200	0.05004200	0.17990300
C	-0.16367100	0.24157100	-1.91404300
H	-1.06044400	0.31096900	-2.52776900
H	0.34595800	-0.69246600	-2.14088600
H	0.49234500	1.07763500	-2.16152300
C	4.79375100	-1.76158000	-0.40653000
H	3.97037900	-2.37617200	-0.74723000
C	-4.43841300	-0.57704100	-0.08407200
C	0.29488600	0.35097900	2.00360100
H	1.19278600	0.45880300	2.60988900
H	-0.20517600	-0.57746400	2.26998500

H	-0.37224000	1.18790700	2.20943900
C	5.63482000	0.30883600	0.50618300
H	5.46469800	1.29442500	0.91656800
C	6.92588300	-0.17844000	0.42221000
H	7.75762100	0.43095000	0.74773500
C	7.14490900	-1.45301400	-0.08329900
C	6.08513000	-2.24824700	-0.49691400
H	6.26588400	-3.23755400	-0.89409300
C	-5.52266200	0.15147000	-0.58404600
H	-5.36310200	1.11824300	-1.04126700
C	-4.65975100	-1.83744300	0.47060600
H	-3.83326000	-2.41037000	0.87136300
C	-5.94082200	-2.36069700	0.53878000
H	-6.10629200	-3.33399900	0.97874600
C	-6.80024200	-0.36914800	-0.52052100
H	-7.63650200	0.19596000	-0.91070500
C	-7.00476200	-1.62308200	0.04466700
N	0.03722600	4.88237500	0.00631100
C	-0.00616100	6.33321100	0.01281800
H	1.00900900	6.71647000	0.04412100
H	-0.56333900	6.67252500	0.88388600
H	-0.50916600	6.67708300	-0.88865300
H	2.09816700	4.53598100	0.19952000
C	-8.39919200	-2.18141900	0.07246300
F	-8.78957700	-2.59393700	-1.14399100
F	-9.29355200	-1.26596000	0.46793400
F	-8.51445900	-3.22835500	0.89353000
C	8.54538400	-1.99836600	-0.13751200
F	8.86426300	-2.64498100	0.99437800
F	9.45508500	-1.03233600	-0.29926400
F	8.70685600	-2.86966700	-1.13831700

***c*-2d** (acetonitrile)

Imaginary frequency: 0

G = -2159.575614 hartree

S	-1.59878800	-2.66375900	-0.11532500
S	1.94413800	-2.49131300	0.27879300
O	-2.38889900	2.95798700	-0.18203800
C	-0.73561100	1.17710100	-0.07316300
C	-1.37309900	-0.00969300	-0.23019500
C	1.02369900	2.61679900	0.11267700
C	-1.26688100	2.52993300	-0.07496100
C	0.70784000	1.27165700	0.06286600
C	1.48899300	0.12648700	0.21601700
C	-2.75526700	-0.31391700	-0.22583000
H	-3.51527200	0.45207700	-0.19276900
C	2.86016700	-0.04925800	0.13417900
H	3.55627300	0.76199300	-0.01589400
C	4.61525100	-1.86686500	0.02359800
C	-3.01924300	-1.64781100	-0.14288300
C	-0.49811300	-1.23877700	-0.43835500
C	0.72525200	-1.15136300	0.50389700
C	3.24772700	-1.38070200	0.13792200
C	-0.09229800	-1.28130700	-1.92308400
H	-0.98603600	-1.24824300	-2.54421900
H	0.45572300	-2.19460400	-2.14595000
H	0.53126200	-0.41960800	-2.16656400
C	4.87526700	-3.19377000	-0.33849100
H	4.05730700	-3.86903100	-0.55759500
C	-4.34250100	-2.26684300	-0.06190000
C	0.33095200	-1.13626000	1.99709100
H	1.22055300	-1.00221900	2.61027700
H	-0.14995200	-2.07413800	2.26624600
H	-0.35770800	-0.31413500	2.18963700
C	5.68782400	-1.00510400	0.28410700
H	5.50521700	0.01590900	0.58933600
C	6.98861700	-1.46419000	0.18324100
H	7.81156300	-0.79510600	0.39444300
C	7.23582300	-2.78206100	-0.18351000
H	8.25457900	-3.13746900	-0.26460800
C	6.17794000	-3.64547700	-0.44466400
H	6.36994200	-4.66977100	-0.73325900
C	-5.47627300	-1.55219700	-0.46284800
H	-5.37353400	-0.54991300	-0.85641900
C	-4.49490100	-3.57228100	0.41243800
H	-3.62965800	-4.13786800	0.73611100
C	-5.75285200	-4.14685500	0.49439500
H	-5.85840000	-5.15595400	0.86935500
C	-6.73073400	-2.13100700	-0.38320300
H	-7.60005300	-1.57167700	-0.70201800
C	-6.87277500	-3.42806500	0.09737600
H	-7.85487100	-3.87810400	0.15839000
N	-0.09369700	3.36539000	0.03615300
C	-0.12250400	4.78668500	0.02274000
C	0.81274100	5.47583800	-0.73982800
C	-1.07407100	5.46451300	0.77535500
C	0.80340500	6.86240200	-0.73537600
H	1.52902100	4.93128400	-1.34171600

C	-1.07917500	6.85094200	0.76212400
H	-1.79062800	4.91209900	1.36548400
C	-0.14258200	7.55137500	0.01208600
H	1.53043800	7.40239900	-1.32678200
H	-1.81517500	7.38510400	1.34788900
H	-0.15166000	8.63310100	0.00851100
H	1.98683000	3.08383200	0.25695800

***c*-2e** (acetonitrile)

Imaginary frequency: 0

G = -2833.761708 hartree

S	-1.83014000	-1.84131000	-0.28174400
S	1.72220400	-1.87172000	0.13175900
O	2.27378300	3.78220700	0.21039100
C	-1.47260300	0.79507200	-0.23683200
C	-2.84425600	0.56719000	-0.19394400
H	-3.57793100	1.35037200	-0.07420700
C	1.17611700	3.30452800	0.09237400
C	1.38411600	0.77146700	0.24991500
C	-0.65863600	-0.45705800	-0.50361900
C	-0.74214400	1.96390100	-0.06951800
C	-3.17338100	-0.77305600	-0.19097400
C	0.70204300	1.92968600	0.08295400
C	0.55887800	-0.49357600	0.44769600
C	2.78002200	0.52478700	0.26802000
H	3.51008200	1.32002600	0.24812800
C	-0.25446300	-0.43550800	-1.99499900
H	0.25916700	-1.35790300	-2.25656600
H	0.40747500	0.40872100	-2.18626700
H	-1.14374600	-0.33392900	-2.61479400
C	-1.11410500	3.29988800	-0.11847500
H	-2.09647200	3.72331600	-0.26789400
C	3.09481800	-0.79552900	0.18595500
C	0.14464400	-0.55492700	1.92981300
H	-0.36647300	-1.49047300	2.14750400
H	-0.51648300	0.27967300	2.16880300
H	1.03142600	-0.48489900	2.55776800
C	-4.53064200	-1.30974600	-0.10962500
C	-4.75861100	-2.60343700	0.36146300
C	-5.61364000	-0.52165100	-0.51520300
C	-6.04731100	-3.10424600	0.43602900
H	-3.93189500	-3.21846100	0.69312900
C	-6.89824900	-1.02258800	-0.44828400
H	-5.44972600	0.47222700	-0.90750000
C	-7.10876100	-2.31161400	0.02917200
C	4.44797000	-1.35550000	0.12331300
C	4.67313200	-2.61909900	-0.42153100
C	5.53080800	-0.61825900	0.61491200
C	5.95649500	-3.13798800	-0.48898500
H	3.84805800	-3.19972700	-0.81402900
C	6.80972300	-1.13436200	0.55244400
H	5.36847200	0.35061300	1.06659300
C	7.01782000	-2.39316800	-0.00187900
H	7.64413400	-0.56461200	0.94054400
H	6.12432100	-4.11550200	-0.91815800
H	-6.22035000	-4.10367800	0.80849500
H	-7.73442400	-0.41672500	-0.77207300
N	-0.03555000	4.09202900	-0.03001700
C	-8.52194400	-2.82150800	0.10252300
F	-9.14558100	-2.71135600	-1.07808600
F	-9.24947000	-2.12290800	0.98585800
F	-8.58566300	-4.10355400	0.46618800
C	8.42316800	-2.91989900	-0.06945000
F	9.02532600	-2.87780900	1.12749300
F	9.18292800	-2.19193000	-0.90217600
F	8.47773900	-4.18430600	-0.49440800
C	-0.06389100	5.51451400	-0.01765800
C	-1.02812000	6.16539000	0.74202900
C	0.86211900	6.22728100	-0.76944000
C	-1.07363300	7.55111500	0.73567300
H	-1.72302200	5.59331300	1.34336100
C	0.81139300	7.61269700	-0.75849000
H	1.60100000	5.70314000	-1.35792400
C	-0.15412900	8.27572600	-0.01110200
H	-1.82252500	8.06271000	1.32494100
H	1.52645800	8.17512200	-1.34359900
H	-0.18797800	9.35694100	-0.00898300

TS-1a (acetonitrile)

Imaginary frequency: 1

G = -2043.828463 hartree

C	-0.62150400	2.04766000	-0.23972100
C	-1.37344700	0.82011900	-0.46412000
C	-0.62301200	-0.37337400	-0.79624100
C	0.52501500	-0.41138200	0.73990500
C	1.33481000	0.81390300	0.58909700
C	0.66317200	1.99668000	0.23620000
S	1.65197800	-1.78252400	0.65082500

C	3.07111900	-0.75854000	0.35503000
C	2.71207200	0.55366200	0.39223700
C	-2.70246900	0.59631800	-0.19914200
C	-3.07469800	-0.75355600	-0.33348000
S	-1.76497500	-1.71518600	-0.81457100
C	0.31839000	-0.37782800	-1.98405900
C	-0.41184400	-0.49737600	1.93116000
C	1.21004200	3.40915800	0.29207800
C	-1.01257800	3.43258400	-0.44754600
H	-3.37716400	1.36605800	0.14492400
H	1.05182500	0.41877700	-1.87568700
H	0.84421000	-1.33119600	-2.04394400
H	-0.23467700	-0.22221200	-2.91005600
H	-1.01207000	0.40688900	2.01581200
H	-1.07137700	-1.36400100	1.87892600
H	0.19320300	-0.58635300	2.83252500
H	3.41489900	1.35524300	0.20105800
O	-2.06105300	3.87252000	-0.90390900
H	2.00236600	3.55213300	-0.45154300
O	1.79134900	3.75284600	1.52039100
H	1.16513300	3.53982600	2.22434000
C	4.36794400	-1.35180500	0.08171000
C	4.52108500	-2.73585900	-0.08048400
C	5.51857400	-0.55247000	-0.03150200
C	5.76210000	-3.29388200	-0.35431200
H	3.65889100	-3.38657200	0.00285500
C	6.75259400	-1.11347400	-0.30463200
H	5.44374600	0.51893600	0.10200800
C	6.88701300	-2.49000200	-0.47030300
H	5.84650800	-4.36642500	-0.47655500
H	7.62097600	-0.47174100	-0.38603800
H	7.85466200	-2.92517800	-0.68163400
C	-4.39139100	-1.31311900	-0.06580500
C	-4.56323600	-2.68388400	0.16253500
C	-5.51207400	-0.47394200	-0.04441400
C	-5.82303600	-3.19987400	0.40660200
H	-3.70431000	-3.34353600	0.16787700
C	-6.77120300	-0.99683700	0.19430500
H	-5.40081500	0.58457300	-0.23630900
C	-6.93019500	-2.35847300	0.42230600
H	-5.94271400	-4.25921600	0.58935700
H	-7.63117900	-0.34077400	0.20072000
H	-7.91501600	-2.76402400	0.61298000
N	0.05398300	4.21054100	-0.04221100
C	0.18898900	5.60188500	-0.39903100
H	0.73901600	5.72702500	-1.33684200
H	-0.80577300	6.02541900	-0.51386900
H	0.71396300	6.13524100	0.39241600

TS-1b (acetonitrile)

Imaginary frequency: 1

G = -2272.826954 hartree

C	-0.61857600	2.48134800	-0.26623000
C	-1.35797800	1.24873500	-0.51748100
C	-0.59350300	0.06062700	-0.82601900
C	0.50229100	0.03617300	0.77709300
C	1.30850200	1.26257100	0.65286300
C	0.64798300	2.43694700	0.26188200
S	1.63545700	-1.33075900	0.73699400
C	3.06071600	-0.30298900	0.49374300
C	2.69880000	1.00587800	0.51146000
C	-2.69268400	1.02059600	-0.29428900
C	-3.06353300	-0.33044300	-0.44673800
S	-1.72862000	-1.28450200	-0.89071500
C	0.40528900	0.05778000	-1.96370200
C	-0.49256700	-0.05320200	1.91848500
C	1.19362000	3.84982500	0.31528500
C	-0.99716700	3.86050200	-0.51215600
H	-3.37608000	1.79103700	0.03009500
H	1.13449300	0.85227700	-1.81698100
H	0.93265300	-0.89612500	-2.00059400
H	-0.09905900	0.21676500	-2.91688500
H	-1.08866400	0.85545200	1.98057600
H	-1.15627800	-0.91324900	1.82475000
H	0.06511000	-0.15524000	2.84877100
H	3.40601600	1.80892100	0.34376800
O	-2.02209900	4.29736900	-1.02420800
H	2.00989300	3.98179400	-0.40438300
O	1.73646600	4.21166900	1.55656600
H	1.09097700	4.00065600	2.24340300
C	4.37059100	-0.89887400	0.27713000
C	4.53836400	-2.27314000	0.10524300
C	5.52913700	-0.10188000	0.23046500
C	5.78943900	-2.84292600	-0.11536700
H	3.67710800	-2.92973100	0.13561800
C	6.77151000	-0.65346500	0.01199100
H	5.45291300	0.96811800	0.37458900
C	6.91579800	-2.03291700	-0.16525500

H	5.86335200	-3.91301200	-0.24427100
H	7.65629500	-0.03059000	-0.02112600
C	-4.37917500	-0.89009000	-0.22601400
C	-4.58038600	-2.27125200	-0.13251000
C	-5.49989900	-0.04852300	-0.11074200
C	-5.83783300	-2.80769000	0.06710400
H	-3.73579000	-2.94593700	-0.20089900
C	-6.75648300	-0.56939200	0.08126100
H	-5.38547600	1.02357800	-0.19232700
C	-6.93890300	-1.95451700	0.17360700
H	-5.95186800	-3.87851700	0.14244100
H	-7.62205600	0.07409700	0.16153700
N	0.05008100	4.64755500	-0.06762700
C	0.20578200	6.02721000	-0.45994200
H	-0.78187400	6.45990000	-0.59961200
H	0.72602800	6.57463300	0.32497300
H	0.77010800	6.12285500	-1.39310100
C	-8.44116500	-3.76903800	0.45507900
H	-7.90822300	-4.20052600	1.30389300
H	-9.51111200	-3.87877400	0.60083200
H	-8.14139000	-4.27357200	-0.46492200
C	8.35881100	-3.87404700	-0.55146000
H	9.42342500	-4.02898700	-0.70145000
H	8.03018300	-4.42857900	0.33066200
H	7.81139100	-4.23028400	-1.42723900
O	-8.19971600	-2.37190300	0.36524900
O	8.18126100	-2.48195100	-0.37234900

TS-1c (acetonitrile)

Imaginary frequency: 1

G = -2718.020038 hartree

C	-0.61798200	2.69020400	-0.28682200
C	-1.34542200	1.45498800	-0.54017600
C	-0.56385600	0.26159500	-0.80583200
C	0.48884100	0.24275600	0.76472000
C	1.30016800	1.47404100	0.64535500
C	0.63310900	2.65701900	0.25907900
S	1.63323000	-1.11953400	0.75381900
C	3.05548200	-0.08609000	0.52052300
C	2.67844900	1.22854700	0.52255300
C	-2.68677500	1.22499900	-0.35717100
C	-3.03408600	-0.13077200	-0.48969500
S	-1.69434800	-1.09080800	-0.86991300
C	0.42757600	0.25231200	-1.95484200
C	-0.49737500	0.16261500	1.91757100
C	1.15452100	4.07656200	0.35735900
C	-1.02102600	4.07530300	-0.51120900
H	-3.38987600	1.99340900	-0.07167400
H	1.14023500	1.06527100	-1.83134700
H	0.97173600	-0.69219000	-1.97322800
H	-0.09030700	0.38010400	-2.90472200
H	-1.12465100	1.05174900	1.95424700
H	-1.13058900	-0.72293500	1.85907100
H	0.07029800	0.11173300	2.84557500
H	3.38216800	2.03594600	0.36176700
O	-2.05330900	4.49422900	-1.01676500
H	1.99272800	4.23411800	-0.33043800
O	1.64455700	4.42198000	1.62308100
H	0.97454700	4.20083900	2.28280800
C	4.36469300	-0.65825800	0.32416900
C	4.55346300	-2.04609600	0.22833900
C	5.50792600	0.16182400	0.22168600
C	5.81150100	-2.59137200	0.03030400
H	3.70422200	-2.71306600	0.30595800
C	6.75774500	-0.38033700	0.02611600
H	5.41006900	1.23585200	0.30120400
C	6.91791100	-1.76344000	-0.07275600
H	5.92585000	-3.66443900	-0.04243700
H	7.62029900	0.27065700	-0.04943600
C	-4.36358700	-0.69719400	-0.29690800
C	-4.53549300	-2.05105100	0.00242500
C	-5.49014000	0.12548500	-0.42209300
C	-5.80419300	-2.57647100	0.17441800
H	-3.67434000	-2.69574200	0.12190300
C	-6.75618100	-0.39916900	-0.25614100
H	-5.37627500	1.17111800	-0.67169000
C	-6.90867800	-1.74854800	0.04328500
H	-5.92947900	-3.62313600	0.41233900
H	-7.62497100	0.23741800	-0.36221800
N	0.01163700	4.86171300	-0.05307200
C	0.13365000	6.26666800	-0.35750200
H	0.75807700	6.43379300	-1.23988400
H	-0.86090100	6.66294500	-0.54720500
H	0.57130000	6.79139800	0.49073700
C	8.28947000	-2.31610400	-0.27531000
F	9.11408900	-2.02386200	0.74887800
F	8.88377100	-1.81358700	-1.37370000
F	8.29933400	-3.64780100	-0.40683300

C	-8.30018300	-2.28332700	0.23084500
F	-8.31968900	-3.60072900	0.44450000
F	-9.06926400	-2.04458000	-0.84116700
F	-8.91389100	-1.70512700	1.27425500

TS-1d (acetonitrile)

Imaginary frequency: 1

G = -2235.513876 hartree

C	-0.31885400	1.32461400	-0.13329500
C	-1.38111500	0.36400300	-0.41164000
C	-0.98780900	-0.97144900	-0.80602800
C	0.09035500	-1.39521900	0.73551700
C	1.20806600	-0.43574600	0.63913300
C	0.89669000	0.89507500	0.33589600
S	0.79325100	-3.01875700	0.58100000
C	2.44595800	-2.41568200	0.35252500
C	2.46723300	-1.06041700	0.44859800
C	-2.72057600	0.50240000	-0.14332900
C	-3.44935500	-0.68516600	-0.33789800
S	-2.45292300	-1.94438200	-0.87821600
C	-0.06536600	-1.18654600	-1.98846300
C	-0.84878600	-1.27145600	1.92079000
C	1.82718400	2.08154800	0.41981300
C	-0.31156600	2.75738500	-0.31377100
H	-3.15888900	1.40963300	0.24514400
H	0.85644100	-0.62620400	-1.84444900
H	0.18052500	-2.24432500	-2.08685000
H	-0.54065600	-0.84859000	-2.90895600
H	-1.17989900	-0.24222100	2.04659600
H	-1.71861700	-1.92248700	1.83046300
H	-0.30122300	-1.56152500	2.81674500
H	3.37006400	-0.48043100	0.30248900
O	-1.20827600	3.46597000	-0.74642800
H	2.63124100	1.98272600	-0.31522600
O	2.45775500	2.22630000	1.65858400
H	1.79126400	2.16794200	2.35533100
N	0.96037800	3.20363900	0.07563000
C	3.53558100	-3.33467000	0.06588300
C	3.29969000	-4.68957400	-0.20131100
C	4.86702200	-2.88750700	0.04683200
C	4.34536300	-5.55625300	-0.48769200
H	2.28626000	-5.07248900	-0.19260600
C	5.90541600	-3.75463800	-0.24009500
H	5.08886200	-1.85132200	0.26681400
C	5.65454200	-5.09738500	-0.51144500
H	4.13123600	-6.59756000	-0.69281800
H	6.92194700	-3.38183100	-0.24768800
H	6.46973900	-5.77341900	-0.73248000
C	-4.86954300	-0.87438000	-0.08300700
C	-5.40861800	-2.15422300	0.09523900
C	-5.71894000	0.23706400	-0.02330600
C	-6.76227100	-2.31640500	0.32796800
H	-4.76126100	-3.02217500	0.07164900
C	-7.07379700	0.06809800	0.20360400
H	-5.32240100	1.23154800	-0.17668500
C	-7.59837800	-1.20648700	0.38177300
H	-7.16675800	-3.30908600	0.47250000
H	-7.72264300	0.93278400	0.23965100
H	-8.65713800	-1.33527900	0.56371900
C	1.46388800	4.50725000	-0.05282000
C	2.84640700	4.71950300	-0.08887000
C	0.61185200	5.61592700	-0.11235000
C	3.35752000	6.00320200	-0.20579100
H	3.53219800	3.88857400	-0.01049700
C	1.13956200	6.89263200	-0.23355200
H	-0.45470300	5.47087500	-0.06514300
C	2.51150600	7.10031700	-0.28542500
H	4.43100200	6.14043000	-0.23258700
H	0.46222800	7.73606500	-0.28038300
H	2.91428900	8.10008000	-0.37682200

TS-1e (acetonitrile)

Imaginary frequency: 1

G = -2909.705889 hartree

C	-0.60918600	1.95911900	-0.18860600
C	-1.36904200	0.75217600	-0.48982000
C	-0.61837000	-0.44594700	-0.80937100
C	0.43368700	-0.55174500	0.77146600
C	1.27434400	0.66276800	0.70014300
C	0.64247600	1.87006500	0.35333000
S	1.54150100	-1.94082500	0.70664600
C	2.99090500	-0.93397600	0.53349400
C	2.65165300	0.38677200	0.58583300
C	-2.71342000	0.54607300	-0.30451200
C	-3.09299900	-0.79502500	-0.49101000
S	-1.77822400	-1.76733200	-0.92244300
C	0.38071800	-0.43496500	-1.95072800
C	-0.55849800	-0.65138900	1.91676800

C	1.21933400	3.26048000	0.47121000
C	-0.97447400	3.34714900	-0.39077200
H	-3.39619000	1.31743800	0.01968900
H	1.11273200	0.35435400	-1.79164200
H	0.90140700	-1.39133100	-2.00308800
H	-0.12694200	-0.25695800	-2.89798500
H	-1.15992700	0.25304000	1.98983100
H	-1.21600400	-1.51566000	1.82077900
H	0.00526500	-0.75695300	2.84265100
H	3.37855500	1.18043200	0.46587800
O	-2.00276600	3.78538200	-0.88022700
H	2.06214100	3.37635600	-0.21608200
O	1.71424700	3.56863000	1.73976400
H	1.04504300	3.34496100	2.39953600
N	0.10784800	4.11167500	0.05796200
C	4.28918300	-1.53392500	0.32614600
C	4.43837700	-2.91824500	0.15713800
C	5.45464200	-0.74236200	0.28722100
C	5.68382300	-3.48882900	-0.05147600
H	3.56915700	-3.56303800	0.18421000
C	6.69223300	-1.30902700	0.08078600
H	5.38537600	0.32779900	0.42621000
C	6.81387200	-2.68838800	-0.09158000
H	5.76921900	-4.55908500	-0.18153800
H	7.57413700	-0.68059700	0.05503200
C	-4.43283900	-1.34012400	-0.30910400
C	-4.63031000	-2.70484900	-0.06473500
C	-5.54043600	-0.49205500	-0.38845700
C	-5.90577100	-3.20631700	0.09607500
H	-3.78170900	-3.37146900	0.01863000
C	-6.82068500	-0.99537800	-0.23213800
H	-5.40710100	0.56053600	-0.59556700
C	-6.99757400	-2.34876700	0.01014500
H	-6.05414900	-4.26052100	0.29018600
H	-7.67389600	-0.33592200	-0.30334400
C	0.25087100	5.50463300	-0.05569000
C	1.52662900	6.07709500	-0.03212700
C	-0.86344100	6.34375700	-0.15946700
C	1.68062000	7.45141600	-0.13347000
H	2.40527600	5.45848700	0.07912100
C	-0.69163400	7.71592600	-0.26470300
H	-1.85334500	5.91819600	-0.15854200
C	0.57603000	8.28236800	-0.25667200
H	2.67825500	7.87108300	-0.11411100
H	-1.56681400	8.34798400	-0.34675200
H	0.70065000	9.35394600	-0.33611300
C	8.17302900	-3.26868100	-0.30666600
F	8.78438800	-2.74442100	-1.38498900
F	8.99761800	-3.03098100	0.73068100
F	8.14977100	-4.59469000	-0.48315400
C	-8.37248600	-2.92104200	0.20958900
F	-8.56066800	-3.31992300	1.47695700
F	-9.33859600	-2.04406200	-0.07211200
F	-8.57672900	-3.99803000	-0.56135200

TS-2a (acetonitrile)

Imaginary frequency: 1

G = -1967.841601 hartree

C	-0.73358200	2.10710200	-0.29373600
C	-1.28358700	0.91216000	-0.62267700
C	-0.43688900	-0.28426000	-0.80925000
C	0.80470600	-0.04562200	1.11286400
C	1.40779100	1.10385500	0.54429300
C	0.59518300	2.28205800	0.24889400
S	1.95905400	-1.33699600	1.15370200
C	3.17386600	-0.39472200	0.39763200
C	2.72621600	0.89473700	0.15053600
C	-2.67848800	0.57402700	-0.54986400
C	-2.89619900	-0.75278200	-0.44148400
S	-1.40714000	-1.69393000	-0.62895600
C	0.63765000	-0.32051500	-1.84889900
C	-0.30757200	-0.07752600	2.11678600
C	0.74225500	3.60090000	0.50130700
C	-1.38192000	3.45718700	-0.30167800
H	-3.43787800	1.32882200	-0.40864500
H	1.09322300	0.65634800	-1.97888500
H	1.40364500	-1.06366600	-1.61913200
H	0.17257000	-0.61032800	-2.79303300
H	-1.00608200	0.74030700	1.95342700
H	-0.84730500	-1.02534700	2.07567200
H	0.10511500	0.03118400	3.12042900
H	3.30904100	1.63728300	-0.37466100
O	-2.50432200	3.75634900	-0.65216100
H	1.56864800	4.11854500	0.96330600
C	4.47450500	-0.95610600	0.05133500
C	4.66077300	-2.33848500	-0.05163700
C	5.55922200	-0.10299000	-0.18003300
C	5.90194700	-2.85436600	-0.38170100

H	3.82749100	-3.01198000	0.10772300
C	6.79892300	-0.62419600	-0.50722300
H	5.43658300	0.96748800	-0.08341300
C	6.97357800	-1.99932900	-0.61041500
H	6.03283200	-3.92481300	-0.46505600
H	7.63254000	0.04359800	-0.67818900
H	7.94331600	-2.40406200	-0.86812000
C	-4.15564400	-1.44887300	-0.18961300
C	-4.17404500	-2.72374700	0.38040100
C	-5.36676600	-0.82911500	-0.51487200
C	-5.37938000	-3.36028800	0.63295100
H	-3.24605800	-3.21596500	0.64528300
C	-6.56701500	-1.46897200	-0.26138200
H	-5.36374000	0.14701100	-0.98200000
C	-6.57728800	-2.73518000	0.31450600
H	-5.38144300	-4.34527800	1.08008400
H	-7.49812300	-0.98279500	-0.52039300
H	-7.51748600	-3.23405200	0.50879700
N	-0.39992600	4.31061600	0.14200200
C	-0.57466100	5.73960600	0.30190900
H	0.18030000	6.27674300	-0.26963800
H	-1.56203800	5.99563300	-0.07268600
H	-0.50318800	6.01769300	1.35277900

TS-2b (acetonitrile)

Imaginary frequency: 1

G = -2196.843244 hartree

C	-0.69383200	2.57467500	-0.31214100
C	-1.26551700	1.39467400	-0.66851900
C	-0.44738400	0.18180200	-0.84474800
C	0.73710600	0.38458900	1.17537200
C	1.38398900	1.51441600	0.62346200
C	0.61310200	2.71188900	0.28880400
S	1.85893300	-0.93083200	1.26835000
C	3.12949200	-0.01970600	0.55548400
C	2.71279800	1.27665400	0.28402100
C	-2.66831700	1.09338800	-0.64664600
C	-2.92805800	-0.23061600	-0.56924800
S	-1.45346100	-1.20265700	-0.72302200
C	0.69185900	0.12593300	-1.80948400
C	-0.43386700	0.37048000	2.10885700
C	0.78486900	4.02635200	0.55176200
C	-1.30490000	3.93931400	-0.34340900
H	-3.40995600	1.86775300	-0.51935000
H	1.16345500	1.09785100	-1.91709300
H	1.43527900	-0.61902100	-1.51779300
H	0.29238700	-0.17224500	-2.78063100
H	-1.09416500	1.21424200	1.92046600
H	-1.00180400	-0.55744600	2.01603100
H	-0.08171100	0.44585900	3.13853100
H	3.32775900	2.00739700	-0.22044300
O	-2.40322100	4.27053800	-0.74220900
H	1.60302400	4.52063500	1.05234400
C	4.42532400	-0.60594700	0.26929500
C	4.62130000	-1.98881200	0.28251500
C	5.52431200	0.21709200	-0.02920200
C	5.85630500	-2.54760900	0.00695500
H	3.79132400	-2.65178100	0.49502400
C	6.75731300	-0.32472700	-0.30094600
H	5.41280000	1.29300500	-0.02902500
C	6.93599700	-1.71352800	-0.28772600
H	5.96639600	-3.62148200	0.01908500
H	7.60772700	0.30539400	-0.52368700
C	-4.20524900	-0.90037800	-0.37804800
C	-4.28066900	-2.22203400	0.05829500
C	-5.40403200	-0.21242600	-0.62648800
C	-5.50045700	-2.84991800	0.25881600
H	-3.37604700	-2.78135200	0.26446100
C	-6.61919300	-0.82352900	-0.43308100
H	-5.37673000	0.80671200	-0.98892500
C	-6.67951300	-2.14946500	0.01461500
H	-5.51800900	-3.87306200	0.60278700
H	-7.54513100	-0.29948100	-0.62836600
N	-0.32119300	4.76671800	0.14438200
C	-0.46318700	6.19995000	0.29484900
H	-1.43228600	6.48025300	-0.10905200
H	-0.41511700	6.48012400	1.34651000
H	0.32158100	6.71606400	-0.25577800
O	8.17406200	-2.15130600	-0.56854000
O	-7.91309100	-2.66244900	0.17386600
C	-8.02637200	-4.00540100	0.61912500
H	-9.09010500	-4.21377500	0.67771500
H	-7.55630300	-4.69016800	-0.08907800
H	-7.57341000	-4.12737700	1.60469200
C	8.41065100	-3.55173700	-0.56078500
H	9.46018900	-3.67939000	-0.80634600
H	8.20985800	-3.97331300	0.42555800
H	7.79456900	-4.05310600	-1.30904700

TS-2c (acetonitrile)

Imaginary frequency: 1

G = -2642.028625 hartree

C	-0.66773100	2.80651900	-0.33967000
C	-1.22676900	1.61959700	-0.67625800
C	-0.40379700	0.39340000	-0.76627600
C	0.70446700	0.64143100	1.19434300
C	1.38292900	1.76453400	0.65234000
C	0.62750800	2.95903700	0.28436100
S	1.81294800	-0.68484500	1.33292700
C	3.09906700	0.20744900	0.64553800
C	2.71674000	1.50705200	0.35119300
C	-2.63371300	1.32360300	-0.69477700
C	-2.89672600	0.00807000	-0.56399600
S	-1.43127500	-0.98340800	-0.61475100
C	0.71832100	0.29352800	-1.75163900
C	-0.45782900	0.66956400	2.14163500
C	0.79554900	4.27936600	0.51526900
C	-1.27439200	4.17500000	-0.42316900
H	-3.37767700	2.10419200	-0.63267300
H	1.22905000	1.24452200	-1.86806600
H	1.43143100	-0.48720100	-1.48157200
H	0.28264400	0.01990800	-2.71457700
H	-1.12725000	1.49695300	1.91666200
H	-1.01699700	-0.26667100	2.10455900
H	-0.09146700	0.80367000	3.15994500
H	3.35971600	2.21910900	-0.14552800
O	-2.36119000	4.49479100	-0.85469300
H	1.60570100	4.78563500	1.01701400
C	4.40170600	-0.40029900	0.38503900
C	4.53269300	-1.78468300	0.23146800
C	5.53411700	0.41024400	0.28667800
C	5.77007100	-2.34346400	-0.01944800
H	3.66127600	-2.42444400	0.28758000
C	6.77602300	-0.14927300	0.03732300
H	5.45141200	1.47949600	0.42520300
C	6.88798200	-1.52233200	-0.11630000
H	5.86669500	-3.41412300	-0.14471600
H	7.65021000	0.48226400	-0.03194300
C	-4.19580400	-0.63761700	-0.37934500
C	-4.29805100	-1.88573600	0.23316700
C	-5.35772800	0.00901500	-0.81626900
C	-5.53767300	-2.47796700	0.42032400
H	-3.41147800	-2.39809500	0.58459300
C	-6.59220500	-0.57861300	-0.63026200
H	-5.28966000	0.96540100	-1.31653000
C	-6.67825500	-1.82171200	-0.01018600
H	-5.60919900	-3.44284800	0.90181600
H	-7.48850000	-0.07650200	-0.97099800
N	-0.29903600	5.01110200	0.06605600
C	-0.44202100	6.44835700	0.18098400
H	-0.43150900	6.75004400	1.22755800
H	0.36429400	6.94923300	-0.35177000
H	-1.39476400	6.72185800	-0.26422100
C	8.21839300	-2.16172300	-0.39693800
F	8.21690000	-2.80538000	-1.57374900
F	8.53398300	-3.07395400	0.53377400
F	9.21607900	-1.27598100	-0.43475500
C	-8.03511700	-2.44224000	0.15965900
F	-8.59567900	-2.73691000	-1.02364900
F	-8.88439600	-1.61338100	0.78402600
F	-7.99738400	-3.57406800	0.86693700

TS-2d (acetonitrile)

Imaginary frequency: 1

G = -2159.525659 hartree

C	-1.05221400	0.84978600	-0.37522300
C	-1.10819400	-0.47219500	-0.67304600
C	0.12884000	-1.26571400	-0.82843100
C	1.15958500	-0.52836900	1.10905800
C	1.29507000	0.74593800	0.50597500
C	0.10555400	1.52507300	0.16635500
S	2.71309200	-1.28861200	1.19494800
C	3.49697700	0.01973600	0.41361000
C	2.60126000	1.03867500	0.12495700
C	-2.27320200	-1.30921900	-0.59531300
C	-1.97503800	-2.61749600	-0.45500400
S	-0.23911700	-2.93100400	-0.61461300
C	1.15869300	-0.91479100	-1.85367800
C	0.12107000	-0.95506700	2.10131000
C	-0.25141200	2.80574900	0.38901000
C	-2.16283500	1.84682400	-0.42147000
H	-3.26322300	-0.89523800	-0.47437800
H	1.20904500	0.15817600	-2.01154500
H	2.14511000	-1.30171700	-1.58985900
H	0.86307000	-1.38599100	-2.79301300
H	-0.82846500	-0.45852400	1.91412900

H	-0.02703100	-2.03627200	2.07631800
H	0.44636800	-0.68398300	3.10637500
H	2.86951500	1.93157800	-0.42060400
O	-3.29869800	1.68940800	-0.80675200
H	0.31068100	3.59725500	0.85844200
C	4.91801600	-0.02122000	0.08886000
C	5.61494000	-1.23318900	0.04554500
C	5.60261900	1.16847500	-0.18290600
C	6.96342100	-1.25407000	-0.26528800
H	5.09661900	-2.16488600	0.23670400
C	6.95170400	1.14233200	-0.49067800
H	5.08306900	2.11594700	-0.13354300
C	7.63498600	-0.06735800	-0.53425900
H	7.49055500	-2.19782000	-0.30249400
H	7.47286400	2.06828500	-0.69327600
H	8.68918800	-0.08523900	-0.77706800
C	-2.88138200	-3.73186900	-0.19154500
C	-2.42398300	-4.90724200	0.40837600
C	-4.23249600	-3.62173800	-0.53683100
C	-3.30301100	-5.94644300	0.67083400
H	-1.38222800	-5.00671100	0.68848000
C	-5.10550500	-4.66213200	-0.27317400
H	-4.59151200	-2.72666400	-1.02783500
C	-4.64407600	-5.82626300	0.33258800
H	-2.93915400	-6.85007500	1.14109000
H	-6.14782900	-4.56935900	-0.54754300
H	-5.32873400	-6.63928900	0.53470100
N	-1.58222500	3.02957500	0.01853200
C	-2.22410600	4.29208900	0.06830900
C	-3.55681300	4.38665700	0.45591600
C	-1.50268700	5.43395100	-0.26459500
C	-4.16293100	5.63339500	0.50341900
H	-4.10629300	3.49533900	0.72024900
C	-2.11650300	6.67578100	-0.19923100
H	-0.47218600	5.34962100	-0.58477000
C	-3.44801600	6.77970300	0.18072600
H	-5.19939500	5.70719500	0.80511900
H	-1.55224600	7.56219400	-0.45686600
H	-3.92621500	7.74900200	0.22507400

TS-2e (acetonitrile)

Imaginary frequency: 1

G = -2833.712076 hartree

C	-0.67691900	1.98111200	-0.38921100
C	-1.20605900	0.77634700	-0.71111700
C	-0.35113000	-0.42895100	-0.79147400
C	0.74831100	-0.12740900	1.18011000
C	1.39756900	1.00261700	0.61935400
C	0.61489200	2.17311300	0.23048500
S	1.88979500	-1.42151200	1.34003800
C	3.15380000	-0.50829300	0.63804800
C	2.73778500	0.77581500	0.32221200
C	-2.60415000	0.44284500	-0.72454300
C	-2.83087400	-0.87813700	-0.58000100
S	-1.33930200	-1.83043900	-0.62345100
C	0.77824700	-0.50789700	-1.76940400
C	-0.42040400	-0.11881700	2.11931300
C	0.75443200	3.49509700	0.45358600
C	-1.32308700	3.32566200	-0.48658700
H	-3.36945100	1.20286600	-0.66947400
H	1.25845400	0.45707000	-1.89936900
H	1.51512900	-1.26025000	-1.48249900
H	0.35724500	-0.81221600	-2.72970700
H	-1.10838000	0.69017200	1.88380700
H	-0.95599000	-1.06908800	2.08738200
H	-0.06364500	0.03280600	3.13855100
H	3.36147200	1.49687300	-0.18594100
O	-2.40705300	3.60583200	-0.94218100
H	1.54461100	4.01862000	0.96790100
C	4.47217400	-1.08701000	0.39124100
C	4.64128600	-2.47076700	0.27860600
C	5.58263200	-0.24888800	0.26862900
C	5.89412400	-3.00349300	0.04597700
H	3.78814400	-3.13262900	0.35498300
C	6.83891100	-0.78161000	0.03628600
H	5.47146200	0.82125900	0.37658700
C	6.98903800	-2.15594300	-0.07370200
H	6.02055300	-4.07430800	-0.04303600
H	7.69621900	-0.12903600	-0.04983800
C	-4.11184600	-1.55658200	-0.38816100
C	-4.17971600	-2.80259700	0.23328100
C	-5.29109800	-0.94392200	-0.82787900
C	-5.40286800	-3.42627000	0.42660100
H	-3.27945000	-3.28882000	0.58695700
C	-6.50903600	-1.56307800	-0.63600600
H	-5.24947600	0.01035000	-1.33495200
C	-6.56086100	-2.80368400	-0.00712500
H	-5.44810800	-4.38952800	0.91444200

H	-7.41885900	-1.08787800	-0.97948400
N	-0.36690300	4.20294800	0.00877400
C	-0.48478800	5.61543300	0.04136900
C	-1.70242000	6.21036900	0.35471700
C	0.63364400	6.39532500	-0.23356400
C	-1.79256600	7.59412800	0.38661900
H	-2.56279100	5.59556300	0.57420900
C	0.53357300	7.77753800	-0.18381600
H	1.57166900	5.92394800	-0.49733000
C	-0.67896000	8.38107200	0.12219400
H	-2.73928100	8.05778300	0.63039000
H	1.40538800	8.38207700	-0.39573700
H	-0.75588200	9.45958700	0.15436100
C	8.33615400	-2.75756700	-0.35884300
F	8.57270500	-3.83081000	0.40660500
F	8.43109600	-3.16979700	-1.63275600
F	9.33483100	-1.89548900	-0.15290400
C	-7.90135600	-3.45670000	0.17181300
F	-7.82885600	-4.59831600	0.86018400
F	-8.75886300	-2.65643100	0.82183100
F	-8.47233300	-3.74409600	-1.00802800

***o*-TS-1a** (acetonitrile)

Imaginary frequency: 1

G = -2899.923436 hartree

S	3.15723900	-2.19697300	1.43584200
S	-1.72029400	-3.48785900	-1.54524000
O	-2.09100100	1.70687600	-1.63055900
O	1.32515500	2.22128300	1.51017100
H	1.45261500	1.36300300	1.93520400
C	1.93803400	-0.44432700	0.05986400
C	3.31250600	-0.36143600	-0.31542000
H	3.68373000	0.31512100	-1.07329900
C	-1.02295900	1.46839700	-1.17492300
C	-1.08134300	-1.08589200	-1.02274300
C	1.69859400	-1.39893300	1.02031000
C	0.90540200	0.42292100	-0.49010200
C	4.10233800	-1.26258900	0.33346000
C	-0.35915000	0.15969700	-0.87002000
C	-0.54720600	-2.24105100	-1.54557900
C	-2.44836200	-1.22797300	-0.63366400
H	-3.00477500	-0.42582900	-0.17117400
C	0.41252300	-1.75787400	1.69053200
H	-0.08057700	-2.58410700	1.17070900
H	-0.26930800	-0.90534700	1.68273000
H	0.58460500	-2.06333700	2.72195200
C	1.09598500	1.88584400	-0.54820800
H	2.04682500	2.39311000	-0.58337600
C	-2.93585300	-2.48274100	-0.83654400
C	0.81978900	-2.48786800	-2.09182000
H	1.49019300	-2.86784100	-1.31610400
H	1.24714900	-1.56059200	-2.47316600
H	0.79124700	-3.21678300	-2.90051500
C	5.54821100	-1.47227700	0.19097600
C	6.13529100	-2.70345000	0.48925100
C	6.36419600	-0.42884000	-0.25394900
C	7.50228700	-2.88743200	0.34373000
H	5.51756300	-3.52863300	0.82300900
C	7.72855800	-0.61785800	-0.40689600
H	5.92895100	0.53969900	-0.46439900
C	8.30380300	-1.84716900	-0.10776600
H	7.94043700	-3.84887200	0.57772900
H	8.34645200	0.20117300	-0.75141200
H	9.36987400	-1.99182800	-0.22310800
C	-4.27817500	-2.99492200	-0.53575800
C	-4.50911400	-4.35759000	-0.33657500
C	-5.35625900	-2.11089400	-0.43810700
C	-5.78271400	-4.82380500	-0.04576200
H	-3.68485800	-5.05850700	-0.39412000
C	-6.62604200	-2.57808800	-0.13862100
H	-5.19977200	-1.05411100	-0.61267700
C	-6.84573300	-3.93649900	0.05762600
H	-5.94227500	-5.88326600	0.10696300
H	-7.44947500	-1.87932700	-0.06757500
H	-7.83867800	-4.30025700	0.28677100
N	-0.01011500	2.48117800	-0.93176200
S	-2.06107300	2.28211700	2.23324900
O	-3.24295100	2.96003800	1.73025100
O	-1.67182300	1.11117300	1.44958600
O	-0.92062200	3.20240500	2.41155200
H	0.45876100	2.58398000	1.86102300
C	-2.45741700	1.69076500	3.85247300
H	-3.29449000	1.00199900	3.76660300
H	-1.58480000	1.18302700	4.25652400
H	-2.72626700	2.54249300	4.47260200
C	-0.18266600	3.86952900	-1.21677800
C	-1.30503300	4.52071200	-0.72538900
C	0.76913000	4.53306500	-1.97847000

C	-1.46530100	5.87083900	-1.00159600
H	-2.02765900	3.98369100	-0.12472900
C	0.60232700	5.88577200	-2.23405000
H	1.62068900	3.99760700	-2.37817200
C	-0.51417300	6.55418700	-1.74855500
H	-2.33457300	6.39096600	-0.62213500
H	1.34065300	6.41235300	-2.82342600
H	-0.64429200	7.60809700	-1.95529200

***o*-TS-1b** (acetonitrile)

Imaginary frequency: 1

G = -2937.239162 hartree

S	2.92476400	-1.24889400	1.55054500
S	-2.02336900	-2.74082000	-1.21792500
O	-2.02440800	2.36730300	-2.27530100
O	1.40106300	3.17164400	0.78360100
H	1.25235600	2.40358800	1.35151300
C	1.83293500	0.29796600	-0.14269800
C	3.21306300	0.22275000	-0.50154700
H	3.63270000	0.72603700	-1.36221900
C	-0.97948900	2.14396400	-1.75333200
C	-1.21692100	-0.33417400	-1.13963900
C	1.52346400	-0.44924200	0.96828100
C	0.86260500	1.11765000	-0.85468900
C	3.93777400	-0.59423400	0.31373900
C	-0.41228000	0.86949300	-1.20475700
C	-0.76511500	-1.59759900	-1.43582000
C	-2.58879300	-0.30878400	-0.73953900
H	-3.08930000	0.60071900	-0.43868500
C	0.21295100	-0.59662000	1.67060800
H	-0.32913300	-1.47430400	1.30810300
H	-0.41492400	0.27794000	1.48946600
H	0.35840400	-0.70882600	2.74434900
C	1.14313000	2.54378000	-1.16219600
H	2.12312800	2.97357100	-1.29811400
C	-3.16394300	-1.54273900	-0.71322400
C	0.58258600	-2.03280900	-1.90736800
H	1.22207800	-2.31318500	-1.06591500
H	1.07591700	-1.21970200	-2.43989500
H	0.50574500	-2.89026100	-2.57466600
C	5.36657700	-0.91651500	0.24398100
C	5.87717000	-2.09932100	0.76978600
C	6.26152800	-0.02681300	-0.36398100
C	7.23116100	-2.40278600	0.70022800
H	5.20947400	-2.81536500	1.23412800
C	7.60622200	-0.31773500	-0.44686200
H	5.89837400	0.91259200	-0.76101300
C	8.10379000	-1.50938400	0.08644300
H	7.58527000	-3.33329900	1.11863100
H	8.29779800	0.37221400	-0.91231100
C	-4.53739900	-1.89928800	-0.34280200
C	-4.86943100	-3.17295600	0.10831900
C	-5.56106300	-0.94711400	-0.43283800
C	-6.17152900	-3.50480500	0.46276100
H	-4.09917500	-3.92924800	0.20324600
C	-6.85564300	-1.25943200	-0.07729800
H	-5.33882300	0.04628600	-0.80129500
C	-7.17311100	-2.54331200	0.37282700
H	-6.38462800	-4.50484900	0.81051100
H	-7.64616400	-0.52412300	-0.15106400
N	0.07542700	3.11233400	-1.66563700
C	-0.08224500	4.47508900	-2.14644300
H	-0.89551700	4.94491100	-1.59649200
H	0.84391500	5.01351500	-1.96705300
H	-0.30943100	4.46196000	-3.21024400
S	-1.89194300	3.93460200	1.14324100
O	-2.90118500	4.50942400	0.27369900
O	-1.61703400	2.52114900	0.89107100
O	-0.64126100	4.72406900	1.13980400
H	0.62347100	3.78765100	0.95189900
C	-2.51521600	4.03835600	2.79522800
H	-3.43896700	3.46671100	2.84445200
H	-1.77230500	3.62280400	3.47162900
H	-2.70164900	5.08434100	3.02636100
O	-8.47060200	-2.75918700	0.69325700
C	-8.83344400	-4.05353700	1.13999200
H	-9.90135600	-4.01877900	1.33410500
H	-8.62519100	-4.80416100	0.37453400
H	-8.30340200	-4.31347800	2.05873900
O	9.43679000	-1.70654700	-0.03647900
C	9.98138000	-2.89727200	0.50494200
H	11.04866800	-2.85866200	0.30834900
H	9.80971000	-2.95126100	1.58208900
H	9.55253600	-3.77821100	0.02270900

***o*-TS-1c** (acetonitrile)

Imaginary frequency: 1

G = -3382.434246 hartree

S	-2.82504500	-1.09553000	-1.59371200
S	2.00586200	-2.52118000	1.31294900
O	1.96311100	2.59537700	2.35402900
O	-1.30836600	3.37497900	-0.85087800
H	-1.17889100	2.60064500	-1.41449000
C	-1.81087400	0.49518300	0.10898900
C	-3.19567200	0.39553500	0.43315500
H	-3.64679300	0.89834000	1.27786900
C	0.93730700	2.36705300	1.79852300
C	1.19761200	-0.11515200	1.20926800
C	-1.45969500	-0.25788300	-0.98724200
C	-0.87040700	1.33198900	0.84265400
C	-3.88006900	-0.44660500	-0.39195700
C	0.38903100	1.08726500	1.24298900
C	0.74380800	-1.38013900	1.50042500
C	2.57659700	-0.08625200	0.84412800
H	3.07756100	0.82499500	0.54969900
C	-0.12890200	-0.38411300	-1.65503800
H	0.41408300	-1.25567400	-1.27958800
H	0.48158200	0.49882000	-1.45606200
H	-0.24469500	-0.49752500	-2.73220300
C	-1.15862500	2.76330500	1.11808100
H	-2.14151300	3.20065500	1.19796400
C	3.15317100	-1.32029800	0.83529800
C	-0.61273000	-1.81459800	1.94658200
H	-1.23063000	-2.10681600	1.09333200
H	-1.11974300	-0.99721800	2.45912400
H	-0.54819500	-2.66479700	2.62413200
C	-5.30182000	-0.80267700	-0.34332700
C	-5.76900000	-1.99601900	-0.89358600
C	-6.21717700	0.06297000	0.26562100
C	-7.11487900	-2.32399700	-0.83849300
H	-5.07652400	-2.68665100	-1.35810600
C	-7.55747500	-0.26399100	0.33025800
H	-5.87805200	1.00513000	0.67466700
C	-8.00540100	-1.45849900	-0.22430100
H	-7.46304800	-3.25282000	-1.26820900
H	-8.25825400	0.41393900	0.80094300
C	4.53339500	-1.66848500	0.48438700
C	4.87613000	-2.95683100	0.07390400
C	5.53674800	-0.69509600	0.55348200
C	6.18357400	-3.27089200	-0.26337100
H	4.11467500	-3.72314900	0.00109000
C	6.83894500	-1.00155000	0.21033700
H	5.29610000	0.30326400	0.89307600
C	7.16178100	-2.29196400	-0.19699700
H	6.43409500	-4.27347600	-0.58089700
H	7.60766000	-0.24144100	0.27007200
N	-0.11219800	3.33536200	1.65925600
C	0.03395400	4.70639900	2.12006800
H	0.26193600	4.70841800	3.18352300
H	0.84251900	5.17581600	1.56289400
H	-0.89682000	5.23452900	1.93454300
S	2.03200800	4.01794400	-1.11320700
O	3.06542600	4.57673600	-0.26251200
O	1.71041500	2.62052100	-0.82689400
O	0.80816800	4.84799900	-1.12192900
H	-0.49751700	3.95393200	-0.99097100
C	2.64839400	4.06148600	-2.77049400
H	3.55141900	3.45701100	-2.81148300
H	1.88726000	3.65682400	-3.43315900
H	2.86947500	5.09485900	-3.02650500
C	-9.46518800	-1.78704500	-0.13275300
F	-9.86171000	-1.95015700	1.14064200
F	-10.23088300	-0.80743000	-0.63917100
F	-9.78353000	-2.90900100	-0.78497700
C	8.58006200	-2.59066100	-0.57820500
F	8.79289100	-3.89223000	-0.79544800
F	8.94285400	-1.94516400	-1.70005700
F	9.44669900	-2.20384200	0.37108000

***o*-TS-1d** (acetonitrile)

Imaginary frequency: 1

G = -2899.923436 hartree

S	3.15723900	-2.19697300	1.43584200
S	-1.72029400	-3.48785900	-1.54524000
O	-2.09100100	1.70687600	-1.63055900
O	1.32515500	2.22128300	1.51017100
H	1.45261500	1.36300300	1.93520400
C	1.93803400	-0.44432700	0.05986400
C	3.31250600	-0.36143600	-0.31542000
H	3.68373000	0.31512100	-1.07329900
C	-1.02295900	1.46839700	-1.17492300
C	-1.08134300	-1.08589200	-1.02274300
C	1.69859400	-1.39893300	1.02031000
C	0.90540200	0.42292100	-0.49010200
C	4.10233800	-1.26258900	0.33346000
C	-0.35915000	0.15969700	-0.87002000

C	-0.54720600	-2.24105100	-1.54557900
C	-2.44836200	-1.22797300	-0.63366400
H	-3.00477500	-0.42582900	-0.17117400
C	0.41252300	-1.75787400	1.69053200
H	-0.08057700	-2.58410700	1.17070900
H	-0.26930800	-0.90534700	1.68273000
H	0.58460500	-2.06333700	2.72195200
C	1.09598500	1.88584400	-0.54820800
H	2.04682500	2.39311000	-0.58337600
C	-2.93585300	-2.48274100	-0.83654400
C	0.81978900	-2.48786800	-2.09182000
H	1.49019300	-2.86784100	-1.31610400
H	1.24714900	-1.56059200	-2.47316600
H	0.79124700	-3.21678300	-2.90051500
C	5.54821100	-1.47227700	0.19097600
C	6.13529100	-2.70345000	0.48925100
C	6.36419600	-0.42884000	-0.25394900
C	7.50228700	-2.88743200	0.34373000
H	5.51756300	-3.52863300	0.82300900
C	7.72855800	-0.61785800	-0.40689600
H	5.92895100	0.53969900	-0.46439900
C	8.30380300	-1.84716900	-0.10776600
H	7.94043700	-3.84887200	0.57772900
H	8.34645200	0.20117300	-0.75141200
H	9.36987400	-1.99182800	-0.22310800
C	-4.27817500	-2.99492200	-0.53575800
C	-4.50911400	-4.35759000	-0.33657500
C	-5.35625900	-2.11089400	-0.43810700
C	-5.78271400	-4.82380500	-0.04576200
H	-3.68485800	-5.05850700	-0.39412000
C	-6.62604200	-2.57808800	-0.13862100
H	-5.19977200	-1.05411100	-0.61267700
C	-6.84573300	-3.93649900	0.05762600
H	-5.94227500	-5.88326600	0.10696300
H	-7.44947500	-1.87932700	-0.06757500
H	-7.83867800	-4.30025700	0.28677100
N	-0.01011500	2.48117800	-0.93176200
S	-2.06107300	2.28211700	2.23324900
O	-3.24295100	2.96003800	1.73025100
O	-1.67182300	1.11117300	1.44958600
O	-0.92062200	3.20240500	2.41155200
H	0.45876100	2.58398000	1.86102300
C	-2.45741700	1.69076500	3.85247300
H	-3.29449000	1.00199900	3.76660300
H	-1.58480000	1.18302700	4.25652400
H	-2.72626700	2.54249300	4.47260200
C	-0.18266600	3.86952900	-1.21677800
C	-1.30503300	4.52071200	-0.72538900
C	0.76913000	4.53306500	-1.97847000
C	-1.46530100	5.87083900	-1.00159600
H	-2.02765900	3.98369100	-0.12472900
C	0.60232700	5.88577200	-2.23405000
H	1.62068900	3.99760700	-2.37817200
C	-0.51417300	6.55418700	-1.74855500
H	-2.33457300	6.39096600	-0.62213500
H	1.34065300	6.41235300	-2.82342600
H	-0.64429200	7.60809700	-1.95529200

***o*-TS-1e** (acetonitrile)

Imaginary frequency: 1

G = -3574.115008 hartree

S	2.81722100	-1.90812300	1.49356300
S	-2.02195600	-2.74497300	-1.63932700
O	-1.96460200	2.46443700	-1.68609900
O	1.36596900	2.66257300	1.58224200
H	1.40505600	1.79533200	2.00621800
C	1.81099000	-0.03242600	0.10601200
C	3.19475300	-0.08085200	-0.23473800
H	3.64812900	0.56125700	-0.97768000
C	-0.93628300	2.13690300	-1.19655900
C	-1.20788300	-0.40580400	-1.07434000
C	1.45642500	-0.96745700	1.05091300
C	0.87618800	0.92969400	-0.46238900
C	3.87470600	-1.06096100	0.42478100
C	-0.39160300	0.77557600	-0.88641100
C	-0.75530900	-1.59584000	-1.59731400
C	-2.59037000	-0.44021400	-0.72241300
H	-3.09072300	0.40080100	-0.26488100
C	0.12563200	-1.20449200	1.68663400
H	-0.42581200	-1.98430400	1.15410000
H	-0.47484600	-0.29337400	1.65962100
H	0.24194200	-1.52164300	2.72221800
C	1.18639500	2.37316200	-0.49238900
H	2.17493500	2.80376800	-0.48491400
C	-3.17014000	-1.65088900	-0.95226600
C	0.60053100	-1.94467300	-2.11494300
H	1.21818800	-2.38820800	-1.32937800
H	1.10951900	-1.04949200	-2.47175800

H	0.53362700	-2.65788300	-2.93516700
C	5.29423400	-1.41089700	0.31052100
C	5.75171100	-2.69022500	0.62481400
C	6.21635200	-0.45204000	-0.12326200
C	7.09530300	-3.01173100	0.50853900
H	5.05302000	-3.45097700	0.94937000
C	7.55425800	-0.77086600	-0.24915500
H	5.88428600	0.55293500	-0.34643600
C	7.99251400	-2.05238000	0.06837100
H	7.43602000	-4.00800800	0.75328800
H	8.26046400	-0.02180400	-0.58459300
C	-4.55450900	-2.05377000	-0.68612300
C	-4.90700100	-3.39621600	-0.54815900
C	-5.55219400	-1.07987300	-0.56097200
C	-6.21860700	-3.76390700	-0.28988300
H	-4.15058800	-4.16677600	-0.62826000
C	-6.85814100	-1.44124300	-0.29508400
H	-5.30401800	-0.03475100	-0.68741100
C	-7.19081300	-2.78554900	-0.16076600
H	-6.47640100	-4.80841900	-0.18421400
H	-7.62202900	-0.67955300	-0.20125000
N	0.14658200	3.06101300	-0.90422600
S	-2.03258100	3.00171800	2.16352400
O	-3.13444900	3.77289800	1.61540600
O	-1.70886400	1.80207400	1.39294800
O	-0.82894800	3.82582800	2.38860900
H	0.51939400	3.09497700	1.90054800
C	-2.53977000	2.44529100	3.76398700
H	-3.42739500	1.82884900	3.64310800
H	-1.72887900	1.86651400	4.19985800
H	-2.76078900	3.31645200	4.37596000
C	0.09927500	4.46224000	-1.17609300
C	-0.99265400	5.19579700	-0.73469200
C	1.14096200	5.05591700	-1.87526100
C	-1.02991000	6.55730100	-0.99881000
H	-1.78629800	4.71241200	-0.18005500
C	1.09620900	6.42020000	-2.11893400
H	1.96827600	4.45841700	-2.23593400
C	0.01126900	7.17041100	-1.68391900
H	-1.87427000	7.14124200	-0.65786900
H	1.90509100	6.89234800	-2.65979700
H	-0.02359600	8.23345200	-1.88165300
C	9.45299800	-2.36236400	-0.06708200
F	9.73922000	-3.63584200	0.21875300
F	9.89960600	-2.12972000	-1.31189400
F	10.20285800	-1.60089400	0.74685300
C	-8.61773300	-3.14439600	0.12431000
F	-8.81187800	-4.46407700	0.20686600
F	-9.04582700	-2.61332300	1.28165800
F	-9.44852300	-2.68521500	-0.82601400

***c*-TS-1a** (acetonitrile)

Imaginary frequency: 1

G = -2899.906715 hartree

S	-3.36699500	1.63782600	0.03522200
S	-0.37325100	3.64511800	-0.21128300
O	3.05009000	-0.75473300	-1.22493800
O	-0.26485600	-2.91965200	0.89467400
H	0.27086000	-2.23559100	1.41483600
C	-1.62956500	-0.34573900	-0.34163400
C	-2.92239900	-0.92895400	-0.23519700
H	-3.09520100	-1.99180800	-0.32241300
C	1.88132200	-0.96873100	-1.05195200
C	0.71815900	1.27936900	-0.77159700
C	-1.61338200	1.11092500	0.11393500
C	-0.43867500	-0.87702100	-0.69732800
C	-3.91754200	-0.02386100	-0.05048100
C	0.75752600	-0.06972800	-0.80737900
C	-0.66401600	1.92623000	-0.78178300
C	1.77051600	2.23620000	-0.75250700
H	2.80699800	1.95683900	-0.86933400
C	-1.18131300	1.10031400	1.59381000
H	-1.22852400	2.10224100	2.01490300
H	-0.16410300	0.71526000	1.68532900
H	-1.84990500	0.44888500	2.15588700
C	-0.03459500	-2.26003500	-0.87440000
H	-0.66738600	-3.05218400	-1.24414200
C	1.35632800	3.49607300	-0.46368700
C	-1.12688500	1.98901300	-2.24956500
H	-2.06314500	2.53589900	-2.33679500
H	-1.26605300	0.98049100	-2.64157200
H	-0.36626800	2.49349000	-2.84395900
C	-5.35144000	-0.31264600	0.04814300
C	-6.23449700	0.61397100	0.60790800
C	-5.85787100	-1.52778200	-0.42590100
C	-7.58768500	0.32766700	0.70406500
H	-5.86052700	1.55673300	0.98689600
C	-7.20950300	-1.80922700	-0.33042600

H	-5.19516200	-2.24669500	-0.88859300
C	-8.07877400	-0.88365500	0.23678500
C	2.20556500	4.68186100	-0.32589500
C	1.74953600	5.81521300	0.35151800
C	3.49335000	4.69281800	-0.87224700
C	2.56438300	6.92787900	0.49068100
H	0.75792000	5.82420300	0.78732600
C	4.30360000	5.80636600	-0.73389000
H	3.85392800	3.83422700	-1.42283200
C	3.84302100	6.92636300	-0.05033400
H	5.29567200	5.80367900	-1.16556200
H	2.19991100	7.79609000	1.02336600
H	-8.25832300	1.05248000	1.14599000
H	-7.58808400	-2.75077200	-0.70561500
H	-9.13534100	-1.10556100	0.30921300
H	4.47816400	7.79593400	0.05578600
N	1.28837500	-2.27735200	-1.15028000
S	2.42405700	-2.26513500	2.61040900
O	3.77061500	-1.90309900	2.21178100
O	1.40458900	-1.34493100	2.04835900
O	2.06968100	-3.65452900	2.33451900
H	0.26177700	-3.72754400	1.02914200
C	2.33097300	-2.05048700	4.36298200
H	2.56189700	-1.01323900	4.59322800
H	1.32404500	-2.30054000	4.68791400
H	3.05815500	-2.71459400	4.82411800
C	2.02355900	-3.45619800	-1.47286300
C	3.20393600	-3.73158900	-0.79536300
C	1.54007500	-4.31242100	-2.45423800
C	3.90482000	-4.88678500	-1.11174300
H	3.55440600	-3.05815300	-0.02478900
C	2.24324000	-5.47007000	-2.75131600
H	0.63026100	-4.06962200	-2.98847800
C	3.42692900	-5.75676900	-2.08327300
H	4.82447400	-5.11050300	-0.58761200
H	1.86989800	-6.14127300	-3.51300100
H	3.97691300	-6.65766900	-2.32097000

***c*-TS-1b** (acetonitrile)

Imaginary frequency: 1

G = -2937.245965 hartree

S	1.37008800	-2.12511100	0.13728000
S	-2.19963000	-1.92799200	-0.11543700
O	-2.26105900	3.55386400	-1.68108000
O	4.05306000	2.80890700	0.00354300
H	3.40011800	2.50619600	0.66325000
C	1.22109000	0.40558900	-0.66058800
C	2.57028600	0.06530100	-0.64334700
H	3.34660000	0.74078900	-0.97157500
C	-1.20335100	2.98629600	-1.53993700
C	-1.65487600	0.53118900	-0.99025100
C	0.32506900	-0.63088300	-0.00963100
C	0.58190200	1.53005200	-1.14821100
C	2.80712700	-1.23469700	-0.24851900
C	-0.86608400	1.61023700	-1.20366800
C	-0.95084100	-0.81589300	-0.86087100
C	-3.06247200	0.43174200	-0.85816800
H	-3.71422700	1.27529000	-1.02864000
C	0.02377400	-0.12989200	1.41959800
H	-0.59067600	-0.85706100	1.94688200
H	-0.48743500	0.83252100	1.37480300
H	0.95909400	0.02113700	1.95416400
C	1.07035600	2.78919200	-1.48537500
H	2.09755100	3.12289800	-1.50414200
C	-3.49017500	-0.77621300	-0.39752000
C	-0.64366500	-1.33202700	-2.27720200
H	-0.22688400	-2.33663900	-2.23842900
H	0.06825700	-0.66869400	-2.77090300
H	-1.56189900	-1.35406100	-2.86245600
C	4.10974000	-1.86289300	-0.14963100
C	4.24379600	-3.24793000	-0.02902500
C	5.27696200	-1.07860200	-0.16607700
C	5.48582100	-3.84880500	0.06263600
H	3.36347800	-3.87922900	-0.02163100
C	6.51604400	-1.66185700	-0.06862400
H	5.20662800	-0.00060300	-0.23207500
C	6.63333000	-3.05371000	0.04362400
C	-4.86701100	-1.16556100	-0.11854100
C	-5.16184800	-2.31813100	0.60866400
C	-5.93822100	-0.38365400	-0.58032900
C	-6.46823800	-2.69064900	0.88329100
H	-4.36048000	-2.94145300	0.98648400
C	-7.23894600	-0.74234500	-0.31872900
H	-5.74838000	0.50589900	-1.16565000
C	-7.51704600	-1.89990200	0.41818700
H	-8.06601700	-0.14571900	-0.67948900
H	-6.65398900	-3.58757400	1.45477200
H	5.55090100	-4.92306400	0.14605400

H	7.41750400	-1.06429800	-0.07002900
N	0.06302000	3.62672000	-1.72896600
C	0.19138600	5.04098000	-2.02386600
H	0.94145300	5.46481200	-1.36010600
H	0.47261400	5.18619700	-3.06574200
H	-0.77436800	5.50469700	-1.84222600
S	1.20399100	3.69632500	1.69057400
O	-0.20177100	3.45842700	1.39071300
O	1.97495000	2.45706300	1.85079500
O	1.84615100	4.61844700	0.75069200
H	3.85649700	3.75328300	-0.03353600
C	1.24682500	4.49622600	3.27129500
H	0.78900000	3.83430400	4.00266800
H	2.28434700	4.69191200	3.53134000
H	0.68929900	5.42715700	3.19985900
O	7.88306600	-3.53285600	0.13038200
C	8.06024500	-4.93699600	0.25596500
H	9.13180900	-5.09887300	0.31552700
H	7.58083300	-5.30781100	1.16333100
H	7.65731600	-5.45731500	-0.61440800
O	-8.81911000	-2.17016600	0.62407800
C	-9.15152000	-3.33930800	1.35686500
H	-10.23576500	-3.36710400	1.40261500
H	-8.78213800	-4.23294200	0.85054500
H	-8.74243100	-3.29387300	2.36776100

***c*-TS-1c** (acetonitrile)

Imaginary frequency: 1

G = -3382.412450 hartree

S	1.96837200	-1.87691500	0.08267800
S	-1.64618200	-2.03185000	-0.06310400
O	-2.25313600	3.31774700	-1.87042300
O	1.77880800	3.73253500	0.06219500
H	1.37918700	3.12537500	0.71210400
C	1.51914900	0.64506800	-0.66212500
C	2.93123100	0.47730400	-0.55418500
H	3.63735800	1.25252600	-0.81568400
C	-1.14382600	2.89935600	-1.66729200
C	-1.33484000	0.43831100	-1.01560500
C	0.75097600	-0.50703100	-0.01625800
C	0.78067800	1.65704700	-1.16318100
C	3.30300900	-0.77288000	-0.18718400
C	-0.66305100	1.58540700	-1.23592000
C	-0.50233000	-0.82981500	-0.84874500
C	-2.73562400	0.18908900	-0.93616000
H	-3.47118500	0.94734200	-1.16070000
C	0.42055400	-0.05820200	1.42086300
H	-0.05577900	-0.86226600	1.97740300
H	-0.24097700	0.81018700	1.39889400
H	1.34389600	0.22151600	1.92793700
C	1.15589000	3.01325200	-1.56428700
H	2.08919300	3.28450100	-2.03508400
C	-3.03928900	-1.03930100	-0.45199500
C	-0.17175800	-1.34879200	-2.26039600
H	0.33064300	-2.31232200	-2.21081700
H	0.47302900	-0.63758700	-2.77869400
H	-1.09543100	-1.46065900	-2.82670700
C	4.67933700	-1.25457500	-0.02979600
C	4.97107100	-2.61621200	-0.09895000
C	5.71985500	-0.34564300	0.19365000
C	6.27499700	-3.06742200	0.03746100
H	4.18031100	-3.33415300	-0.27561600
C	7.01884500	-0.79143800	0.33220300
H	5.50815600	0.71116900	0.28039200
C	7.29286700	-2.15325400	0.25131800
C	-4.38697400	-1.56722300	-0.21417800
C	-4.59337800	-2.62962700	0.67041900
C	-5.48420600	-1.01039200	-0.87378800
C	-5.86737500	-3.11513300	0.89891700
H	-3.75634000	-3.07134700	1.19584100
C	-6.76142400	-1.49488700	-0.64859300
H	-5.34039100	-0.20637800	-1.58223300
C	-6.94814100	-2.54500500	0.23793100
H	-7.60439100	-1.06090600	-1.16747600
H	-6.02010400	-3.93495000	1.58908000
H	6.49197600	-4.12442600	-0.02351200
H	7.81886300	-0.08440700	0.51069600
N	0.03141800	3.66088900	-1.91884500
C	-0.03259800	5.01007300	-2.45249400
H	-0.24194100	5.71549700	-1.64935900
H	0.91971900	5.24878400	-2.91919300
H	-0.82693400	5.05074300	-3.19341600
S	-0.87943300	4.75896900	1.56037300
O	-2.25061400	5.13725700	1.29098600
O	-0.61183000	3.32577300	1.41996600
O	0.09272000	5.54793900	0.76791000
H	1.23504400	4.56691700	0.24592400
C	-0.55164300	5.16674600	3.24943200

H	-1.23664500	4.59800000	3.87372800
H	0.47916400	4.90382300	3.47458000
H	-0.71240100	6.23400800	3.38100500
C	-8.31963700	-3.09292500	0.50753100
F	-9.26352800	-2.50453100	-0.23153500
F	-8.38645000	-4.40928400	0.25658300
F	-8.67237900	-2.93591400	1.79297800
C	8.71604200	-2.60426200	0.40961600
F	8.85050300	-3.92905600	0.31038500
F	9.51543600	-2.05663700	-0.51872000
F	9.22018800	-2.24527800	1.60023500

***c*-TS-1d** (acetonitrile)

Imaginary frequency: 1

G = -2899.906715 hartree

S	-3.36699500	1.63782600	0.03522200
S	-0.37325100	3.64511800	-0.21128300
O	3.05009000	-0.75473300	-1.22493800
O	-0.26485600	-2.91965200	0.89467400
H	0.27086000	-2.23559100	1.41483600
C	-1.62956500	-0.34573900	-0.34163400
C	-2.92239900	-0.92895400	-0.23519700
H	-3.09520100	-1.99180800	-0.32241300
C	1.88132200	-0.96873100	-1.05195200
C	0.71815900	1.27936900	-0.77159700
C	-1.61338200	1.11092500	0.11393500
C	-0.43867500	-0.87702100	-0.69732800
C	-3.91754200	-0.02386100	-0.05048100
C	0.75752600	-0.06972800	-0.80737900
C	-0.66401600	1.92623000	-0.78178300
C	1.77051600	2.23620000	-0.75250700
H	2.80699800	1.95683900	-0.86933400
C	-1.18131300	1.10031400	1.59381000
H	-1.22852400	2.10224100	2.01490300
H	-0.16410300	0.71526000	1.68532900
H	-1.84990500	0.44888500	2.15588700
C	-0.03459500	-2.26003500	-0.87440000
H	-0.66738600	-3.05218400	-1.24414200
C	1.35632800	3.49607300	-0.46368700
C	-1.12688500	1.98901300	-2.24956500
H	-2.06314500	2.53589900	-2.33679500
H	-1.26605300	0.98049100	-2.64157200
H	-0.36626800	2.49349000	-2.84395900
C	-5.35144000	-0.31264600	0.04814300
C	-6.23449700	0.61397100	0.60790800
C	-5.85787100	-1.52778200	-0.42590100
C	-7.58768500	0.32766700	0.70406500
H	-5.86052700	1.55673300	0.98689600
C	-7.20950300	-1.80922700	-0.33042600
H	-5.19516200	-2.24669500	-0.88859300
C	-8.07877400	-0.88365500	0.23678500
C	2.20556500	4.68186100	-0.32589500
C	1.74953600	5.81521300	0.35151800
C	3.49335000	4.69281800	-0.87224700
C	2.56438300	6.92787900	0.49068100
H	0.75792000	5.82420300	0.78732600
C	4.30360000	5.80636600	-0.73389000
H	3.85392800	3.83422700	-1.42283200
C	3.84302100	6.92636300	-0.05033400
H	5.29567200	5.80367900	-1.16556200
H	2.19991100	7.79609000	1.02336600
H	-8.25832300	1.05248000	1.14599000
H	-7.58808400	-2.75077200	-0.70561500
H	-9.13534100	-1.10556100	0.30921300
H	4.47816400	7.79593400	0.05578600
N	1.28837500	-2.27735200	-1.15028000
S	2.42405700	-2.26513500	2.61040900
O	3.77061500	-1.90309900	2.21178100
O	1.40458900	-1.34493100	2.04835900
O	2.06968100	-3.65452900	2.33451900
H	0.26177700	-3.72754400	1.02914200
C	2.33097300	-2.05048700	4.36298200
H	2.56189700	-1.01323900	4.59322800
H	1.32404500	-2.30054000	4.68791400
H	3.05815500	-2.71459400	4.82411800
C	2.02355900	-3.45619800	-1.47286300
C	3.20393600	-3.73158900	-0.79536300
C	1.54007500	-4.31242100	-2.45423800
C	3.90482000	-4.88678500	-1.11174300
H	3.55440600	-3.05815300	-0.02478900
C	2.24324000	-5.47007000	-2.75131600
H	0.63026100	-4.06962200	-2.98847800
C	3.42692900	-5.75676900	-2.08327300
H	4.82447400	-5.11050300	-0.58761200
H	1.86989800	-6.14127300	-3.51300100
H	3.97691300	-6.65766900	-2.32097000

***c*-TS-1e** (acetonitrile)

Imaginary frequency: 1

G = -3574.094464 hartree

S	1.99366500	-2.43216000	-0.07550500
S	-1.61219100	-2.58870700	-0.27885400
O	-2.26484600	2.96140800	-1.20134000
O	1.70915000	3.04375700	0.90535000
H	0.89741000	2.72206600	1.41412100
C	1.53228600	0.17271600	-0.40436900
C	2.94248700	-0.00081800	-0.31302700
H	3.64262000	0.81846700	-0.38904900
C	-1.15394200	2.53725000	-1.04467300
C	-1.31899300	0.00686500	-0.81015700
C	0.76841000	-1.07292100	0.03823900
C	0.78733100	1.25055000	-0.73399700
C	3.32118000	-1.29329600	-0.15264100
C	-0.65465700	1.18043000	-0.83236400
C	-0.47559900	-1.26424600	-0.84686200
C	-2.71700900	-0.26312400	-0.78151500
H	-3.45857900	0.51545000	-0.88216900
C	0.42244700	-0.86339600	1.52622200
H	-0.05161500	-1.75117700	1.93881600
H	-0.24585600	-0.00781600	1.63941000
H	1.33865400	-0.66220500	2.08064800
C	1.15388400	2.64810300	-0.88566600
H	2.10344400	3.01271500	-1.24591700
C	-3.01145200	-1.55704800	-0.50471500
C	-0.13035700	-1.53998800	-2.32238100
H	0.38335500	-2.49292700	-2.42826000
H	0.50852500	-0.74592100	-2.71160600
H	-1.04911800	-1.56724400	-2.90669300
C	4.70089300	-1.78600100	-0.06619700
C	4.98589600	-3.01722100	0.52321700
C	5.75230500	-1.01832500	-0.58078300
C	6.29300500	-3.47124400	0.61432700
H	4.18671300	-3.62100800	0.93256300
C	7.05416000	-1.46823800	-0.49319700
H	5.54892000	-0.07479900	-1.06784800
C	7.32122200	-2.69430000	0.10812400
C	-4.35490400	-2.12636400	-0.35731500
C	-4.55298900	-3.31869100	0.33821600
C	-5.45933400	-1.47193000	-0.91445000
C	-5.82626500	-3.84573200	0.48916400
H	-3.71251700	-3.83624800	0.78273000
C	-6.72852400	-1.99465200	-0.76764800
H	-5.32201800	-0.56032100	-1.47927200
C	-6.90845500	-3.18051700	-0.06255400
H	-7.57852600	-1.48511700	-1.20284900
H	-5.97012900	-4.76634000	1.03687900
H	6.50408300	-4.42327400	1.08042800
H	7.86234000	-0.87097400	-0.89541800
N	0.03062900	3.35243000	-1.13389200
S	-0.94985100	3.81974000	2.62897900
O	-2.28369800	4.22625600	2.22983200
O	-0.55203400	2.52493300	2.02321300
O	0.07835700	4.83118600	2.40105800
H	1.67985400	4.00288300	1.06920800
C	-1.00124600	3.52429900	4.37149100
H	-1.73923800	2.74975900	4.56552100
H	-0.01438700	3.20373700	4.69607400
H	-1.28363100	4.45202900	4.86351600
C	0.00512500	4.74949300	-1.42374100
C	-0.85296300	5.57646800	-0.71134100
C	0.84331200	5.25590900	-2.40879400
C	-0.86296000	6.93470800	-0.99569700
H	-1.48758600	5.16221800	0.06081600
C	0.83200300	6.61696700	-2.67404000
H	1.48772900	4.59145900	-2.97031700
C	-0.02222800	7.45643700	-1.97047300
H	-1.52629800	7.58791900	-0.44454300
H	1.48393300	7.01760800	-3.43855300
H	-0.03323600	8.51715800	-2.18334000
C	-8.29790000	-3.73553700	0.06124300
F	-8.76614500	-4.16666700	-1.12118200
F	-8.36580600	-4.76750000	0.90636100
F	-9.16564600	-2.81048700	0.49581600
C	8.74668000	-3.16101900	0.17476000
F	9.54286700	-2.24363100	0.74324300
F	8.88619000	-4.29036100	0.87352400
F	9.24990300	-3.39145400	-1.04830900

MA (acetonitrile)

Imaginary frequency: 0

G = -664.349692 hartree

S	0.85852900	1.87996400	1.33946400
O	2.25297700	1.58494600	1.26064000
O	0.43228700	3.21982900	1.60845700
O	0.26056000	1.43714600	-0.05526900
H	-0.57576900	1.89527000	-0.23577400

C	0.09069000	0.77955000	2.47209100
H	0.49368600	1.01220200	3.45549400
H	-0.98260000	0.94869700	2.44758300
H	0.34007500	-0.23749000	2.18222300

Water (acetonitrile)

Imaginary frequency: 0

G = -76.429766 hartree

O	0.27175100	1.24806000	0.00764300
H	0.43823700	1.86100300	-0.71466100
H	1.14493300	0.98708100	0.31518500

MA-anion (acetonitrile)

Imaginary frequency: 0

G = -663.927111 hartree

S	0.70153200	1.88014400	1.28221500
O	2.13322500	1.61145300	1.17249000
O	0.41077300	3.22453400	1.77340900
O	-0.03504300	1.54728400	0.06544400
C	0.09618000	0.77011000	2.53076400
H	0.61422200	0.98053200	3.46372100
H	-0.97313100	0.93067400	2.64869000
H	0.29182100	-0.25133400	2.21243600

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