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Supplementary Materials

π-Extended Chalcogenoviologens with Stable Radical State Enable Enhanced Visible-Light-Driven Hydrogen Evolution and Statically/Dynamically Electrochromic Displays

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Experimental Procedures

1. Materials and instrumentation

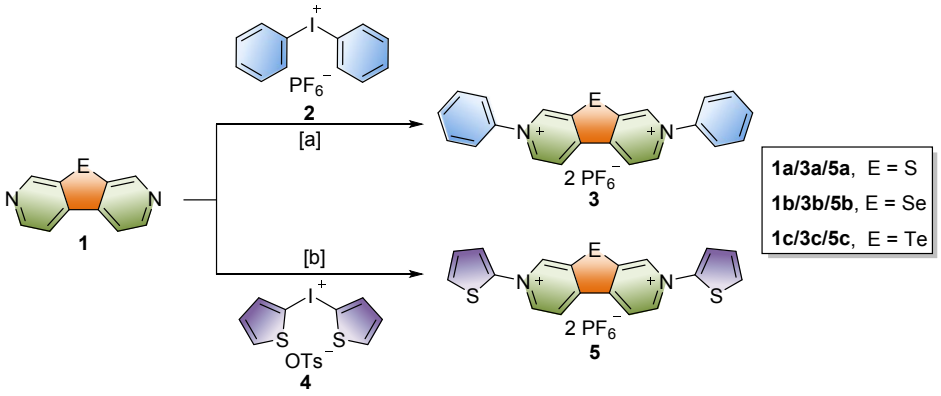
General. All reactions were performed using standard Schlenk and glovebox (Vigor) techniques under argon atmosphere. Safedry DMF was purchased from Adamas-beta®.Anhydrous $Cu(OAc)_2$ (97%), diphenyliodonium hexafluorophosphate (97%), thiophene (99%), 3-Chloroperoxybenzoic acid (85%), I_2 (99.8%) were purchased from Energy Chemical Inc. *p*-Toluenesulfonic acid monohydrate (98%) was purchased from Bide Pharmatech Ltd. Chalcogenoviologens (**1a**-**1c**) and dithienyliodonium tosylate were synthesized according to the references.[1, 2] If no other special indicated, other reagents and solvents were used as commercially available without further purification. NMR spectra were measured on a Bruker Avance-400 spectrometer in the solvents indicated; chemical shifts are reported in units (ppm) by assigning TMS resonance in the ^1H spectrum as 0.00 ppm, DMSO-d_6 resonance in the ^{13}C spectrum as 39.50 ppm. Coupling constants are reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). UV-vis measurements were performed using DH-2000-BAL Scan spectrophotometer. The cyclic voltammetry (CV) in solution were measured using CHI660E B157216, with a polished gold electrode as the working electrode, a Pt-net as counter electrode, and an Ag wire as reference electrode, using ferrocene/ferrocenium (Fc/Fc^+) as internal standard. EPR was measured using a Bruker EMX PLUS6/1 instrument at room temperature in dry degassed DMF. Thermogravimetric analysis (TGA) measurements were carried out in the temperature range of 30-700 °C by using of a Mettler-Toledo TGA1 thermal analyzer in air, at a heating rate of 10 $K \bullet min^{-1}$. High-resolution mass spectra (HRMS) were collected on a Bruker maxis UHR-TOF mass spectrometer in an ESI positive mode. Elemental analysis was conducted on a machine of Euro Vector EA3000. Analytical gas chromatography (GC) for gas sample were carried out on a SHIMDZU GC-2014ATF/SPL (TDX-01 60/80 mesh, 2.0 mm x 3.2mm x 2.1 mm-FID, TCD permanent gases, N_2 carrier gas). Nitrogen as the carrier gas. The 300 W xenon lamp (PLS-SXE300D) used for irradiation and the optical power meter were supplied by Beijing Perfectlight Technology Co., Ltd.. Photographs were taken using a Nikon D5100 digital camera.

In the solution-based ECD, Indium tin oxide (ITO)-coated glass (~ 15 Ω/sq) was utilized as the electrodes and **3/5** was used as active component. The two pieces of ITO glass were sealed together with a UV-cured gasket with 50 μm-thick intervals introduced by Baumgartner group.

In the gel-based electrochromic writing board, indium-tin oxide (ITO)-coated glass (~ 10 Ω/sq) was utilized as the electrodes and **5b** was used as active component, free-standing EC gel consists of **5b**, P(VDF-co-HFP), and [EMI][TFSI] in weight fraction of 3:4:36 introduced by Moon group.[3]

All the computational calculations reported in this work were performed using the Gaussian 09 code. To simulate the experimental UV-Vis in N,N-dimethylformamide (DMF), the Polarizable Continuum Model (PCM)[4] as a self-consistent reaction field (SCRF) was used for the calculation of equilibrium geometries, vibrational frequencies and excited state calculations. The geometries for the ground state of these compounds in the DMF solution were optimized at the B3LYP level[5] with the LANL08d basis set[6] applied for the Te atom and 6-311G(d,p) basis set for all other atoms. And the keyword “opt=tight” was used.

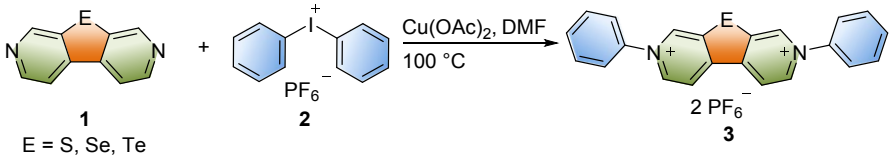
2. Synthetic procedures



Conditions: [a] $Cu(OAc)_2$, DMF, 100 °C. [b]$Cu(OAc)_2$, DMF, 40 °C; then NH_4PF_6, H_2O.

Scheme S1. Synthesis of π-extended chalcogenoviologens **3** and **5**.

Synthesis of arylated chalcogenoviologens E-PhV^{2+}.



1 (1.0 mmol), diphenyliodonium hexafluorophosphate **2** (1278 mg, 3.0 mmol) and $Cu(OAc)_2$·(9 mg, 0.05 mmol, 5 mol %) were dissolved in dried and degassed DMF (30 mL) and heated to 100 °C for 8 h while stirring. The solvent were removed via decompression, the residual oil was taken up in acetone/chloroform/diethyl ether (1:1:1), and filtered. The residue was taken up in chloroform (30 mL) and acetone (6 mL) and stirred for 2 h. The filtered solid was washed with cold water and dried under a vacuum to obtain **3**.

Sulfur-bridged arylviologen analogue.

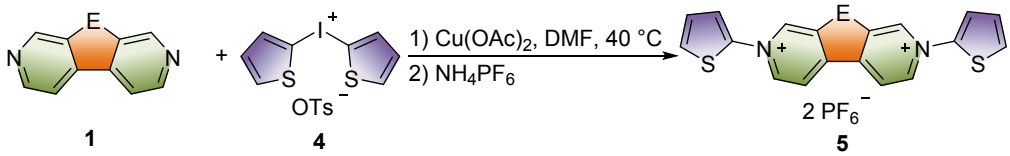
3a: a primrose yellow solid. Yield: 472 mg (75%). ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.55 (s, 2H, Py*H*), 9.70 (s, 4H, Py*H*), 8.06–8.04 (m, 4H, *o*-Ph*H*), 7.89–7.84 (m, 6H, *p*-/*m*-Ph*H*); ^{13}C{H} NMR (DMSO-d_6, 100 MHz): δ 144.35, 143.08, 142.59, 141.99, 140.08, 131.74, 130.47, 124.91, 123.24; ^{19}F NMR (DMSO-d_6, 376 MHz): δ 69.20, 71.09; ^{31}P NMR (DMSO-d_6, 162 MHz): δ −144.222 (hept); HRMS (ESI) m/z: [M-2PF_6^-] calcd for $C_{22}H_{16}N_2S$ 340.1019; found 340.1028; elemental analysis calcd (%) for $C_{22}H_{16}F_{12}N_2P_2S$: C 42.20, H 2.79, N 4.61; found: C 41.92, H 2.56, N 4.44; UV/vis (in DMF): λ_{max} (ε) = 402 nm (4.964 × 10^3 M^{-1} cm^{-1}); Mp (°C): > 300 (changed to dark at 243 °C).

Selenium-bridged arylviologen analogue.

3b: a yellow green solid. Yield: 528 mg (78%). ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.31 (s, 2H, Py*H*), 9.71–9.66 (m, 4H, Py*H*), 8.05–8.03 (m, 4H, *o*-Ph*H*), 7.89–7.83 (m, 6H, *p*-/*m*-Ph*H*); ^{13}C{H} NMR (DMSO-d_6, 100 MHz): δ 145.89, 145.67, 143.63, 143.05, 140.30, 131.67, 130.47, 124.81, 124.17; ^{19}F NMR (DMSO-d_6, 376 MHz): δ 69.18, 71.07; ^{31}P NMR (DMSO-d_6, 162 MHz): δ −144.223 (hept); HRMS (ESI) m/z: [M-2PF_6^-] calcd for $C_{22}H_{16}N_2Se$ 388.0465; found 388.0473; elemental analysis calcd (%) for $C_{22}H_{16}F_{12}N_2P_2Se$: C 39.55, H 2.72, N 4.61; found: C 39.02, H 2.38, N 4.14; UV/vis (in DMF): λ_{max} (ε) = 431 nm (4.559 × 10^3 M^{-1} cm^{-1}); Mp (°C): > 300 (changed to dark at 260 °C).

Tellurium-bridged arylviologen analogue.

3c: a red solid. Yield: 508 mg (70%). ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.97 (s, 2H, Py*H*), 9.64–9.60 (m, 4H, Py*H*), 8.03–8.01 (m, 4H, *o*-Ph*H*), 7.87–7.82 (m, 6H, *p*-/*m*-Ph*H*); ^{13}C{H} NMR (DMSO-d_6, 100 MHz): δ 151.17, 149.63, 143.01, 140.17, 139.63, 131.49, 130.44, 125.37, 124.74; ^{19}F NMR (DMSO-d_6, 376 MHz): δ 69.22, 71.11; ^{31}P NMR (DMSO-d_6, 162 MHz): δ −144.200 (hept); HRMS (ESI) m/z: [M-2PF_6^-] calcd for $C_{22}H_{16}N_2Te$ 438.0373; found 438.0369; elemental analysis calcd (%) for $C_{22}H_{16}F_{12}N_2P_2Se$: C 36.79, H 2.51, N 3.99; found: C 36.40, H 2.22, N 3.86; UV/vis (in DMF): λ_{max} (ε) = 506 nm (3.517 × 10^3 M^{-1} cm^{-1}); Mp (°C): > 300 (changed to dark at 235 °C).



1 (0.3 mmol), di(2-thienyl)-iodonium tosylate **4** (464 mg, 1.0 mmol) and $Cu(OAc)_2$·(3 mg, 0.017 mmol, 5 mol %) were dissolved in dried and degassed DMF (30 mL) and heated to 40 °C for 36 h while stirring. The solvent were removed via decompression, the residual oil was taken up in THF/CH_2Cl_2/diethyl ether (1:1:1), and filtered. The filtered solid was washed with CH_2Cl_2 and dried under a vacuum. The solid was dispersed in H_2O (20 mL) and saturated NH_4PF_6 solution (3 mL) was dropped into the dispersion while stirring. After reacted for 8 h at room temperature, the precipitate was isolated via vacuum filtration and washed with H_2O (10 mL) and DCM (10 mL) for at least 3 times, respectively. The precipitate was collected and dried under high vacuum to obtain **5**.

Sulfur-bridged thienylviologen analogue

5a: a green solid. Yield: 154 mg (80%). ^{1}H NMR (DMSO-d_6, 600 MHz): δ 10.56 (s, 2H, Py*H*), 9.71–9.59 (m, 4H, Py*H*), 8.00 (s, 4H, Th*H*), 7.39 (s, 2H, Th*H*); ^{13}C{H} NMR (DMSO-d_6, 150 MHz): δ 143.78, 143.34, 142.31, 139.58, 129.78, 127.64, 125.84, 123.21; ^{19}F NMR (DMSO-d_6, 564 MHz): δ 69.17, 71.06; ^{31}P NMR (DMSO-d_6, 243 MHz): δ −144.215 (qui); HRMS (ESI) m/z: [M-2PF_6^-] calcd for $C_{18}H_{12}N_2S_3$ 352.0163; found 352.0156; elemental analysis calcd (%) for $C_{18}H_{12}F_{12}N_2P_2S_3$: C 33.92, H 2.27, N 4.14; found: C 33.65, H 1.88, N 4.36; UV/vis (in DMF): λ_{max} (ε) = 345 nm (14.410 × 10^3 M^{-1} cm^{-1}); Mp (°C): > 300 (changed to dark at 236 °C).

Selenium-bridged thienylviologen analogue.

5b: a green solid. Yield: 170 mg (82%). ^{1}H NMR (DMSO-d_6, 600 MHz): δ 10.32 (s, 2H, Py*H*), 9.72–9.56 (m, 4H, Py*H*), 7.99 (s, 4H, Th*H*), 7.38 (s, 2H, Th*H*); ^{13}C{H} NMR (DMSO-d_6, 150 MHz): δ 145.40, 145.28, 143.94, 143.34, 139.70, 129.63, 127.70, 125.67, 124.14; ^{19}F NMR (DMSO-d_6, 564 MHz): δ 69.17, 71.06; ^{31}P NMR (DMSO-d_6, 243 MHz): δ −144.222 (qui); HRMS (ESI) m/z: [M-2PF_6^-] calcd for $C_{18}H_{12}N_2S_2Se$ 399.9584; found 399.9601; elemental analysis calcd (%) for $C_{18}H_{12}F_{12}N_2P_2S_2Se$: C 31.76, H 1.99, N 3.95; found: C 31.36, H 1.75, N 4.06; UV/vis (in DMF): λ_{max} (ε) = 359 nm (14.500 × 10^3 M^{-1} cm^{-1}); Mp (°C): > 300.

Tellurium-bridged thienylviologen analogue.

5c: a black red solid. Yield: 170 mg (77%). ^{1}H NMR (DMSO-d_6, 600 MHz): δ 10.00 (s, 2H, Py*H*), 9.66–9.49 (m, 4H, Py*H*), 7.98 (s, 4H, Th*H*), 7.37 (s, 2H, Th*H*); ^{13}C{H} NMR (DMSO-d_6, 150 MHz): δ 150.89, 148.98, 143.31, 140.04, 139.50, 129.30, 127.72, 125.40; ^{19}F NMR (DMSO-d_6, 564 MHz): δ 69.18, 71.07; ^{31}P NMR (DMSO-d_6, 243 MHz): δ −144.221 (qui); HRMS (ESI) m/z: [M-2PF_6^-] calcd for $C_{18}H_{12}N_2S_2Te$ 449.9487; found 449.9498; elemental analysis calcd (%) for $C_{18}H_{12}F_{12}N_2P_2S_2Te$: C 29.75, H 1.98, N 3.59; found: C 29.30, H 1.64, N 3.80; UV/vis (in DMF): λ_{max} (ε) = 394 nm (14.248 × 10^3 M^{-1} cm^{-1}); Mp (°C): > 300.

3. Resonance structure analysis of 3 (left) and 5 (right).

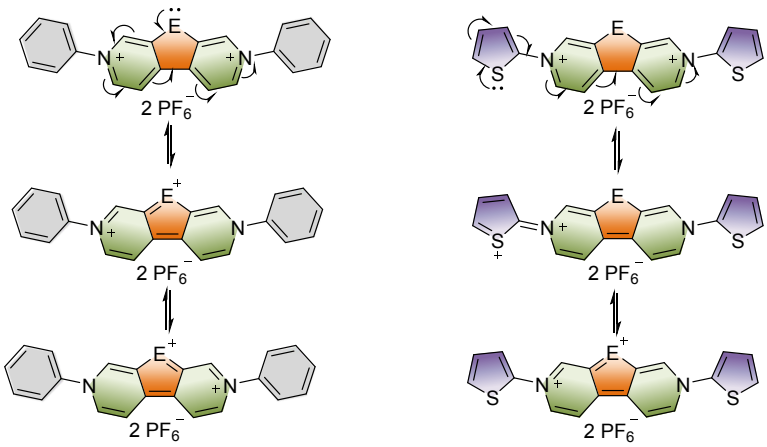


Figure S1. Resonance structure analysis of **3** and **5**.

4. TGA of π-Extended Chalcogenoviologens

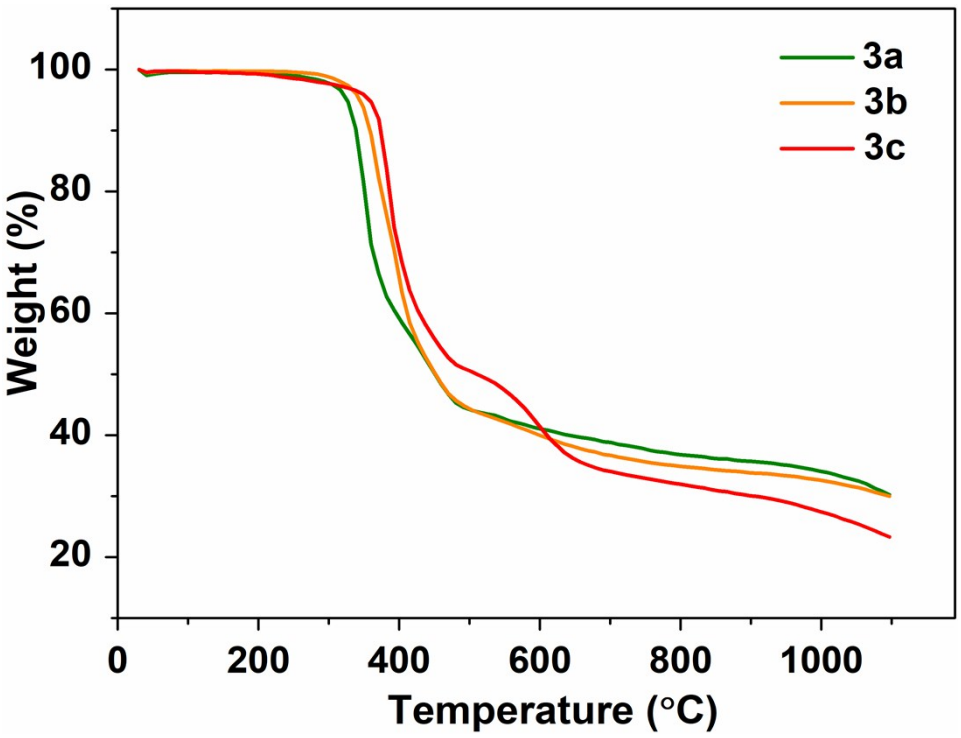


Figure S2. TGA of compounds **3a**, **3b** and **3c**.

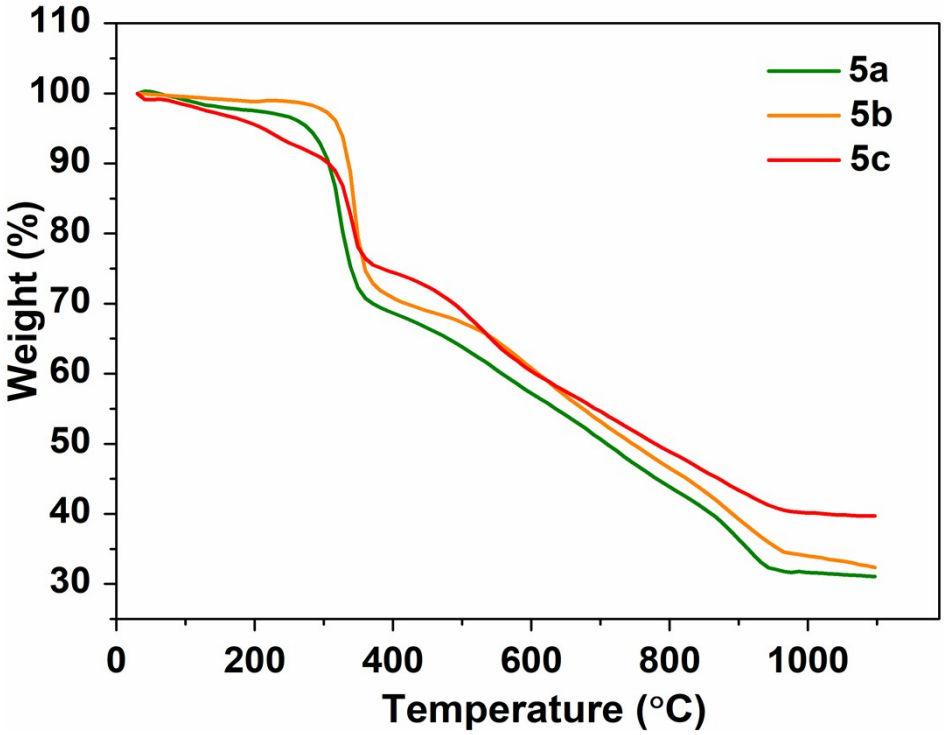


Figure S3. TGA of compounds **5a**, **5b** and **5c**.

5. The cyclic voltammogram

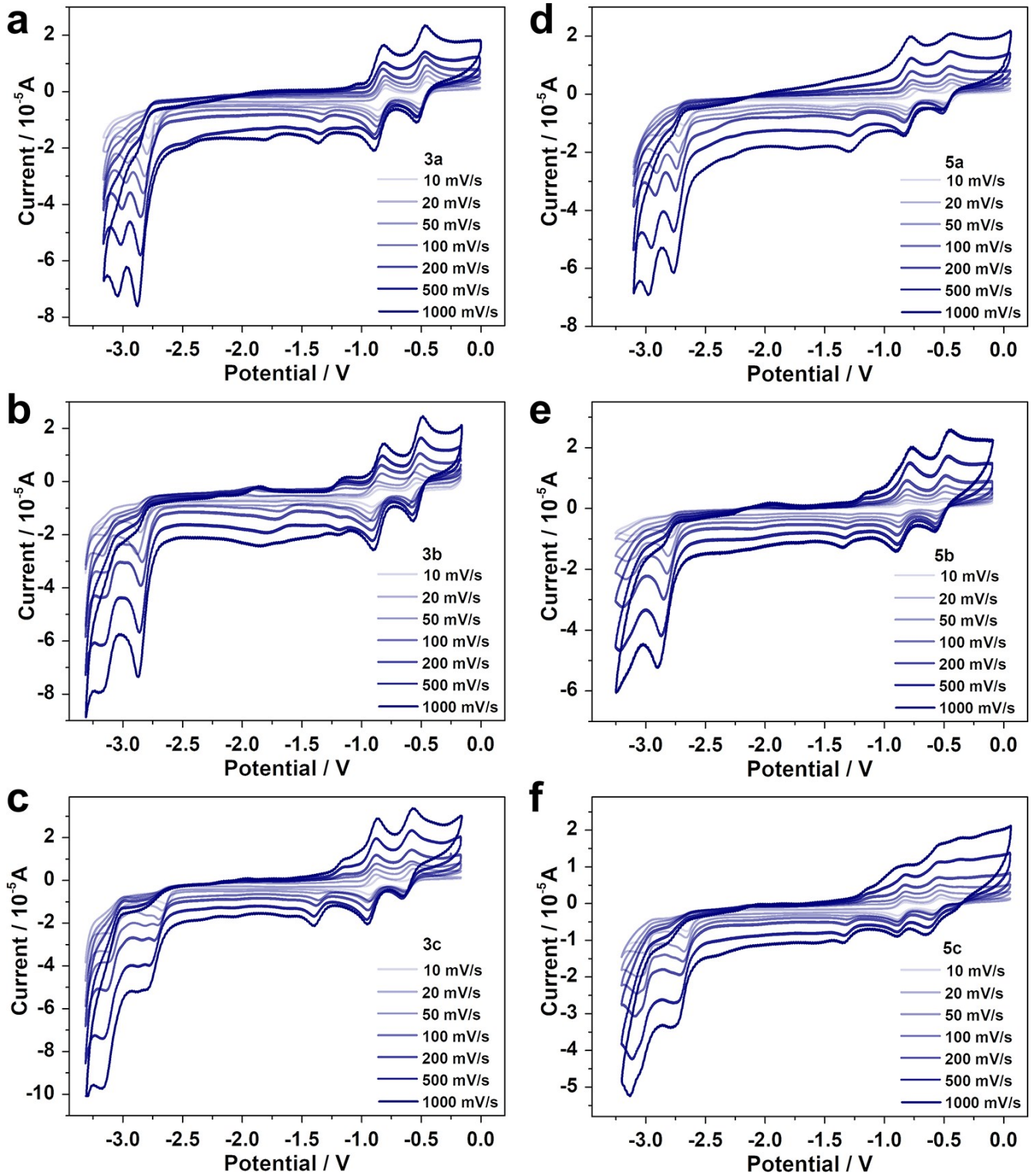


Figure S4. The cyclic voltammogram at different scan rates in DMF solution with tetrabutylammonium hexafluorophosphate (0.05M) as supporting electrolyte, potential E referenced to Fc/Fc^{+}, c~10^{-3} M

Table S1. Optical and Electronic Properties of Chalcogen-Bridged Viologens.

compd	λ_{max} [nm] (ε [$M^{-1}\bullet cm^{-1}$])	E_{red} [V]	E_g [eV][a] (calcd)[b]	E_{LUMO} [eV][c] (calcd)	E_{HOMO} [eV] (calcd)
3a	334 (15820), 402 (4950)	-0.41, -0.77,-2.65	2.94 (3.62)	-4.39 (-4.03)	-7.33 (-7.65)
3b	336 (15450), 431 (4570)	-0.47, -0.79, -2.73	2.73 (3.46)	-4.33 (-4.01)	-7.06 (-7.47)
3c	337 (13590), 506 (3470)	-0.52, -0.82, -2.60, -3.01	2.28 (3.06)	-4.28 (-3.95)	-6.56 (-7.01)
5a	345 (14410), 410 (6230)	-0.40, -0.73, -2.61, -2.85	2.77 (3.06)	-4.40 (-4.15)	-7.17 (-7.20)
5b	359 (14500), 408 (2460)	-0.44, -0.77, -2.69, -3.02	2.63 (3.06)	-4.36 (-4.13)	-6.99 (-7.19)
5c	394 (14248), 523 (3159)	-0.48, -0.79, -2.57, -2.95	2.21 (2.96)	-4.32 (-4.07)	-6.53 (-7.03)
S-BnV	271 (12079), 395 (5670)	−0.60, −1.05	3.00 (3.40)	−4.20 (−3.88)	−7.20 (−7.283)
Se-BnV	273 (11782), 422 (3851)	−0.63, −1.05, −2.64	2.78 (3.48)	−4.17 (−3.86)	−6.95 (−7.281)
Te-BnV	278 (16300), 491 (3680)	−0.68, −1.10, −2.66	2.33 (3.17)	−4.12 (−3.80)	−6.45 (−6.97)
BnV	279 (13458)	−0.74, −1.08	3.78	−4.06	−7.84
P-BnV	257 (10700), 298 (8270)	−0.53, −0.97	3.5	−4.3	−7.8

[a] Energy gap values were calculated from the absorption spectra. [b] Theoretical calculations have been carried out by using the GAUSSIAN09 suite of programs. [c] Energy levels vs vacuum level were calculated from CV data and from the optically determined energy gap.

6. Electrochromism of 3a, 3c, 5a, 5b and 5c

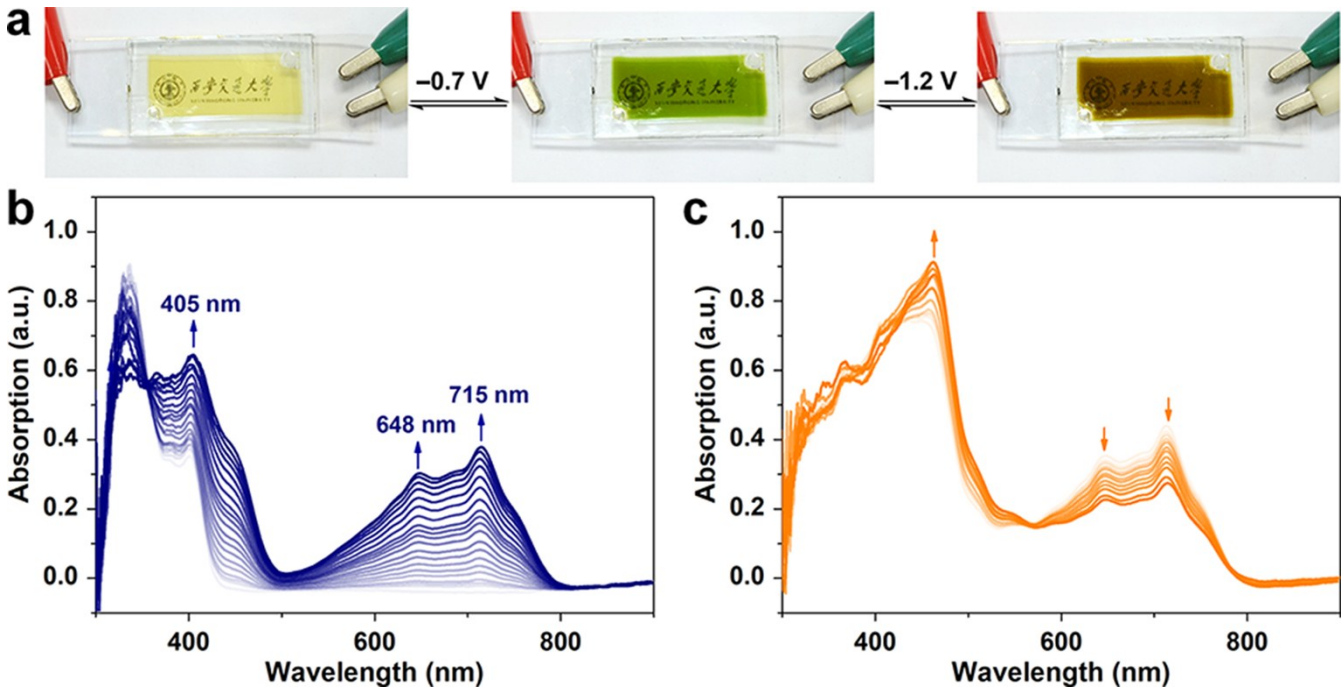


Figure S5. (a) Solution-based electrochromic device with **3a** (no electrolyte). (b) Spectroelectrochemistry of **3a** for first reduction. (b) Spectroelectrochemistry of **3a** for second reduction.

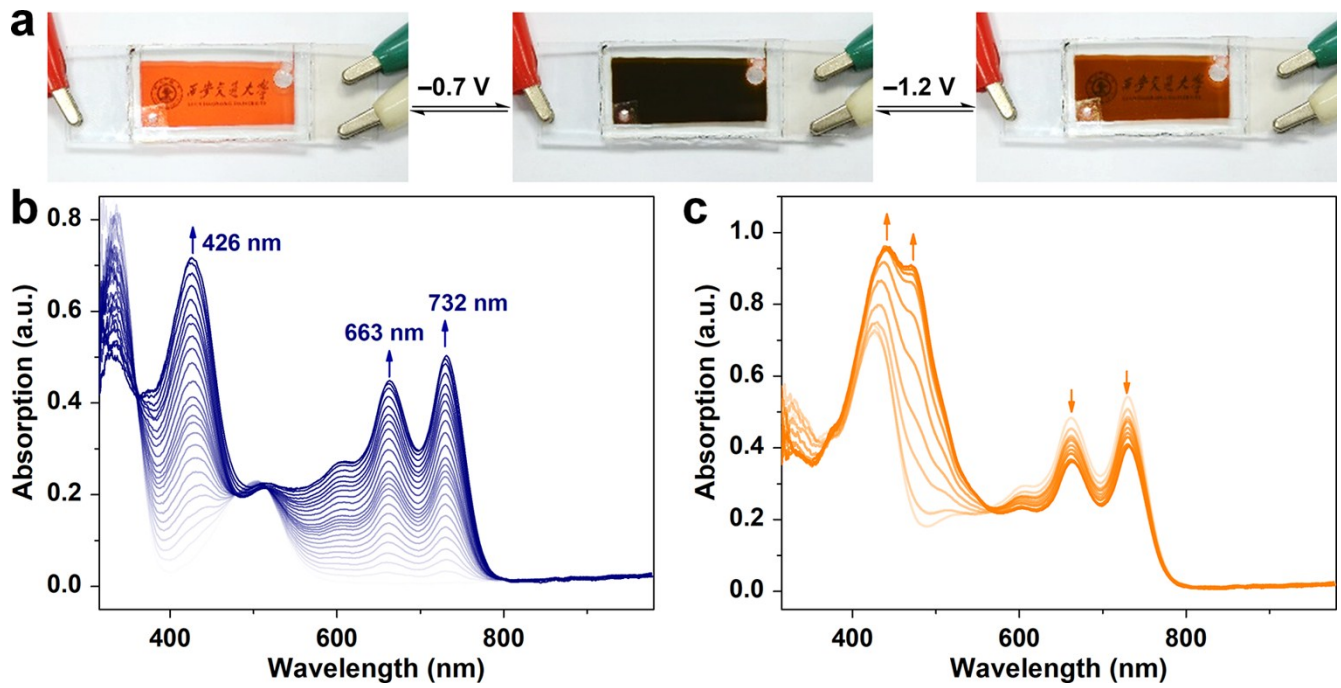


Figure S6. (a) Solution-based electrochromic device with **3c** (no electrolyte). (b) Spectroelectrochemistry of **3c** for first reduction. (b) Spectroelectrochemistry of **3c** for second reduction.

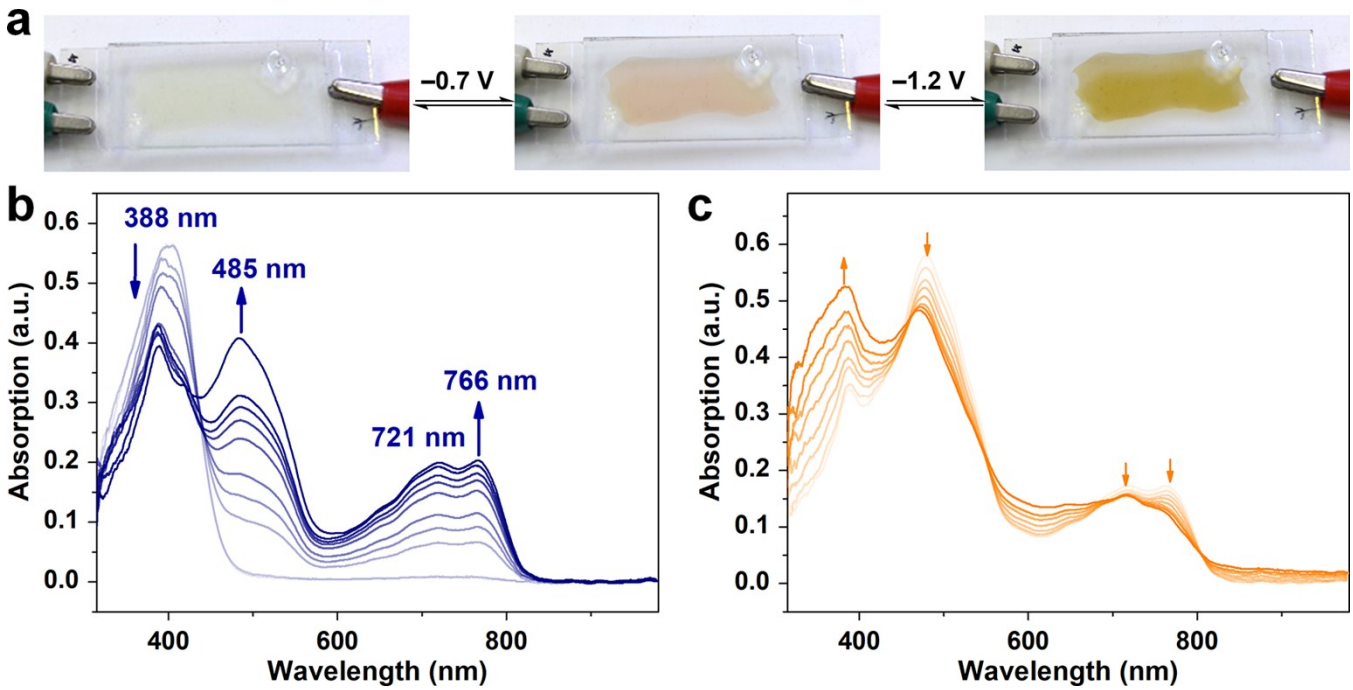


Figure S7. (a) Solution-based electrochromic device with **5a** (no electrolyte). (b) Spectroelectrochemistry of **5a** for first reduction. (b) Spectroelectrochemistry of **5a** for second reductio

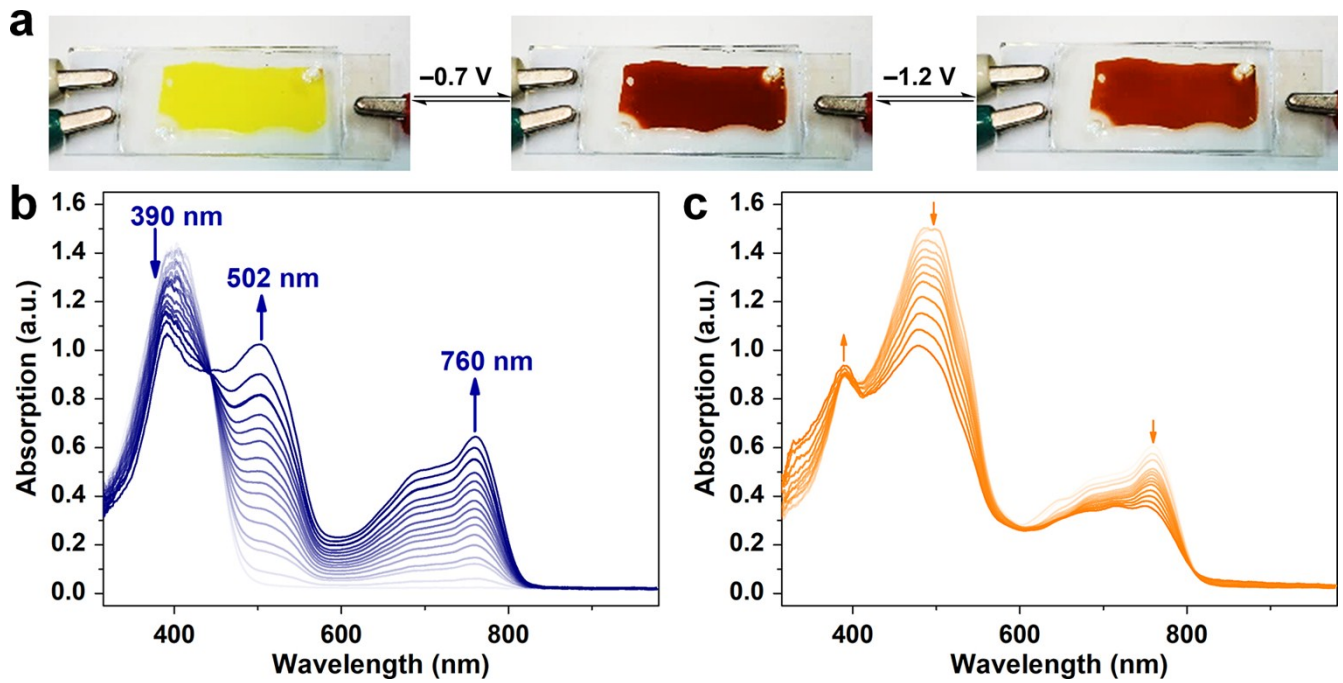


Figure S8. (a) Solution-based electrochromic device with **5b** (no electrolyte). (b) Spectroelectrochemistry of **5b** for first reduction. (b) Spectroelectrochemistry of **5b** for second reduction.

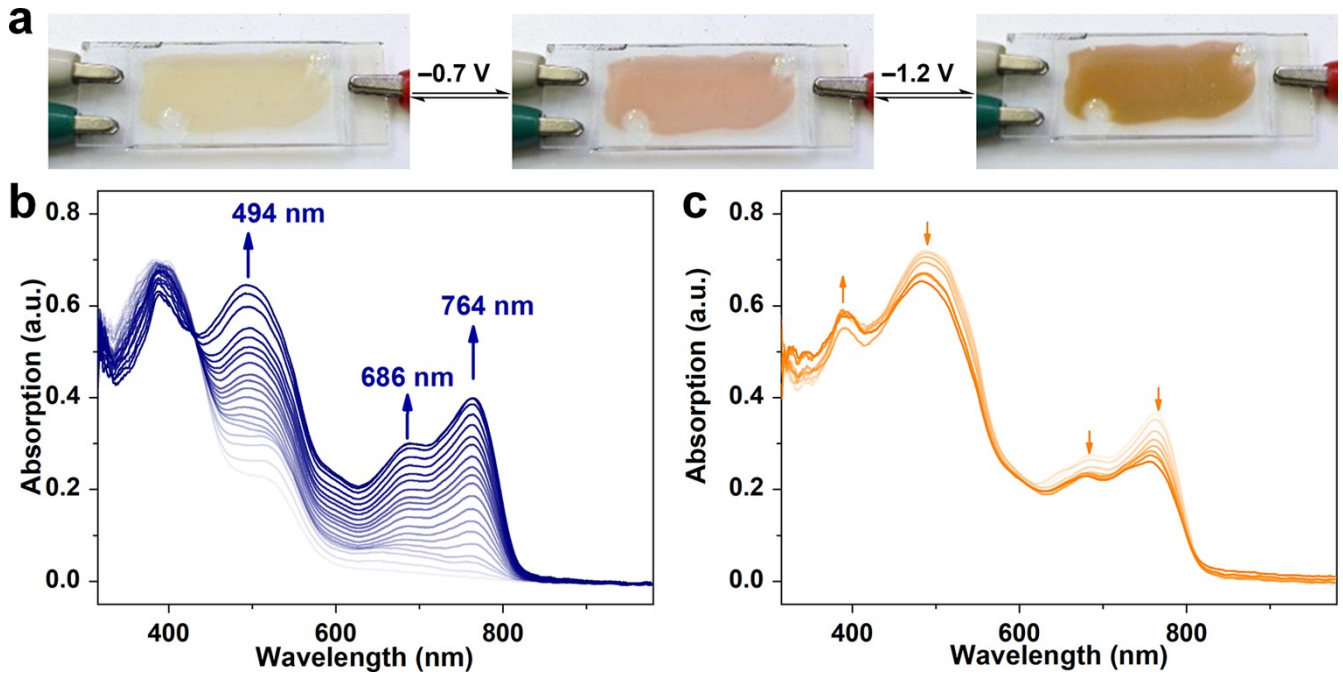


Figure S9. (a) Solution-based electrochromic device with **5c** (no electrolyte). (b) Spectroelectrochemistry of **5c** for first reduction. (b) Spectroelectrochemistry of **5c** for second reduction.

7. Colorful display of ECDs

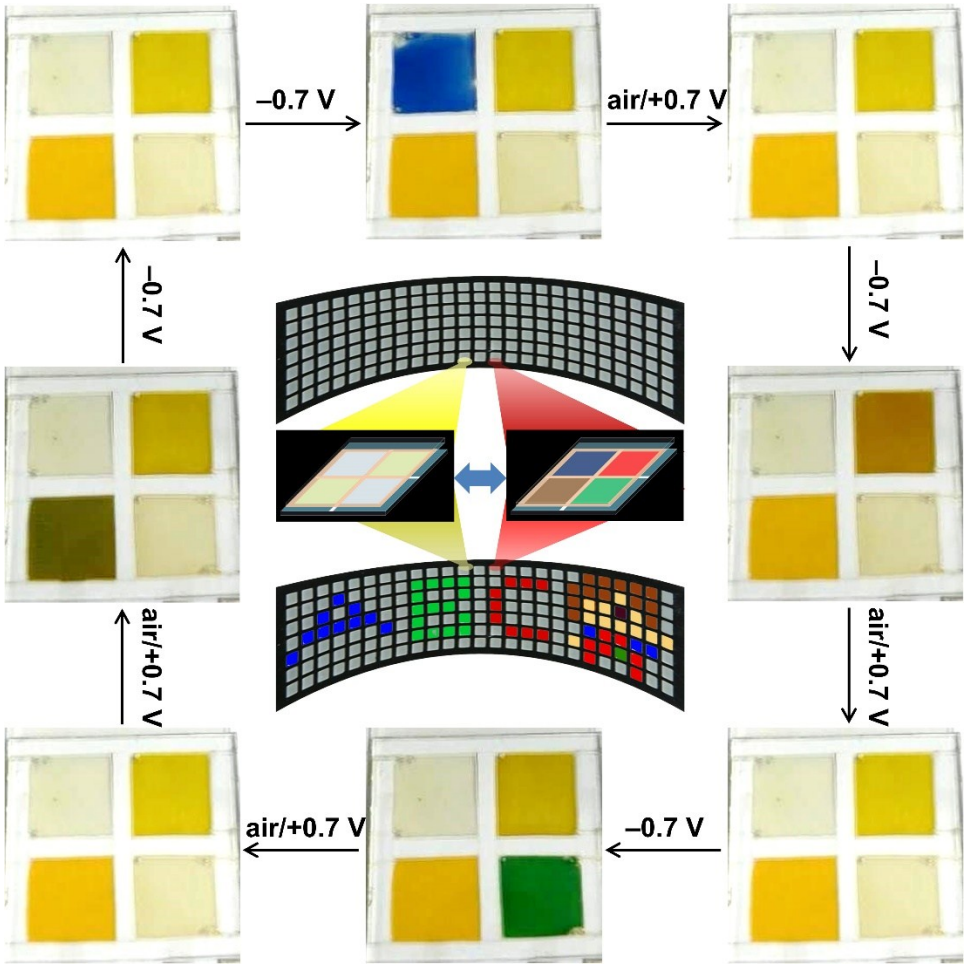


Figure S10. Colorful display of ECDs with four-latticed pixel matrix and schematic diagram of flexible E-link in the center.

Table S2. The comparison of ECD color retention.

Active materials	Retention time	Color Management	Reference
PR-Br[7]	1.5 h	Blue colour display	*Energy Environ. Sci.* **2016**, *9*, 117-122.
Bi–Cu electrolyte composition[8]	24 h	Black colour display	*ACS Energy Lett.* **2017**, *3*, 104-111
TiO_2 nanoparticle (TNP) layer with PR-Br[9]	2.7 h	Blue colour display	*Adv. Funct. Mater.* **2017**, *27*, 1701192.
Urea-N+ Rh-M[10]	1 h	Multicolour display	Nat. Commun. **2019**, *10*, 1559
π-Extended Chalcogenoviologens	**8 h without deoxygenization lasting for weeks after deoxygenization**	**Multicolour display**	**This work**

8. H_2 normalized curve

The system in which H_2 was 2.0 percent (volume fraction) and protected by Argon was chosen as the"standard H_2". 20 μL, 40 μL, 60 μL, 80 μL, 100 μL, 120 μL, 160 μL, 200 μL gas from the "standard H_2" was injected to GC respectively, every volume for three times. The curve figure was the H_2 peak area verse the number of moles of hydrogen, and the equation was fitted by origin.

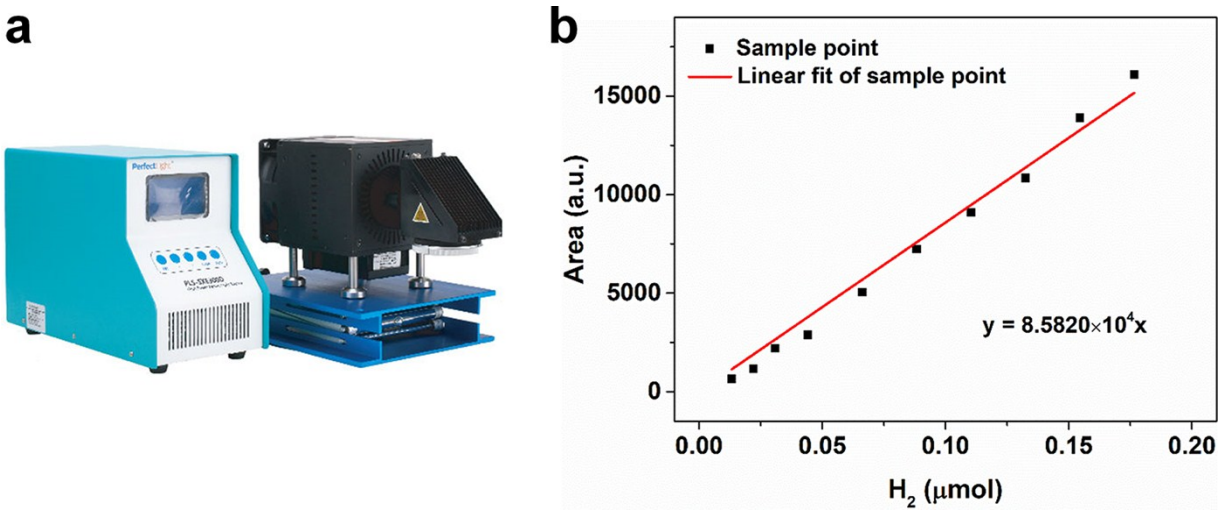


Figure S11. (a) The used xenon lamp PLS-SXE300D. (b) H2 peak area verse the number of moles of hydrogen and polynomial fit of sample point to be H_2 normalized curve.

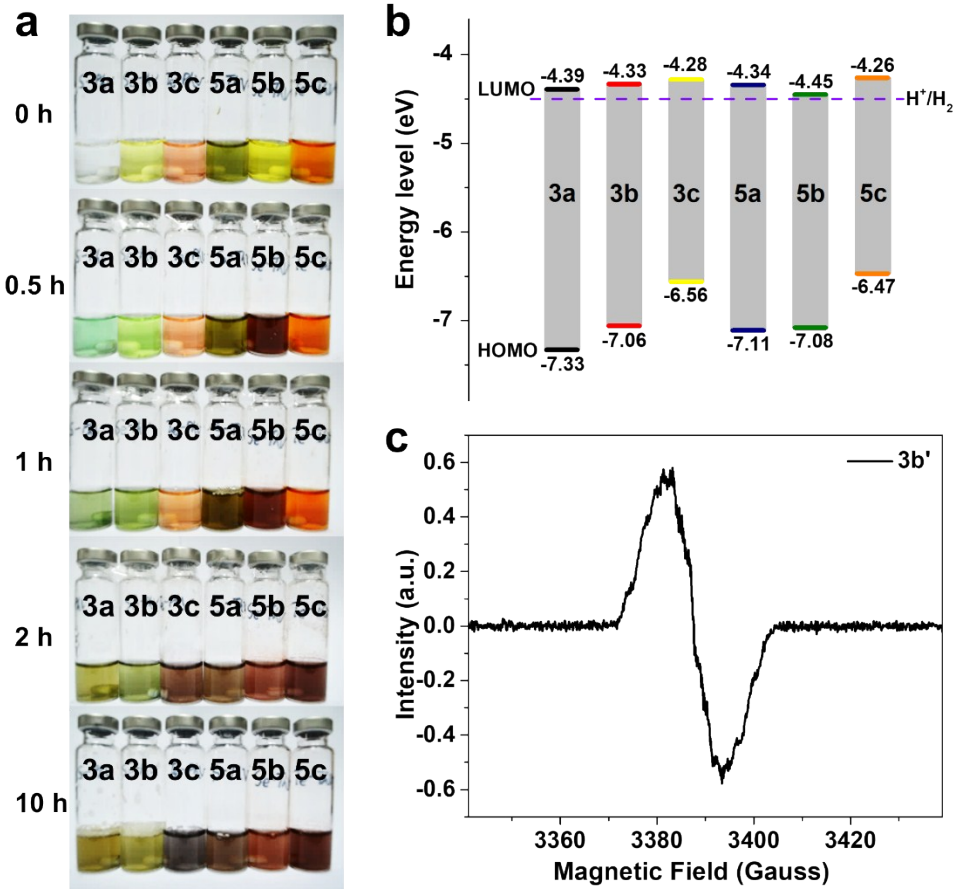


Figure S12. (a) Color changes of different samples under xenon lamp with proceeding time. (b) Experimental energy levels of the LUMO and HOMO orbitals for **3** and **5**. (c) EPR spectrum of hydrogen generation system of **5b** after 0.5 h light exposure

9. Hydrogen generation under xenon lamp

The solution was bubbled with Argon for 30 min, after that it was irradiated under Xenon lamp (> 400 nm) with light power of 100 mW. Then 200 μL upper gas of the reactor was injected to gas chromatography per hour to measure hydrogen generation. The production of the hydrogen was calculated according to the H_2 normalized curve (Fig. S11).

Apparent quantum yield (AQY) calculation:

For the max of the absorption of **3b** is 431nm, in the equation (1), λ = 431 nm. E is measured 100 mW. The number of incident photons (N_0) is calculated to be 2.17×10^{17} s^{-1} by equation (1). The H_2 molecules generated in 24 h under Xenon light was 16.9 μmol. The photons number of collected to be H_2 is 1.18×10^{14} s^{-1} as calculated by equation (2). The AQY is 1.09×10^{-3} calculated by equation (3):

$N_0 = \lambda E/hc = 431 \times 10^{-9} \times 100 \times 10^{-3} / (6.63 \times 10^{-34} \times 3 \times 10^{8})$ $s^{-1} = 2.17 \times 10^{17}$ s^{-1} (1)

$N = nNA/t = 16.9 \times 10^{-6} \times 6.02 \times 10^{23} / 24 \times 3600$ $s^{-1} = 1.18 \times 10^{14}$ s^{-1} (2)

$AQY_{\mathbf{3b}} = 2N/N_0 = 1.09 \times 10^{-3}$ (3)

Table S3. Hydrogen generation activities of some organic photocatalytic system.[11]

Classify	Catalysts	Hydrogen generation rate	TON	Conditions	Reference
metal-bearing organic small molecule	PPDI-bpy (~60% $CoCl_2$)[12]	0.36 mmol•h^{-1}•g^{-1}	---	30 vol% diethylamine/water	*Chem. Mater.* **2016**, *28*, 5394−5399
	$[PtCl_2(bpy\ MV_4)]Cl_8 \bullet 16H_2O$[13]	0.13 mmol•h^{-1}•g^{-1}	18	aqueous acetate buffer solution (0.03 M CH_3COOH and 0.07 M CH_3COONa)	*Chem. Commun.* **2016**, *52*, 1385−1388
	Zn(II)PPIX/C_3N_4 hybrid system; MV^{2+} (PT)[14]	5.67 mmol•h^{-1}•g^{-1}	2.2	Tris-buffer	*Nano Lett.* **2019**, *19*, 9121-9130
organic small molecule with photosensitizer	MV^{2+} (PT)[15]	0.074 mmol•h^{-1}•g^{-1}	---	Pure aqueous λ > 420 nm	*ACS Appl. Mater. Interfaces.* **2017**, *9*, 10355−10359
	SWCNT/ dendrimer nanohybrids; MV^{2+} (PT)[16]	0.040 mmol•h^{-1}•g^{-1}	---	Tris-HCl buffer	*Chem. Commun.* **2018**, *54*, 393-396
	Thiocarbonyl dye/SWCNT/C60; MV^{2+} (PT)[17]	0.098 mmol•h^{-1}•g^{-1}	7.6	Tris-HCl buffer	*J. Am. Chem. Soc.* **2018**, *140*, 3821-3824
organic small molecule without metal	Se-BnV^{2+} 1	0.31 mmol•h^{-1}•g^{-1}	0.17%	Pure aqueous λ > 400 nm	*Angew. Chem. Int. Ed.* **2018**, *57*, 4897-4901
	S-PhV (3a)	**0.68 mmol•h^{-1}•g^{-1}**	**2.3**	**aqueous acetate buffer solution λ > 400 nm**	***This work***
	Se-PhV (3b)	**0.71 mmol•h^{-1}•g^{-1}**	**11.4**	**aqueous acetate buffer solution λ > 400 nm**	***This work***

10. Mulliken charge distribution

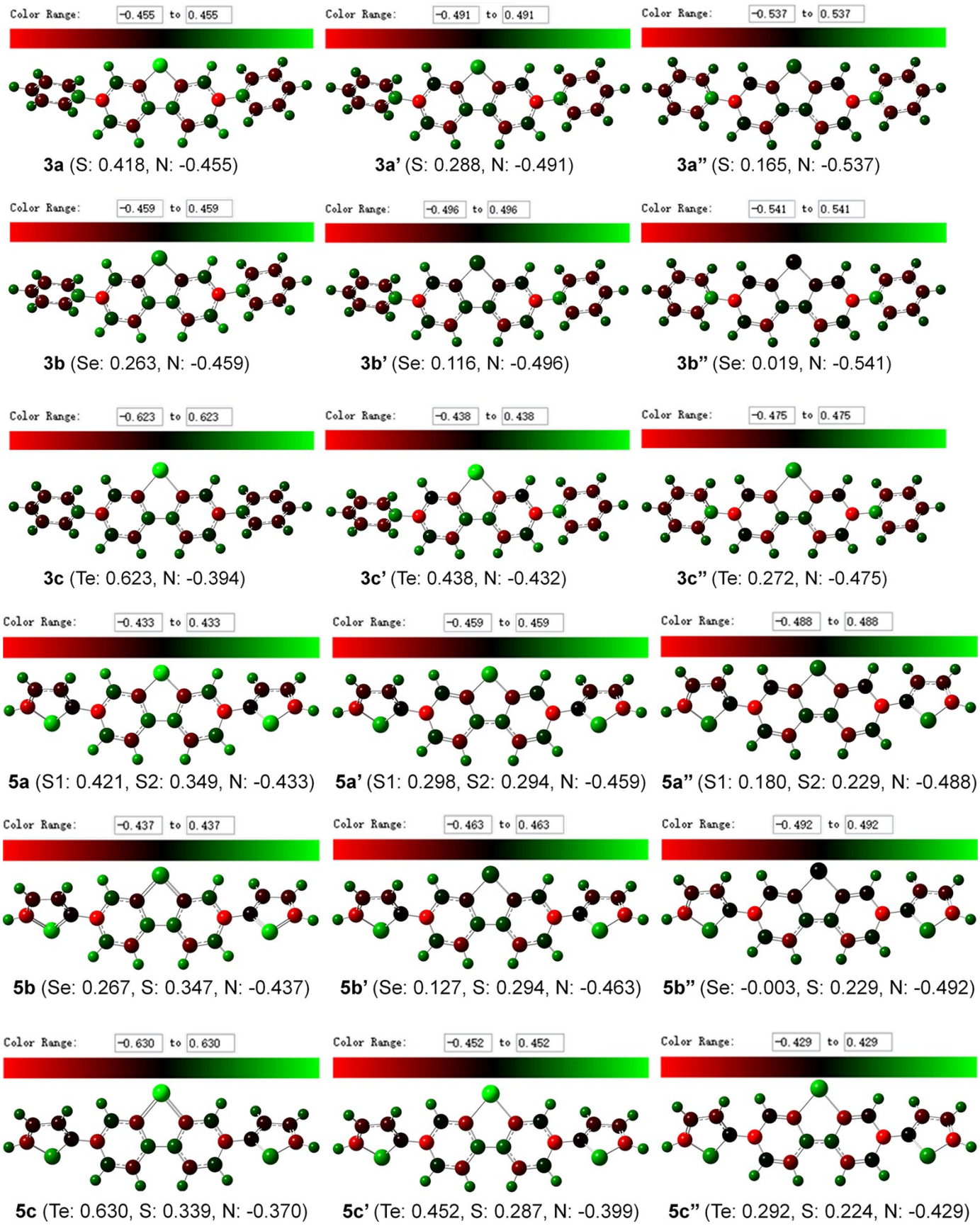
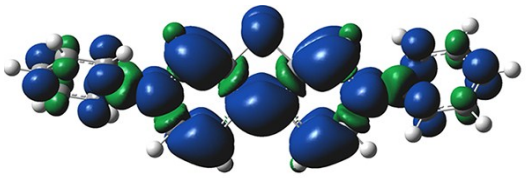
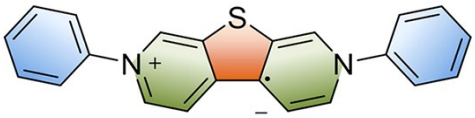


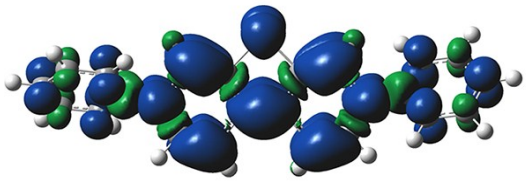
Figure S13. Mulliken charge distribution in π-extended chalcogenoviologens **3** and **5**.

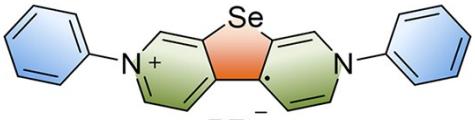
11. Calculated spin density plots for the radical species



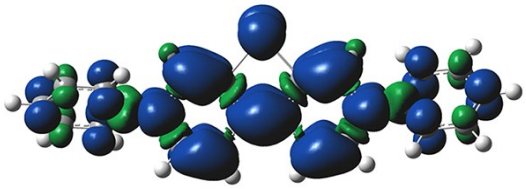


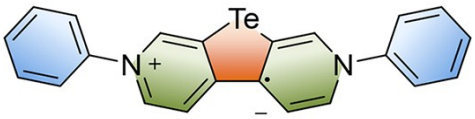
3a'



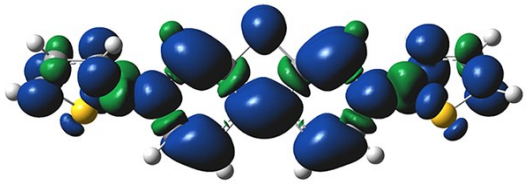


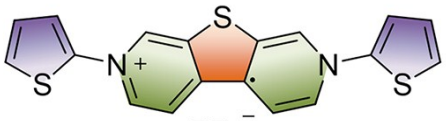
3b'



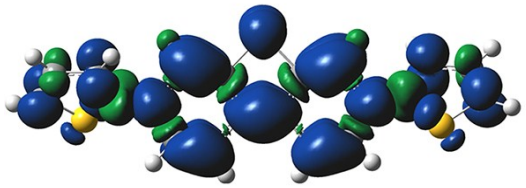


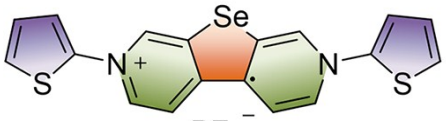
3c'



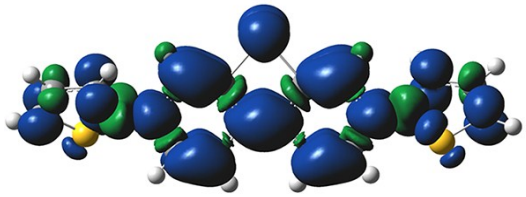


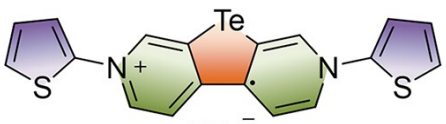
5a'





5b'





5c'

Figure S14. Calculated spin density plots for the radical species of π-extended chalcogenoviologens.

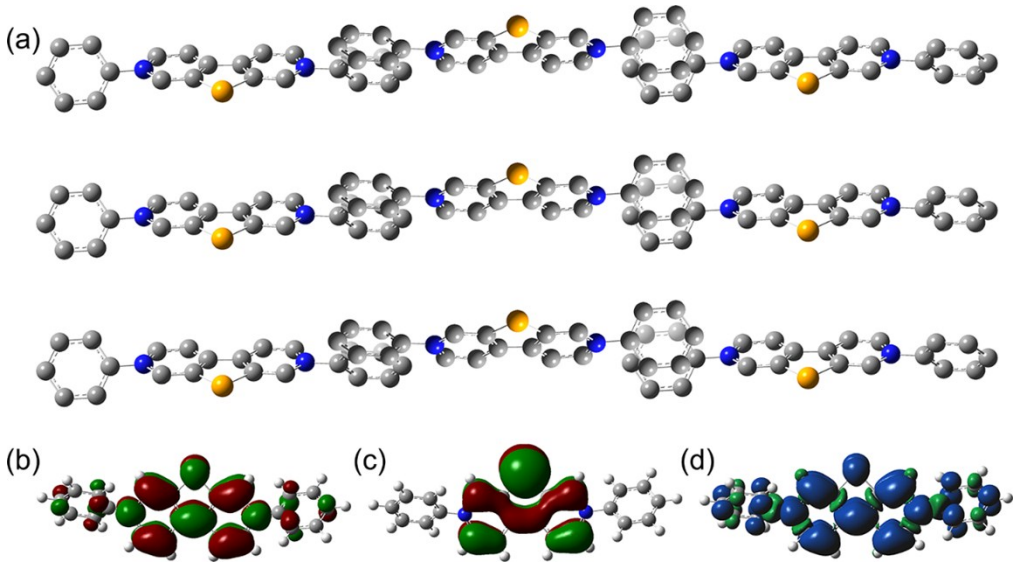


Figure S15. Calculated stacking manner (a) of **3b**, SOMO-α (b), SOMO-β (c) and spin density (d) of **3b'**.

12. Computed UV-vis spectra

The simulated UV–Vis spectra for optimized molecules were performed at the time dependent density functional theory (TD-DFT) at the ground-state equilibrium geometries, both low-lying singlet and triplet states were determined using the B3LYP in association with the LANL08d basis set applied for the Te atom and 6-311++G(d,p) basis set for all other atoms.

The calculated maximum absorption wavelength ($\lambda_{TD\text{-}DFT}$), oscillator strength (f), molecular orbitals (MOs) involved in the main transitions, and the difference between the experimental and calculated wavelengths (Δλ) of **3** and **5** in DMF are reported in Table S2. To make it well suitable for efficiently and reasonably accurate determination of the excited state properties, the structures and frequencies of compounds **3** and **5** in the DMF solution were optimized at the B3LYP level with the LANL08d basis set applied for the Te atom and 6-31G(d) basis set for all other atoms, the keyword "opt=tight" was used. And the following discussions for the absorption are based on PCM/TD-B3LYP method with the LANL08d basis set applied for the Te atom and 6-311++G(d,p) basis set for other atoms.

It should be pointed out that the structures of all stationary points in DMF solvent were fully optimized, and frequency calculations were performed at the same level. The frequency calculations confirmed the nature of all revealed equilibrium geometries: there were no imaginary frequencies.[18]

Table S2. Calculated ($\lambda_{TD\text{-}DFT}$) and experimental (λ_{exp}) wavelengths (nm) of **3** and **5**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength.

	λ_{exp}	$\lambda_{TD\text{-}DFT}$		f	MOs				Δ(nm)
3a	402	B3LYP	394.99	0.5791	87 -> 89	HOMO-1->LUMO	0.70291	49.4%	-8.41
3b	431	B3LYP	393.59	0.5807	96 -> 98	HOMO-1->LUMO	0.70297	49.4%	-37.41
3c	506	B3LYP	511.37	0.0588	83 -> 84	HOMO-> LUMO	0.70090	49.1%	5.37
5a	410	B3LYP	475.69	0.7478	90 -> 91	HOMO-> LUMO	0.70374	49.5%	65.69
5b	408	B3LYP	474.03	0.7468	99 ->100	HOMO-> LUMO	0.70372	49.5%	66.03
5c	523	B3LYP	528.08	0.0571	85 -> 86	HOMO-> LUMO	0.70109	49.2%	5.08

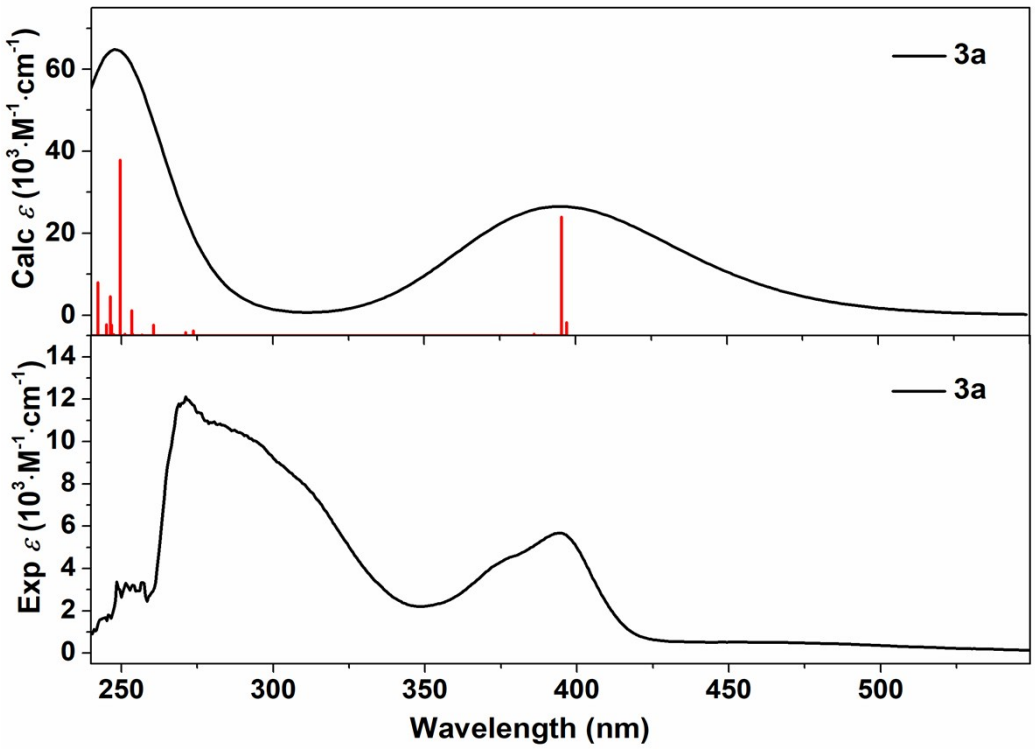


Figure S16. Computed, at the TD-B3LYP/6-311++G(d,p) level of theory in the DMF, and experimental UV-vis spectra of **3a**.

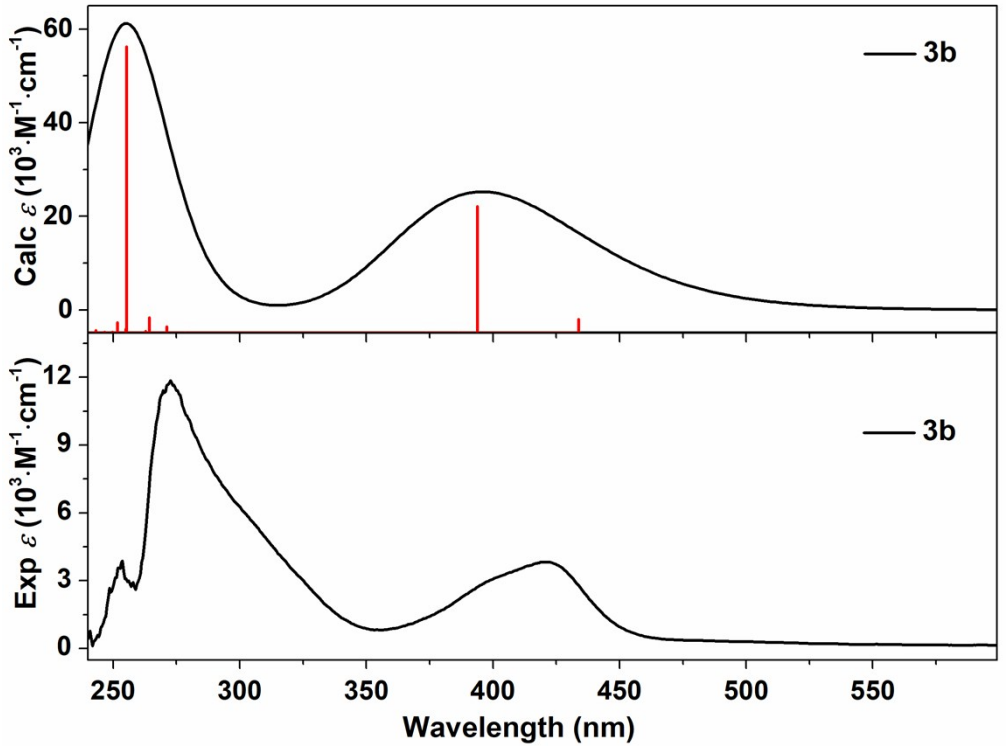


Figure S17. Computed, at the TD-B3LYP/6-311++G(d,p) level of theory in the DMF, and experimental UV-vis spectra of **3b**.

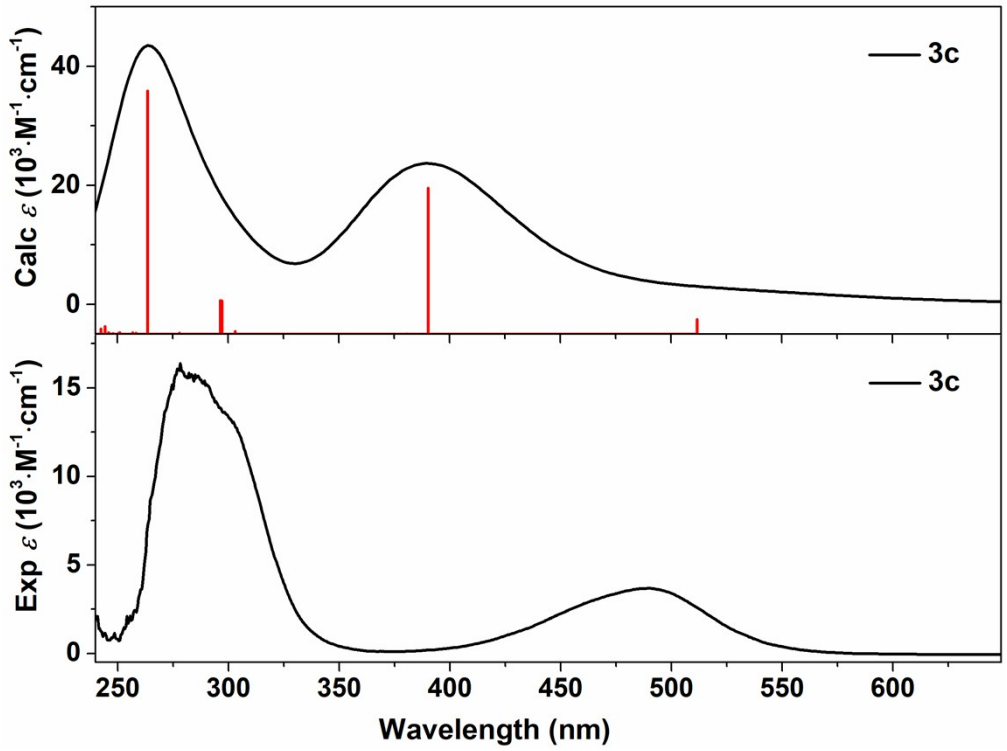


Figure S18. Computed, at the TD-B3LYP/GenECP level of theory in the DMF, and experimental UV-vis spectra of **3c**.

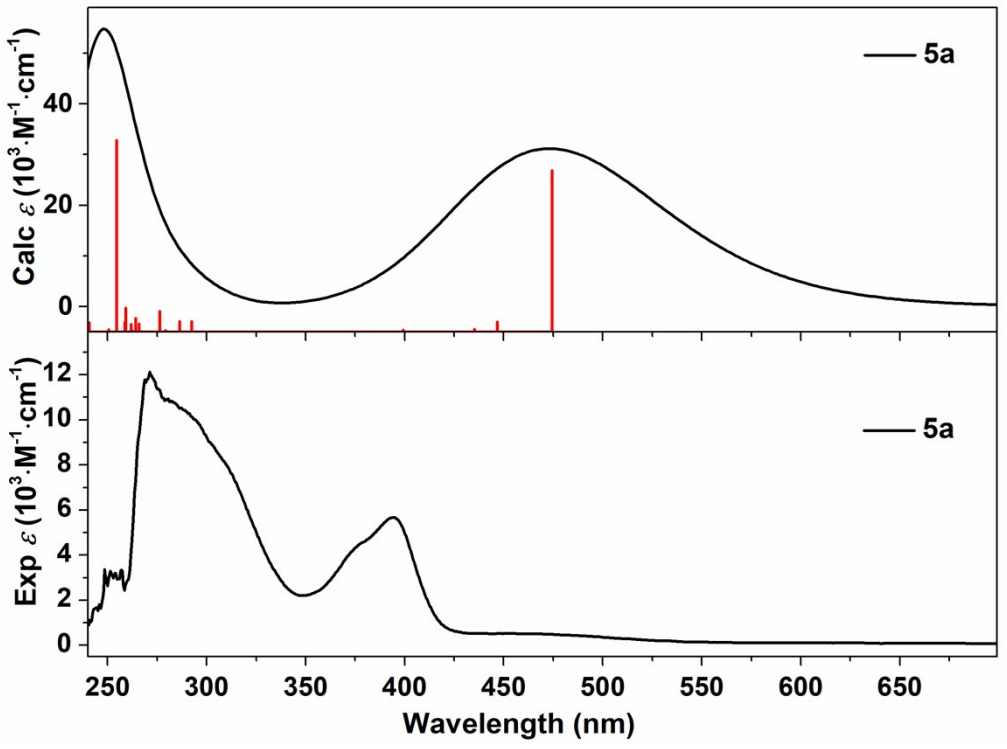


Figure S19. Computed, at the TD-B3LYP/6-311++G(d,p) level of theory in the DMF, and experimental UV-vis spectra of **5a**.

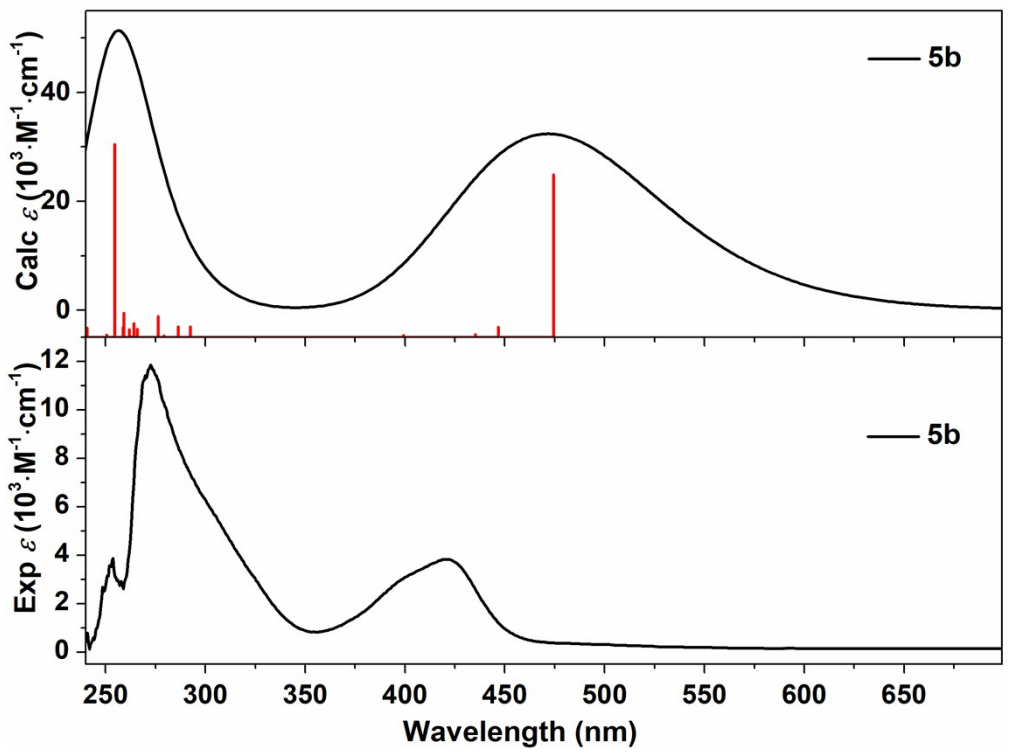


Figure S20. Computed, at the TD-B3LYP/6-311++G(d,p) level of theory in the DMF, and experimental UV-vis spectra of **5b**.

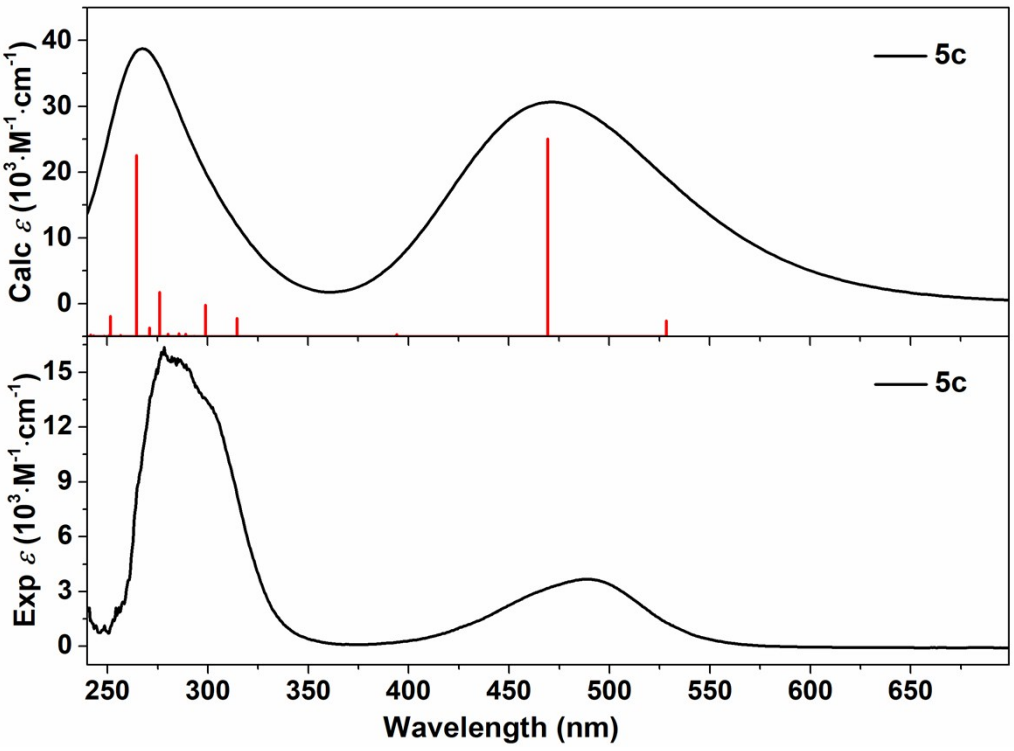
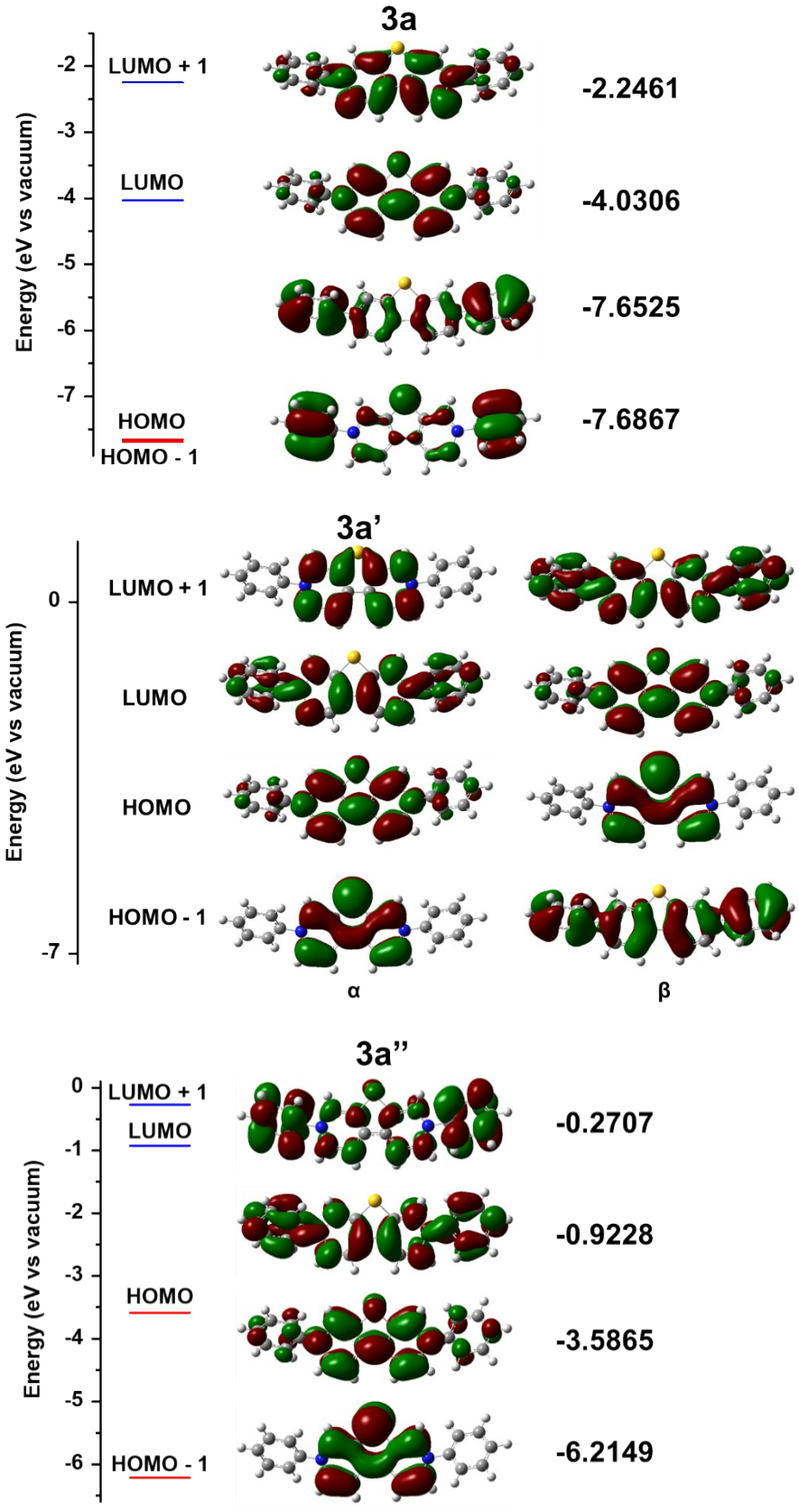
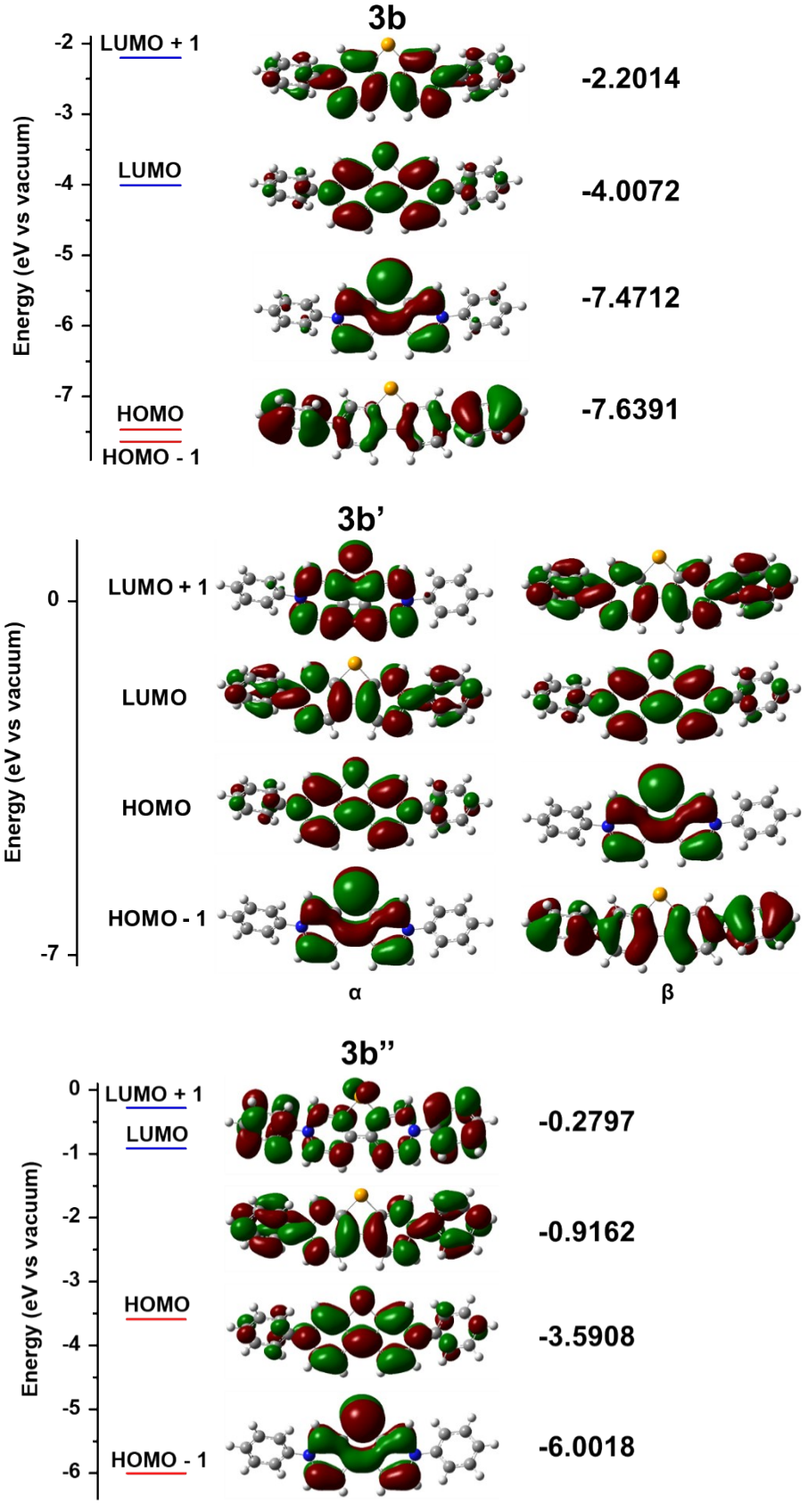
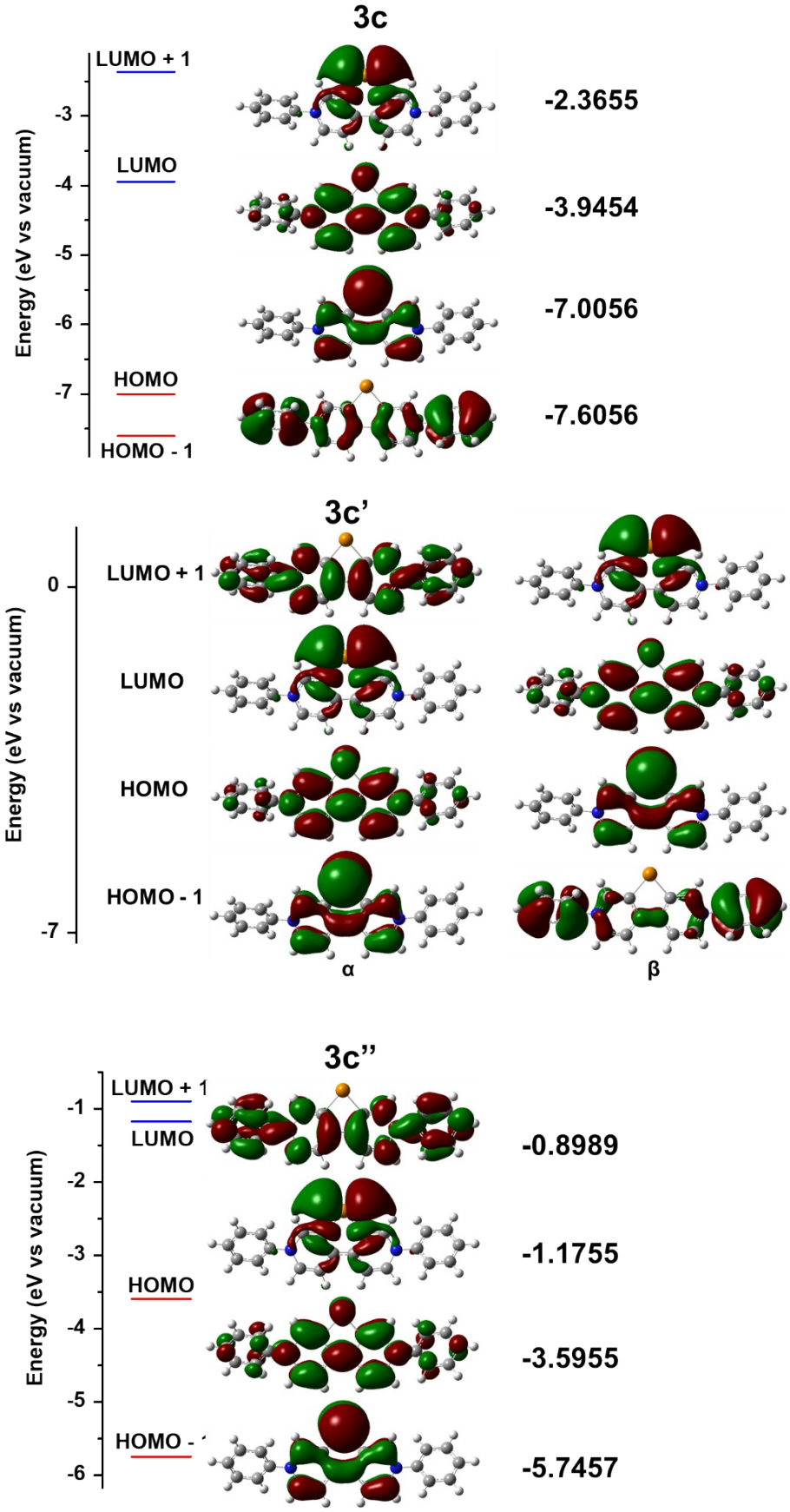


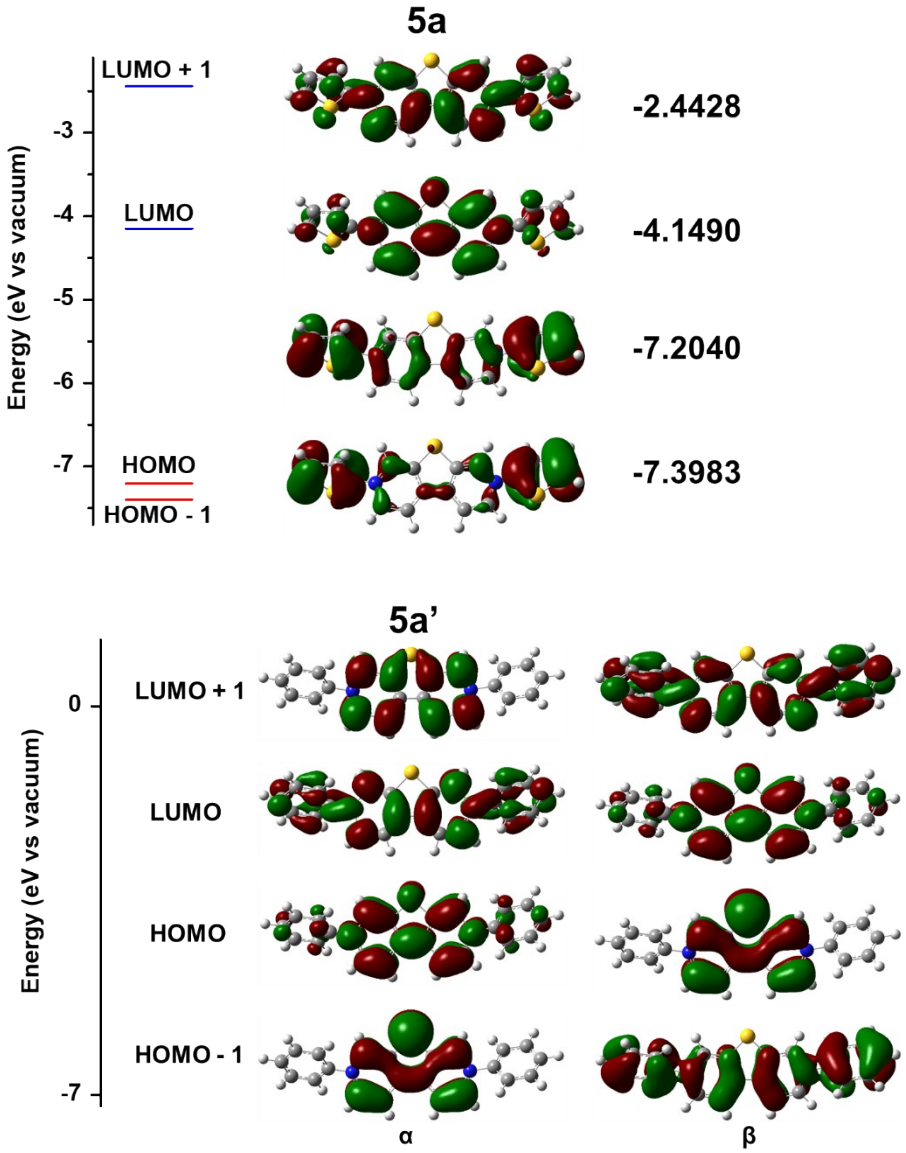
Figure S21. Computed, at the TD-B3LYP/GenECP level of theory in the DMF, and experimental UV-vis spectra of **5c**.

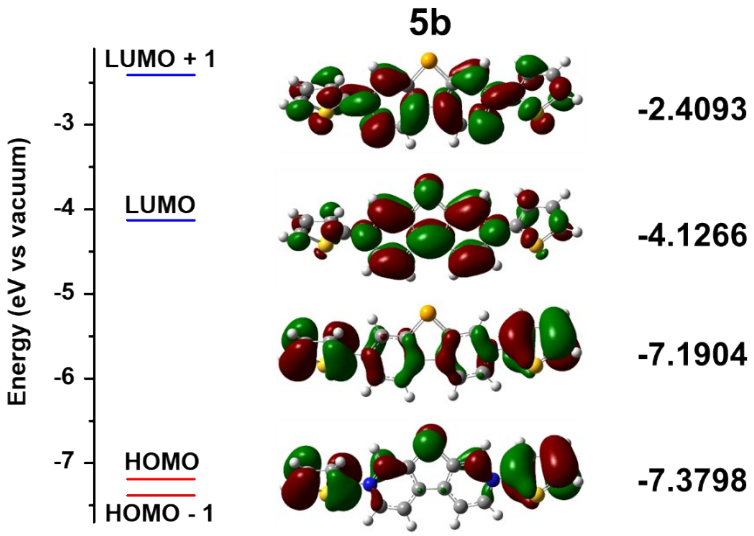
13. DFT Calculations

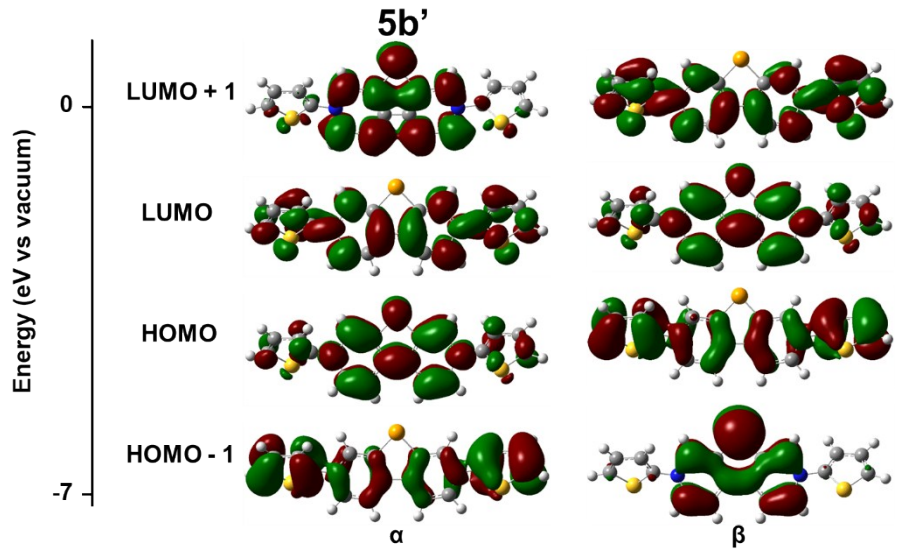


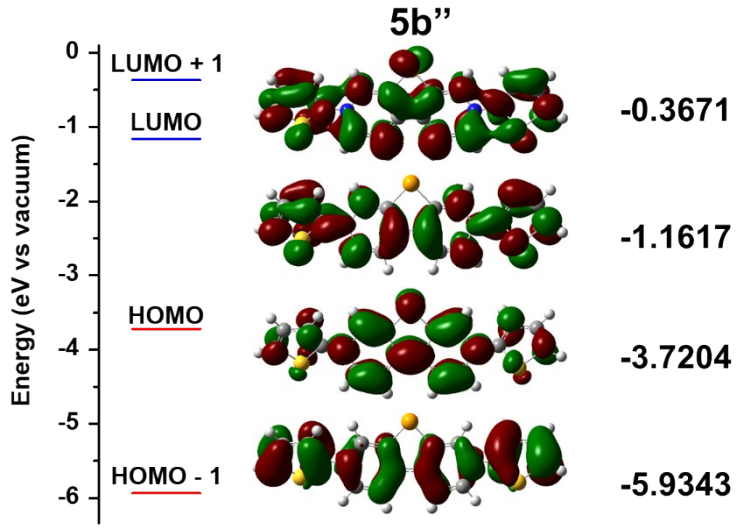

3b
-2
-3
-4
-5
-6
-7
Energy (eV vs vacuum)
LUMO + 1
LUMO
HOMO
HOMO - 1
-2.2014
-4.0072
-7.4712
-7.6391
3b'
0
-7
Energy (eV vs vacuum)
LUMO + 1
LUMO
HOMO
HOMO - 1
α
β
3b''
0
-1
-2
-3
-4
-5
-6
Energy (eV vs vacuum)
LUMO + 1
LUMO
HOMO
HOMO - 1
-0.2797
-0.9162
-3.5908
-6.0018

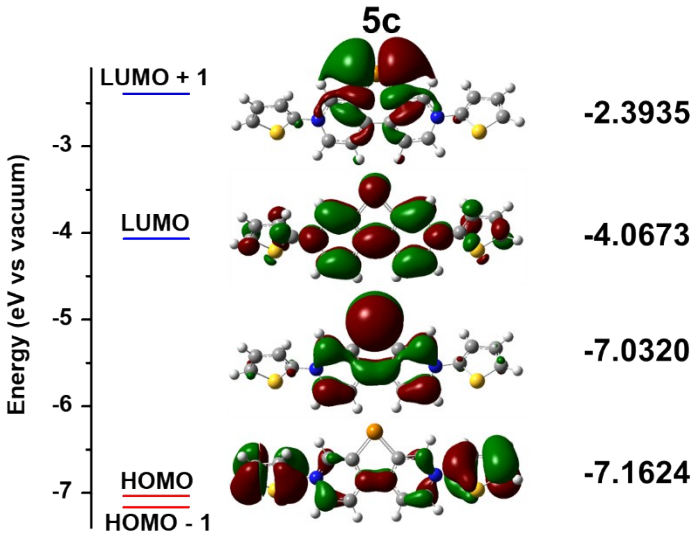

3c
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-3
-4
-5
-6
-7
-2.3655
-3.9454
-7.0056
-7.6056
3c'
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
0
-7
α
β
3c''
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-1
-2
-3
-4
-5
-6
-0.8989
-1.1755
-3.5955
-5.7457

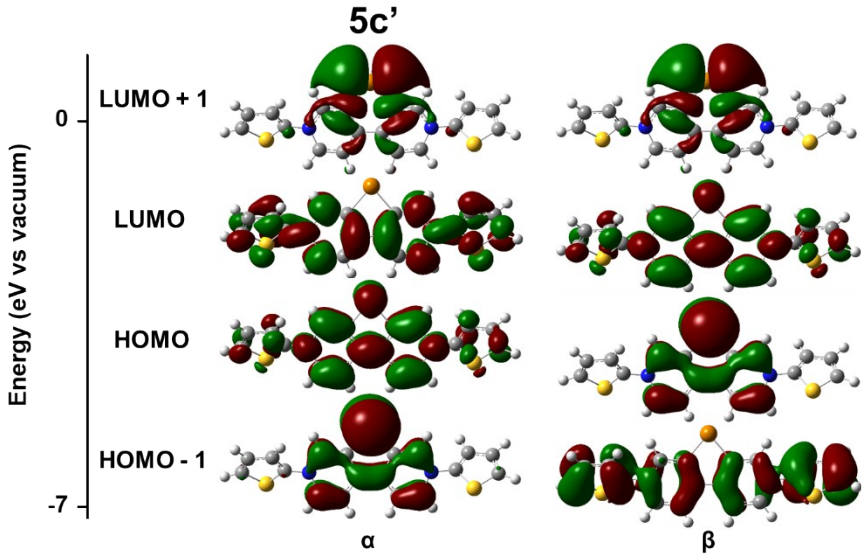

5a
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-3
-4
-5
-6
-7
-2.4428
-4.1490
-7.2040
-7.3983
5a'
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
0
-7
α
β
5a''
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-1
-2
-3
-4
-5
-6
-0.363
-1.1701
-3.7177
-5.9419

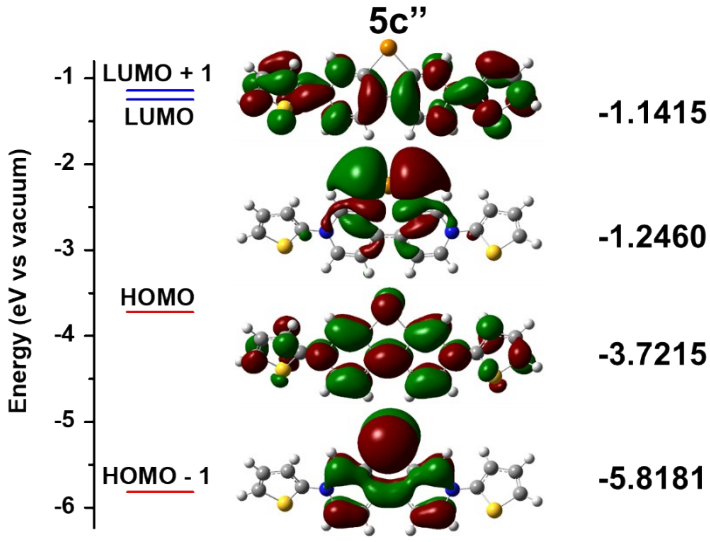

5b
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-3
-4
-5
-6
-7
-2.4093
-4.1266
-7.1904
-7.3798


5b'
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
0
-7
α
β


5b''
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
0
-1
-2
-3
-4
-5
-6
-0.3671
-1.1617
-3.7204
-5.9343


5c
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-3
-4
-5
-6
-7
-2.3935
-4.0673
-7.0320
-7.1624


5c'
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
0
-7
α
β


5c''
LUMO + 1
LUMO
HOMO
HOMO - 1
Energy (eV vs vacuum)
-1
-2
-3
-4
-5
-6
-1.1415
-1.2460
-3.7215
-5.8181

14. Cartesian coordinates of optimized structures studied in this work

3a

Symbol	X	Y	Z
N	3.4416502	0.2767882	-0.0001602
C	2.9755956	1.5619343	-0.0007011
C	1.6236378	1.8274980	-0.0065614
C	0.7227887	0.7548687	0.0043339
C	1.2353020	-0.5638276	0.0103336
C	2.6045214	-0.7838367	-0.0023921
C	-0.7229793	0.7548625	0.0072677
C	-1.2354458	-0.5638587	0.0024737
S	-0.0000728	-1.8086828	0.0079742
C	-1.6238267	1.8275296	0.0154899
C	-2.9757696	1.5619624	0.0062694
N	-3.4417314	0.2768055	0.0051099
C	-2.6047070	-0.7838451	0.0118089
C	4.8777498	0.0434970	0.0064611
C	-4.8777255	0.0432368	-0.0093958
C	-5.4155493	-0.7992419	-0.9835212
C	-6.7926867	-1.0187930	-0.9879828
C	-7.6070784	-0.4020583	-0.0352652
C	-7.0483436	0.4393210	0.9300781
C	-5.6732708	0.6693737	0.9509791
C	5.4214325	-0.8003977	0.9760925
C	6.7986167	-1.0196465	0.9722248
C	7.6073793	-0.4011811	0.0158506
C	7.0428899	0.4415652	-0.9449364
C	5.6676662	0.6712275	-0.9575729
H	3.7274935	2.3380221	0.0253021
H	1.2902912	2.8582006	-0.0056941
H	3.0575205	-1.7656975	-0.0345616
H	-1.2904496	2.8582218	0.0144119
H	-3.7276607	2.3379709	-0.0226831
H	-3.0579138	-1.7656326	0.0435449
H	-4.7796612	-1.2507753	-1.7382831
H	-7.2263550	-1.6644249	-1.7446454
H	-8.6783617	-0.5765787	-0.0454137
H	-7.6786461	0.9118301	1.6763424
H	-5.2272207	1.2993221	1.7133968
H	4.7902024	-1.2533786	1.7338460

H	7.2367615	-1.6664382	1.7253069
H	8.6787399	-0.5754792	0.0195480
H	7.6687593	0.9153957	-1.6940864
H	5.2170510	1.3020690	-1.7165729

3a'

Symbol	X	Y	Z
N	-3.4706890	0.2761166	-0.0085792
C	-2.9747062	1.5636414	-0.0126887
C	-1.6345862	1.8238824	-0.0081085
C	-0.7038828	0.7453536	-0.0041758
C	-1.2536776	-0.5777145	-0.0100142
C	-2.6039052	-0.7990863	-0.0072614
C	0.7038814	0.7453538	0.0042266
C	1.2536770	-0.5777139	0.0100754
S	-0.0000002	-1.8252879	0.0000398
C	1.6345851	1.8238824	0.0081503
C	2.9747050	1.5636416	0.0127221
N	3.4706893	0.2761168	0.0086129
C	2.6039044	-0.7990861	0.0073137
C	-4.8919398	0.0494067	-0.0113755
C	4.8919392	0.0494082	0.0113641
C	5.4435601	-0.8748214	0.9043210
C	6.8211658	-1.0927721	0.8965321
C	7.6426182	-0.3870183	0.0143200
C	7.0818656	0.5380377	-0.8694361
C	5.7044816	0.7568246	-0.8804224
C	-5.4435313	-0.8748073	-0.9043666
C	-6.8211371	-1.0927592	-0.8966241
C	-7.6426165	-0.3870222	-0.0144238
C	-7.0818922	0.5380179	0.8693669
C	-5.7045087	0.7568064	0.8803993
H	-3.7185801	2.3479648	-0.0453964
H	-1.3028147	2.8554498	-0.0226890
H	-3.0554385	-1.7808621	0.0255702
H	1.3028142	2.8554499	0.0227306
H	3.7185782	2.3479657	0.0454257
H	3.0554360	-1.7808627	-0.0255119
H	4.8086979	-1.3978480	1.6122878
H	7.2513532	-1.8064660	1.5924810
H	8.7149360	-0.5572361	0.0155353
H	7.7132414	1.0832783	-1.5642950

H	5.2636176	1.4508466	-1.5887536
H	-4.8086450	-1.3978209	-1.6123214
H	-7.2513031	-1.8064408	-1.5925989
H	-8.7149342	-0.5572407	-0.0156752
H	-7.7132905	1.0832448	1.5642164
H	-5.2636660	1.4508172	1.5887547

3a''

Symbol	X	Y	Z
N	-3.5080679	-0.2780322	-0.0014547
C	-2.9814079	-1.5697641	0.0069627
C	-1.6507737	-1.8265109	0.0119885
C	-0.6881195	-0.7472778	0.0047140
C	-1.2732221	0.5827060	0.0104936
C	-2.6062992	0.8065117	0.0090200
C	0.6881194	-0.7472779	-0.0047176
C	1.2732221	0.5827059	-0.0104989
S	0.0000000	1.8346996	-0.0000035
C	1.6507735	-1.8265110	-0.0119917
C	2.9814078	-1.5697642	-0.0069664
N	3.5080678	-0.2780323	0.0014499
C	2.6062992	0.8065116	-0.0090260
C	-4.9070206	-0.0553404	0.0060206
C	4.9070206	-0.0553407	-0.0060200
C	5.4526850	1.0332905	-0.7090501
C	6.8296008	1.2511729	-0.7050514
C	7.6873995	0.3871347	-0.0199067
C	7.1466126	-0.6987611	0.6736289
C	5.7702423	-0.9177217	0.6930660
C	-5.4526824	1.0332906	0.7090530
C	-6.8295983	1.2511731	0.7050590
C	-7.6873994	0.3871351	0.0199171
C	-7.1466149	-0.6987606	-0.6736206
C	-5.7702448	-0.9177213	-0.6930625
H	-3.7143221	-2.3642348	0.0519537
H	-1.3240719	-2.8607205	0.0416064
H	-3.0503659	1.7908247	-0.0342411
H	1.3240717	-2.8607206	-0.0416096
H	3.7143219	-2.3642350	-0.0519576
H	3.0503658	1.7908247	0.0342329
H	4.8063409	1.6899473	-1.2821317
H	7.2327260	2.0952945	-1.2579799

H	8.7597418	0.5580543	-0.0247490
H	7.7970262	-1.3740668	1.2228835
H	5.3649647	-1.7391116	1.2749315
H	-4.8063362	1.6899472	1.2821324
H	-7.2327215	2.0952946	1.2579891
H	-8.7597416	0.5580548	0.0247632
H	-7.7970305	-1.3740661	-1.2228730
H	-5.3649691	-1.7391111	-1.2749296

3b

Symbol	X	Y	Z
N	-3.4615733	0.4585640	-0.0020720
C	-2.9512852	1.7258331	-0.0041140
C	-1.5907841	1.9398521	0.0031660
C	-0.7241961	0.8383911	-0.0029410
C	-1.2817411	-0.4616110	-0.0078330
C	-2.6574242	-0.6278610	0.0021570
C	0.7242081	0.8383991	-0.0024960
C	1.2817581	-0.4615880	0.0035590
C	1.5908001	1.9398602	-0.0088840
C	2.9512942	1.7258671	0.0001160
N	3.4615983	0.4585950	-0.0000240
C	2.6574562	-0.6278290	-0.0047990
C	-4.9042084	0.2733040	-0.0068450
C	4.9041954	0.2732030	0.0084170
C	5.4745634	-0.5529680	0.9779791
C	6.8583155	-0.7262301	0.9759501
C	7.6474636	-0.0800750	0.0215030
C	7.0565505	0.7442991	-0.9393091
C	5.6743994	0.9277721	-0.9537901
C	-5.4772244	-0.5536150	-0.9741821
C	-6.8609905	-0.7267101	-0.9683371
C	-7.6475236	-0.0796620	-0.0123400
C	-7.0539735	0.7454201	0.9462391
C	-5.6717684	0.9287281	0.9569101
H	-3.6740463	2.5289822	-0.0327150
H	-1.2236971	2.9588982	-0.0006760
H	-3.1475522	-1.5920741	0.0328730
H	1.2237041	2.9589072	-0.0062340
H	3.6739893	2.5290682	0.0290220
H	3.1475932	-1.5920731	-0.0342390
H	4.8578504	-1.0278231	1.7342731

H	7.3167155	-1.3589221	1.7289761
H	8.7240497	-0.2185130	0.0267300
H	7.6673496	1.2396031	-1.6870251
H	5.2039414	1.5438921	-1.7128911
H	-4.8625894	-1.0292231	-1.7316751
H	-7.3214586	-1.3599881	-1.7196061
H	-8.7241367	-0.2179830	-0.0145910
H	-7.6627386	1.2413901	1.6951721
H	-5.1991774	1.5453631	1.7142881
Se	0.0000210	-1.8407731	-0.0019930

3b'

Symbol	X	Y	Z
N	-3.4903732	0.4593419	-0.0086243
C	-2.9492062	1.7281769	-0.0097235
C	-1.6005903	1.9366697	-0.0047040
C	-0.7047468	0.8281787	-0.0035698
C	-1.3012857	-0.4743090	-0.0103571
C	-2.6578055	-0.6424307	-0.0088260
C	0.7047477	0.8281785	0.0035335
C	1.3012859	-0.4743093	0.0103267
C	1.6005908	1.9366698	0.0046621
C	2.9492068	1.7281770	0.0096890
N	3.4903729	0.4593420	0.0086020
C	2.6578060	-0.6424306	0.0088028
C	-4.9179690	0.2806585	-0.0098958
C	4.9179696	0.2806576	0.0099058
C	5.5015219	-0.6263689	0.9002501
C	6.8856805	-0.7977313	0.8908088
C	7.6822049	-0.0625617	0.0097129
C	7.0896814	0.8450604	-0.8713575
C	5.7057046	1.0170863	-0.8807886
C	-5.5015414	-0.6263863	-0.9002087
C	-6.8856998	-0.7977476	-0.8907351
C	-7.6822060	-0.0625590	-0.0096386
C	-7.0896633	0.8450813	0.8713999
C	-5.7056861	1.0171063	0.8807990
H	-3.6634747	2.5396509	-0.0404287
H	-1.2333725	2.9562332	-0.0157704
H	-3.1459853	-1.6069456	0.0199047
H	1.2333724	2.9562332	0.0157171
H	3.6634755	2.5396511	0.0403882

H	3.1459869	-1.6069452	-0.0199234
H	4.8852787	-1.1719581	1.6075863
H	7.3402809	-1.4981272	1.5847630
H	8.7596604	-0.1964573	0.0097879
H	7.7016081	1.4130975	-1.5653665
H	5.2411748	1.6975271	-1.5872150
H	-4.8853143	-1.1719906	-1.6075473
H	-7.3403144	-1.4981582	-1.5846654
H	-8.7596616	-0.1964540	-0.0096887
H	-7.7015746	1.4131340	1.5654097
H	-5.2411424	1.6975609	1.5872030
Se	0.0000001	-1.8554718	-0.0000151

3b''

Symbol	X	Y	Z
N	3.5280191	-0.4625126	0.0027053
C	2.9561860	-1.7353552	-0.0030966
C	1.6173914	-1.9413476	-0.0081704
C	0.6885711	-0.8314268	-0.0035005
C	1.3215017	0.4764286	-0.0091152
C	2.6609954	0.6486055	-0.0072666
C	-0.6885712	-0.8314267	0.0034984
C	-1.3215017	0.4764286	0.0091131
C	-1.6173914	-1.9413475	0.0081678
C	-2.9561861	-1.7353552	0.0030941
N	-3.5280191	-0.4625125	-0.0027074
C	-2.6609954	0.6486056	0.0072646
C	4.9334167	-0.2861830	-0.0041277
C	-4.9334167	-0.2861828	0.0041283
C	-5.5150163	0.7836822	0.7072174
C	-6.8982891	0.9563945	0.7023700
C	-7.7268746	0.0646698	0.0167764
C	-7.1504002	-1.0030451	-0.6762299
C	-5.7675292	-1.1767285	-0.6949416
C	5.5150175	0.7836823	-0.7072154
C	6.8982903	0.9563946	-0.7023655
C	7.7268746	0.0646696	-0.0167709
C	7.1503990	-1.0030455	0.6762339
C	5.7675280	-1.1767290	0.6949431
H	3.6598908	-2.5559088	-0.0459493
H	1.2552008	-2.9638570	-0.0351168
H	3.1405456	1.6165298	0.0320984

H	-1.2552008	-2.9638570	0.0351137
H	-3.6598909	-2.5559088	0.0459463
H	-3.1405456	1.6165298	-0.0321007
H	-4.8908899	1.4612928	1.2805576
H	-7.3292005	1.7867707	1.2551543
H	-8.8042600	0.2002489	0.0211121
H	-7.7780200	-1.6995186	-1.2255858
H	-5.3352555	-1.9846608	-1.2762214
H	4.8908921	1.4612933	-1.2805563
H	7.3292027	1.7867711	-1.2551488
H	8.8042601	0.2002487	-0.0211048
H	7.7780178	-1.6995193	1.2255905
H	5.3352532	-1.9846615	1.2762220
Se	0.0000000	1.8613251	-0.0000011

3c

Symbol	X	Y	Z
N	3.4886605	-0.6661633	-0.0067705
C	2.9195743	-1.9072790	-0.0212571
C	1.5504492	-2.0536093	-0.0133088
C	0.7274744	-0.9158399	-0.0059032
C	1.3445575	0.3612484	-0.0063902
C	2.7293500	0.4533938	0.0048044
C	-0.7275290	-0.9158085	0.0005096
C	-1.3445545	0.3613068	0.0030816
C	-1.5505410	-2.0535589	0.0067116
C	-2.9196492	-1.9071883	0.0163985
N	-3.4886910	-0.6660252	0.0048258
C	-2.7293622	0.4535191	-0.0063235
C	4.9375914	-0.5453959	-0.0059274
C	-4.9376139	-0.5451646	0.0073850
C	-5.5480050	0.2649282	0.9667298
C	-6.9383338	0.3774452	0.9592832
C	-7.6954509	-0.3128821	0.0093702
C	-7.0653608	-1.1203433	-0.9413186
C	-5.6760196	-1.2426345	-0.9503687
C	5.5502646	0.2663574	-0.9624040
C	6.9405685	0.3788802	-0.9514473
C	7.6954326	-0.3131140	-0.0009493
C	7.0630889	-1.1222220	0.9468343
C	5.6737279	-1.2445003	0.9524024
H	3.6013309	-2.7452159	-0.0603656

H	1.1399614	-3.0557901	-0.0300310
H	3.2677558	1.3911546	0.0433003
H	-1.1400786	-3.0557801	0.0214794
H	-3.6013883	-2.7451657	0.0550248
H	-3.2677922	1.3913560	-0.0426158
H	-4.9552138	0.7741106	1.7198228
H	-7.4264696	0.9971739	1.7044049
H	-8.7771386	-0.2221898	0.0101892
H	-7.6514808	-1.6499278	-1.6853261
H	-5.1769171	-1.8454109	-1.7020442
H	4.9592727	0.7768581	-1.7160156
H	7.4304706	0.9999289	-1.6943065
H	8.7771183	-0.2224120	0.0009753
H	7.6474488	-1.6530838	1.6913154
H	5.1728527	-1.8484954	1.7019366
Te	0.0000486	1.9564034	-0.0009924

3c'

Symbol	X	Y	Z
N	-3.5171589	0.6669042	-0.0101550
C	-2.9165916	1.9083382	-0.0164121
C	-1.5596212	2.0495264	-0.0110276
C	-0.7072622	0.9038225	-0.0043730
C	-1.3660840	-0.3736414	-0.0090828
C	-2.7313243	-0.4686900	-0.0067894
C	0.7072626	0.9038227	0.0044205
C	1.3660842	-0.3736415	0.0091146
C	1.5596210	2.0495267	0.0110943
C	2.9165915	1.9083380	0.0164689
N	3.5171583	0.6669045	0.0101836
C	2.7313246	-0.4686899	0.0068110
C	-4.9507844	0.5535362	-0.0081615
C	4.9507844	0.5535377	0.0081478
C	5.5768444	-0.3381761	0.8858198
C	6.9675740	-0.4472745	0.8727987
C	7.7294084	0.3348166	0.0009581
C	7.0949158	1.2269411	-0.8671372
C	5.7042906	1.3366999	-0.8731858
C	-5.5768192	-0.3381615	-0.8858682
C	-6.9675490	-0.4472610	-0.8728888
C	-7.7294091	0.3348130	-0.0010551
C	-7.0949416	1.2269209	0.8670756

C	-5.7043165	1.3366800	0.8731659
H	-3.5896310	2.7540765	-0.0527252
H	-1.1492911	3.0524324	-0.0284273
H	-3.2685783	-1.4069634	0.0253444
H	1.1492906	3.0524320	0.0285225
H	3.5896322	2.7540743	0.0528003
H	3.2685781	-1.4069630	-0.0253339
H	4.9874837	-0.9201684	1.5871156
H	7.4539068	-1.1358809	1.5569974
H	8.8117830	0.2495585	-0.0017899
H	7.6795729	1.8315203	-1.5537773
H	5.2096167	2.0051938	-1.5706036
H	-4.9874382	-0.9201399	-1.5871584
H	-7.4538616	-1.1358552	-1.5571142
H	-8.8117836	0.2495545	0.0016600
H	-7.6796177	1.8314870	1.5537111
H	-5.2096637	2.0051608	1.5706112
Te	0.0000003	-1.9697478	0.0000116

3c’’

Symbol	X	Y	Z
N	-3.5543860	-0.6693306	-0.0035506
C	-2.9234664	-1.9146169	0.0011106
C	-1.5768174	-2.0544307	0.0063664
C	-0.6899962	-0.9062208	0.0022843
C	-1.3873747	0.3749793	0.0064577
C	-2.7358434	0.4758792	0.0046682
C	0.6899962	-0.9062209	-0.0022885
C	1.3873748	0.3749793	-0.0064607
C	1.5768173	-2.0544308	-0.0063721
C	2.9234663	-1.9146170	-0.0011158
N	3.5543860	-0.6693308	0.0035473
C	2.7358435	0.4758791	-0.0046707
C	-4.9664829	-0.5572112	0.0016841
C	4.9664829	-0.5572114	-0.0016830
C	5.5970792	0.4830340	-0.7076329
C	6.9870622	0.5929286	-0.7013292
C	7.7734409	-0.3337411	-0.0116708
C	7.1481775	-1.3724266	0.6837944
C	5.7584434	-1.4830842	0.7010445
C	-5.5970772	0.4830335	0.7076370
C	-6.9870602	0.5929281	0.7013374

C	-7.7734410	-0.3337408	0.0116801
C	-7.1481795	-1.3724255	-0.6837880
C	-5.7584454	-1.4830832	-0.7010422
H	-3.5864671	-2.7684371	0.0441321
H	-1.1711995	-3.0605485	0.0341933
H	-3.2643072	1.4184516	-0.0353069
H	1.1711993	-3.0605485	-0.0342010
H	3.5864670	-2.7684372	-0.0441386
H	3.2643072	1.4184514	0.0353049
H	5.0050134	1.1860028	-1.2845842
H	7.4560947	1.4009754	-1.2561489
H	8.8558950	-0.2474408	-0.0151142
H	7.7429902	-2.0952687	1.2355685
H	5.2890243	-2.2691609	1.2835025
H	-5.0050097	1.1860016	1.2845874
H	-7.4560911	1.4009743	1.2561594
H	-8.8558950	-0.2474405	0.0151268
H	-7.7429939	-2.0952670	-1.2355612
H	-5.2890280	-2.2691592	-1.2835024
Te	0.0000000	1.9727000	-0.0000011

5a

Symbol	X	Y	Z
N	3.4447162	-0.1766636	-0.1133011
C	2.9742337	-1.4653461	-0.1204348
C	1.6254169	-1.7297060	-0.0640823
C	0.7212953	-0.6588121	-0.0282428
C	1.2347167	0.6603957	-0.0465051
C	2.6018301	0.8846022	-0.0641263
C	-0.7212960	-0.6588118	0.0282355
C	-1.2347166	0.6603963	0.0465006
C	-1.6254174	-1.7297056	0.0640767
C	-2.9742342	-1.4653454	0.1204325
N	-3.4447157	-0.1766628	0.1133018
C	-2.6018299	0.8846031	0.0641262
H	3.7214543	-2.2429338	-0.1941826
H	1.2961252	-2.7616421	-0.0691136
H	3.0546583	1.8655881	-0.0201909
H	-1.2961256	-2.7616416	0.0691086
H	-3.7214552	-2.2429325	0.1941813
H	-3.0546584	1.8655891	0.0201931
C	4.8502422	0.0663936	-0.1696645

C	5.4760012	0.9990805	-0.9570417
S	5.9617446	-0.8155209	0.8465150
C	6.8830595	1.0010236	-0.7485726
H	4.9626559	1.6295885	-1.6737395
C	7.2856669	0.0808820	0.1828793
H	7.5669551	1.6525723	-1.2787955
H	8.2882661	-0.1312735	0.5292623
C	-4.8502422	0.0663936	0.1696684
C	-5.4760003	0.9990752	0.9570527
S	-5.9617435	-0.8155049	-0.8465263
C	-6.8830580	1.0010259	0.7485780
H	-4.9626528	1.6295832	1.6737490
C	-7.2856712	0.0808561	-0.1828436
H	-7.5669526	1.6525755	1.2788011
H	-8.2882735	-0.1313157	-0.5292075
S	0.0000001	1.9052461	-0.0000066

5a’

Symbol	X	Y	Z
N	-3.4680860	-0.1813843	0.1220237
C	-2.9707728	-1.4725498	0.1157237
C	-1.6323921	-1.7291428	0.0621991
C	-0.7032726	-0.6501355	0.0269427
C	-1.2519496	0.6734639	0.0475765
C	-2.6008716	0.8967975	0.0806145
C	0.7032727	-0.6501356	-0.0269442
C	1.2519499	0.6734638	-0.0475780
C	1.6323919	-1.7291431	-0.0622006
C	2.9707727	-1.4725504	-0.1157250
N	3.4680860	-0.1813849	-0.1220248
C	2.6008719	0.8967971	-0.0806159
H	-3.7129426	-2.2570547	0.1769580
H	-1.2997971	-2.7604829	0.0643858
H	-3.0583924	1.8757439	0.0570836
H	1.2997967	-2.7604832	-0.0643875
H	3.7129425	-2.2570553	-0.1769591
H	3.0583931	1.8757433	-0.0570856
C	-4.8623359	0.0552833	0.1852170
C	-5.5038413	0.9818020	0.9656604
S	-5.9754905	-0.8117026	-0.8537035
C	-6.9124262	0.9899266	0.7426242
H	-4.9959695	1.6116785	1.6870256

C	-7.3131172	0.0756615	-0.1920906
H	-7.5986425	1.6393034	1.2737636
H	-8.3153690	-0.1466149	-0.5326089
C	4.8623361	0.0552824	-0.1852171
C	5.5038425	0.9817976	-0.9656636
S	5.9754891	-0.8116986	0.8537091
C	6.9124273	0.9899227	-0.7426262
H	4.9959714	1.6116712	-1.6870320
C	7.3131169	0.0756617	0.1920934
H	7.5986445	1.6392967	-1.2737678
H	8.3153682	-0.1466134	0.5326138
S	0.0000002	1.9209659	-0.0000009

5a”

Symbol	X	Y	Z
N	-0.0000158	3.5027288	-0.1568572
C	-0.0067975	2.9769216	-1.4513458
C	-0.0046418	1.6461548	-1.7029795
C	-0.0026243	0.6886055	-0.6212869
C	-0.0051083	1.2719836	0.7090904
C	0.0000000	2.6046563	0.9336091
C	0.0026243	-0.6886055	-0.6212869
C	0.0051083	-1.2719836	0.7090904
C	0.0046418	-1.6461548	-1.7029795
C	0.0067975	-2.9769216	-1.4513458
N	0.0000158	-3.5027288	-0.1568572
C	0.0000000	-2.6046563	0.9336091
H	-0.0416107	3.7122016	-2.2452601
H	-0.0201074	1.3162772	-2.7362741
H	0.0357788	3.0584256	1.9137480
H	0.0201074	-1.3162772	-2.7362741
H	0.0416107	-3.7122016	-2.2452601
H	-0.0357788	-3.0584256	1.9137480
C	-0.0164503	4.8786992	0.0755864
C	-0.5815043	5.5499350	1.1349033
S	0.8411954	5.9923134	-0.9920907
C	-0.3487561	6.9577892	1.0833151
H	-1.1718561	5.0638078	1.9027219
C	0.3776478	7.3526783	-0.0033529
H	-0.7387926	7.6515943	1.8203366
H	0.6506996	8.3522618	-0.3124657
C	0.0164503	-4.8786992	0.0755864

C	0.5815043	-5.5499350	1.1349033
S	-0.8411954	-5.9923134	-0.9920907
C	0.3487561	-6.9577892	1.0833151
H	1.1718561	-5.0638078	1.9027219
C	-0.3776478	-7.3526783	-0.0033529
H	0.7387926	-7.6515943	1.8203366
H	-0.6506996	-8.3522618	-0.3124657
S	0.0000000	0.0000000	1.9604263

5b

Symbol	X	Y	Z
N	-3.4640970	0.3659550	-0.1037704
C	-2.9489638	1.6367744	-0.1012462
C	-1.5911742	1.8483168	-0.0481882
C	-0.7224906	0.7475554	-0.0235672
C	-1.2811770	-0.5524107	-0.0423304
C	-2.6547869	-0.7219965	-0.0613313
C	0.7224896	0.7475553	0.0236228
C	1.2811739	-0.5524088	0.0423804
C	1.5911736	1.8483158	0.0482389
C	2.9489650	1.6367762	0.1012857
N	3.4641005	0.3659558	0.1038155
C	2.6547814	-0.7219928	0.0613684
H	-3.6672355	2.4419160	-0.1660174
H	-1.2245818	2.8676161	-0.0467190
H	-3.1446625	-1.6854461	-0.0256631
H	1.2245783	2.8676139	0.0467734
H	3.6672325	2.4419241	0.1660559
H	3.1446411	-1.6854441	0.0256676
C	-4.8764486	0.1693365	-0.1653792
C	-5.5300381	-0.7366821	-0.9611904
S	-5.9618758	1.0804416	0.8529739
C	-6.9372996	-0.6932978	-0.7578075
H	-5.0352542	-1.3792784	-1.6802250
C	-7.3126732	0.2332101	0.1785354
H	-7.6403580	-1.3181049	-1.2951403
H	-8.3089368	0.4764472	0.5227553
C	4.8764563	0.1693512	0.1653900
C	5.5301071	-0.7365271	0.9613134
S	5.9618376	1.0804523	-0.8530219
C	6.9373389	-0.6932927	0.7577045
H	5.0353841	-1.3790182	1.6804821

C	7.3126498	0.2330925	-0.1787853
H	7.6404262	-1.3180931	1.2950068
H	8.3088874	0.4762218	-0.5231579
Se	-0.0000011	-1.9315907	0.0000162

5b'

Symbol	X	Y	Z
N	3.4876765	-0.3710425	-0.1183960
C	2.9454603	-1.6436370	-0.1068131
C	1.5985958	-1.8485386	-0.0541718
C	0.7041774	-0.7395718	-0.0249525
C	1.2994278	0.5634289	-0.0468552
C	2.6545804	0.7337408	-0.0804436
C	-0.7041775	-0.7395723	0.0249606
C	-1.2994286	0.5634283	0.0468613
C	-1.5985951	-1.8485397	0.0541814
C	-2.9454598	-1.6436389	0.1068210
N	-3.4876766	-0.3710448	0.1184008
C	-2.6545815	0.7337392	0.0804484
H	3.6584893	-2.4550757	-0.1629949
H	1.2301494	-2.8676885	-0.0514770
H	3.1482786	1.6952959	-0.0615442
H	-1.2301477	-2.8676893	0.0514890
H	-3.6584888	-2.4550777	0.1630029
H	-3.1482808	1.6952937	0.0615488
C	4.8886627	-0.1809158	-0.1829022
C	5.5606227	0.7199728	-0.9677958
S	5.9728278	-1.0800226	0.8594856
C	6.9687751	0.6820790	-0.7451926
H	5.0738156	1.3632294	-1.6918817
C	7.3390809	-0.2407174	0.1936426
H	7.6760658	1.3057165	-1.2795464
H	8.3334996	-0.4948092	0.5348563
C	-4.8886634	-0.1809191	0.1829018
C	-5.5606278	0.7199591	0.9678032
S	-5.9728222	-1.0800123	-0.8595041
C	-6.9687789	0.6820678	0.7451918
H	-5.0738243	1.3632065	1.6918998
C	-7.3390789	-0.2407144	-0.1936596
H	-7.6760729	1.3056978	1.2795499
H	-8.3334955	-0.4948008	-0.5348834
Se	-0.0000008	1.9444696	0.0000026

5b''

Symbol	X	Y	Z
N	-3.5207888	-0.3494139	0.1079131
C	-2.9497830	-1.6249467	0.0955441
C	-1.6117051	-1.8256288	0.0523344
C	-0.6886906	-0.7132661	0.0231553
C	-1.3195099	0.5949666	0.0450204
C	-2.6581168	0.7678118	0.0811912
C	0.6886906	-0.7132661	-0.0231553
C	1.3195099	0.5949666	-0.0450204
C	1.6117051	-1.8256289	-0.0523345
C	2.9497830	-1.6249467	-0.0955442
N	3.5207888	-0.3494140	-0.1079131
C	2.6581169	0.7678118	-0.0811912
H	-3.6544753	-2.4450237	0.1505952
H	-1.2459298	-2.8469847	0.0551594
H	-3.1483286	1.7310320	0.0636288
H	1.2459298	-2.8469847	-0.0551596
H	3.6544753	-2.4450237	-0.1505954
H	3.1483286	1.7310320	-0.0636287
C	-4.9025739	-0.1629880	0.1627221
C	-5.5933868	0.8724822	0.7479343
S	-6.0026967	-1.2667356	-0.6663776
C	-7.0044770	0.7743047	0.5526455
H	-5.1175223	1.6557127	1.3262744
C	-7.3822774	-0.3243531	-0.1647780
H	-7.7117287	1.4874925	0.9623540
H	-8.3780025	-0.6664850	-0.4112572
C	4.9025739	-0.1629881	-0.1627222
C	5.5933867	0.8724821	-0.7479345
S	6.0026967	-1.2667353	0.6663780
C	7.0044770	0.7743045	-0.5526458
H	5.1175222	1.6557124	-1.3262747
C	7.3822774	-0.3243533	0.1647777
H	7.7117287	1.4874922	-0.9623546
H	8.3780026	-0.6664852	0.4112567
Se	0.0000000	1.9792722	0.0000001

5c

Symbol	X	Y	Z
N	3.4904372	-0.5804438	-0.1070299

C	2.9171749	-1.8250519	-0.0959320
C	1.5507130	-1.9687435	-0.0439399
C	0.7257822	-0.8312783	-0.0236286
C	1.3437765	0.4458114	-0.0478756
C	2.7266509	0.5413751	-0.0718352
C	-0.7257824	-0.8312782	0.0236207
C	-1.3437765	0.4458114	0.0478733
C	-1.5507135	-1.9687433	0.0439304
C	-2.9171753	-1.8250519	0.0959258
N	-3.4904373	-0.5804438	0.1070292
C	-2.7266508	0.5413751	0.0718358
H	3.5953042	-2.6650045	-0.1528339
H	1.1412334	-2.9714716	-0.0390101
H	3.2662038	1.4784240	-0.0461018
H	-1.1412341	-2.9714715	0.0389976
H	-3.5953043	-2.6650047	0.1528271
H	-3.2662033	1.4784243	0.0461054
C	4.9103517	-0.4469935	-0.1673427
C	5.6058939	0.4143509	-0.9772810
S	5.9510954	-1.3830917	0.8734113
C	7.0097127	0.3140476	-0.7660674
H	5.1421333	1.0638855	-1.7105706
C	7.3405667	-0.6090938	0.1905309
H	7.7414066	0.8972514	-1.3119115
H	8.3239760	-0.8885329	0.5441739
C	-4.9103515	-0.4469942	0.1673467
C	-5.6058912	0.4143536	0.9772837
S	-5.9510974	-1.3830887	-0.8734081
C	-7.0097085	0.3140714	0.7660528
H	-5.1421287	1.0638965	1.7105647
C	-7.3405687	-0.6091220	-0.1904931
H	-7.7413997	0.8972930	1.3118816
H	-8.3239802	-0.8885807	-0.5441143
Te	-0.0000000	2.0412099	-0.0000016

5c'

Symbol	X	Y	Z
N	-3.5142023	-0.5836713	0.1207097
C	-2.9130984	-1.8288869	0.1041067
C	-1.5579550	-1.9667848	0.0515839
C	-0.7066993	-0.8207010	0.0248019
C	-1.3638865	0.4575561	0.0496651

C	-2.7276634	0.5551094	0.0858252
C	0.7066993	-0.8207010	-0.0248018
C	1.3638864	0.4575562	-0.0496650
C	1.5579550	-1.9667847	-0.0515837
C	2.9130984	-1.8288868	-0.1041065
N	3.5142023	-0.5836712	-0.1207096
C	2.7276634	0.5551094	-0.0858251
H	-3.5853184	-2.6748165	0.1563796
H	-1.1470727	-2.9695431	0.0468015
H	-3.2704981	1.4902597	0.0719420
H	1.1470728	-2.9695431	-0.0468013
H	3.5853184	-2.6748164	-0.1563794
H	3.2704981	1.4902598	-0.0719419
C	-4.9223491	-0.4571967	0.1823804
C	-5.6374043	0.4071037	0.9710868
S	-5.9613483	-1.3972579	-0.8689347
C	-7.0420017	0.3064030	0.7432774
H	-5.1829628	1.0667488	1.7014500
C	-7.3666637	-0.6263665	-0.2031613
H	-7.7787157	0.8935264	1.2792411
H	-8.3474799	-0.9234019	-0.5491804
C	4.9223490	-0.4571965	-0.1823803
C	5.6374042	0.4071044	-0.9710863
S	5.9613485	-1.3972574	0.8689350
C	7.0420016	0.3064030	-0.7432778
H	5.1829625	1.0667501	-1.7014489
C	7.3666639	-0.6263679	0.2031595
H	7.7787156	0.8935263	-1.2792418
H	8.3474802	-0.9234045	0.5491772
Te	-0.0000000	2.0539089	0.0000000

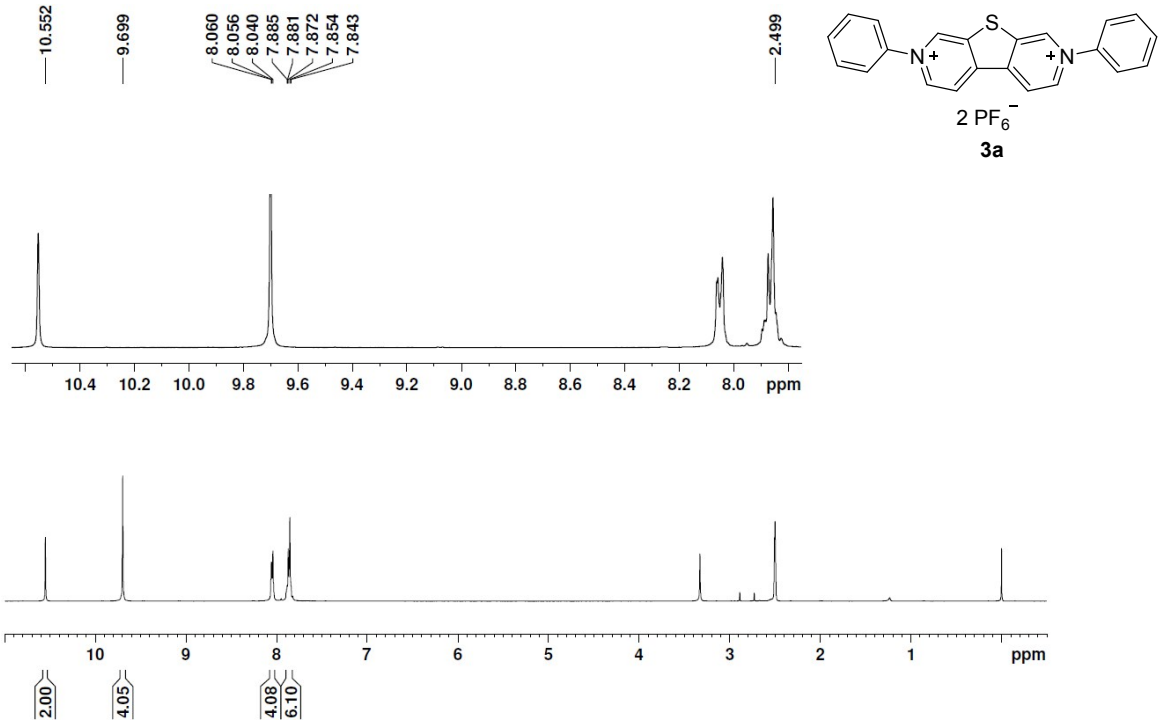
5c''

Symbol	X	Y	Z
N	-3.5471250	-0.5629530	0.1084759
C	-2.9172381	-1.8108425	0.0907820
C	-1.5715297	-1.9456945	0.0474949
C	-0.6902430	-0.7954338	0.0218756
C	-1.3852212	0.4862935	0.0448907
C	-2.7326815	0.5882700	0.0823902
C	0.6902430	-0.7954338	-0.0218755
C	1.3852212	0.4862935	-0.0448907
C	1.5715297	-1.9456945	-0.0474948

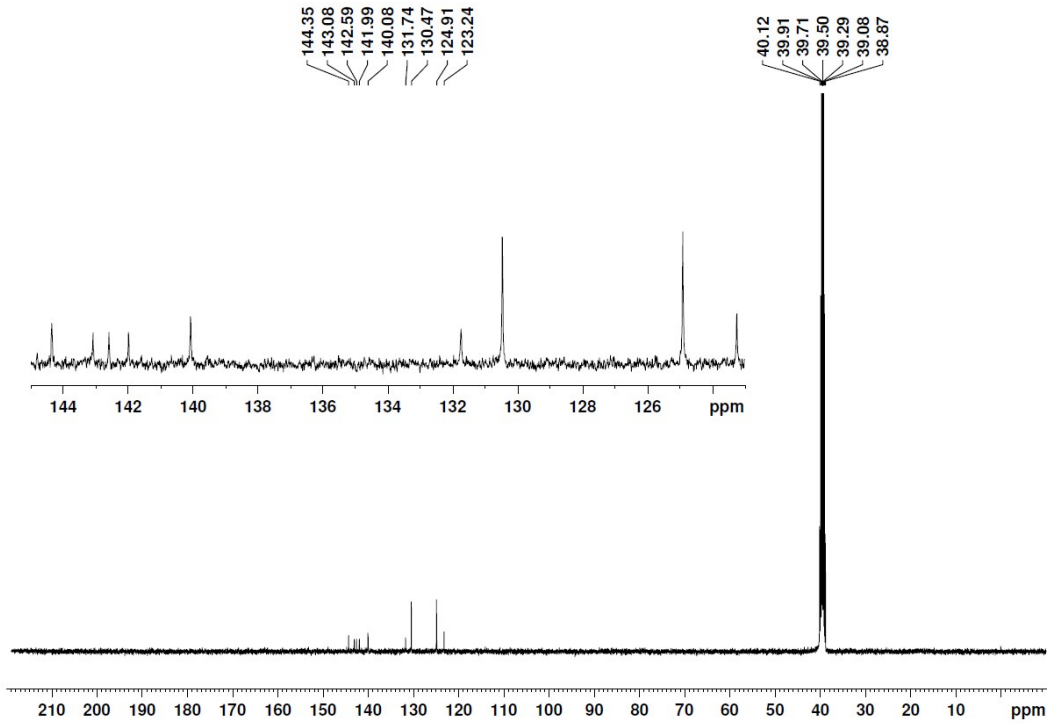
C	2.9172381	-1.8108425	-0.0907820
N	3.5471250	-0.5629530	-0.1084758
C	2.7326815	0.5882700	-0.0823902
H	-3.5815816	-2.6642262	0.1422267
H	-1.1629723	-2.9507502	0.0474155
H	-3.2714206	1.5258024	0.0677465
H	1.1629723	-2.9507502	-0.0474155
H	3.5815816	-2.6642262	-0.1422267
H	3.2714205	1.5258024	-0.0677464
C	-4.9362654	-0.4400482	0.1615291
C	-5.6754843	0.5591222	0.7516473
S	-5.9823333	-1.5888743	-0.6746122
C	-7.0803831	0.3965540	0.5526974
H	-5.2378558	1.3600493	1.3359479
C	-7.4049667	-0.7150744	-0.1715991
H	-7.8208475	1.0737886	0.9646745
H	-8.3833335	-1.1017826	-0.4218658
C	4.9362654	-0.4400482	-0.1615290
C	5.6754843	0.5591224	-0.7516471
S	5.9823333	-1.5888742	0.6746123
C	7.0803830	0.3965540	-0.5526975
H	5.2378557	1.3600495	-1.3359476
C	7.4049667	-0.7150748	0.1715985
H	7.8208474	1.0737885	-0.9646748
H	8.3833335	-1.1017832	0.4218647
Te	0.0000000	2.0838808	0.0000000

15. NMR spectra

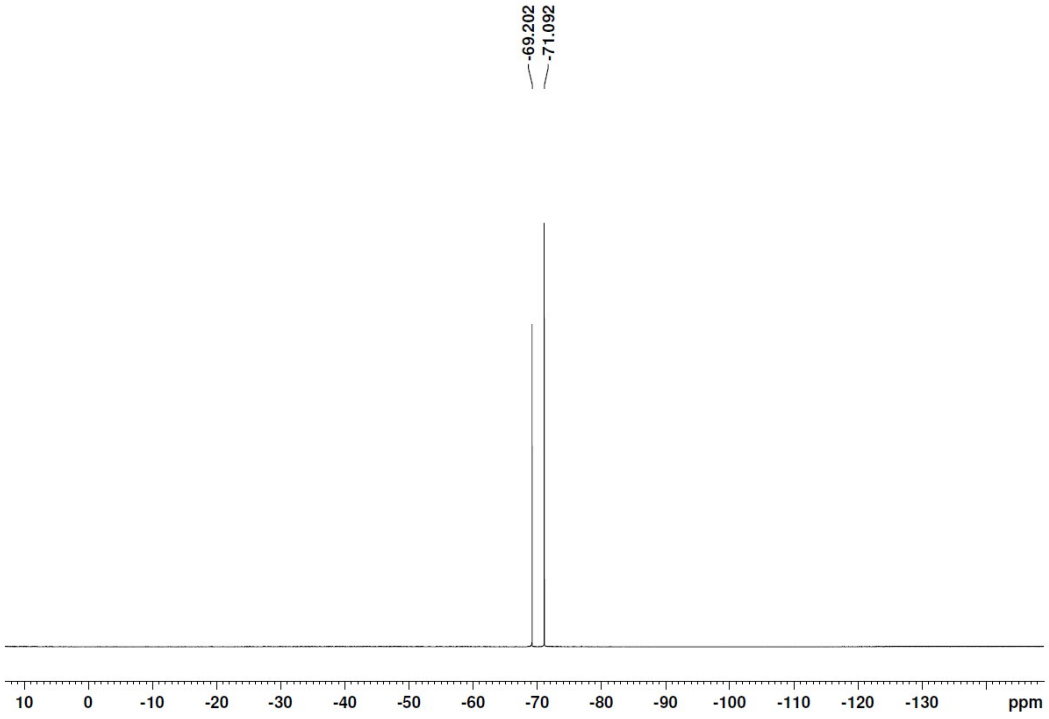
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **3a**



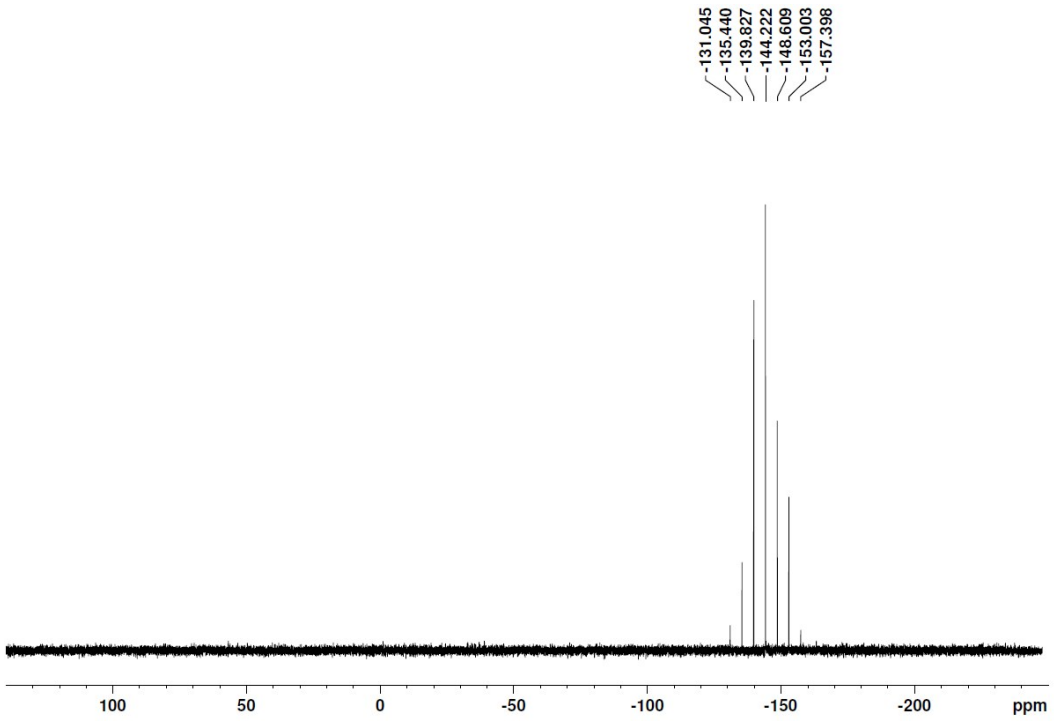
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **3a**



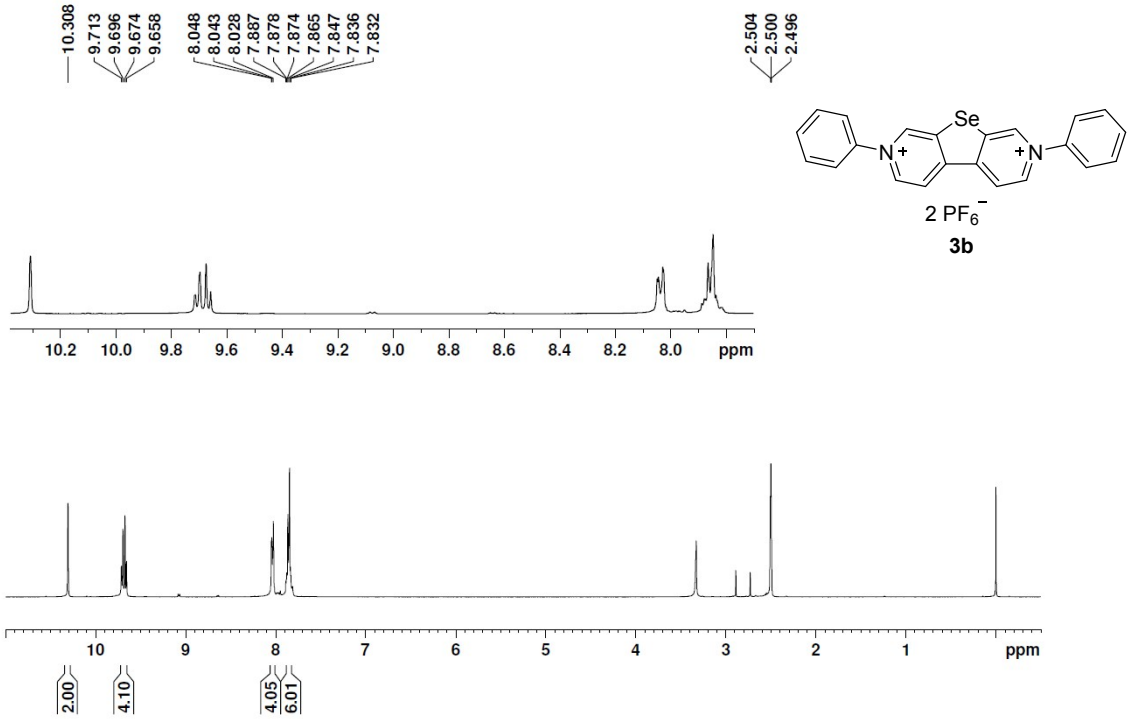
^{19}F NMR (DMSO-d_6, 376 MHz) spectrum of **3a**



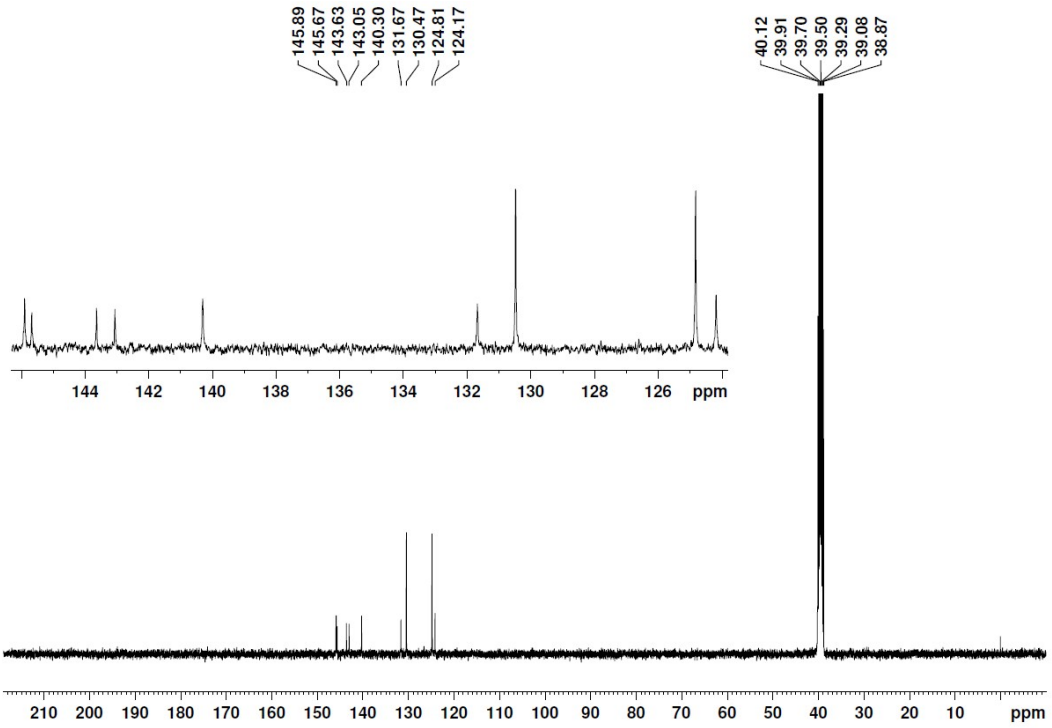
^{31}P NMR (DMSO-d_6, 162 MHz) spectrum of **3a**



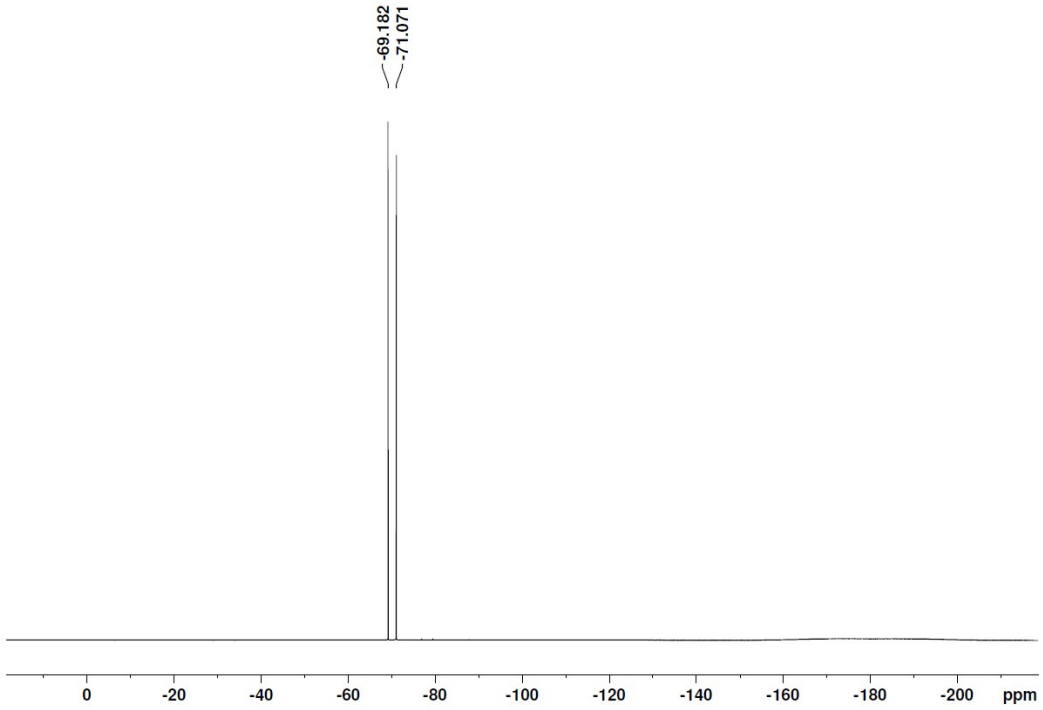
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **3b**



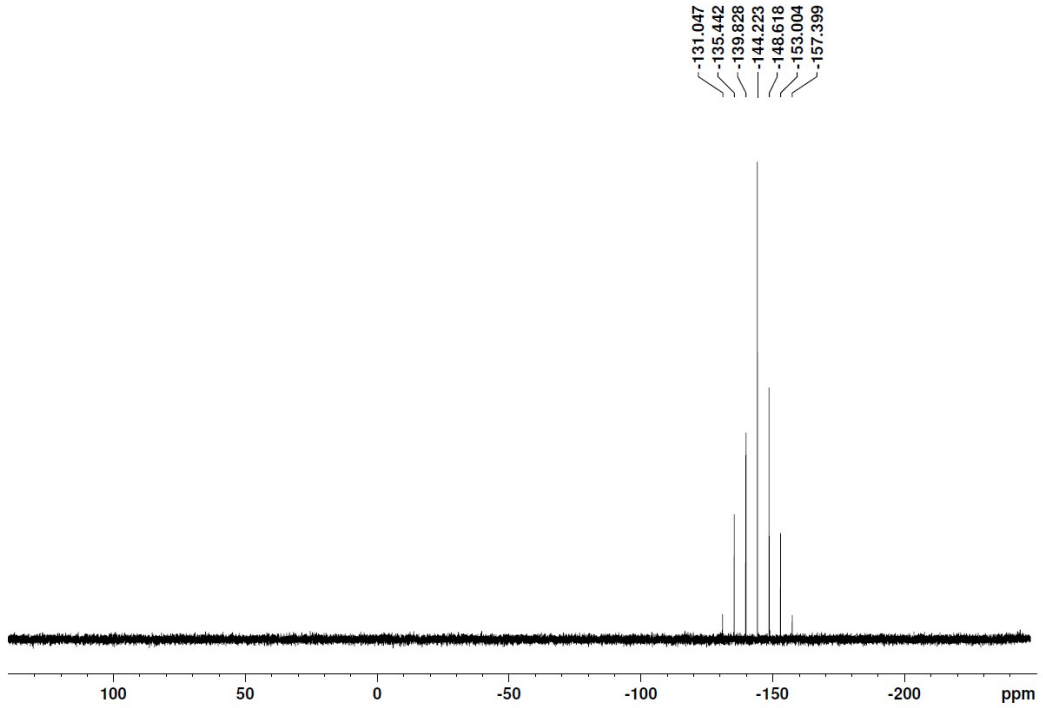
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **3b**



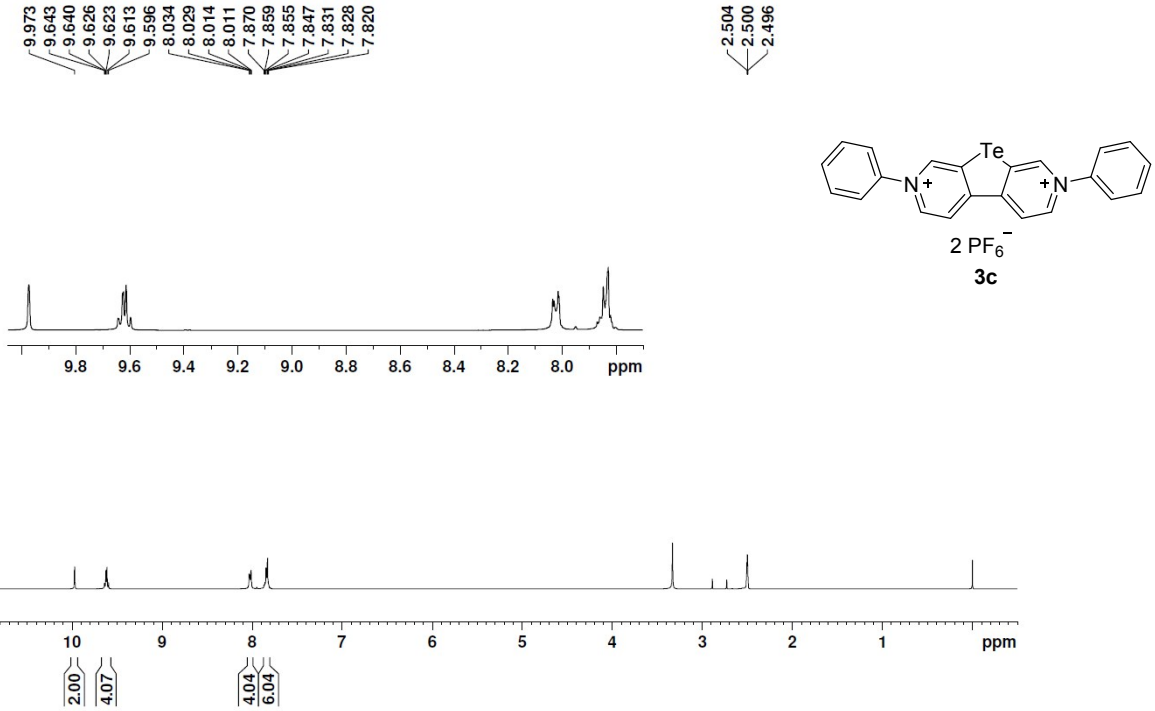
^{19}F NMR (DMSO-d_6, 376 MHz) spectrum of **3b**



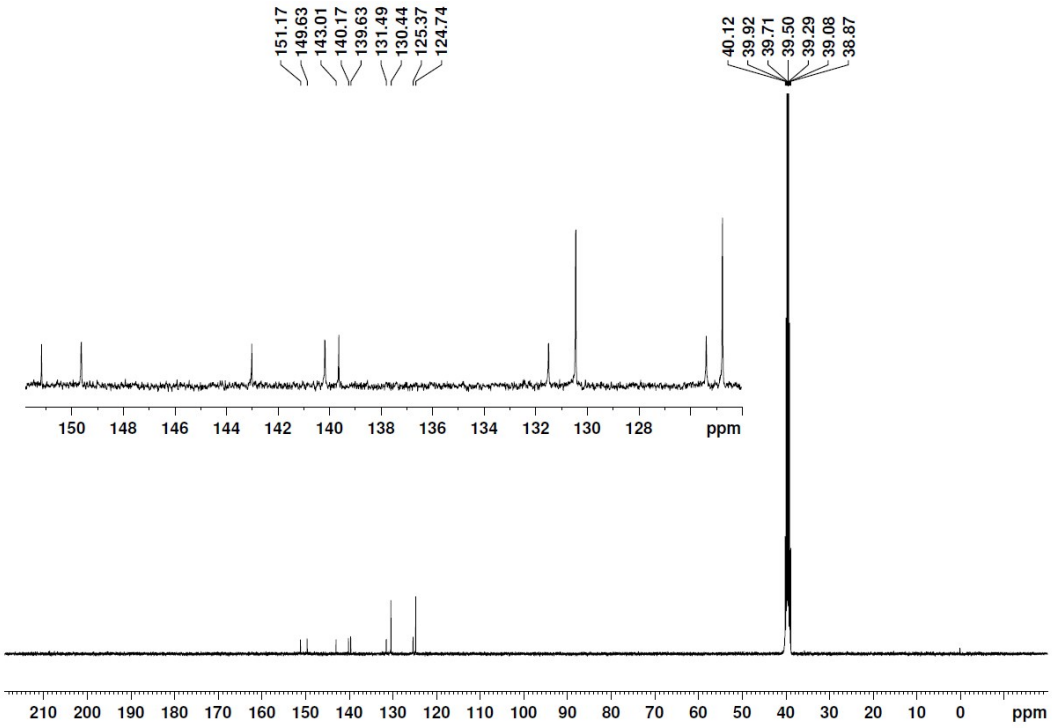
^{31}P (DMSO-d_6, 162 MHz) NMR spectrum of **3b**



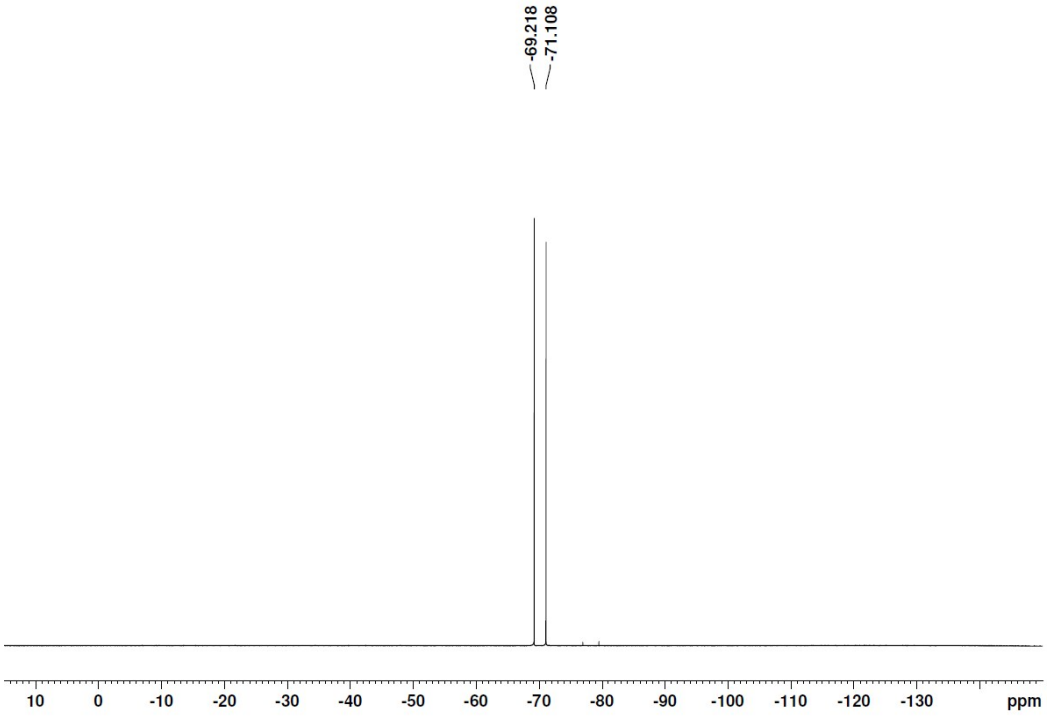
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **3c**



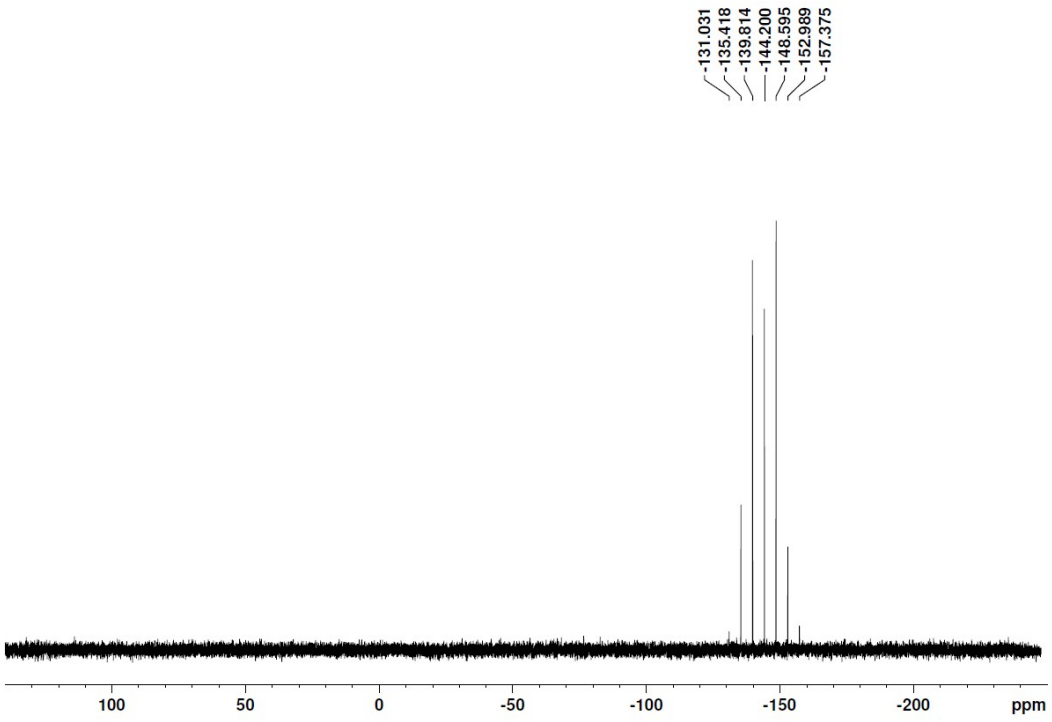
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of **3c**



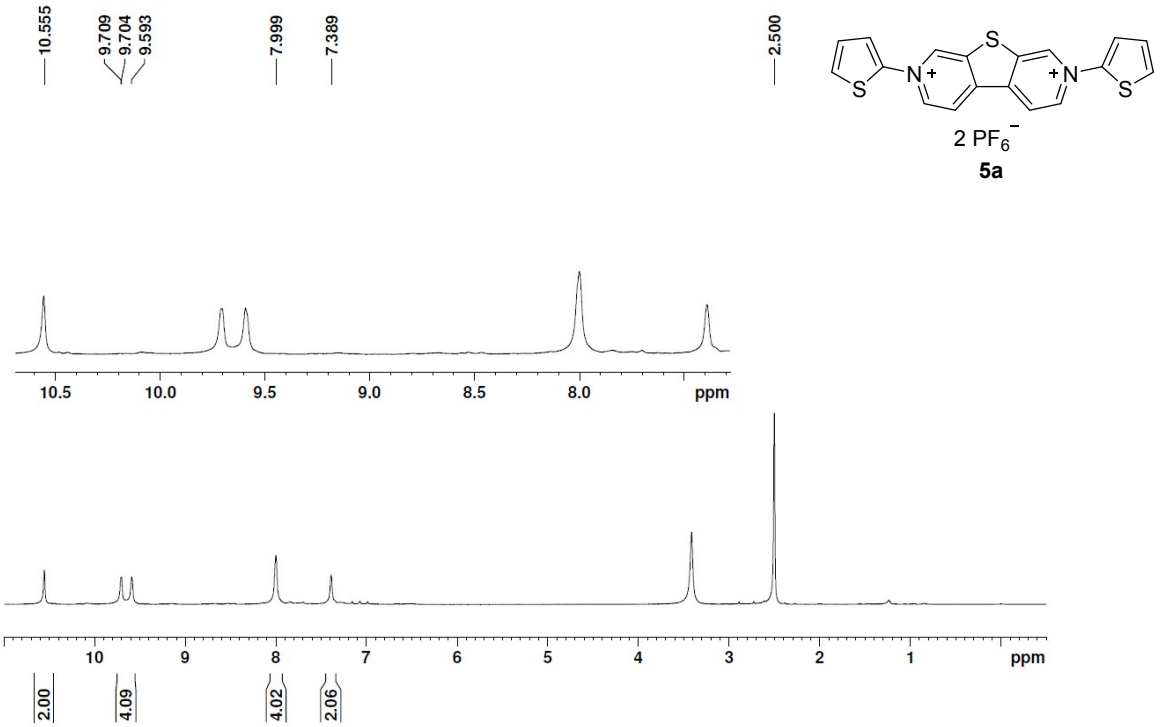
^{19}F NMR (DMSO-d_6, 376 MHz) spectrum of **3c**



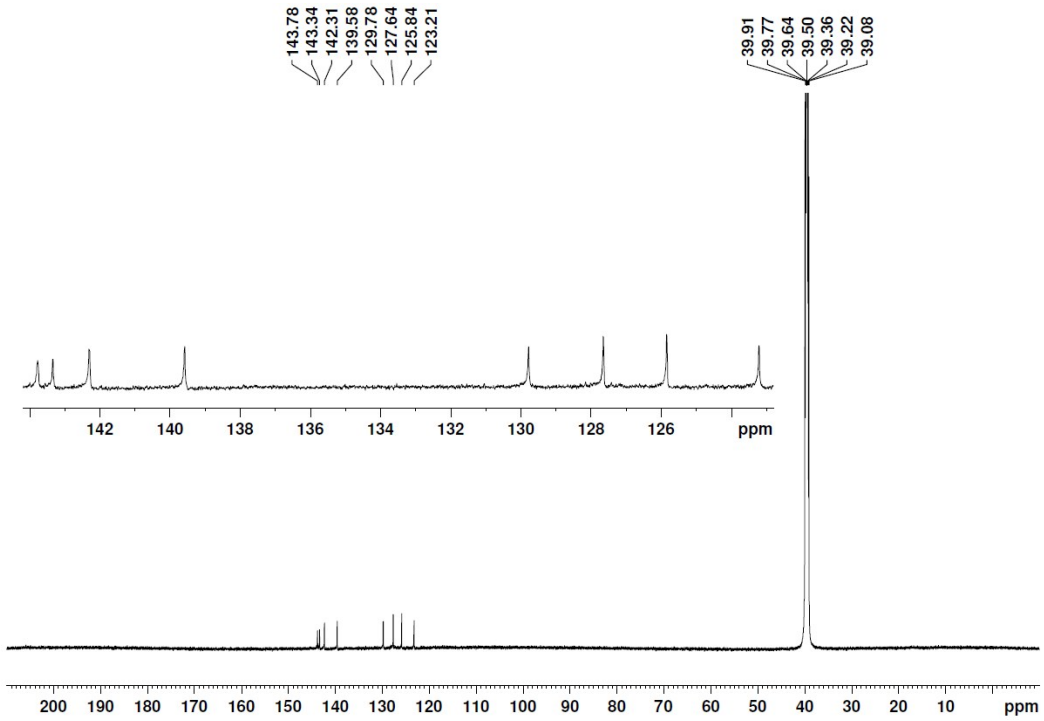
^{31}P NMR (DMSO-d_6, 162 MHz) spectrum of **3c**



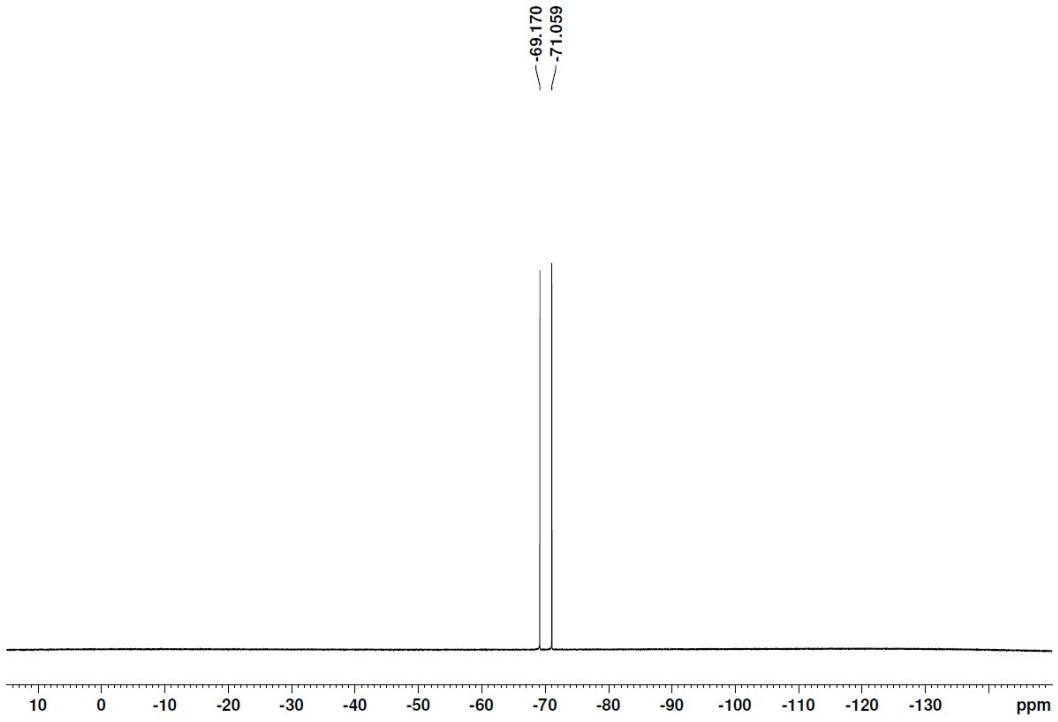
^{1}H NMR (DMSO-d_6, 600 MHz) spectrum of **5a**



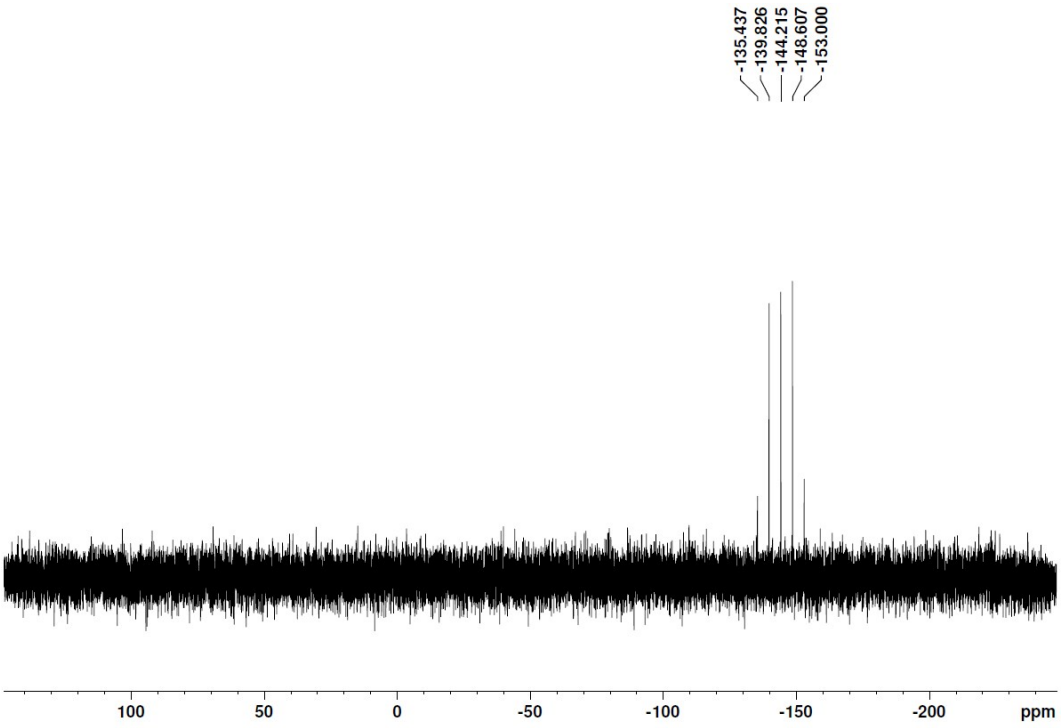
^{13}C NMR (DMSO-d_6, 150 MHz) spectrum of **5a**



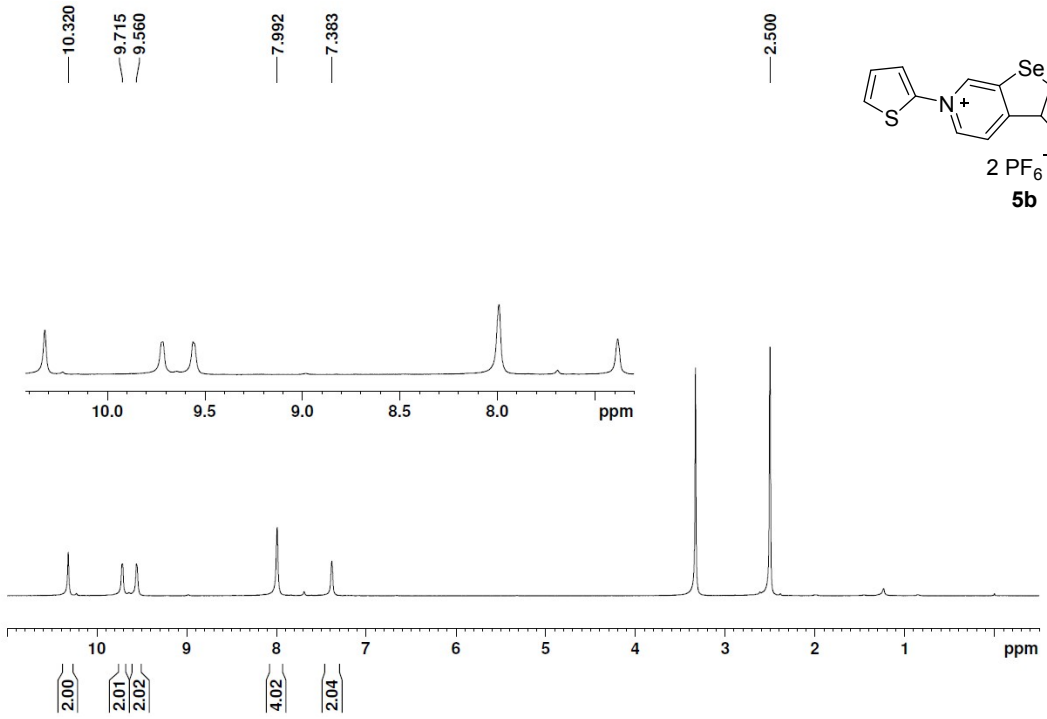
^{19}F NMR (DMSO-d_6, 564 MHz) spectrum of **5a**



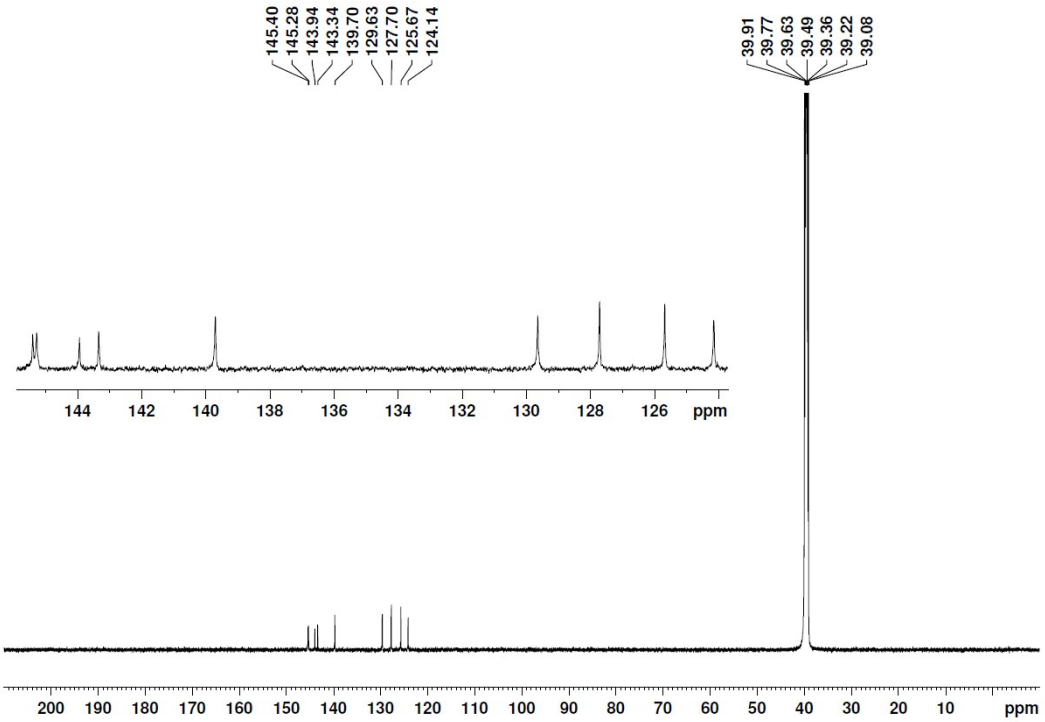
^{31}P NMR (DMSO-d_6, 243 MHz) spectrum of **5a**



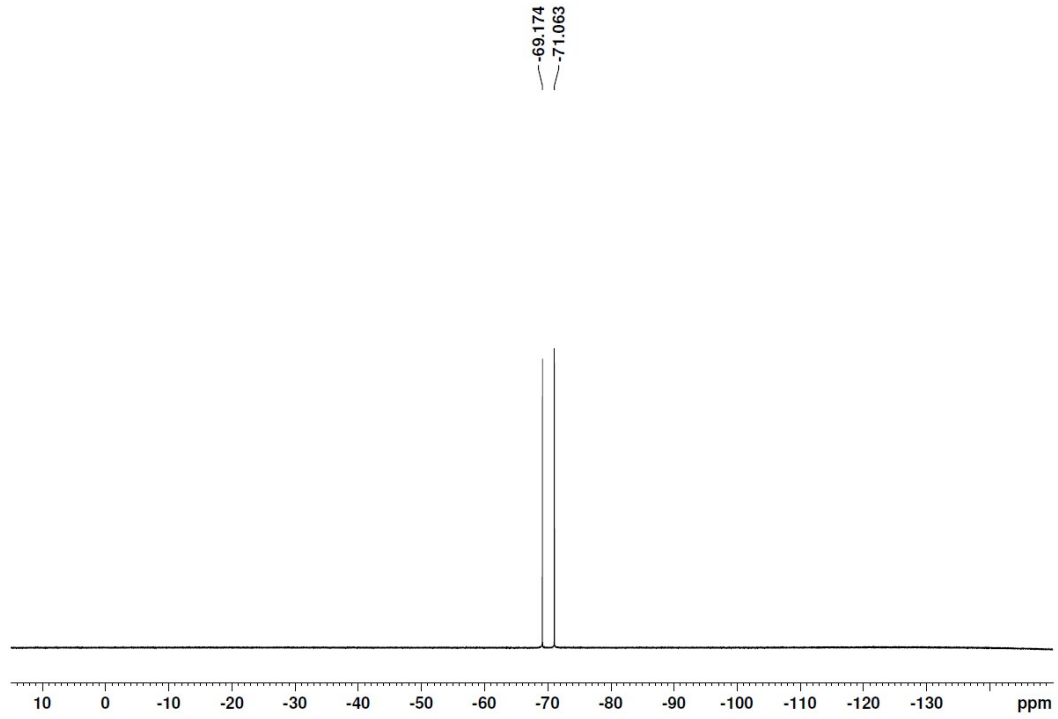
^{1}H NMR (DMSO-d_6, 600 MHz) spectrum of **5b**



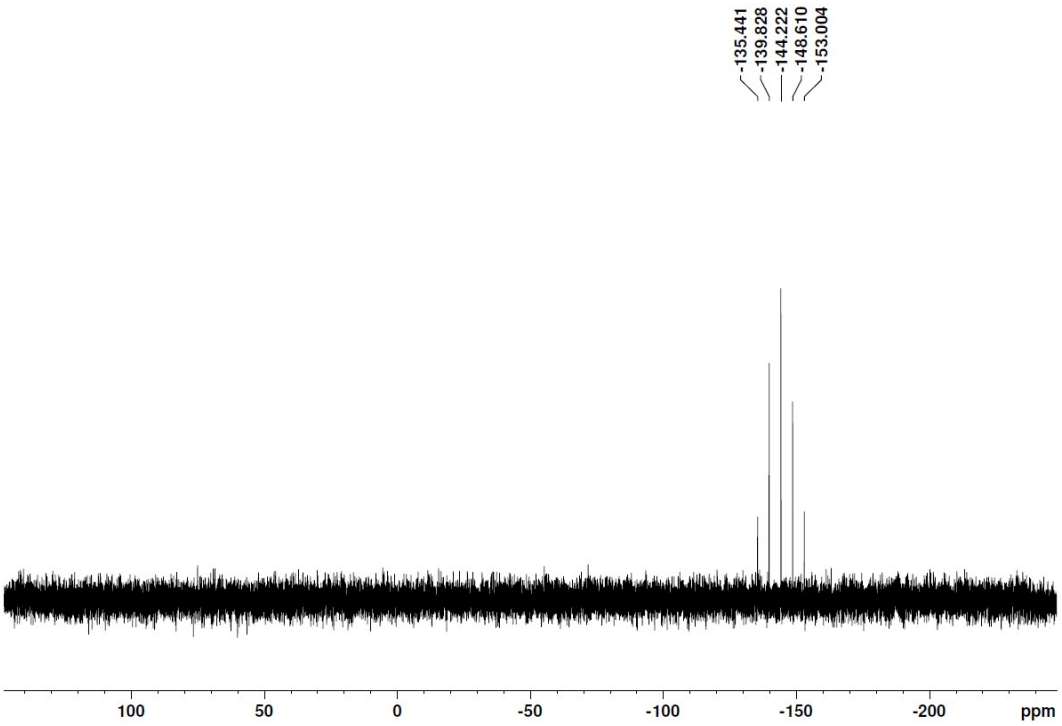
^{13}C NMR (DMSO-d_6, 150 MHz) spectrum of **5b**



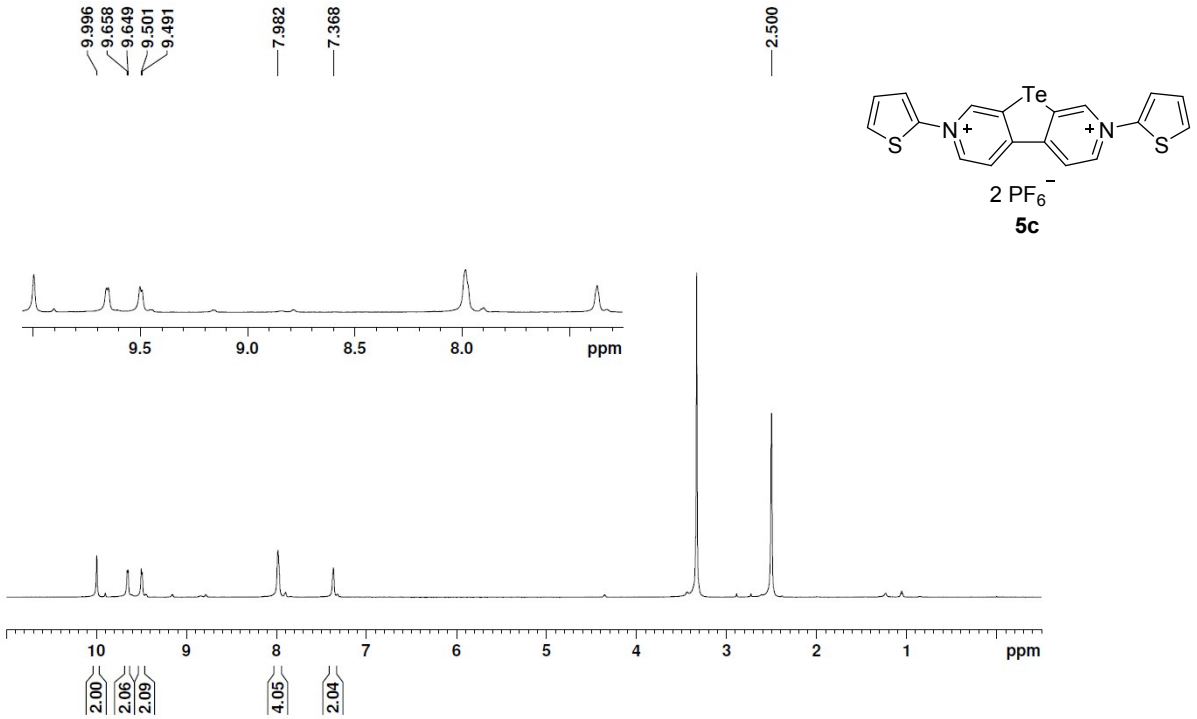
^{19}F NMR (DMSO-d_6, 564 MHz) spectrum of **5b**



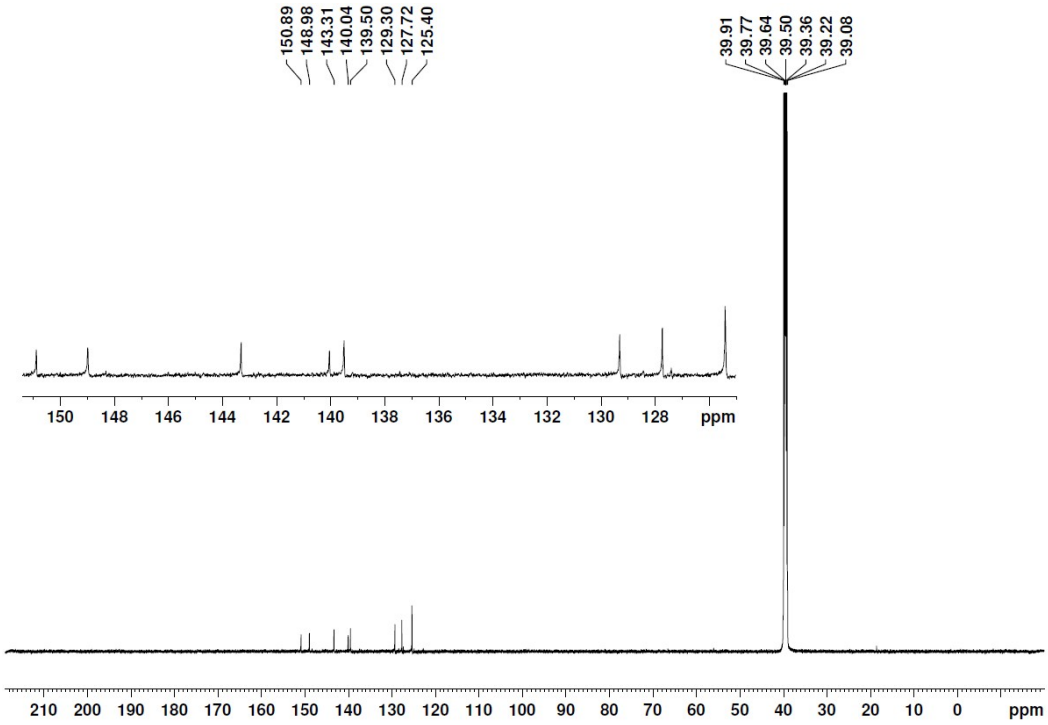
^{31}P NMR (DMSO-d_6, 243 MHz) spectrum of **5b**



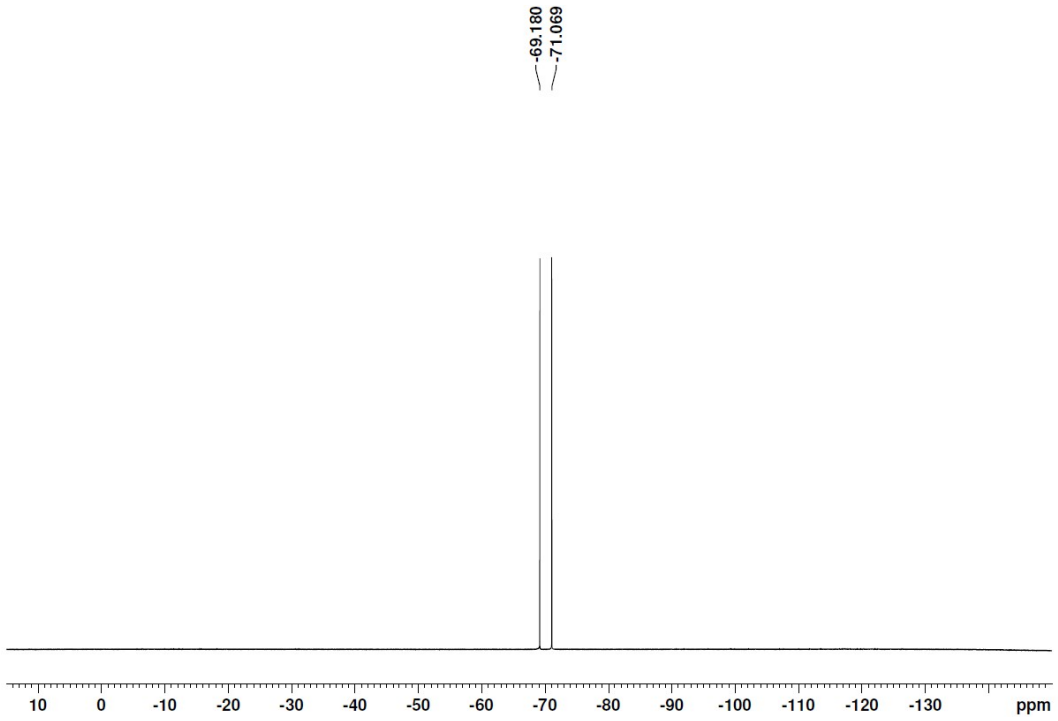
^{1}H NMR (DMSO-d_6, 600 MHz) spectrum of **5c**



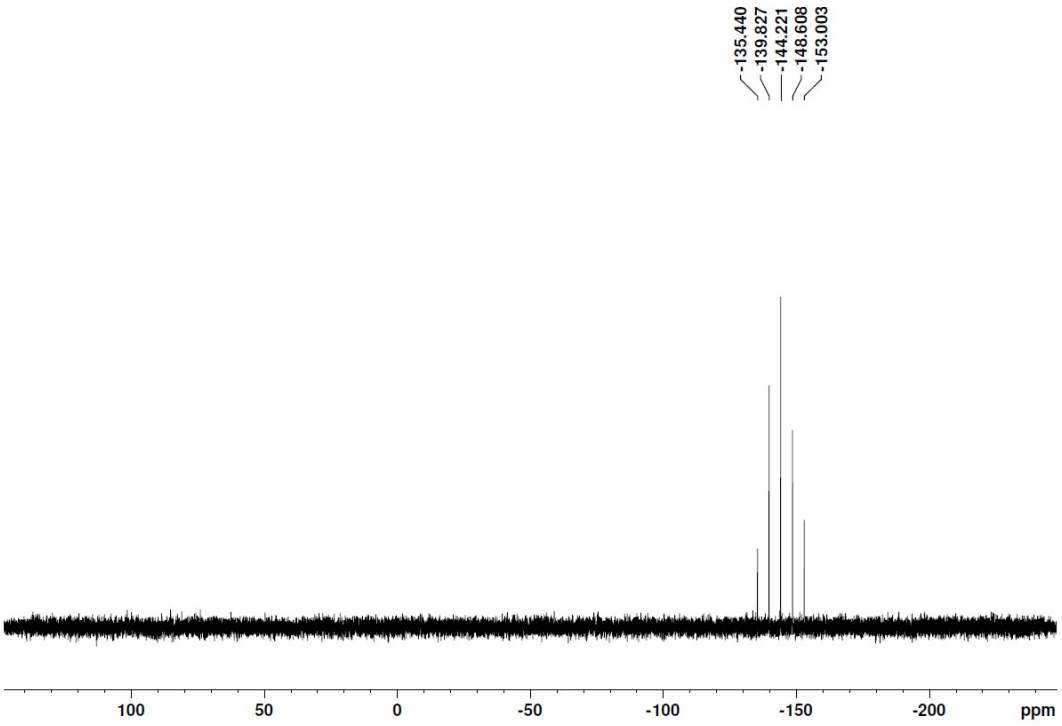
^{13}C NMR (DMSO-d_6, 150 MHz) spectrum of **5c**



^{19}F NMR (DMSO-d_6, 564 MHz) spectrum of **5c**



^{31}P NMR (DMSO-d_6, 243 MHz) spectrum of **5c**



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