Supplementary Information

Electrochemical and photocatalytic generation of *cis*-olefin-bridged carbodication for umpolung [4+1] cycloaddition with primary amines or H_2O

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1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on JEOL JNM AL 400 (400 MHz) and JEOL JNM AL 600 (600 MHz) spectrometers. ^{1}H NMR spectra are reported as follows: chemical shift in ppm (δ) relative to the chemical shift of $CDCl_3$ at 7.26 ppm, CD_2Cl_2 at 5.32 ppm, multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, bs = broad singlet), and coupling constants (Hz). ^{13}C NMR spectra were recorded on JEOL JNM AL 400 (101 MHz) spectrometer with complete proton decoupling, and chemical shift reported in ppm (δ) relative to the central line for $CDCl_3$ at 77 ppm, and CD_2Cl_2 at 53.8 ppm. High-resolution mass spectra were obtained on a Bruker Daltonics SolariX spectrometer using dithranol (DIT) as an exact matrix and FT-ICR-MS analyzer and a JEOL JMST100GCV Time-of-Flight Mass Spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University. UV/Vis absorption spectra were recorded on a JASCO V-770 iRMAOR spectrometer at 25 °C in analytical-grade solvents (con. 1 x 10^{-5} M). Redox potential values are measured by cyclic voltammograms (CV) with a IviumStat.h. potentiostat connected to a traditional three-electrode cell. The values are versus $Ag/AgNO_3$ reference electrode; Pt wire as a counter electrode and glassy carbon as a working electrode; 0.1 M $TBAPF_6$ as a supporting electrolyte in dichloromethane (DCM) or DCM/HFIP (5:1 v/v); scan rate is 50 mV s^{-1}, and the energy level of Fc/Fc+ as -4.80 eV. Column chromatography was carried out employing silica gel 60 N (spherical, neutral, 40~50 μm, KANTO Chemical Co.) and Silica gel 60 (Merck). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm precoated plate Kieselgel 60 F254 (Merck). Photoredox catalyzed reaction were conducted using the Kessil PR160 L 440 nm LED lamp and PR160 w/ Fan Kit. Electrochemical reactions were carried out on the IKA ElectraSyn 2.0 and electrodes were purchased from IKA com.

Computational studies were performed using the Gaussian 16 program package[1] with density functional theory (DFT). Unless otherwise noted, the M06-2X functional and the def2-SVP basis set were employed for all atoms. Solvent effects were taken into account using the SMD solvation model with hexafluoroisopropanol (HFIP) as the solvent. Intrinsic reaction coordinate (IRC) calculations were carried out for all optimized transition states to confirm their connectivity to the corresponding reactants and products.

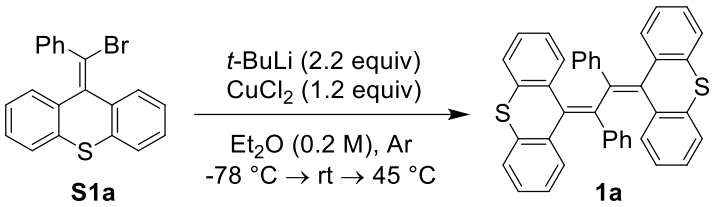
1. Gaussian 16, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R.

Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

Materials

Unless otherwise noted, materials were purchased from Wako, TCI, Kanto, Aldrich, and other commercial suppliers and were used without purification. Dehydrated THF and Et_2O were purchased from Kanto and dichloroethane was purchased from Aldrich. Other solvents were purchased from commercial suppliers as dehydrated solvents, and used under argon or nitrogen atmosphere. All air- and moisture-sensitive manipulations were performed under argon atmosphere using oven-dried glassware, including standard Schlenk and glovebox techniques. The representative structures of **2a** (CCDC 2453063) and **3a** (CCDC 2453062) were confirmed by means of X-ray crystallography. The structures of starting substrates and products were determined by ^1H, ^{13}C NMR, high resolution mass spectrometry (HRMS).
DFT calculations were performed at the SMD(HFIP)/M06-2X/def2-SVP level.

2. General procedure for synthesis of substrates 1



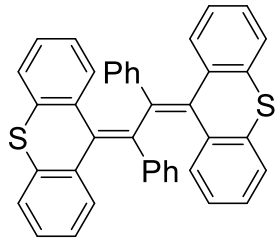
Compound **S1a** was prepared via bromination of 9-benzylidene-9*H*-thioxanthene, which was synthesized from 9*H*-thioxanthen-9-one following the reported methods.[1-3] A suspension of **S1a** (1.8 g, 5 mmol) in Et_2O (0.2 M) was cooled to -78 °C. *t*-BuLi (1.6 M in pentane, 7 mL, 2.2 equiv) was added dropwise to the reaction mixture at -78 °C and stirred for 2 h. Anhydrous $CuCl_2$ (806.7 mg, 6 mmol) was added to the resulting solution and the reaction was stirred at 45 °C for 2 h while the temperature was gradually increased (over 1 h). The reaction was filtered with short pad of celite and washed with dichloromethane (DCM). The filtrate was washed with sat. NH_4Cl (20 mL) and brine (20 mL), dried over $MgSO_4$. After filtration and concentration in vacuo, the residue was purified by flash column chromatography using hexane/DCM (50/1 → 10/1 → 5/1) as an eluent to give 1,2-dialkyl-1,2-di(9*H*-thioxanthen-9-ylidene)ethane **1a** in 67% yield (955 mg, 3.35 mmol) as white solid.

References

1. Hertz, V. M., Bolte, M., Lerner, H.-W. & Wagner, M. *Angew. Chem. Int. Ed.* **54**, 8800−8804 (2015).
2. Bhanuchandra, M., Yorimitsu, H. & Osuka, A. *Org. Lett.* **18**, 384−387 (2016).
3. Zhang, S. Matsuyama, H., Nakamura, I., Terada, M. & Jin, T. *Org. Lett.* **25**, 5027−503 (2023).

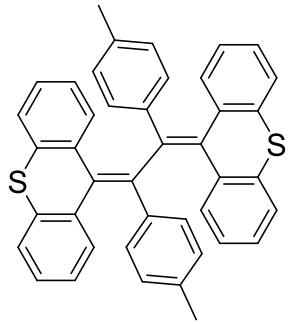
3. Analytical data of substrates 1

1,2-diphenyl-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1a)



Yield: 67% (3.35 mmol, 955 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.64 (brs, 2H), 7.78 (brs, 2H), 7.49 (d, *J* = 7.8 Hz, 2H), 7.37 (brs, 4H), 7.11 (t, *J* = 7.3 Hz, 2H), 6.97 (d, *J* = 7.8 Hz, 2H), 6.88 (d, *J* = 6.9 Hz, 2H), 6.84 (d, *J* = 6.9 Hz, 2H), 6.79-6.76 (m, 4H), 6.51 (d, *J* = 6.8 Hz, 4H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 141.7, 138.8, 137.8, 136.8, 136.4, 135.2, 134.7, 130.7, 130.4, 128.1, 127.5, 127.4, 127.2, 126.9, 126.8, 126.5, 126.2 (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] Calcd. for $C_{40}H_{26}S_2$, 570.1476; found 570.1475. m.p. 269 °C~270 °C.

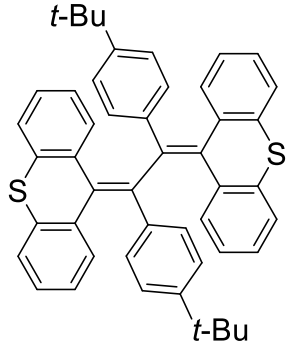
1,2-di(9*H*-thioxanthen-9-ylidene)-1,2-di-*p*-tolylethane (1b)



Yield: 55% (2.74 mmol, 822.5 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.62 (brs, 2H), 7.71 (brs, 2H), 7.50 (d, *J* = 7.3 Hz, 2H), 7.34 (brs, 4H), 7.12 (t, *J* = 7.3 Hz, 2H), 6.99 (d, *J* = 7.3 Hz, 2H), 6.92-6.88 (m, 2H), 6.59 (d, *J* = 7.8 Hz, 4H), 6.45 (d, *J* = 7.8 Hz, 4H), 2.04 (s, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 141.6, 138.3, 137.1, 136.6, 135.8, 135.6, 135.3, 134.8, 130.6, 130.4, 128.3, 128.1, 127.4, 127.1, 126.8, 126.7, 126.3, 21.1 (one sp^2 peak was not

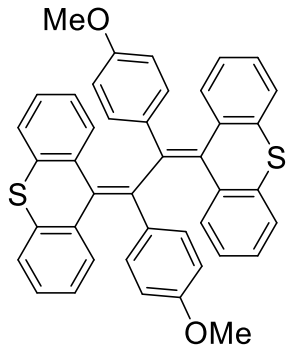
shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{42}H_{30}S_2$, 598.1789; found 598.1788. m.p. 177 °C~179 °C.

1,2-bis(4-(*tert*-butyl)phenyl)-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1c)



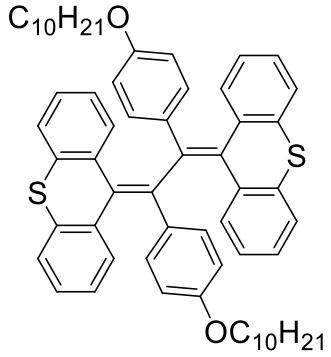
Yield: 65% (3.25 mmol, 1.1 g), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.61 (brs, 2H), 7.72 (brs, 2H), 7.49 (d, *J* = 6.9 Hz, 2H), 7.34 (brs, 4H), 7.13-7.09 (m, 2H), 6.96 (d, *J* = 7.3 Hz, 2H), 6.87-6.85 (m ,2H), 6.77 (d, *J* = 7.3 Hz, 4H), 1.07 (s, 18H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 149.6, 141.4, 138.3, 137.2, 135.7, 135.3(6), 135.3(0), 134.8, 130.7, 130.1, 128.1, 127.4, 127.0, 126.7, 126.6, 126.1, 124.2, 34.3, 31.1 (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{48}H_{42}S_2$, 682.2728; found 682.2727. m.p. 192 °C~193 °C.

1,2-bis(4-methoxyphenyl)-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1d)



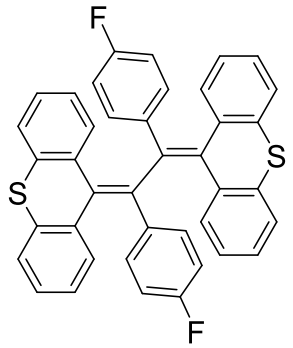
Yield: 43% (2.15 mmol, 677.4 mg), pale yellow solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.60 (brs, 2H), 7.71 (brs, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 7.34 (brs, 4H), 7.12 (t, *J* = 7.3 Hz, 2H), 7.00 (d, *J* = 7.3 Hz, 2H), 6.93-6.92 (m, 2H), 6.50 (d, *J* = 8.2 Hz, 4H), 6.33 (d,*J* = 8.2 Hz, 4H), 3.57 (s, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.4, 141.3, 138.3, 137.0, 135.3, 135.2, 134.8, 131.7, 130.7, 130.6, 128.0, 127.4, 127.0, 126.7(9), 126.7(4), 126.4, 112.9, 54.9 (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{42}H_{30}O_2S_2$, 630.1687; found 630.1686. m.p. 229 °C~231 °C.

1,2-bis(4-(decyloxy)phenyl)-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1e)



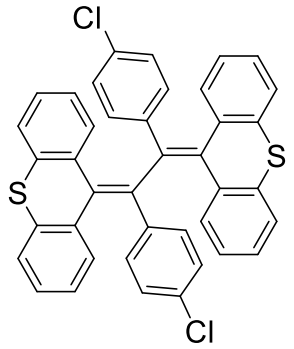
Yield: 49% (2.45 mmol, 1.08 g), pale yellow solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.60 (brs, 2H), 7.70 (brs, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 7.33 (brs, 4H), 7.12 (t, *J* = 7.3 Hz, 2H), 7.01 (d, *J* = 7.3 Hz, 2H), 6.93-6.89 (m, 2H), 6.48 (d, *J* = 8.2 Hz, 4H), 6.31 (d,*J* = 8.2 Hz, 4H), 3.69 (t, *J* = 6.4 Hz, 4H), 1.62-1.57 (m, 4H), 1.28-1.23 (m, 32H), 0.87 (t, *J* = 6.4 Hz, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.0, 141.4, 138.4, 137.1, 135.2, 135.1, 134.8, 131.7, 130.6, 130.4, 128.0, 127.3, 127.0, 126.7, 126.3, 113.4, 67.6, 31.9, 29.6, 29.4, 29.3, 26.0, 22.7, 14.2 (two sp^2 peaks and two sp^3 peaks were not show due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{60}H_{66}O_2S_2$, 882.4504; found 882.4503. m.p. 91 °C~93 °C.

1,2-bis(4-fluorophenyl)-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1f)



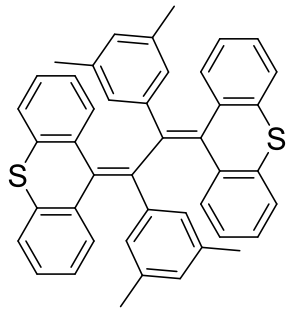
Yield: 61% (3.05 mmol, 924.4 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.58 (brs, 2H), 7.75-7.73 (m, 2H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.38 (brs, 4H), 7.17-7.13 (m, 2H), 6.94-6.90 (m, 4H), 6.77 (d, *J* = 7.8 Hz, 4H), 6.41 (d, *J* = 8.2 Hz, 4H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 161.71 (d, J_F = 247.3 Hz), 140.4, 137.4, 136.7, 136.4, 135.1, 134.7, 132.0 (d, J_F = 7.7 Hz), 130.5, 127.9, 127.5, 127.4, 127.1, 126.9, 126.7, 126.4, 114.6 (d, J_F = 21.1 Hz) (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{24}F_2S_2$, 606.1286; found 626.1287. m.p. 207 °C~209 °C.

1,2-bis(4-chlorophenyl)-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1g)



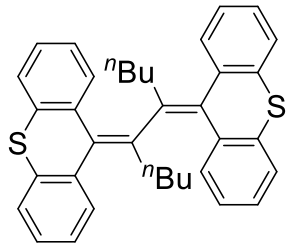
Yield: 58% (2.9 mmol, 925.2 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.61 (brs, 2H), 7.74 (brs, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 7.39-7.38 (m, 4H), 7.13 (t, *J* = 6.9 Hz, 2H), 6.95-6.89 (m, 4H), 6.54-6.45 (m, 8H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 139.9, 137.2, 137.2, 137.1, 136.3, 135.1, 134.6, 132.9, 131.6, 130.5, 127.9, 127.5, 127.2, 126.9, 126.7, 126.5 (two sp^2 peaks were not show due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{24}Cl_2S_2$, 638.0697; found 638.0696. m.p. 284 °C~286 °C.

1,2-bis(3,5-dimethylphenyl)-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1h)



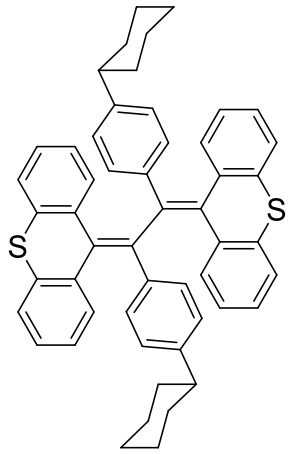
Yield: 36% (1.8 mmol, 563.5 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.61 (brs, 2H), 7.72 (brs, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 7.35-7.33 (m, 4H), 7.12 (t, *J* = 7.3 Hz, 2H), 6.97 (d, *J* = 7.3 Hz, 2H), 6.92-6.88 (m, 2H), 6.48 (s, 2H), 6.16 (s, 4H), 1.87 (s, 12H). ^{13}C NMR ($CDCl_3$,101 MHz) δ 141.4, 138.3, 137.7, 137.4, 136.3, 135.8, 135.5, 134.7, 130.3, 128.5, 128.4, 128.2, 127.1, 127.0, 126.7, 126.5, 126.1, 21.1 (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{44}H_{34}S_2$, 626.2102; found 626.2102. m.p. 250 °C~252 °C.

9,9'-(decane-5,6-diylidene)bis(9*H*-thioxanthene) (1i)



Yield: 29% (1.45 mmol, 384.4 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.22 (d, *J* = 7.8 Hz, 2H), 7.54 (d, *J* = 7.3 Hz, 2H), 7.50 (d, *J* = 6.9 Hz, 2H), 7.39-7.34 (m, 4H), 7.30-7.18 (m, 6H), 2.39-2.31 (m, 2H), 1.61-1.56 (m,2H), 1.11-0.74 (m, 8H), 0.56 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 141.3, 138.6, 137.4, 135.0, 134.9, 133.0, 128.7, 127.8, 127.1, 127.0, 126.7, 126.5, 126.1, 125.9, 33.5, 29.4, 23.0, 13.6. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{36}H_{34}S_2$, 530.2102; found 530.2101. m.p. 273 °C~275 °C.

1,2-dicyclohexyl-1,2-di(9*H*-thioxanthen-9-ylidene)ethane (1j)



Yield: 31% (1.55 mmol, 451.2 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.32 (d, *J* = 7.8 Hz, 2H), 7.57-7.53 (m, 6H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.29-7.19 (m, 6H), 2.74-2.67 (m, 2H), 1.44-1.36 (m, 6H),1.12-1.06 (m, 4H), 0.94-0.74 (m,10H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 143.9, 139.4, 138.5, 136.2, 135.7, 134.3, 128.6, 128.0, 127.6, 127.3, 126.6, 126.3, 126.1, 126.0, 41.6, 33.4, 28.5, 27.6, 26.9, 26.1 (four sp^2 peaks were not show due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{38}S_2$, 582.2415; found 582.2414. m.p. 130 °C~132 °C.

4. Electrochemical [4+1] cycloaddition of 1 with primary amines

4.1 Reaction setup for electrochemical synthesis

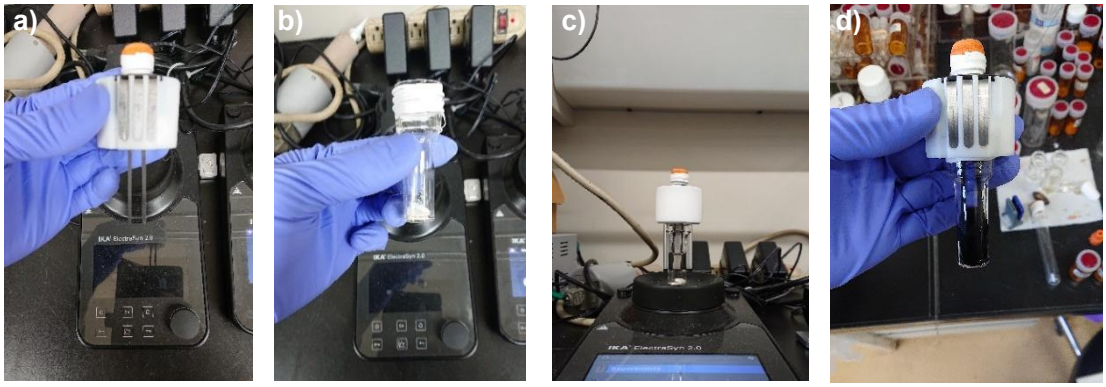
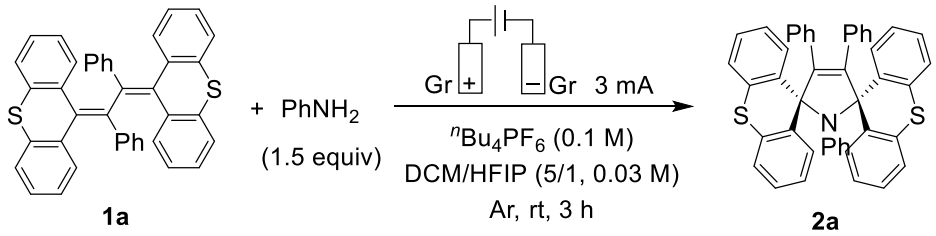


Fig. S1. Reaction setup for electrochemical synthesis with ElectraSyn 2.0. a) ElectraSyn 2.0 cap equipped with anode (Graphite) and cathode (Graphite). b) 5 mL ElectraSyn 2.0 vial with a stirring bar, substrates, and $^{n}Bu_4NPF_6$. c) 5 mL ElectraSyn 2.0 vial after all reagents are added. d) 5 mL Electrasyn 2.0 vial after electrochemical [4+1] cycloaddition was finished.

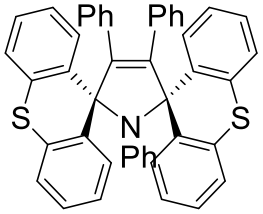
4.2 Representative procedure for the electrochemical [4+1] cycloaddition of 1a with aniline



To an undivided ElectraSyn cell (5 mL) vial equipped with a stirring bar was added **1a** (57 mg, 0.1 mmol, 1.0 equiv) and $^{n}Bu_4NPF_6$ (116.2 mg, 0.3 mmol, 0.1 M). The cell was equipped with (+) graphite/ (–) graphite electrodes and sealed with a cap. The cell was charged with argon via a balloon. A mixture of DCM/HFIP (v/v = 5:1, 3.0 mL) and aniline (14 mg, 0.15 mmol, 1.5 equiv) were added to the cell via syringe. The reaction mixture was subjected to the programmed electrolysis at room temperature for 3 h at a constant current of 3 mA and a stirring speed of 400 rpm. Upon completion, the electrodes were washed with DCM, which was combined with the reaction mixture. After concentration in vacuo, the residue was purified by flash column chromatography using hexane/DCM (5/1) as an eluent to give desired product **2a** in 98% yield (64.8 mg, 0.098 mmol) as white solid.

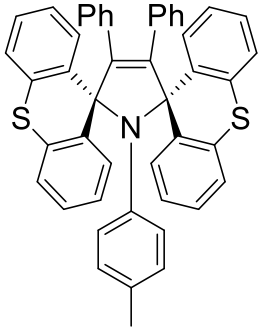
5. Analytical data of products 2

1',3',4'-triphenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2a)



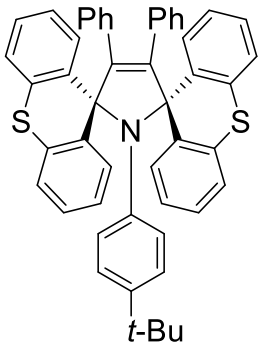
Yield: 98% (0.098 mmol, 64.8 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.75 (d, *J* = 7.8 Hz, 4H), 7.25-7.20 (m, 8H), 7.17-7.12 (m, 4H), 7.00-6.96 (m, 2H), 6.86-6.80 (m, 6H), 6.56-6.47 (m, 7H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.8, 140.7, 133.7, 133.4, 132.6, 131.5, 130.9, 127.7(9), 127.7(1), 127.2, 127.0, 125.7, 125.1, 117.8, 116.8, 78.5. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{46}H_{31}NS_2$, 661.1898; found 661.1897. m.p. 328 °C~330 °C.

3',4'-diphenyl-1'-(*p*-tolyl)-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2b)



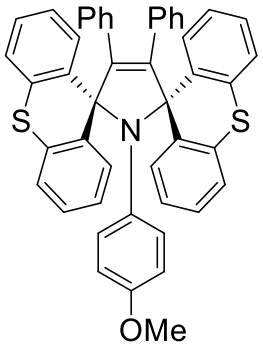
Yield: 89% (0.089 mmol, 60.1 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.75 (d, *J* = 7.8 Hz, 4H), 7.21-7.19 (m, 9H), 7.16-7.12 (m, 4H), 6.98 (t, *J* = 7.6 Hz, 2H), 6.83 (t, *J* = 7.6 Hz, 4H), 6.64 (d, *J* = 8.7 Hz, 2H), 6.56-6.54 (m, 4H), 6.39 (d, *J* = 8.7 Hz, 2H), 2.02 (s, 3H). ^{13}C NMR δ 140.8, 140.4, 136.7, 133.4, 132.6, 131.7, 130.8, 130.7, 127.9, 127.6(5), 125.6(4), 125.1, 118.1, 116.9, 78.4, 21.2 (one sp^2 peak was not show due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{47}H_{33}NS_2$, 675.2054; found 675.2054. m.p. 326 °C~328 °C.

1'-(4-(*tert*-butyl)phenyl)-3',4'-diphenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2c)



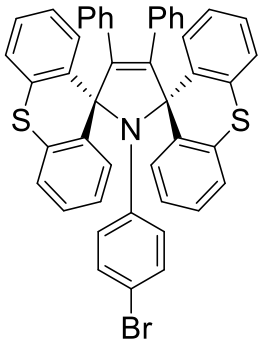
Yield: 91% (0.091 mmol, 65.2 mg, colorless solid); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 (d, J = 7.8 Hz, 4H), 7.25-7.20 (m, 8H), 7.17-7.12 (m, 5H), 6.97 (t, *J* = 7.6 Hz, 2H), 6.81 (q, *J* = 8.2 Hz, 6H), 6.52 (d, *J* = 7.3 Hz, 4H), 6.44-6.40 (m, 2H), 1.07 (s, 9H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.8, 138.8, 138.1, 133.8, 133.4, 132.8, 131.8, 130.9, 127.7, 127.1, 127.0, 125.6, 125.1, 124.5, 116.9, 78.4, 33.5, 31.4. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{50}H_{39}NS_2$, 717.2524; found 717.2523. m.p. 325 °C~327 °C.

1'-(4-methoxyphenyl)-3',4'-diphenyl-1'H-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2d)



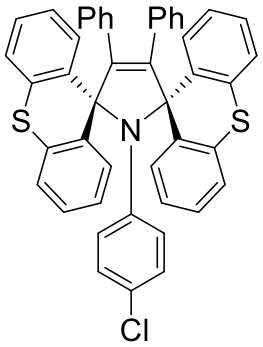
Compound **2d** was synthesized under the standard conditions using $^{n}Bu_4NI$ (3.7 mg, 0.01 mmol) additive. Yield: 91% (0.091 mmol, 63 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.81 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.20-7.12 (m, 12H), 7.02 (t, *J* = 7.3 Hz, 2H), 6.90 (t, *J* = 7.8 Hz, 4H), 6.78-6.76 (m, 4H), 6.36-6.31 (m, 2H), 6.07-6.02 (m, 2H), 3.57 (s, 3H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 153.0, 141.4, 134.2, 134.1, 133.4, 132.4, 132.2, 131.0, 127.4, 127.3(7), 127.3(4), 125.5, 125.1, 122.5, 113.0, 78.2, 55.2. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{47}H_{33}NOS_2$, 691.2003; found 691.2003. m.p. 336 °C~338 °C.

1'-(4-bromophenyl)-3',4'-diphenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2e)



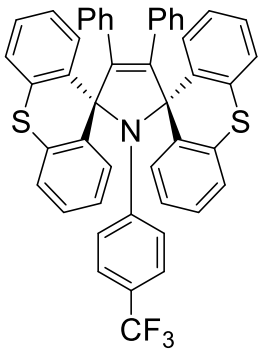
Yield: 97% (0.097 mmol, 71.8 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.71 (d, *J* = 7.8 Hz, 4H), 7.26-7.21 (m, 8H), 7.18-7.14 (m, 4H), 6.99 (t, *J* = 7.3 Hz, 2H), 6.92-6.88 (m, 2H), 6.84 (t, *J* = 7.8 Hz, 4H), 6.55-6.53 (m, 4H), 6.41-6.36 (m, 2H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.6, 139.9, 133.5, 133.4, 132.5, 131.0, 130.9, 130.5, 128.0, 127.3, 127.1, 125.8, 125.2, 119.3, 109.6, 78.6. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{46}H_{30}BrNS_2$, 739.1003; found 739.1002. m.p. 330 °C~332 °C.

1'-(4-chlorophenyl)-3',4'-diphenyl-1'H-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2f)



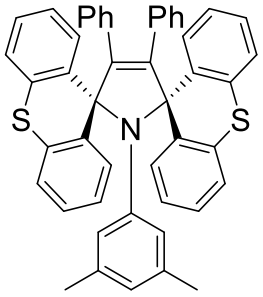
Yield: 75% (52.1 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.71 (d, *J* = 7.8 Hz, 4H), 7.24-7.20 (m, 8H), 7.18-7.14 (m, 4H), 6.99 (t, *J* = 7.6 Hz, 2H), 6.84 (t, *J* = 7.8 Hz, 4H), 6.79-6.74 (m, 2H), 6.56-6.54 (m, 4H), 6.40 (m, 2H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.7, 139.4, 133.5, 133.4, 132.5, 131.1, 130.9, 127.9, 127.6, 127.3, 127.1, 125.8, 125.2, 122.3, 118.9, 78.6. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{46}H_{30}ClNS_2$, 695.1508; found 695.1507. m.p. 345 °C~347 °C.

3',4'-diphenyl-1'-(4-(trifluoromethyl)phenyl)-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2g)



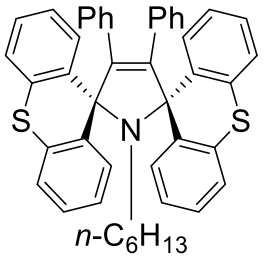
Yield: 77% (0.077 mmol, 56.2 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.69 (d, *J* = 7.8 Hz, 4H), 7.28-7.23 (m, 8H), 7.19-7.15 (m, 4H), 7.06 (d, *J* = 8.7 Hz, 2H), 6.99 (t, *J* = 7.6 Hz, 2H), 6.84 (t, *J* = 7.8 Hz, 4H), 6.59 (d, *J* = 8.7 Hz, 2H), 6.52 (d, *J* = 7.3 Hz, 4H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 143.7, 140.5, 133.4, 133.3, 132.5, 130.9, 130.6, 128.1, 127.3, 127.1, 125.9, 125.3, 125.0 (q, J_F = 3.8 Hz), 124.9 (q, J_F = 270.3 Hz), 118.3 (q, J_F = 32.6 Hz), 116.7, 78.9. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{47}H_{30}F_3NS_2$, 729.1772; found 729.1771. m.p. 326 °C~328 °C.

1'-(3,5-dimethylphenyl)-3',4'-diphenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2h)



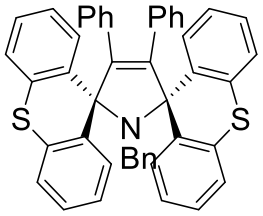
Yield: 86% (59.3 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.75 (d, *J* = 8.2 Hz, 4H), 7.23-7.19 (m, 8H), 7.18-7.12 (m, 4H), 6.97 (t, *J* = 7.6 Hz, 2H), 6.82 (t, *J* = 7.6 Hz, 4H), 6.53 (d, *J* = 7.3 Hz, 4H), 6.16 (s, 3H), 1.90 (s, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.8, 140.7, 136.8, 133.8, 133.3, 132.7, 131.7, 130.9, 127.6, 127.1, 127.0, 125.5, 125.1, 118.7, 115.6, 78.5, 21.4. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{48}H_{35}NS_2$, 689.2211; found 689.2211. m.p. >350 °C (Out of the measuring range).

1'-hexyl-3',4'-diphenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2i)



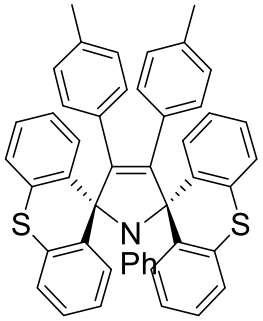
Yield: 74% (0.074 mmol, 51.7 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.57 (d, *J* = 8.2 Hz, 4H), 7.23-7.20 (m, 8H), 7.15-7.10 (m, 4H), 7.05 (t, J = 7.6 Hz, 2H), 6.90 (t, *J* = 7.8 Hz, 4H), 6.63-6.60 (m, 4H), 2.69-2.65 (m, 2H), 1.02 (q, *J* = 7.2 Hz, 2H), 0.92-0.79 (m, 6H), 0.72 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.4, 134.8, 134.4, 133.0, 132.4, 130.5, 127.5, 127.3, 127.0, 125.3, 125.2, 79.4, 46.3, 31.5, 30.0, 28.1, 22.5, 14.0. HRMS (FD+(eiFi) m/z: [M] calcd. for $C_{46}H_{39}NS_2$, 699.2524; found, 699.2523. m.p. 218 °C~220 °C.

1'-benzyl-3',4'-diphenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2j)



Yield: 93% (0.093 mmol, 62.8 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.64 (d, *J* = 7.8 Hz, 4H), 7.20-7.15 (m, 8H), 7.06-7.02 (m, 6H), 6.91 (t, *J* = 7.8 Hz, 4H), 6.70-6.65 (m, 5H), 6.56 (t, *J* = 7.6 Hz, 2H), 6.04-6.02 (m, 2H), 4.13 (s, 2H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.8, 138.8, 134.4, 134.3, 132.7, 132.2, 130.5, 129.6, 127.7, 127.1(9), 127.1(3), 126.9, 125.6, 125.4, 125.1, 78.7, 48.8. HRMS (FD+(eiFi) m/z: [M] calcd. for $C_{47}H_{33}NS_2$, 675.2054; found 675.2054. m.p. 304 °C~306 °C.

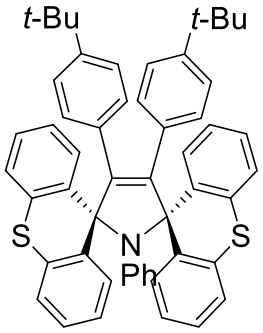
1'-phenyl-3',4'-di-p-tolyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2k)



Yield: 71% (0.071 mmol, 48.9 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 (d, J = 8.2 Hz, 4H), 7.23-7.19 (m, 8H), 7.15-7.09 (m, 4H), 6.83-6.79 (m, 2H), 6.65 (d, *J* = 8.2 Hz, 4H),

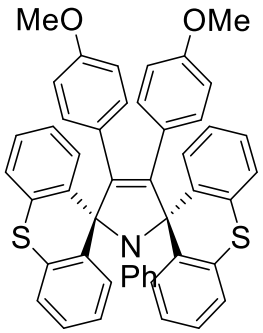
6.51-6.44 (m, 7H), 2.12 (s, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.8, 140.4, 136.7, 133.4, 132.6, 131.7, 130.8, 130.7, 127.9, 127.6, 125.6, 125.1, 118.1, 116.9, 78.4, 21.2 (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{48}H_{35}NS_2$, 689.2211; found 689.2210. m.p. 348 °C~350 °C.

3',4'-bis(4-(tert-butyl)phenyl)-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2l)



Yield: 85% (0.085 mmol, 65.7 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.71 (d, J = 7.8 Hz, 4H), 7.22-7.18 (m, 8H), 7.14-7.07 (m, 4H), 6.85 (d, *J* = 8.2 Hz, 4H), 6.80 (dd, *J* = 8.7, 7.3 Hz, 2H), 6.52-6.43 (m, 7H), 1.14 (s, 18H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 150.0, 140.8, 140.2, 133.4, 132.5, 131.9, 130.8, 130.5, 127.6, 127.5, 125.5, 125.1, 124.0, 118.7, 117.2, 78.4, 34.3, 31.2. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{54}H_{47}NS_2$, 773.3150; found 773.3150. m.p. 333 °C~335 °C.

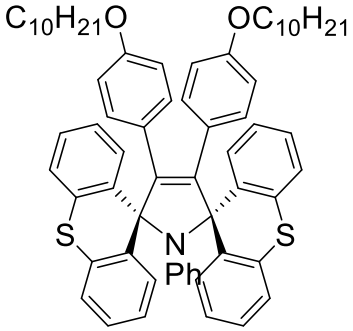
3',4'-bis(4-methoxyphenyl)-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2m)



Yield: 91% (0.091 mmol, 65.6 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.70 (d, *J* = 8.2 Hz, 4H), 7.21-7.18 (m, 8H), 7.15-7.09 (m, 4H), 6.81 (dd, *J* = 8.7, 7.3 Hz, 2H), 6.51-6.46 (m, 7H), 6.40 (d, *J* = 8.7 Hz, 4H), 3.63 (s, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.6, 140.8, 140.1, 133.4, 132.5, 132.0, 131.8, 127.6, 126.2, 125.6, 125.1, 118.3, 117.0, 112.7, 78.3, 54.9 (one

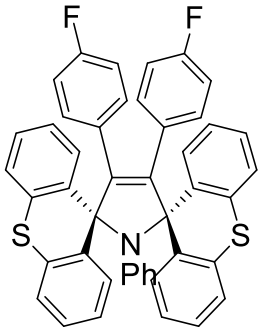
sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{48}H_{35}NO_2S_2$, 721.2109; found 721.2109. m.p. 299 °C~301 °C.

3',4'-bis(4-(decyloxy)phenyl)-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2n)



Yield: 91% (0.091 mmol, 88.7 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.71 (d, *J* = 8.2 Hz, 4H), 7.20-7.18 (m, 8H), 7.14-7.09 (m, 4H), 6.81 (dd, *J* = 8.7, 7.3 Hz, 2H), 6.51-6.45 (m, 7H), 6.39 (d, *J* = 8.7 Hz, 4H), 3.75 (t, *J* = 6.9 Hz, 4H), 1.66 (quint, *J* = 6.9 Hz, 4H), 1.37-1.25 (m, 28H), 0.87 (t, *J* = 6.4 Hz, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.2, 140.8, 140.0, 133.3, 132.5, 132.0, 131.8, 127.6, 126.0, 125.6, 125.1, 118.3, 117.0, 113.2, 78.3, 67.7, 31.9, 29.6, 29.4, 29.3(9), 29.3(2), 27.0, 22.7, 14.2. (one sp^2 peak and one sp^3 peak were not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{66}H_{71}NO_2S_2$, 973.4926; found 973.4925. m.p. 99 °C~101 °C.

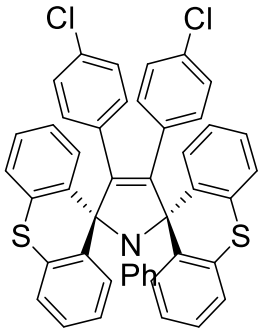
3',4'-bis(4-fluorophenyl)-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2o)



Yield: 84% (0.084 mmol, 58.6 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.71-7.67 (m, 4H), 7.24-7.23 (m, 8H), 7.18-7.13 (m, 4H), 6.85-6.80 (m, 5H), 6.56 (t, *J* = 8.7 Hz, 1H), 6.51-6.43 (m, 7H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 162.1 (d, J_F = 247.3 Hz), 140.7, 140.3, 133.4, 132.5 (d, J_F = 7.7 Hz), 131.2, 129.4 (d, J_F = 2.9 Hz), 127.9, 127.7, 125.8, 125.2, 117.5, 116.9, 114.3 (d, J_F = 21.1 Hz), 78.4 (one sp^2 peak was not shown due to superimposition). HRMS

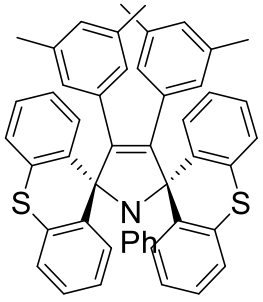
(FD+(eiFi)) m/z: [M] calcd. for $C_{46}H_{29}F_2NS_2$, 697.1710; found 697.1710. m.p. >350 °C (Out of the measuring range).

3',4'-bis(4-chlorophenyl)-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2p)



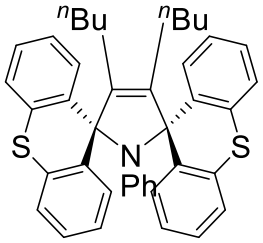
Yield: 41% (0.041 mmol, 29.9 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.70 (d, J = 8.2 Hz, 4H), 7.24-7.22 (m, 8H), 7.18-7.12 (m, 4H), 6.83 (dd, *J* = 8.7, 7.3 Hz, 2H), 6.59-6.53 (m, 4H), 6.51-6.45 (m, 7H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.6, 140.2, 133.6, 133.4, 132,5, 132.0, 131.9, 131.0, 128.0, 127.7. 127.5, 125.9, 125.3, 117.5, 117.0, 78.4. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{46}H_{29}Cl_2NS_2$, 729.1118; found 729.1118. m.p. >350 °C (Out of the measuring range).

3',4'-bis(3,5-dimethylphenyl)-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2q)



Compound **2q** was synthesized under the standard condition at 55 °C. Yield: 65% (0.065 mmol, 46.6 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.69 (d, *J* = 8.2 Hz, 4H), 7.21-7.19 (m, 8H), 7.15-7.11 (m, 4H), 6.82 (dd, *J* = 8.9, 7.1 Hz, 2H), 6.62 (s, 2H), 6.56 (d, *J* = 8.2 Hz, 2H), 6.48-6.45 (m, 1H), 6.14 (s, 4H), 1.93 (s, 12H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.9, 140.0, 136.0, 133.5, 133.4, 132.6, 131.6, 128.9, 128.6, 127.6, 125.3, 125.0, 117.5, 116.5, 78.5, 21.1 (one sp^2 peak was not shown due to superimposition). HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{50}H_{39}NS_2$, 717.2524; found 717.2523. m.p. >350 °C (Out of the measuring range).

3',4'-dibutyl-1'-phenyl-1'*H*-dispiro[thioxanthene-9,2'-pyrrole-5',9''-thioxanthene] (2r)



Yield: 76% (0.076 mmol, 47.2 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39-7.36 (m, 8H), 7.24-7.20 (m, 4H), 7.07-7.03 (m, 4H), 6.75 (dd, *J* = 9.2, 7.3 Hz, 2H), 6.41-6.36 (m, 3H), 2.10-2.06 (m, 4H), 1.10 (td, J = 14.4, 7.0 Hz, 4H), 0.99-0.92 (m, 4H), 0.69 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 140.7, 139.8, 132.7, 132.6, 132.4, 127.6, 127.5, 125.8, 125.30, 117.1, 116.1, 78.1, 31.5, 26.8, 23.6, 13.6. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{42}H_{39}NS_2$, 621.2524; found 621.2524. m.p. 231 °C~232 °C.

6. Photoredox catalytic [4+1] cycloaddition of 1 with H_2O

6.1 Reaction setup for photocatalysis

Two test tubes are placed in the stainless steel test tube stand at the center of a magnetic stirrer. Two parallel Blue LED lamps (Kessil PR 160L-440) are placed at an oblique angle to the side of the test tubes. The magnetic stirrer, test tube, and LEDs are covered with PR 160 Rig w/ Fan kit. A fan over the test tube is always turned on when the reaction is running.

a) b)

b) d)

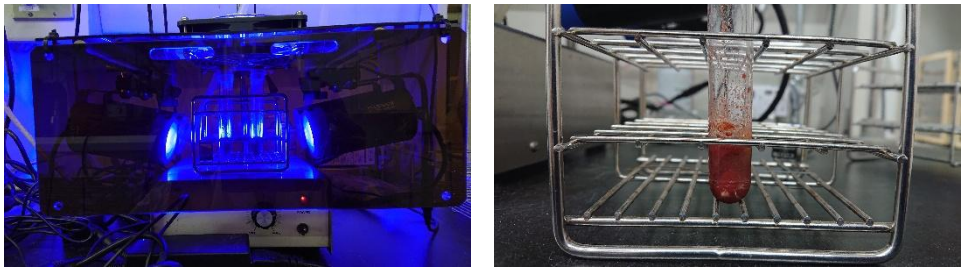
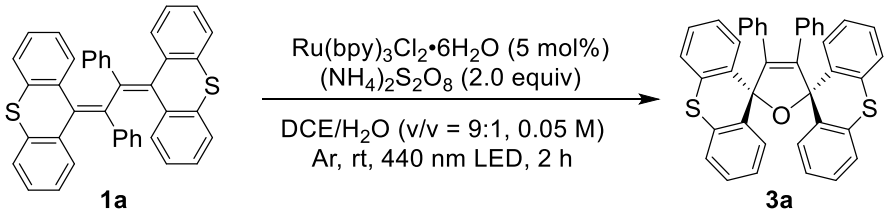


Fig. S2. a) Setup the stainless steel test tube stand, magnetic stirrer, and LED lamp. b) Steup the PR 160 Rig w/ Fan kit. c) Light irradiation. d) Test tube after reaction.

6.2 Representative procedure for the photocatalytic [4+1] cycloaddition of 1a with H_2O

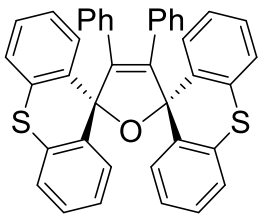


To a transparent test tube (Ø15 x 105 mm) was added substrate **1a** (57 mg, 0.1 mmol, 1.0 equiv), $Ru(bpy)_3Cl_2 \cdot 6H_2O$ (3.7 mg, 5.0 mol%), anhydrous $(NH_4)_2S_2O_8$ (45.6 mg, 0.2 mmol, 2.0 equiv) and anhydrous DCE/H_2O (v/v = 9:1, 2 mL, 0.05M). The test tube was stirred for 2 h under an Ar atmosphere under irradiation of a Kessil lamp (440 nm, 75% intensity) placed 5–7 cm away from the test tube. A regular fan was equipped to maintain the ambient temperature at 25 °C. Upon completion, the reaction mixture was diluted with DCM (10 mL),

poured into water (20 mL) and extracted with DCM (2 × 10 mL). The combined organic layer was washed with brine (3 × 10 mL) and dried over $MgSO_4$. After filtration and concentration in vacuo, the residue was purified by flash column chromatography using hexane/DCM (5/1) as an eluent to give desired product **3a** in 98% yield (57.4 mg, 0.098 mmol) as white solid.

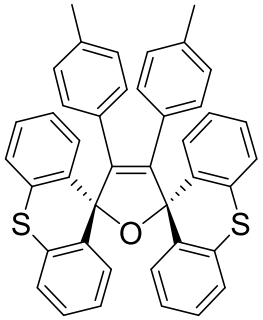
7. Analytical data of products 3

3',4'-diphenyldispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3a)



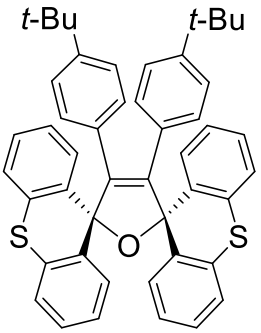
Yield: 98% (0.098 mmol, 57.4 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.25 (td, *J* = 7.3, 1,4 Hz, 4H), 7.22-7.16 (m, 6H), 7.06-7.00 (m, 8H), 6.78 (dd, *J* = 8.5, 1,4 Hz, 4H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 138.3, 135.0, 133.7, 132.8, 130.1, 129.8, 128.0, 127.7, 127.6, 125.9, 125.6, 92.9. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{26}OS_2$, 586.1425; found 586.1423. m.p. 336 °C~338 °C.

3',4'-di-*p*-tolyldispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3b)



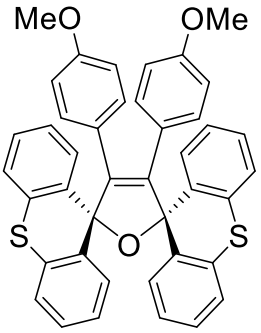
Yield: 93% (0.093mmol, 57.1 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.26-7.22 (m, 4H), 7.19 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.05-7.00 (m, 4H), 6.83 (d, *J* = 8.2 Hz, 4H), 6.65 (d, *J* = 8.2 Hz, 4H), 2.25 (s, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 137.9, 137.3, 135.2, 132.8, 130.8, 129.9, 129.8, 128.7, 127.6, 125.8, 125.6, 92.8, 21.3. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{42}H_{30}OS_2$, 614.1738; found 614.1737. m.p. 326 °C~328 °C.

3',4'-bis(4-(*tert*-butyl)phenyl)dispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3c)



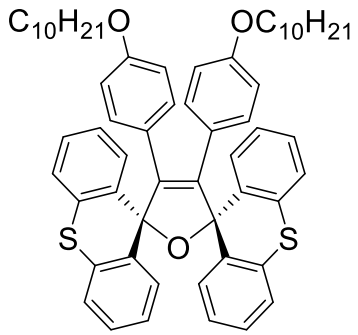
Yield: 93% (0.093 mmol, 64.9 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.26-7.21 (m, 4H), 7.19 (dd, *J* = 8.2, 1.4 Hz, 4H), 7.05-7.00 (m, 8H), 6.67 (dd, *J* = 6.9, 1.8 Hz, 4H), 1.23 (s, 18H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 150.6, 137.7, 135.3, 132.8, 130.7, 129.8, 129.6, 127.5, 125.7, 125.5, 124.8, 92.9, 34.5, 31.3. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{48}H_{42}OS_2$, 698.2677; found 698.2676. m.p. 303 °C~305 °C.

3',4'-bis(4-methoxyphenyl)dispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3d)



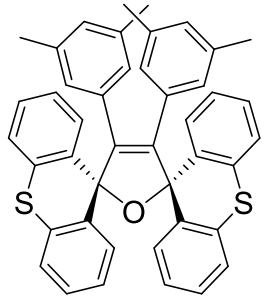
Yield: 67% (0.067 mmol, 43.3 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 (dd, *J* = 7.8, 0.9 Hz, 4H), 7.28-7.21 (m, 4H), 7.18 (dd, *J* = 8.0, 1.1 Hz, 4H), 7.05-7.01 (m, 4H), 6.70 (dt, *J* = 9.5, 2.5 Hz, 4H), 6.57 (dt, *J* = 9.5, 2.5 Hz, 4H), 3.72 (s, 6H) ^{13}C NMR ($CDCl_3$, 101 MHz) δ 159.0, 137.0, 135.3, 132.7, 131.4, 129.8, 127.6, 126.1, 125.8, 125.6, 113.5, 92.7, 55.1. HRMS (FE+(eiFi)) m/z: calcd. for $C_{42}H_{30}O_3S_2$, 646.1636; found 646.1635. m.p. >199 °C (decomposition).

3',4'-bis(4-(decyloxy)phenyl)dispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3e)



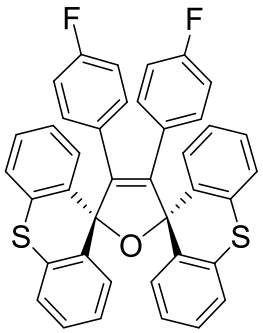
Yield: 78% (0.078 mmol, 70.1 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 (d, *J* = 7.8 Hz, 4H), 7.25-7.23 (m, 4H), 7.18 (dd, *J* = 8.0 Hz, 4H), 7.04-7.00 (m, 4H), 6.68 (d, *J* = 9.2 Hz, 4H), 6.55 (d, *J* = 8.7 Hz, 4H), 3.85 (t, *J* = 6.6 Hz, 4H), 1.72 (quint, *J* = 6.9 Hz, 4H), 1.41-1.26 (m, 28H), 0.92-0.82 (m, 6H) ^{13}C NMR ($CDCl_3$, 101 MHz) δ 158.6, 137.0, 135.3, 132.7, 131.3, 129.8, 127.5, 125.9, 125.8, 125.5, 114.0, 92.7, 67.9, 31.9, 29.6, 29.4, 29.4, 29.3, 26.1, 22.7, 14.2 (one sp^3 peak was not shown due to superimposition). HRMS (FE+(eiFi)) m/z: calcd. for $C_{60}H_{66}O_3S_2$, 898.4453; found 898.4452. m.p. 72 °C~74 °C.

3',4'-bis(3,5-dimethylphenyl)dispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3f)



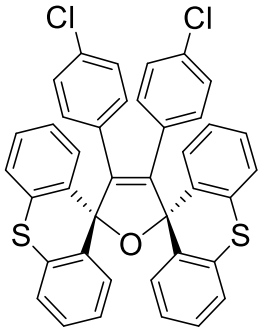
Yield: 75% (0.075 mmol, 48.2 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.26-7.22 (m, 4H), 7.19 (dd, *J* = 8.0, 1.1 Hz, 4H), 7.06-7.02 (m, 4H), 6.80 (s, 2H), 6.39 (s, 4H), 1.99 (s, 12H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 138.1, 137.0, 135.2, 133.7, 132.8, 129.8, 128.9, 128.0, 127.5, 125.6, 125.5, 92.8, 21.3. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{44}H_{34}OS_2$, 642.2051; found 642.2052. m.p. 297 °C~299 °C.

3',4'-bis(4-fluorophenyl)dispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3g)



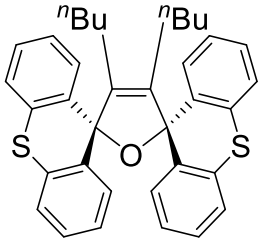
Yield: 77% (0.77 mmol, 47.9 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37 (dd, *J* = 7.8, 0.9 Hz, 4H), 7.28-7.24 (m, 4H), 7.15 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.07-7.03 (m, 4H), 6.76 (s, 4H), 6.74 (s, 4H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 162.3 (d, J_F = 249.2 Hz), 137.4, 134.7, 132.8, 131.8 (d, J_F = 7.7 Hz), 129.6, 129.5 (d, J_F = 3.8 Hz), 127.9, 126.0, 125.7, 115.2 (d, J_F = 21.1 Hz), 92.8. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{24}F_2OS_2$, 622.1237, found 622.1236. m.p. 317 °C~319 °C.

3',4'-bis(4-chlorophenyl)dispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3h)



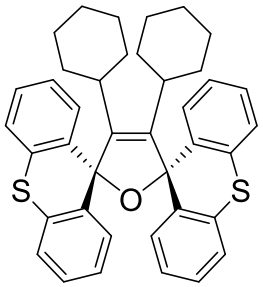
Yield: 77% (0.077 mmol, 50.4 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.38 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.29-7.25 (m, 4H), 7.14 (dd, *J* = 8.0, 1.4 Hz, 4H), 7.07-7.01 (m, 8H), 6.71 (dt, *J* = 9.0, 2.3 Hz, 4H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 137.8, 134.6, 134.1, 132.8, 131.8, 131.3, 129.6, 128.4, 127.9, 126.1, 125.8, 92.8. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{24}Cl_2OS_2$, 654.0646; found 654.0645. m.p. 346 °C~348 °C.

3',4'-dibutyldispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3i)



Yield: 73% (0.073 mmol, 39.9 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.44 (dd, *J* = 7.8, 0.9 Hz, 4H), 7.28-7.24 (m, 4H), 7.16 (dd, *J* = 8.0, 1.1 Hz, 4H), 7.10-7.06 (m, 4H), 2.31-2.27 (m, 4H), 1.33-1.19 (m, 8H), 0.80 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 139.2, 135.7, 132.2, 129.8, 127.6, 126.1, 125.6, 92.8, 31.1, 27.2, 23.8, 13.7. HRMS (FD+(eiFi) m/z: [M] calcd. for $C_{36}H_{34}OS_2$, 546.2051; found 546.2051. m.p. 174 °C~176 °C.

3',4'-dicyclohexyldispiro[thioxanthene-9,2'-furan-5',9''-thioxanthene] (3j)



Yield: 68% (0.068 mmol, 40.7 mg), white solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.38 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.35 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.27-7.23 (m, 4H), 7.10-7.05 (m, 4H), 2.84 (tt, *J* = 11.9, 2.7 Hz, 2H), 1.62-1.51 (m, 12H), 1.38-1.00 (m, 10H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ 143.1. 135.6, 131.5, 131.2, 127.6, 125.9, 125.0, 92.8, 38.4, 32.7, 27.6, 26.2. HRMS (FD+(eiFi)) m/z: [M] calcd. for $C_{40}H_{38}OS_2$, 598.2364, found 598.2363. m.p. 283 °C~284 °C.

8. Summary of single crystals

8.1 Summary of single crystal 2a

Single crystal **2a** was prepared by slow diffusion of hexane into a $CHCl_3$ solution of **2a** at room temperature. CCDC 2453063

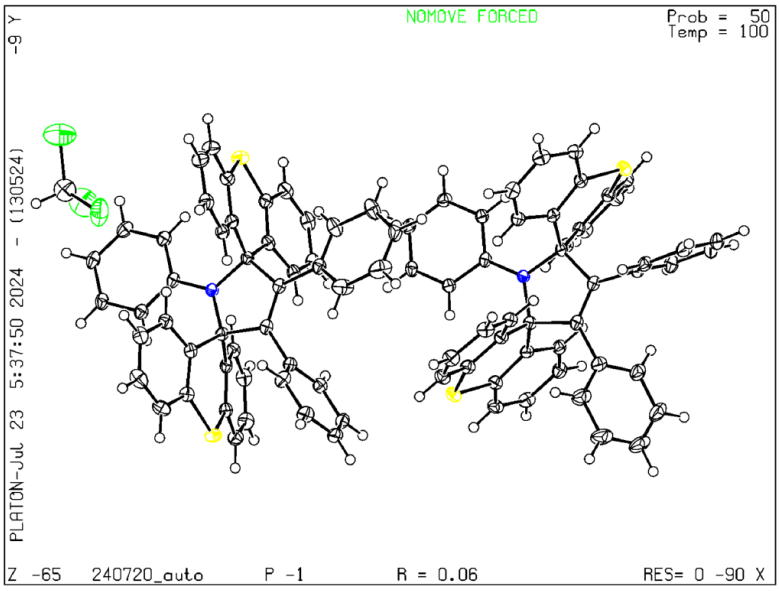


Fig. S3. ORTEP drawing of **2a**. Thermal ellipsoids are shown at 50% probability. A colorless prism crystal of $C_{40}H_{37}OS_2$ having approximate dimensions of 0.3 x 0.2 x 0.2 mm was mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS RAPID diffractometer using multi-layer mirror mono chromated Mo-K$^{\alpha}$radiation.

Table S1. Crystal data and structure refinement for **2a**

Identification code	**2a**
Empirical formula	$C_{93}H_{63}Cl_3N_2S_4$
Formula weight	1443.04
Temperature/K	99.90(14)
Crystal system	triclinic
Space group	P-1
a/Å	11.2066(2)
b/Å	16.8166(2)
c/Å	20.3126(2)
α /°	70.0750(10)
β /°	79.4680(10)
γ /°	76.9960(10)
Volume/Å^3	3483.01(9)
Z	2
ρ_{calc}g/cm^3	1.376
μ /mm^{-1}	0.305

F(000)	1500.0
Crystal size/mm^3	0.22 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.538 to 61.804
Index ranges	-15 ≤ h ≤ 15, -23 ≤ k ≤ 23, -28 ≤ l ≤ 28
Reflections collected	189638
Independent reflections	19410 [R_{int} = 0.0756, R_{sigma} = 0.0372]
Data/restraints/parameters	19410/0/919
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0623, wR_2 = 0.1622
Final R indexes [all data]	R_1 = 0.0832, wR_2 = 0.1750
Largest diff. peak/hole / e Å^{-3}	0.93/-0.97

8.2 Summary of single crystal 3a

Single crystal of **3a** was prepared by slow diffusion of hexane into a $CHCl_3$ solution of **3a** at room temperature. CCDC 2453062

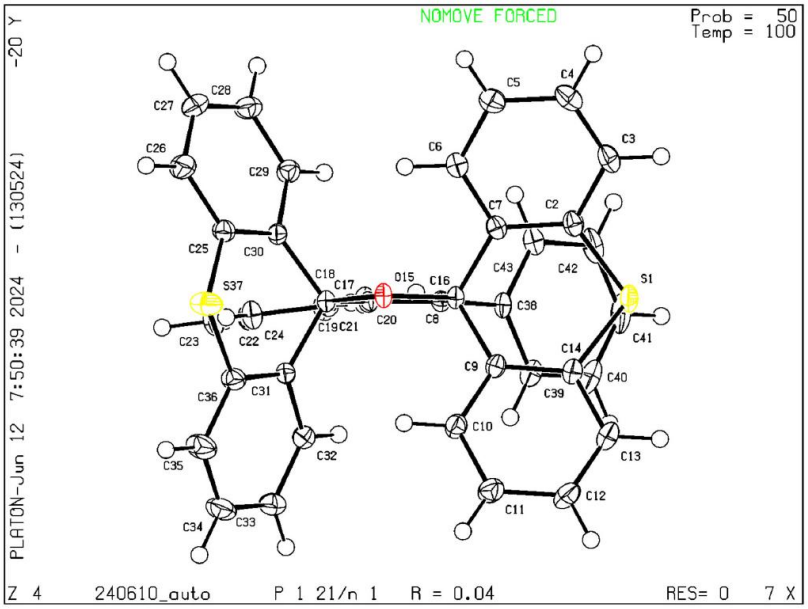


Fig. S4. ORTEP drawing of **3a**.

Thermal ellipsoids are shown at 50% probability. A colorless prism crystal of $C_{40}H_{37}OS_2$ having approximate dimensions of 0.3 x 0.2 x 0.2 mm was mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS RAPID diffractometer using multi-layer mirror mono chromated Mo-K$^{\alpha}$radiation.

Table S2. Crystal data and structure refinement for **3a**

Identification code	**3a**
Empirical formula	$C_{40}H_{37}O_{6.5}S_2$
Formula weight	685.81
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	16.0424(2)
b/Å	11.17230(10)
c/Å	19.0872(2)
α /°	90
β /°	91.6550(10)
γ /°	90
Volume/Å^3	3419.58(6)
Z	4
ρ_{calc}g/cm^3	1.332
μ /mm^{-1}	0.206
F(000)	1444.0
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	? (λ = 0.71073)
2Θ range for data collection/°	4.898 to 62.76
Index ranges	-22 ≤ h ≤ 22, -15 ≤ k ≤ 16, -26 ≤ l ≤ 27
Reflections collected	85415
Independent reflections	10053 [R_{int} = 0.0342, R_{sigma} = 0.0203]
Data/restraints/parameters	10053/0/388
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0360, wR_2 = 0.1016
Final R indexes [all data]	R_1 = 0.0422, wR_2 = 0.1050
Largest diff. peak/hole / e Å^{-3}	0.38/-0.23

Table S3. Solvent masks information for **3a**

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	-0.170	0.500	383.2	111.3	11 water
2	0.000	0.500	0.000	0.0	0.0	?
3	0.500	-0.251	0.000	383.2	111.3	11 water
4	0.500	0.000	0.500	0.0	0.0	?

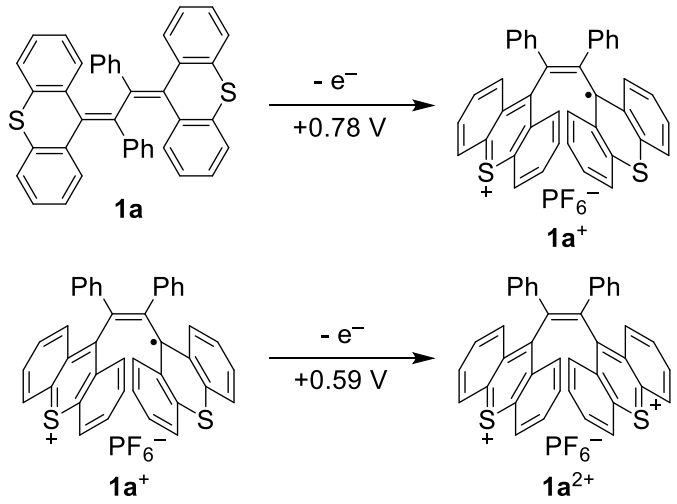
9. DFT calculations

9.1. Calculations of the redox potentials of 1a

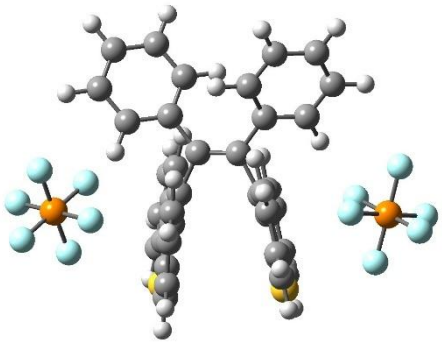
Gas phase free energies were computed using M06-2X/aug-cc-pVTZ//M06-2X/6-31G(d,p). Solvation free energies were computed at the SMD/M06-2X/6-31G(d,p) level of theory. The computational procedure was based on previous studies (for example, Psciuk, B. T.; Lord, R. L.; Munk, B. H.; Schlegel, H. B. Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. J. Chem. Theory Comput. 2012, *8*, 5107–5123). The SHE (standard hydrogen electrode) was set to 4.281 V.

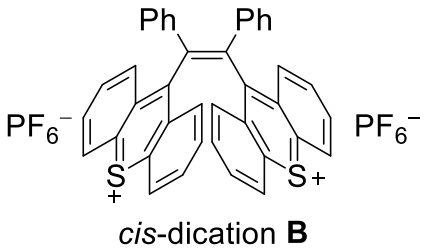
Table S4. Calculated free energies:

	1a	**1a**$^{+}$	**1a**$^{+}$ · PF_6^-	**1a**$^{2+}$ · PF_6^-
SMD/M06-2X/6-31G(d,p)	-2335.197670	-2335.016997	-3275.535062	-3275.361495
M06-2X/6-31G(d,p)	-2335.153570	-2334.929914	-3275.463910	-3275.234850
M06-2X/aug-cc-pVTZ	-2336.212453	-2335.980703	-3276.876313	-3276.643538



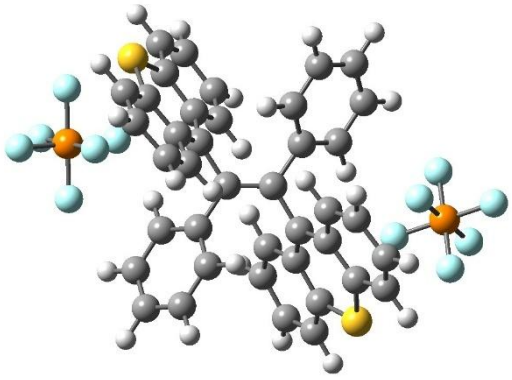
9.2. Stability energy difference between *cis*- and *trans*-dication conformers

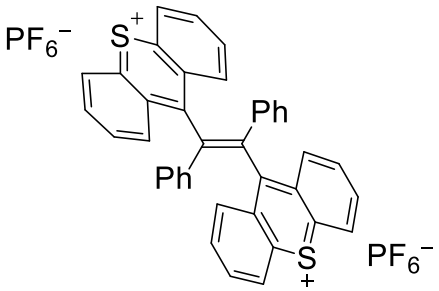




cis-dication **B**

ΔG = 0 kcal/mol; stable





trans-dication **B**

ΔG = 3.4 kcal/mol

Fig. S5. Stability energy difference between *cis*- and *trans*-dication conformers.

Table S5. Single-point calculation for *cis/trans* relative stability

calculation level	$\Delta E_{cis\text{-}trans}$ (kcal/mol)
HF	+6.0
MP2	-9.2
B3LYP	+4.1
B3LYP-D3(BJ)	-4.7

All single-point calculations were performed using the SMD solvation model and the def2-SVP basis set. The results indicate that the relative stability of the *cis* and *trans* isomers is strongly affected by dispersion interactions. Consequently, methods that do not incorporate dispersion effects, such as HF and B3LYP without Grimme's dispersion correction, tend to overestimate the stability of the trans isomer.

Table S6 Calculation data of dications

trans-dication **B**

Sum of electronic and thermal Free Energies= -4213.446971

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.633669	0.295404	0.275315
2	6	0	-0.625492	-0.113840	0.558659
3	6	0	1.801968	-0.641265	0.401771
4	6	0	2.744530	-0.340897	1.422666
5	6	0	1.937636	-1.741647	-0.488058
6	6	0	3.935330	-1.100231	1.610061
7	6	0	2.525635	0.751709	2.320782
8	6	0	3.024091	-2.663105	-0.395094
9	6	0	0.975619	-1.985339	-1.516498
10	6	0	4.884942	-0.737297	2.588913
11	16	0	4.305851	-2.506346	0.719783
12	6	0	3.447462	1.085444	3.276305
13	1	0	1.605012	1.328128	2.252215
14	6	0	3.109677	-3.777977	-1.256863
15	6	0	1.071144	-3.067703	-2.350361
16	1	0	0.143719	-1.299511	-1.639728
17	6	0	4.647599	0.346361	3.398899
18	1	0	5.801138	-1.320951	2.696228
19	1	0	3.256928	1.924851	3.945924
20	1	0	3.947950	-4.471314	-1.162047
21	6	0	2.144076	-3.977886	-2.214729
22	1	0	0.318331	-3.225292	-3.123384
23	1	0	5.385513	0.628768	4.151656
24	1	0	2.214907	-4.839979	-2.880112
25	6	0	-1.814074	0.803067	0.518414
26	6	0	-2.332016	1.258862	-0.719793
27	6	0	-2.400355	1.119240	1.777881
28	6	0	-3.533861	2.025867	-0.801580

29	6	0	-1.669457	0.964003	-1.951927
30	6	0	-3.615640	1.852215	1.892214
31	6	0	-1.753951	0.737362	2.995244
32	6	0	-4.038384	2.455671	-2.046584
33	16	0	-4.472046	2.469776	0.551312
34	6	0	-2.161811	1.398227	-3.152504
35	1	0	-0.742935	0.398531	-1.934715
36	6	0	-4.179738	2.130927	3.156687
37	6	0	-2.303039	1.028078	4.216627
38	1	0	-0.794441	0.223660	2.954500
39	6	0	-3.360630	2.146942	-3.200909
40	1	0	-4.966632	3.028266	-2.085407
41	1	0	-1.630304	1.163016	-4.075243
42	1	0	-5.119871	2.682618	3.220046
43	6	0	-3.535576	1.716564	4.298114
44	1	0	-1.786121	0.731232	5.129887
45	1	0	-3.753852	2.482113	-4.162204
46	1	0	-3.973914	1.935156	5.273347
47	6	0	0.970054	1.671443	-0.186788
48	6	0	1.875174	1.821837	-1.246368
49	6	0	0.389323	2.814639	0.384791
50	6	0	2.151716	3.088989	-1.758195
51	1	0	2.368392	0.947802	-1.678080
52	6	0	0.672189	4.076954	-0.127257
53	1	0	-0.262703	2.726084	1.256117
54	6	0	1.544271	4.215894	-1.208377
55	1	0	2.856787	3.189687	-2.583687
56	1	0	0.216864	4.958226	0.328402
57	1	0	1.763849	5.207131	-1.609856
58	6	0	-0.963644	-1.517368	0.937467
59	6	0	-1.995547	-2.165458	0.244871
60	6	0	-0.254595	-2.214559	1.926365
61	6	0	-2.286741	-3.502050	0.513405
62	1	0	-2.566019	-1.634013	-0.519988
63	6	0	-0.551138	-3.548583	2.192024
64	1	0	0.524308	-1.710713	2.503463

65	6	0	-1.561818	-4.196953	1.480490
66	1	0	-3.089577	-3.993458	-0.037291
67	1	0	0.006210	-4.082141	2.964265
68	1	0	-1.791718	-5.243617	1.689409
69	15	0	5.589391	0.819880	-1.061951
70	9	0	4.764726	1.491477	0.166695
71	9	0	4.871715	1.835107	-2.105655
72	9	0	4.372046	-0.248284	-1.281234
73	9	0	6.401623	0.135968	-2.285339
74	9	0	6.790711	1.882111	-0.841622
75	9	0	6.298493	-0.208150	-0.021941
76	15	0	-5.512153	-1.053113	-0.936628
77	9	0	-4.271925	-0.680172	-1.926371
78	9	0	-4.914680	-2.554651	-0.771687
79	9	0	-6.385608	-1.534895	-2.211309
80	9	0	-6.732978	-1.423420	0.058638
81	9	0	-6.095935	0.453684	-1.101950
82	9	0	-4.622949	-0.563432	0.340774

cis-dication **B**

Sum of electronic and thermal Free Energies= -4213.452446

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.676632	1.524881	0.067634
2	6	0	0.677666	1.575621	0.201748
3	6	0	-1.311921	0.164259	0.108044
4	6	0	-1.793693	-0.390406	-1.105234
5	6	0	-1.310813	-0.533833	1.345509
6	6	0	-2.134495	-1.769884	-1.211283
7	6	0	-1.905403	0.401063	-2.291141
8	6	0	-1.506069	-1.943615	1.417621
9	6	0	-1.063884	0.161161	2.567980

10	6	0	-2.582615	-2.315247	-2.431466
11	16	0	-1.951254	-2.893048	0.067071
12	6	0	-2.358284	-0.136377	-3.466161
13	1	0	-1.643404	1.456321	-2.259907
14	6	0	-1.324074	-2.633063	2.634749
15	6	0	-0.942973	-0.514584	3.755125
16	1	0	-0.976766	1.248861	2.546337
17	6	0	-2.700162	-1.505239	-3.537448
18	1	0	-2.842290	-3.374121	-2.489631
19	1	0	-2.451901	0.493243	-4.351608
20	1	0	-1.435547	-3.718846	2.667150
21	6	0	-1.036826	-1.925103	3.780985
22	1	0	-0.762344	0.034390	4.680347
23	1	0	-3.058973	-1.928588	-4.477234
24	1	0	-0.906676	-2.460321	4.723360
25	6	0	1.398074	0.272695	0.404081
26	6	0	1.461561	-0.627574	-0.687778
27	6	0	1.898032	-0.026457	1.702993
28	6	0	1.816047	-1.999278	-0.522624
29	6	0	1.142568	-0.185087	-2.009631
30	6	0	2.276622	-1.350802	2.066450
31	6	0	1.959770	0.971432	2.722994
32	6	0	1.777957	-2.889510	-1.614594
33	16	0	2.252136	-2.677299	0.983241
34	6	0	1.122170	-1.057111	-3.064969
35	1	0	0.930137	0.872611	-2.171860
36	6	0	2.656802	-1.659242	3.389677
37	6	0	2.373328	0.667691	3.994766
38	1	0	1.683364	1.997696	2.489521
39	6	0	1.422925	-2.423419	-2.860471
40	1	0	2.035718	-3.940123	-1.468218
41	1	0	0.880870	-0.698319	-4.066477
42	1	0	2.922802	-2.685395	3.652135
43	6	0	2.710339	-0.660335	4.335680
44	1	0	2.428289	1.452921	4.749634
45	1	0	1.395526	-3.116423	-3.703432

46	1	0	3.019446	-0.900387	5.354479
47	6	0	-1.614107	2.653565	-0.162673
48	6	0	-2.904822	2.565330	0.381324
49	6	0	-1.291522	3.744262	-0.987249
50	6	0	-3.842350	3.568951	0.140190
51	1	0	-3.192106	1.698893	0.983094
52	6	0	-2.230743	4.741569	-1.224129
53	1	0	-0.312823	3.797956	-1.467317
54	6	0	-3.504653	4.662055	-0.654226
55	1	0	-4.843000	3.481809	0.565934
56	1	0	-1.972340	5.582353	-1.870647
57	1	0	-4.238942	5.446516	-0.847387
58	6	0	1.547810	2.779666	0.183550
59	6	0	2.804926	2.686663	-0.433391
60	6	0	1.187959	3.971713	0.832567
61	6	0	3.669852	3.780671	-0.435998
62	1	0	3.119631	1.756381	-0.913421
63	6	0	2.056839	5.057136	0.830550
64	1	0	0.232547	4.040707	1.356809
65	6	0	3.295894	4.967863	0.189535
66	1	0	4.642791	3.693798	-0.922543
67	1	0	1.770556	5.978135	1.341935
68	1	0	3.974672	5.822957	0.192340
69	15	0	-5.448616	-0.571501	0.010526
70	9	0	-4.631800	0.081717	-1.232486
71	9	0	-5.765068	0.917551	0.578715
72	9	0	-4.074758	-0.601871	0.893249
73	9	0	-6.253845	-1.222103	1.256158
74	9	0	-6.809704	-0.539989	-0.864483
75	9	0	-5.107830	-2.057867	-0.549771
76	15	0	5.267088	-0.636400	-1.046768
77	9	0	4.019914	-0.381841	-2.061812
78	9	0	5.666746	0.933890	-1.161698
79	9	0	6.222261	-0.982852	-2.306690
80	9	0	6.500834	-0.884654	-0.028884
81	9	0	4.842929	-2.199939	-0.926567

82	9	0	4.299541	-0.286649	0.218213

9.3. Non-covalent interaction (NCI) analysis

a) b)

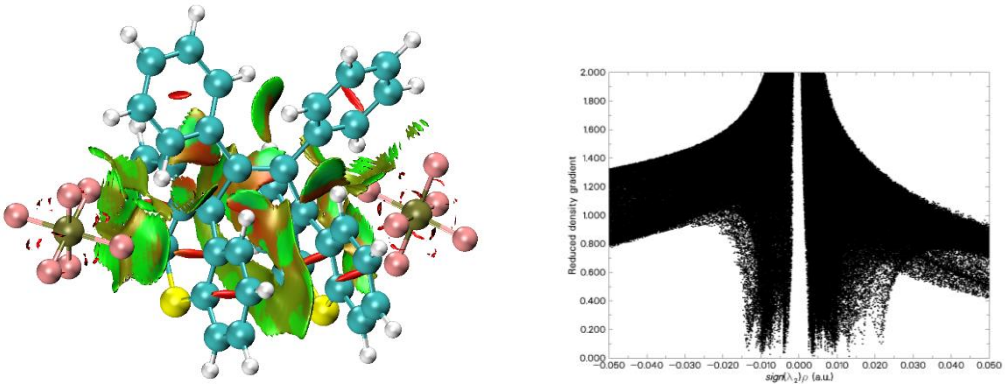


Fig. S6. a) NCI surface (0.5 isovalue) of **1a**$^{2+}$ · 2PF_6^-. b) NCI plot of **1a**$^{2+}$ · 2PF_6^-.

9.4. HOMO and LUMO distribution of products 2a and 3a

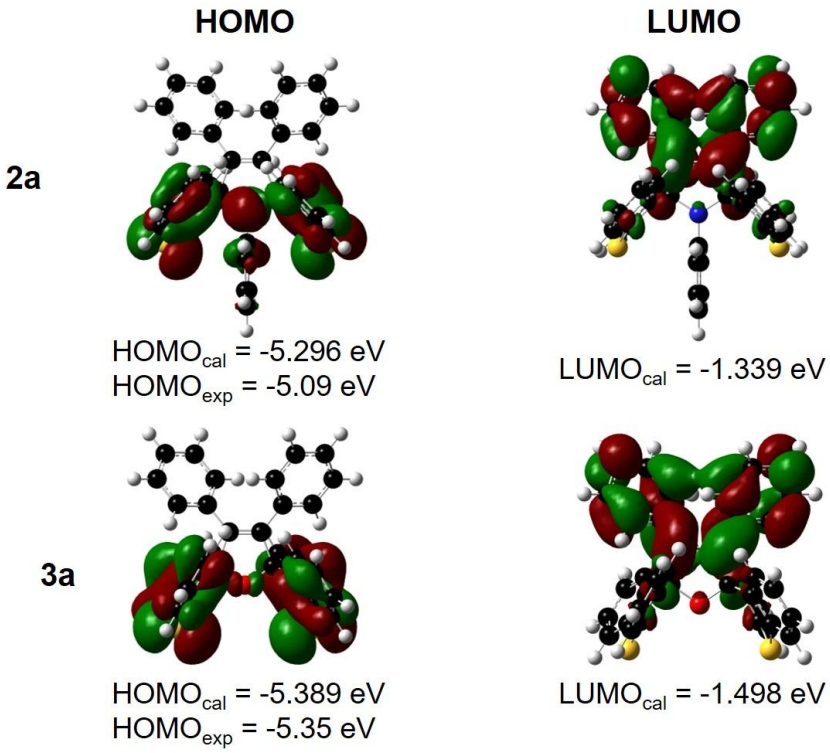
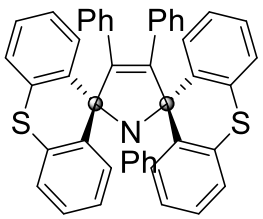


Fig. S7. HOMO and LUMO distribution of products **2a** and **3a**. DFT calculations were performed at the B3LYP/6-31G(d,p) level.

Table S7



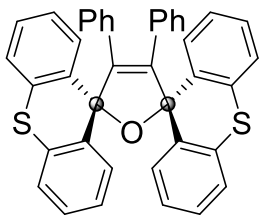
2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.242950	0.016797	0.114936
2	6	0	-1.242944	0.016719	-0.114997
3	6	0	-0.678475	-1.412780	-0.000310
4	6	0	0.678579	-1.412734	0.000151
5	6	0	-1.574249	-2.589642	0.160637
6	6	0	-1.208528	-3.630115	1.039241
7	6	0	-2.830239	-2.680371	-0.466109
8	6	0	-2.043600	-4.721036	1.257796
9	1	0	-0.258446	-3.577435	1.559388
10	6	0	-3.665576	-3.776529	-0.248415
11	1	0	-3.159743	-1.894719	-1.133349
12	6	0	-3.277977	-4.803945	0.609654
13	1	0	-1.732613	-5.504280	1.943129
14	1	0	-4.626882	-3.819976	-0.752108
15	1	0	-3.931868	-5.654036	0.780433
16	6	0	1.574435	-2.589534	-0.160783
17	6	0	1.208813	-3.630037	-1.039394
18	6	0	2.830419	-2.680167	0.465989
19	6	0	2.043972	-4.720896	-1.257925
20	1	0	0.258743	-3.577428	-1.559571
21	6	0	3.665843	-3.776262	0.248319
22	1	0	3.159850	-1.894485	1.133231
23	6	0	3.278339	-4.803712	-0.609753
24	1	0	1.733059	-5.504164	-1.943263

25	1	0	4.627142	-3.819634	0.752033
26	1	0	3.932296	-5.653756	-0.780513
27	6	0	-3.830537	1.048708	3.268300
28	6	0	-4.001040	1.691379	2.051084
29	6	0	-3.208256	1.349275	0.942197
30	6	0	-2.223095	0.350644	1.034512
31	6	0	-2.091884	-0.292642	2.277240
32	6	0	-2.869511	0.041714	3.379426
33	6	0	-1.876399	0.246952	-1.516713
34	6	0	-2.821750	1.254893	-1.777575
35	6	0	-3.260345	1.514646	-3.087881
36	1	0	-3.994435	2.298228	-3.252694
37	6	0	-2.780949	0.772338	-4.156961
38	6	0	-1.867428	-0.256993	-3.917940
39	6	0	-1.434259	-0.504251	-2.620750
40	1	0	-4.450735	1.320270	4.117294
41	1	0	-4.759265	2.461385	1.940889
42	1	0	-1.356140	-1.077018	2.384741
43	1	0	-2.728589	-0.484969	4.318228
44	1	0	-3.130562	0.981443	-5.163487
45	1	0	-1.495596	-0.865724	-4.736431
46	1	0	-0.732445	-1.310168	-2.450888
47	6	0	3.830574	1.049215	-3.268211
48	6	0	4.000953	1.691848	-2.050958
49	6	0	3.208160	1.349604	-0.942121
50	6	0	2.223110	0.350869	-1.034525
51	6	0	2.092033	-0.292381	-2.277285
52	6	0	2.869671	0.042114	-3.379422
53	6	0	1.876358	0.246982	1.516680
54	6	0	2.821595	1.255008	1.777632
55	6	0	3.260139	1.514712	3.087964
56	1	0	3.994140	2.298362	3.252847
57	6	0	2.780805	0.772272	4.156981
58	6	0	1.867402	-0.257142	3.917869
59	6	0	1.434282	-0.504352	2.620653
60	1	0	4.450778	1.320885	-4.117166

61	1	0	4.759089	2.461932	-1.940693
62	1	0	1.356395	-1.076847	-2.384853
63	1	0	2.728853	-0.484547	-4.318252
64	1	0	3.130376	0.981343	5.163529
65	1	0	1.495624	-0.865974	4.736309
66	1	0	0.732558	-1.310334	2.450721
67	16	0	-3.529752	2.283046	-0.525764
68	16	0	3.529500	2.283330	0.525904
69	7	0	-0.000024	0.815029	-0.000016
70	6	0	-0.000082	2.240357	0.000027
71	6	0	0.157400	2.952807	-1.198865
72	6	0	-0.157620	2.952720	1.198963
73	6	0	0.158465	4.347240	-1.197024
74	1	0	0.278668	2.403240	-2.125658
75	6	0	-0.158794	4.347152	1.197209
76	1	0	-0.278841	2.403084	2.125720
77	6	0	-0.000192	5.046987	0.000114
78	1	0	0.282050	4.887153	-2.131594
79	1	0	-0.282421	4.886998	2.131813
80	1	0	-0.000234	6.133401	0.000148



3a

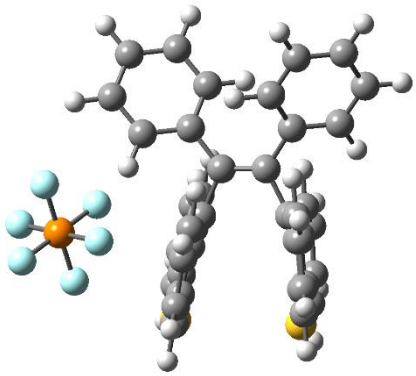
Standard orientation:

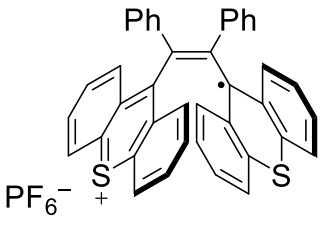
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.193186	-0.363895	0.153186
2	8	0	0.000028	-1.174265	-0.000938
3	6	0	1.193322	-0.363776	-0.153912

4	6	0	0.677813	1.076607	-0.020526
5	6	0	-0.677873	1.076583	0.019726
6	6	0	1.600513	2.233824	0.105538
7	6	0	1.268876	3.315082	0.948171
8	6	0	2.861932	2.257239	-0.517160
9	6	0	2.142002	4.382241	1.132299
10	1	0	0.317701	3.312906	1.468535
11	6	0	3.734612	3.330371	-0.334749
12	1	0	3.167008	1.434823	-1.151602
13	6	0	3.380166	4.399649	0.485681
14	1	0	1.857985	5.198521	1.790172
15	1	0	4.698985	3.322161	-0.834183
16	1	0	4.062933	5.231659	0.630114
17	6	0	-1.600755	2.233596	-0.105840
18	6	0	-1.269351	3.315517	-0.947722
19	6	0	-2.862259	2.256225	0.516729
20	6	0	-2.142779	4.382521	-1.131239
21	1	0	-0.318161	3.313910	-1.468057
22	6	0	-3.735246	3.329216	0.334944
23	1	0	-3.167137	1.433323	1.150638
24	6	0	-3.381025	4.399139	-0.484730
25	1	0	-1.858957	5.199326	-1.788544
26	1	0	-4.699668	3.320359	0.834270
27	1	0	-4.063996	5.231065	-0.628689
28	6	0	3.737371	-1.716104	3.115481
29	6	0	3.687437	-2.434121	1.927296
30	6	0	2.904312	-1.980236	0.855621
31	6	0	2.159087	-0.792580	0.957649
32	6	0	2.236612	-0.084842	2.166965
33	6	0	3.009798	-0.531269	3.233995
34	6	0	1.719666	-0.667157	-1.569909
35	6	0	2.427083	-1.850469	-1.844725
36	6	0	2.778510	-2.189081	-3.160318
37	1	0	3.334642	-3.104053	-3.342235
38	6	0	2.433249	-1.358086	-4.218713
39	6	0	1.742084	-0.172346	-3.965120

40	6	0	1.394732	0.157736	-2.658725
41	1	0	4.348786	-2.074118	3.938453
42	1	0	4.263288	-3.348079	1.815241
43	1	0	1.672496	0.831489	2.280762
44	1	0	3.041734	0.044181	4.153973
45	1	0	2.712660	-1.628939	-5.232470
46	1	0	1.470795	0.491819	-4.779920
47	1	0	0.848110	1.075597	-2.477246
48	6	0	-3.739051	-1.716257	-3.114794
49	6	0	-3.688410	-2.434330	-1.926700
50	6	0	-2.904762	-1.980408	-0.855390
51	6	0	-2.159691	-0.792716	-0.957798
52	6	0	-2.237927	-0.084905	-2.167056
53	6	0	-3.011662	-0.531318	-3.233663
54	6	0	-1.718562	-0.667589	1.569480
55	6	0	-2.425976	-1.850854	1.844568
56	6	0	-2.776796	-2.189437	3.160339
57	1	0	-3.332909	-3.104369	3.342516
58	6	0	-2.431027	-1.358448	4.218578
59	6	0	-1.740018	-0.172692	3.964681
60	6	0	-1.393262	0.157391	2.658123
61	1	0	-4.350870	-2.074276	-3.937465
62	1	0	-4.264094	-3.348360	-1.814389
63	1	0	-1.673837	0.831422	-2.281064
64	1	0	-3.044221	0.044167	-4.153597
65	1	0	-2.710034	-1.629282	5.232452
66	1	0	-1.468460	0.491525	4.779349
67	1	0	-0.846893	1.075346	2.476324
68	16	0	2.885990	-3.009267	-0.587187
69	16	0	-2.885707	-3.009366	0.587350

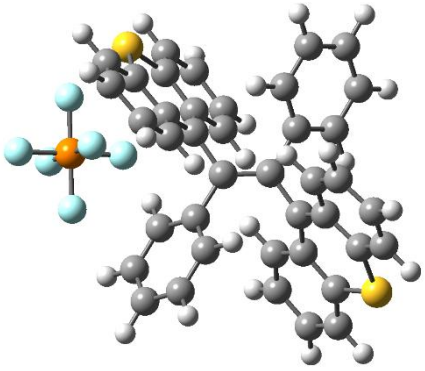
9.5. Stability energy difference between *cis*- and *trans*-radical cation conformers

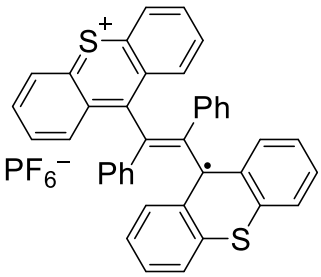




cis-radical cation **A**

ΔG = 0 kcal/mol; stable





trans-radical cation **A**

ΔG = 5.7 kcal/mol

Fig. S8. Stability energy difference between *cis*- and *trans*-radical cation conformers.

Table S8. Calculation data of radical cations

cis-radical cation **A**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.665216	1.301212	0.039601
2	6	0	-1.997570	1.077268	0.203880
3	6	0	0.186710	0.069951	-0.001751
4	6	0	1.046419	-0.204047	1.103446
5	6	0	0.114376	-0.767531	-1.158432
6	6	0	1.745551	-1.434998	1.229475
7	6	0	1.203781	0.743252	2.158805

8	6	0	0.677303	-2.073172	-1.188505
9	6	0	-0.551577	-0.320549	-2.336331
10	6	0	2.569543	-1.687344	2.341918
11	16	0	1.610287	-2.728685	0.102838
12	6	0	2.024492	0.495727	3.231062
13	1	0	0.669183	1.690359	2.109488
14	6	0	0.481278	-2.917364	-2.295224
15	6	0	-0.704526	-1.140943	-3.430886
16	1	0	-0.939465	0.698420	-2.366554
17	6	0	2.711081	-0.730988	3.325018
18	1	0	3.101349	-2.638230	2.415787
19	1	0	2.136513	1.245126	4.015659
20	1	0	0.893649	-3.928614	-2.284017
21	6	0	-0.210672	-2.458696	-3.399875
22	1	0	-1.215703	-0.770368	-4.320646
23	1	0	3.361132	-0.930094	4.179015
24	1	0	-0.351164	-3.116770	-4.259276
25	6	0	-2.359908	-0.350422	0.459958
26	6	0	-1.976358	-0.939034	1.715411
27	6	0	-2.994012	-1.113187	-0.584387
28	6	0	-1.788618	-2.336995	1.875407
29	6	0	-1.710693	-0.116845	2.841038
30	6	0	-2.898709	-2.529154	-0.628167
31	6	0	-3.639088	-0.477211	-1.679687
32	6	0	-1.280548	-2.861255	3.070319
33	16	0	-2.091567	-3.482624	0.592465
34	6	0	-1.239095	-0.645096	4.028611
35	1	0	-1.884182	0.957999	2.757700
36	6	0	-3.401458	-3.251565	-1.721277
37	6	0	-4.157555	-1.197834	-2.736576
38	1	0	-3.732290	0.607971	-1.687209
39	6	0	-0.996228	-2.020794	4.138652
40	1	0	-1.112767	-3.937126	3.160056
41	1	0	-1.040904	0.015533	4.874406
42	1	0	-3.299232	-4.339240	-1.740715
43	6	0	-4.025613	-2.594006	-2.768675

44	1	0	-4.655714	-0.675255	-3.554608
45	1	0	-0.601577	-2.439878	5.065734
46	1	0	-4.417816	-3.167577	-3.610285
47	6	0	0.040570	2.599938	-0.085202
48	6	0	1.208241	2.662885	-0.860592
49	6	0	-0.372319	3.744425	0.618599
50	6	0	1.929407	3.852954	-0.958249
51	1	0	1.569982	1.773663	-1.382778
52	6	0	0.348991	4.928679	0.516620
53	1	0	-1.249698	3.699813	1.267057
54	6	0	1.497927	4.989086	-0.277738
55	1	0	2.838802	3.878953	-1.560222
56	1	0	0.021539	5.809790	1.072050
57	1	0	2.063695	5.920078	-0.350509
58	6	0	-3.075543	2.092606	0.121645
59	6	0	-4.169536	2.004357	0.993395
60	6	0	-3.060137	3.103549	-0.853524
61	6	0	-5.211049	2.929299	0.916414
62	1	0	-4.204780	1.206656	1.740177
63	6	0	-4.103840	4.019185	-0.932468
64	1	0	-2.231978	3.160190	-1.563553
65	6	0	-5.178772	3.939726	-0.042659
66	1	0	-6.053072	2.855209	1.607265
67	1	0	-4.084108	4.797031	-1.698375
68	1	0	-5.996117	4.660761	-0.106921
69	15	0	4.381389	0.289946	-0.821615
70	9	0	3.704005	0.941487	0.501877
71	9	0	4.206194	1.705927	-1.602694
72	9	0	2.907889	-0.169429	-1.349095
73	9	0	5.050457	-0.357840	-2.148449
74	9	0	5.845039	0.750054	-0.301184
75	9	0	4.541101	-1.127204	-0.046431

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trans-radical cation **A**

Standard orientation:

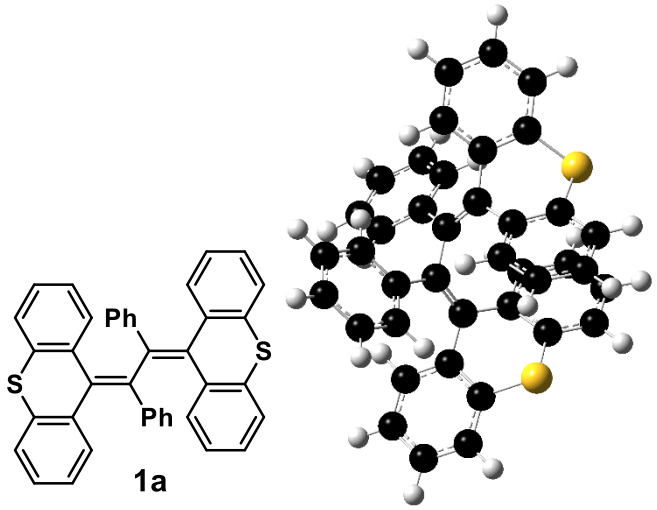
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.459122	0.145435	0.333374
2	6	0	1.599117	0.543128	-0.288107
3	6	0	-0.831956	0.887424	0.194333
4	6	0	-1.323426	1.543562	1.363699
5	6	0	-1.533082	0.875403	-1.041880
6	6	0	-2.578946	2.211803	1.396908
7	6	0	-0.529897	1.594686	2.551588
8	6	0	-2.802905	1.505259	-1.203047
9	6	0	-1.000396	0.197161	-2.181997
10	6	0	-3.033715	2.847372	2.572963
11	16	0	-3.618641	2.336873	0.045936
12	6	0	-0.977502	2.222564	3.685338
13	1	0	0.458785	1.138658	2.553348
14	6	0	-3.486019	1.460419	-2.435629
15	6	0	-1.668203	0.169438	-3.377290
16	1	0	-0.041934	-0.307780	-2.099161
17	6	0	-2.247237	2.842698	3.701031
18	1	0	-4.006594	3.343128	2.577950
19	1	0	-0.349612	2.247897	4.576675
20	1	0	-4.462519	1.939131	-2.530595
21	6	0	-2.922888	0.806462	-3.505520
22	1	0	-1.235684	-0.355962	-4.229469
23	1	0	-2.603016	3.334364	4.608057
24	1	0	-3.456381	0.772196	-4.457025
25	6	0	2.898507	-0.176916	-0.164588
26	6	0	3.081960	-1.489844	-0.730760
27	6	0	3.951070	0.532507	0.525541
28	6	0	4.351087	-2.129061	-0.775010
29	6	0	1.997904	-2.221070	-1.287162
30	6	0	5.296448	0.086385	0.560576
31	6	0	3.661055	1.716438	1.256393

32	6	0	4.502867	-3.413141	-1.312916
33	16	0	5.838577	-1.370754	-0.243130
34	6	0	2.153181	-3.488173	-1.818655
35	1	0	1.004412	-1.781246	-1.286390
36	6	0	6.285394	0.809208	1.239215
37	6	0	4.641035	2.427185	1.926734
38	1	0	2.631470	2.071421	1.306734
39	6	0	3.413169	-4.098317	-1.830276
40	1	0	5.493502	-3.874190	-1.324877
41	1	0	1.285232	-4.008499	-2.227122
42	1	0	7.313707	0.439864	1.241173
43	6	0	5.967745	1.980843	1.911863
44	1	0	4.371773	3.332252	2.473867
45	1	0	3.544659	-5.099589	-2.243386
46	1	0	6.747544	2.535422	2.436271
47	6	0	0.375667	-1.070699	1.191530
48	6	0	-0.699301	-1.951193	1.005676
49	6	0	1.352072	-1.374477	2.151843
50	6	0	-0.783521	-3.127744	1.749250
51	1	0	-1.469260	-1.727849	0.264447
52	6	0	1.263393	-2.550000	2.892376
53	1	0	2.176768	-0.681239	2.332377
54	6	0	0.199704	-3.432013	2.688982
55	1	0	-1.625929	-3.801799	1.587860
56	1	0	2.027259	-2.775894	3.638967
57	1	0	0.134731	-4.353054	3.271780
58	6	0	1.635606	1.751302	-1.165372
59	6	0	2.237353	1.640353	-2.427682
60	6	0	1.068290	2.977063	-0.790242
61	6	0	2.235539	2.718790	-3.309484
62	1	0	2.693748	0.693071	-2.726607
63	6	0	1.076951	4.057894	-1.669998
64	1	0	0.637667	3.099587	0.205919
65	6	0	1.652129	3.929426	-2.934224
66	1	0	2.693644	2.612746	-4.294746
67	1	0	0.638049	5.008659	-1.361351

68	1	0	1.655187	4.776334	-3.623258
69	15	0	-4.461103	-1.564131	-0.020401
70	9	0	-3.676002	-2.857538	0.573093
71	9	0	-5.403194	-2.537818	-0.906769
72	9	0	-3.387112	-1.487021	-1.243080
73	9	0	-5.231772	-0.265534	-0.617324
74	9	0	-5.517328	-1.635734	1.204111
75	9	0	-3.505024	-0.585125	0.867017

9.6. DFT calculation data of 1a, intermediates, and transition states (TS) for the electrochemical cycloaddition mechanism

Table S9. DFT calculation for mechanism

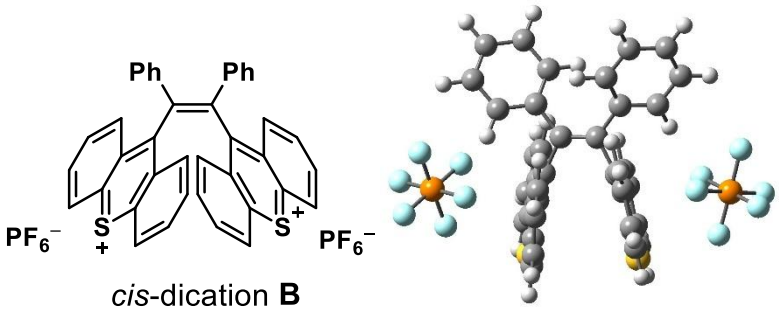


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.752568	-0.946308	0.054032
2	6	0	-0.752568	-0.946309	-0.054031
3	6	0	1.517462	-0.100882	-0.685496
4	6	0	2.992700	-0.221399	-0.798585
5	6	0	0.964545	1.115611	-1.342639
6	6	0	3.809687	0.892153	-0.552165
7	6	0	3.595129	-1.431107	-1.169295
8	6	0	1.580206	2.348372	-1.046421
9	6	0	-0.155478	1.119853	-2.183755
10	6	0	5.202646	0.780337	-0.608893
11	16	0	3.076277	2.436063	-0.093188
12	6	0	4.979693	-1.546144	-1.228300
13	1	0	2.958493	-2.290356	-1.393571
14	6	0	1.021305	3.549684	-1.493223
15	6	0	-0.702678	2.314863	-2.642098
16	1	0	-0.603013	0.171844	-2.482370

17	6	0	5.783913	-0.442303	-0.932461
18	1	0	5.827907	1.652934	-0.407749
19	1	0	5.435691	-2.497849	-1.506725
20	1	0	1.503174	4.497659	-1.243003
21	6	0	-0.132490	3.532889	-2.271788
22	1	0	-1.584893	2.293302	-3.284495
23	1	0	6.871415	-0.527398	-0.975360
24	1	0	-0.565982	4.473779	-2.616387
25	6	0	-1.517462	-0.100883	0.685496
26	6	0	-0.964546	1.115611	1.342640
27	6	0	-2.992701	-0.221400	0.798584
28	6	0	-1.580206	2.348371	1.046420
29	6	0	0.155476	1.119853	2.183757
30	6	0	-3.809687	0.892152	0.552163
31	6	0	-3.595130	-1.431108	1.169295
32	6	0	-1.021306	3.549683	1.493223
33	16	0	-3.076276	2.436062	0.093186
34	6	0	0.702675	2.314863	2.642101
35	1	0	0.603010	0.171843	2.482374
36	6	0	-5.202646	0.780336	0.608889
37	6	0	-4.979694	-1.546144	1.228299
38	1	0	-2.958494	-2.290357	1.393572
39	6	0	0.132487	3.532889	2.271790
40	1	0	-1.503175	4.497659	1.243002
41	1	0	1.584889	2.293302	3.284499
42	1	0	-5.827907	1.652933	0.407744
43	6	0	-5.783914	-0.442304	0.932458
44	1	0	-5.435693	-2.497849	1.506723
45	1	0	0.565979	4.473778	2.616390
46	1	0	-6.871416	-0.527398	0.975356
47	6	0	1.302504	-1.881257	1.088254
48	6	0	2.487215	-1.579245	1.789906
49	6	0	0.575780	-3.008509	1.508954
50	6	0	2.954904	-2.404233	2.806903
51	1	0	3.037023	-0.664750	1.567294
52	6	0	1.047489	-3.839002	2.526003

53	1	0	-0.381653	-3.251360	1.047380
54	6	0	2.246684	-3.550900	3.171214
55	1	0	3.874874	-2.137906	3.331308
56	1	0	0.461901	-4.713095	2.817658
57	1	0	2.615846	-4.198560	3.968826
58	6	0	-1.302503	-1.881259	-1.088253
59	6	0	-0.575778	-3.008510	-1.508953
60	6	0	-2.487214	-1.579248	-1.789906
61	6	0	-1.047487	-3.839004	-2.526001
62	1	0	0.381655	-3.251360	-1.047378
63	6	0	-2.954902	-2.404236	-2.806902
64	1	0	-3.037023	-0.664753	-1.567294
65	6	0	-2.246681	-3.550903	-3.171213
66	1	0	-0.461897	-4.713096	-2.817656
67	1	0	-3.874872	-2.137911	-3.331307
68	1	0	-2.615843	-4.198563	-3.968825



cis-dication **B**

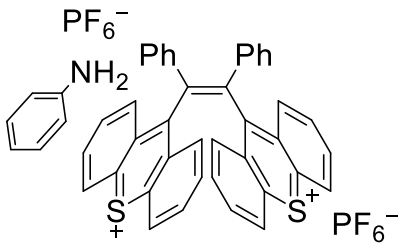
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.486457	2.276284	-0.174012
2	6	0	2.248477	1.170686	0.047648
3	6	0	-0.000542	2.087486	-0.041610
4	6	0	-0.784821	1.987100	-1.225340
5	6	0	-0.521047	1.769563	1.242797

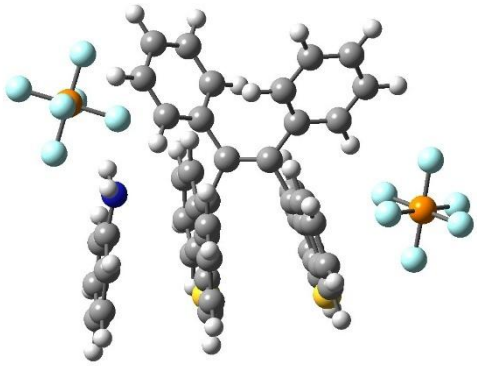
6	6	0	-1.998381	1.239241	-1.249013
7	6	0	-0.340793	2.541966	-2.465447
8	6	0	-1.711850	1.004358	1.408110
9	6	0	0.176778	2.164335	2.425440
10	6	0	-2.695364	1.018663	-2.460708
11	16	0	-2.668265	0.449848	0.109739
12	6	0	-1.053597	2.363407	-3.623122
13	1	0	0.569034	3.137959	-2.489189
14	6	0	-2.126730	0.577620	2.691551
15	6	0	-0.268547	1.791619	3.667716
16	1	0	1.077588	2.773116	2.327451
17	6	0	-2.232072	1.580350	-3.625830
18	1	0	-3.601416	0.410097	-2.449822
19	1	0	-0.702912	2.818448	-4.550329
20	1	0	-3.018723	-0.046249	2.785940
21	6	0	-1.413863	0.968292	3.800409
22	1	0	0.271605	2.113777	4.559290
23	1	0	-2.778914	1.421927	-4.556974
24	1	0	-1.740423	0.649583	4.792005
25	6	0	1.567825	-0.111068	0.438341
26	6	0	0.820770	-0.802461	-0.545260
27	6	0	1.676122	-0.536666	1.792175
28	6	0	-0.047112	-1.889222	-0.217664
29	6	0	0.911412	-0.426933	-1.924193
30	6	0	0.864635	-1.585551	2.309956
31	6	0	2.557513	0.119863	2.705024
32	6	0	-0.819121	-2.524050	-1.212271
33	16	0	-0.263114	-2.467772	1.372996
34	6	0	0.160781	-1.055355	-2.880310
35	1	0	1.606344	0.363832	-2.210097
36	6	0	0.912719	-1.927871	3.678980
37	6	0	2.625460	-0.251412	4.023213
38	1	0	3.196990	0.925623	2.348793
39	6	0	-0.721991	-2.100902	-2.517060
40	1	0	-1.491417	-3.338233	-0.940692
41	1	0	0.247900	-0.757738	-3.926461

42	1	0	0.267393	-2.721882	4.060798
43	6	0	1.786709	-1.274694	4.517751
44	1	0	3.319477	0.254228	4.695579
45	1	0	-1.328681	-2.590195	-3.281426
46	1	0	1.831866	-1.555132	5.571535
47	6	0	2.040208	3.588744	-0.605244
48	6	0	1.693839	4.748981	0.095730
49	6	0	2.910230	3.681810	-1.702472
50	6	0	2.221609	5.983935	-0.283079
51	1	0	1.016077	4.681192	0.947797
52	6	0	3.426742	4.915902	-2.083254
53	1	0	3.174361	2.782090	-2.263568
54	6	0	3.087605	6.069403	-1.371535
55	1	0	1.953555	6.881877	0.277018
56	1	0	4.097827	4.979189	-2.941900
57	1	0	3.496957	7.036193	-1.670906
58	6	0	3.729304	1.079182	-0.068964
59	6	0	4.580564	2.097625	0.391085
60	6	0	4.289801	-0.096212	-0.592091
61	6	0	5.960273	1.950591	0.297389
62	1	0	4.161869	2.998536	0.843852
63	6	0	5.674034	-0.235135	-0.687967
64	1	0	3.649562	-0.915158	-0.928493
65	6	0	6.510972	0.788607	-0.249935
66	1	0	6.612898	2.745653	0.663076
67	1	0	6.090922	-1.155761	-1.099161
68	1	0	7.594874	0.678234	-0.320290
69	1	0	-1.191680	5.272602	1.152839
70	1	0	-1.320723	5.320904	-0.547453
71	7	0	-1.533678	4.822040	0.310452
72	6	0	-2.752622	4.191761	0.391077
73	6	0	-3.508628	3.927624	-0.768639
74	6	0	-3.251405	3.752980	1.635098
75	6	0	-4.703054	3.220271	-0.683926
76	1	0	-3.139042	4.277974	-1.736727
77	6	0	-4.447327	3.047722	1.704409

78	1	0	-2.679739	3.965802	2.543141
79	6	0	-5.176147	2.759116	0.547116
80	1	0	-5.268389	3.017355	-1.596803
81	1	0	-4.810790	2.708298	2.677464
82	1	0	-6.106141	2.191178	0.605359
83	15	0	3.048381	-3.934679	-0.683615
84	9	0	2.464346	-2.886711	-1.785032
85	9	0	3.298265	-5.025415	-1.852996
86	9	0	4.539470	-3.330099	-0.918653
87	9	0	2.799311	-2.829701	0.488689
88	9	0	1.550977	-4.514105	-0.446772
89	9	0	3.632758	-4.966010	0.418594
90	15	0	-4.467620	-2.693563	-0.308758
91	9	0	-5.125318	-3.633973	0.832337
92	9	0	-3.168824	-2.448283	0.646786
93	9	0	-5.182238	-1.389175	0.338220
94	9	0	-5.750537	-2.936584	-1.264724
95	9	0	-3.798432	-1.748391	-1.459857
96	9	0	-3.727184	-3.986500	-0.959414



cis-dication **B** + $PhNH_2$ (H-bonding)



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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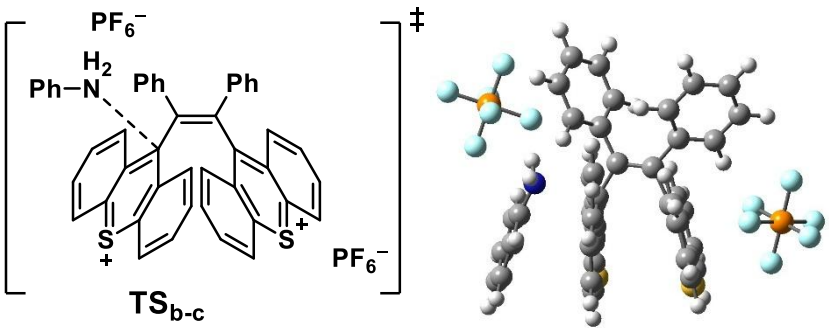
2	6	0	0.884163	1.309220	0.695445
3	6	0	-0.786396	-0.438464	0.409254
4	6	0	-1.231233	-0.796002	-0.897593
5	6	0	-0.395474	-1.415557	1.370454
6	6	0	-1.020574	-2.098126	-1.434994
7	6	0	-1.842173	0.167157	-1.753247
8	6	0	-0.125002	-2.769555	1.021070
9	6	0	-0.220027	-1.043819	2.737100
10	6	0	-1.353973	-2.392480	-2.774256
11	16	0	-0.282597	-3.385309	-0.571397
12	6	0	-2.218501	-0.148163	-3.035091
13	1	0	-2.057278	1.159319	-1.367069
14	6	0	0.368217	-3.678446	1.982179
15	6	0	0.218781	-1.947903	3.671815
16	1	0	-0.434045	-0.016697	3.035962
17	6	0	-1.952614	-1.431903	-3.558295
18	1	0	-1.159546	-3.390531	-3.173395
19	1	0	-2.721623	0.599313	-3.649928
20	1	0	0.596881	-4.705197	1.688254
21	6	0	0.538304	-3.269741	3.286007
22	1	0	0.337503	-1.641980	4.712251
23	1	0	-2.229825	-1.670848	-4.586585
24	1	0	0.911450	-3.977797	4.028208
25	6	0	1.883413	0.209414	0.479326
26	6	0	2.013114	-0.328006	-0.823626
27	6	0	2.612245	-0.261744	1.607110
28	6	0	2.749311	-1.522544	-1.082343
29	6	0	1.396398	0.322055	-1.940043
30	6	0	3.375753	-1.461917	1.553845
31	6	0	2.548211	0.418910	2.860948
32	6	0	2.810158	-2.062458	-2.383415
33	16	0	3.559554	-2.405113	0.135233
34	6	0	1.470815	-0.207938	-3.199371
35	1	0	0.876821	1.267136	-1.777081
36	6	0	4.009873	-1.967712	2.707736
37	6	0	3.204963	-0.060127	3.965588

38	1	0	1.974907	1.341158	2.942076
39	6	0	2.170355	-1.418349	-3.417598
40	1	0	3.369471	-2.982387	-2.564747
41	1	0	0.999500	0.306163	-4.038243
42	1	0	4.575859	-2.899826	2.651673
43	6	0	3.929717	-1.269467	3.892161
44	1	0	3.155610	0.486966	4.907605
45	1	0	2.222095	-1.839320	-4.423363
46	1	0	4.436263	-1.655951	4.778272
47	6	0	-1.504759	2.035427	0.854903
48	6	0	-2.428357	1.933723	1.900618
49	6	0	-1.563703	3.139745	-0.007756
50	6	0	-3.397069	2.920304	2.082545
51	1	0	-2.379259	1.090299	2.590978
52	6	0	-2.543601	4.112322	0.164708
53	1	0	-0.841032	3.229760	-0.823163
54	6	0	-3.460940	4.006505	1.212058
55	1	0	-4.109761	2.832671	2.904620
56	1	0	-2.590713	4.959732	-0.522128
57	1	0	-4.230520	4.769314	1.344213
58	6	0	1.482136	2.659610	0.882958
59	6	0	0.974176	3.584777	1.810140
60	6	0	2.637131	2.986852	0.155206
61	6	0	1.594832	4.817977	1.978831
62	1	0	0.103611	3.331109	2.417548
63	6	0	3.251234	4.226992	0.325366
64	1	0	3.070389	2.276183	-0.552434
65	6	0	2.729172	5.146470	1.232202
66	1	0	1.194461	5.526420	2.706451
67	1	0	4.147128	4.462499	-0.250965
68	1	0	3.212230	6.115796	1.370194
69	1	0	-3.627246	-0.690468	2.204244
70	1	0	-4.061949	-0.220275	0.619042
71	7	0	-3.572025	-0.886180	1.210497
72	6	0	-3.571519	-2.203176	0.833185
73	6	0	-3.914229	-2.576467	-0.483582

74	6	0	-3.164135	-3.206679	1.738815
75	6	0	-3.823736	-3.906180	-0.878632
76	1	0	-4.255187	-1.805494	-1.178707
77	6	0	-3.077991	-4.530872	1.327044
78	1	0	-2.913348	-2.926547	2.766046
79	6	0	-3.389675	-4.891397	0.012558
80	1	0	-4.091168	-4.176189	-1.903130
81	1	0	-2.755302	-5.292543	2.041184
82	1	0	-3.317077	-5.932745	-0.306357
83	15	0	5.629471	0.789320	-1.459057
84	9	0	4.215798	0.897254	-2.260345
85	9	0	6.430888	1.080196	-2.834473
86	9	0	5.562229	2.383294	-1.149556
87	9	0	4.813776	0.499293	-0.076707
88	9	0	5.670981	-0.806118	-1.759602
89	9	0	7.027880	0.683268	-0.651813
90	15	0	-5.970802	1.402336	-0.731204
91	9	0	-5.856579	1.378218	0.892012
92	9	0	-5.873091	3.017542	-0.719648
93	9	0	-7.582668	1.478692	-0.627452
94	9	0	-6.040654	-0.225001	-0.730804
95	9	0	-6.057350	1.406014	-2.348377
96	9	0	-4.340921	1.304429	-0.826982



$TS_{b\text{-}c}$

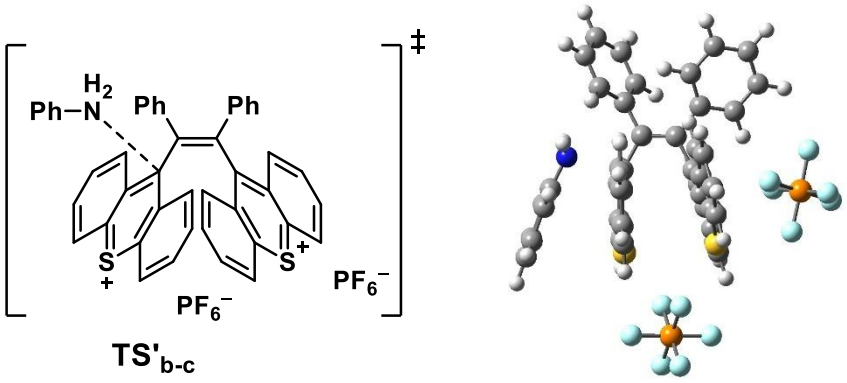
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.548895	0.987520	0.529188
2	6	0	0.774972	1.299483	0.571391
3	6	0	-0.899718	-0.475944	0.328015
4	6	0	-1.167793	-0.908150	-1.023227
5	6	0	-0.445726	-1.399775	1.337810
6	6	0	-0.857605	-2.209596	-1.485394
7	6	0	-1.760752	-0.010860	-1.951288
8	6	0	-0.086688	-2.741092	1.059994
9	6	0	-0.375160	-0.965615	2.689160
10	6	0	-1.081354	-2.569048	-2.829968
11	16	0	-0.135511	-3.445268	-0.515406
12	6	0	-2.007334	-0.379035	-3.254381
13	1	0	-2.068799	0.975908	-1.613932
14	6	0	0.393433	-3.581939	2.086180
15	6	0	0.064690	-1.800433	3.690094
16	1	0	-0.674535	0.056615	2.928463
17	6	0	-1.649288	-1.664359	-3.702444
18	1	0	-0.817168	-3.572756	-3.171075
19	1	0	-2.483687	0.326537	-3.936256
20	1	0	0.688846	-4.606775	1.850421
21	6	0	0.471922	-3.114211	3.381224
22	1	0	0.108279	-1.442820	4.719833
23	1	0	-1.830207	-1.954523	-4.738938
24	1	0	0.839144	-3.772235	4.170947
25	6	0	1.804200	0.209964	0.475539
26	6	0	2.031937	-0.384775	-0.787885
27	6	0	2.488760	-0.170469	1.663988
28	6	0	2.820615	-1.563825	-0.940142
29	6	0	1.476652	0.196407	-1.973035
30	6	0	3.294212	-1.342233	1.718763
31	6	0	2.344090	0.582646	2.868213
32	6	0	2.985689	-2.159775	-2.207295
33	16	0	3.576584	-2.358943	0.368852
34	6	0	1.660187	-0.382259	-3.199079
35	1	0	0.917007	1.128812	-1.890430

36	6	0	3.891207	-1.753772	2.928597
37	6	0	2.966590	0.196880	4.028145
38	1	0	1.737501	1.487123	2.864885
39	6	0	2.406167	-1.579565	-3.312111
40	1	0	3.581065	-3.069535	-2.306451
41	1	0	1.238167	0.081309	-4.091850
42	1	0	4.491074	-2.665936	2.954745
43	6	0	3.734535	-0.987313	4.062129
44	1	0	2.856739	0.798942	4.930790
45	1	0	2.542329	-2.041763	-4.291705
46	1	0	4.214230	-1.299102	4.991584
47	6	0	-1.587815	2.058993	0.575642
48	6	0	-2.462681	2.157257	1.662353
49	6	0	-1.629815	3.039753	-0.425201
50	6	0	-3.370729	3.212074	1.743197
51	1	0	-2.409497	1.430919	2.475930
52	6	0	-2.547977	4.082377	-0.350906
53	1	0	-0.933964	2.985676	-1.266363
54	6	0	-3.420363	4.171800	0.734584
55	1	0	-4.045699	3.278955	2.598092
56	1	0	-2.578193	4.833395	-1.142647
57	1	0	-4.140596	4.989896	0.792258
58	6	0	1.357807	2.669543	0.677865
59	6	0	0.811183	3.662362	1.508771
60	6	0	2.537354	2.952018	-0.030044
61	6	0	1.414891	4.912281	1.598995
62	1	0	-0.077782	3.452440	2.105163
63	6	0	3.134288	4.209039	0.060309
64	1	0	3.006339	2.193867	-0.661102
65	6	0	2.572059	5.193674	0.868950
66	1	0	0.981239	5.671901	2.252202
67	1	0	4.049164	4.405193	-0.500853
68	1	0	3.040768	6.176883	0.943429
69	1	0	-3.229435	-0.451683	1.938500
70	1	0	-3.668986	-0.031000	0.352139
71	7	0	-3.194192	-0.707097	0.953510

72	6	0	-3.417799	-2.044018	0.681151
73	6	0	-3.807213	-2.450552	-0.608872
74	6	0	-3.133546	-3.016326	1.658812
75	6	0	-3.867317	-3.804764	-0.917552
76	1	0	-4.062735	-1.691933	-1.351475
77	6	0	-3.197054	-4.366292	1.334771
78	1	0	-2.855758	-2.696750	2.667148
79	6	0	-3.543063	-4.767367	0.041698
80	1	0	-4.164625	-4.111684	-1.922664
81	1	0	-2.967384	-5.113418	2.097539
82	1	0	-3.585178	-5.828617	-0.210236
83	15	0	5.682192	0.762504	-1.270022
84	9	0	4.320865	0.807911	-2.163141
85	9	0	6.566678	0.991805	-2.605740
86	9	0	5.578487	2.369303	-1.051667
87	9	0	4.783066	0.534393	0.071333
88	9	0	5.760861	-0.845676	-1.482292
89	9	0	7.027414	0.718412	-0.371472
90	15	0	-6.032607	1.252957	-0.534695
91	9	0	-5.597878	1.215879	1.032421
92	9	0	-5.997846	2.870329	-0.512649
93	9	0	-7.592261	1.260721	-0.111663
94	9	0	-6.032979	-0.373141	-0.551969
95	9	0	-6.435268	1.272493	-2.100972
96	9	0	-4.444449	1.228353	-0.951884



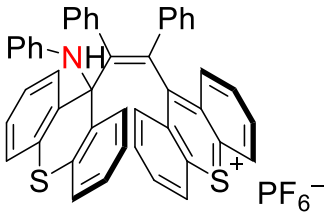
TS'$_{b\text{-}c}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.927537	1.946295	-0.164005
2	6	0	2.362674	0.670380	0.015909
3	6	0	0.429956	2.195620	-0.015082
4	6	0	-0.362849	2.101846	-1.229522
5	6	0	-0.148076	1.880594	1.276843
6	6	0	-1.699249	1.642939	-1.241210
7	6	0	0.200644	2.493023	-2.471690
8	6	0	-1.466958	1.397685	1.439311
9	6	0	0.623095	2.094378	2.449512
10	6	0	-2.419120	1.548521	-2.451632
11	16	0	-2.564065	1.087921	0.146971
12	6	0	-0.513646	2.423971	-3.647132
13	1	0	1.217429	2.879837	-2.497326
14	6	0	-1.959519	1.075922	2.723371
15	6	0	0.125351	1.812308	3.701279
16	1	0	1.639127	2.480185	2.347887
17	6	0	-1.834174	1.937844	-3.638020
18	1	0	-3.440814	1.164468	-2.432476
19	1	0	-0.052879	2.743997	-4.582610
20	1	0	-2.969500	0.670216	2.820571
21	6	0	-1.173215	1.280823	3.837043
22	1	0	0.740095	1.986673	4.585625
23	1	0	-2.400996	1.868640	-4.568189
24	1	0	-1.563481	1.035552	4.826525
25	6	0	1.398069	-0.405296	0.430990
26	6	0	0.508789	-0.929025	-0.534074
27	6	0	1.436935	-0.840794	1.785990
28	6	0	-0.580283	-1.782758	-0.179392
29	6	0	0.685973	-0.627768	-1.922843
30	6	0	0.415202	-1.667213	2.330745
31	6	0	2.477814	-0.417437	2.667128
32	6	0	-1.474637	-2.256227	-1.160337

33	16	0	-0.915636	-2.251549	1.426761
34	6	0	-0.180196	-1.108206	-2.866238
35	1	0	1.541106	-0.022489	-2.226339
36	6	0	0.421866	-2.016115	3.699041
37	6	0	2.497762	-0.802641	3.983388
38	1	0	3.279850	0.212866	2.285837
39	6	0	-1.278288	-1.912815	-2.477130
40	1	0	-2.313173	-2.888911	-0.870025
41	1	0	-0.022950	-0.878046	-3.921085
42	1	0	-0.382430	-2.634767	4.102820
43	6	0	1.454561	-1.597807	4.507089
44	1	0	3.314901	-0.483128	4.631221
45	1	0	-1.976511	-2.280649	-3.231501
46	1	0	1.465924	-1.888274	5.559025
47	6	0	2.879456	3.023046	-0.578240
48	6	0	3.194309	4.077543	0.288815
49	6	0	3.554082	2.930342	-1.803760
50	6	0	4.152549	5.025598	-0.069249
51	1	0	2.727206	4.140588	1.274128
52	6	0	4.507100	3.880026	-2.162041
53	1	0	3.339042	2.095454	-2.475575
54	6	0	4.808109	4.931546	-1.296010
55	1	0	4.393747	5.835629	0.621520
56	1	0	5.022496	3.792839	-3.120330
57	1	0	5.558503	5.673769	-1.574655
58	6	0	3.762313	0.180584	-0.166535
59	6	0	4.885616	0.917421	0.246218
60	6	0	3.955441	-1.100309	-0.709009
61	6	0	6.165487	0.396677	0.084716
62	1	0	4.762702	1.893581	0.716981
63	6	0	5.241391	-1.614170	-0.873509
64	1	0	3.103793	-1.715562	-1.006916
65	6	0	6.349277	-0.865547	-0.484219
66	1	0	7.027701	0.979422	0.414575
67	1	0	5.364933	-2.611458	-1.298054
68	1	0	7.356179	-1.268847	-0.608590

69	1	0	0.747880	4.660868	1.005879
70	1	0	0.651367	4.779544	-0.676935
71	7	0	0.218278	4.409959	0.171380
72	6	0	-1.159306	4.599999	0.278924
73	6	0	-1.943597	4.738265	-0.877130
74	6	0	-1.775384	4.519877	1.538856
75	6	0	-3.330678	4.750359	-0.771697
76	1	0	-1.456762	4.825463	-1.851962
77	6	0	-3.162976	4.532699	1.629469
78	1	0	-1.158766	4.438064	2.438026
79	6	0	-3.945153	4.627196	0.476122
80	1	0	-3.937107	4.847959	-1.674400
81	1	0	-3.638409	4.460196	2.609688
82	1	0	-5.033948	4.625519	0.552010
83	15	0	1.886853	-4.541390	-0.609305
84	9	0	1.492887	-3.432466	-1.734690
85	9	0	1.814428	-5.706461	-1.730881
86	9	0	3.459818	-4.303978	-0.947034
87	9	0	1.962497	-3.363454	0.515007
88	9	0	0.313887	-4.753894	-0.271636
89	9	0	2.286656	-5.634517	0.515812
90	15	0	-5.065050	-1.635850	-0.289898
91	9	0	-5.929032	-2.412251	0.838722
92	9	0	-3.758352	-1.684982	0.681802
93	9	0	-5.486925	-0.209890	0.354300
94	9	0	-6.360451	-1.592976	-1.261412
95	9	0	-4.193794	-0.860855	-1.430026
96	9	0	-4.620549	-3.060662	-0.938076



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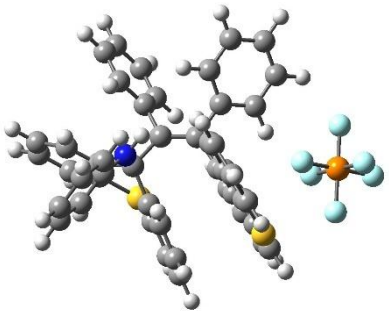
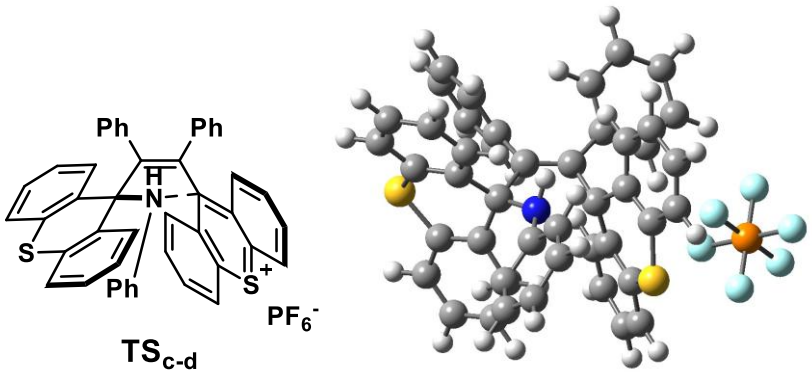


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.401550	-1.032141	-0.294991
2	6	0	-0.073258	-0.921835	-0.536450
3	6	0	-2.346574	0.157061	0.105431
4	6	0	-3.605585	-0.430410	0.776974
5	6	0	-1.665246	1.117405	1.095334
6	6	0	-3.514341	-0.980934	2.060765
7	6	0	-4.830262	-0.522753	0.108082
8	6	0	-1.468123	0.719765	2.423949
9	6	0	-1.210105	2.385881	0.710800
10	6	0	-4.596946	-1.649083	2.641928
11	16	0	-2.002618	-0.876294	2.976466
12	6	0	-5.915892	-1.178093	0.682721
13	1	0	-4.929037	-0.104507	-0.893491
14	6	0	-0.803652	1.547751	3.334562
15	6	0	-0.559259	3.220070	1.615854
16	1	0	-1.340248	2.718506	-0.319692
17	6	0	-5.796351	-1.756209	1.946394
18	1	0	-4.498164	-2.071041	3.644325
19	1	0	-6.857115	-1.245195	0.134301
20	1	0	-0.658183	1.213416	4.364169
21	6	0	-0.343665	2.795930	2.928039
22	1	0	-0.215080	4.203876	1.291216

23	1	0	-6.641608	-2.277298	2.399740
24	1	0	0.171602	3.442546	3.641283
25	6	0	0.786115	0.264066	-0.215066
26	6	0	1.428837	0.297298	1.049409
27	6	0	0.998024	1.237880	-1.230762
28	6	0	2.277045	1.372145	1.444678
29	6	0	1.249130	-0.772913	1.980786
30	6	0	1.773449	2.408966	-1.004422
31	6	0	0.386663	1.094084	-2.512955
32	6	0	2.894815	1.377123	2.712029
33	16	0	2.602569	2.726376	0.456746
34	6	0	1.867816	-0.763680	3.202980
35	1	0	0.610200	-1.611151	1.703485
36	6	0	1.882111	3.405618	-1.998014
37	6	0	0.503213	2.066414	-3.473199
38	1	0	-0.159955	0.178977	-2.740978
39	6	0	2.691561	0.323528	3.572702
40	1	0	3.540826	2.209720	2.996566
41	1	0	1.722619	-1.594976	3.894187
42	1	0	2.471188	4.304027	-1.801745
43	6	0	1.247603	3.238153	-3.207646
44	1	0	0.031767	1.931538	-4.447434
45	1	0	3.178815	0.327117	4.549430
46	1	0	1.333296	4.012938	-3.971537
47	6	0	-2.065350	-2.356761	-0.504289
48	6	0	-3.074992	-2.546093	-1.456937
49	6	0	-1.668627	-3.440877	0.287571
50	6	0	-3.666587	-3.796402	-1.619088
51	1	0	-3.388557	-1.712490	-2.088612
52	6	0	-2.264369	-4.691334	0.128216
53	1	0	-0.883145	-3.299497	1.034246
54	6	0	-3.264238	-4.872560	-0.826307
55	1	0	-4.445454	-3.931997	-2.372244
56	1	0	-1.943442	-5.527122	0.753108
57	1	0	-3.730149	-5.851678	-0.954269
58	6	0	0.711206	-1.993952	-1.244728

59	6	0	0.195229	-2.559959	-2.423982
60	6	0	1.979960	-2.399407	-0.808363
61	6	0	0.896968	-3.545152	-3.108782
62	1	0	-0.765815	-2.219148	-2.811987
63	6	0	2.678105	-3.395735	-1.494015
64	1	0	2.450563	-1.946425	0.064542
65	6	0	2.137896	-3.978274	-2.636556
66	1	0	0.474674	-3.972898	-4.020194
67	1	0	3.660759	-3.698933	-1.131196
68	1	0	2.688542	-4.755040	-3.170895
69	1	0	-2.139976	0.510224	-1.957093
70	7	0	-2.678340	0.802948	-1.152023
71	6	0	-3.449181	1.938689	-1.338535
72	6	0	-3.495891	2.498668	-2.631295
73	6	0	-4.184801	2.562852	-0.314250
74	6	0	-4.254029	3.634576	-2.888758
75	1	0	-2.926302	2.025126	-3.435586
76	6	0	-4.939530	3.702792	-0.589562
77	1	0	-4.167994	2.168491	0.701456
78	6	0	-4.985480	4.250031	-1.870367
79	1	0	-4.271163	4.044026	-3.901340
80	1	0	-5.500676	4.168863	0.223543
81	1	0	-5.579869	5.142143	-2.073546
82	15	0	5.178993	-0.292741	-0.054092
83	9	0	4.235890	-0.953719	1.099194
84	9	0	6.499032	-0.793628	0.739924
85	9	0	5.140576	-1.689393	-0.878792
86	9	0	3.844222	0.208142	-0.845327
87	9	0	5.209384	1.104196	0.774985
88	9	0	6.106468	0.368169	-1.205418



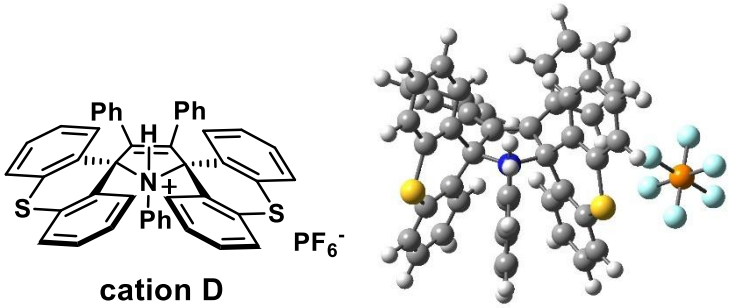
$TS_{c\text{-}d}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.627223	-0.970240	-0.304207
2	6	0	-0.308700	-1.055102	-0.585704
3	6	0	-2.194788	0.432348	0.066615
4	6	0	-3.514101	0.689499	-0.687352
5	6	0	-2.370689	0.534824	1.590143
6	6	0	-4.744056	0.230958	-0.186790
7	6	0	-3.518469	1.298612	-1.951942
8	6	0	-3.512932	0.017411	2.224556
9	6	0	-1.384512	1.099316	2.410677
10	6	0	-5.918384	0.355053	-0.941184
11	16	0	-4.923385	-0.587095	1.360703
12	6	0	-4.682958	1.419643	-2.704017
13	1	0	-2.606223	1.693368	-2.399579
14	6	0	-3.611406	-0.003164	3.623147
15	6	0	-1.487606	1.101459	3.796900
16	1	0	-0.515326	1.575241	1.963938
17	6	0	-5.889387	0.936662	-2.200844
18	1	0	-6.861455	-0.009057	-0.527133
19	1	0	-4.640973	1.893473	-3.685737
20	1	0	-4.511735	-0.410034	4.088819
21	6	0	-2.596108	0.520979	4.410377
22	1	0	-0.694435	1.555855	4.393050

23	1	0	-6.809533	1.024044	-2.781157
24	1	0	-2.686770	0.503869	5.497866
25	6	0	0.552813	0.166483	-0.366501
26	6	0	1.189199	0.248484	0.948609
27	6	0	1.255239	0.745215	-1.516311
28	6	0	2.067976	1.298617	1.286962
29	6	0	0.918485	-0.729732	1.935645
30	6	0	2.133239	1.838348	-1.367852
31	6	0	0.948796	0.309700	-2.826109
32	6	0	2.577979	1.407679	2.590205
33	16	0	2.571586	2.526828	0.165802
34	6	0	1.458805	-0.643858	3.201441
35	1	0	0.262728	-1.566012	1.694221
36	6	0	2.677037	2.470689	-2.499594
37	6	0	1.493314	0.929340	-3.935109
38	1	0	0.262628	-0.527264	-2.966718
39	6	0	2.271626	0.447608	3.537741
40	1	0	3.245960	2.234100	2.840477
41	1	0	1.237510	-1.414533	3.940936
42	1	0	3.357306	3.315325	-2.370227
43	6	0	2.360569	2.019929	-3.768225
44	1	0	1.247536	0.570142	-4.935202
45	1	0	2.687127	0.533760	4.543619
46	1	0	2.794693	2.513644	-4.639471
47	6	0	-2.537847	-2.143617	-0.243798
48	6	0	-3.516596	-2.370587	-1.220862
49	6	0	-2.433232	-3.020801	0.841940
50	6	0	-4.391091	-3.446467	-1.097673
51	1	0	-3.590473	-1.703292	-2.083233
52	6	0	-3.311660	-4.096109	0.963551
53	1	0	-1.669558	-2.847665	1.604516
54	6	0	-4.296659	-4.304898	-0.000728
55	1	0	-5.151500	-3.616512	-1.862589
56	1	0	-3.228153	-4.770445	1.818082
57	1	0	-4.988222	-5.144309	0.096825
58	6	0	0.398547	-2.287036	-1.048453

59	6	0	-0.226126	-3.167231	-1.949070
60	6	0	1.721273	-2.557551	-0.660920
61	6	0	0.431063	-4.305194	-2.406237
62	1	0	-1.227684	-2.949280	-2.318378
63	6	0	2.374968	-3.701316	-1.120502
64	1	0	2.265221	-1.885290	0.002405
65	6	0	1.731727	-4.583826	-1.984619
66	1	0	-0.075076	-4.972827	-3.106311
67	1	0	3.400947	-3.885481	-0.799469
68	1	0	2.246981	-5.477280	-2.342910
69	1	0	-1.097457	1.065403	-1.462251
70	7	0	-1.128223	1.309564	-0.471779
71	6	0	-1.120244	2.745016	-0.437322
72	6	0	-0.545155	3.375577	-1.554311
73	6	0	-1.641759	3.533318	0.595657
74	6	0	-0.392908	4.756864	-1.586864
75	1	0	-0.231815	2.781426	-2.416199
76	6	0	-1.499460	4.918950	0.542492
77	1	0	-2.177665	3.098422	1.434215
78	6	0	-0.852724	5.536174	-0.526474
79	1	0	0.073139	5.223050	-2.457028
80	1	0	-1.908470	5.520623	1.356159
81	1	0	-0.736705	6.621069	-0.547922
82	15	0	5.093895	-0.761376	0.435976
83	9	0	3.934288	-1.238844	1.472442
84	9	0	6.229427	-1.318561	1.449890
85	9	0	5.029190	-2.215973	-0.290088
86	9	0	3.949558	-0.213561	-0.583078
87	9	0	5.150484	0.688318	1.161041
88	9	0	6.243734	-0.291792	-0.605469



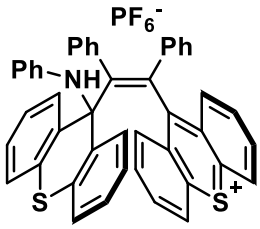
cation D

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.534186	-1.496015	0.072769
2	6	0	-0.226641	-1.369734	-0.238353
3	6	0	-2.317758	-0.194126	-0.045924
4	6	0	-3.291334	-0.204293	-1.227377
5	6	0	-2.945425	0.258242	1.261672
6	6	0	-4.298564	0.762398	-1.359306
7	6	0	-3.095556	-1.110481	-2.283562
8	6	0	-3.938644	1.250672	1.300372
9	6	0	-2.483974	-0.250800	2.486190
10	6	0	-5.078184	0.817959	-2.525169
11	16	0	-4.663666	1.966924	-0.130713
12	6	0	-3.869637	-1.057330	-3.434919
13	1	0	-2.323188	-1.877698	-2.200427
14	6	0	-4.395890	1.757547	2.525039
15	6	0	-2.936644	0.247462	3.700790
16	1	0	-1.748157	-1.051183	2.499333
17	6	0	-4.861390	-0.081648	-3.558249
18	1	0	-5.865726	1.570253	-2.609218
19	1	0	-3.698437	-1.776998	-4.236608
20	1	0	-5.164556	2.533583	2.533386
21	6	0	-3.884954	1.271562	3.719462
22	1	0	-2.546806	-0.164338	4.632763
23	1	0	-5.475940	-0.028988	-4.458627

24	1	0	-4.244782	1.676995	4.666757
25	6	0	0.224697	0.079834	-0.379121
26	6	0	0.946543	0.567993	0.868556
27	6	0	0.952845	0.386968	-1.680761
28	6	0	1.701911	1.751383	0.873450
29	6	0	0.812866	-0.129385	2.079938
30	6	0	1.724015	1.547290	-1.843079
31	6	0	0.744225	-0.437618	-2.799105
32	6	0	2.216192	2.261330	2.073952
33	16	0	2.040004	2.702297	-0.558948
34	6	0	1.328043	0.369212	3.268514
35	1	0	0.303887	-1.092215	2.094962
36	6	0	2.281331	1.853571	-3.093598
37	6	0	1.291830	-0.130585	-4.037708
38	1	0	0.130359	-1.334350	-2.703005
39	6	0	2.011462	1.587183	3.267963
40	1	0	2.796889	3.185764	2.058848
41	1	0	1.199805	-0.194484	4.193857
42	1	0	2.897122	2.749096	-3.202389
43	6	0	2.065666	1.022515	-4.183065
44	1	0	1.115821	-0.791221	-4.887727
45	1	0	2.415284	1.995759	4.196091
46	1	0	2.509794	1.272046	-5.148410
47	6	0	-2.203037	-2.720337	0.586642
48	6	0	-3.552166	-3.013899	0.337272
49	6	0	-1.484190	-3.574417	1.443844
50	6	0	-4.146276	-4.150000	0.888753
51	1	0	-4.162517	-2.363258	-0.288083
52	6	0	-2.079876	-4.703285	1.993974
53	1	0	-0.448096	-3.340562	1.696341
54	6	0	-3.413902	-5.002683	1.709942
55	1	0	-5.195317	-4.361776	0.673644
56	1	0	-1.500943	-5.348399	2.657556
57	1	0	-3.882638	-5.889425	2.141001
58	6	0	0.745229	-2.472931	-0.434683
59	6	0	0.327403	-3.632604	-1.111607

60	6	0	2.083150	-2.374757	-0.028115
61	6	0	1.212670	-4.679293	-1.340602
62	1	0	-0.701698	-3.707080	-1.470838
63	6	0	2.967939	-3.430262	-0.256653
64	1	0	2.455148	-1.481850	0.472885
65	6	0	2.536612	-4.584872	-0.904647
66	1	0	0.870609	-5.570883	-1.869689
67	1	0	4.003340	-3.330394	0.071409
68	1	0	3.232721	-5.406859	-1.083257
69	1	0	-1.299577	0.743869	-1.554331
70	7	0	-1.177444	0.781452	-0.534108
71	6	0	-1.281908	2.203218	-0.214750
72	6	0	-1.463920	3.068919	-1.292542
73	6	0	-1.193238	2.677495	1.094118
74	6	0	-1.554818	4.437620	-1.062131
75	1	0	-1.532198	2.671884	-2.309228
76	6	0	-1.286697	4.050139	1.309764
77	1	0	-1.047912	2.001616	1.936905
78	6	0	-1.464830	4.927824	0.239888
79	1	0	-1.695161	5.119429	-1.902196
80	1	0	-1.216664	4.434228	2.328823
81	1	0	-1.534565	6.001481	0.424080
82	15	0	5.193244	0.045478	0.417140
83	9	0	4.232900	-0.512818	1.609133
84	9	0	6.469578	-0.031654	1.414650
85	9	0	5.476661	-1.484888	-0.056623
86	9	0	3.910817	0.110236	-0.579946
87	9	0	4.909856	1.568300	0.893376
88	9	0	6.147990	0.590181	-0.774525



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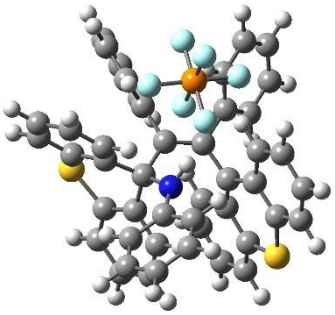
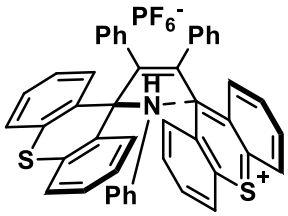


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.136077	0.942698	0.637880
2	6	0	0.383044	0.015435	1.479864
3	6	0	0.231959	0.991619	-0.894243
4	6	0	-0.814734	1.836574	-1.642005
5	6	0	1.635209	1.606421	-1.098506
6	6	0	-0.787754	3.236996	-1.589796
7	6	0	-1.874095	1.218068	-2.314193
8	6	0	1.841363	2.987758	-0.986752
9	6	0	2.744072	0.807245	-1.414347
10	6	0	-1.819909	3.994692	-2.154367
11	16	0	0.502007	4.119739	-0.762099
12	6	0	-2.904904	1.966838	-2.874822
13	1	0	-1.927567	0.130492	-2.357314
14	6	0	3.128065	3.534989	-1.093842
15	6	0	4.017877	1.347173	-1.551407
16	1	0	2.609679	-0.266872	-1.540991
17	6	0	-2.884270	3.358665	-2.784170
18	1	0	-1.782945	5.085087	-2.100483
19	1	0	-3.732590	1.457539	-3.371000
20	1	0	3.262086	4.614935	-0.999535
21	6	0	4.216809	2.715792	-1.363384
22	1	0	4.857329	0.694369	-1.798884
23	1	0	-3.690834	3.953691	-3.216842

24	1	0	5.213901	3.150742	-1.456030
25	6	0	1.512951	-0.910008	1.145023
26	6	0	2.834543	-0.401097	1.279789
27	6	0	1.232324	-2.273442	0.832610
28	6	0	3.987625	-1.172511	0.950832
29	6	0	3.052820	0.932950	1.751320
30	6	0	2.242760	-3.176283	0.401163
31	6	0	-0.105495	-2.765239	0.888130
32	6	0	5.281509	-0.628865	1.082080
33	16	0	3.911155	-2.770378	0.332285
34	6	0	4.316249	1.444998	1.888574
35	1	0	2.191641	1.544968	2.014436
36	6	0	1.916728	-4.488198	-0.000764
37	6	0	-0.408989	-4.053498	0.525248
38	1	0	-0.904520	-2.105685	1.221575
39	6	0	5.438750	0.658423	1.545906
40	1	0	6.153280	-1.231146	0.818442
41	1	0	4.455679	2.461844	2.257255
42	1	0	2.703877	-5.160775	-0.347943
43	6	0	0.609123	-4.916859	0.063752
44	1	0	-1.441437	-4.397940	0.581545
45	1	0	6.444103	1.070951	1.649074
46	1	0	0.363129	-5.936200	-0.238960
47	6	0	-1.090468	1.946902	1.213445
48	6	0	-2.436821	2.042703	0.834502
49	6	0	-0.612512	2.810240	2.209731
50	6	0	-3.272104	2.985816	1.431512
51	1	0	-2.846242	1.361466	0.091388
52	6	0	-1.447098	3.750852	2.806695
53	1	0	0.435252	2.750928	2.513727
54	6	0	-2.782613	3.844390	2.415208
55	1	0	-4.319553	3.040248	1.127503
56	1	0	-1.050968	4.415175	3.577310
57	1	0	-3.441599	4.581153	2.879356
58	6	0	-0.119546	-0.185724	2.881630
59	6	0	-1.496629	-0.349074	3.110565

60	6	0	0.759402	-0.268540	3.969261
61	6	0	-1.978878	-0.546214	4.400053
62	1	0	-2.189327	-0.330695	2.267762
63	6	0	0.270083	-0.459706	5.262650
64	1	0	1.837351	-0.175610	3.823820
65	6	0	-1.098278	-0.592944	5.483251
66	1	0	-3.052030	-0.670484	4.558140
67	1	0	0.969030	-0.507145	6.099968
68	1	0	-1.479553	-0.744778	6.494962
69	1	0	-0.457382	-0.953872	-0.840901
70	7	0	0.232549	-0.391656	-1.331158
71	6	0	0.448193	-0.841740	-2.632654
72	6	0	0.309943	-2.226163	-2.856654
73	6	0	0.822266	-0.021838	-3.710803
74	6	0	0.543334	-2.769668	-4.114054
75	1	0	0.010105	-2.868819	-2.024767
76	6	0	1.061156	-0.583527	-4.965491
77	1	0	0.921846	1.055730	-3.582747
78	6	0	0.926982	-1.953528	-5.181004
79	1	0	0.425392	-3.845693	-4.260144
80	1	0	1.350447	0.072789	-5.789317
81	1	0	1.112260	-2.380704	-6.167934
82	15	0	-3.656202	-1.760790	-0.254769
83	9	0	-2.323834	-0.831925	-0.014246
84	9	0	-2.811337	-2.644749	-1.323289
85	9	0	-3.162111	-2.741675	0.946840
86	9	0	-4.457547	-0.853390	0.824307
87	9	0	-4.125388	-0.763463	-1.443620
88	9	0	-4.959676	-2.682961	-0.486692



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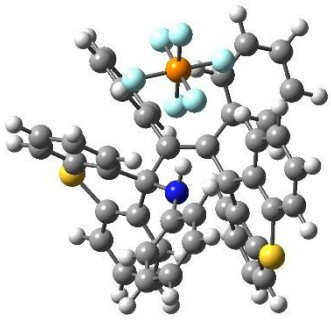
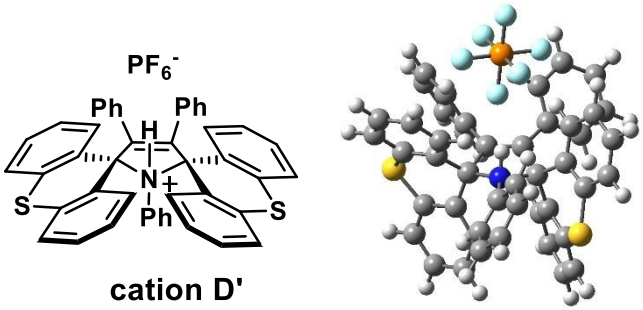


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.280423	0.991795	0.710812
2	6	0	0.081986	-0.098545	1.419818
3	6	0	0.410625	1.194226	-0.676144
4	6	0	-0.575875	1.747499	-1.716896
5	6	0	1.628595	2.128566	-0.550094
6	6	0	-0.879729	3.119718	-1.745290
7	6	0	-1.253282	0.908151	-2.610142
8	6	0	1.442116	3.514658	-0.421059
9	6	0	2.948762	1.658050	-0.555956
10	6	0	-1.853777	3.619667	-2.615891
11	16	0	-0.123743	4.291662	-0.664029
12	6	0	-2.221039	1.404987	-3.478924
13	1	0	-1.067162	-0.164745	-2.623920
14	6	0	2.527940	4.365812	-0.172156
15	6	0	4.033046	2.502543	-0.348580
16	1	0	3.149644	0.606319	-0.737776
17	6	0	-2.530486	2.762823	-3.475723
18	1	0	-2.073624	4.689421	-2.620403
19	1	0	-2.741610	0.719576	-4.148486
20	1	0	2.353027	5.438917	-0.068020
21	6	0	3.819408	3.860201	-0.113554
22	1	0	5.044215	2.092158	-0.364929
23	1	0	-3.290867	3.160452	-4.150347

24	1	0	4.658719	4.533171	0.070774
25	6	0	1.237877	-0.927281	0.920724
26	6	0	2.554079	-0.496350	1.403067
27	6	0	1.048824	-2.351789	0.633961
28	6	0	3.740735	-1.170945	1.040739
29	6	0	2.668957	0.615897	2.272619
30	6	0	2.113029	-3.147960	0.156538
31	6	0	-0.238506	-2.930205	0.689733
32	6	0	4.989796	-0.702798	1.475856
33	16	0	3.755523	-2.579579	0.015570
34	6	0	3.896458	1.042747	2.739596
35	1	0	1.770271	1.147905	2.583372
36	6	0	1.880299	-4.463465	-0.276506
37	6	0	-0.460669	-4.230478	0.276318
38	1	0	-1.078883	-2.341188	1.047357
39	6	0	5.064867	0.393791	2.319415
40	1	0	5.899128	-1.225798	1.172189
41	1	0	3.952711	1.895113	3.417740
42	1	0	2.712061	-5.064979	-0.649657
43	6	0	0.603919	-4.997109	-0.218663
44	1	0	-1.467501	-4.645587	0.327407
45	1	0	6.040717	0.737957	2.667121
46	1	0	0.434350	-6.022423	-0.552425
47	6	0	-1.294254	1.956306	1.210085
48	6	0	-2.547991	2.088081	0.597438
49	6	0	-0.991197	2.736161	2.332989
50	6	0	-3.466649	3.013791	1.086792
51	1	0	-2.812393	1.449801	-0.246874
52	6	0	-1.912834	3.659781	2.819435
53	1	0	-0.017390	2.627189	2.817412
54	6	0	-3.149356	3.806923	2.190495
55	1	0	-4.442542	3.109080	0.606174
56	1	0	-1.663489	4.269140	3.690413
57	1	0	-3.872626	4.532698	2.568197
58	6	0	-0.569657	-0.541233	2.688080
59	6	0	-1.971747	-0.543843	2.786300

60	6	0	0.180843	-1.039624	3.762791
61	6	0	-2.598415	-0.995365	3.943320
62	1	0	-2.574298	-0.225655	1.935746
63	6	0	-0.452609	-1.484612	4.923584
64	1	0	1.269629	-1.088868	3.708180
65	6	0	-1.841713	-1.458145	5.021353
66	1	0	-3.688975	-0.997196	3.995842
67	1	0	0.149629	-1.860247	5.753080
68	1	0	-2.335866	-1.811381	5.928579
69	1	0	-0.083040	-0.737440	-0.879799
70	7	0	0.787427	-0.205068	-0.981143
71	6	0	1.385424	-0.662851	-2.198776
72	6	0	1.104560	-1.993242	-2.549739
73	6	0	2.172519	0.120613	-3.052067
74	6	0	1.699727	-2.565559	-3.669020
75	1	0	0.387673	-2.570841	-1.962049
76	6	0	2.748151	-0.459873	-4.180039
77	1	0	2.325228	1.181836	-2.869045
78	6	0	2.543099	-1.806560	-4.478864
79	1	0	1.482165	-3.606321	-3.916494
80	1	0	3.361138	0.159688	-4.837204
81	1	0	3.009392	-2.251516	-5.359523
82	15	0	-3.532878	-1.723772	-0.743376
83	9	0	-2.143952	-0.896376	-0.446190
84	9	0	-2.686167	-2.776241	-1.643212
85	9	0	-3.258341	-2.631547	0.578231
86	9	0	-4.341730	-0.652467	0.170025
87	9	0	-3.788559	-0.803404	-2.051307
88	9	0	-4.895622	-2.540769	-1.031470



cation D'

Standard orientation:

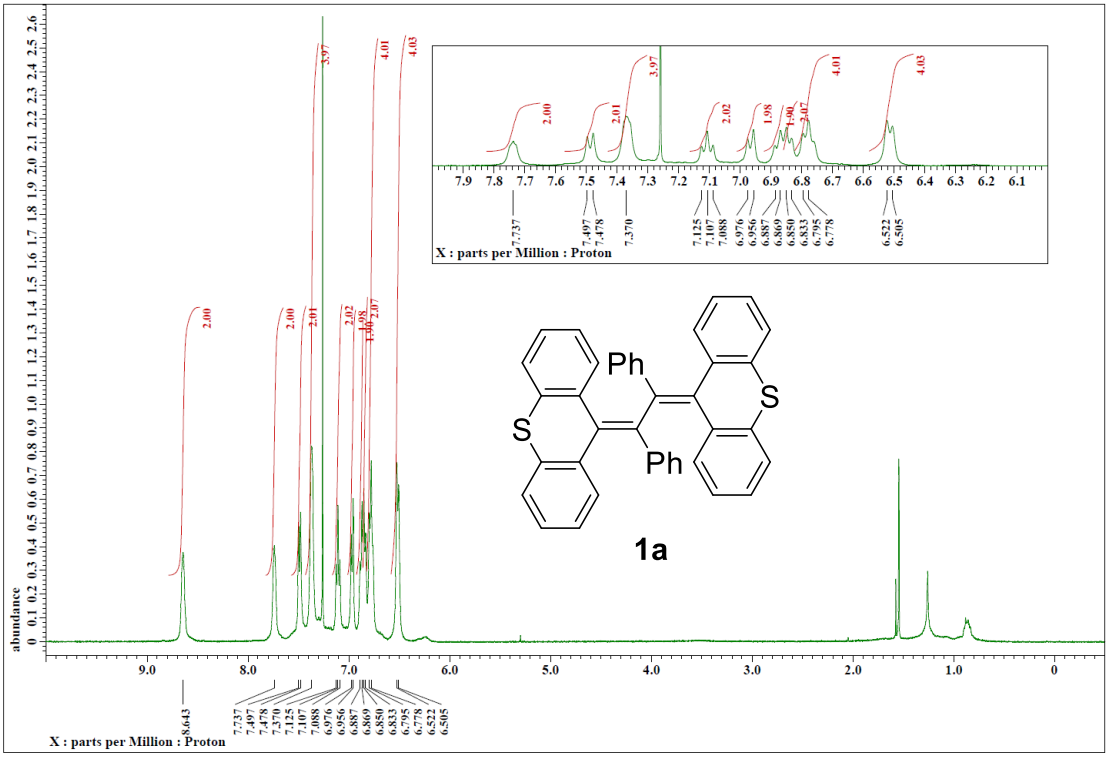
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.397539	0.990854	0.737201
2	6	0	0.062032	-0.105921	1.366473
3	6	0	0.317680	1.278295	-0.609545
4	6	0	-0.672140	1.606148	-1.742401
5	6	0	1.349677	2.413799	-0.438203
6	6	0	-1.205367	2.905298	-1.845272
7	6	0	-1.140238	0.649105	-2.654770
8	6	0	0.897094	3.746593	-0.382761
9	6	0	2.728340	2.215836	-0.277977
10	6	0	-2.183312	3.211194	-2.797982
11	16	0	-0.745569	4.232433	-0.784413
12	6	0	-2.105629	0.955820	-3.608969
13	1	0	-0.791813	-0.381336	-2.647836
14	6	0	1.769538	4.795971	-0.063362
15	6	0	3.603974	3.257951	0.007054
16	1	0	3.158664	1.226456	-0.383108
17	6	0	-2.639676	2.238537	-3.676822
18	1	0	-2.575463	4.228951	-2.852303
19	1	0	-2.445935	0.175193	-4.289645
20	1	0	1.381616	5.816247	-0.025670
21	6	0	3.117984	4.554512	0.153315
22	1	0	4.667742	3.043013	0.120756
23	1	0	-3.401374	2.487118	-4.417698

24	1	0	3.788960	5.380552	0.395055
25	6	0	1.244037	-0.750292	0.646885
26	6	0	2.566973	-0.311990	1.257026
27	6	0	1.178725	-2.257065	0.474282
28	6	0	3.785280	-0.897646	0.874878
29	6	0	2.603934	0.689402	2.243047
30	6	0	2.298389	-2.987880	0.038654
31	6	0	-0.040248	-2.936071	0.612738
32	6	0	4.999953	-0.413699	1.380106
33	16	0	3.881485	-2.266112	-0.224790
34	6	0	3.802935	1.141298	2.775298
35	1	0	1.676642	1.149470	2.585175
36	6	0	2.181656	-4.347621	-0.275174
37	6	0	-0.157791	-4.284851	0.299998
38	1	0	-0.925915	-2.401379	0.942279
39	6	0	5.009728	0.610316	2.317336
40	1	0	5.937160	-0.873139	1.058431
41	1	0	3.795420	1.926031	3.533145
42	1	0	3.061191	-4.899894	-0.613380
43	6	0	0.956578	-4.990847	-0.154440
44	1	0	-1.125567	-4.776584	0.404705
45	1	0	5.960643	0.972760	2.712128
46	1	0	0.876420	-6.050277	-0.404999
47	6	0	-1.459448	1.886615	1.251268
48	6	0	-2.732049	1.905010	0.664672
49	6	0	-1.179258	2.725459	2.335048
50	6	0	-3.701453	2.781171	1.145162
51	1	0	-2.961197	1.224407	-0.157135
52	6	0	-2.152872	3.601954	2.810099
53	1	0	-0.186925	2.700905	2.793256
54	6	0	-3.411347	3.636798	2.209817
55	1	0	-4.693035	2.792490	0.688012
56	1	0	-1.927062	4.261499	3.650370
57	1	0	-4.173885	4.325347	2.579866
58	6	0	-0.475626	-0.677130	2.627424
59	6	0	-1.865531	-0.712981	2.832317

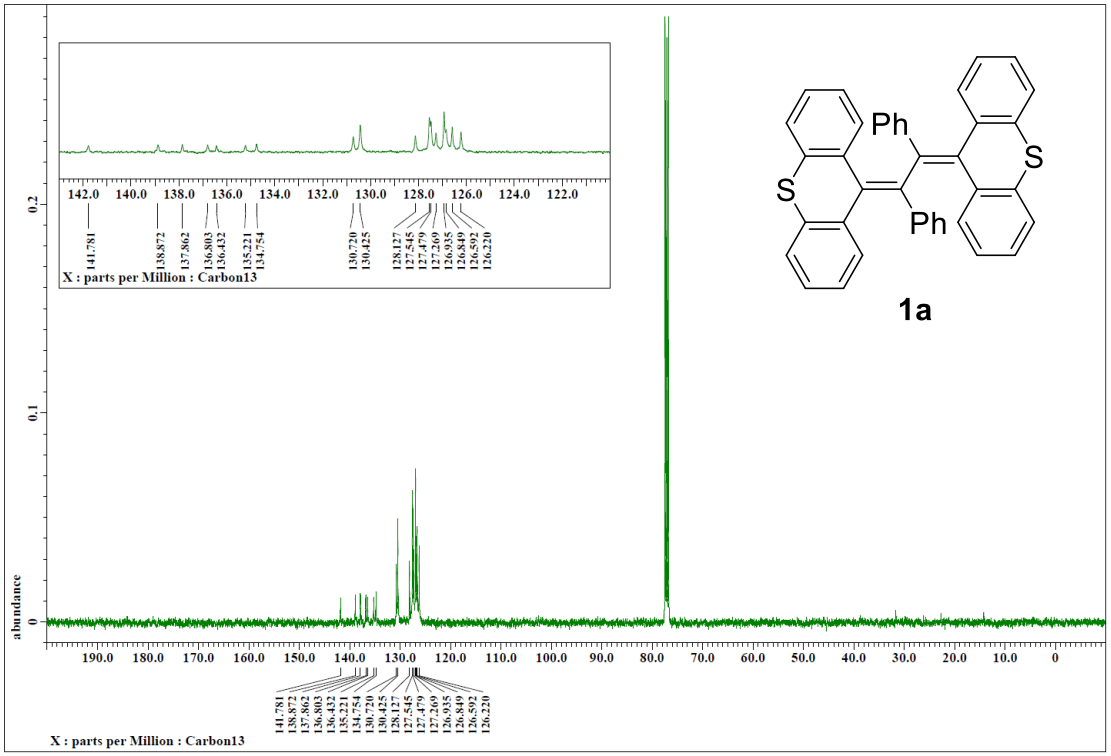
60	6	0	0.359116	-1.268615	3.588505
61	6	0	-2.398258	-1.286393	3.983194
62	1	0	-2.537677	-0.332598	2.063756
63	6	0	-0.179604	-1.836547	4.742253
64	1	0	1.439862	-1.300178	3.445479
65	6	0	-1.557678	-1.841125	4.948525
66	1	0	-3.481440	-1.311943	4.117167
67	1	0	0.487809	-2.285250	5.480516
68	1	0	-1.977319	-2.290851	5.850554
69	1	0	0.009694	-0.650755	-0.933416
70	7	0	0.892496	-0.124661	-0.820704
71	6	0	1.655708	-0.518116	-2.023221
72	6	0	1.361540	-1.792714	-2.523958
73	6	0	2.556536	0.306060	-2.693095
74	6	0	2.060583	-2.285655	-3.619099
75	1	0	0.576032	-2.401956	-2.069367
76	6	0	3.242110	-0.196343	-3.799559
77	1	0	2.727576	1.337681	-2.404304
78	6	0	3.023100	-1.495903	-4.246800
79	1	0	1.836061	-3.287459	-3.988872
80	1	0	3.951985	0.451540	-4.316178
81	1	0	3.574601	-1.881078	-5.106178
82	15	0	-3.410521	-1.954455	-0.747312
83	9	0	-2.079144	-1.025743	-0.479233
84	9	0	-2.489685	-2.989047	-1.593756
85	9	0	-3.090750	-2.782450	0.615077
86	9	0	-4.294249	-0.897817	0.111489
87	9	0	-3.712917	-1.112326	-2.096555
88	9	0	-4.715098	-2.870197	-1.006321

10. ^{1}H and ^{13}C NMR spectra of substrates and products

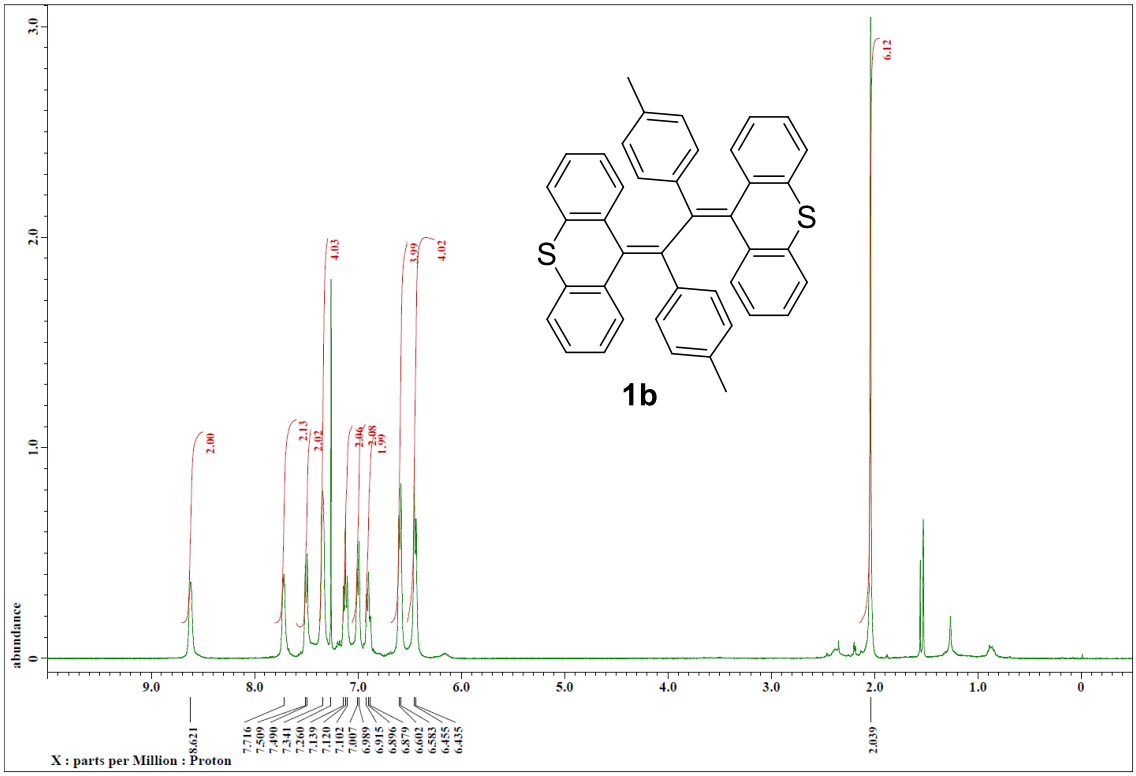
^{1}H NMR ($CDCl_3$, 400 MHz)



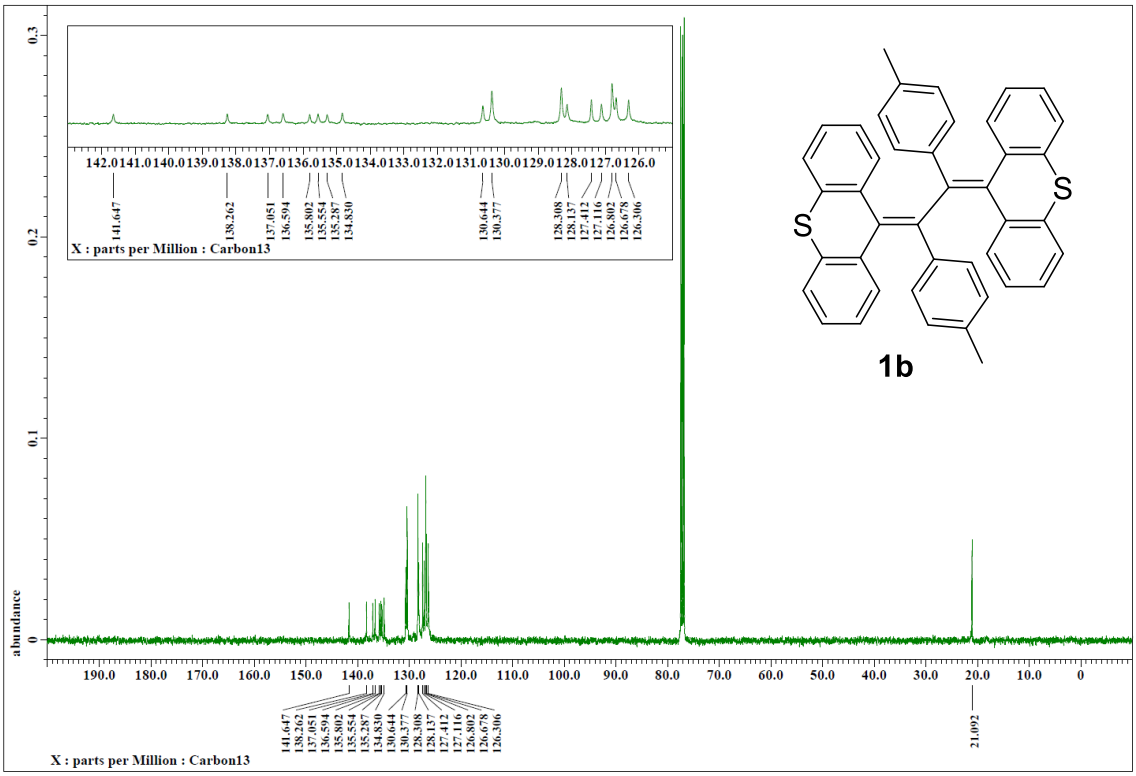
^{13}C NMR ($CDCl_3$, 101 MHz)



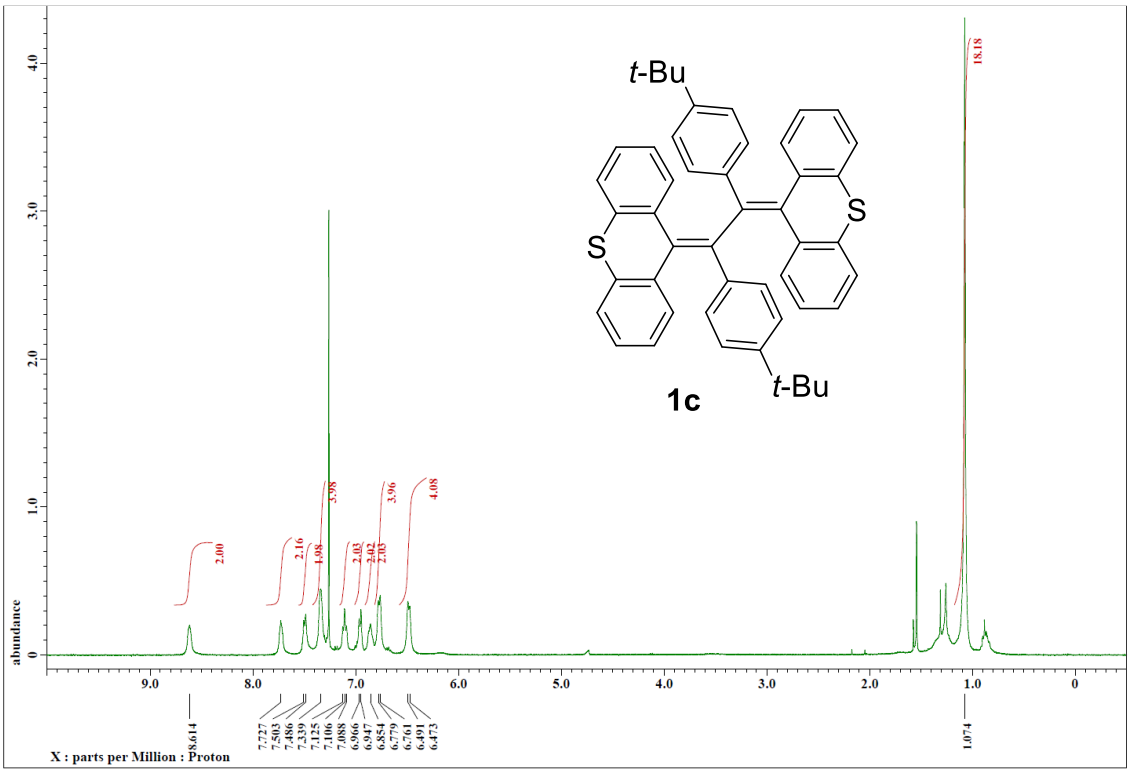
^{1}H NMR ($CDCl_3$, 400 MHz)



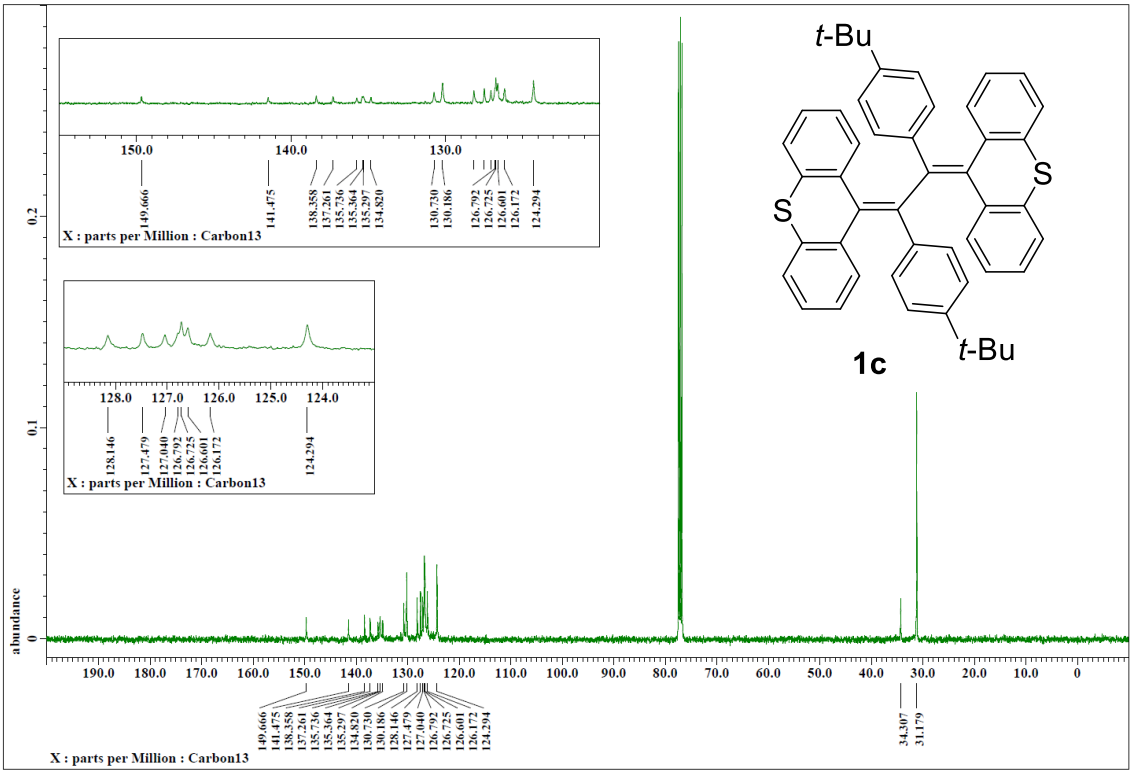
^{13}C NMR ($CDCl_3$, 101 MHz)



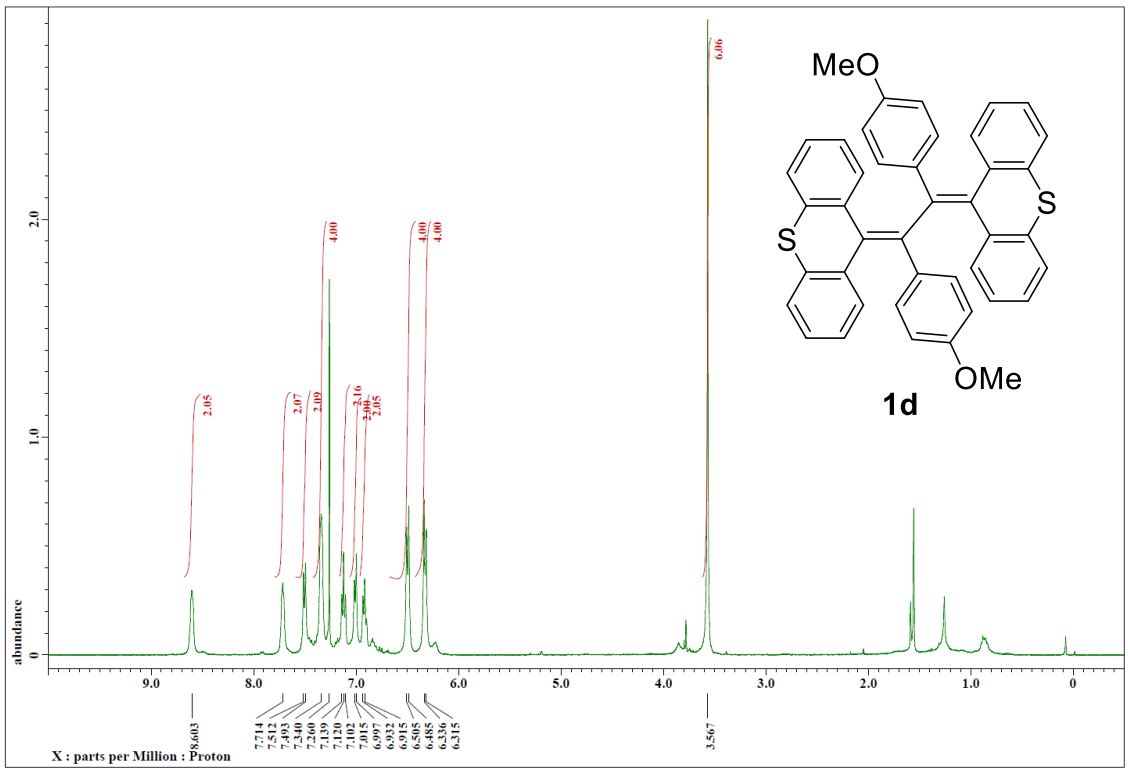
^{1}H NMR ($CDCl_3$, 400 MHz)



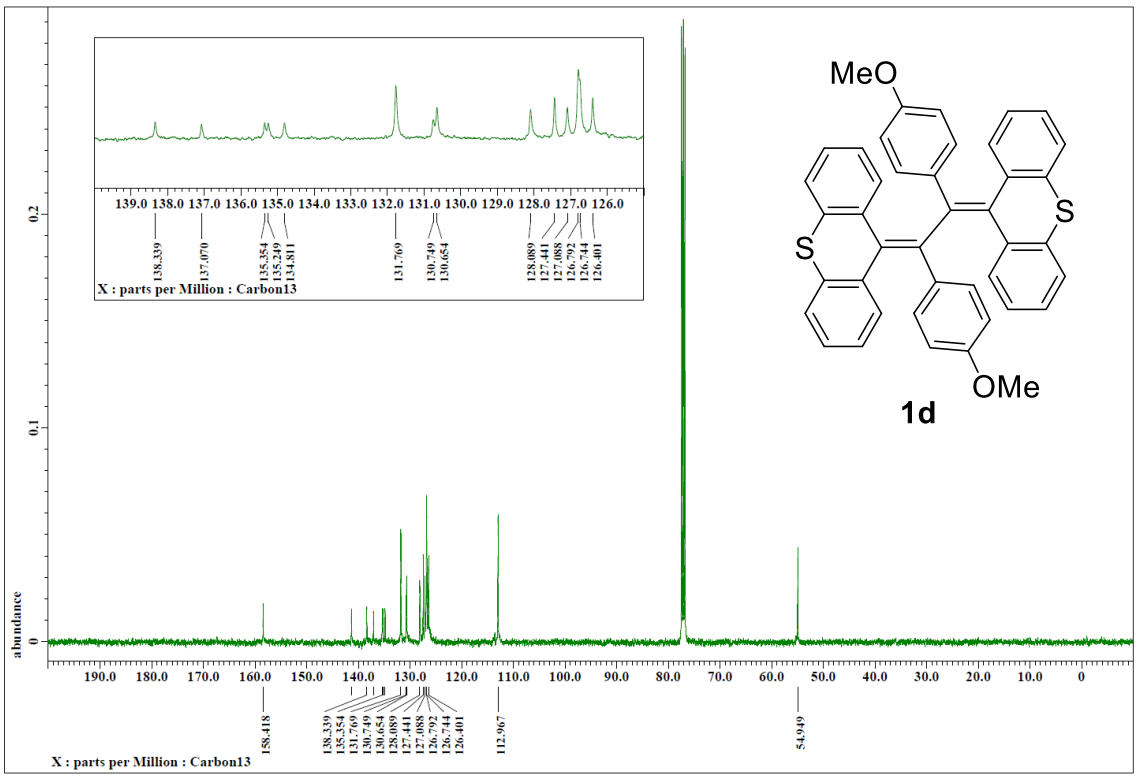
^{13}C NMR ($CDCl_3$, 101 MHz)



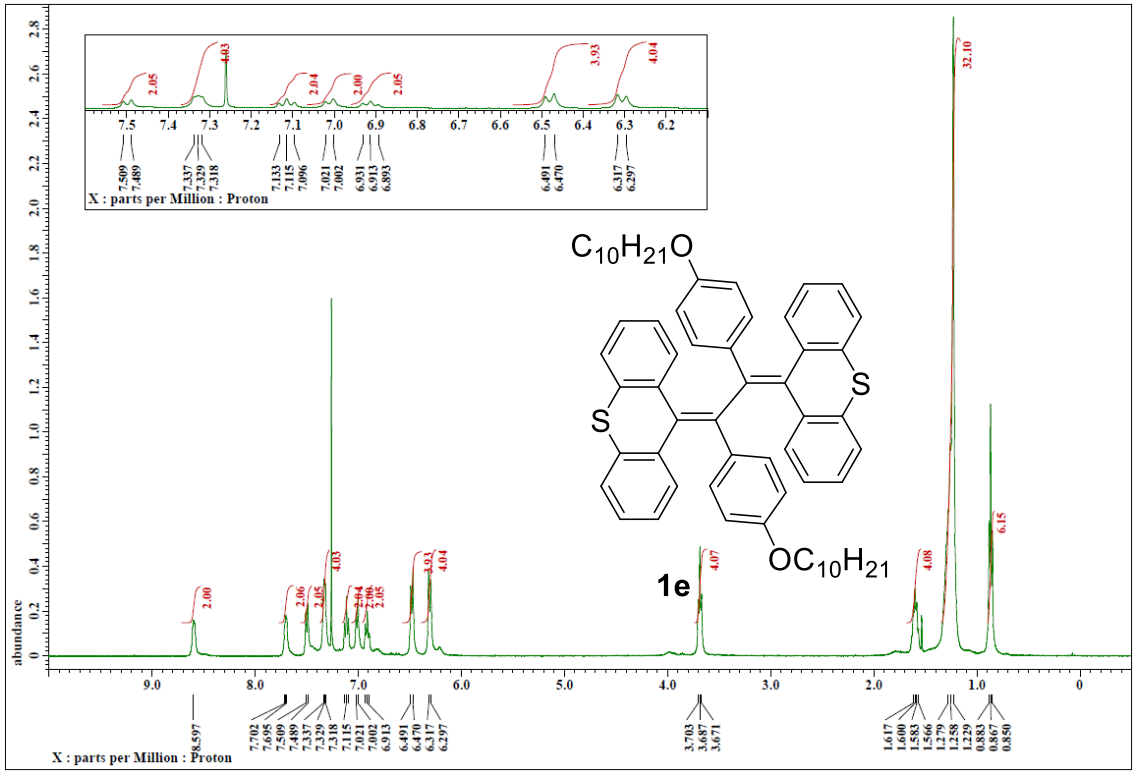
^{1}H NMR ($CDCl_3$, 400 MHz)



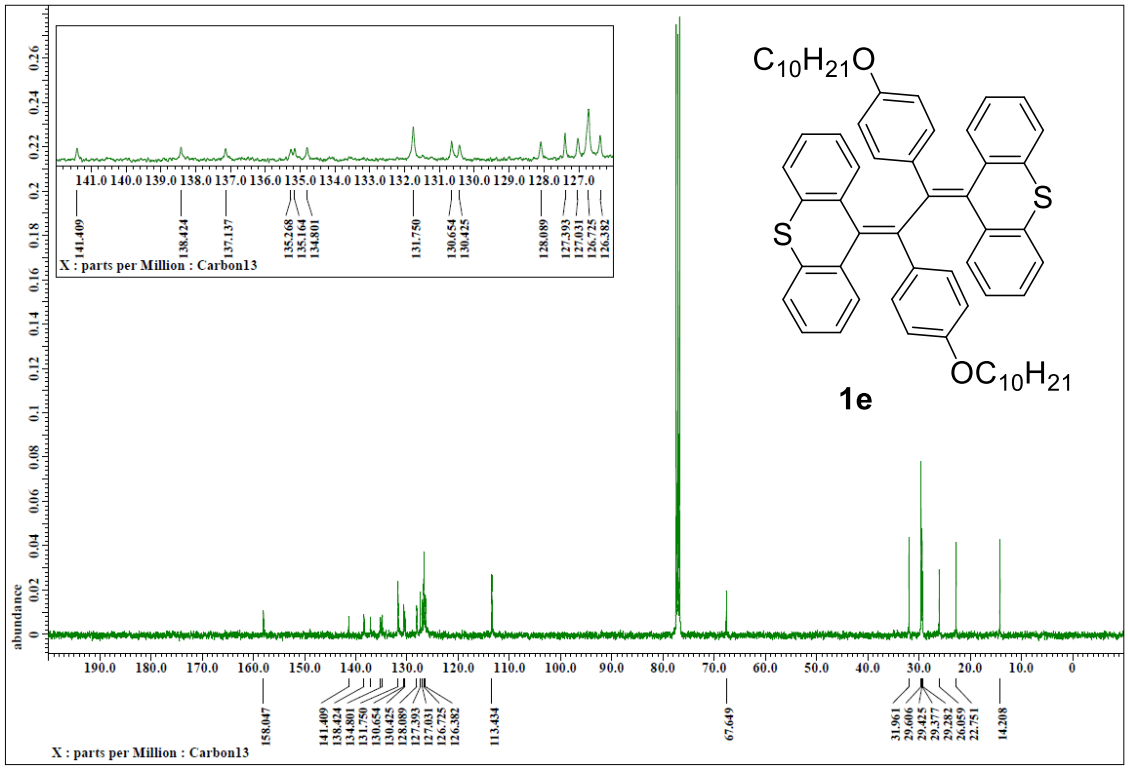
^{13}C NMR (101 MHz)



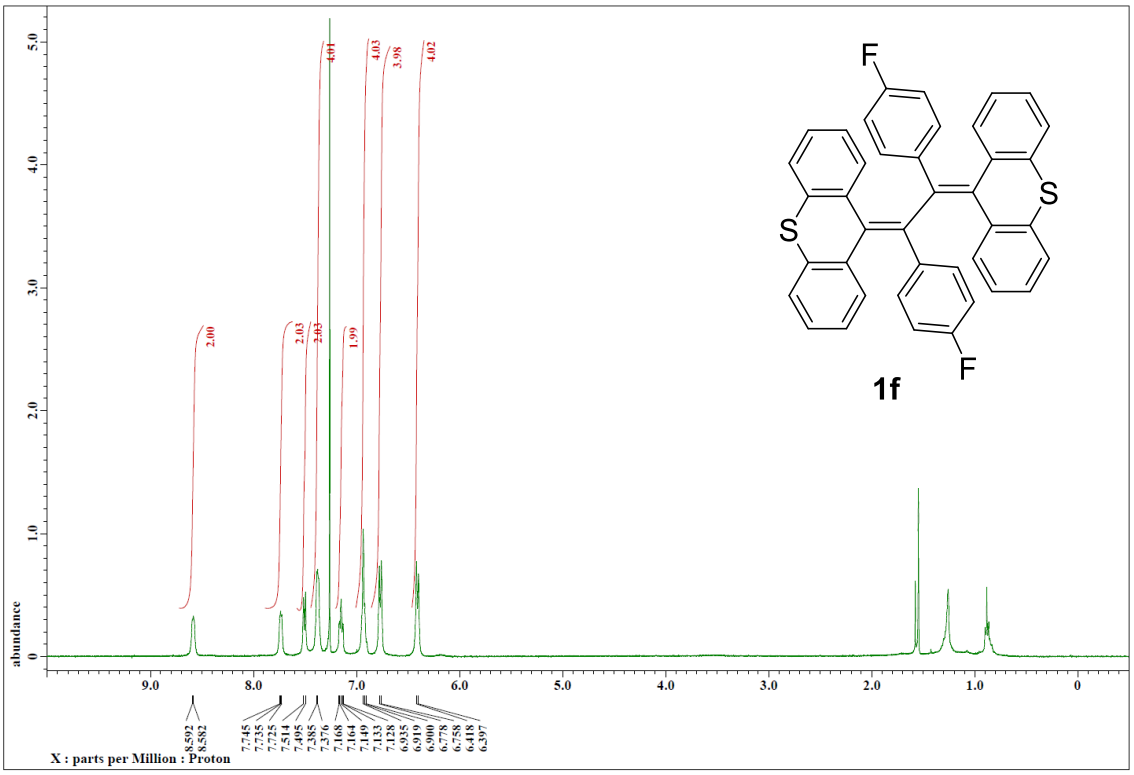
^{1}H NMR ($CDCl_3$, 400 MHz)



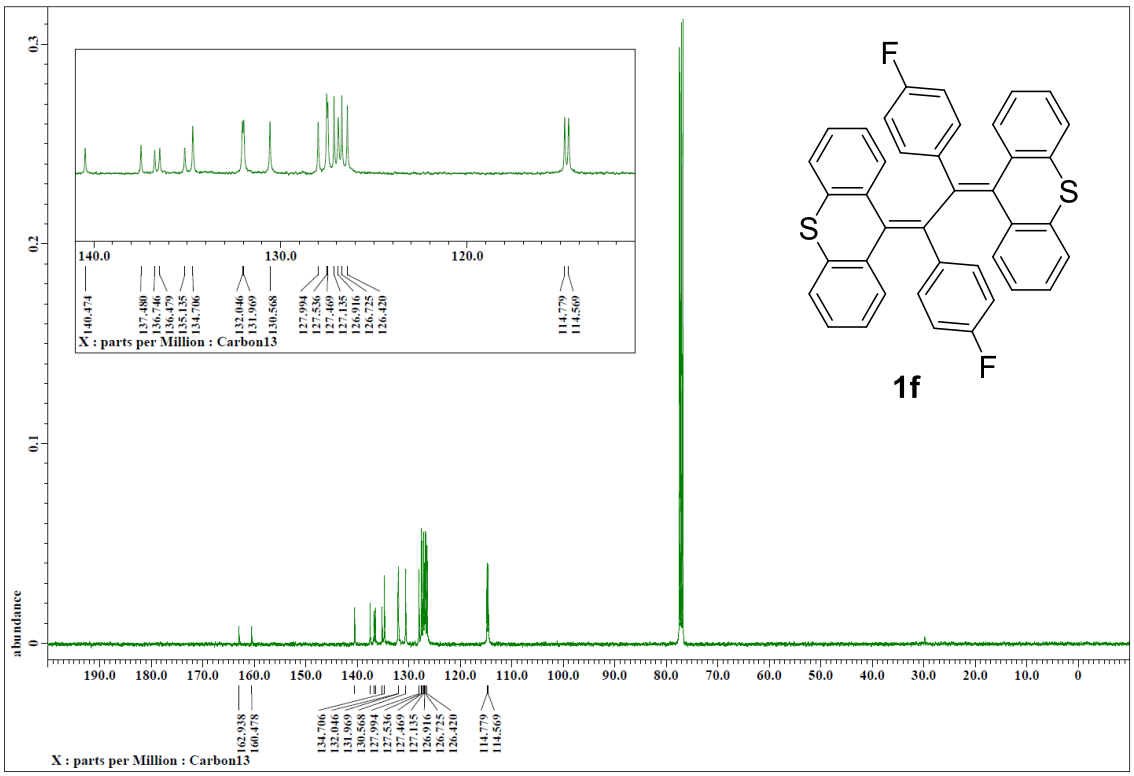
^{13}C NMR ($CDCl_3$, 101 MHz)



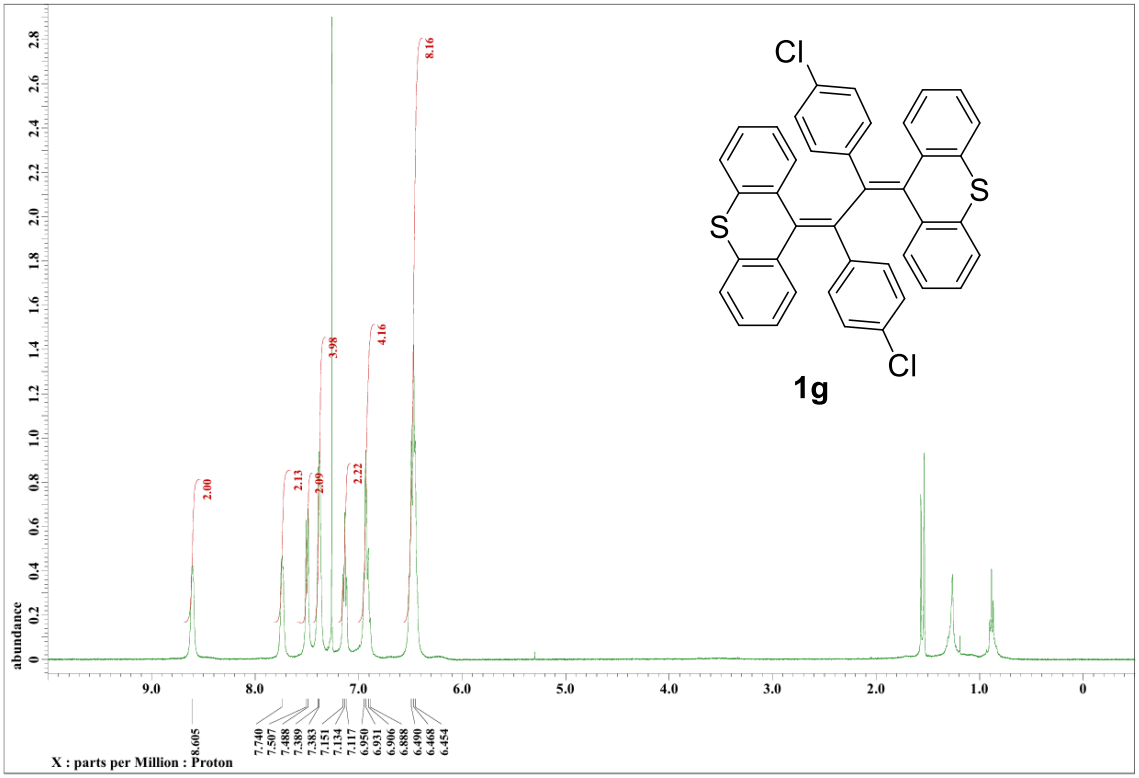
^{1}H NMR ($CDCl_3$, 400 MHz)



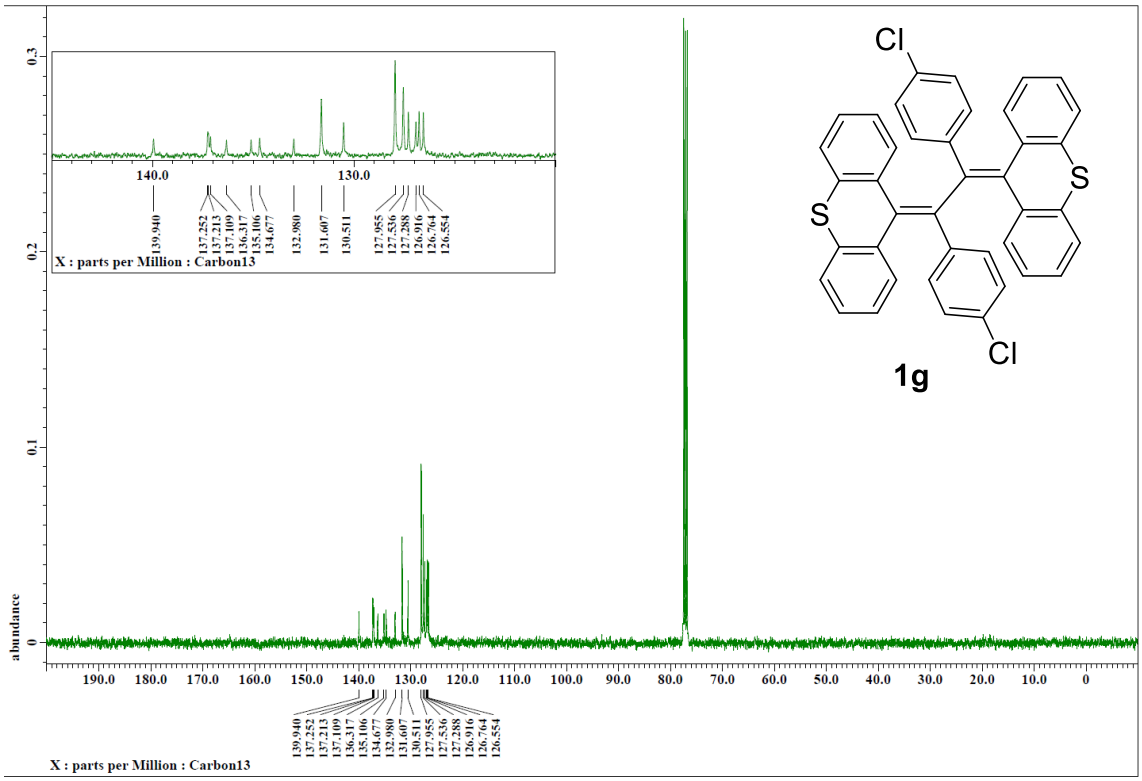
^{13}C NMR ($CDCl_3$, 101 MHz)



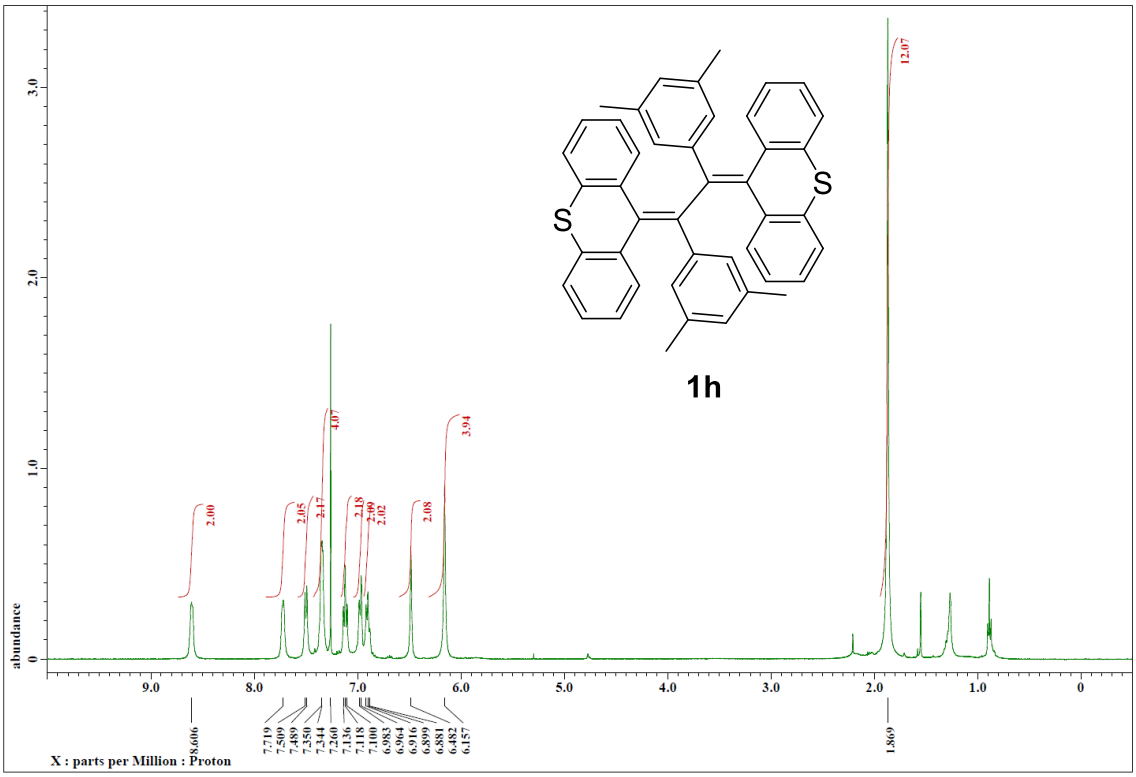
^{1}H NMR ($CDCl_3$, 400 MHz)



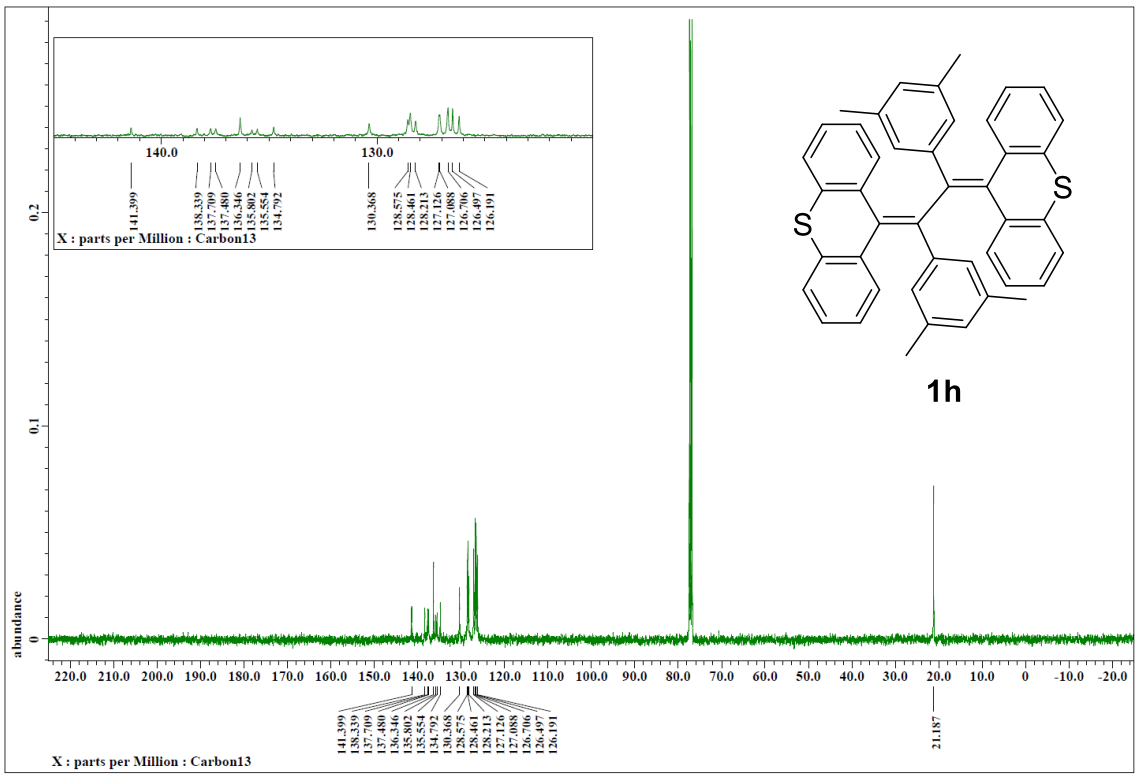
^{13}C NMR ($CDCl_3$, 101 MHz)



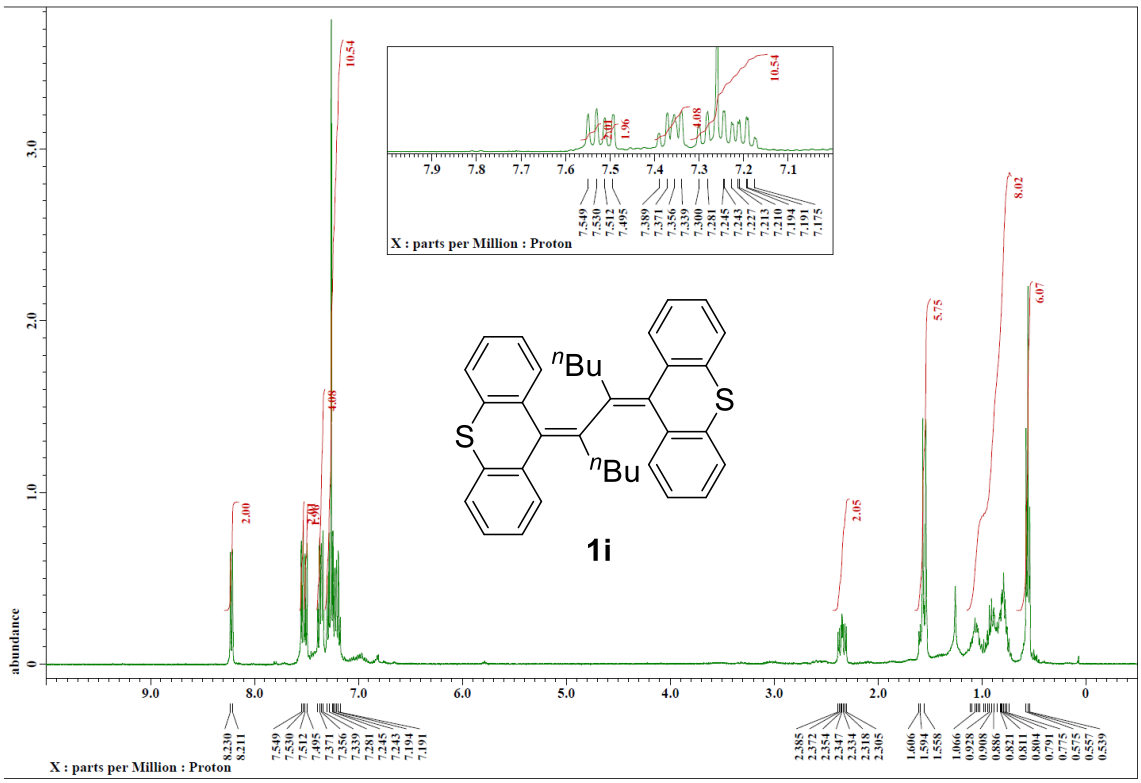
^{1}H NMR ($CDCl_3$, 400 MHz)



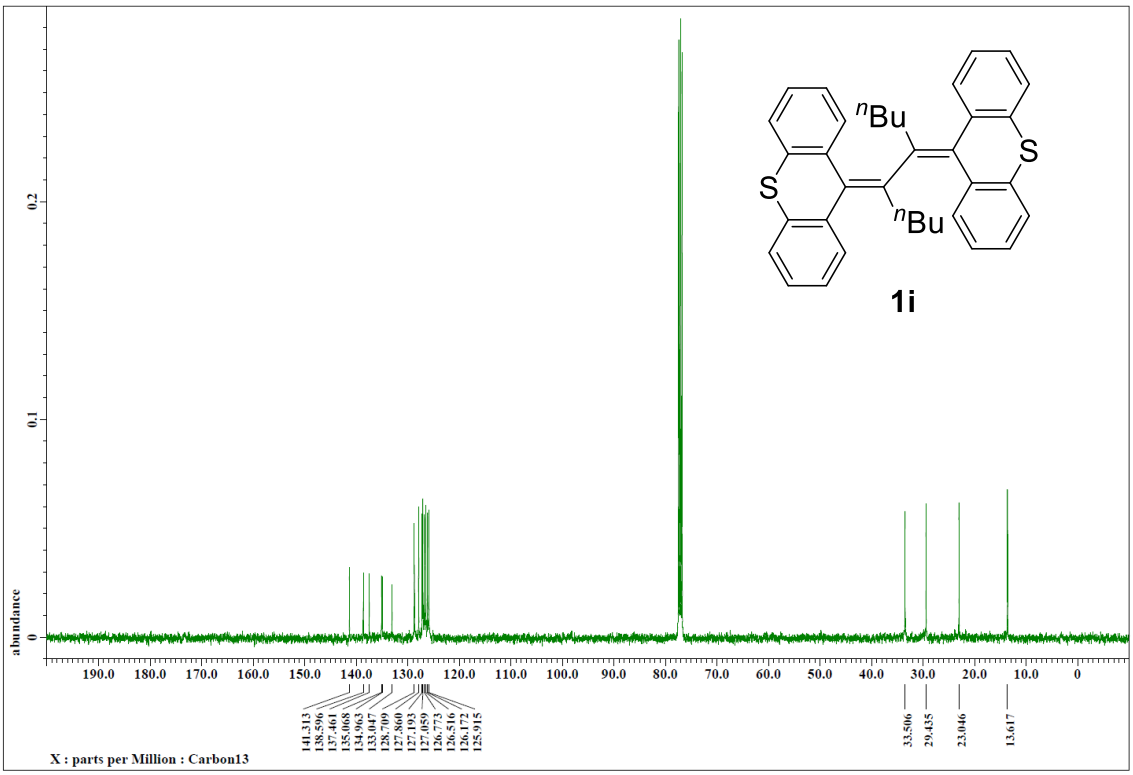
^{13}C NMR ($CDCl_3$, 101 MHz)



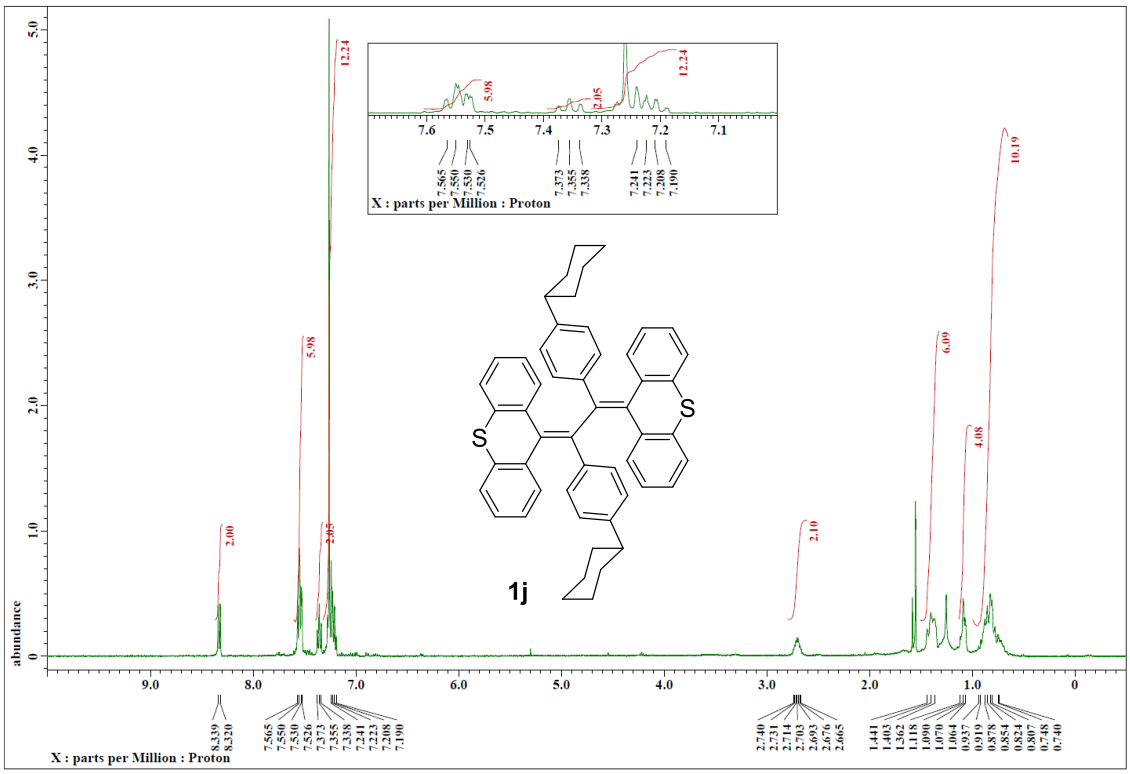
^{1}H NMR ($CDCl_3$, 400 MHz)



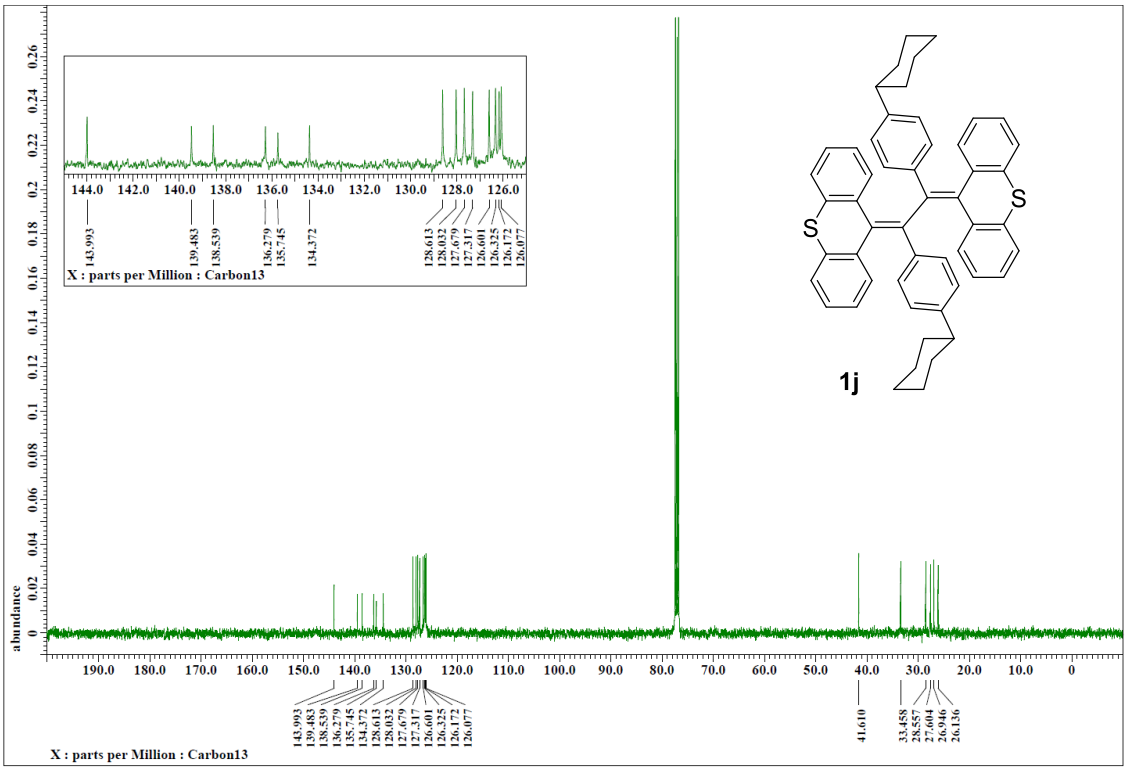
^{13}C NMR ($CDCl_3$, 101 MHz)



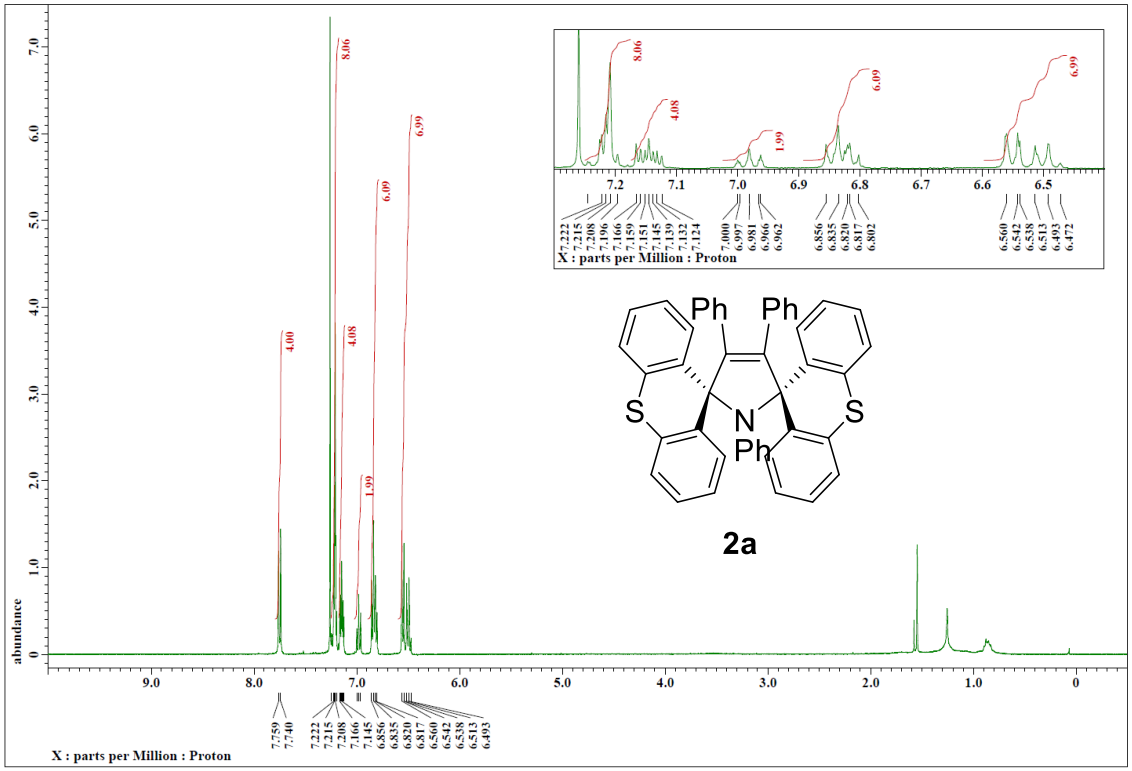
^{1}H NMR ($CDCl_3$, 400 MHz)



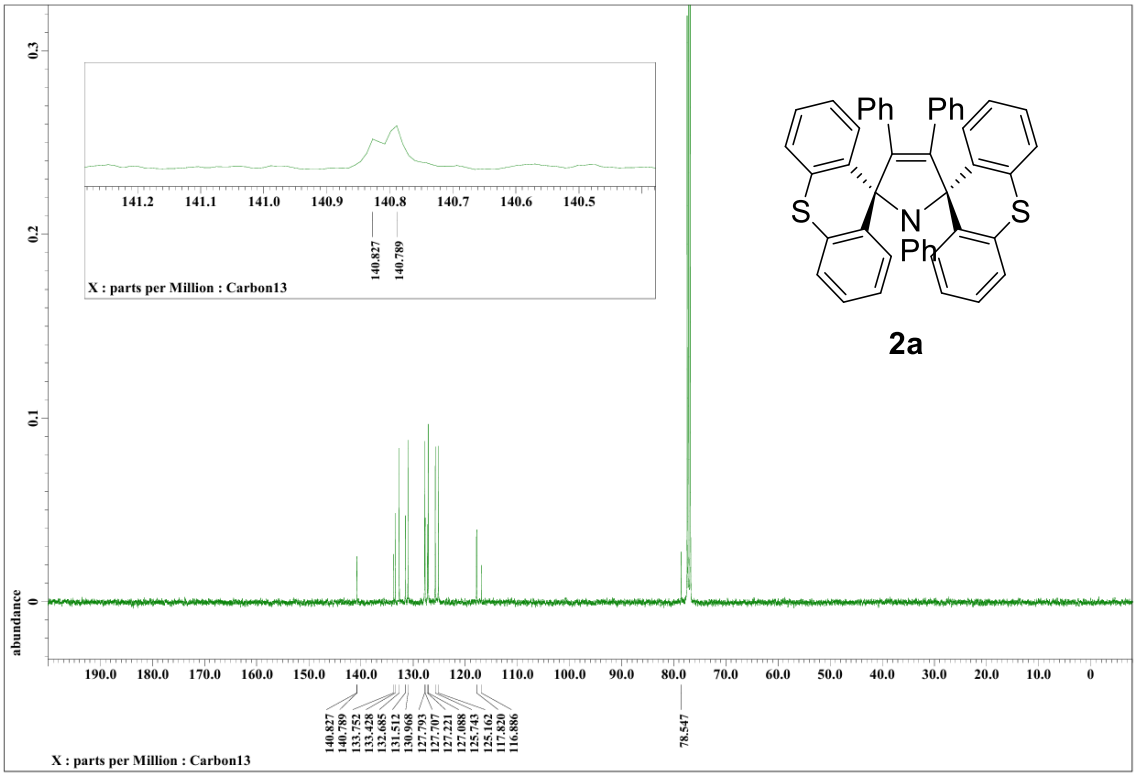
^{13}C NMR ($CDCl_3$, 101 MHz)



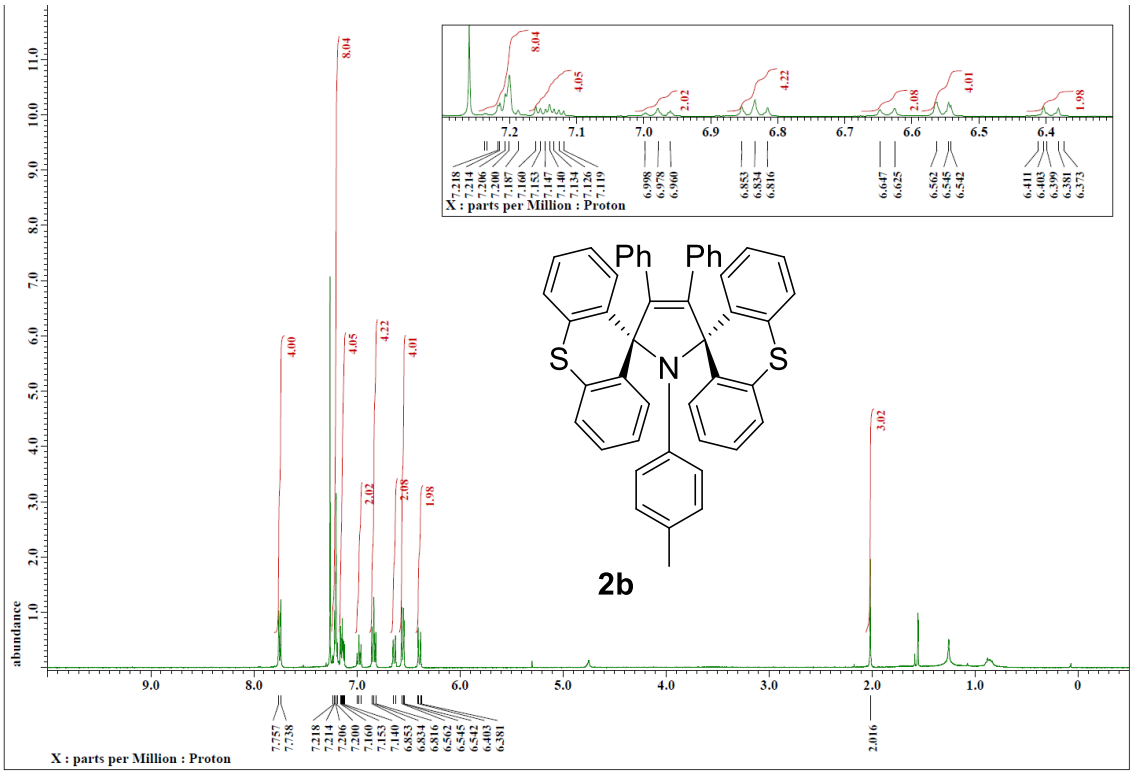
^{1}H NMR ($CDCl_3$, 400 MHz)



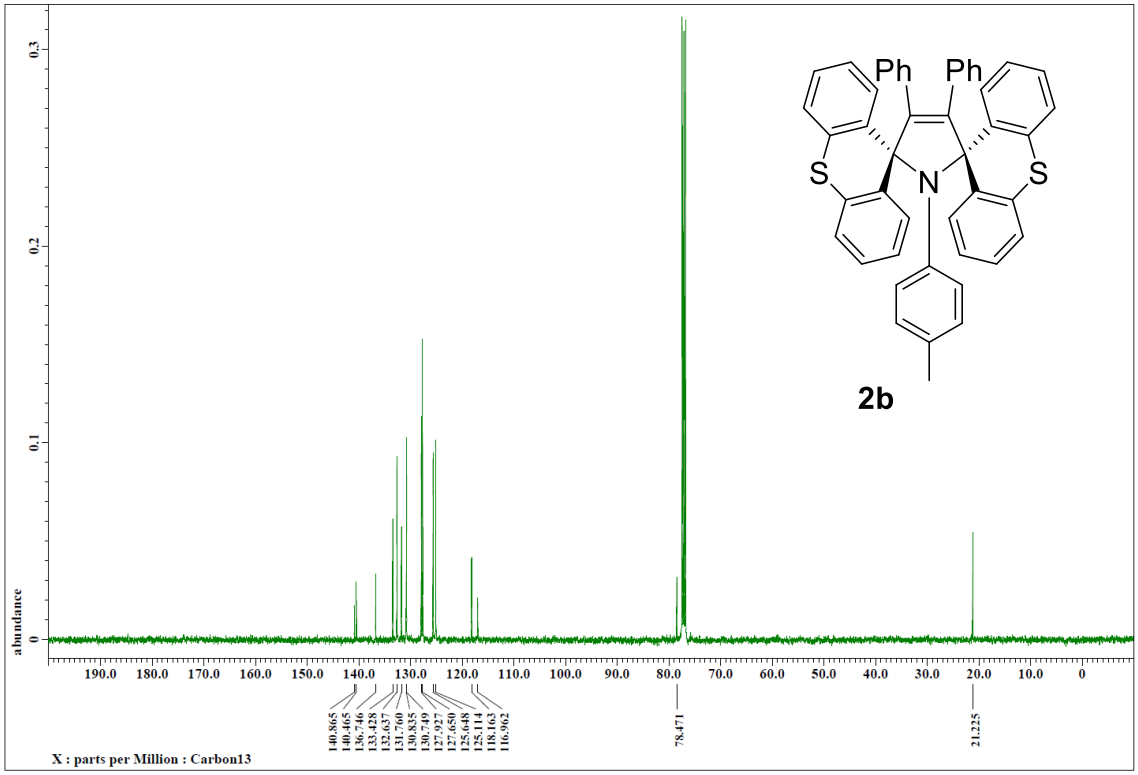
^{13}C NMR ($CDCl_3$, 101 MHz)



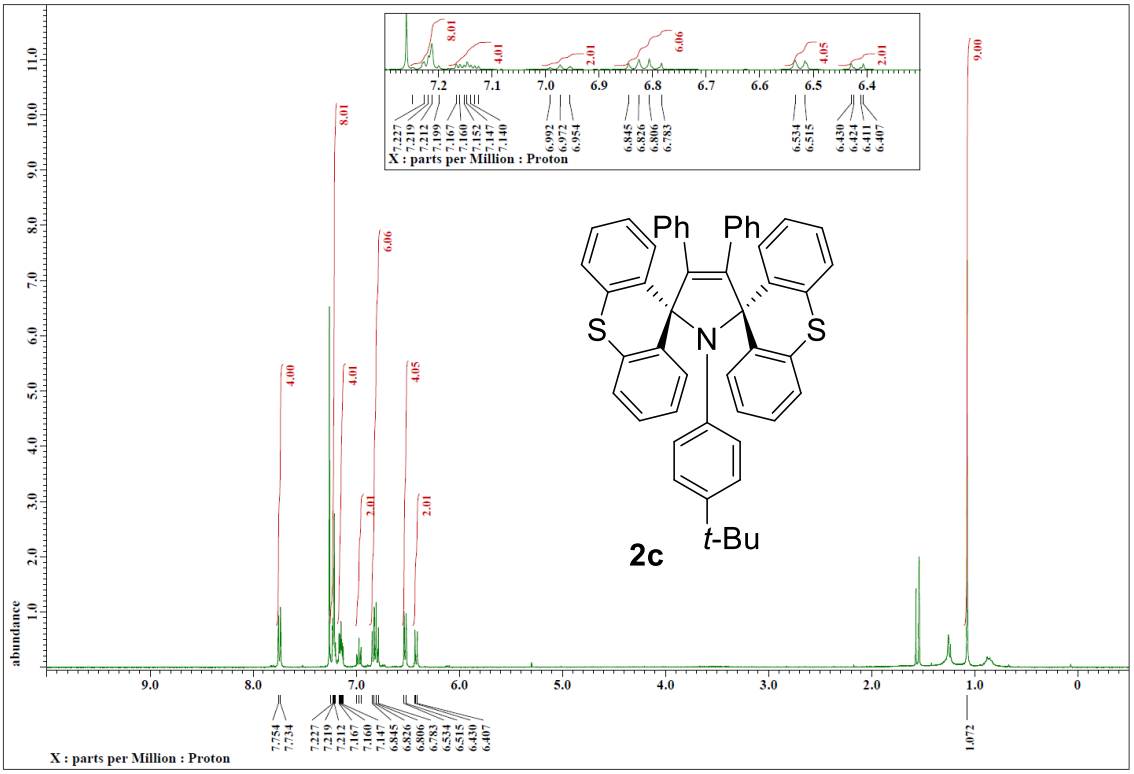
^{1}H NMR ($CDCl_3$, 400 MHz)



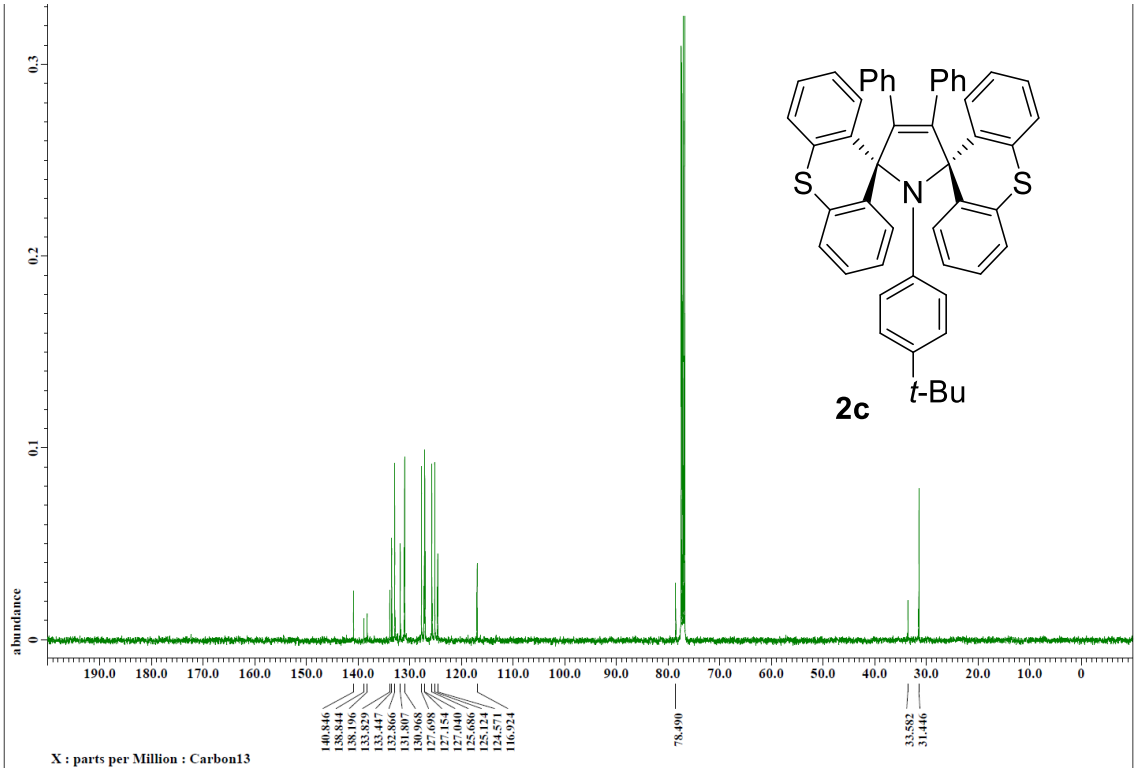
^{13}C NMR ($CDCl_3$, 101 MHz)



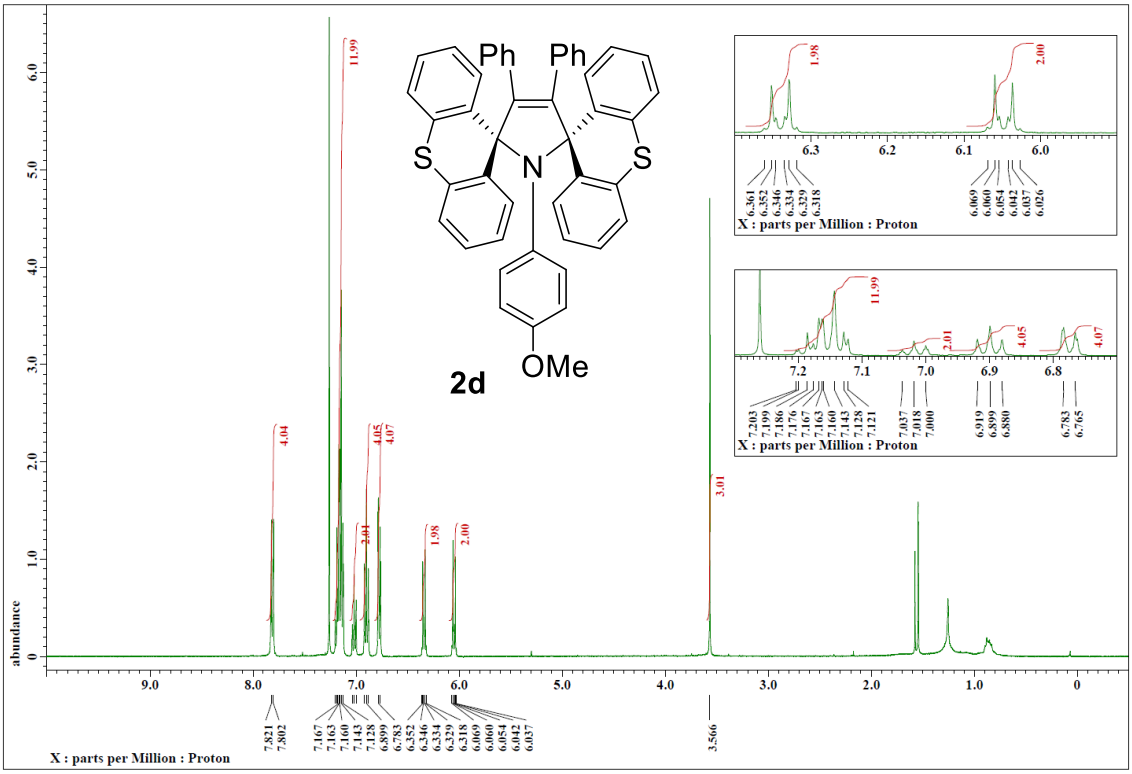
^{1}H NMR ($CDCl_3$, 400 MHz)



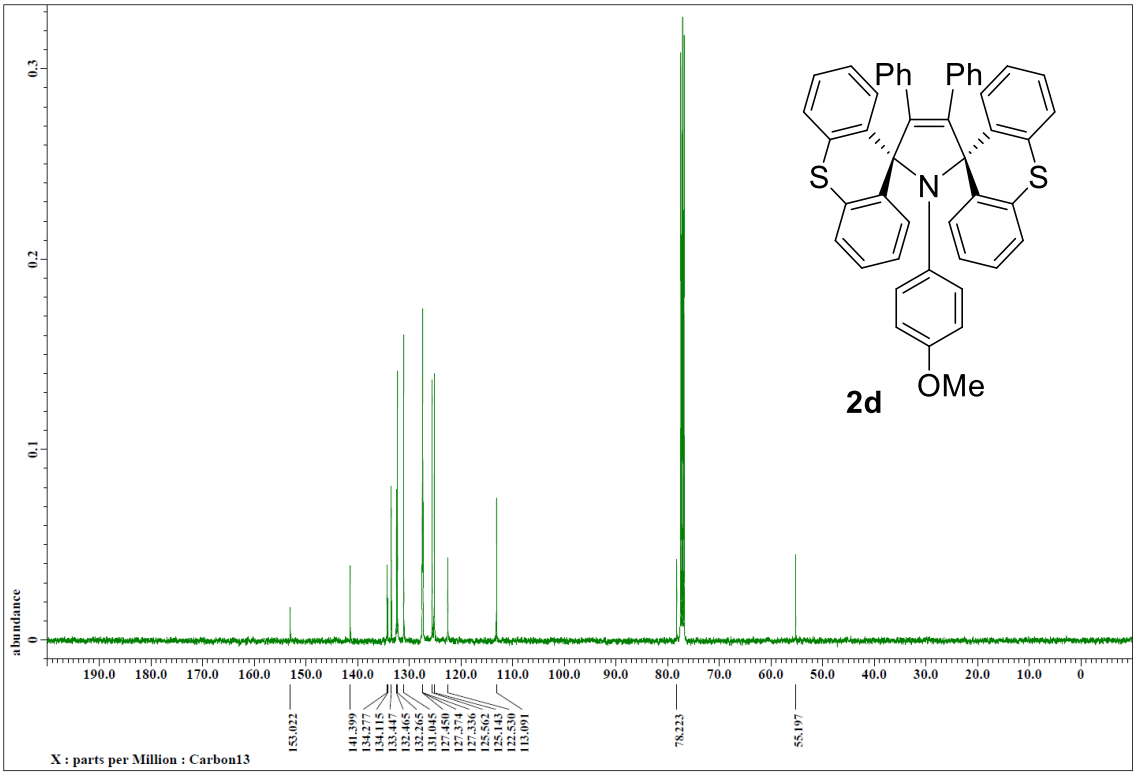
^{13}C NMR ($CDCl_3$, 101 MHz)



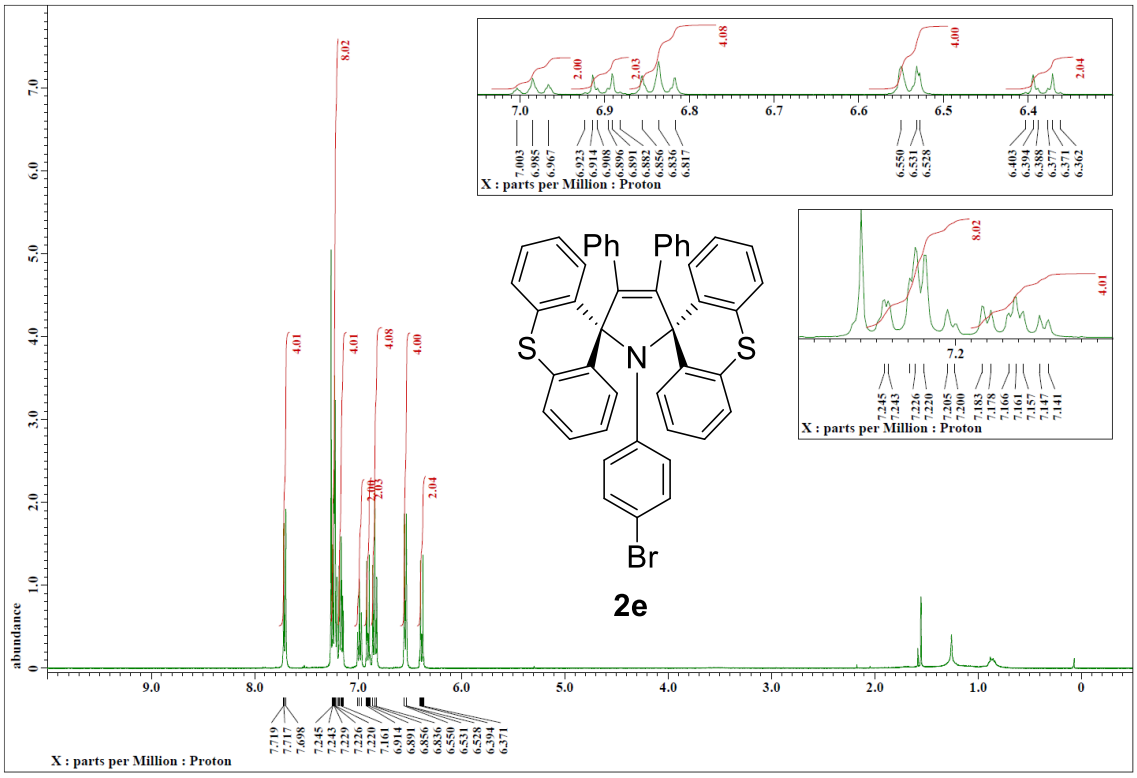
^{1}H NMR ($CDCl_3$, 400 MHz)



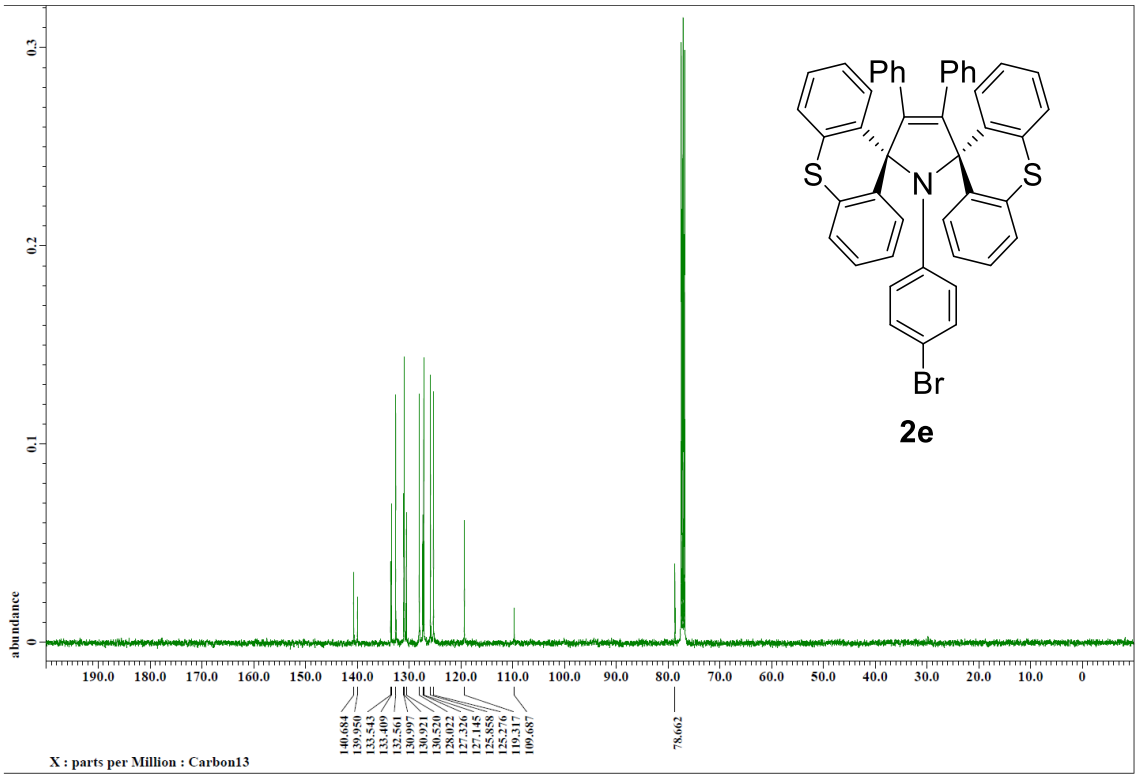
^{13}C NMR ($CDCl_3$, 101 MHz)



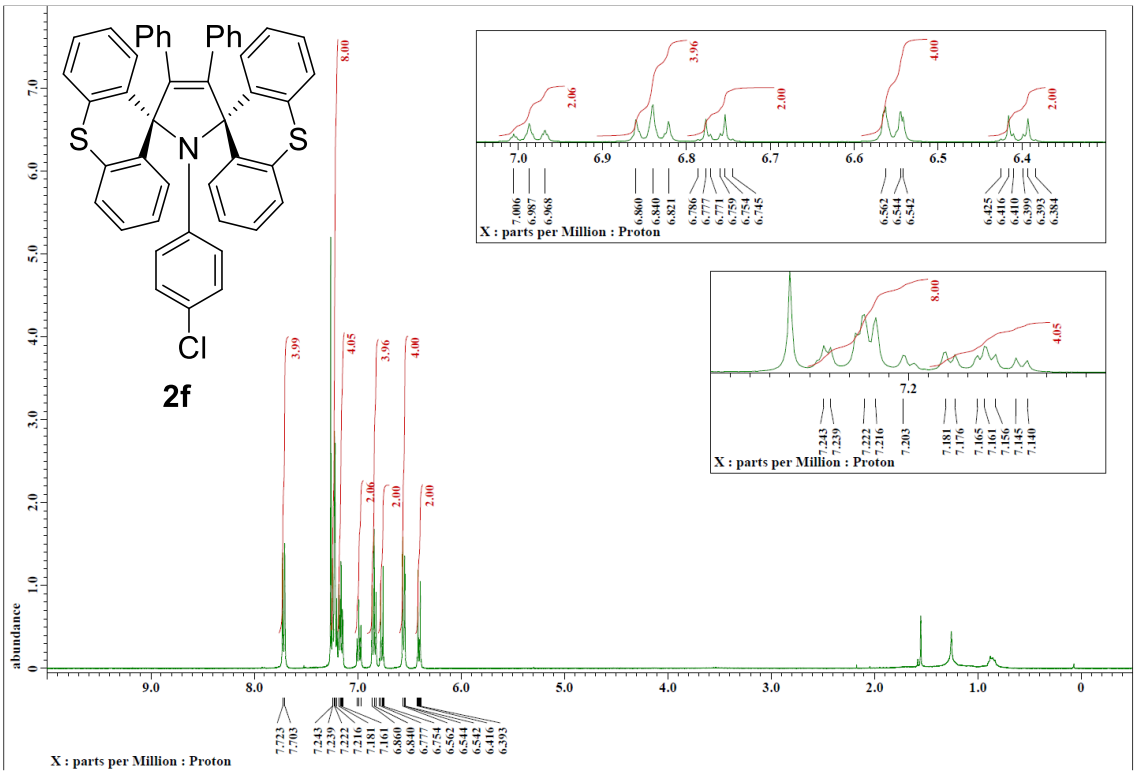
^{1}H NMR ($CDCl_3$, 400 MHz)



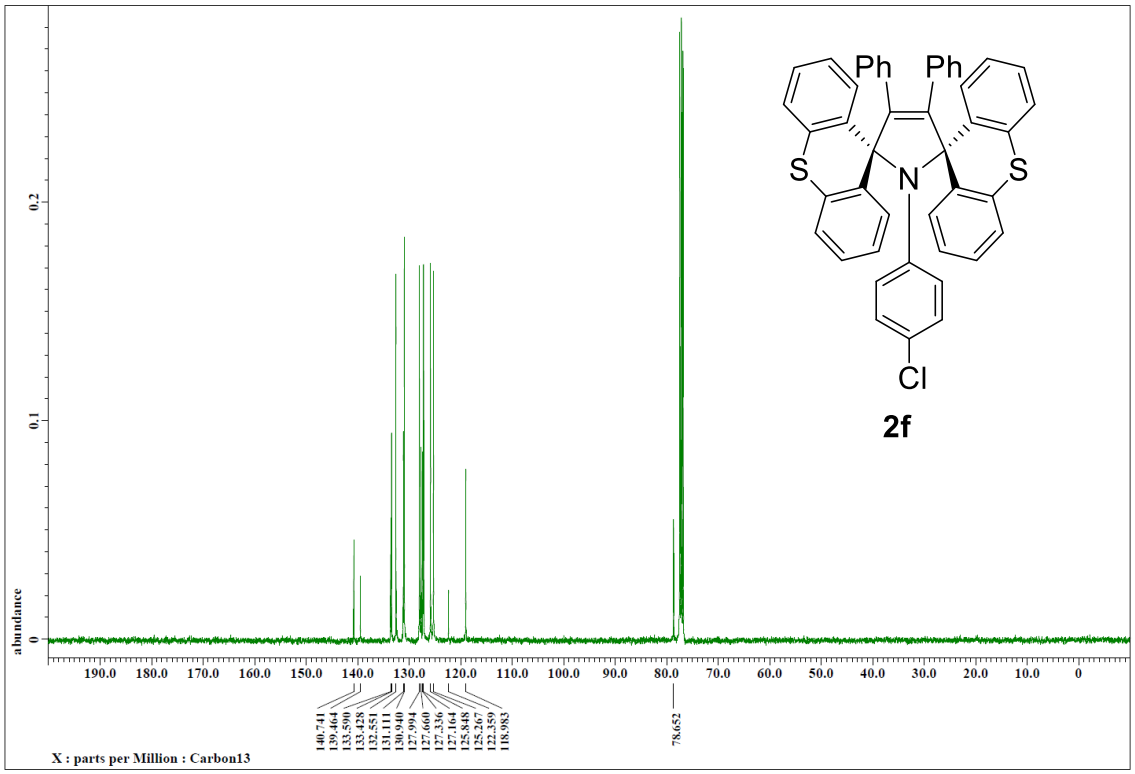
^{13}C NMR ($CDCl_3$, 101 MHz)



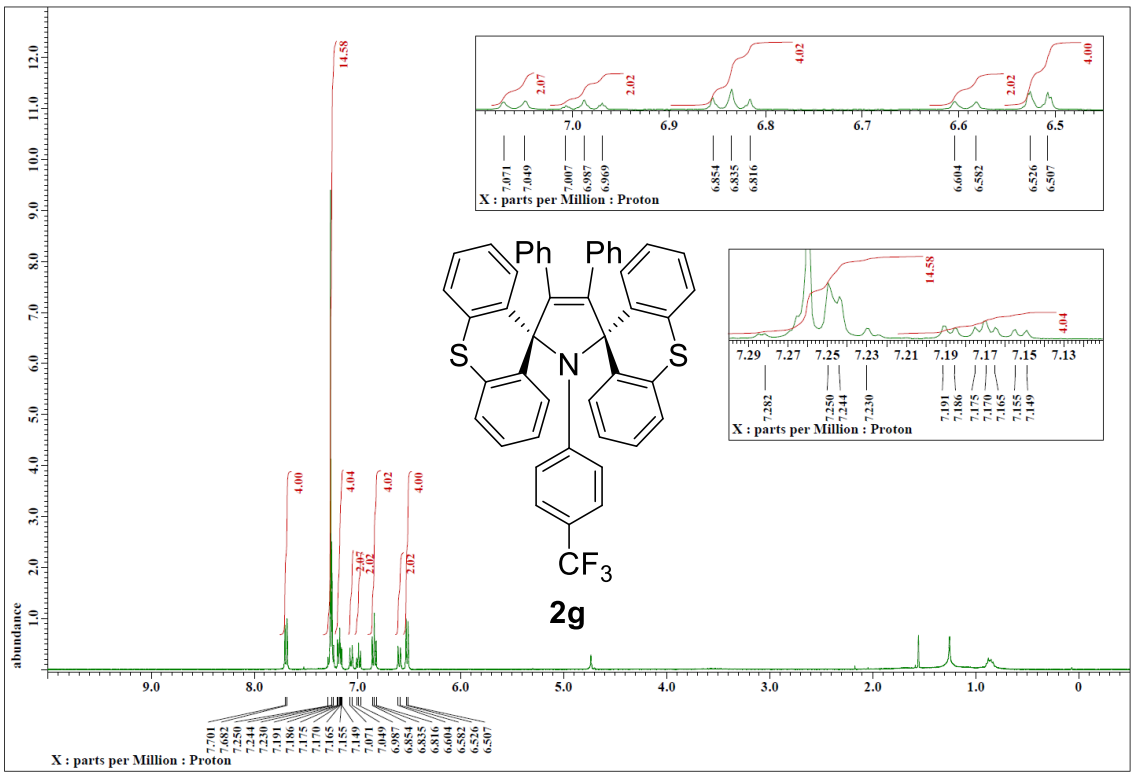
^{1}H NMR ($CDCl_3$, 400 MHz)



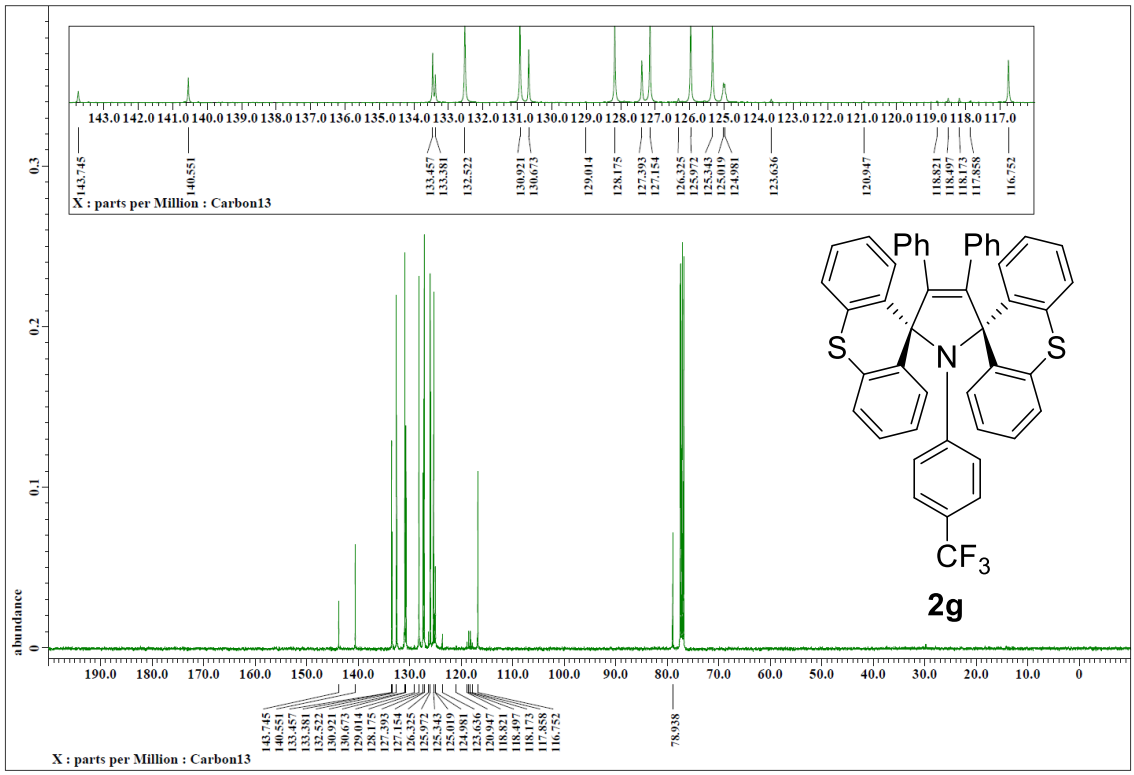
^{13}C NMR ($CDCl_3$, 101 MHz)



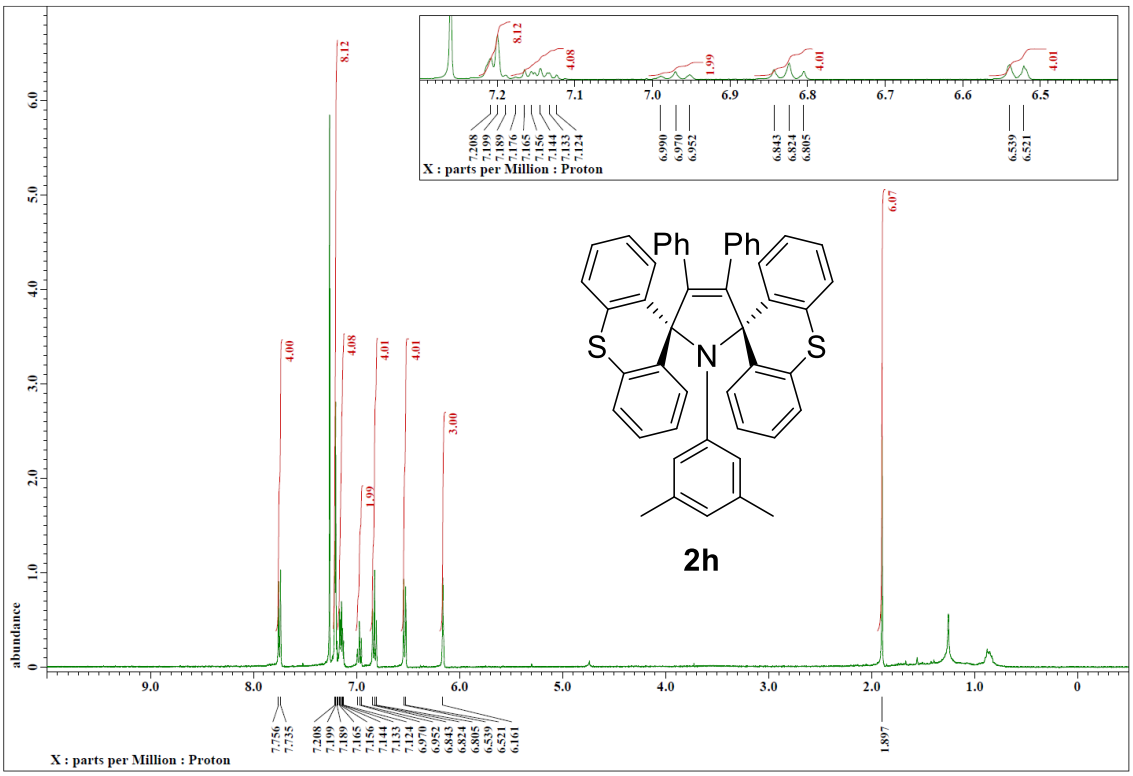
^{1}H NMR ($CDCl_3$, 400 MHz)



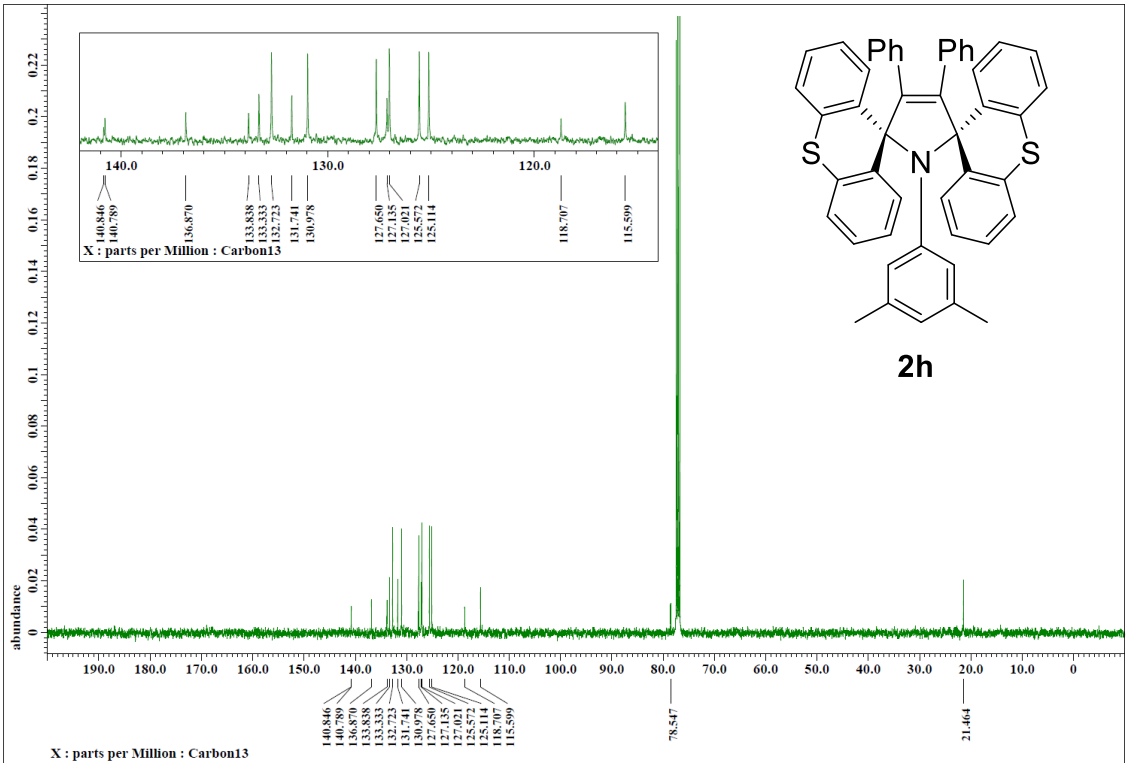
^{13}C NMR ($CDCl_3$, 101 MHz)



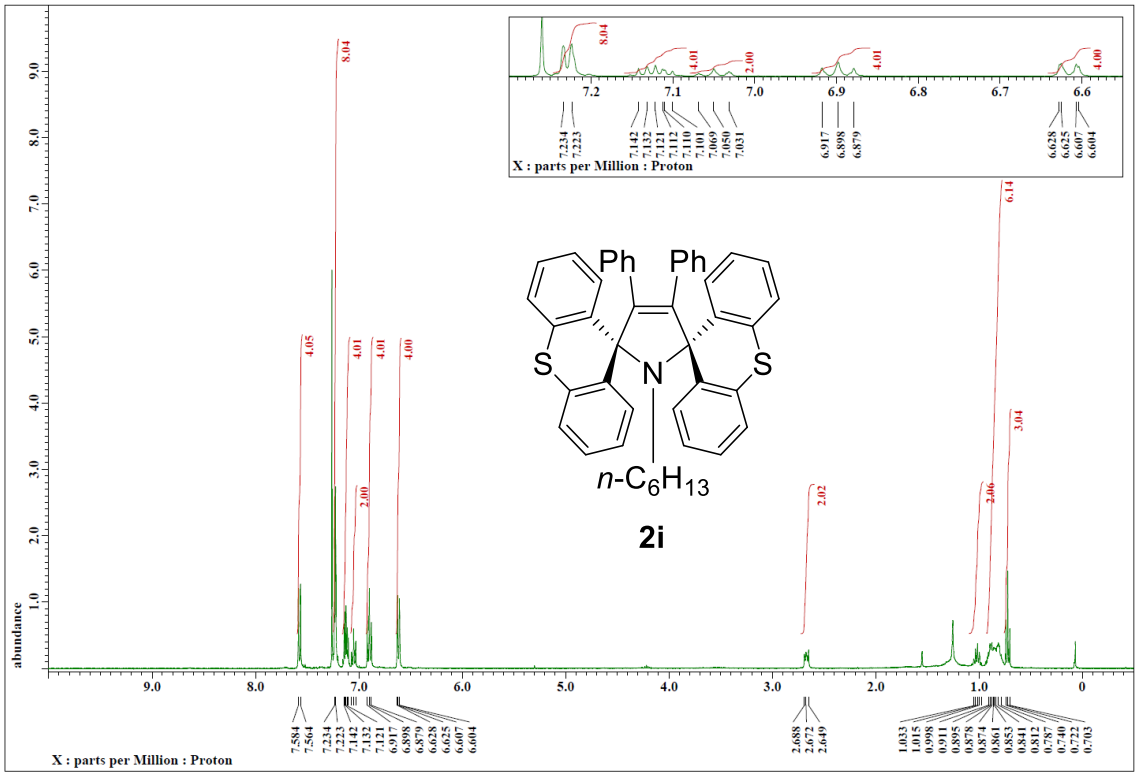
^{1}H NMR ($CDCl_3$, 400 MHz)



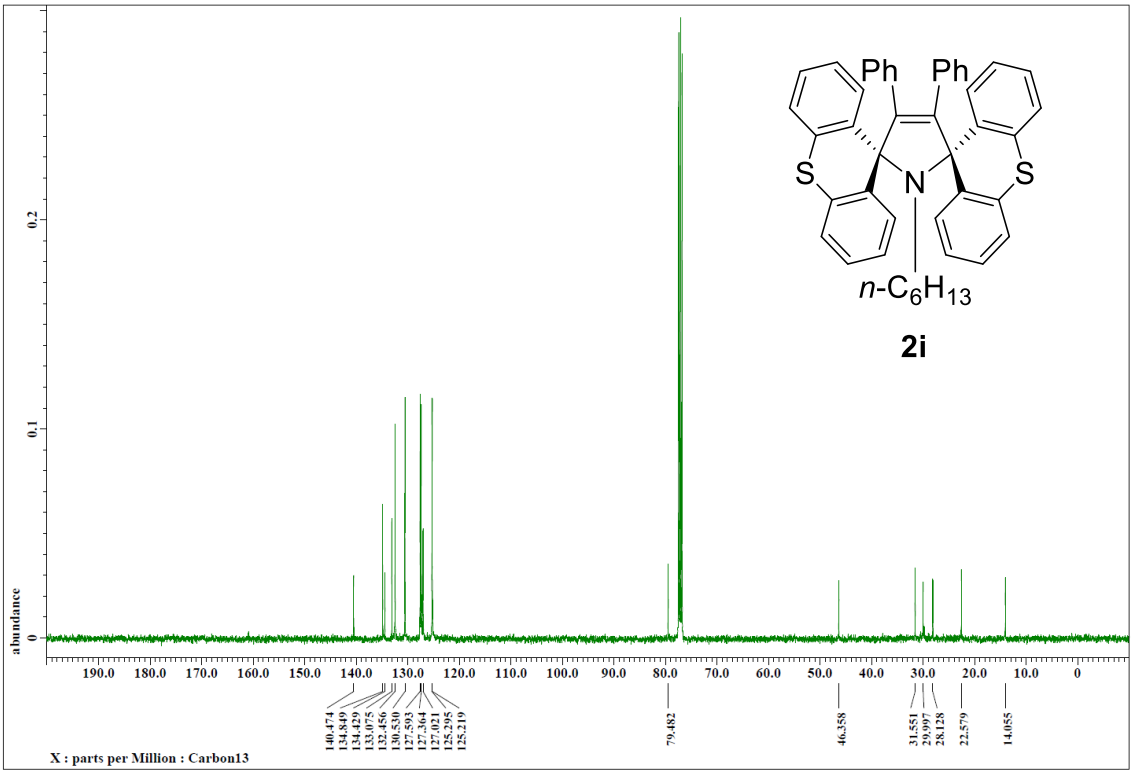
^{13}C NMR ($CDCl_3$, 101 MHz)



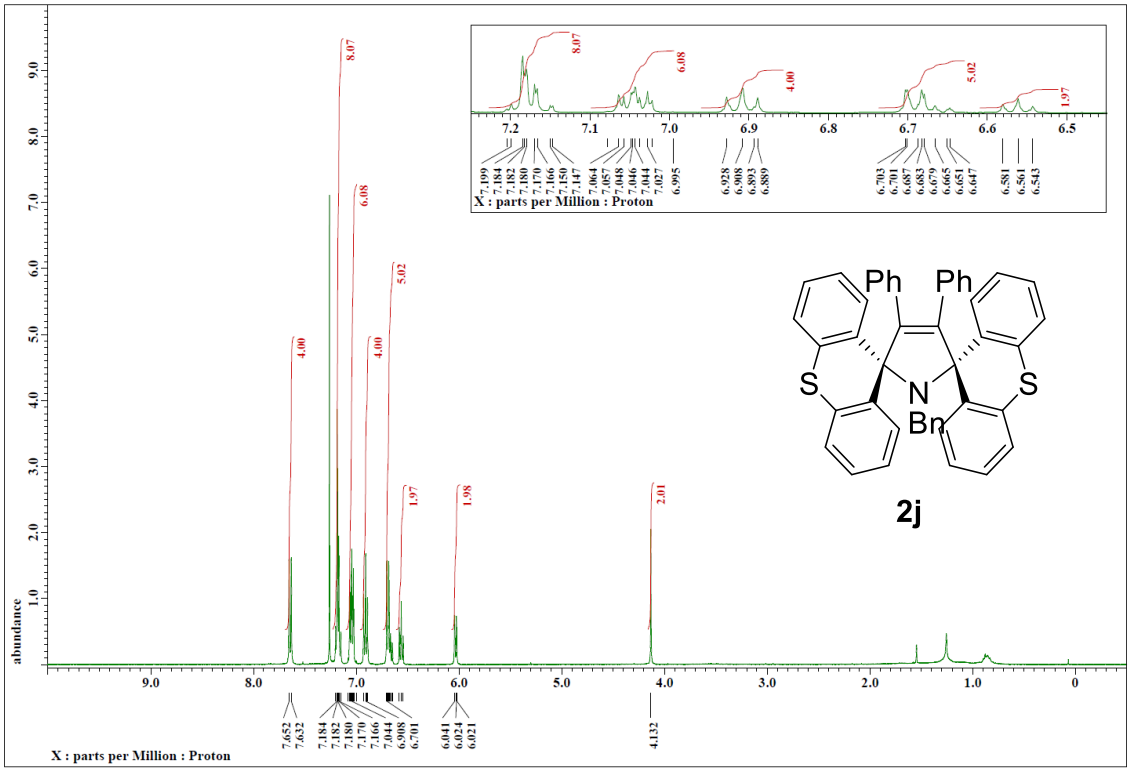
^{1}H NMR ($CDCl_3$, 400 MHz)



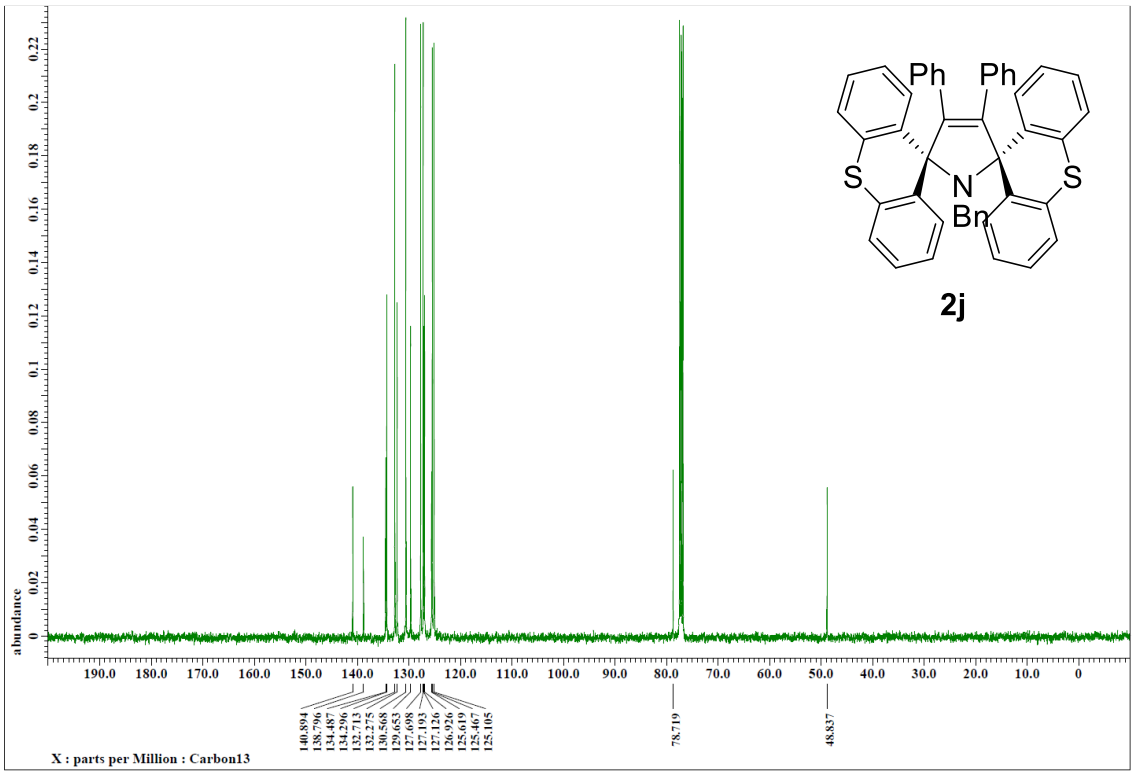
^{13}C NMR ($CDCl_3$, 101 MHz)



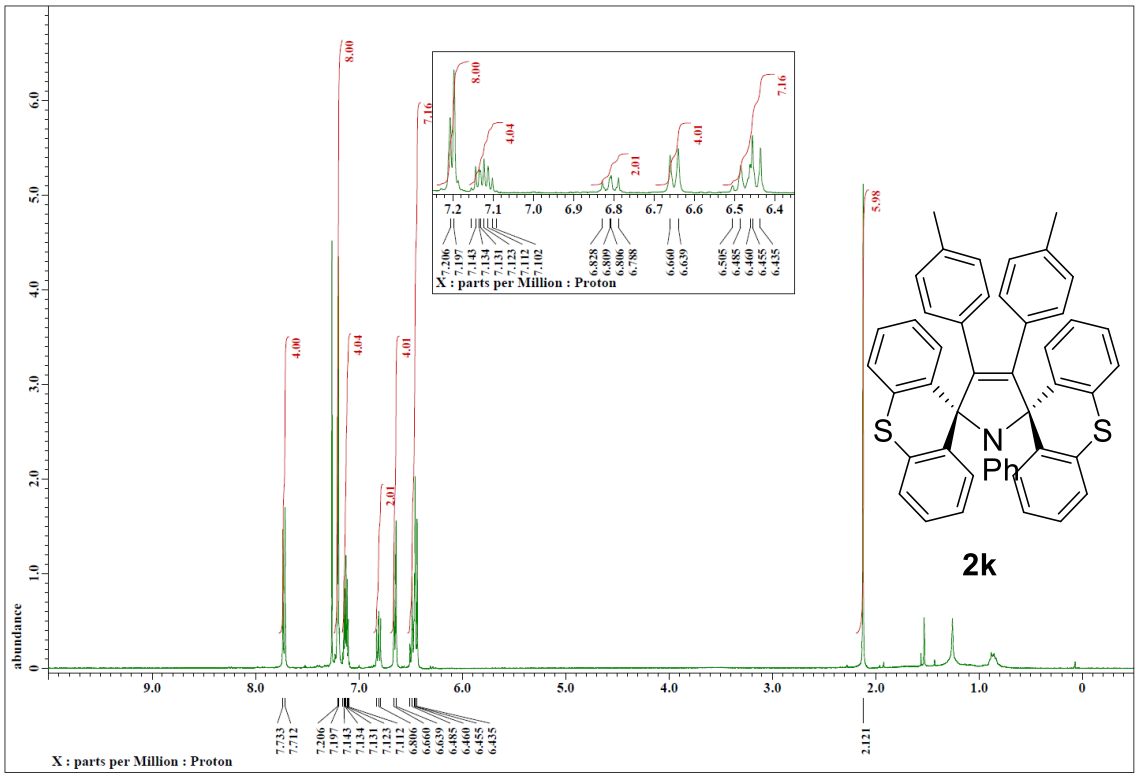
^{1}H NMR ($CDCl_3$, 400 MHz)



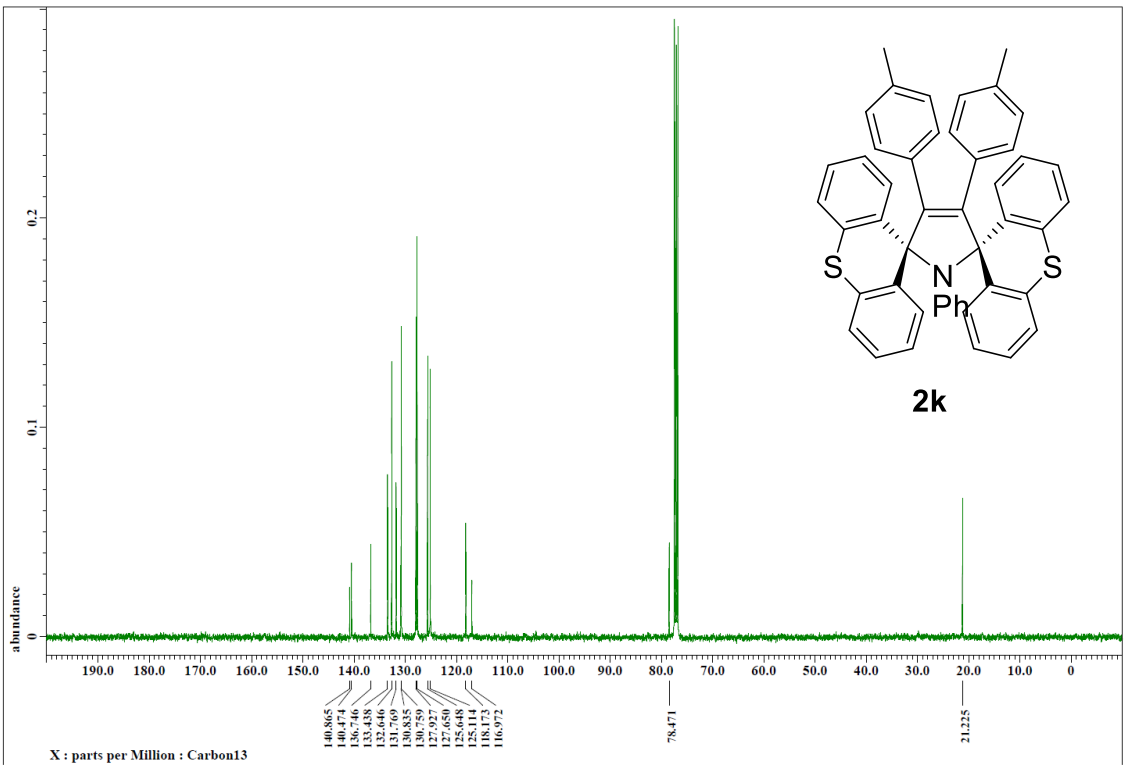
^{13}C NMR ($CDCl_3$, 101 MHz)



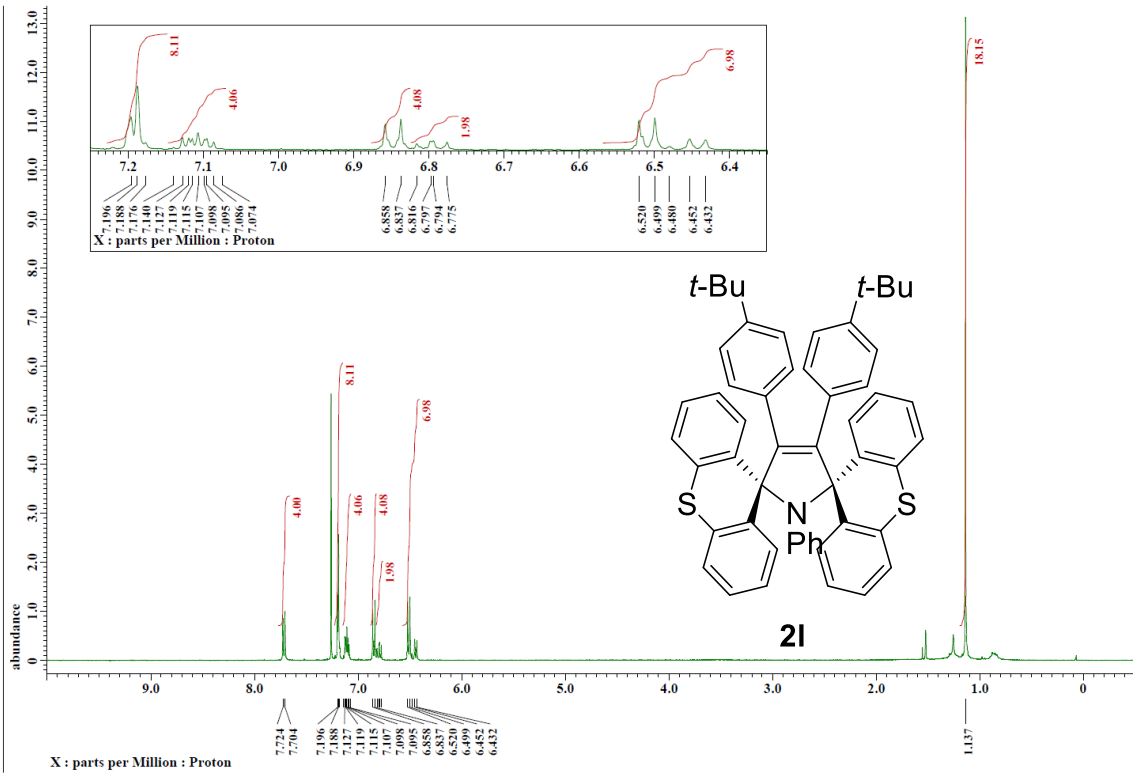
^{1}H NMR ($CDCl_3$, 400 MHz)



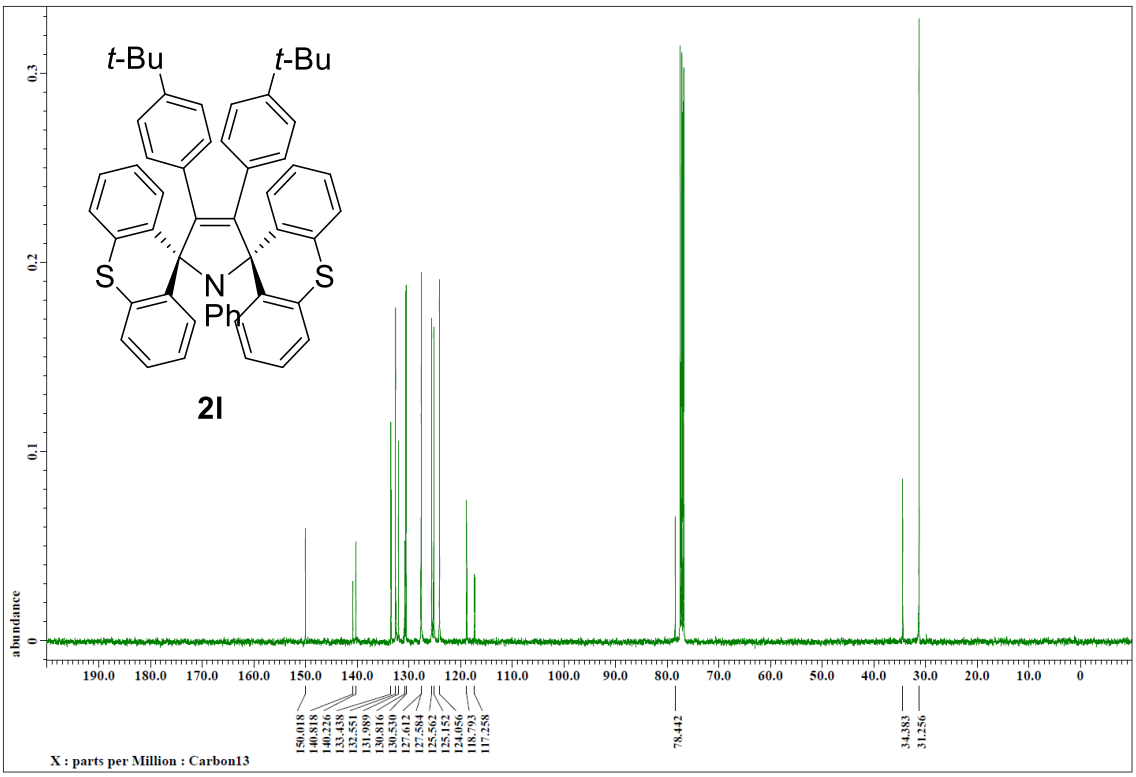
^{13}C NMR ($CDCl_3$, 101 MHz)



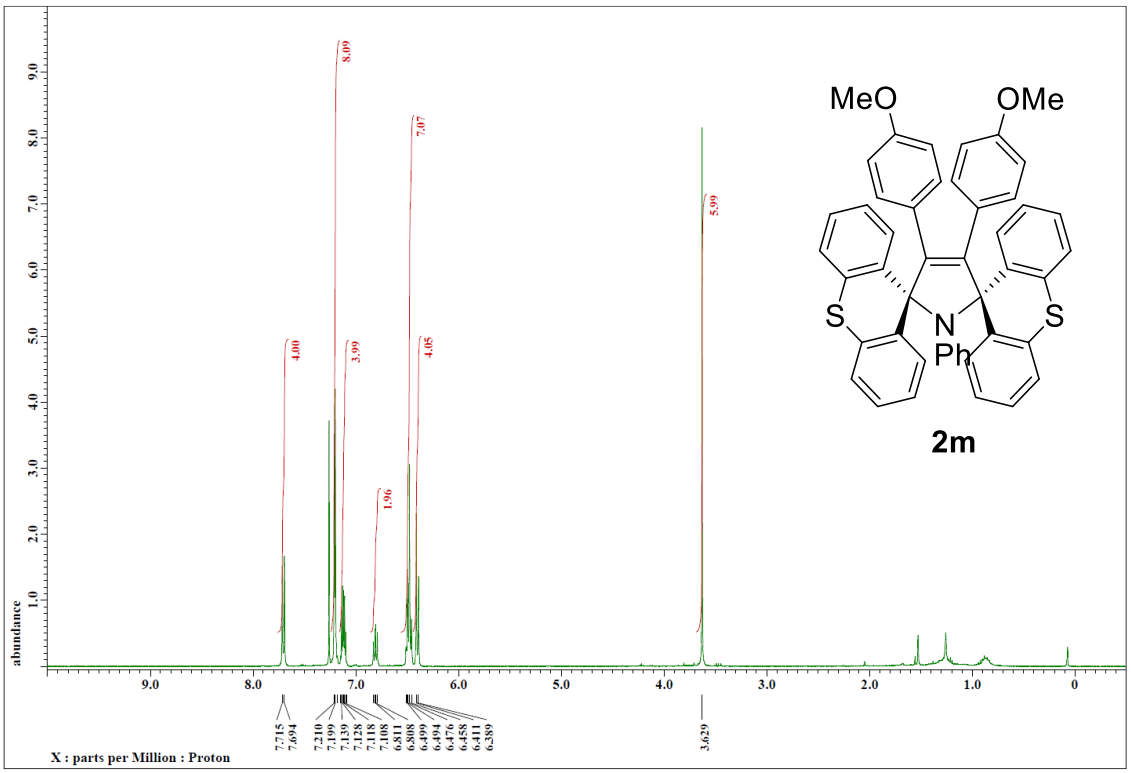
^{1}H NMR ($CDCl_3$, 400 MHz)



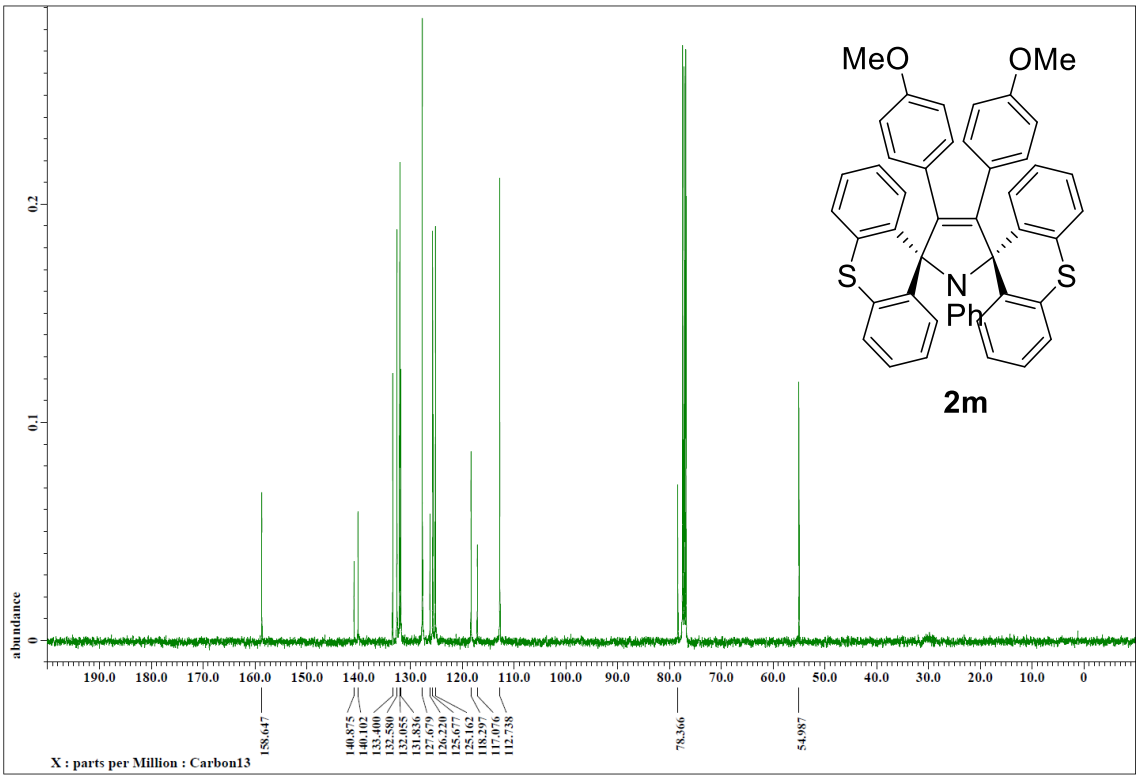
^{13}C NMR ($CDCl_3$, 101 MHz)



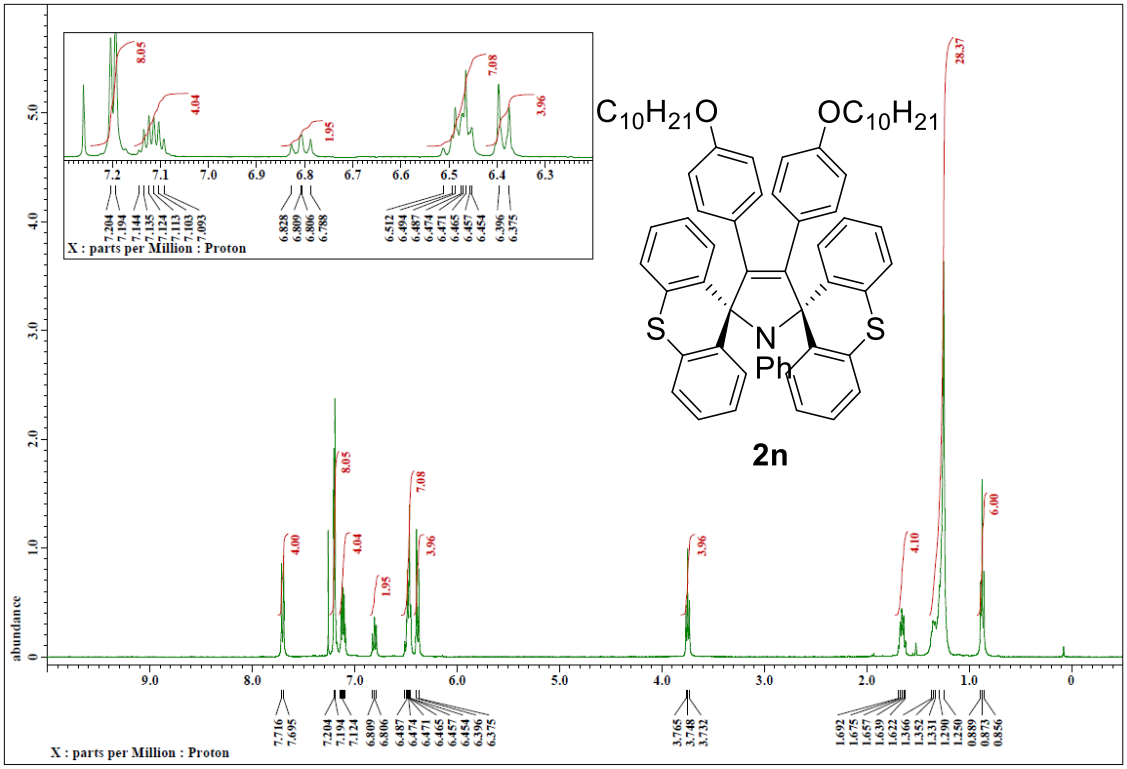
^{1}H NMR ($CDCl_3$, 400 MHz)



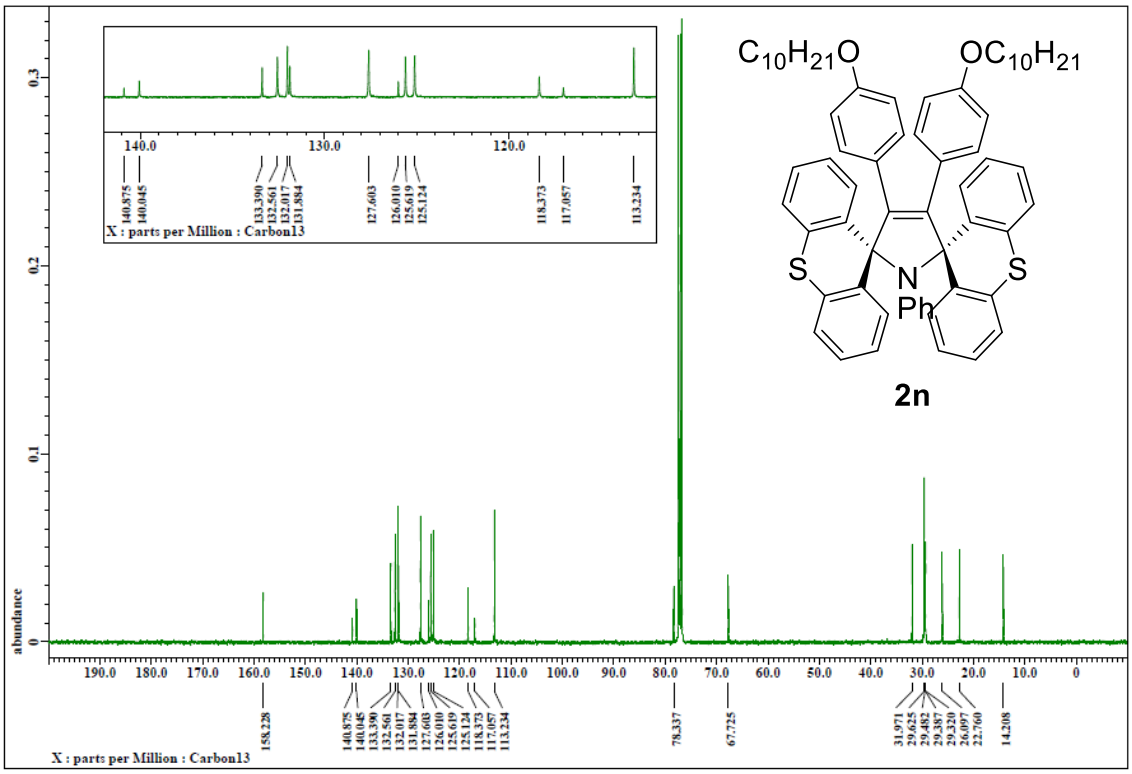
^{13}C NMR ($CDCl_3$, 101 MHz)



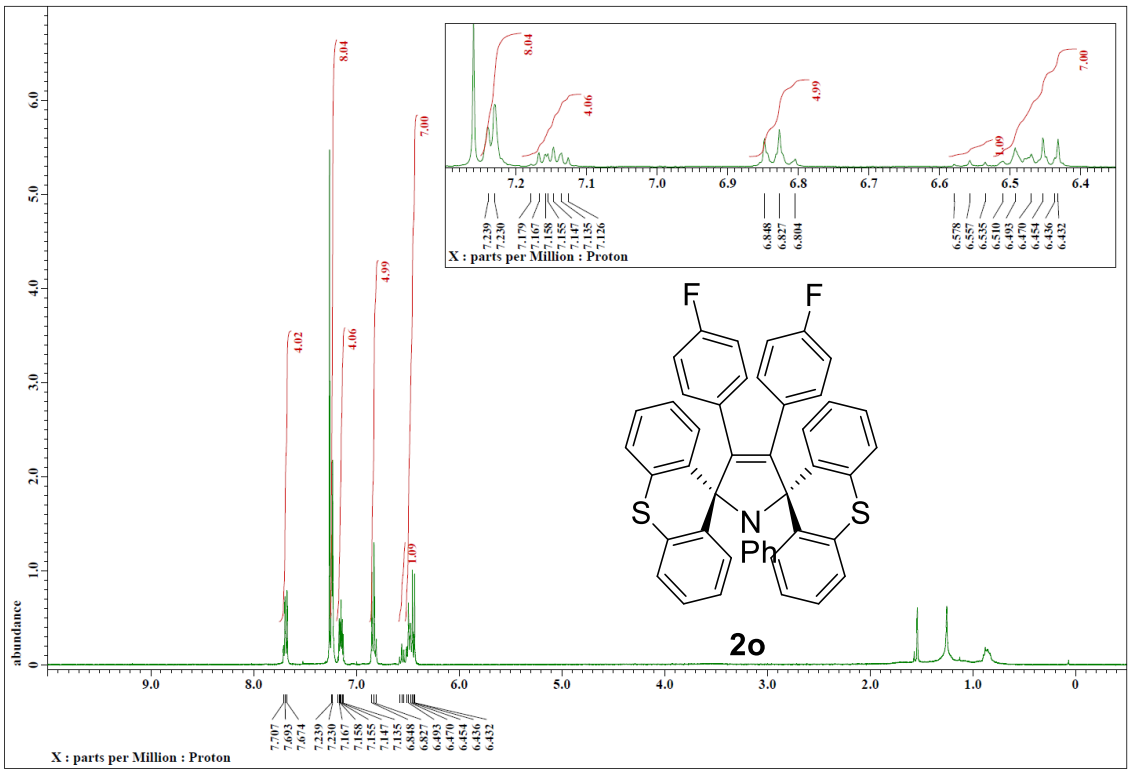
^{1}H NMR ($CDCl_3$, 400 MHz)



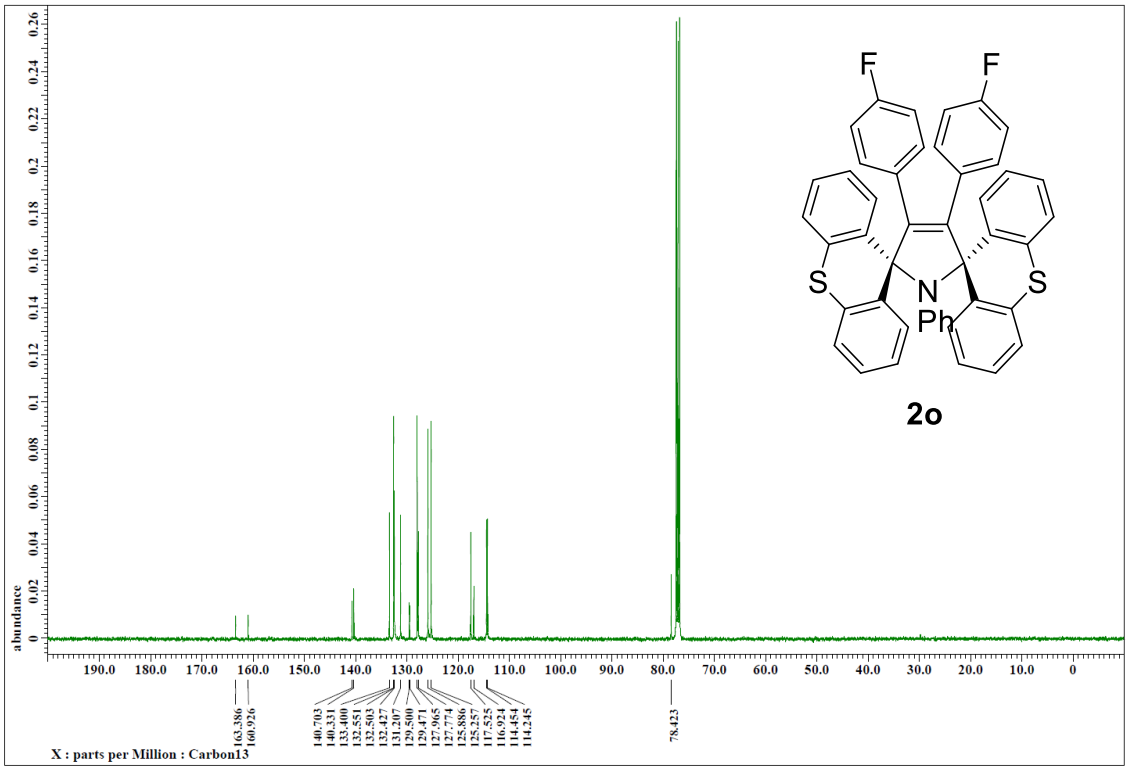
^{13}C NMR ($CDCl_3$, 101 MHz)



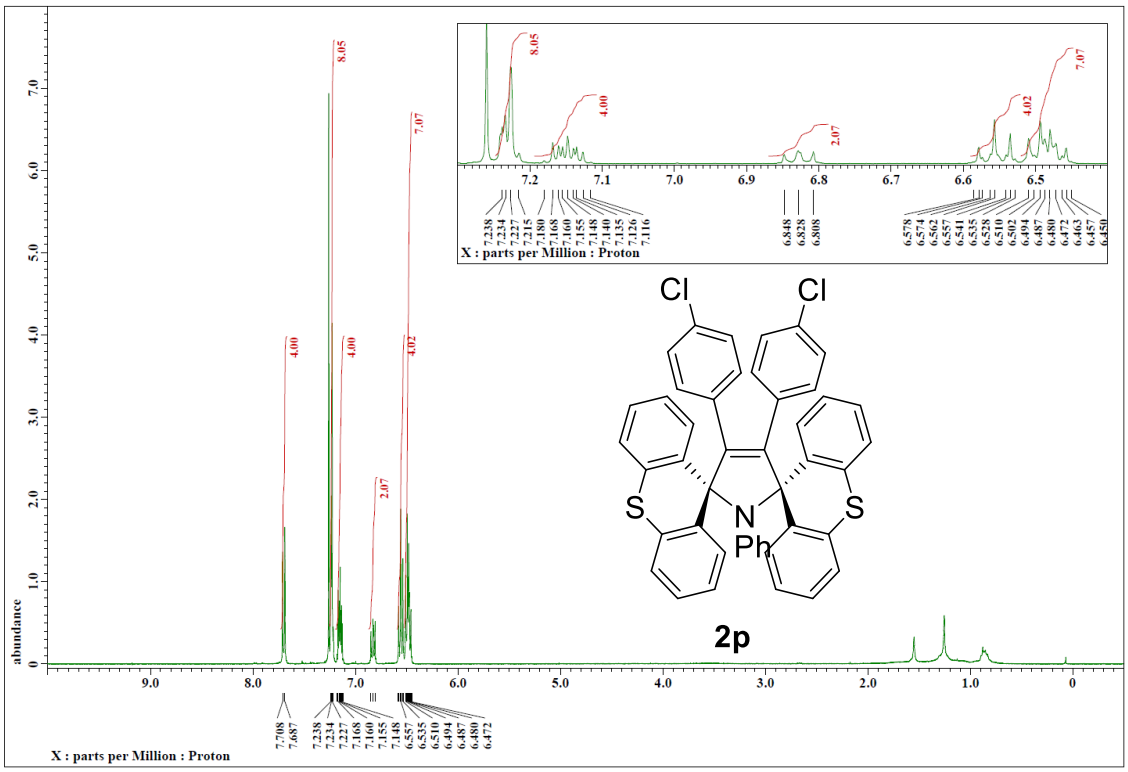
^{1}H NMR ($CDCl_3$, 400 MHz)



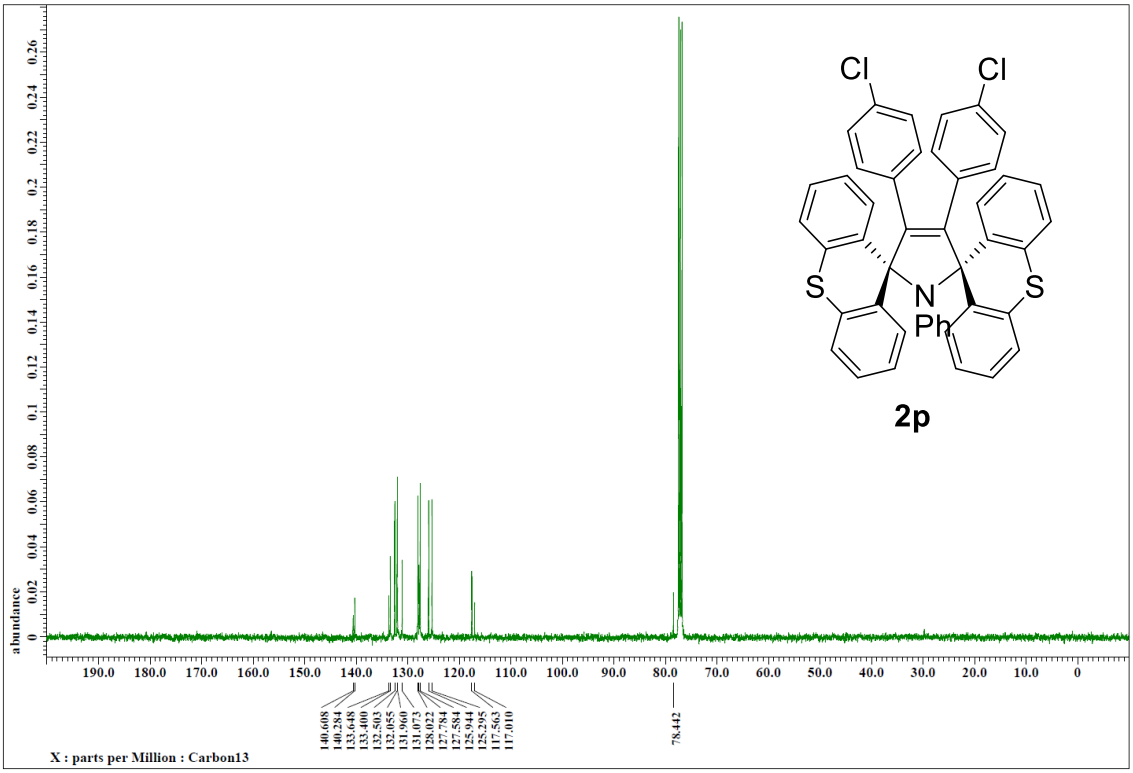
^{13}C NMR ($CDCl_3$, 101 MHz)



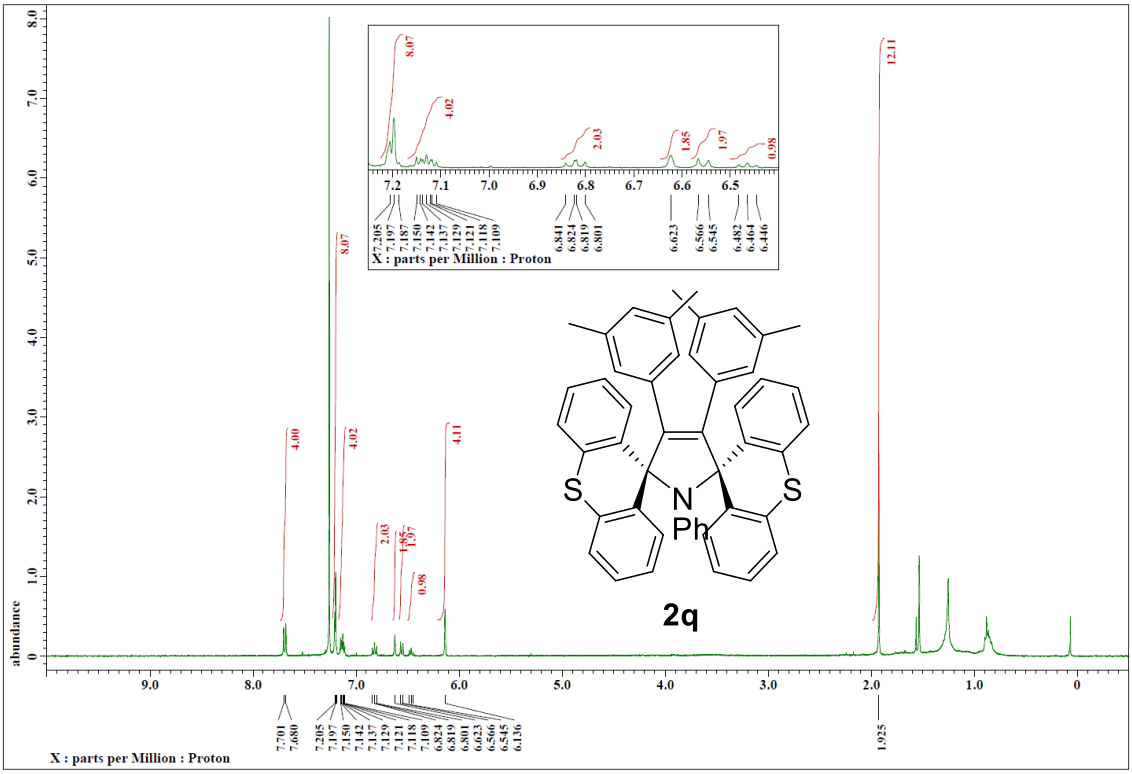
^{1}H NMR ($CDCl_3$, 400 MHz)



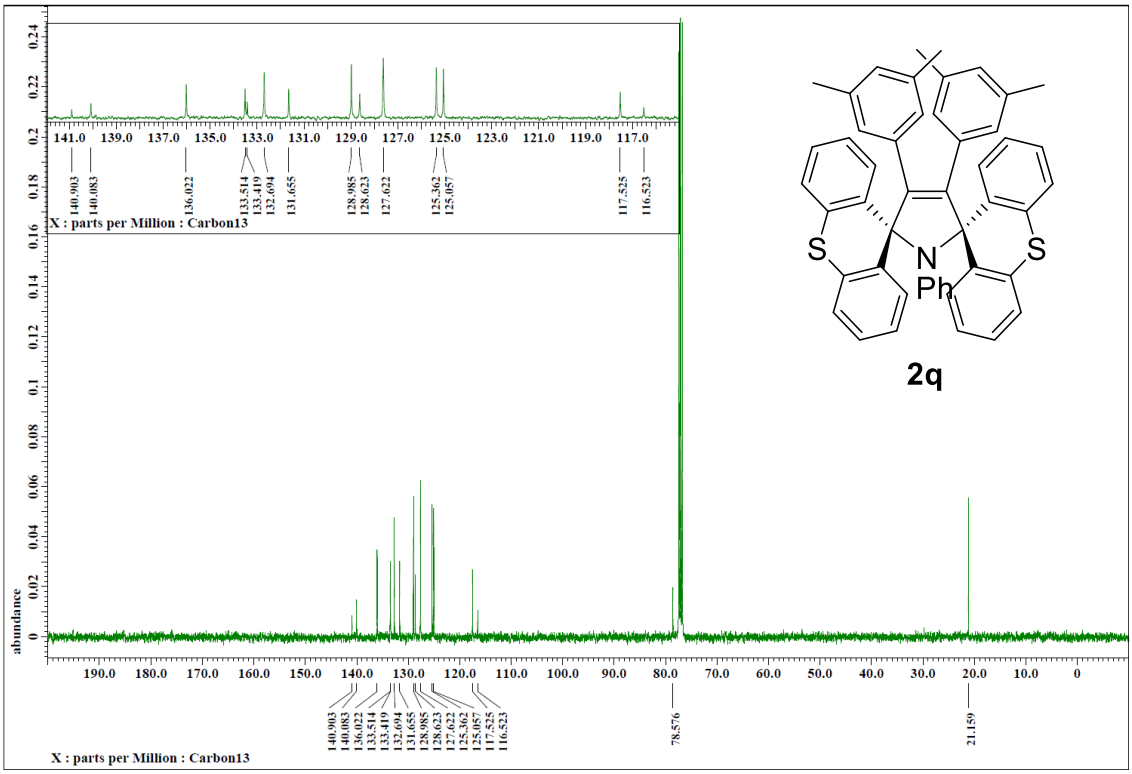
^{13}C NMR ($CDCl_3$, 101 MHz)



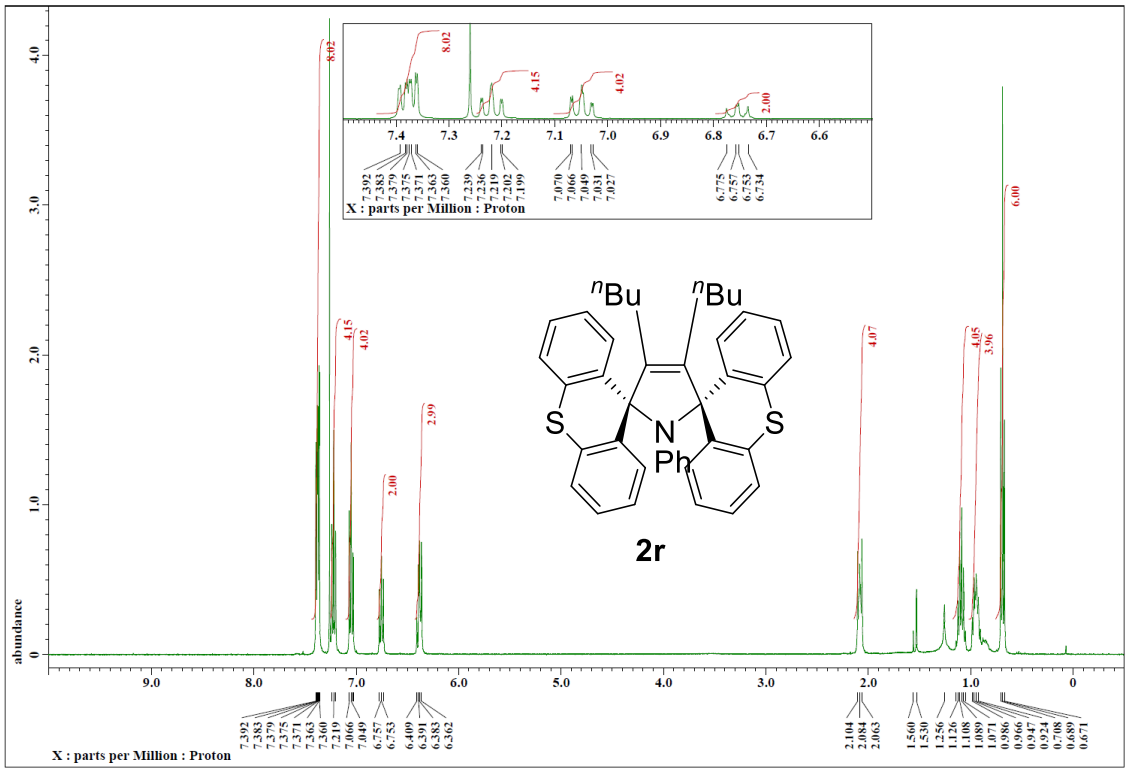
^{1}H NMR ($CDCl_3$, 400 MHz)



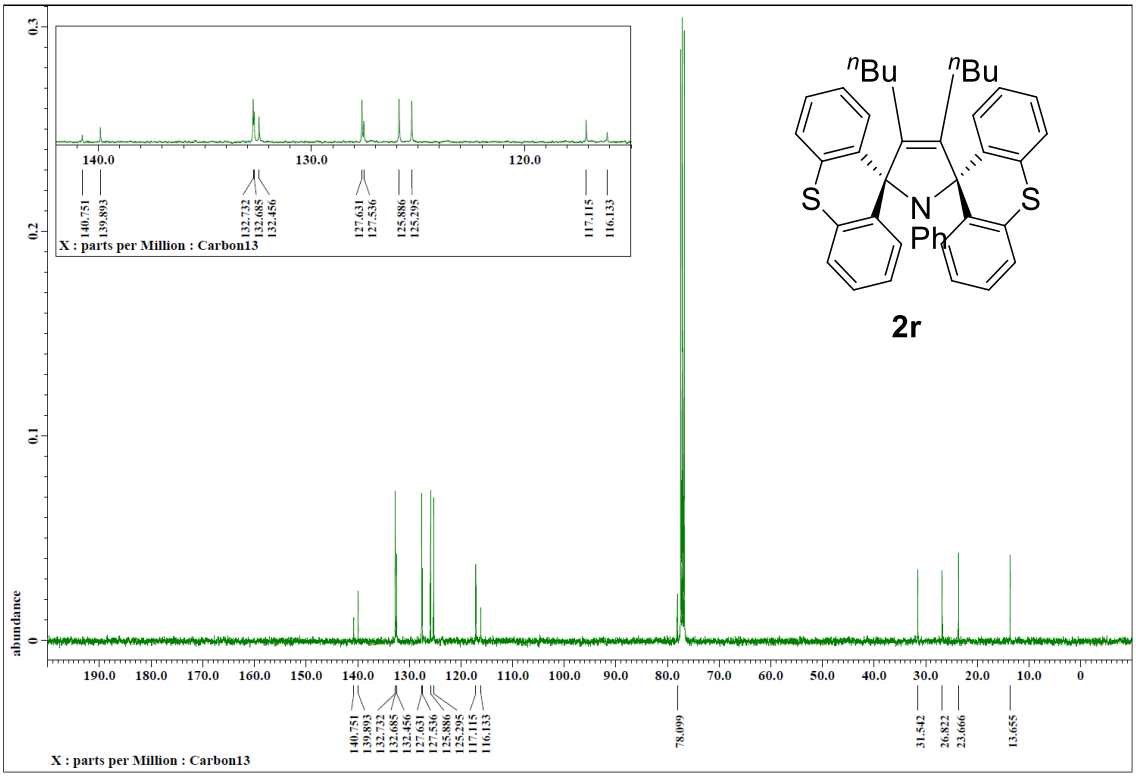
^{13}C NMR ($CDCl_3$, 101 MHz)



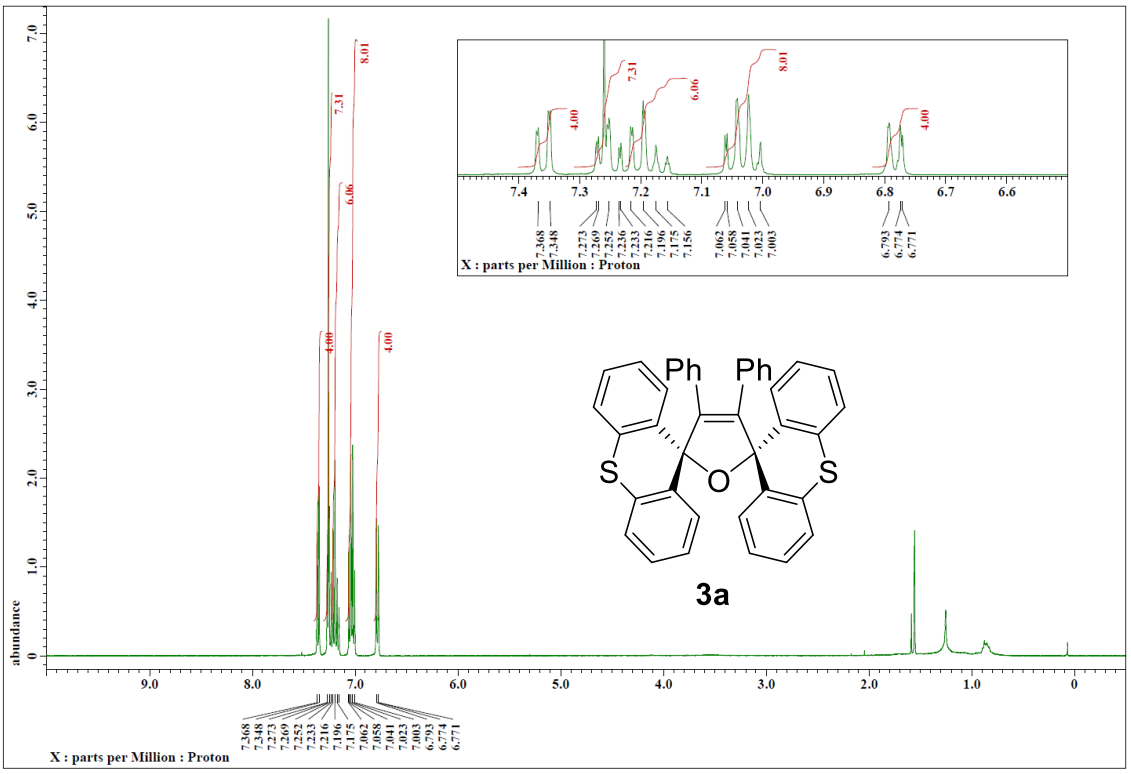
^{1}H NMR ($CDCl_3$, 400 MHz)



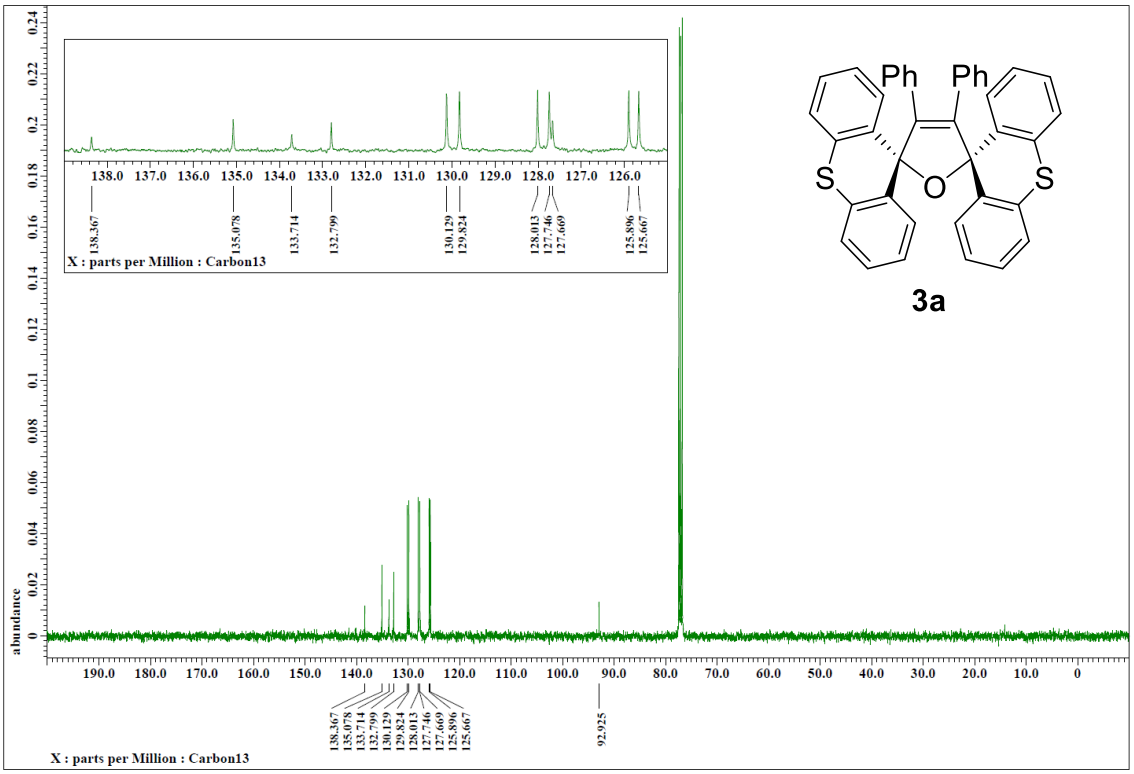
^{13}C NMR ($CDCl_3$, 101 MHz)



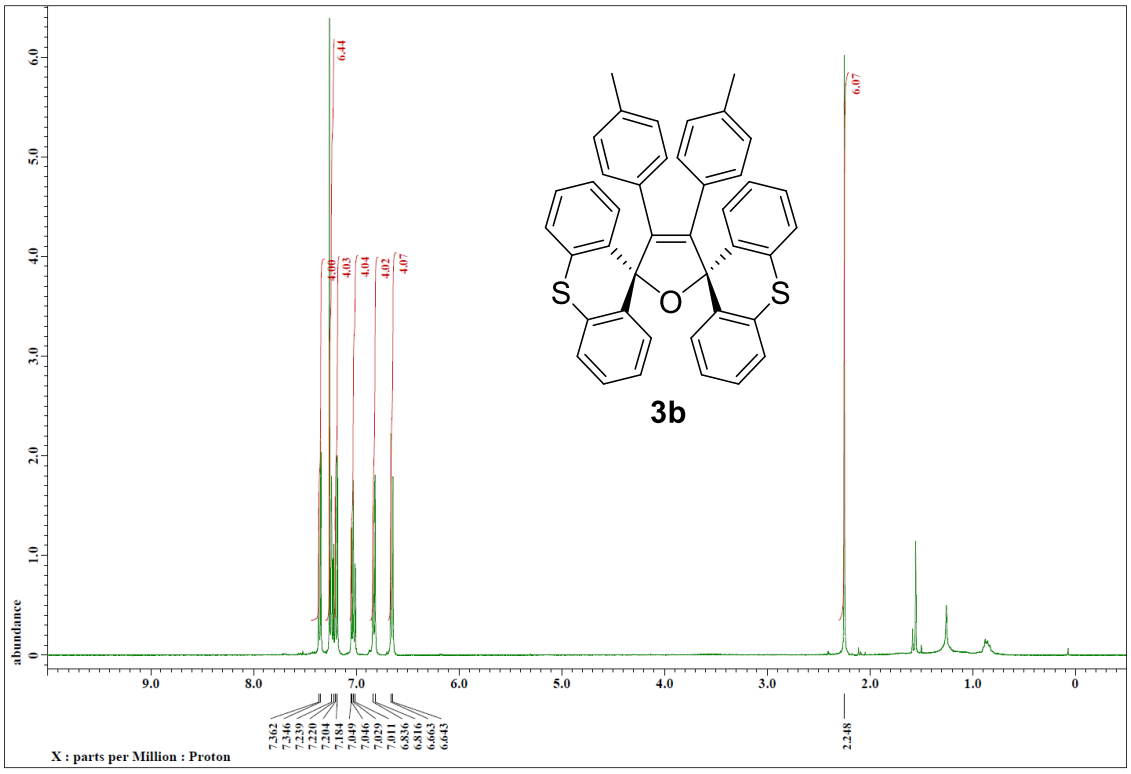
^{1}H NMR ($CDCl_3$, 400 MHz)



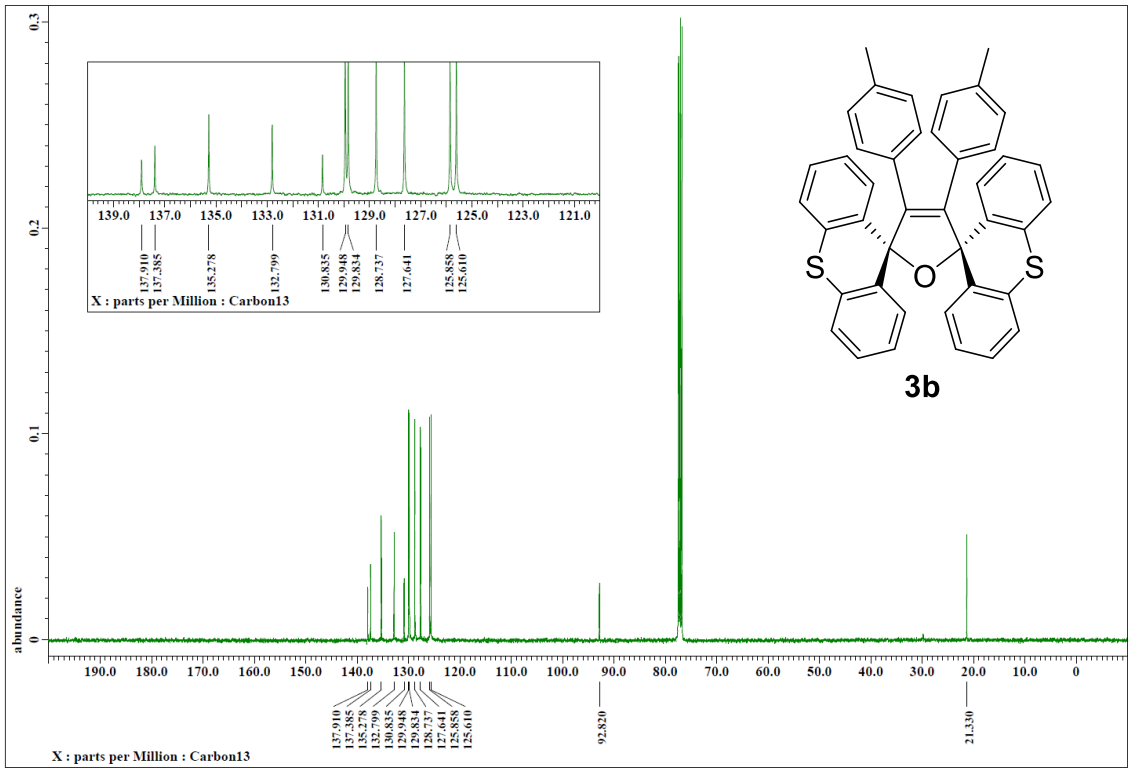
^{13}C NMR ($CDCl_3$, 101 MHz)



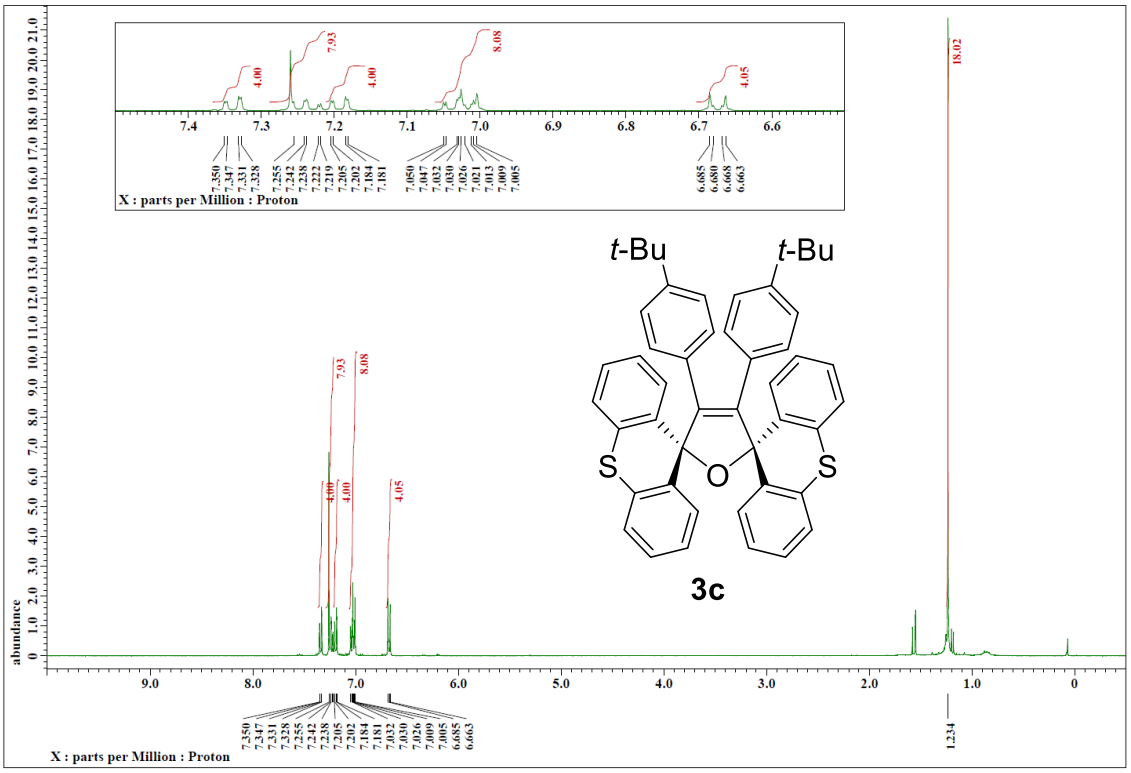
^{1}H NMR ($CDCl_3$, 400 MHz)



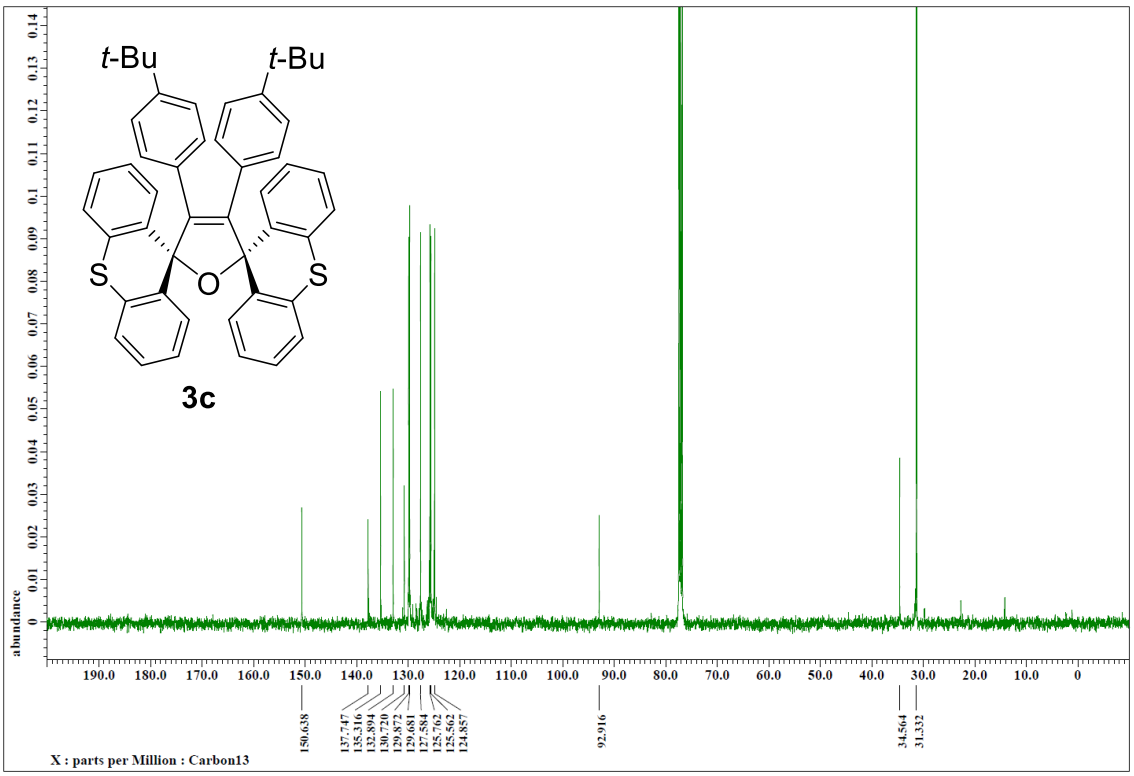
^{13}C NMR ($CDCl_3$, 101 MHz)



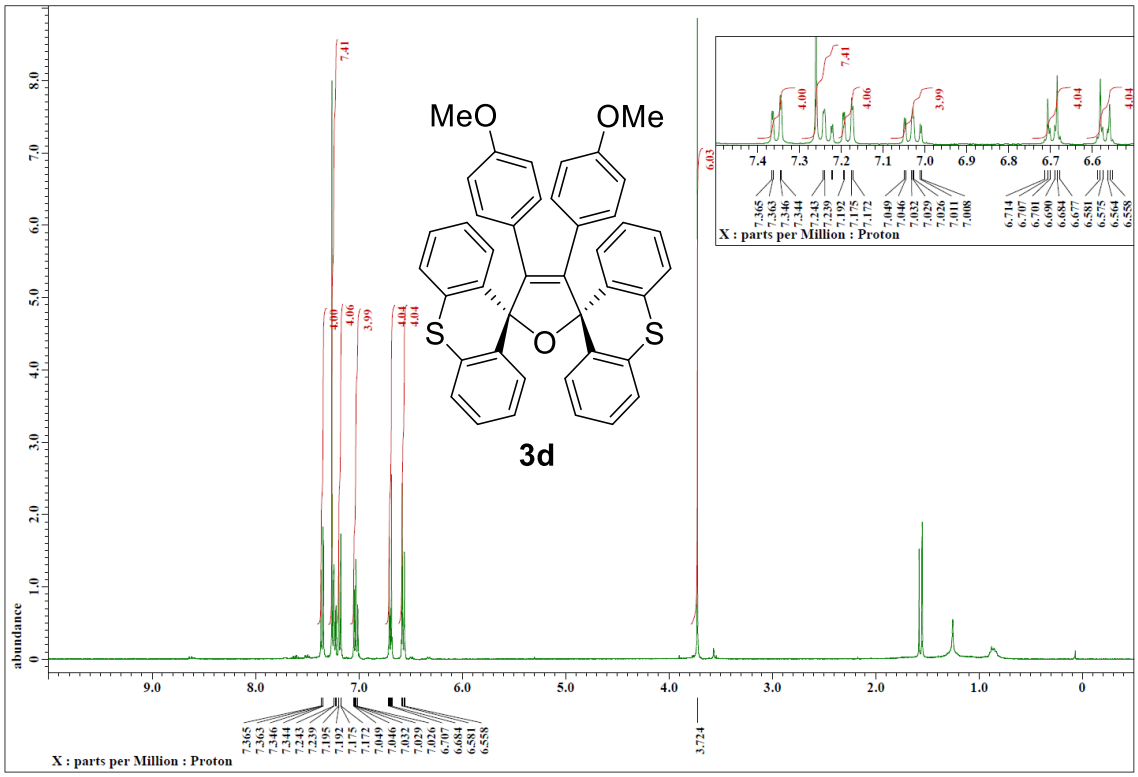
^{1}H NMR ($CDCl_3$, 400 MHz)



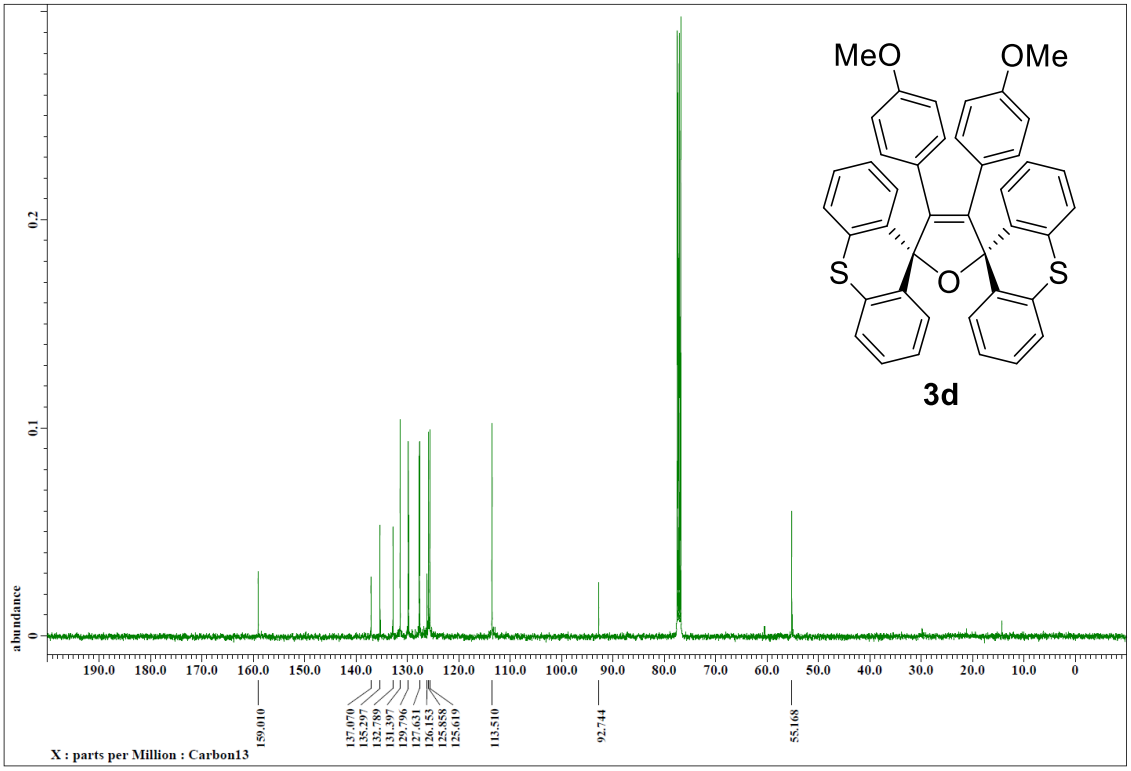
^{13}C NMR ($CDCl_3$, 101 MHz)



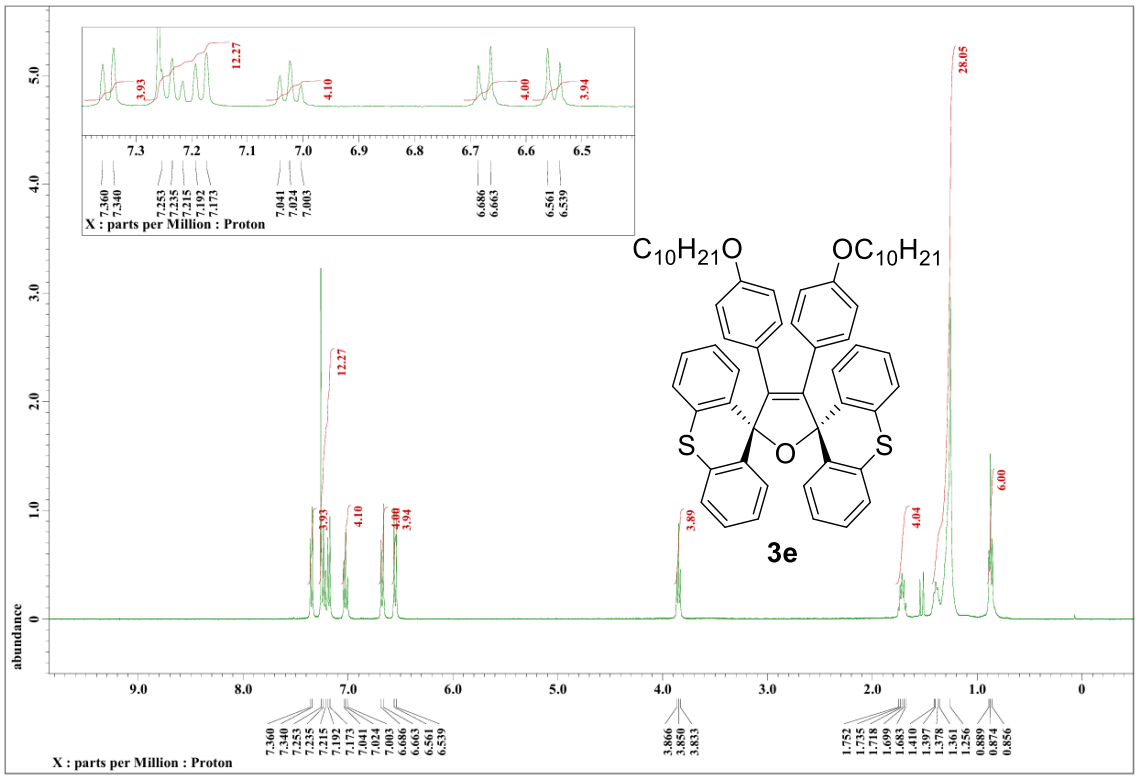
^{1}H NMR ($CDCl_3$, 400 MHz)



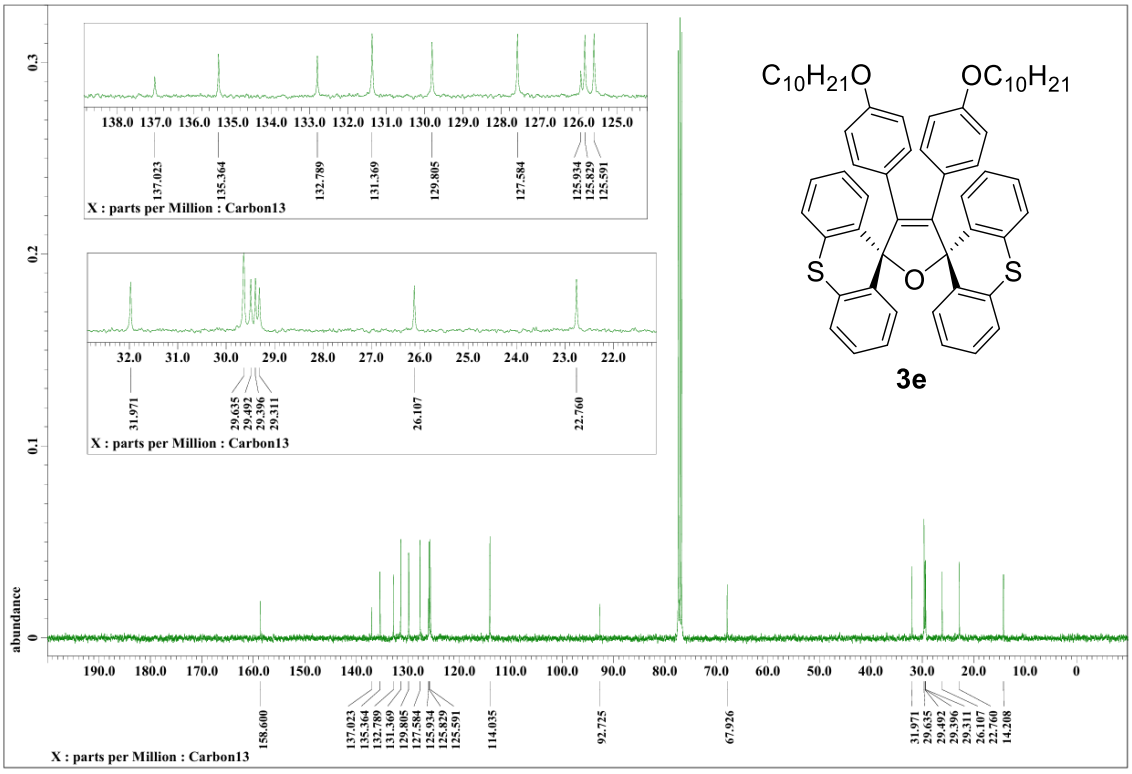
^{13}C NMR ($CDCl_3$, 101 MHz)



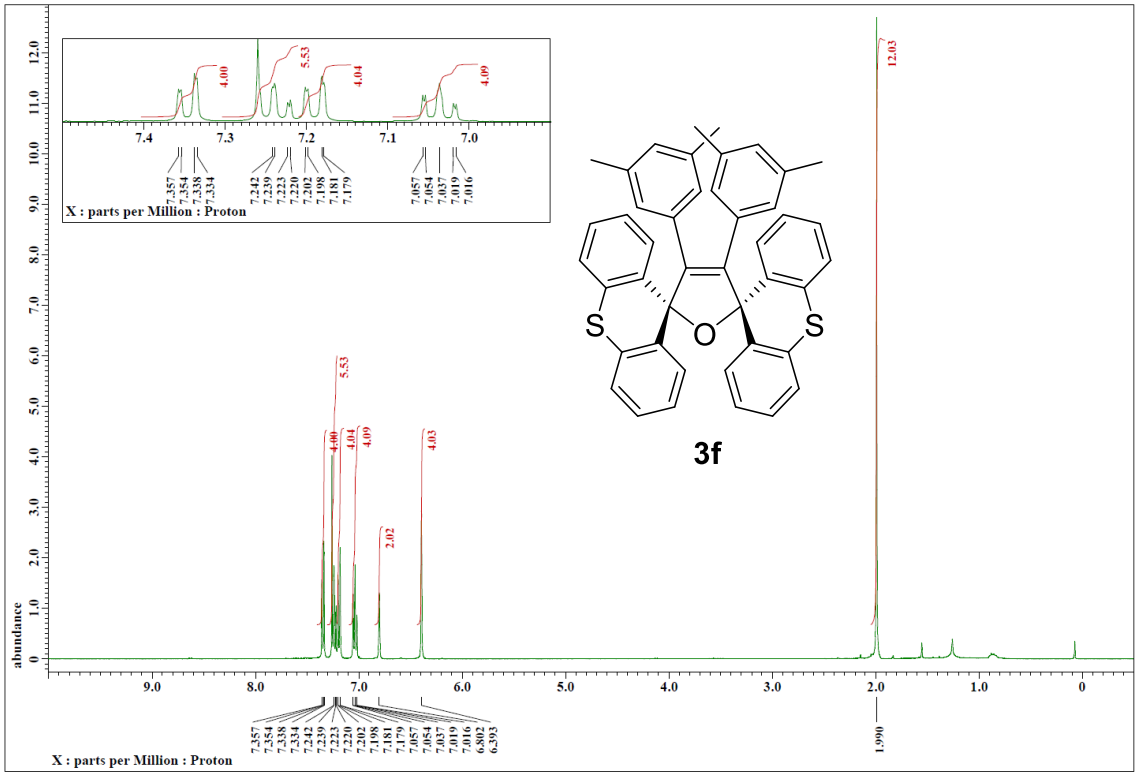
^{1}H NMR ($CDCl_3$, 400 MHz)



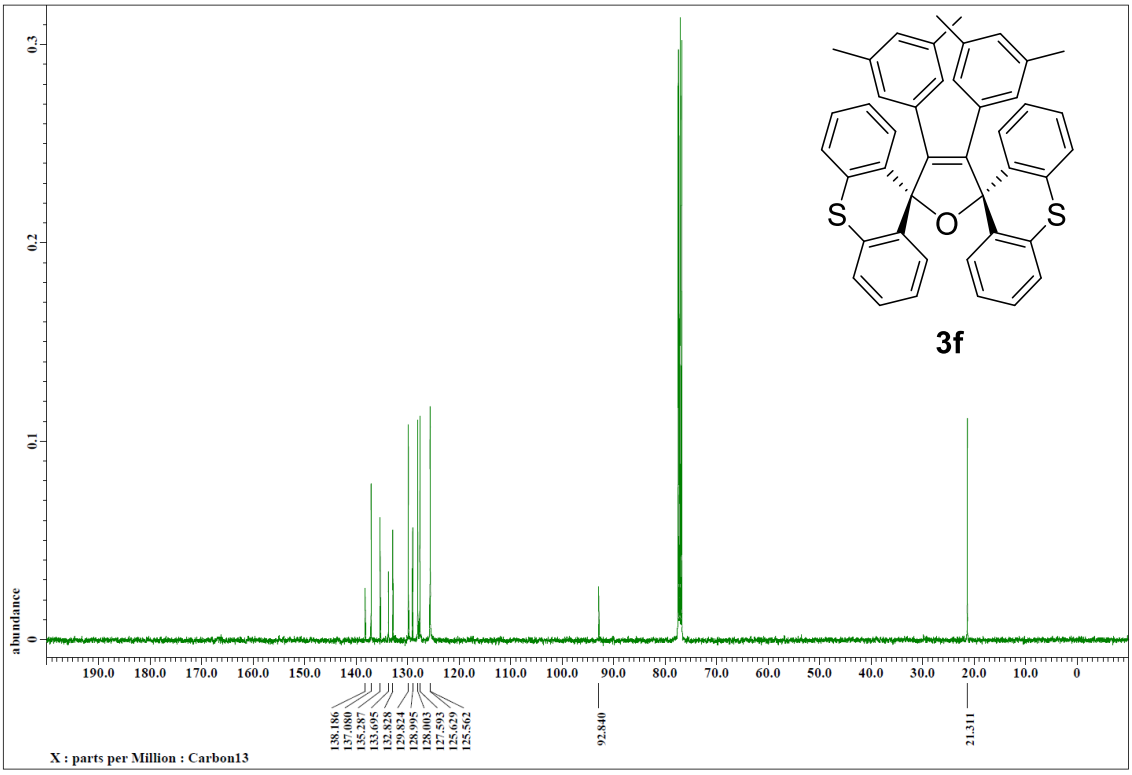
^{13}C NMR ($CDCl_3$, 101 MHz)



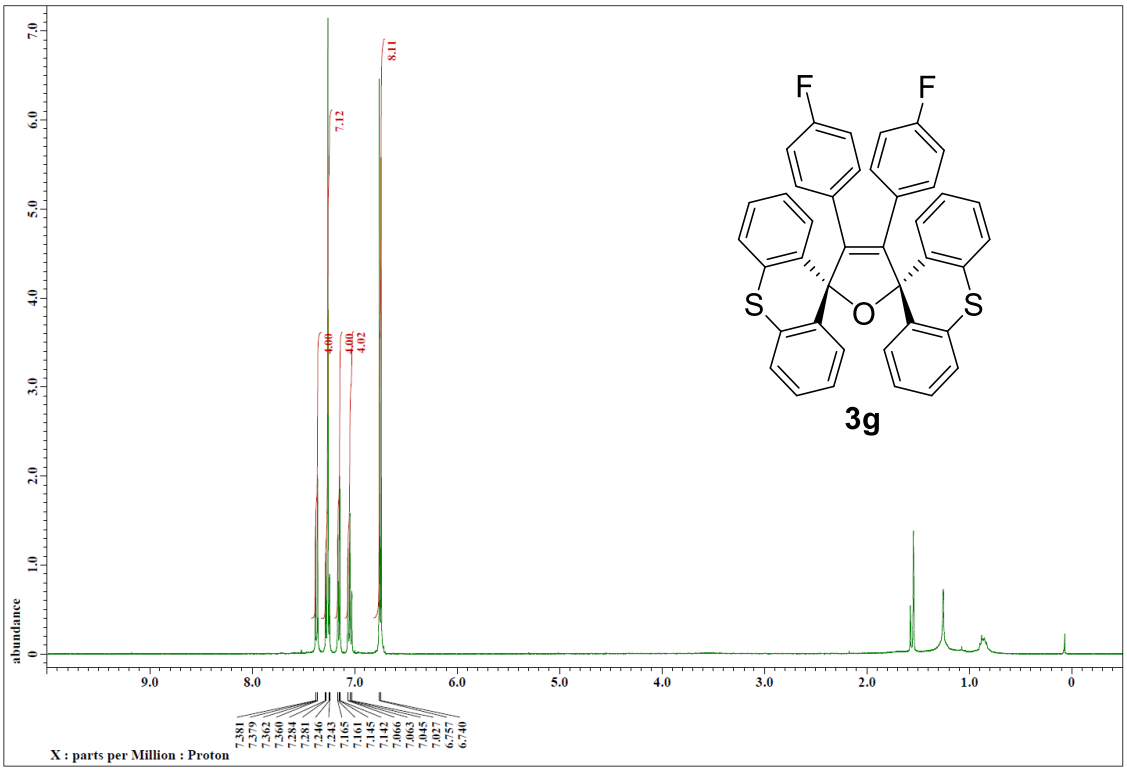
^{1}H NMR ($CDCl_3$, 400 MHz)



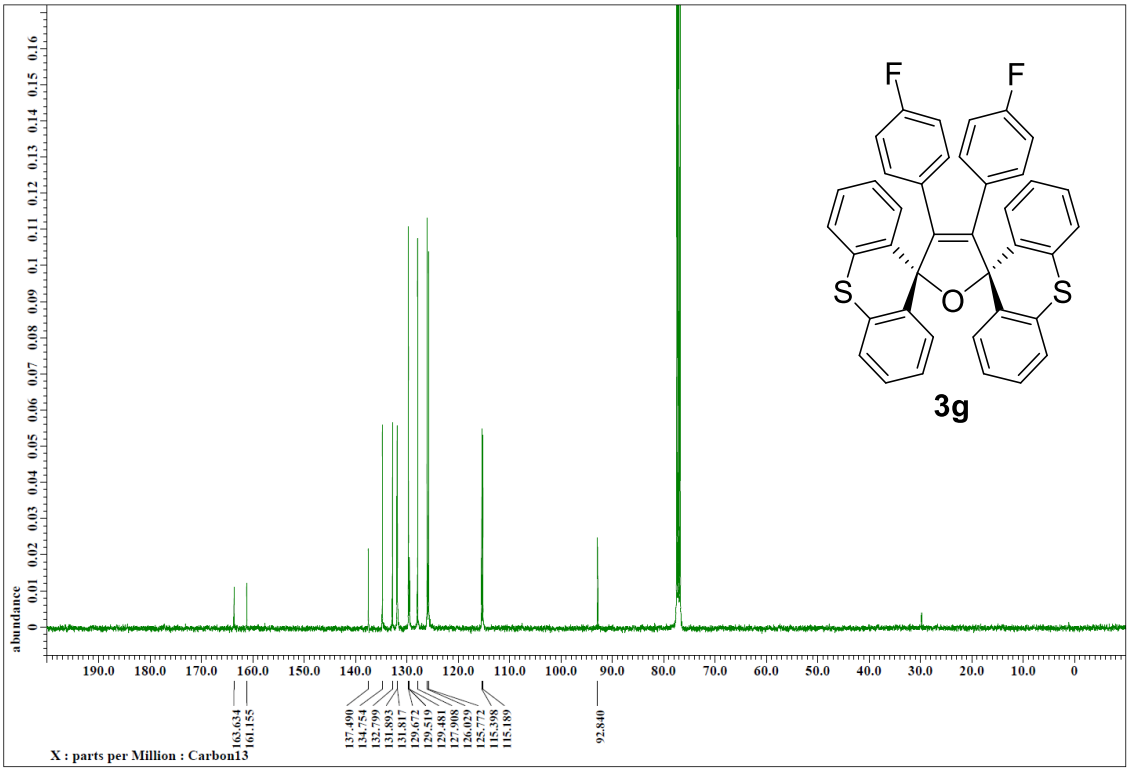
^{13}C NMR ($CDCl_3$, 101 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)



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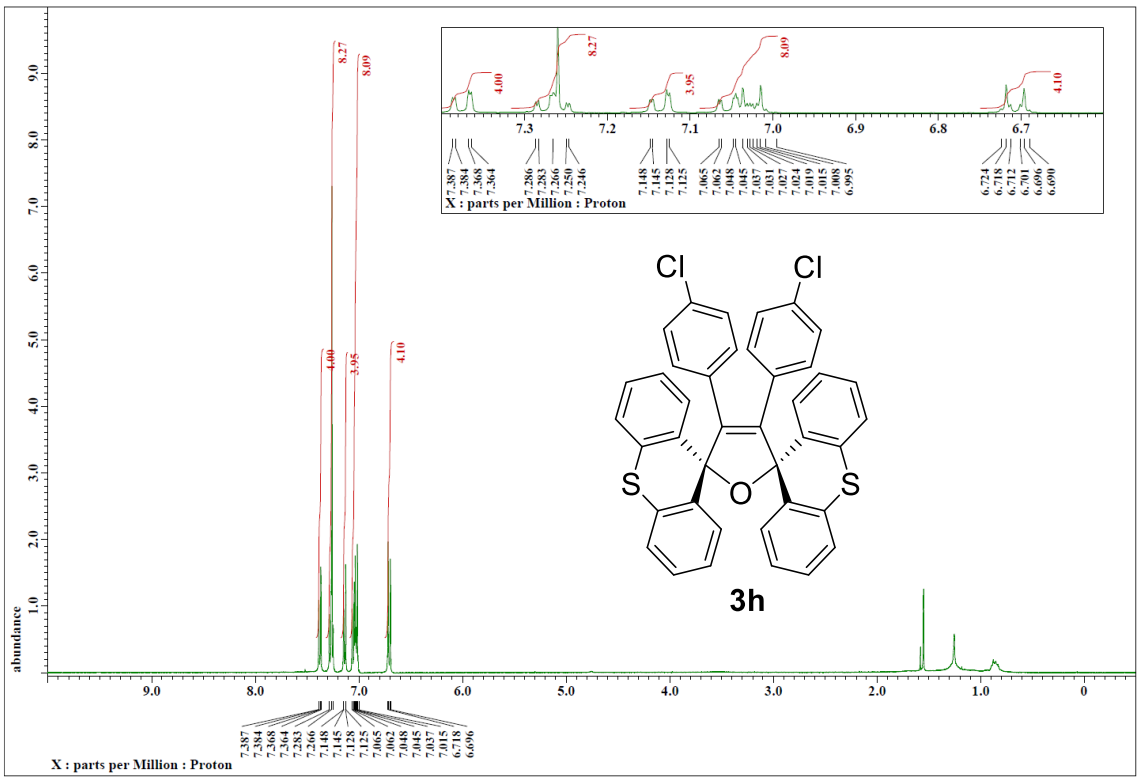

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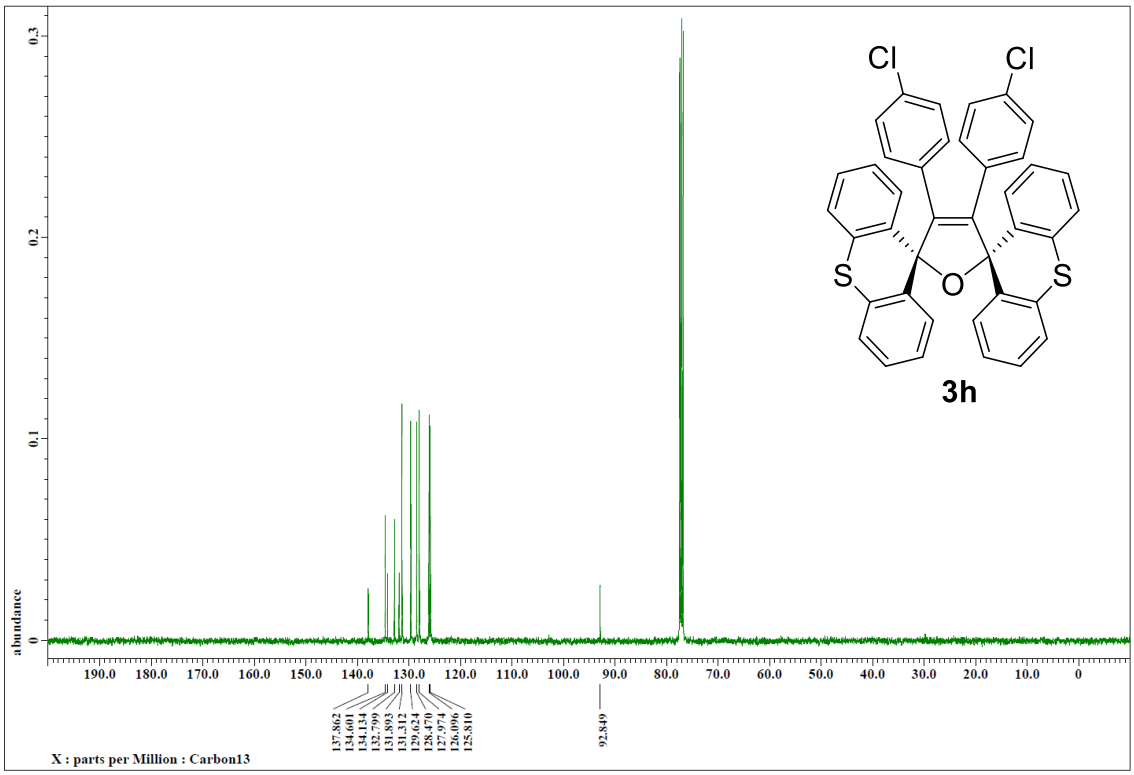
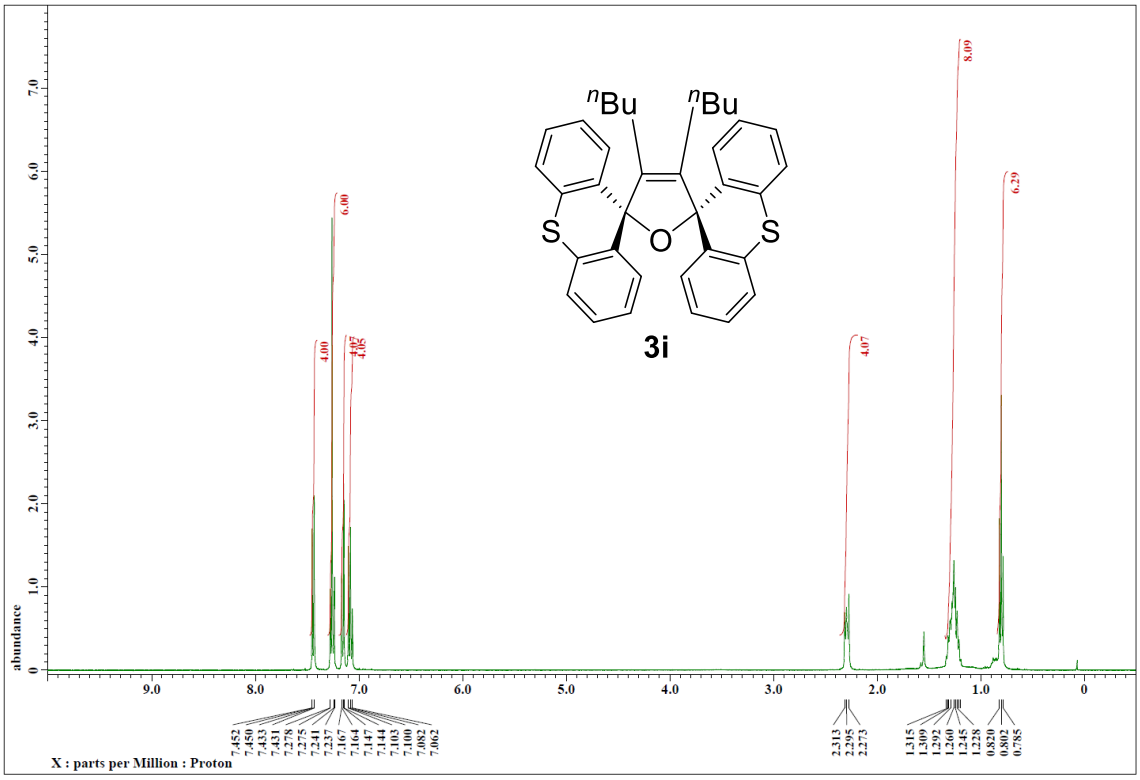
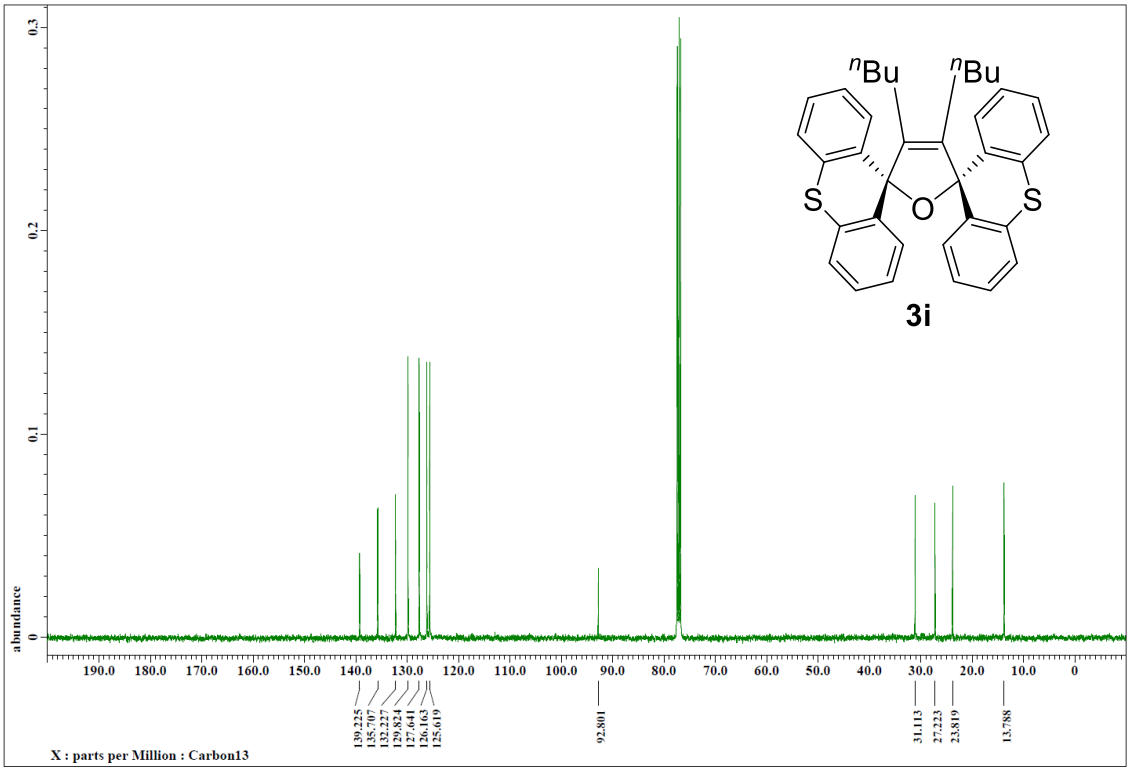


^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)



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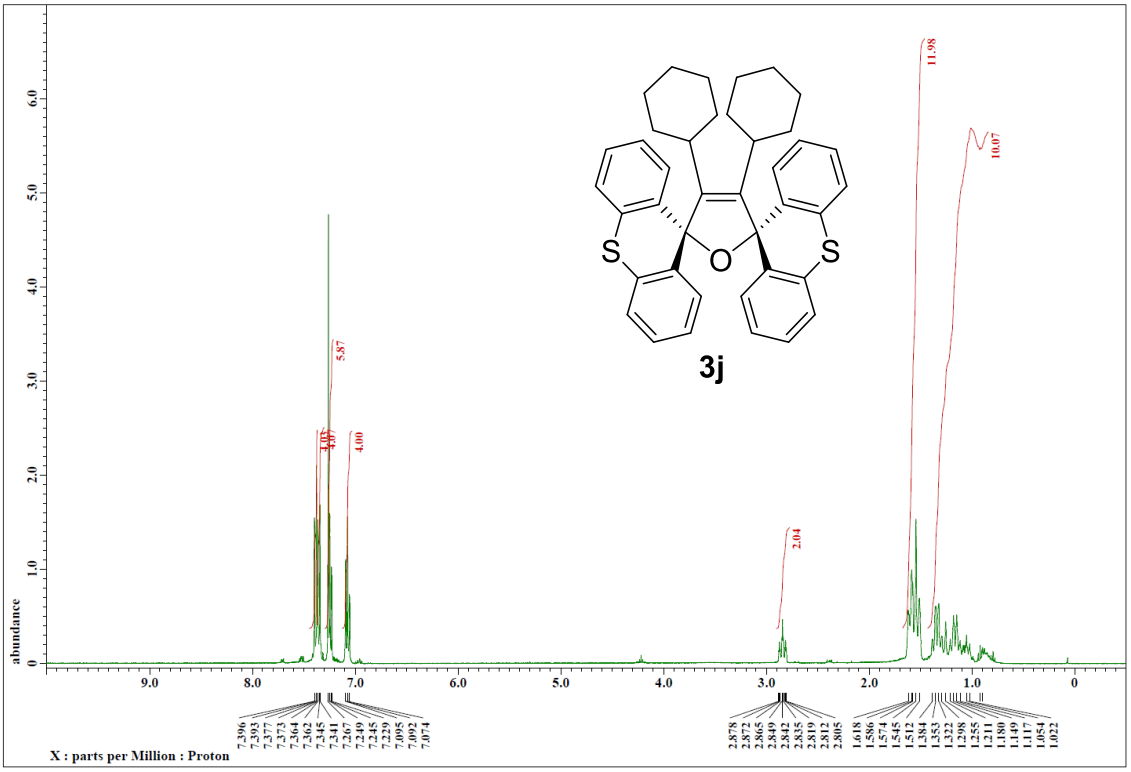

^{13}C NMR ($CDCl_3$, 101 MHz)