Electronic Supplementary Information
Anion Recognition by a Bidentate Chalcogen Bond Donor

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Contents

1.0 Synthetic Procedures

1.1 General Considerations

Commercial reagents were purchased from Sigma Aldrich and were used as received with the following exceptions: Acetonitrile, THF, dimethylformamide, and dichloromethane were purified by passing them through columns of activated alumina under argon (Innovative Technology, Inc). CHROMA SOLV PLUS Acetone was purchased from Sigma Aldrich and used without further purification. Copper iodide, N-iodosuccinimide, and TMS-acetylene were purchased from Alfa Aesar and used without further purification. Potassium carbonate and methanol were purchased from Fisher Scientific and used without further purification. Dichloromethane and hexanes used for work up were purchased from Caledon. $CDCl_3$ was purchased from Cambridge Isotope Laboratories and stored over molecular sieves. Deuterated THF-d_8 was purchased from Sigma Aldrich and was used as received. Unless otherwise noted, all manipulations involving air- or water-sensitive reagents were performed under a dry argon atmosphere using standard Schlenk techniques or under dry nitrogen in a glovebox. Stainless steel needles and gas-tight syringes were used to transfer air and moisture-sensitive liquids.

1.2 Instrumentation

^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra for donor characterization were recorded in $CDCl_3$ either on an Agilent DD2 500 spectrometer equipped with a 5 mm Xsens Cold Probe at 500 and 150.7 MHz or on a Varian 300 or 400 MHz spectrometer as indicated.^{1}H and ^{19}F spectra obtained for NMR titrations were performed on an Agilent DD2 600 spectrometer equipped with a 5 mm OneNMR H/F[X] probe at 600 MHz. Spectral features are tabulated in the following order: chemical shift (δ, ppm); multiplicity (s-singlet, d-doublet, t-triplet, q-quartet, m-complex multiplet); number of protons; coupling constant (J, Hz); assignment. Chemical shifts for ^{1}H are referenced to the residual solvent peaks of δ 7.26 for $CDCl_3$, and δ 1.73 for THF. Chemical shifts for ^{13}C spectra are reported in δ downfield from tetramethylsilane and are referenced to the carbon resonance of $CDCl_3$ (δ 77.16). Absorption spectra were recorded on a Varian Cary 5000 UV-Vis-NIR spectrophotometer at 25 °C. High-resolution mass spectra (HRMS) were obtained on a JEOL AccuTOF JMS-T1000LC equipped with a Direct Analysis in Real Time (DART) ion source.

1.3 Donor Preparation

1.3.1 Previously Reported Compounds

Tellurophene,[1] 2-(tributylstannyl)tellurophene,[2] 2,5-bis(4-cyanophenyl)tellurophene (**1a**), 2,5-bis[(4-trifluoromethyl)phenyl]tellurophene (**1b**), 2-(4-nitrophenyl)-5-(4-(N,N'-dibutylamino)phenyl)tellurophene (**1c**), and 2,5-bis(perfluorophenyl)tellurophene (**1d**) were prepared according to literature procedures.[3]

1.3.2 Bidentate Donor Preparation

1.3.2.1 2-(perfluorophenyl)tellurophene (3)

A 3-neck round-bottom flask was charged with $Pd(PPh_3)_4$ (277 mg, 6.39 mmol), copper iodide (91 mg, 0.48 mmol), and cesium fluoride (1.46 g, 9.63 mmol), equipped with a condenser and subjected to 3 pump/purge cycles with argon. In a separate flask, 2-(tributylstannyl)tellurophene (2.50 g, 5.33 mmol) was dissolved in 15 mL dry DMF, and degassed by purging with argon. The tellurophene solution was added to the reaction flask with stirring. Degassed pentafluoroiodobenzene was added and the reaction mixture was heated at 60 °C for 23 h. After cooling to room temperature, water was added and the mixture was extracted 3 times with DCM. The combined organic layers were washed twice with water and twice with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation, and the crude brown oil was purified by flash chromatography on silica gel (hexanes) to give 750 mg (41% yield) of off-white solid containing ~4% of 2,5-bis(perfluorophenyl)tellurophene impurity.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.26 (td, $^{2}J_{Te,H}$ = 50.0 Hz, $^{3}J_{H,H}$ = 7.2 Hz, 1 H), 8.20 (d, *J* = 4 Hz, 1H), 7.90-7.93 (m, 1H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3 (dm, $^{1}J_{C,F}$ = 247.5 Hz), 140.4 (td, *J* = 6.3, 2.5 Hz), 139.5 (dm, $^{1}J_{C,F}$ = 252.5 Hz), 138.1 (dm, $^{1}J_{C,F}$ = 251.3 Hz), 137.7, 131.8 (t, *J* = 6.3 Hz), 125.2 (m), 115.6 (td, *J* = 13.8, 5.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -140.4 (dd, *J* = 15.4, 6.4 Hz), -156.7 (t, *J* = 21.4 Hz), -162.4 (m).
DART-TOF HRMS calcd for $C_{10}H_4F_5Te$ $[M+H]^+$. Expected: 348.92954. Found: 348.92868. Δ = -2.47 ppm.

1.3.2.2 2-iodo-5-(perfluorophenyl)tellurophene (4)

A Schlenk flask was loaded with **3** (716 mg, 2.07 mmol) and NIS (466 mg, 2.07 mmol). The flask was degassed by three pump/purge cycles. 7.5 mL of dry, degassed DMF was added to the reaction flask and the mixture was stirred at 40 °C for 24 h. After cooling to room temperature, the reaction was quenched by adding water and aqueous sodium thiosulfate. The mixture was extracted 3 times with diethyl ether, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation and the crude mixture was purified by flash chromatography on silica gel (hexanes) to give 290 mg (30% yield) of white solid product, and 225 mg of recovered starting material.
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (m, 1H), 7.70 (d, *J* = 5.0 Hz, 1H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 143.4 (dm, $^{1}J_{C,F}$ = 247.5 Hz), 140.7 (td, *J* = 6.3, 1.3 Hz), 139.7 (dm, $^{1}J_{C,F}$ = 255.0 Hz), 138.1 1 (dm, $^{1}J_{C,F}$ = 252.5 Hz), 131.5 (m), 115.0 (td, *J* = 13.8, 5.0 Hz), 74.9 (td, *J* = 8.8, 1.3 Hz).
^{19}F NMR (282 MHz, $CDCl_3$) δ -140.7 (d, *J* = 16.0 Hz), -155.8 (t, *J* = 20.9 Hz), -161.9 (m).
ESI-TOF HRMS calcd for $C_{10}H_2F_5ITe$ $[M]^+$. Expected: 473.8184. Found: 473.8174. Δ = -2.1 ppm.

1.3.2.3 2-[(trimethylsilyl)ethynyl]-5-(perfluorophenyl)tellurophene (5)

$Pd(PPh_3)_2Cl_2$ (11mg, 0.016 mmol), copper iodide (12 mg, 0.064 mmol), and **4** (150 mg, 0.32 mmol) were added to a Schlenk flask and degassed by three pump/purge cycles. A dry, degassed solution of trimethylsilylacetylene (0.14 mL, 0.95 mmol) in DMF (3 mL) and Et_3N (0.6 mL) were added and the reaction mixture was stirred at 50 °C for 20 h. After cooling to room temperature, water was added and the mixture was extracted 3 times with DCM. The combined organic phase was dried over $MgSO_4$ and filtered, and the solvent was removed by rotary evaporation. The brown solid was purified by flash chromatography on silica gel (hexanes) to give 78 mg of white solid (56% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 4.8 Hz, 1H), 7.88, (m, 1H), 0.25 (s, 9H). [1]
^{3}C NMR (125 MHz, $CDCl_3$) δ 143.5 (dm, $^{1}J_{C,F}$ = 246.3 Hz), 142.9, 139.6 (dm, $^{1}J_{C,F}$ = 255.0 Hz), 139.5 (td, *J* = 6.3, 1.3 Hz), 138.2, (dm, $^{1}J_{C,F}$ = 252.5 Hz), 128.4 (td, *J* = 8.8,1.3 Hz), 127.6 (m), 115.2 (td, *J* = 13.8, 5.0 Hz), 105.7, 103.3.
^{19}F NMR (376 MHz, $CDCl_3$) δ -140.2 (dd, *J* = 15.0, 6.4 Hz), -155.9 (t, *J* = 20.1 Hz), -162.0 (m).
DART-TOF HRMS calcd for $C_{15}H_{12}F_5SiTe$ $(M+H)^+$. Expected: 444.96907. Found: 444.96816. Δ = -2.03 ppm.

1.3.2.4 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)

K_2CO_3 (27 mg, 0.20 mmol) was added to a degassed solution of **5** (78 mg, 0.18 mmol) in 3:1 THF/MeOH (1 mL) and stirred at room temperature for 1 h. The solvent was removed by rotary evaporation and the residue was dissolved in hexane and passed through a plug of silica. The solvent was removed and the crude product was used in the next step. $Pd(PPh_3)_2Cl_2$ (6 mg, 0.009 mmol), copper iodide (7 mg, 0.035 mmol), and **4** (84 mg, 0.18 mmol) were added to a Schlenk flask and degassed by three pump/purge cycles. The deprotected crude product was dissolved in a dry, degassed mixture of DMF (2 mL) and Et_3N (0.4 mL) and added to the reaction flask. The reaction was heated at 50 °C for 20 h and then cooled to room temperature. A shiny off-white precipitate was observed. Water was added and the mixture was extracted 3 times with DCM. The combined organic phase was washed twice with brine, dried over $MgSO_4$ and filtered. The solvent was removed by rotary evaporation. 3 compounds

were observed by TLC and the product was isolated as a yellow solid by flash chromatography on silica gel (19 mg, 15% yield).
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18 (d, *J* = 4.5 Hz, 2H), 7.90, (m, 2H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 143.5 (dm, $^{1}J_{C,F}$ = 245.0 Hz), 141.9, 139.8 (t, *J* = 6.3 Hz), 139.7 (dm, $^{1}J_{C,F}$ = 253.8 Hz), 138.2, (dm, $^{1}J_{C,F}$ = 247.5 Hz), 128.5, 127.7 (t, *J* = 8.8 Hz), 115.1 (td, *J* = 13.8, 3.8 Hz), 98.9.
^{19}F NMR (282 MHz, $CDCl_3$) δ -140.1 (d, *J* = 15.5 Hz), -155.7 (t, *J* = 20.9 Hz), -161.9 (m).
DART-TOF HRMS calcd for $C_{22}H_5F_{10}Te_2$ $(M+H)^+$. Expected: 718.83560. Found: 718.83698. Δ = 1.92 ppm.

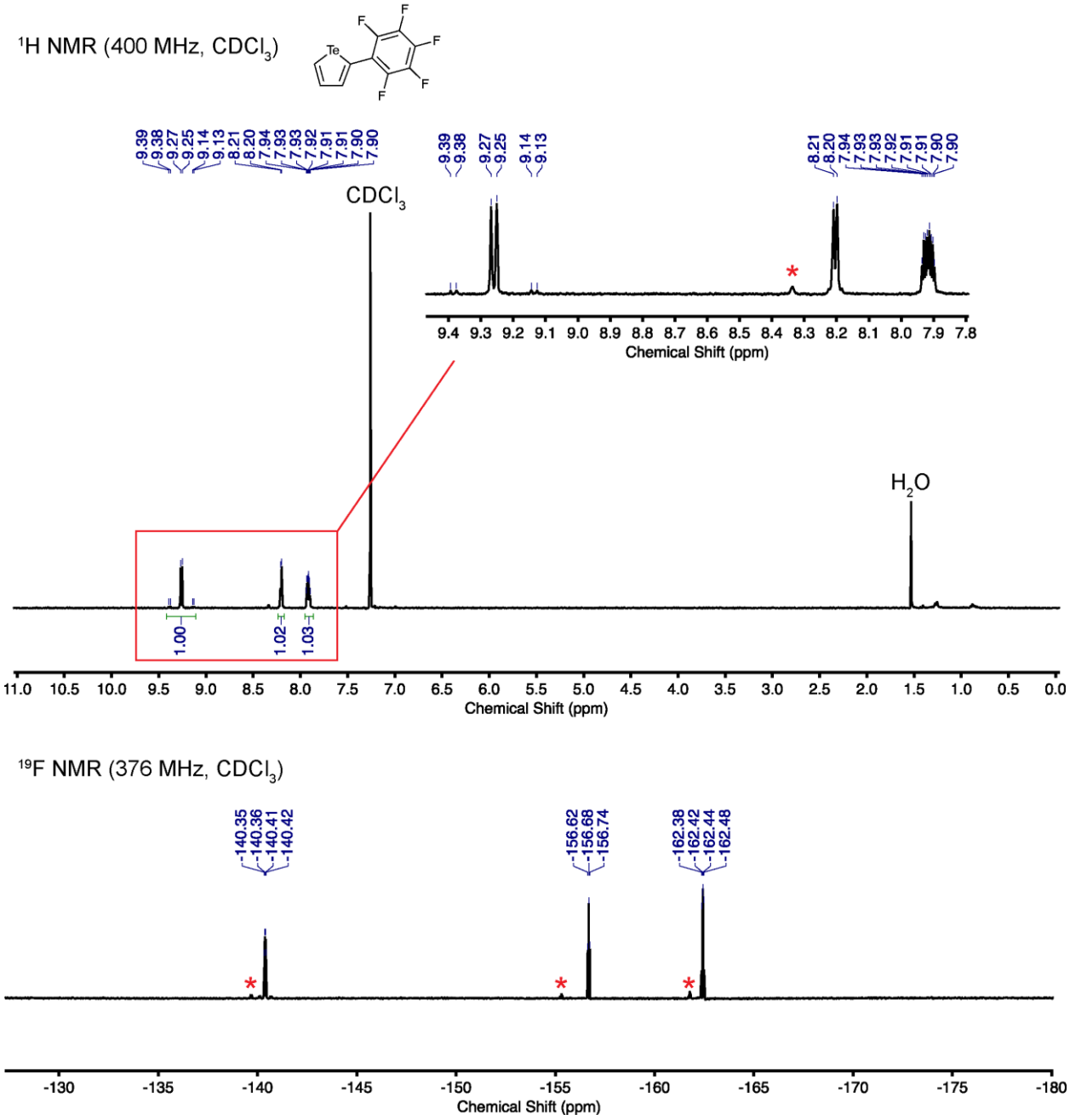
1.3.2.4 2,5-Bis(pentafluorophenyl)thiophene

2,5-Bis(pentafluorophenyl)thiophene was prepared according to a previously reported literature procedure[4] from the 2,5-dibromothiophene and perfluorophenyl boronic acid. This is a known compound.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (m, 2H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 130.37, 129.34, and multiplets in the aromatic region.
^{19}F NMR (564 MHz, $CDCl_3$) δ -139.22 (dd, *J* = 22.1, 7.2 Hz), -154.37 (t, *J* = 21.1 Hz), -161.47 (td, *J* = 21.5, 7.0 Hz).

1.3.3 NMR spectra

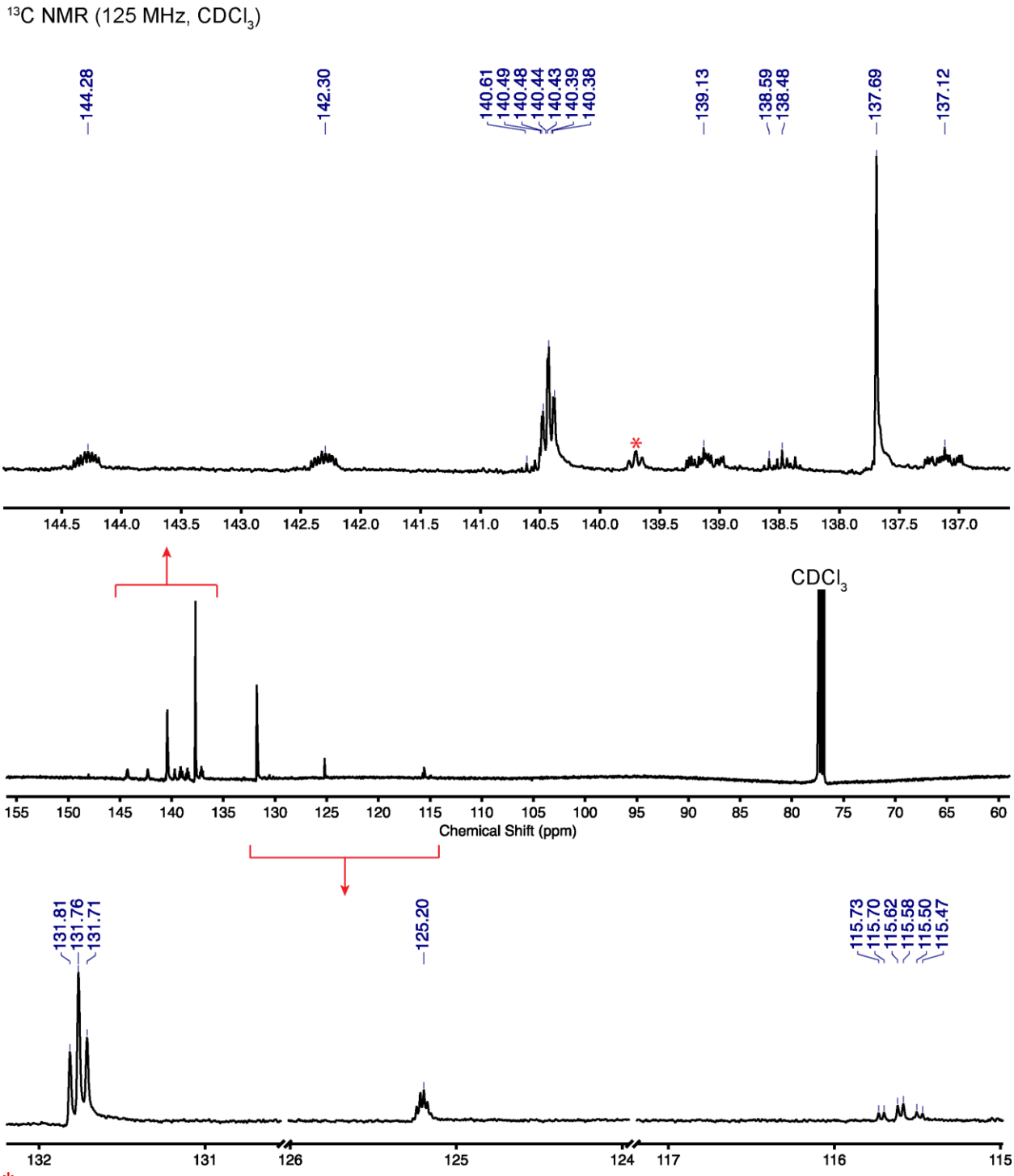
1.3.3.1 2-(perfluorophenyl)tellurophene (3)

Figure S 1: ^{1}H NMR spectrum of **3** at 400 MHz and ^{19}F NMR spectrum at 376 MHz taken in $CDCl_3$.



* denotes 2,5-bis(perfluorophenyl)tellurophene impurity.

Figure S 2: ^{13}C NMR spectrum of **3** taken in $CDCl_3$ at 125 MHz.



* denotes 2,5-bis(perfluorophenyl)tellurophene impurity.

1.3.3.2 2-iodo-5-(perfluorophenyl)tellurophene (4)

Figure S 3: ^{1}H NMR spectrum of **4** at 500 MHz and ^{19}F NMR spectrum at 282 MHz taken in $CDCl_3$.

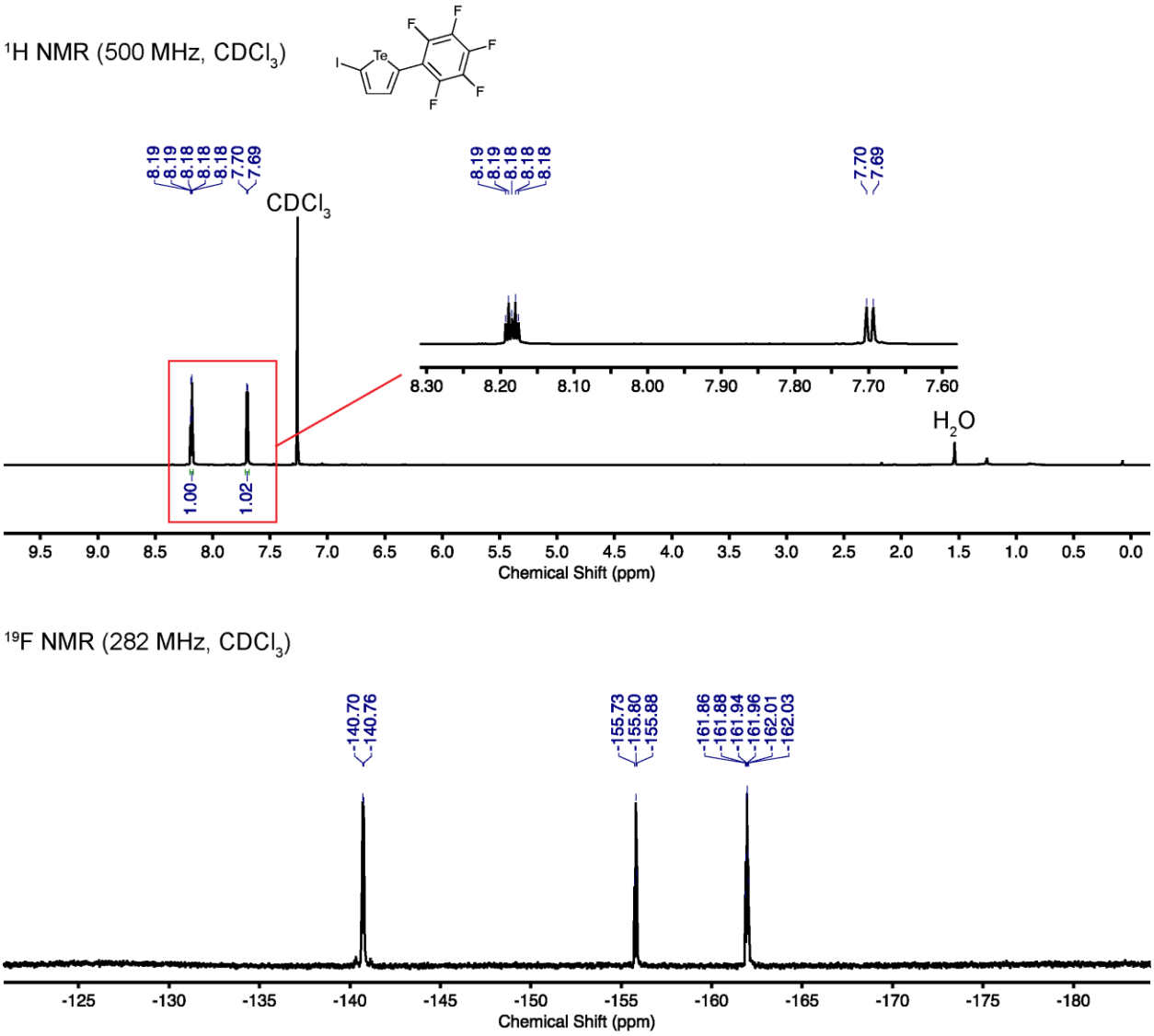
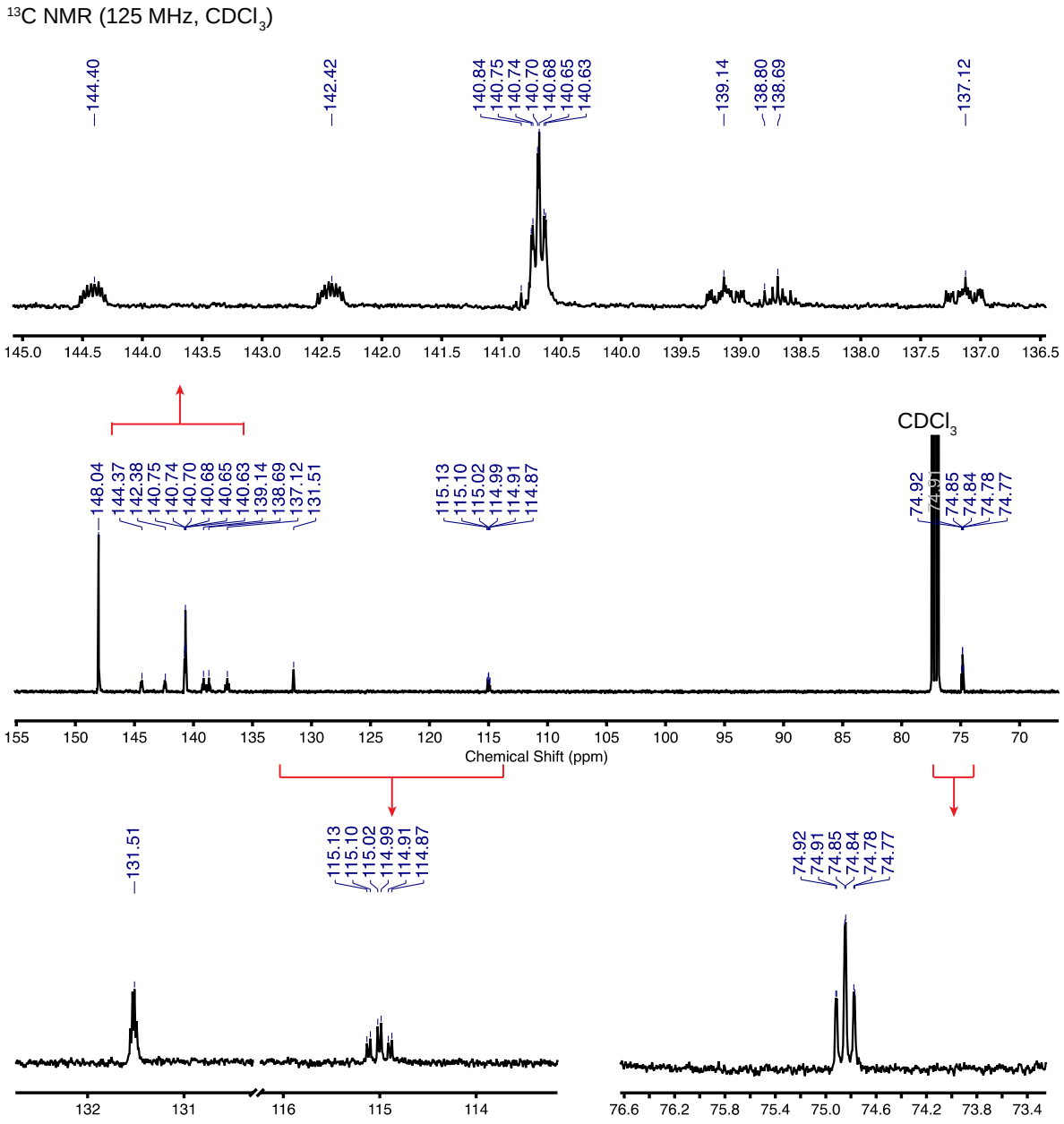
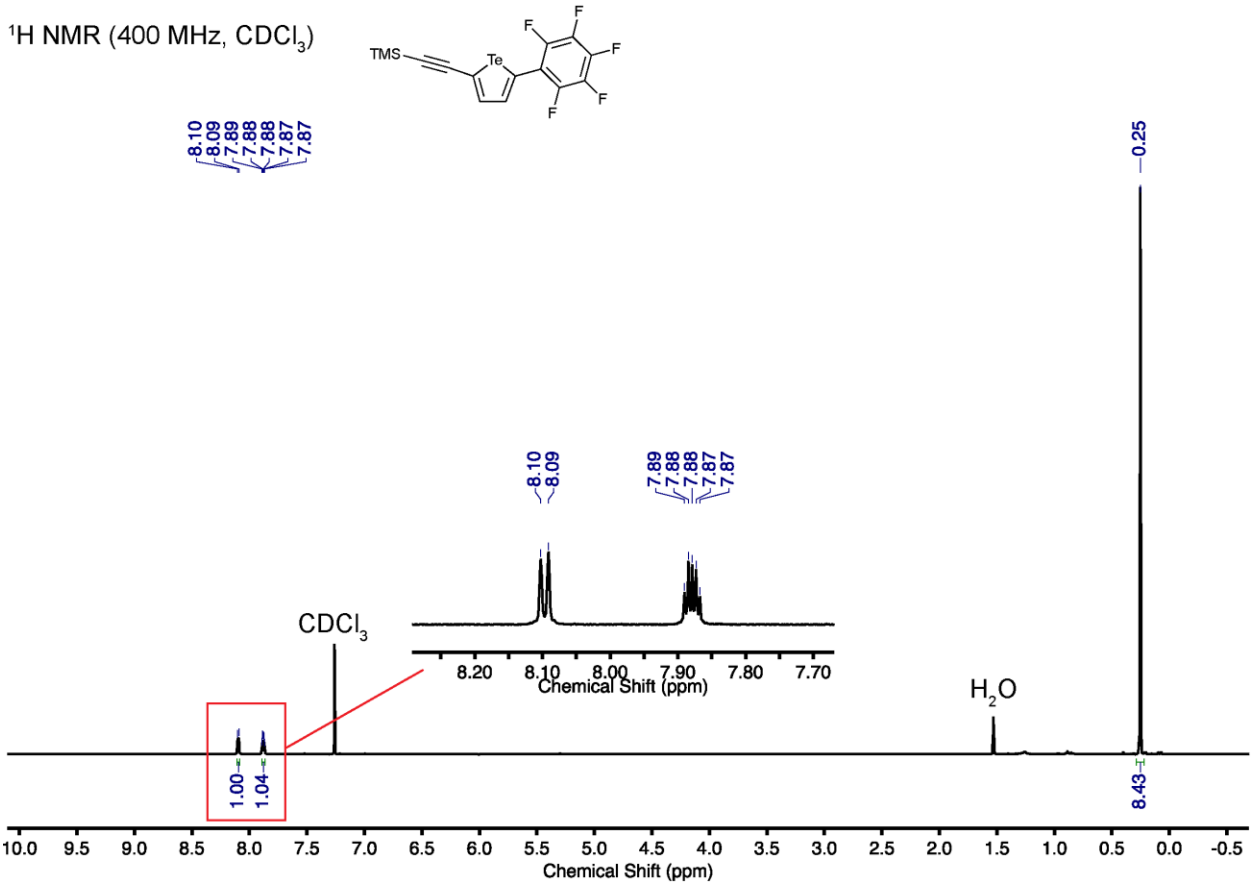


Figure S 4: ^{13}C NMR spectrum of **4** taken in $CDCl_3$ at 125 MHz.



1.3.3.3 2-[(trimethylsilyl)ethynyl]-5-(perfluorophenyl)tellurophene (5)

Figure S 5: ^{1}H NMR spectrum of **5** at 400 MHz and ^{19}F NMR spectrum at 376 MHz taken in $CDCl_3$.



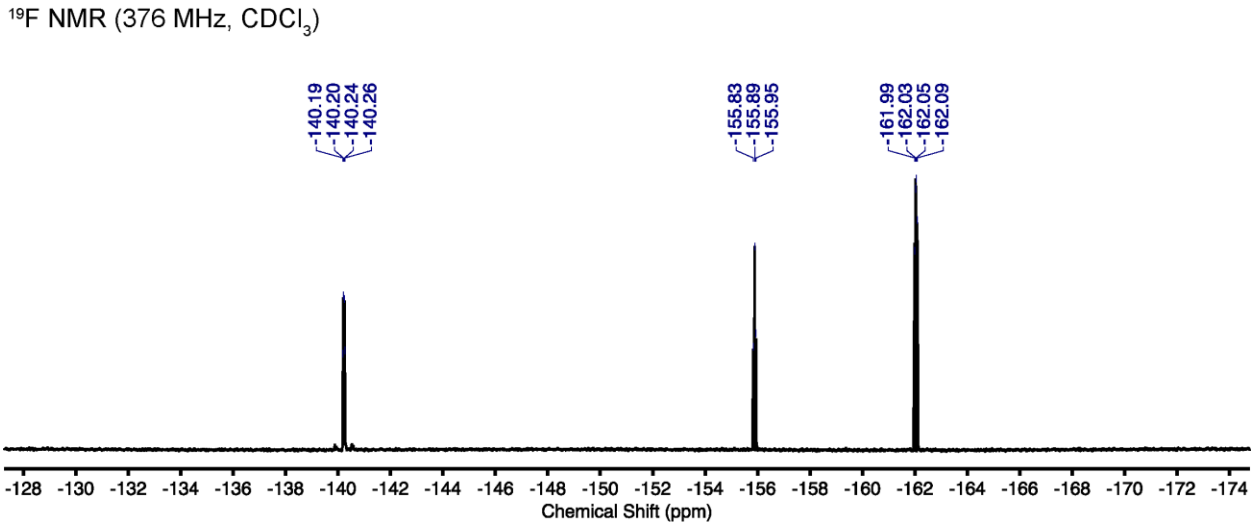
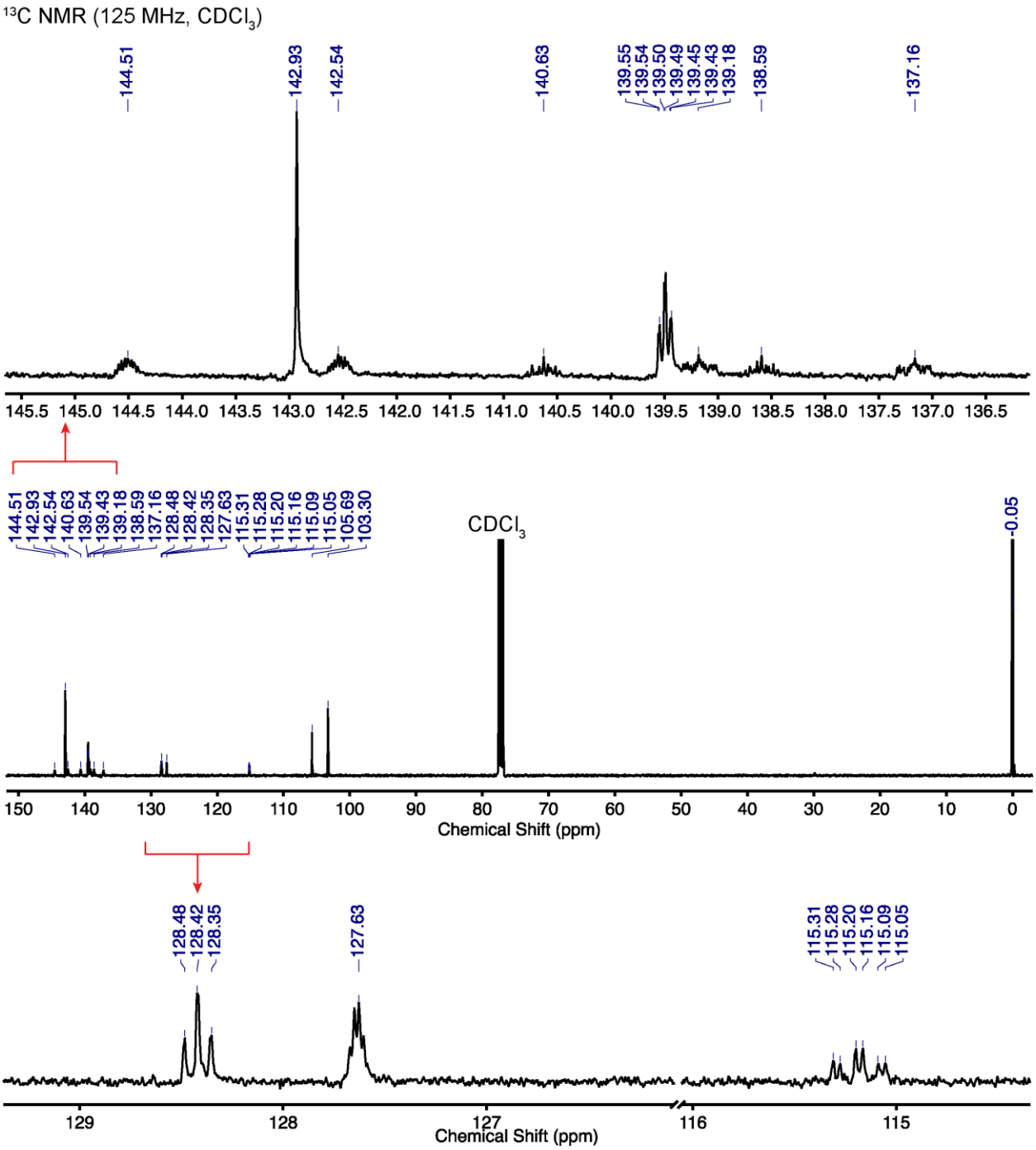
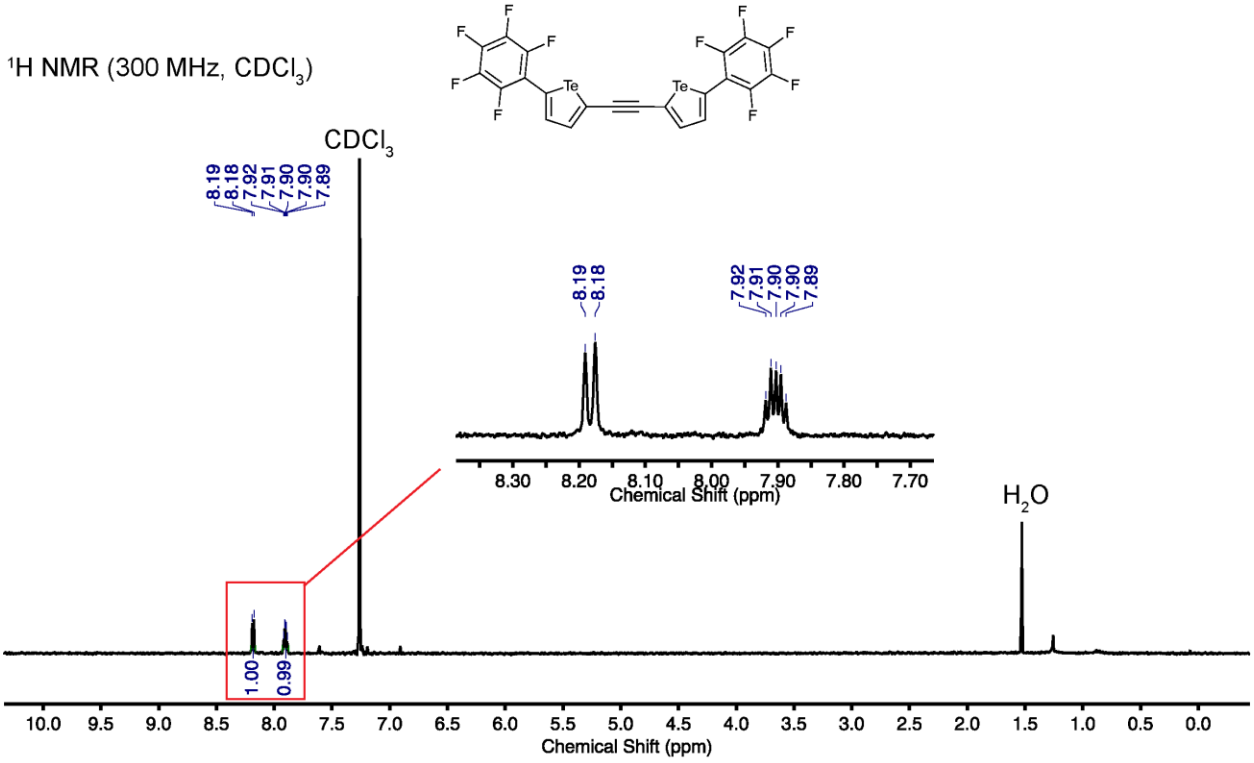


Figure S 6: ^{13}C NMR spectrum of **5** taken in $CDCl_3$ at 125 MHz.



1.3.3.4 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)

Figure S 7: ^{1}H NMR spectrum of **3** at 300 MHz and ^{19}F NMR spectrum at 282 MHz taken in $CDCl_3$.



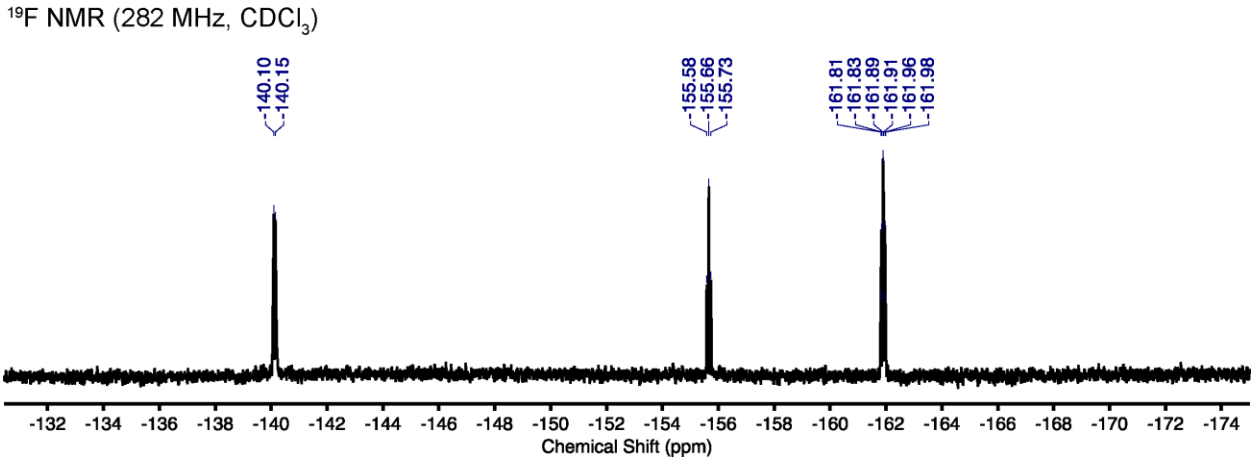


Figure S 8: ^{1}H NMR spectrum of **2** at 600 MHz taken in THF-d_8.

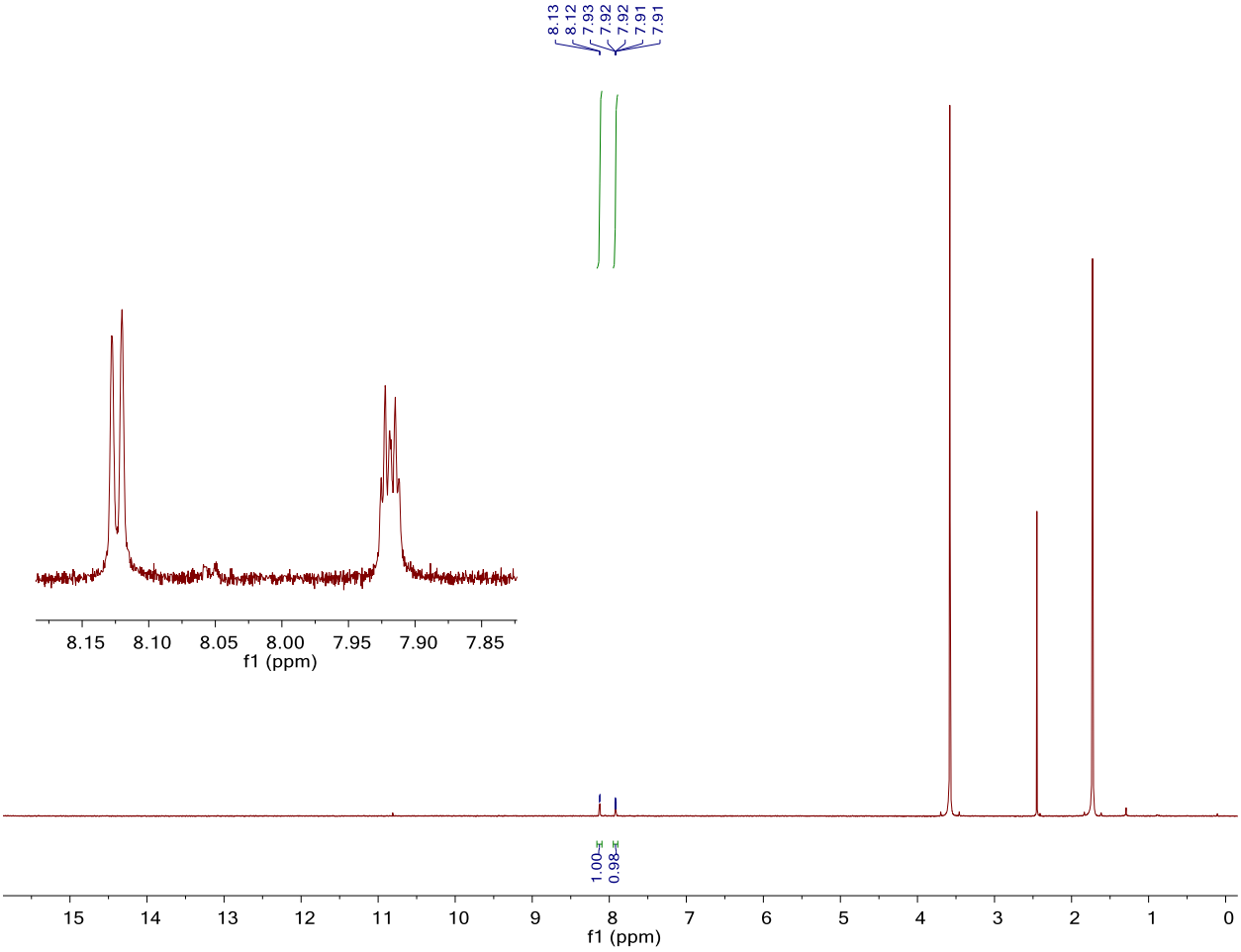


Figure S 9: ^{19}F NMR spectrum of **2** at 564 MHz taken in THF-d_8.

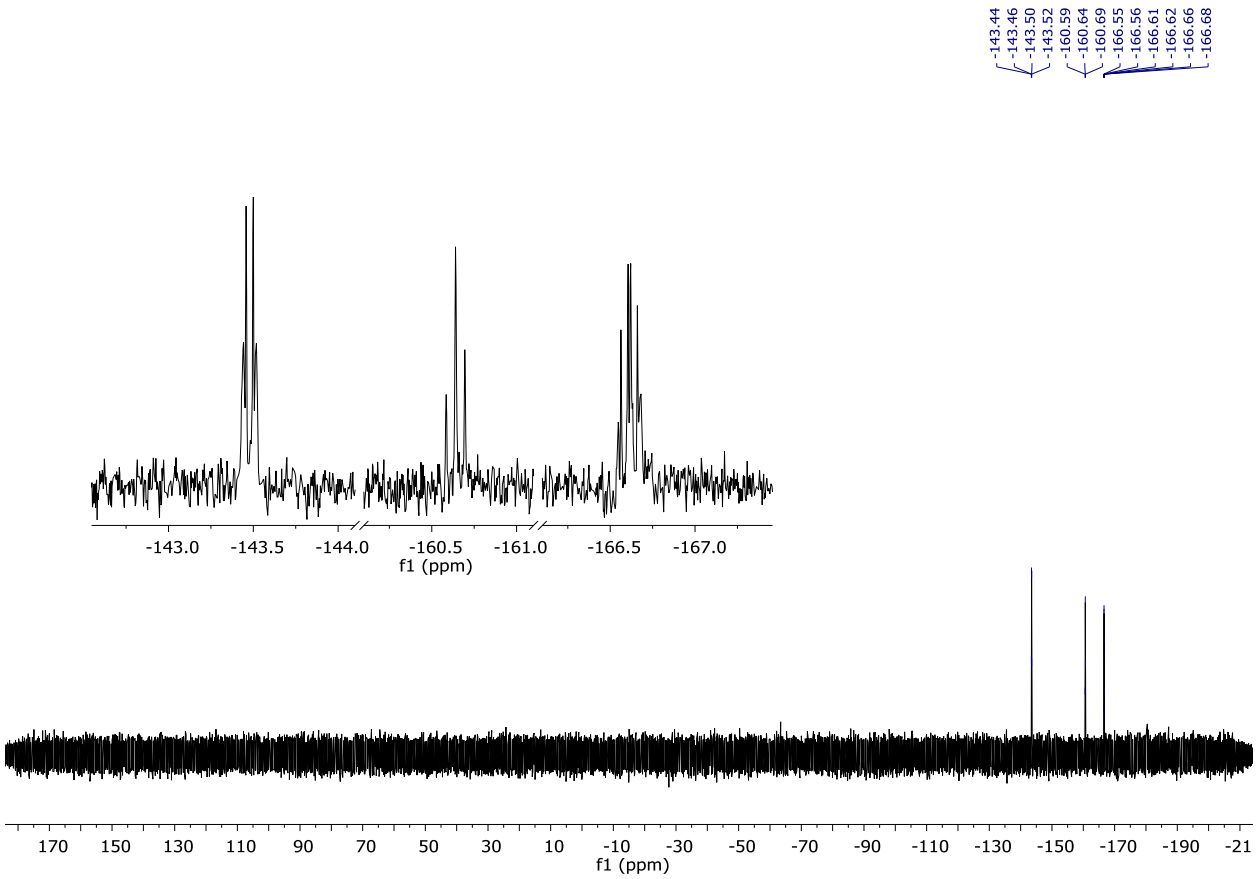
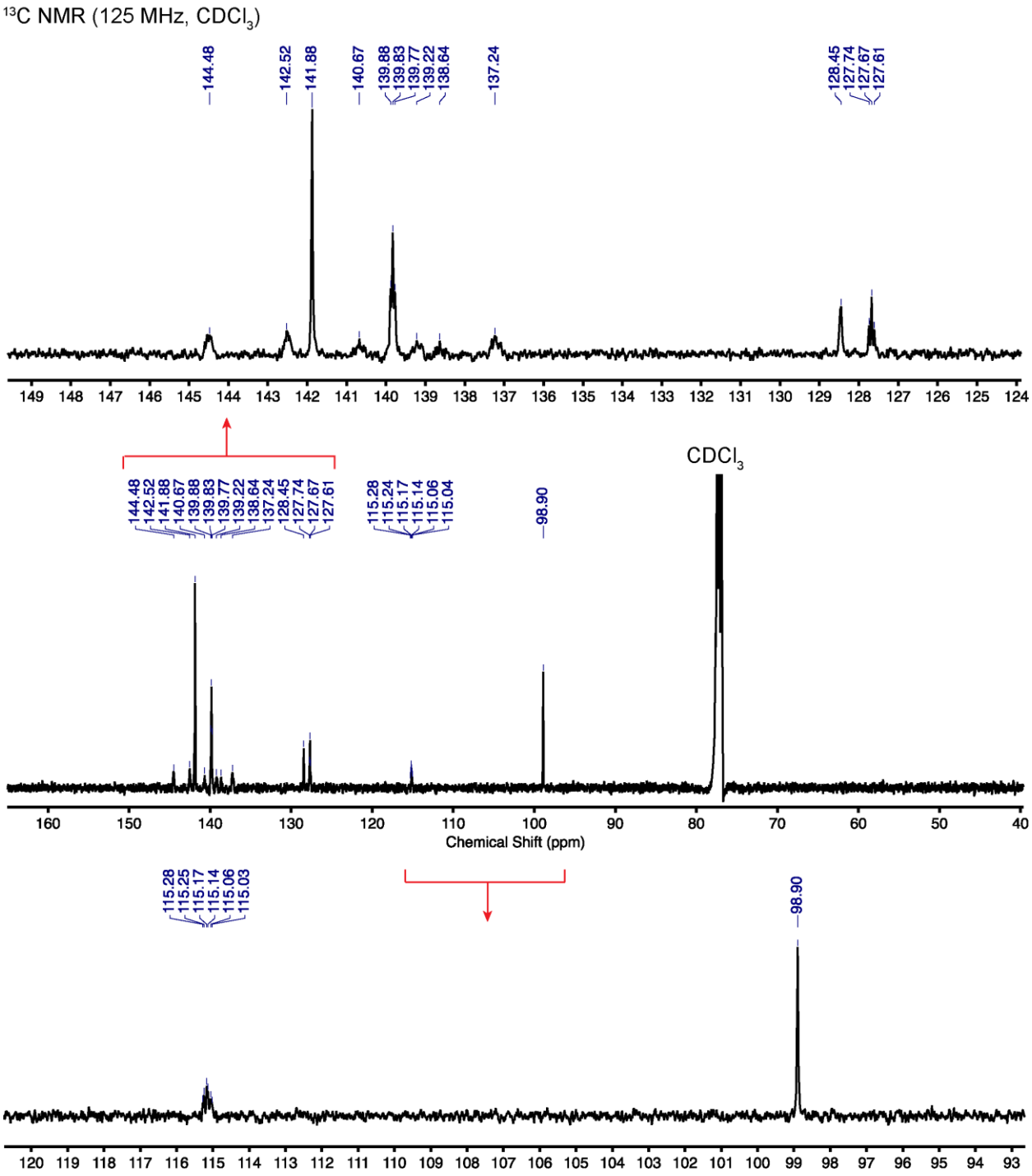


Figure S 10: ^{13}C NMR spectrum of **2** taken in $CDCl_3$ at 125 MHz.



2.0 Association Constants

2.1 Methodology

A solution of chalcogen bond donor was prepared. In order to keep the concentration of the donor constant throughout the titration, the donor solution was then used to prepare the acceptor solution. UV-vis titrations were carried out *via* serial dilution of the acceptor by adding aliquots of the acceptor solution to a known volume of donor solution. NMR titrations were set up in an identical manner. The concentrations of the solutions used in the experiments were chosen such that the complexation ratio (β = [donor]/[acceptor]) would be between 0.2 and 0.8.[5] Taken at the wavelength or peak of greatest change, graphs of ΔAbs or Δδ verses acceptor concentration were curve-fitted to a 1:1 binding isotherm[6] in Origin 9.0 SR1. Stoichiometry of binding was determined using the continuous variation method (Job Plot).[5]

Association constants were determined as averages from repeat experiments. The errors are reported as standard deviations.

Estimates for association constants for acceptor donor combinations that could not be measured due to weak binding affinities or solubility issues were determined using a complexation ratio of 0.2, the experimental host concentration, and either the highest obtainable acceptor concentration during a typical experiment or at the highest allowable acceptor concentration of 0.2 M.

2.2 Association Constant Summary

Table S 1: Association constants (M^{-1}) with various acceptors in THF.

Acceptor	1d	2
TBACl	310 ± 20	2290 ± 30
TBACl[a]		1900 ± 100
TBABr	103 ± 5	614 ± 5
$TBANO_3$	< 5	19.6 ± 0.9
TBAOBz	34 ± 3	66.4 ± 0.5
TBAOTs	< 2	< 2

a) Titration carried out at 112.1 μM, ~10x the concentration of typical experiments.

Table S 2: Association constants (M^{-1}) with TBACl in acetonitrile.

Acceptor	1d	2
TBACl	< 3	19.1 ± 0.3

Table S 3: Association constants (M^{-1}) with TBACl in acetone.

Acceptor	1d	2
TBACl	6.2 ± 0.2	111 ± 1

2.3 Associations Constants Determined by UV/Vis spectroscopy

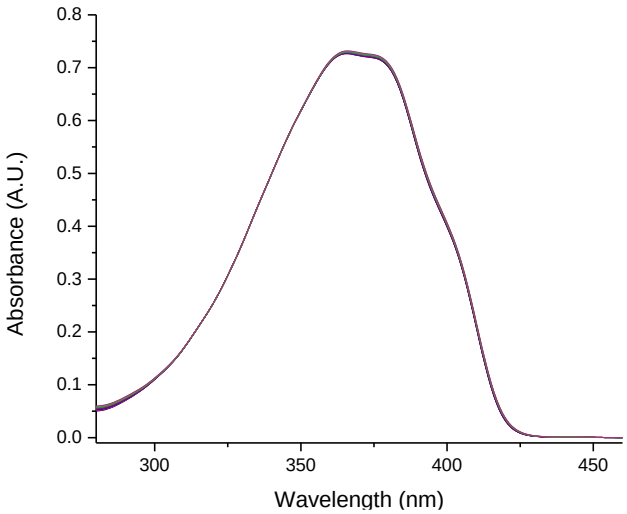
2.3.1 Tetrahydrofuran

2.3.1.1 2,5-bis(4-cyanophenyl)tellurophene (1a)

2.3.1.1.1 TBACl

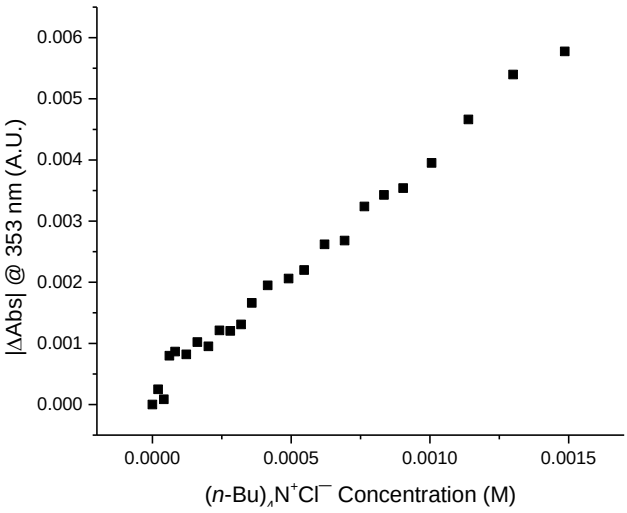
2.3.1.1.1.1 Spectrum

Figure S 11: Spectral change of **1a** upon the addition of TBACl in THF. Titration carried out at 21.0 µM **1a**.



2.3.1.1.1.2 Titrations

Figure S 12: Plot of ΔAbs versus TBACl concentration for the UV/Vis titration of **1a** in THF. Titration carried out at 21.0 µM **1a**.

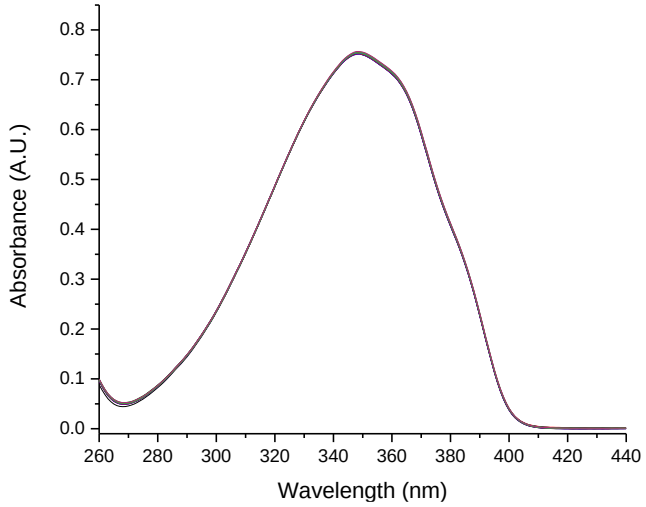


2.3.1.2 2,5-bis[(4-trifluoromethyl)phenyl]tellurophene (1b)

2.3.1.2.1 TBACl

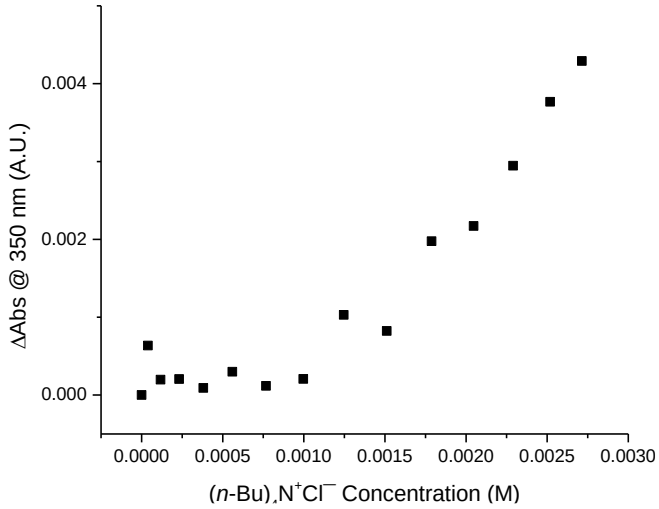
2.3.1.2.1.1 Spectrum

Figure S 13: Spectral change of **1b** upon the addition of TBACl in THF. Titration carried out at 27.4 µM **1b**.



2.3.1.2.1.2 Titrations

Figure S 14: Plot of ΔAbs versus TBACl concentration for the UV/Vis titration of **1b** in THF. Titration carried out at 27.4 µM **1b**.

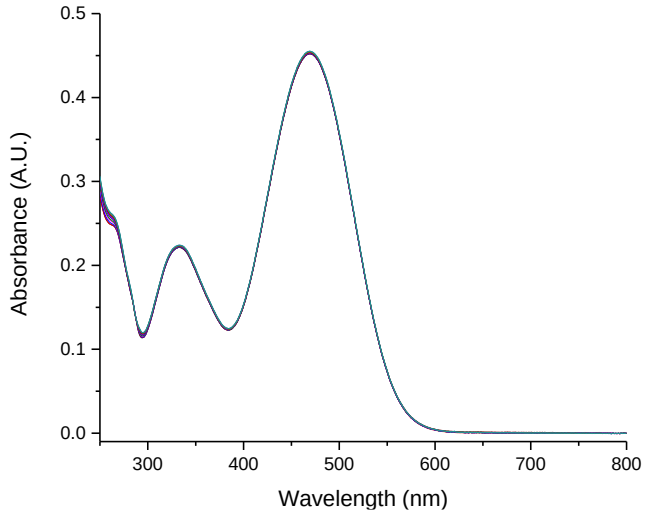


2.3.1.3 2-(4-nitrophenyl)-5-(4-(N,N'-dibutylamino)phenyl)tellurophene (1c)

2.3.1.3.1 TBACl

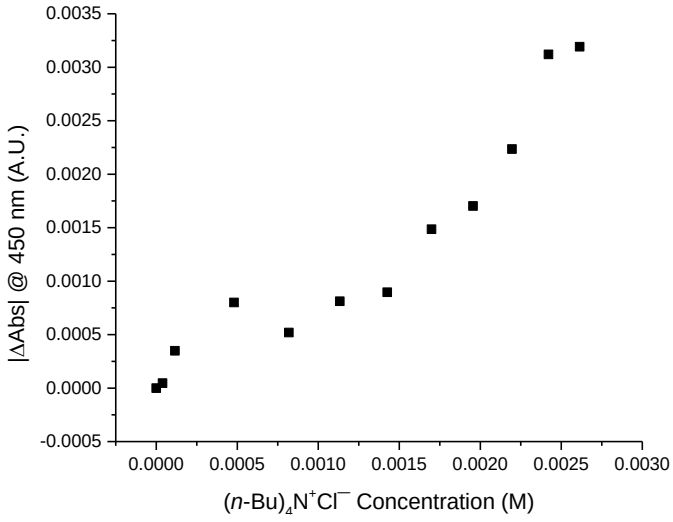
2.3.1.3.1.1 Spectrum

Figure S 15: Spectral change of **1c** upon the addition of TBACl in THF. Titration carried out at 17.9 µM **1c**.



2.3.1.3.1.2 Titrations

Figure S 16: Plot of ΔAbs versus TBACl concentration for the UV/Vis titration of **1c** in THF. Titration carried out at 17.9 µM **1c**.

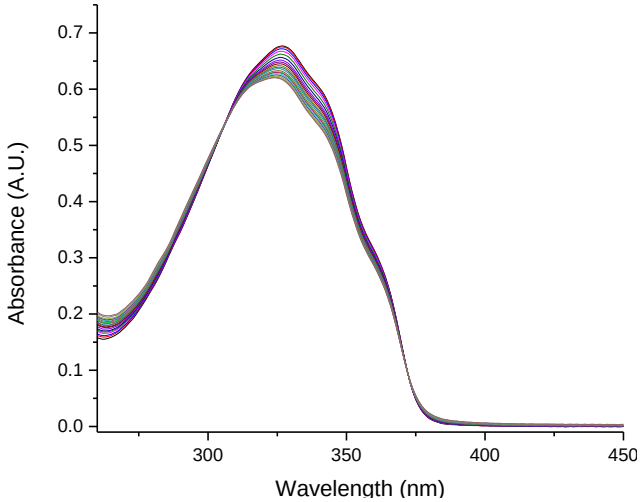


2.3.1.4 2,5-bis(perfluorophenyl)tellurophene (1d)

2.3.1.4.1 TBACl

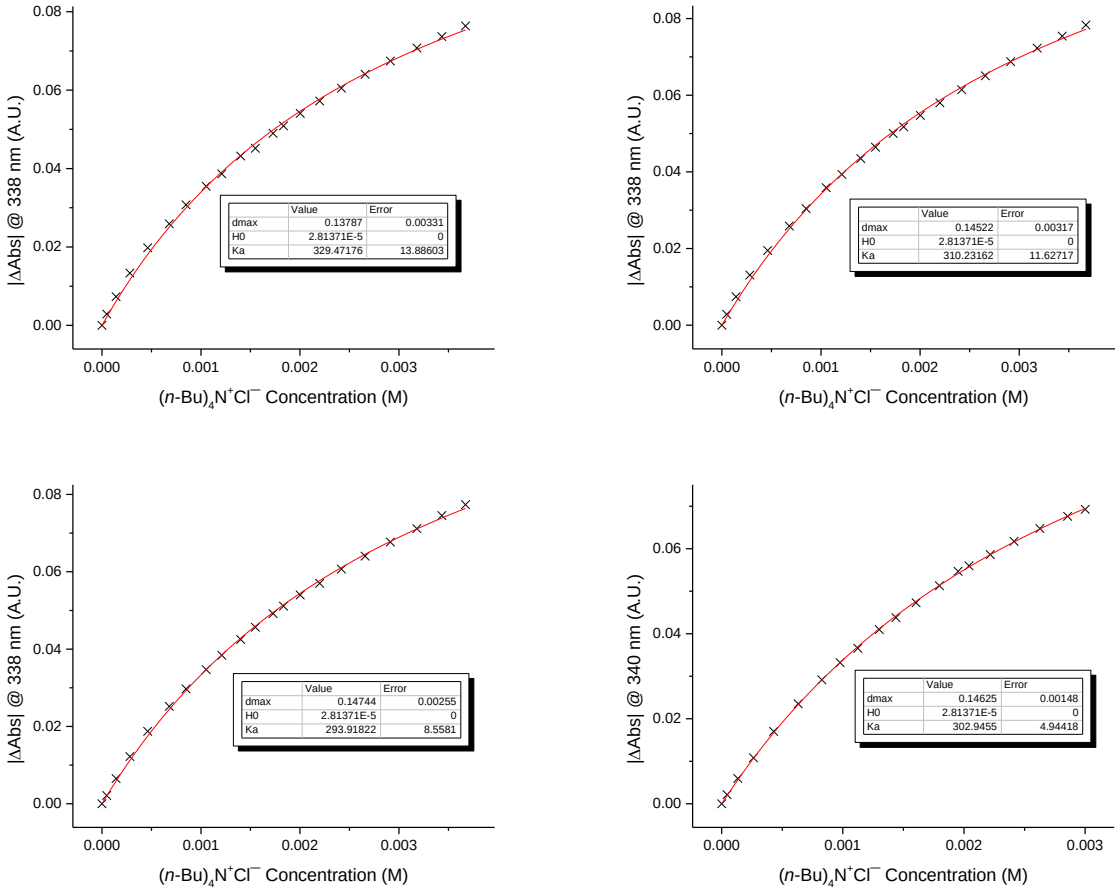
2.3.1.4.1.1 Spectrum

Figure S 17: Spectral change of **1d** upon the addition of TBACl in THF. Titration carried out at 28.1 µM **1d**.



2.3.1.4.1.2 Titrations

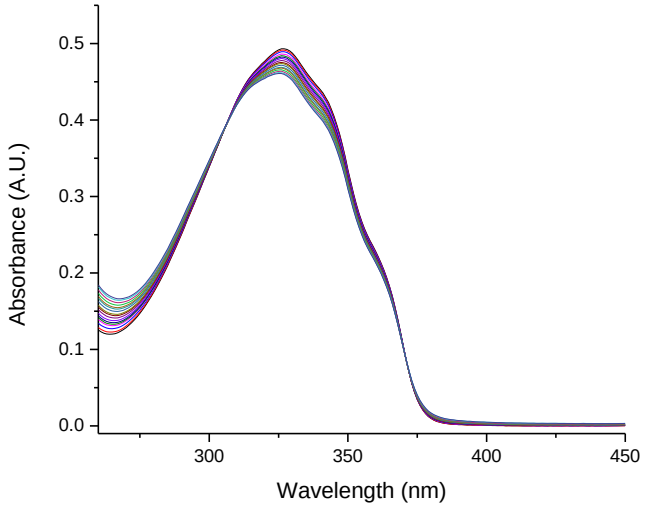
Figure S 18: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **1d** in THF. Titrations carried out at 28.1 µM **1d**. From left to right, K_a = 329 M^{-1}, 310 M^{-1}, 294 M^{-1}, 303 M^{-1}.



2.3.1.4.2 TBABr

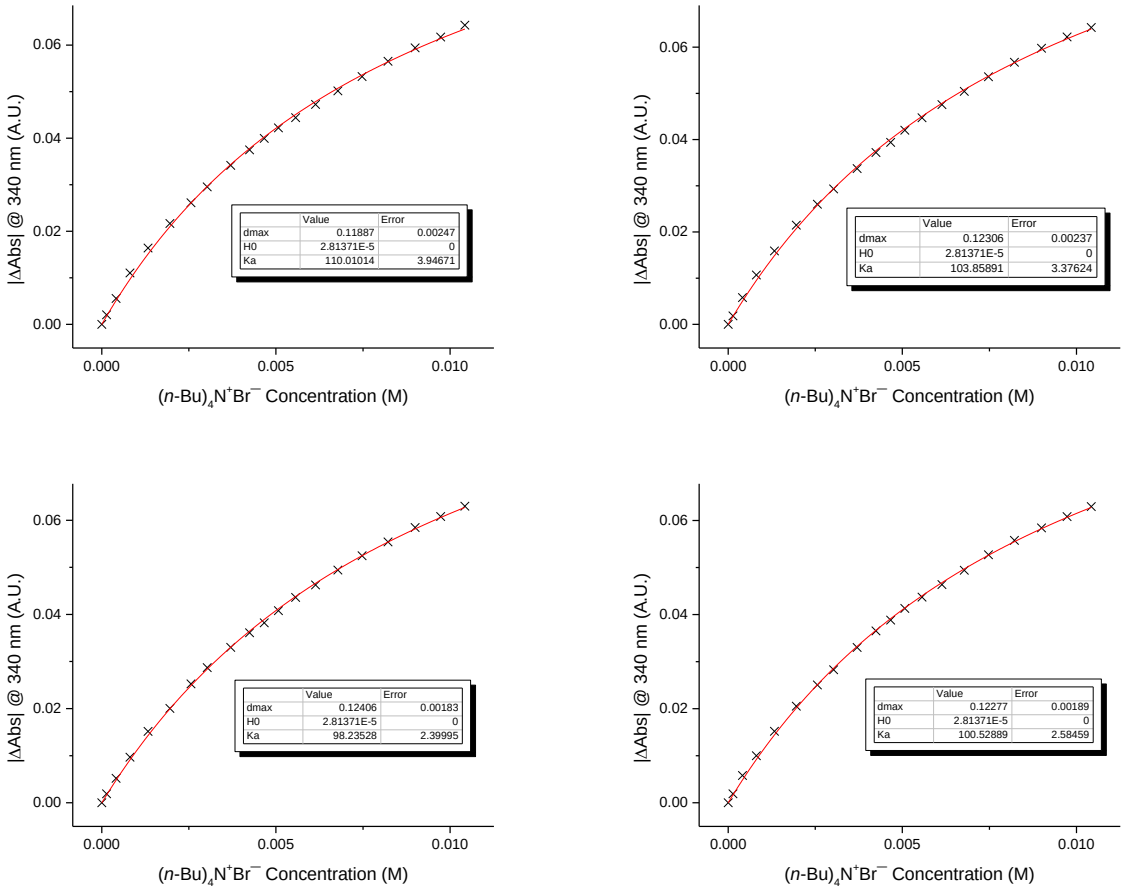
2.3.1.4.2.1 Spectrum

Figure S 19: Spectral change of **1d** upon the addition of TBABr in THF. Titration carried out at 28.1 µM **1d**.



2.3.1.4.2.2 Titrations

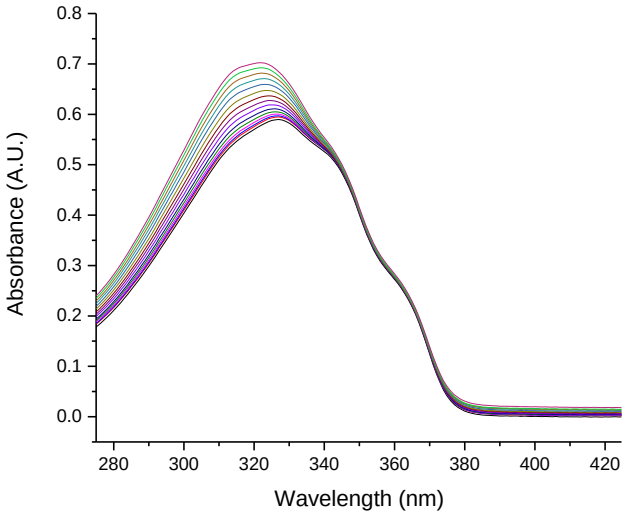
Figure S 20: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **1d** in THF. Titrations carried out at 28.1 µM **1d**. From left to right, K_a = 110 M^{-1}, 104 M^{-1}, 98 M^{-1}, 101 M^{-1}.



2.3.1.4.3 $TBANO_3$

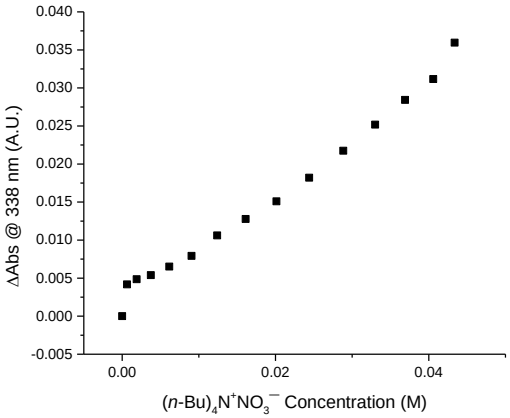
2.3.1.4.3.1 Spectrum

Figure S 21: Spectral change of **1d** upon the addition of $TBANO_3$ in THF. Titration carried out at 28.1 µM **1d**.



2.3.1.4.3.2 Titrations

Figure S 22: Plot of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **1d** in THF. Titration carried out at 28.1 µM **1d**.

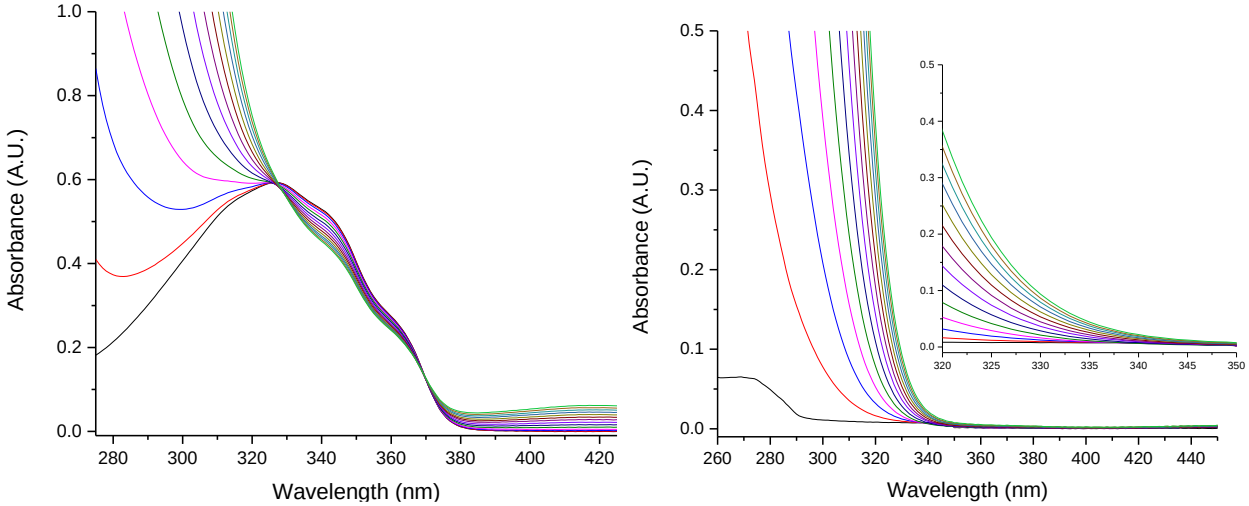


2.3.1.4.4 TBAOBz

Δabs versus [TBAOBz] plots for **1d** were created at 350 nm, but overlapped with the absorbance of the guest. To remedy this, the absorbance changes were corrected for the absorbance of TBAOBz at that concentration of guest.

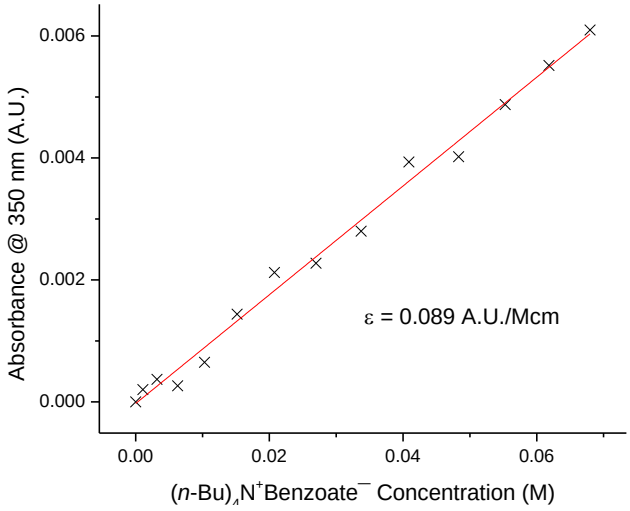
2.3.1.4.4.1 Spectrum

Figure S 23: (left) Representative Spectral change of **1d** upon the addition of TBAOBz in THF. Titration carried out at 17.9 μM **1d**. (right) UV-vis absorbance spectra of THF solutions with different concentrations of TBAOBz.



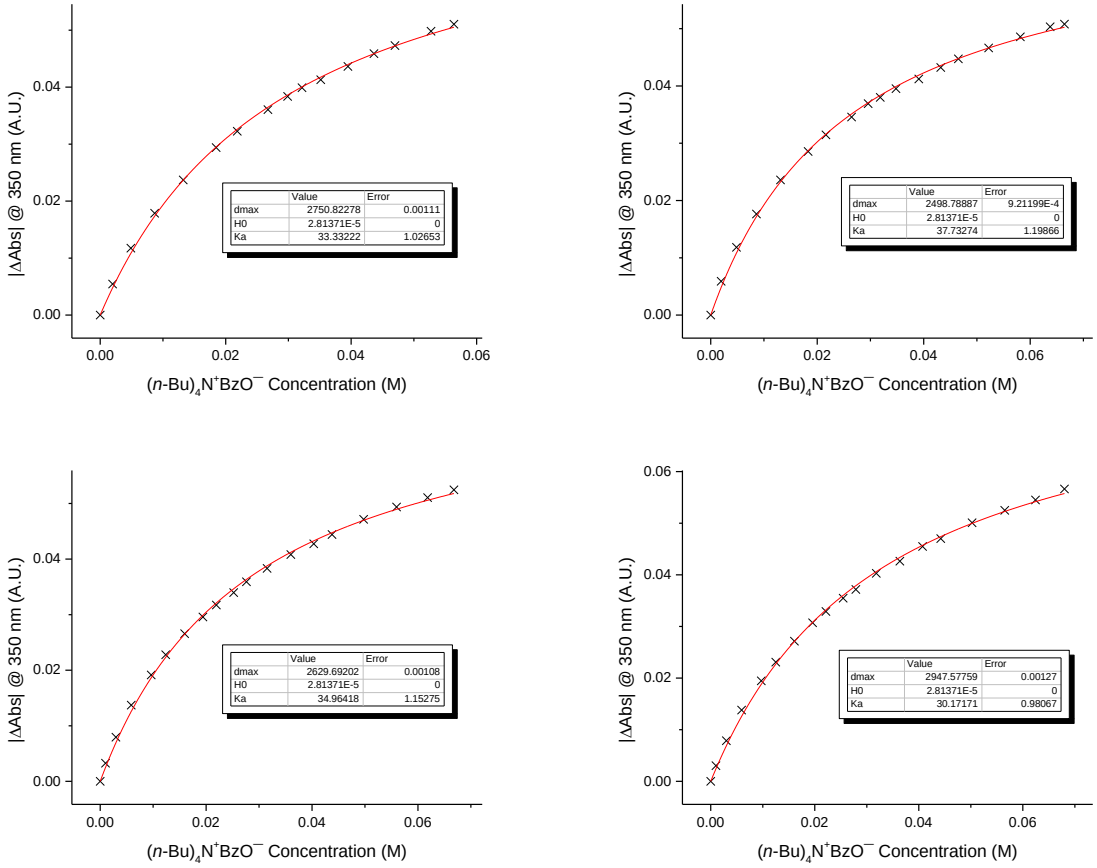
2.3.1.4.4.3 Absorbance Corrections

Figure S 24: Δabs versus [TBAOBz] at 350 nm in THF. Slope of the line represents the molar absorptivity.



2.3.1.4.4.2 Titrations

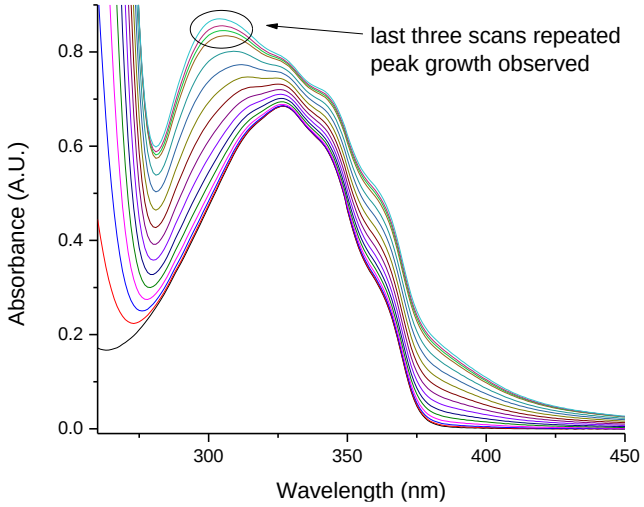
Figure S 25: Plots of ΔAbs versus TBAOBz concentration for the UV/Vis titration of **1d** in THF. Titrations carried out at 28.1 µM **1d**. From left to right, K_a = 33 M^{-1}, 38 M^{-1}, 35 M^{-1}, 30 M^{-1}.



2.3.1.4.5 TBAI

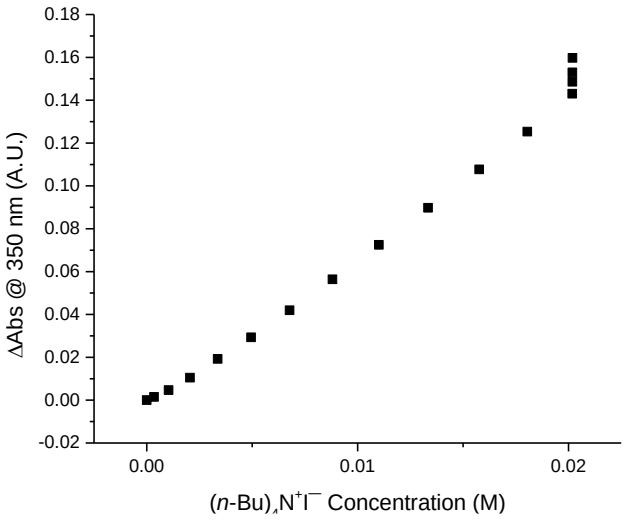
2.3.1.4.5.1 Spectrum

Figure S 26: Spectral change of **1d** upon the addition of TBAI in THF. Titration carried out at 28.1 µM **1d**. Repeated scans at the end of the titration revealed peak growth over time at ~ 300 nm.



2.3.1.4.5.2 Titrations

Figure S 27: Plot of ΔAbs versus TBAI concentration for the UV/Vis titration of **1d** in THF. Titration carried out at 28.1 µM **1d**. Binding to weak to be measured and confounded with decomposition.

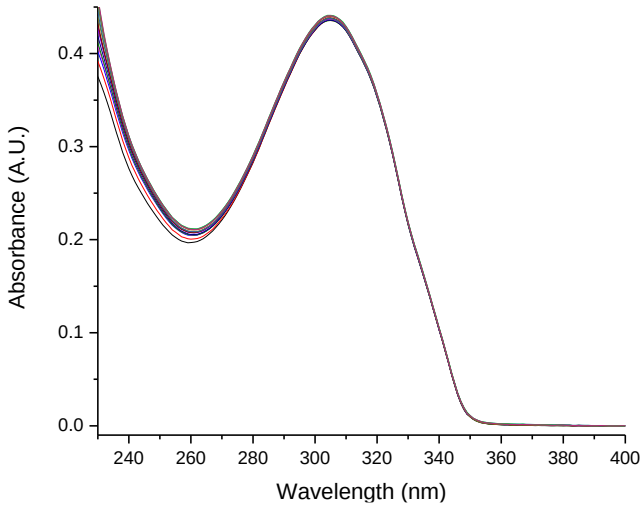


2.3.1.5 2,5-Bis(pentafluorophenyl)thiophene

2.3.1.5.1 TBACl

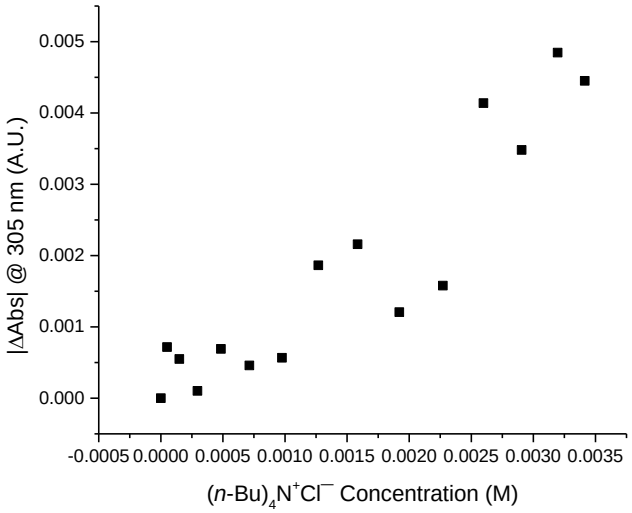
2.3.1.5.1.1 Spectrum

Figure S 28: Spectral change of 2,5-Bis(pentafluorophenyl)thiophene upon the addition of TBACl in THF. Titration carried out at 17.3 µM of 2,5-Bis(pentafluorophenyl)thiophene



2.3.1.5.1.2 Titrations

Figure S 29: Plot of ΔAbs versus TBACl concentration for the UV/Vis titration of 2,5-Bis(pentafluorophenyl)thiophene in THF. Titration carried out at 17.3 µM of 2,5-Bis(pentafluorophenyl)thiophene.

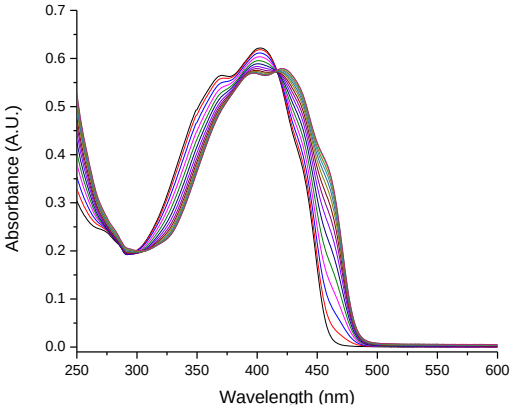


2.3.1.6 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)

2.3.1.6.1 TBACl

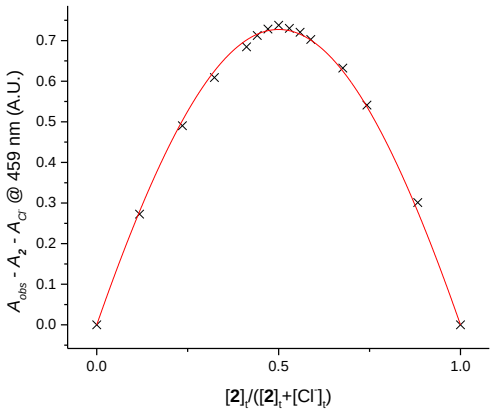
2.3.1.6.1.1 Spectrum

Figure S 30: Spectral change of **2** upon the addition of TBACl in THF. Titration carried out at 17.9 µM **2**.



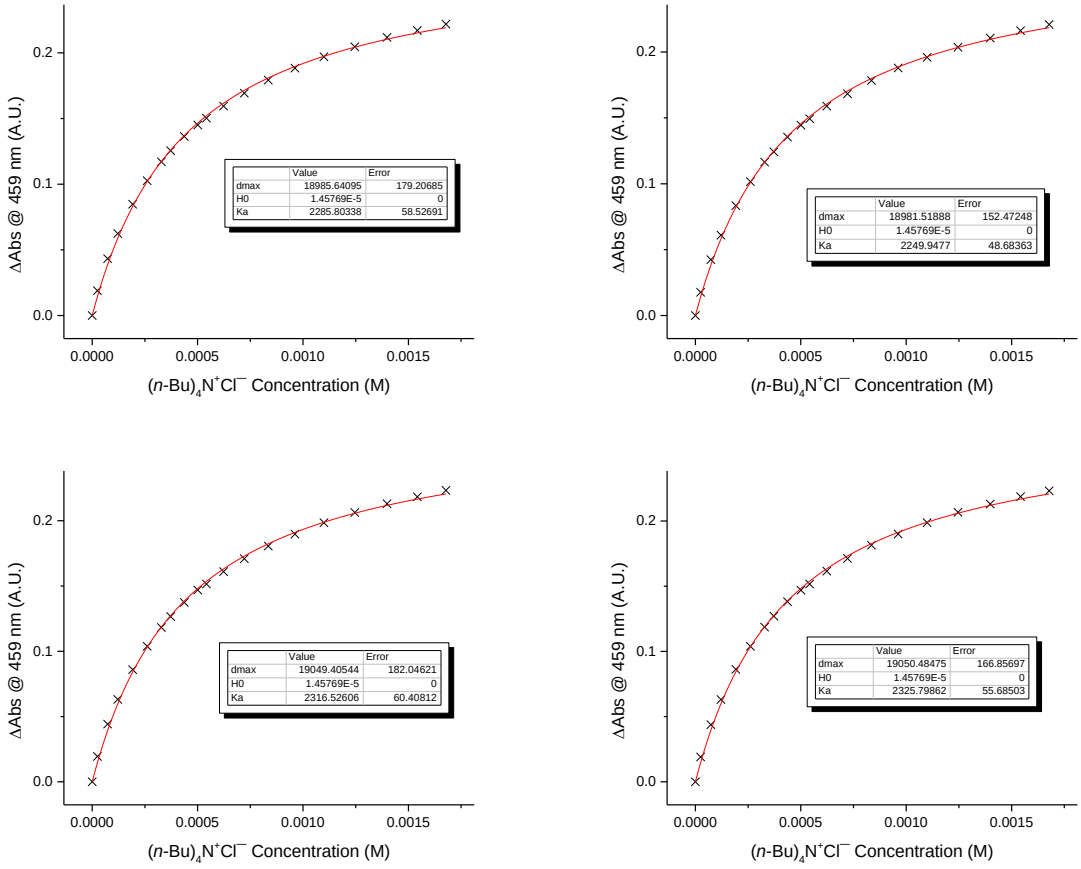
2.3.2.5.1.2 Job Plot

Figure S 31: UV/Vis Job Plot for the **2**-Cl^- complex in THF. [**2** + TBACl] = 353.2 µM.



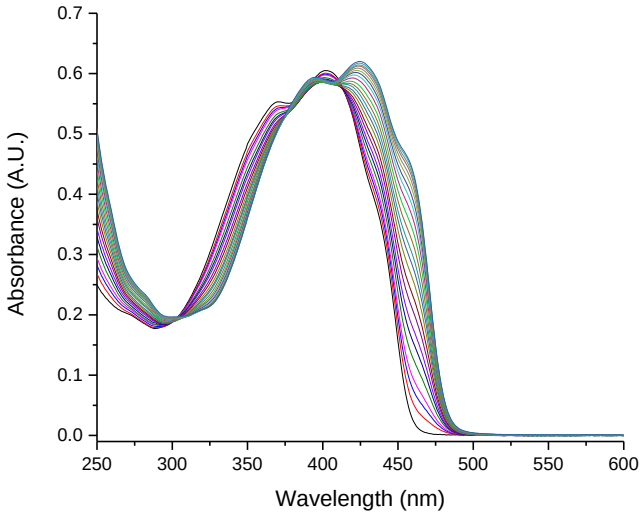
2.3.1.6.1.3 Titrations

Figure S 32: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **2** in THF. Titrations carried out at 14.6 µM **2**. From left to right, K_a = 2286 M^{-1}, 2250 M^{-1}, 2317 M^{-1}, 2326 M^{-1}.



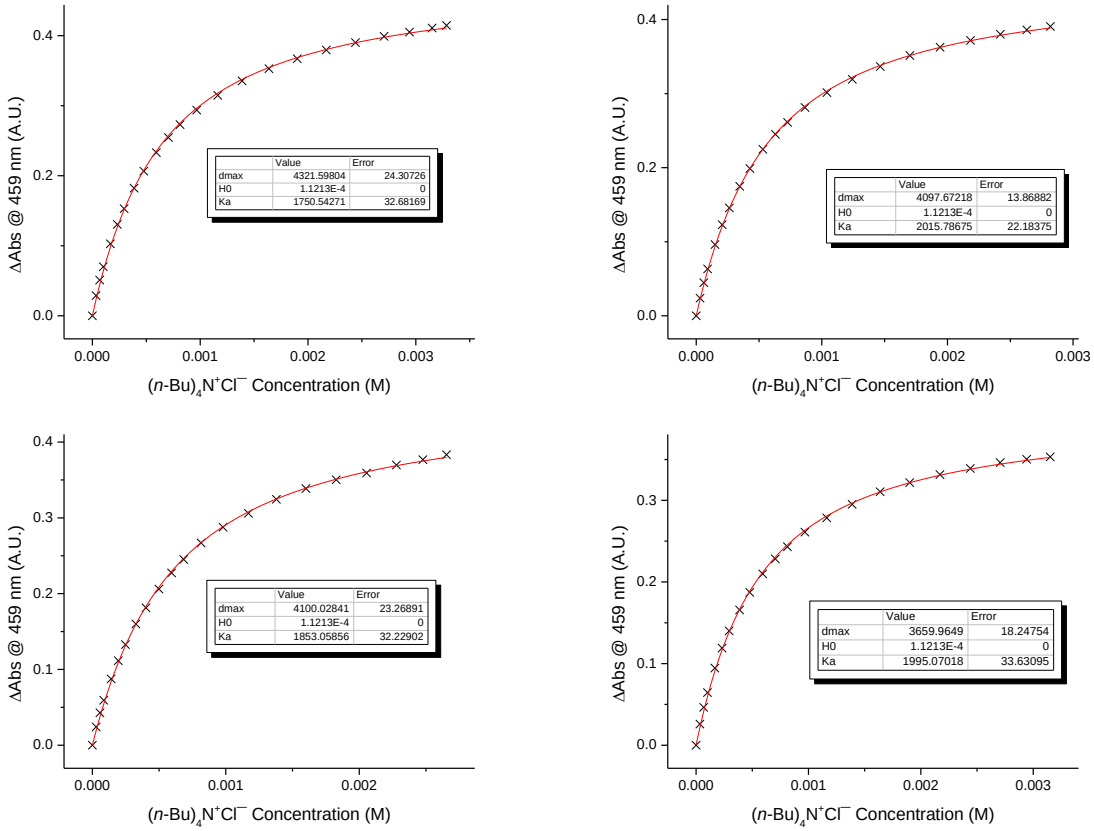
2.3.1.6.1.4 High Concentration Spectrum

Figure S 33: Spectral change of **2** upon the addition of TBACl in THF. Titration carried out at 112.2 µM **2** in a 4 mm path length cuvette.



2.3.1.6.1.5 High Concentration Titrations

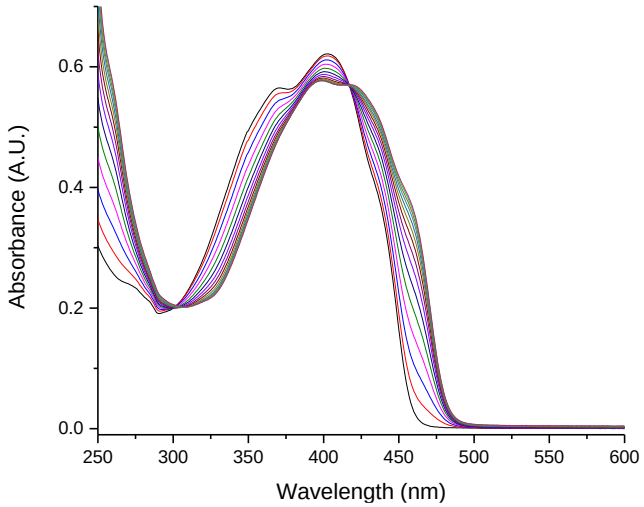
Figure S 34: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **2** in THF. Titrations carried out at 112.1 µM **2** in a 4 mm path length couvetter. From left to right, K_a = 1751 M^{-1}, 2016 M^{-1}, 1853 M^{-1}, 1995 M^{-1}.



2.3.1.6.2 TBABr

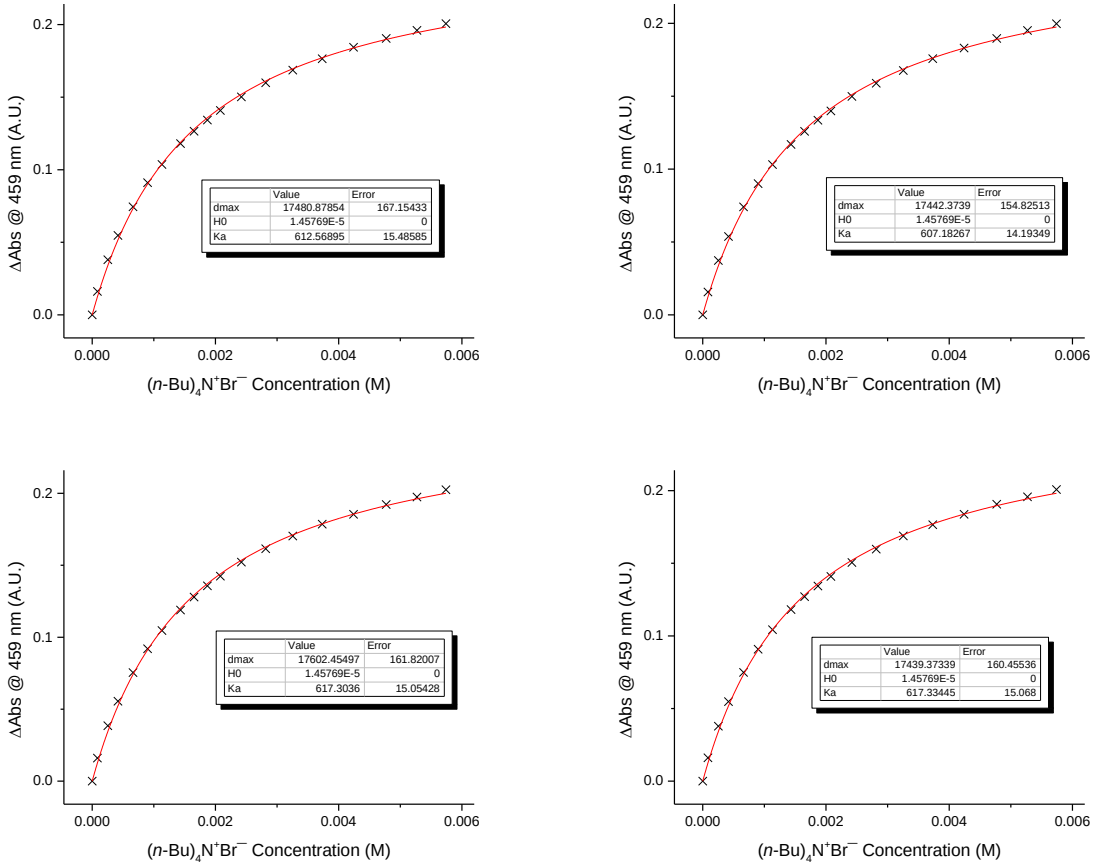
2.3.1.6.2.1 Spectrum

Figure S 35: Spectral change of **2** upon the addition of TBABr in THF. Titration carried out at 17.9 µM **2**.



2.3.1.6.2.2 Titrations

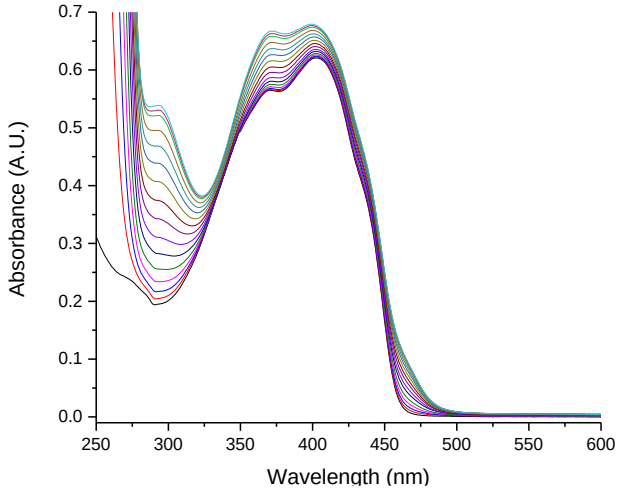
Figure S 36: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **2** in THF. Titrations carried out at 14.6 µM **2**. From left to right, K_a = 613 M^{-1}, 607 M^{-1}, 617 M^{-1}, 617 M^{-1}.



2.3.1.6.3 TBAI

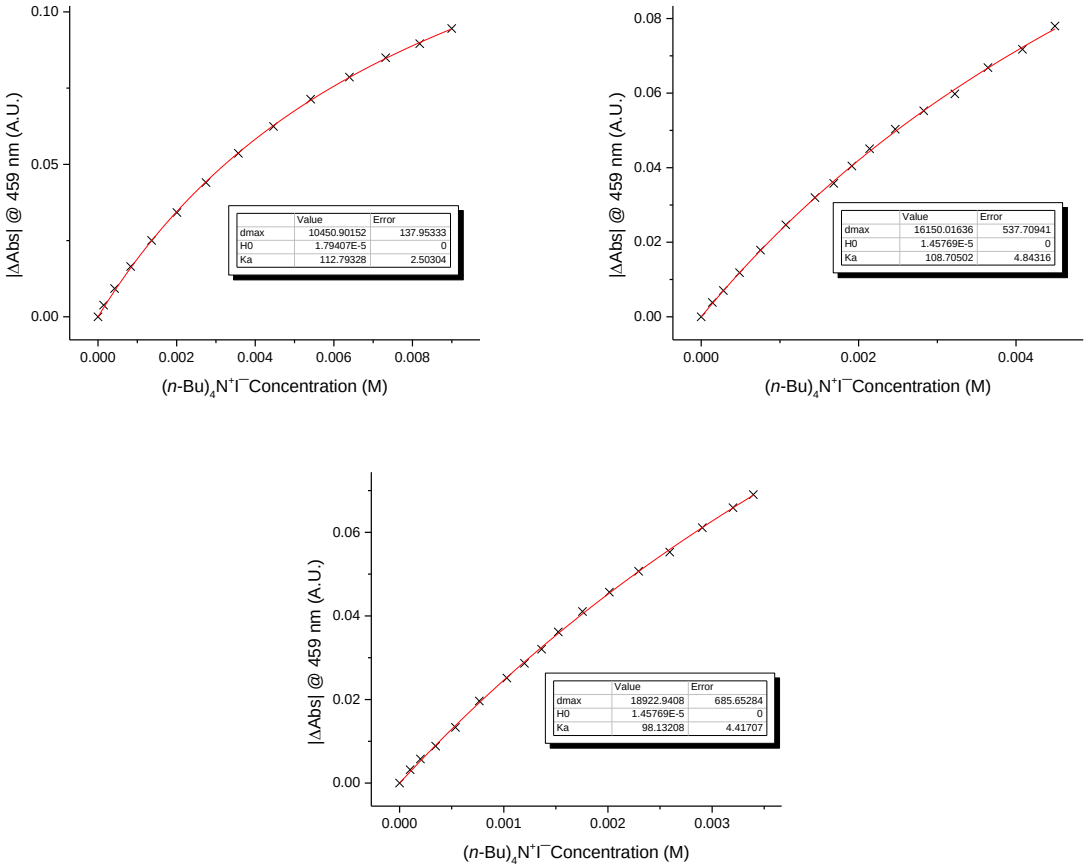
2.3.1.6.3.1 Spectrum

Figure S 37: (right) Spectral change of **2** upon the addition of TBAI in THF. Titration carried out at 17.9 µM **2**.



2.3.1.6.3.2 Titrations

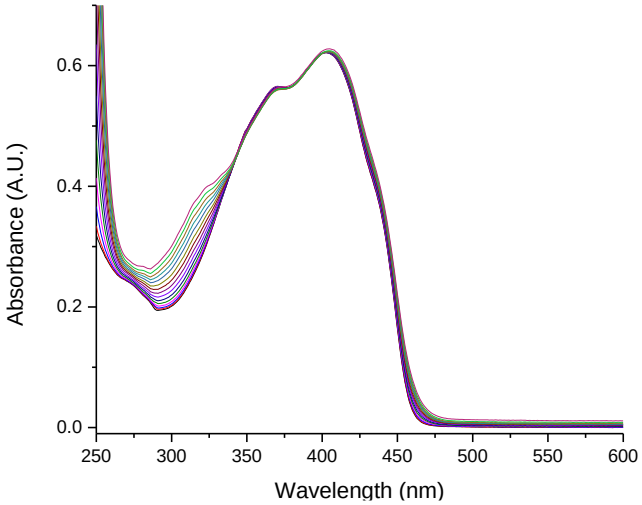
Figure S 38: Plots of ΔAbs versus TBAI concentration for the UV/Vis titration of **2** in THF. From left to right: 17.9 µM **2**, K_a = 113 M^{-1}, 14.6 µM **2**, K_a = 109 M^{-1}, 14.6 µM **2**, K_a = 98 M^{-1}.



2.3.1.6.4 $TBANO_3$

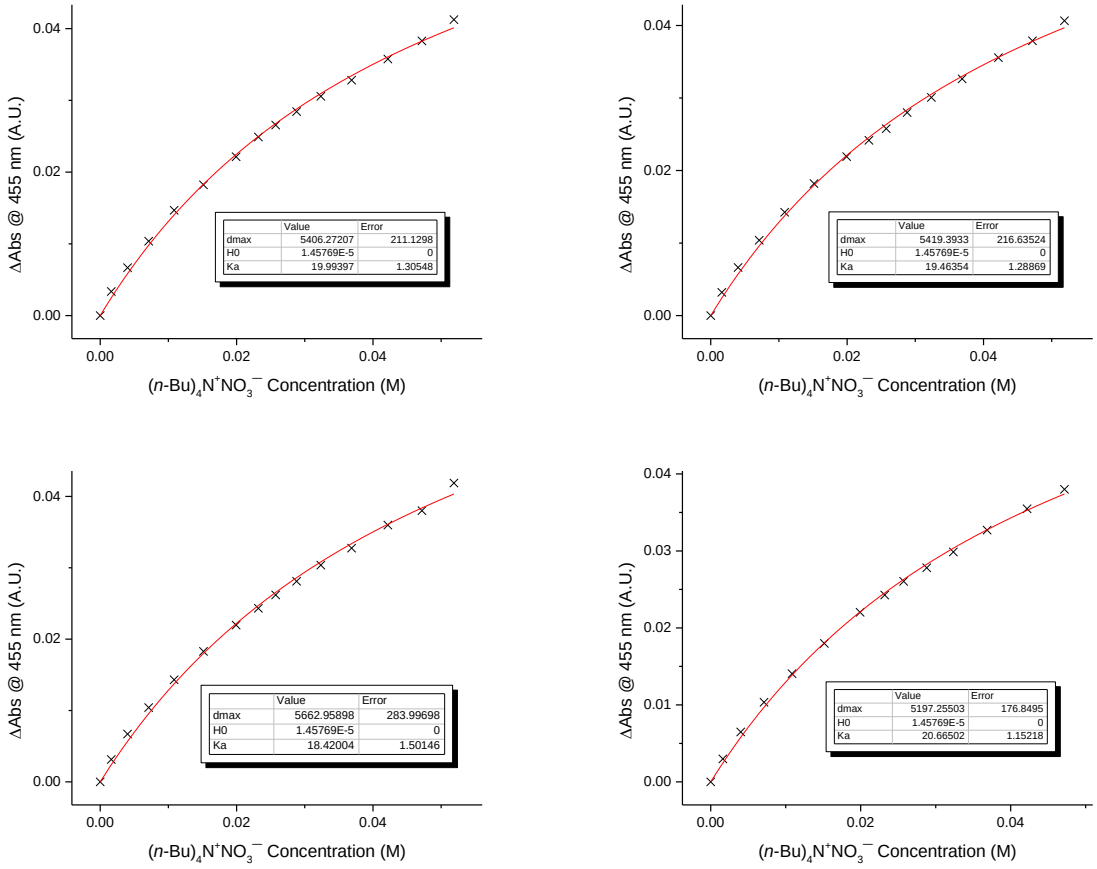
2.3.1.6.4.1 Spectrum

Figure S 39: Spectral change of **2** upon the addition of $TBANO_3$ in THF. Titration carried out at 17.9 µM **2**.



2.3.1.6.4.2 Titrations

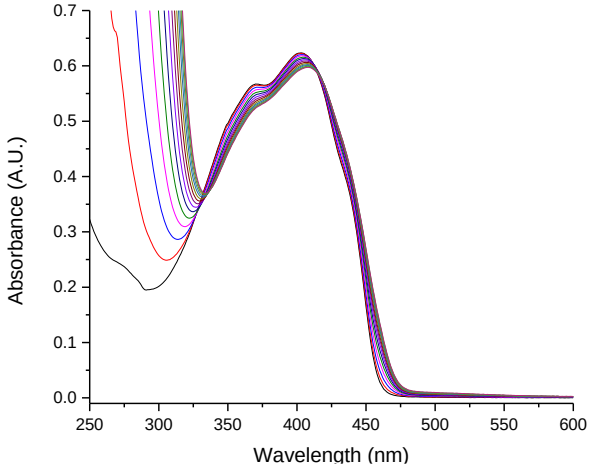
Figure S 40: Plots of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **2** in THF. Titrations carried out at 14.6 µM **2**. From left to right, K_a = 20 M^{-1}, 19 M^{-1}, 18 M^{-1}, 21 M^{-1}.



2.3.1.6.5 TBAOBz

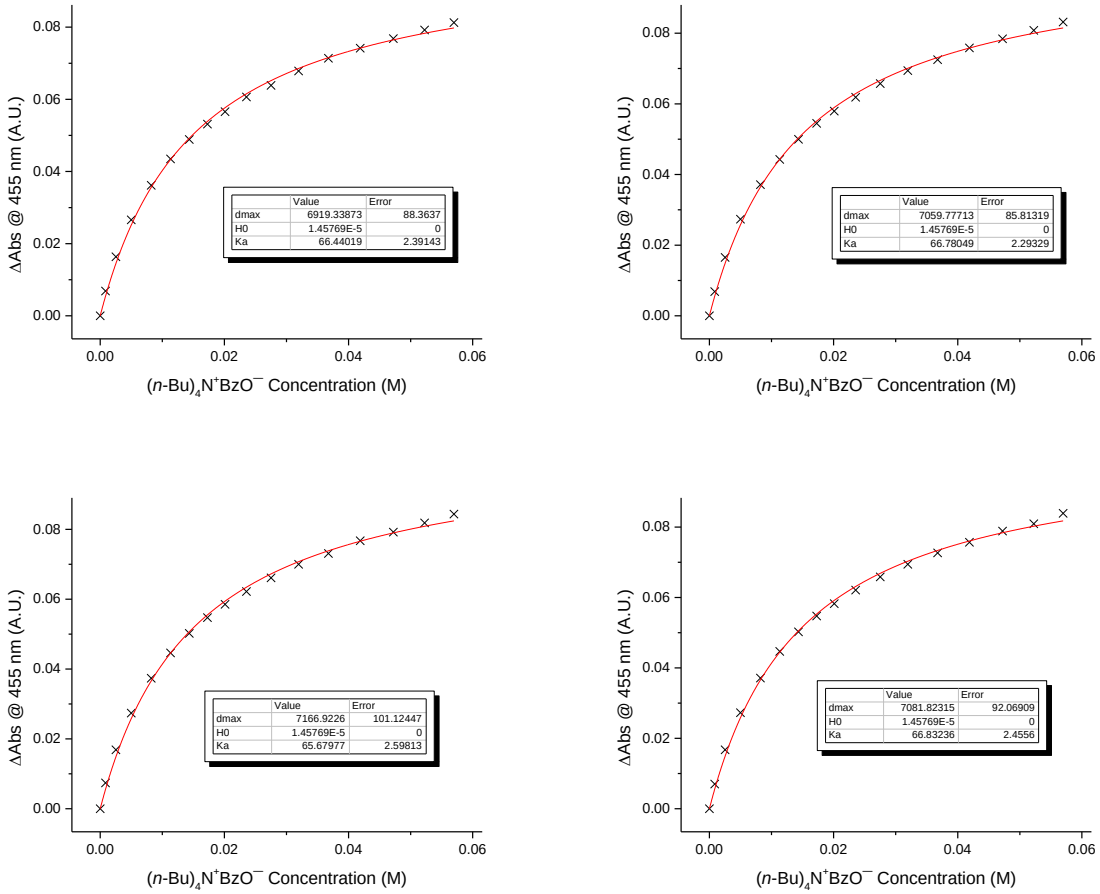
2.3.1.6.5.1 Spectrum

Figure S 41: Spectral change of **2** upon the addition of TBAOBz in THF. Titration carried out at 17.9 µM **2**.



2.3.1.6.5.2 Titrations

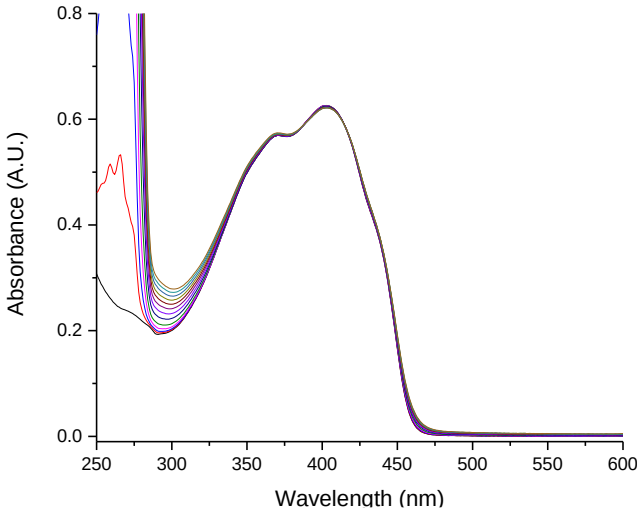
Figure S 42: Plots of ΔAbs versus TBAOBz concentration for the UV/Vis titration of **2** in THF. Titrations carried out at 14.6 µM **2**. From left to right, K_a = 66 M^{-1}, 67 M^{-1}, 66 M^{-1}, 67 M^{-1}.



2.3.1.6.6 TBAOTs

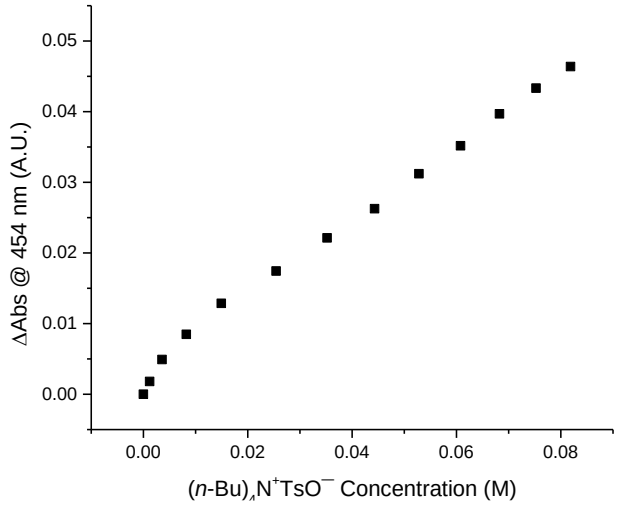
2.3.1.6.6.1 Spectrum

Figure S 43: Spectral change of **2** upon the addition of TBAOTs in THF. Titration carried out at 17.9 µM **2**.

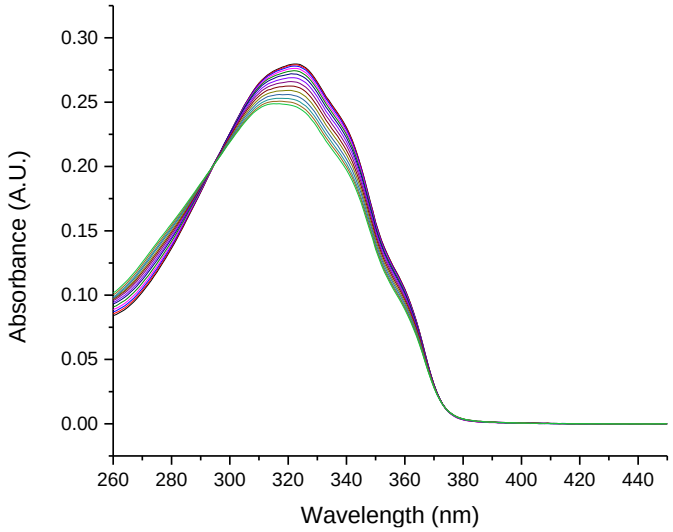


2.3.1.6.6.2 Titrations

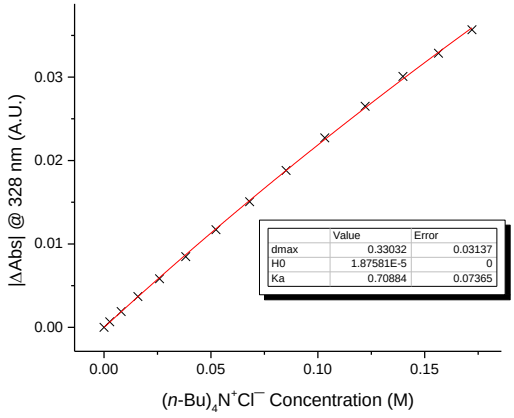
Figure S 44: Plot of ΔAbs versus TBAOTs concentration for the UV/Vis titration of **2** in THF. Titration carried out at 17.9 µM **2**. Binding too weak to be determined accurately.



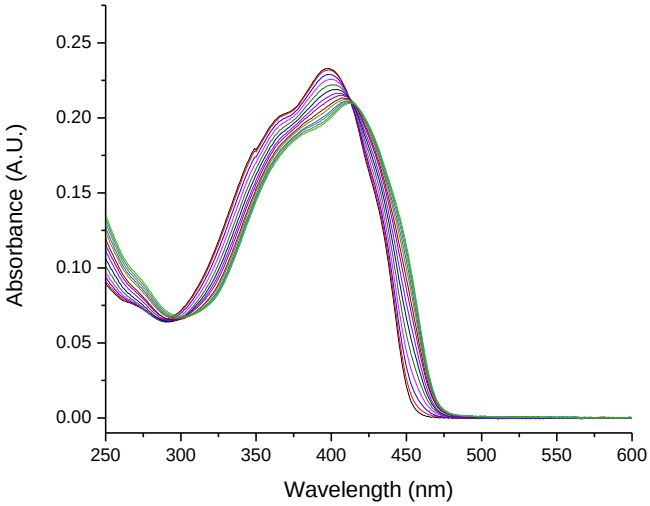
2.3.2 Acetonitrile
2.3.2.1 2,5-bis(perfluorophenyl)tellurophene (1d)
2.3.2.1.1 TBACl
2.3.2.1.1.1 Spectrum
Figure S 45: Spectral change of **1d** upon the addition of TBACl in acetonitrile. Titration carried out at 18.8 µM **1d**.



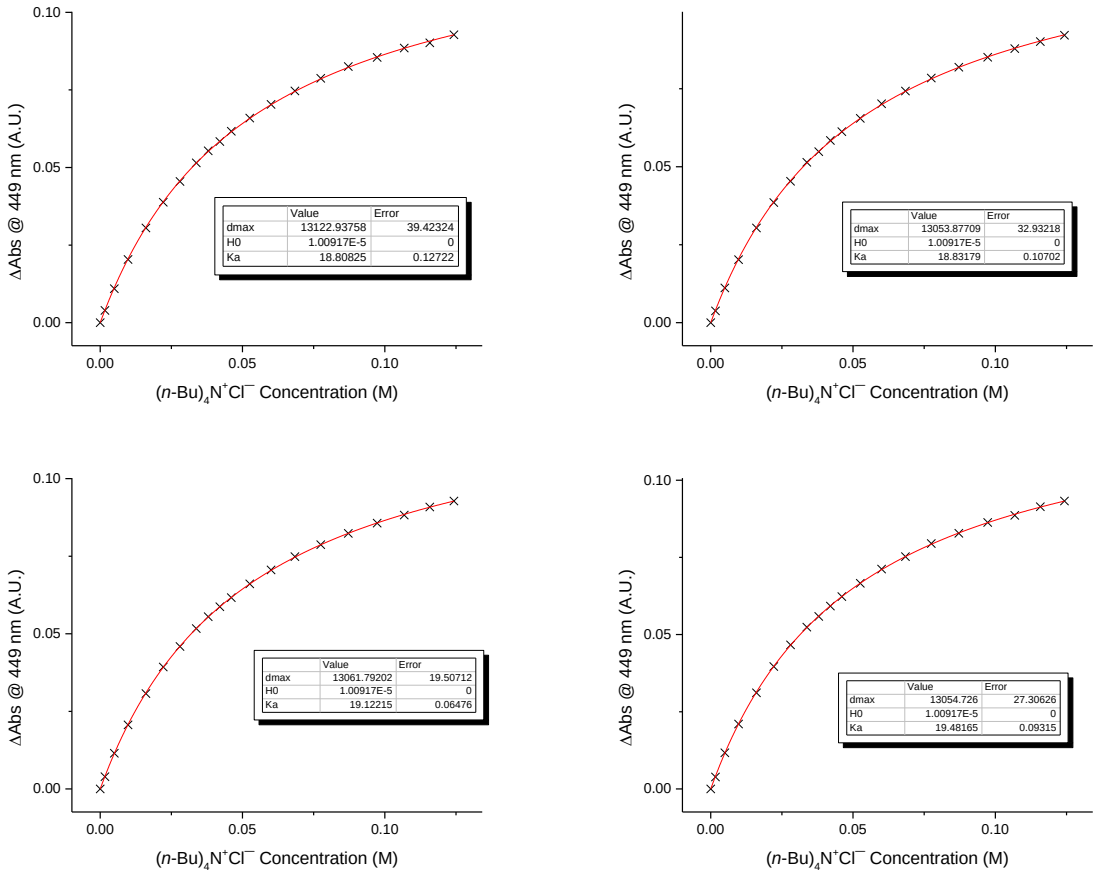
2.3.2.1.1.2 Titrations
Figure S 46: Plot of ΔAbs versus TBACl concentration for the UV/Vis titration of **1d** in acetonitrile. Titration carried out at 18.8 µM **1a**. K_a = 0.71 M^{-1}. Binding too weak to be determined accurately.



2.3.2.2 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)
2.3.2.2.1 TBACl
2.3.2.2.1.1 Spectrum
Figure S 47: Spectral change of **2** upon the addition of TBACl in acetonitrile. Titration carried out at 10.0 µM **2**.

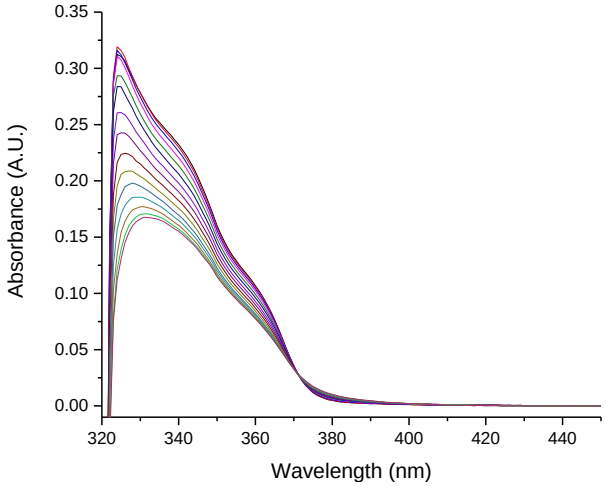


2.3.2.2.1.2 Titrations
Figure S 48: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **2** in acetonitrile. Titrations carried out at 10.1 µM **2**. From left to right, K_a = 18.8 M^{-1}, 18.8 M^{-1}, 19.12 M^{-1}, 19.48 M^{-1}.



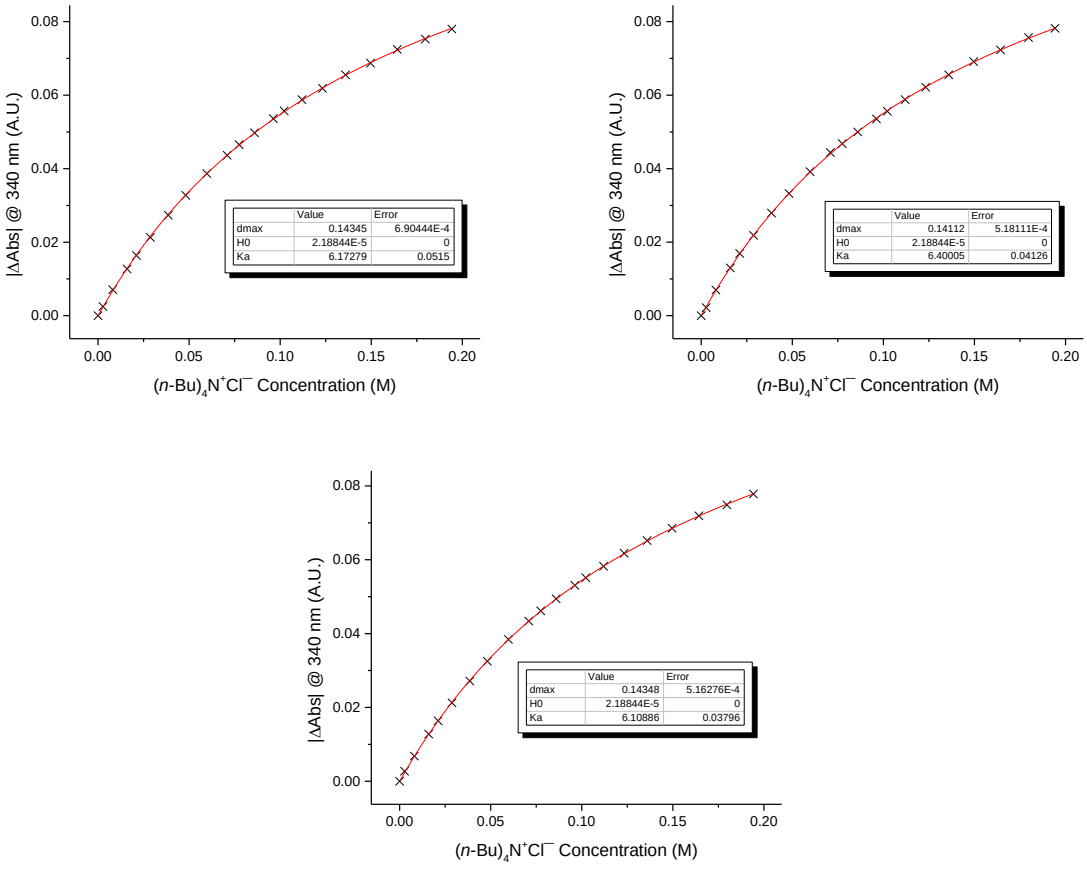
2.3.3 Acetone
2.3.3.1 2,5-bis(perfluorophenyl)tellurophene (1d)
2.3.3.1.1 TBACl
2.3.3.1.1.1 Spectrum

Figure S 49: Spectral change of **1d** upon the addition of TBACl in acetone. Titration carried out at 21.8 µM **1d**.

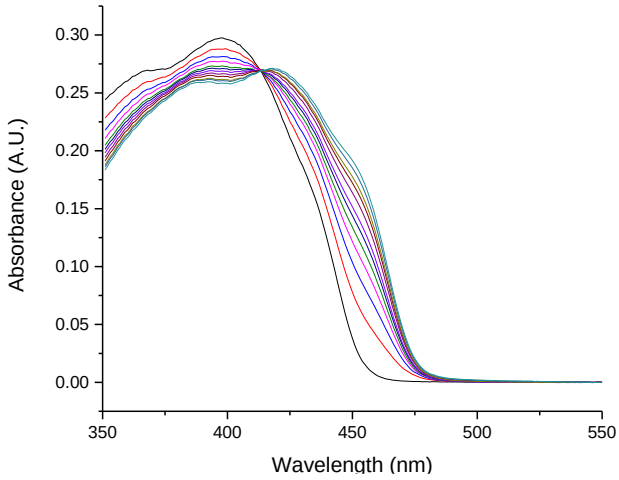


2.3.2.1.1.2 Titrations

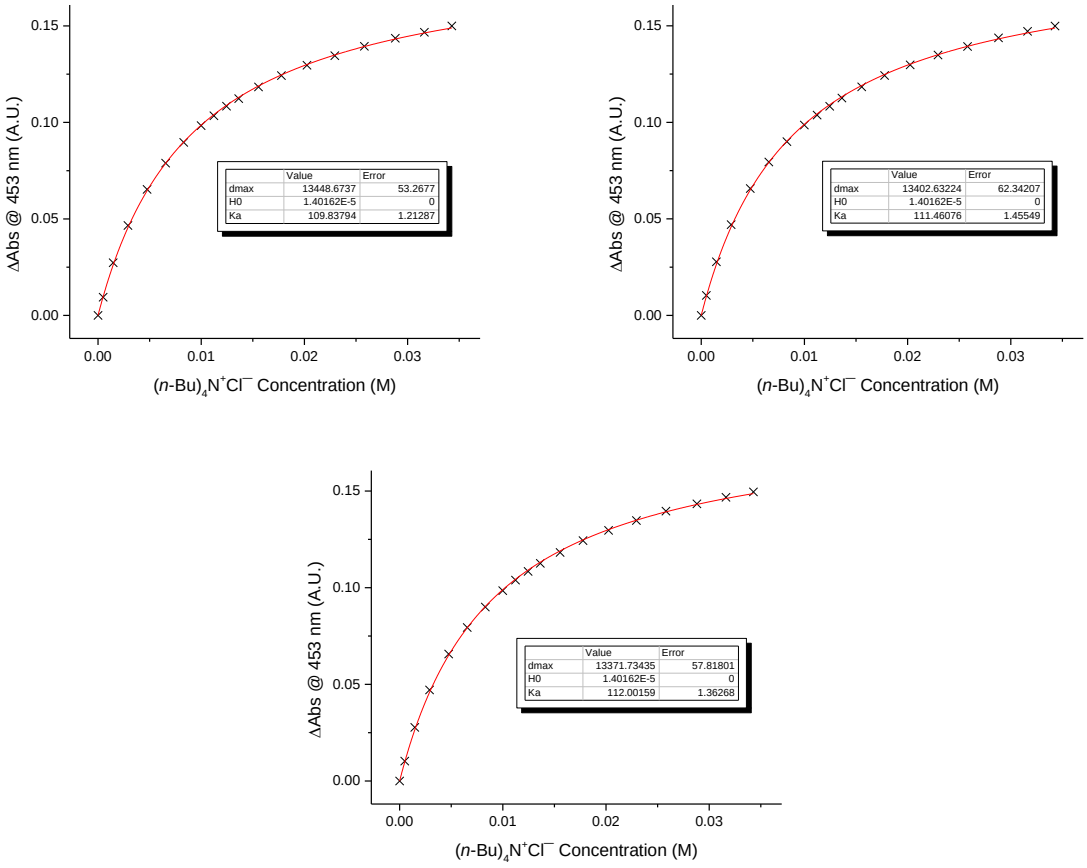
Figure S 50: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **1d** in acetone. Titrations carried out at 21.8 µM **1d**. From left to right, K_a = 6.17 M^{-1}, 6.40 M^{-1}, 6.11 M^{-1}.



2.3.3.2 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)
2.3.3.2.1 TBACl
2.3.3.2.1.1 Spectrum
Figure S 51: Spectral change of **2** upon the addition of TBACl in Acetone. Titration carried out at 14.0 µM **2**.



2.3.2.2.1.2 Titrations
Figure S 52: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **2** in acetone. Titrations carried out at 14.0 µM **2**. From left to right, K_a = 110 M^{-1}, 111 M^{-1}, 112 M^{-1}.



2.4 NMR Titrations with TBACl in THF-d_8

2.4.1 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)

2.4.1.1 NMR Spectra

Figure S 53: ^{1}H NMR spectra of the titration of 949.2 µM **2** with TBACl in THF-d_8. TBACl concentration increases on the y-axis. Upfield peak shift from δ 7.92 represents donor-acceptor binding. Chloride concentration increases moving up the y-axis.

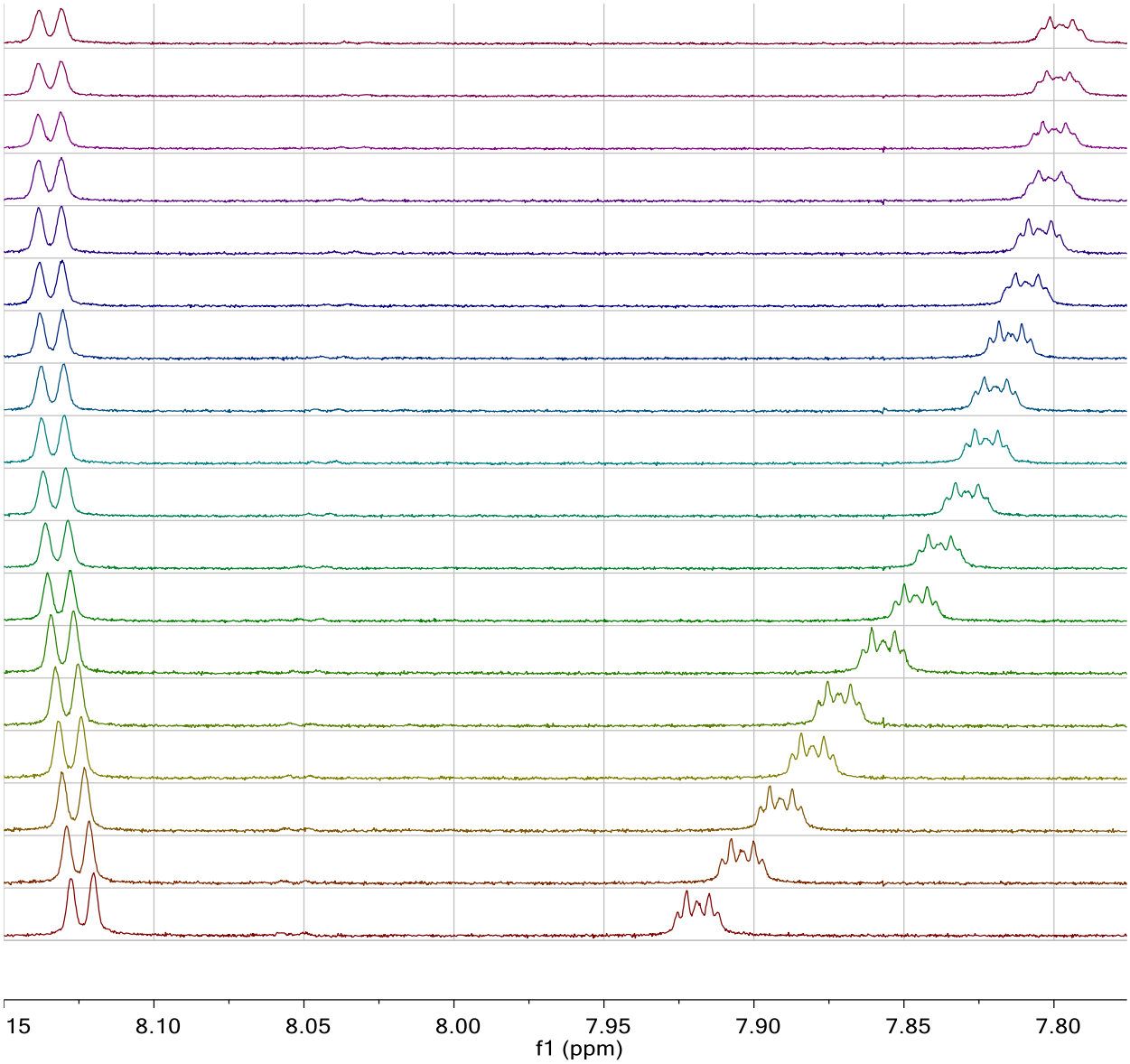
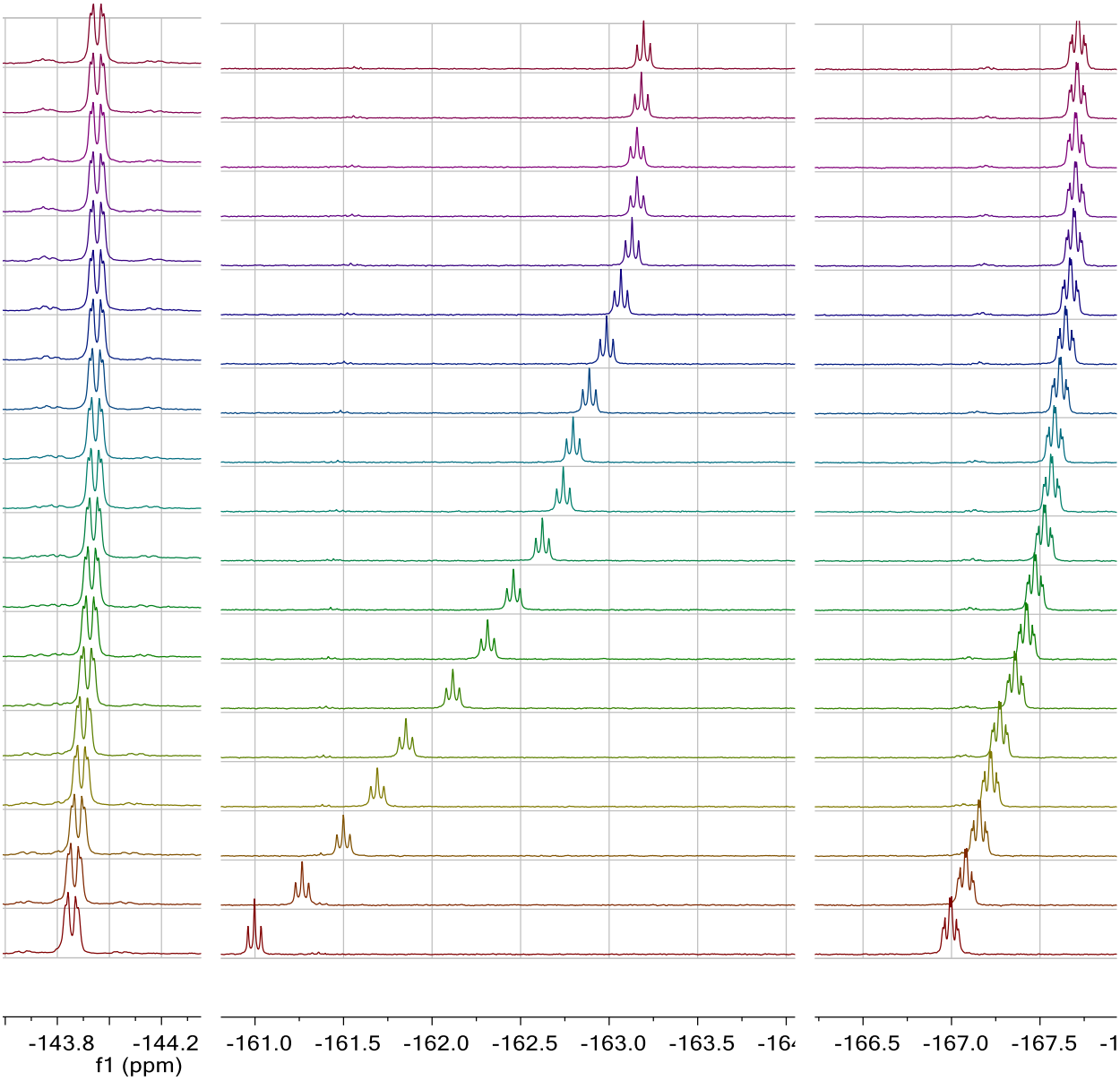


Figure S 54: ^{9}F NMR spectra of the titration of 949.2 µM **2** with TBACl in THF-d_8. TBACl concentration increases on the y-axis. Upfield peak shift from δ -161.0 and δ -167.0 represents donor-acceptor binding. Perfluorohexane used as internal standard. Chloride concentration increases moving up the y-axis.



2.4.1.2 Titration curves

2.4.1.2.1 Individual fitting

Figure S 55: Plot of |Δδ| versus TBACl concentration for the ^{1}H NMR titration of **2** in THF-d$_8$. Titration carried out 949.2 µM **2**. K_a = 3168.

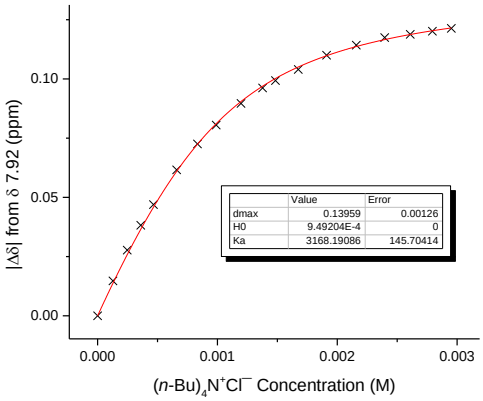
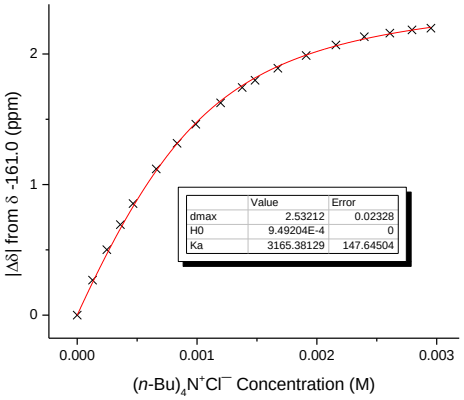
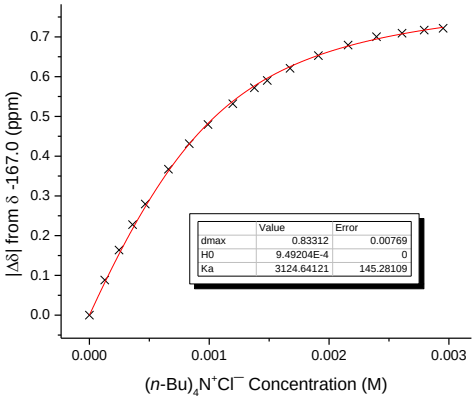


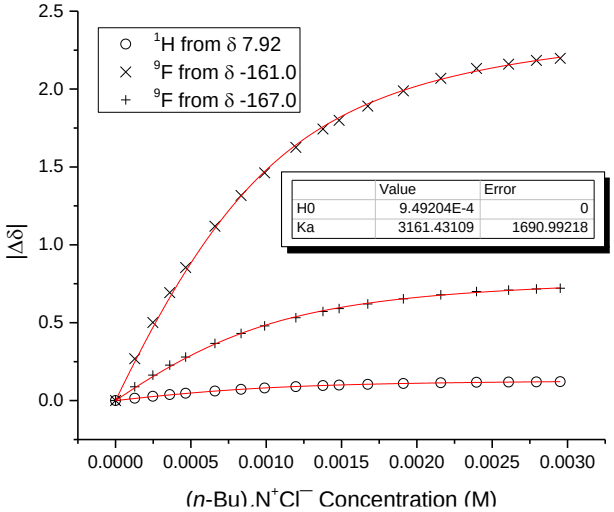
Figure S 56: Plot of |Δδ| versus TBACl concentration for the ^{9}F NMR titration of **2** in THF-d$_8$. Titration carried out 949.2 µM **2**. From left to right, K_a = 3165 M^{-1}, 3125 M^{-1}





2.4.1.2.1 Global Fitting

Figure S 57: Plot of |Δδ| versus TBACl concentration for the ^{1}H and ^{9}F NMR titration of **2** in THF-d_8. Titration carried out 949.2 μM **2**. Peak shifts globally fit to a 1:1 binding isotherm, K_a = 3161 M^{-1}.



2.5 Donor Stability towards Tetrabutylammonium Acetate and Benzoate

2.5.1 2,5-bis(perfluorophenyl)tellurophene (1d)

2.5.1.1 Methodology

Into two quartz UV cuvettes was placed 2.5 mL of a 28.1 μM solution of **1d**. 12.4 mg of TBAOAc (0.04 mmol, 16.4 mM in cuvette) was dissolved into one cuvette. Into the other was dissolved 85.2 mg of TBAOBz (0.23 mmol, 93.7 mM in cuvette) and UV monitoring began. After 80 minutes, ΔAbs vs. time plots were created using the wavelength where the most change in absorbance occurred.

To determine the relative stability of the donor during the course of a UV-vis titration (~10 minutes), one UV cuvette was left over night and the change in absorbance noted.

2.5.1.2 Results

Figure S 58: UV-vis absorption spectra versus time for a 28.1 μM solution of **1d** in THF in the presence of 16.4 mM of TBAOAc (left) and 93.7 mM of TBAOBz (right). Spectra recorded for 80 minutes.

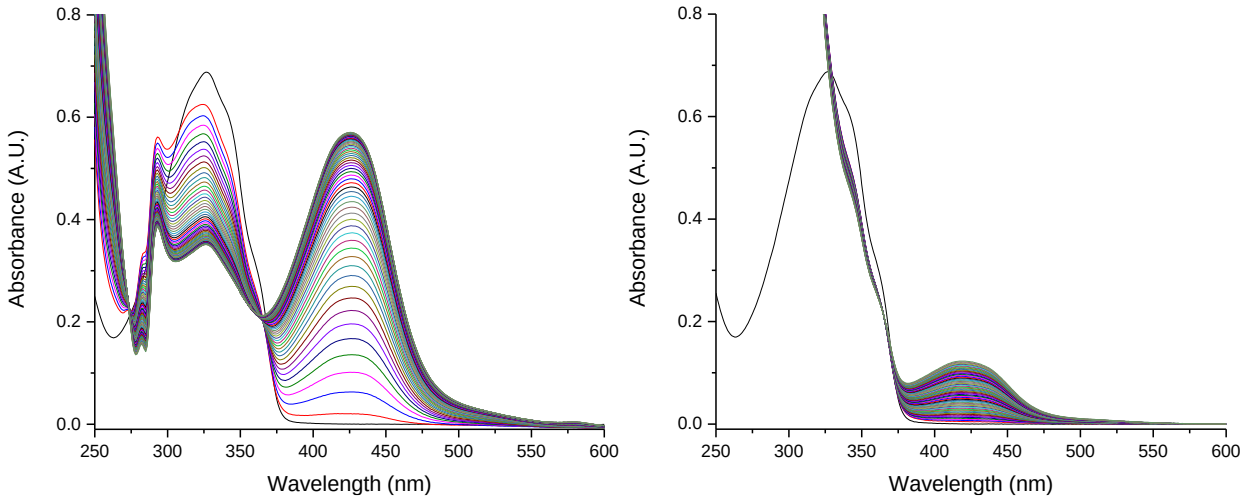
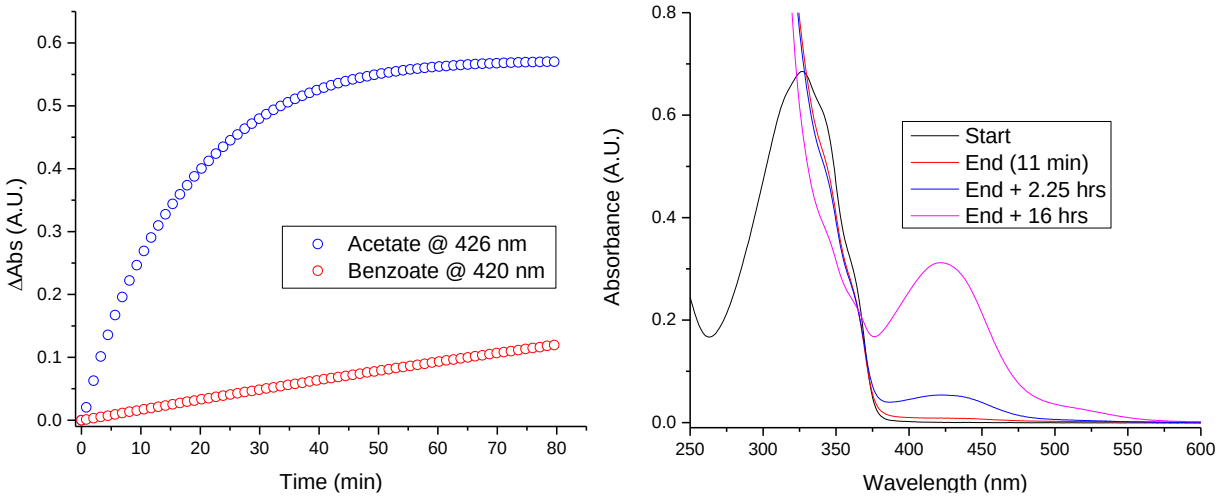


Figure S 59: (Left) ΔAbs versus time profile obtained from a 28.1 µM solution of **1d** in THF in the presence of 16.4 mM of TBAOAc and 93.7 mM of TBAOBz. (Right) TBAOBz Decomposition product growth during the course of a typical titration (11 minutes), and after being left for 2.25 hrs and overnight. Less than 10% decomposition occurs by the end of the titration.



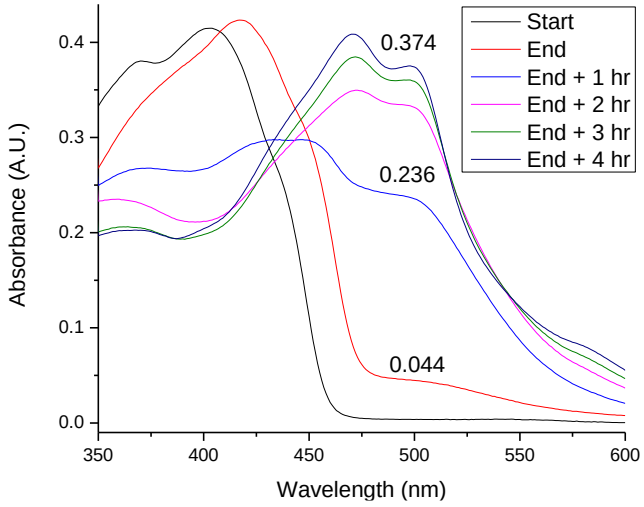
2.5.2 1,2-bis(5-(perfluorophenyl)tellurophen-2-yl)ethyne (2)

2.5.2.1 Methodology

To determine the relative stability of the donor during the course of a UV-vis titration with TBAOAc (~10 minutes), one UV cuvette was left after the titration was complete. The UV-vis spectrum was collected every hour for four hours and the change in absorbance noted. Very little change was noted for the titrations with TBAOBz, and this process was skipped for that system.

2.5.2.2 Results

Figure S 60: TBAOAc Decomposition product growth during the course of a typical titration (10 minutes), and after being left for 4 hrs and overnight. Approximately 12% decomposition occurs by the end of the titration.



3.0 Computational Methods

3.1 Methodology

All thermodynamic calculations were performed using the Gaussian 09 program.[7] DFT calculations were carried out at the B97-D3[8] level with all stationary points optimized using the Def2-TZVP[9] basis set. Electrostatic potential surfaces (ESPs) were optimized and created at the B97-D3/Def2-TZVP level of theory and determined at a electron density of 0.001 electrons/bohr. Vibrational frequency calculations were performed to characterize each stationary point as a minimum (no imaginary frequencies) on the potential energy surface. This held true for all modeled complexes except for the binding structures with benzoate which contained small negative frequencies. These are noted above their Cartesian coordinates. All frequency calculations were carried out at 1 atm and 298.15 K. $V_{S,max}$ values were determined in the standard fashion.[10] For bound complexes, the B97-D3/Def2-TZVP level of theory employed with solvation modeled using a self-consistent reaction field by means of the PCM[11] method. For more complex donor acceptor combinations (NO_3 or OBz) multiple binding geometries were checkd, only the lowest energy structure are shown. Structures and ESPs were visualized using GaussView 5.0, ESP contour plots were visualized using Jmol using a previously described method.[12]

In their most stable configurations, the σ-holes on the tellurium atoms in compounds 1a-d are hidden from view. To remedy this, $V_{S,max}$ were obtained by fixing one of the aromatic rings 90° out of plane of the tellurophene ring and allowing the rest of the structure to optimize around this restriction using the Opt=ModRedundant keyword.

3.2 Electrostatic Potentials

3.2.1 $V_{S,max}$ values

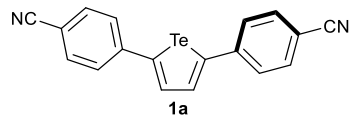
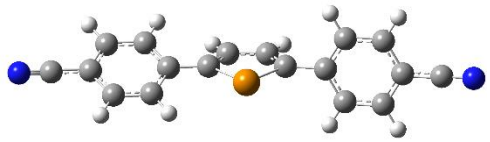
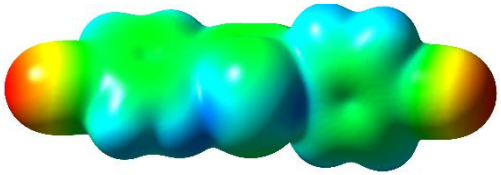
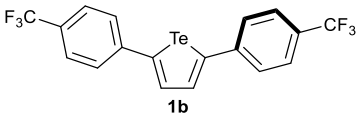
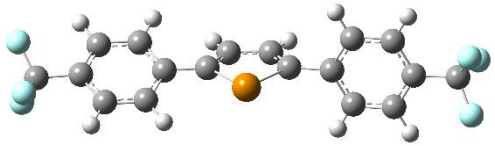
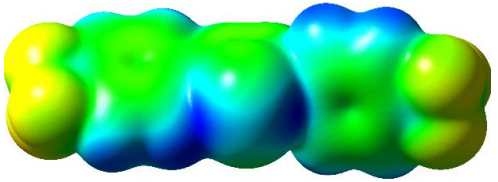
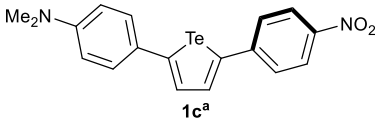
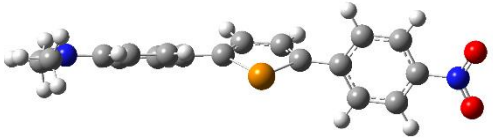
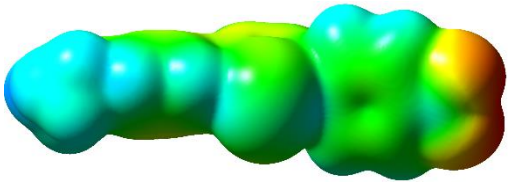
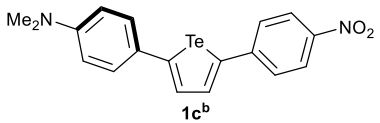
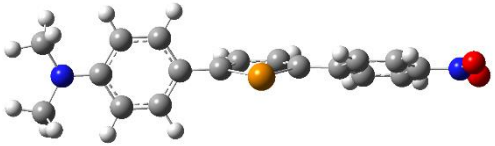
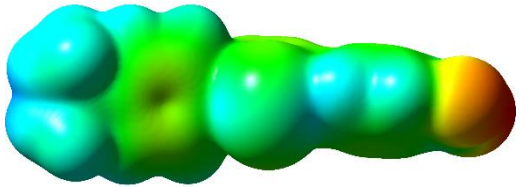
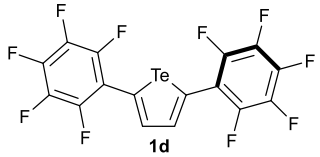
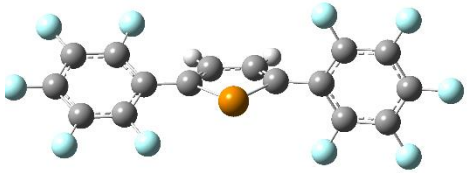
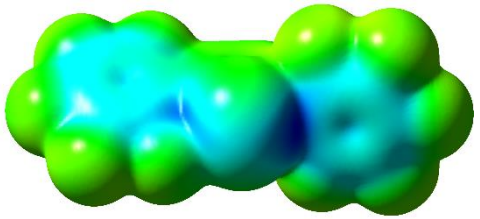
Table S 4: σ-hole electrostatic potentials ($V_{S,max}$) calculated at the B97D3/Def2-TZVP level of theory, presented in kcal/mol. All structures had one of the aryl rings fixed 90° out of plane in order to visualize one of the σ-holes.

Compound	$V_{S,max}$ (kcal/mol)
1a	28.3
1b	23.5
1c[a]	17.1
1c[b]	16.7
1d	29.6
2,5-Bis(pentafluorophenyl)thiophene	18.8
2	24.9

a) value obtained when the 4-NO_2 ring is fixed at 90° b) value obtained when 4-NMe_2 ring is fixed at 90°

3.2.2 ESP Surfaces

Table S 5: Fixed 90° geometries and ESPs obtained using the default scaling values in GaussView 5.0 for each compound.

Donor	Geometry	Default scaling
 **1a**		
 **1b**		
 **1c[a]**		
 **1c[b]**		
 **1d**		

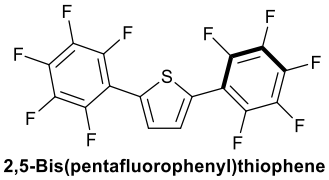
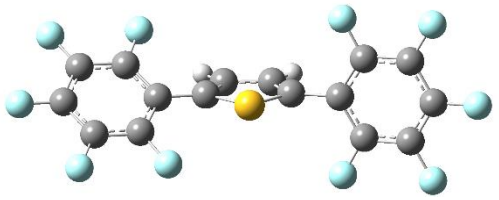
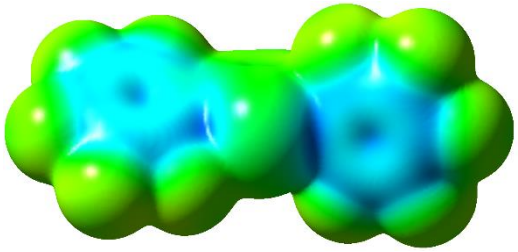
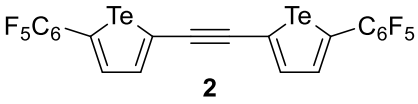
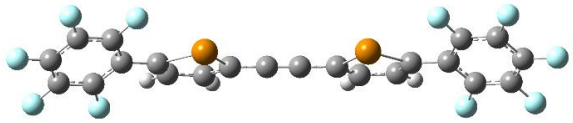
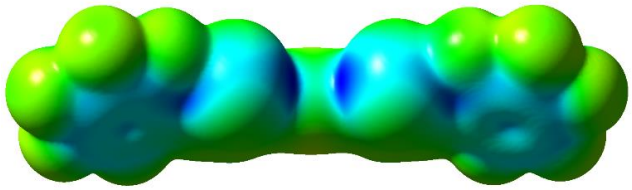
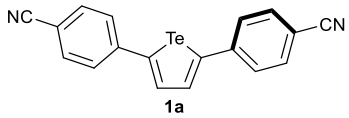
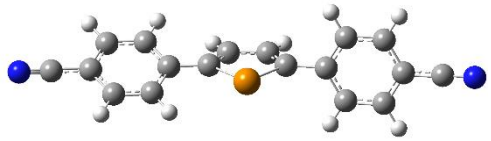
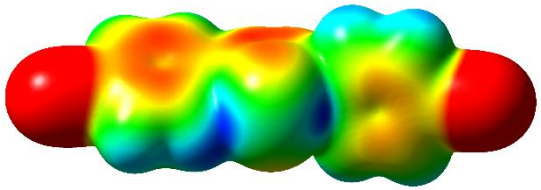
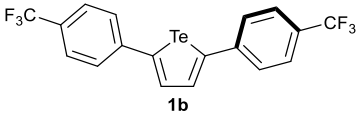
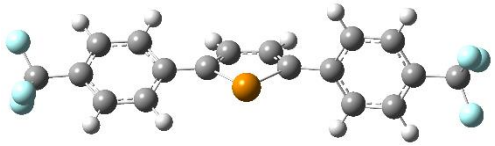
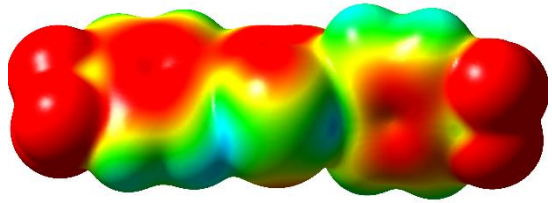
Donor	Geometry	Default scaling
 2,5-Bis(pentafluorophenyl)thiophene		
 2		

Table S 6: Fixed 90° geometries and ESPs obtained when scaling from 0 kcal/mol (red) to 29.6 kcal/mol (blue), the $V_{S,Max}$ of **1d**, the largest in the series.

Donor	Geometry	Scaled 0 – 29.6 kcal/mol
 1a		
 1b		

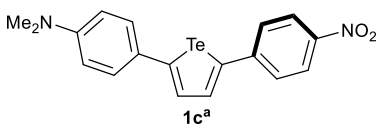
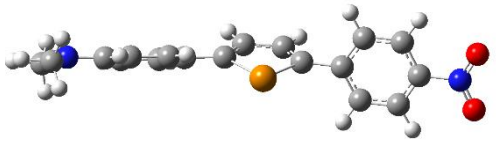
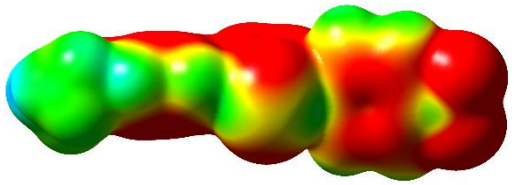
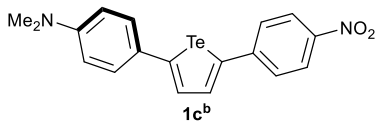
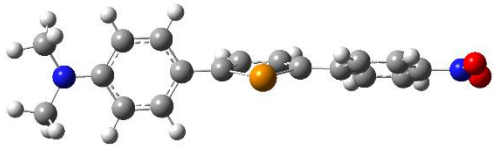
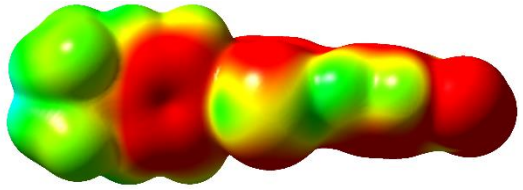
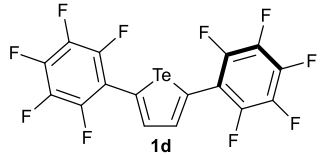
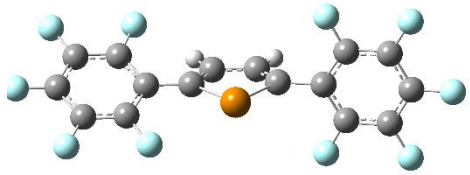
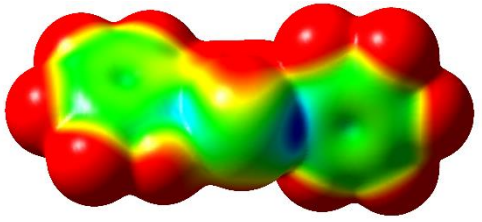
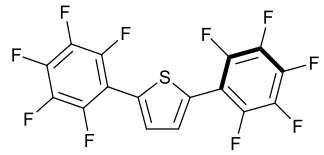
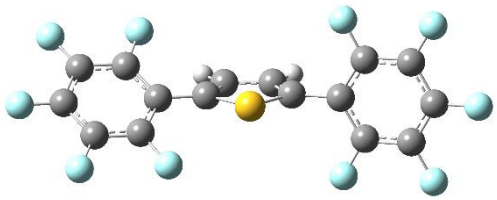
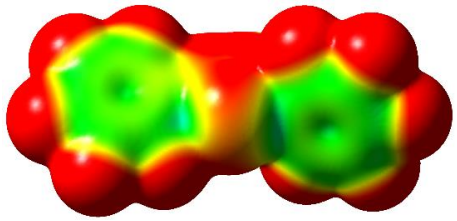
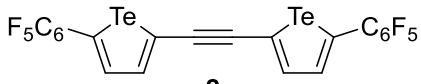
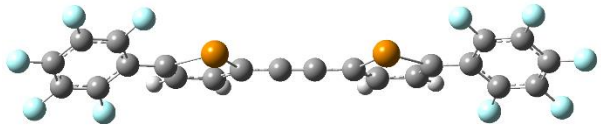
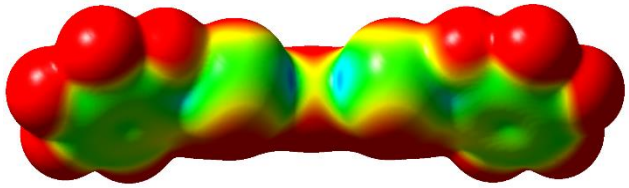
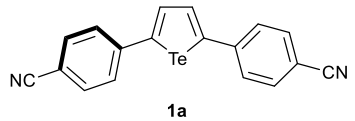
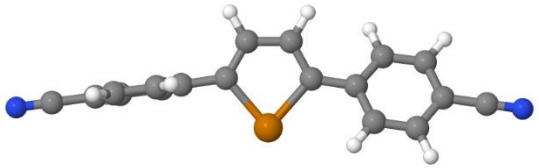
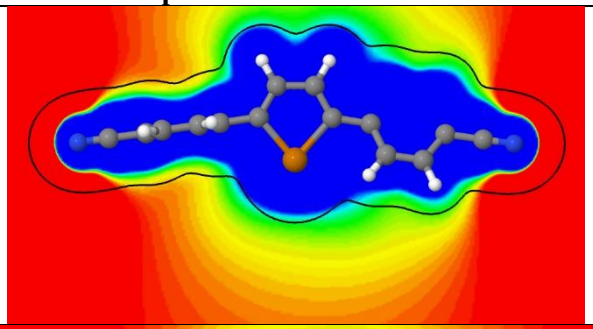
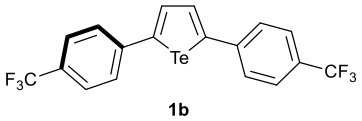
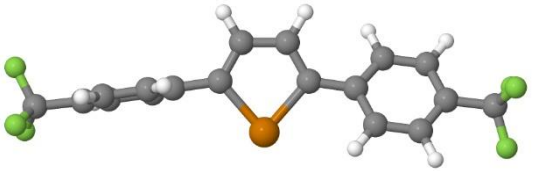
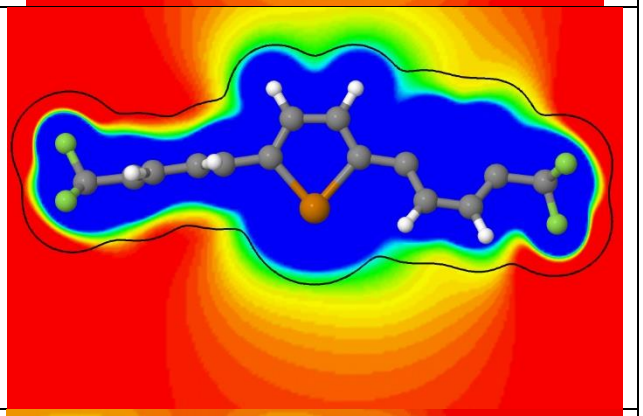
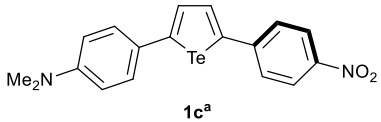
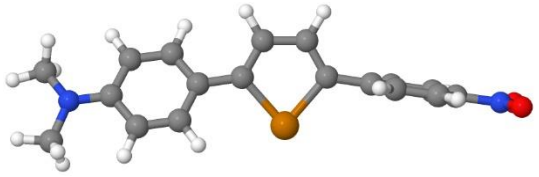
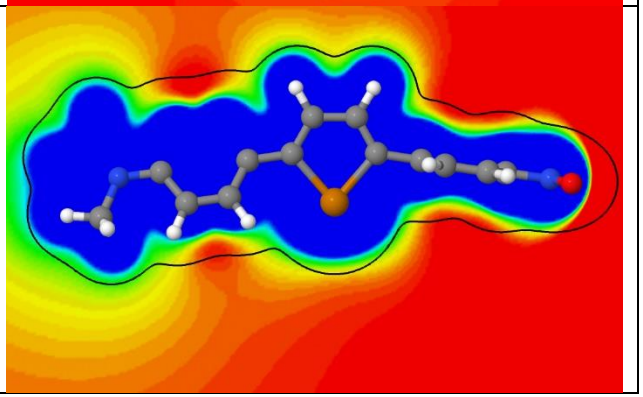
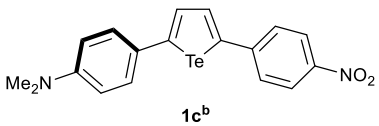
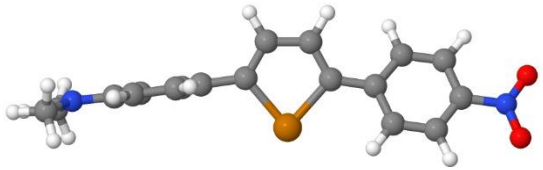
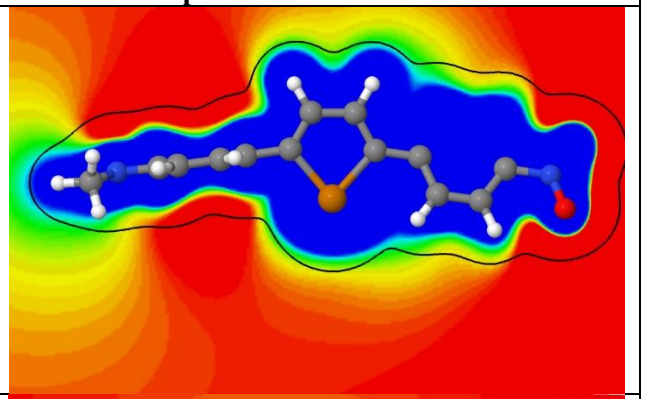
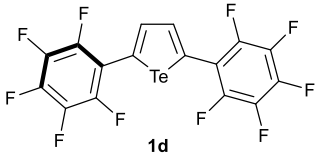
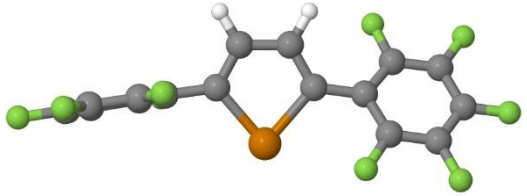
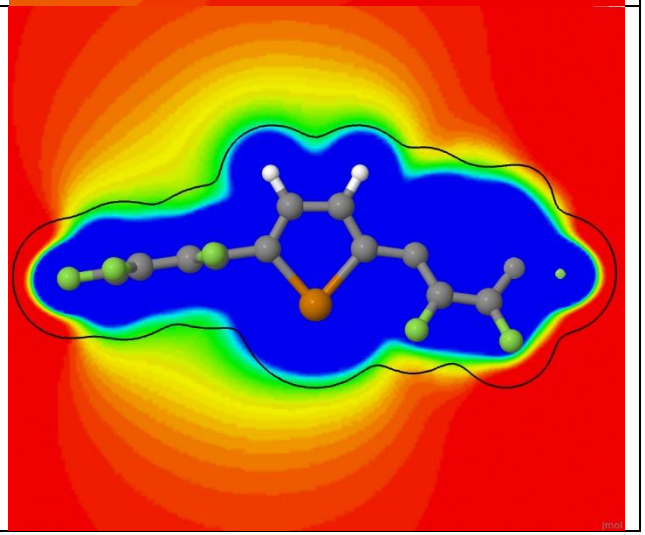
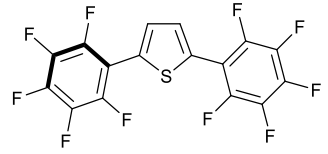
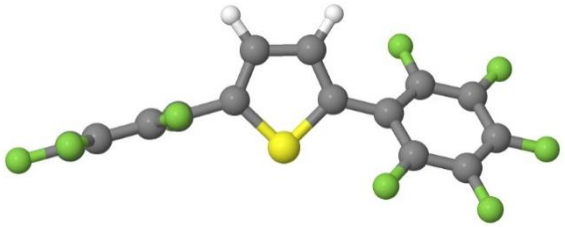
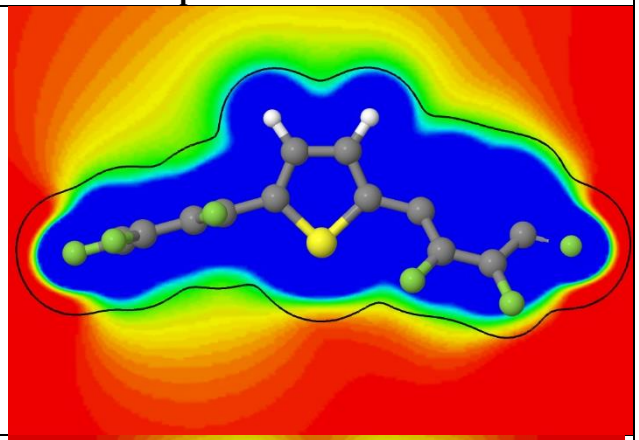
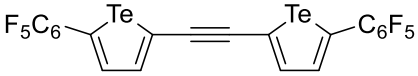
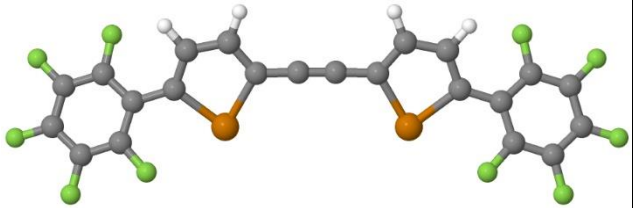
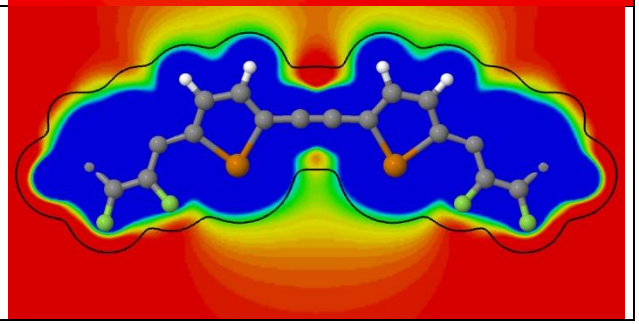
Donor	Geometry	Scaled 0 – 29.6 kcal/mol
 **1c[a]**		
 **1c[b]**		
 **1d**		
 **2,5-Bis(pentafluorophenyl)thiophene**		
 **2**		

Table S 7 Fixed 90° geometries and ESP contour plots obtained when scaling from 0 kcal/mol (red) to 29.6 kcal/mol (blue), the $V_{S,Max}$ of **1d**, the largest in the series.

Donor	Geometry	Contour plot scaled at 0 – 29.6 kcal/mol
 **1a**		
 **1b**		
 **1c**[a]		

Donor	Geometry	Contour plot scaled at 0 – 29.6 kcal/mol
 **1c[b]**		
 **1d**		

Donor	Geometry	Contour plot scaled at 0 – 29.6 kcal/mol
 2,5-Bis(pentafluorophenyl)thiophene		
 **2**		

3.3 Optimized Geometries

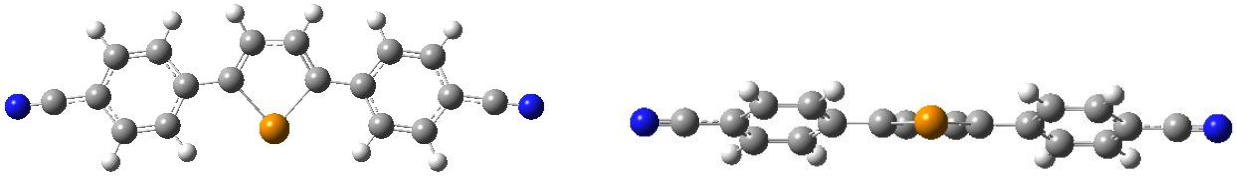
3.3.1 ESP Geometries

Optimized ESP geometries at the B97D3/Def2TZVP level of theory can be seen in section 3.2.2 above.

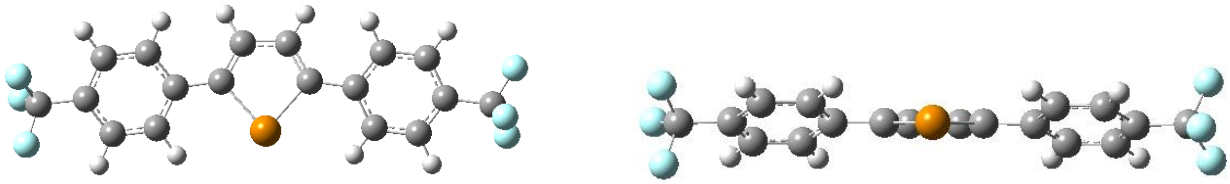
3.3.2 Donor Geometries

Optimized donor geometries at the B97D3/Def2TZVP PCM(THF) level of theory are presented below.

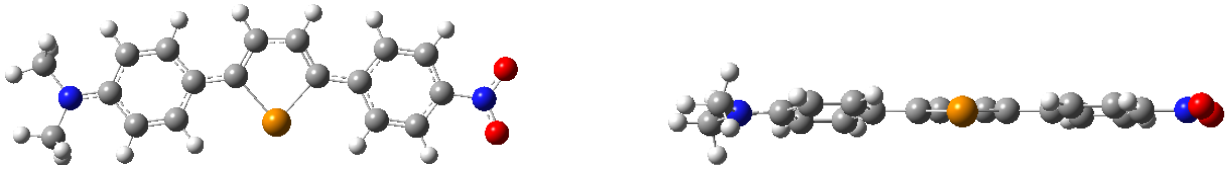
3.3.2.1 1a



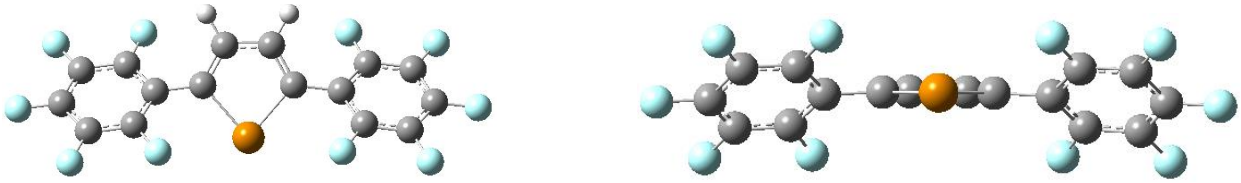
3.3.2.2 1b



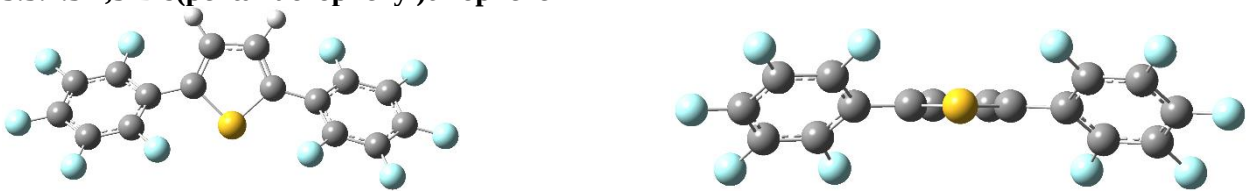
3.3.2.3 1c



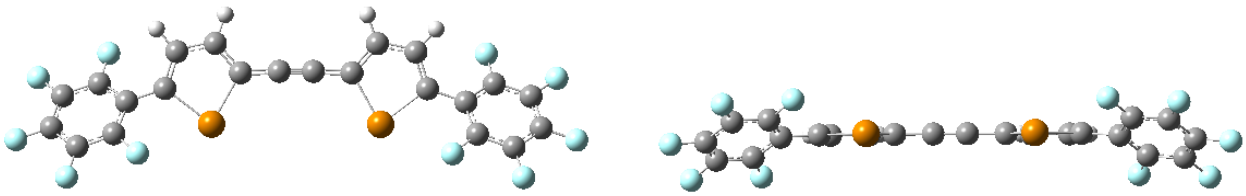
3.3.2.4 1d



3.3.2.5 2,5-Bis(pentafluorophenyl)thiophene



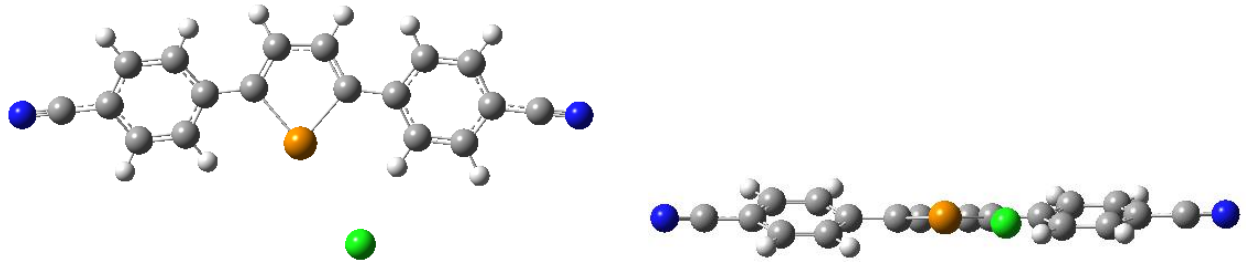
3.3.2.6 2



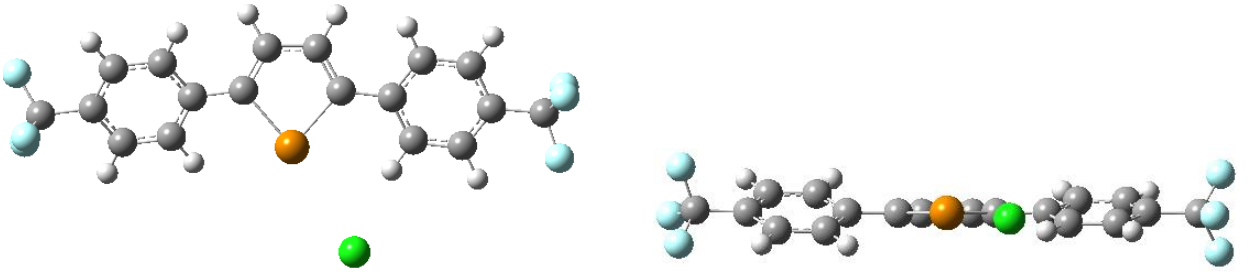
3.3.3 Donor Acceptor Complex Geometries

Optimized donor acceptor complex geometries at the B97D3/Def2TZVP PCM(THF) level of theory are presented below.

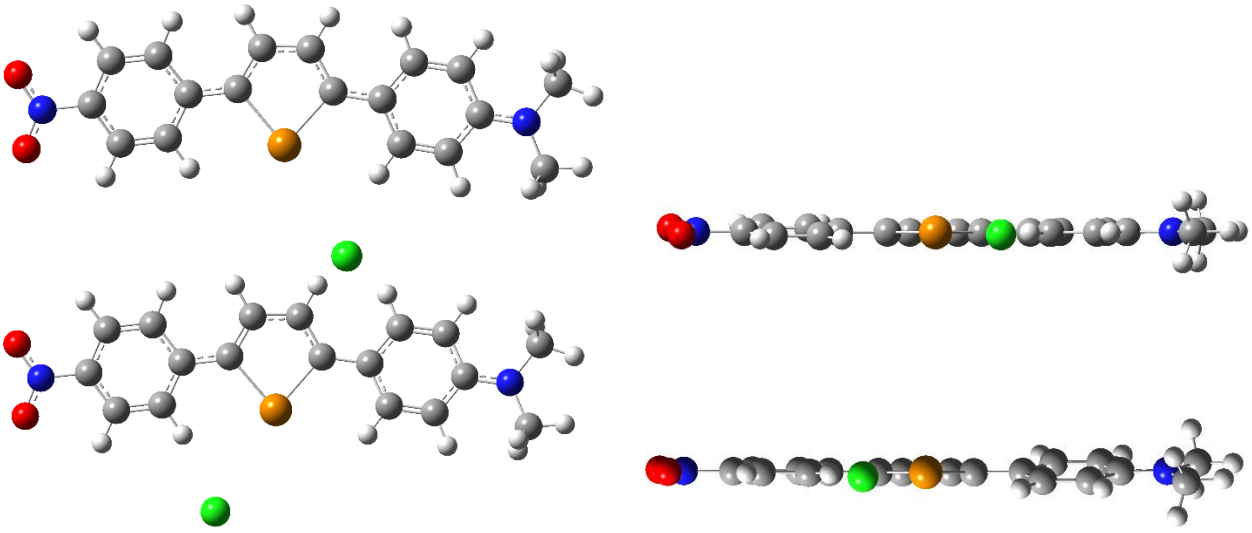
3.3.3.1 1a-Cl



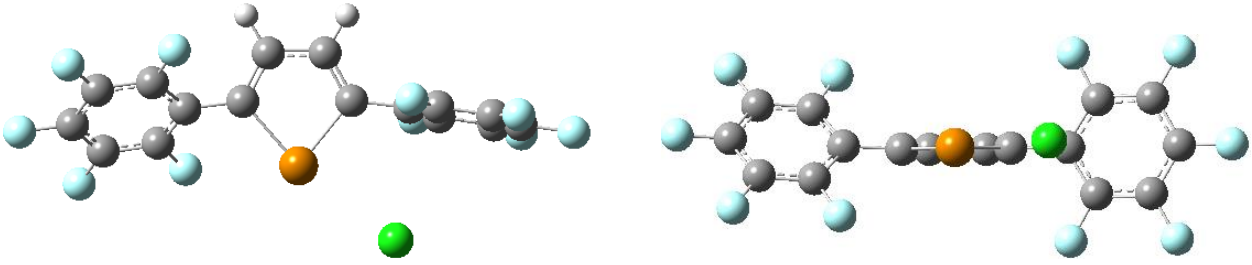
3.3.3.2 1b-Cl



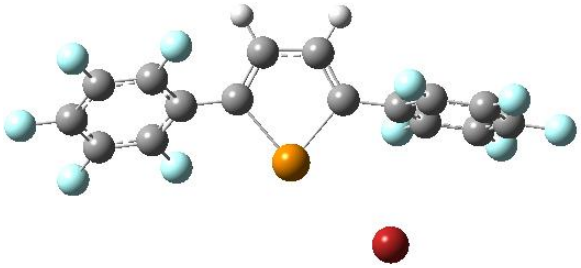
3.3.3.3 1c-Cl

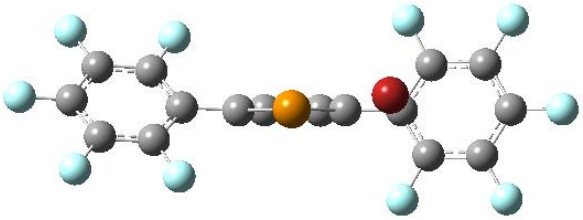


3.3.3.4 1d-Cl

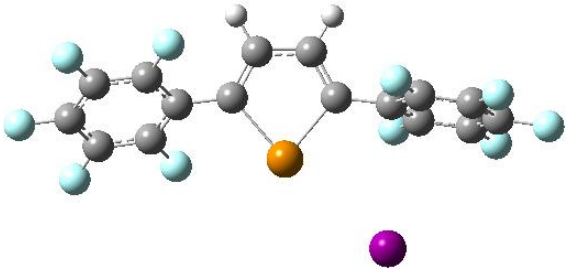


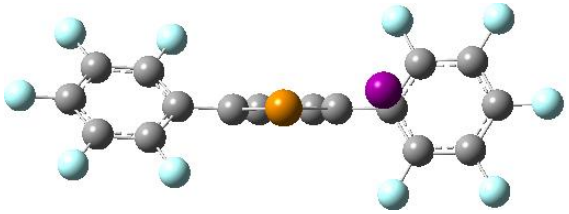
3.3.3.5 1d-Br



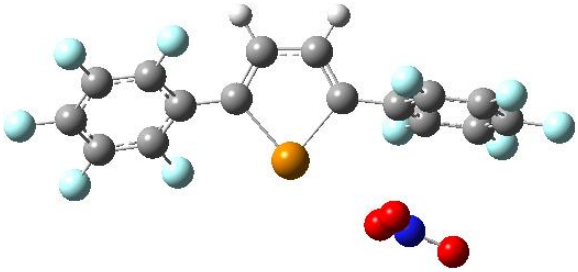


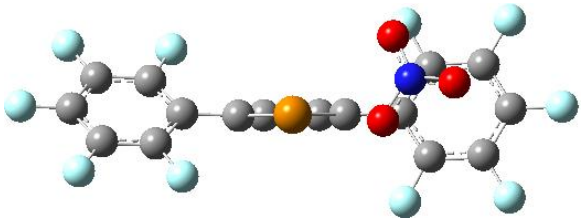
3.3.3.6 1d-I



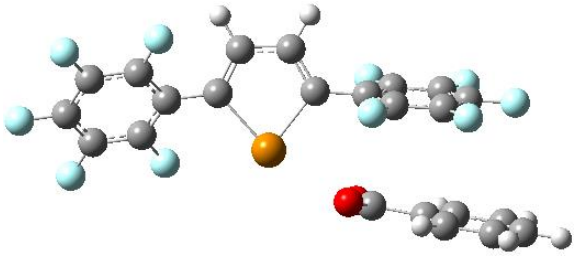


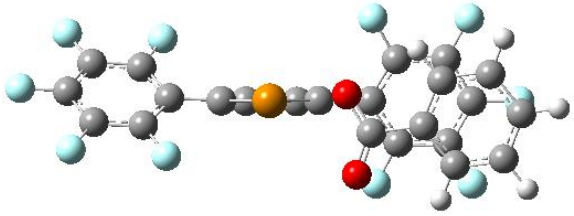
3.3.3.7 1d-NO_3



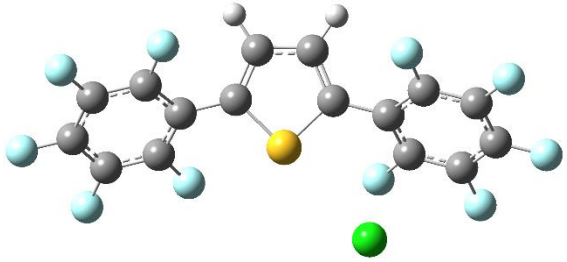


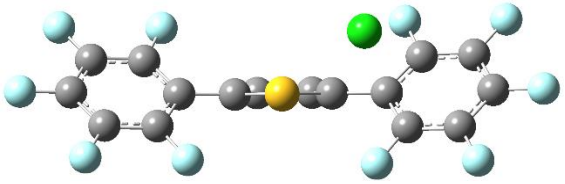
3.3.3.8 1d-OBz



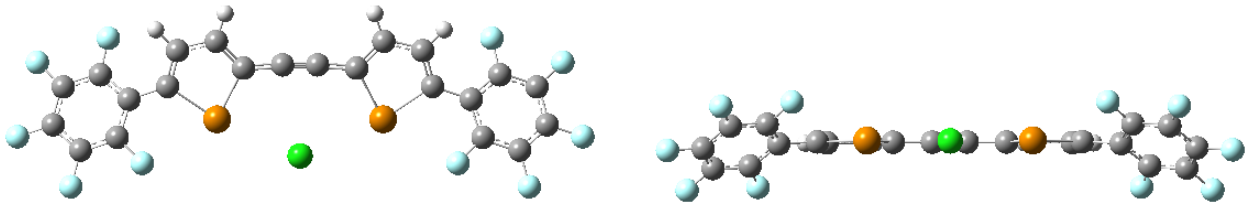


3.3.3.8 2,5-Bis(pentafluorophenyl)thiophene-Cl

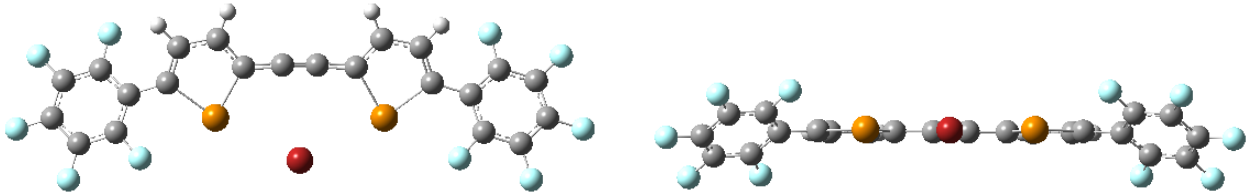




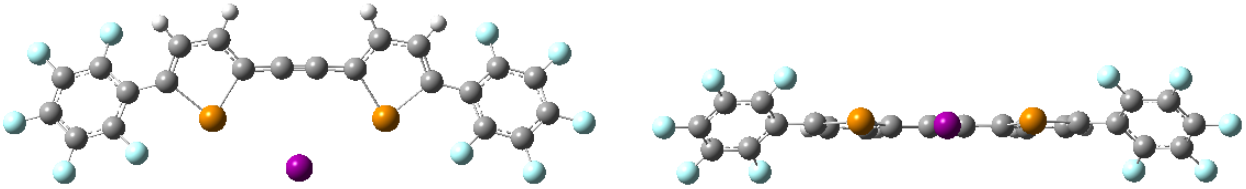
3.3.3.9 2-Cl



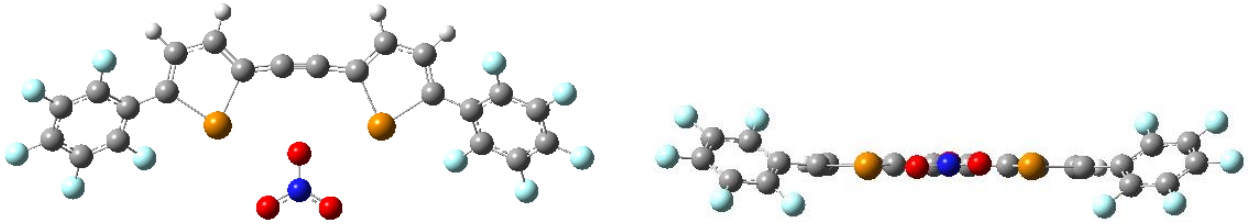
3.3.3.10 2-Br



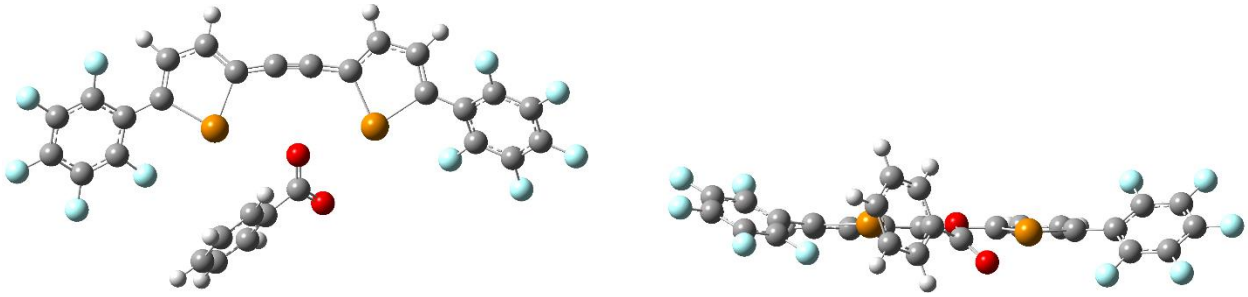
3.3.3.11 2-I



3.3.3.12 2-NO_3



3.3.3.13 2-OBz



3.3.4 Cartesian Coordinates

3.3.4.1 nomenclature

All optimized structures used for modeling chalcogen bonded complexes are reported using the following filename format:

<purpose>_<donor>-<acceptor>_<misc>.out

Where:

<purpose> : ESP, ESP90 (ESP with one aromatic ring fixed at 90°), ESPComplex (ESP with aromatic ring fixed in its binding conformation with chloride), or binding

<donor> : The name of the chalcogen bond donor being modeled; **1a-d**, **2**, or 2,5-Bis(pentafluorophenyl)thiophene.

<acceptor> : The anion being modeled with the donor; Cl, Br, I, NO_3, OBz, or no entry for ESP calculations and donor calculations without acceptor

<misc> : Mainly contains information relevant to donor **1c** and its unsymmetrical nature. NO2 or NMe2 represents which aryl ring is rotated 90° for esp calculations or towards which ring the Cl is located for binding geometries.

3.3.4.2 ESP Coordinates

==========
ESP90_1a.out
==========

C	-0.703216	1.805659	0.407719
C	-1.373498	0.643537	0.140084
C	-2.829639	0.440572	0.092812
C	-3.536406	0.613110	-1.108551
H	-1.256951	2.718520	0.619838
C	1.384524	0.618639	0.157542
C	0.722988	1.794777	0.413748
C	-3.536262	0.066741	1.247717
C	-4.912813	0.428707	-1.157304
C	-4.912651	-0.119790	1.210705
C	-5.611748	0.060225	0.004890
C	2.824852	0.408938	0.103565
C	3.401909	-0.847374	0.375782
C	3.691669	1.472310	-0.227512
C	4.774149	-1.038963	0.331313
C	5.065632	1.294091	-0.268068
C	5.624560	0.033979	0.011589
Te	-0.012883	-0.912045	-0.203614
H	2.760234	-1.680735	0.652762
H	5.200785	-2.013030	0.549518
H	5.718671	2.121264	-0.529095
H	3.274361	2.442312	-0.479061
H	-2.992895	0.895024	-2.005788
H	-5.455764	0.566766	-2.087164
H	-2.992554	-0.073889	2.177541
H	-5.455595	-0.403695	2.106868
C	7.037372	-0.155017	-0.035359
C	-7.026340	-0.131687	-0.039320
N	8.189513	-0.309070	-0.073041
N	-8.177738	-0.287709	-0.075188
H	1.276721	2.700542	0.651987

==========
ESP90_1b.out
==========

C	-0.709793	1.820240	0.422738
C	-1.376699	0.658577	0.147215
C	-2.832893	0.450910	0.102636
C	-3.536164	0.069165	1.255235
C	1.382796	0.644799	0.157112
C	0.717391	1.815025	0.425217
H	-1.266654	2.729071	0.644259
C	-3.544462	0.626708	-1.094271
C	-4.914779	-0.120920	1.217532
C	-4.922483	0.437069	-1.136410
C	-5.610983	0.059281	0.019754
C	2.825555	0.440588	0.098631
C	3.409630	-0.808507	0.381183
C	3.685627	1.501916	-0.248625
C	4.785450	-0.991611	0.328898
C	5.062690	1.325330	-0.293990
C	5.621918	0.075870	-0.009677
Te	-0.009301	-0.887346	-0.215274
H	2.773720	-1.642413	0.669726
H	5.210872	-1.964683	0.552641
H	5.704682	2.155660	-0.570332
H	3.263447	2.467247	-0.510346
H	-2.990920	-0.076919	2.183400
H	-5.446759	-0.413996	2.116830
H	-3.005626	0.913096	-1.993001
H	-5.461551	0.577187	-2.068002
C	7.117287	-0.107732	-0.013790
C	-7.111542	-0.092673	-0.017592
F	7.738998	0.737940	-0.875461
F	7.480371	-1.370397	-0.359323
F	7.653997	0.127384	1.219367
F	-7.551109	-0.557160	-1.215751
F	-7.737191	1.101803	0.191242
F	-7.569276	-0.944802	0.934243
H	1.269066	2.720613	0.669467

==========
ESP90_1c_NMe2.out
==========

Te	0.070858	-0.869940	-0.245075
C	-1.285435	0.676895	0.189250
C	-2.740110	0.490307	0.133328
C	-3.463808	0.071486	1.259896
C	1.484279	0.624567	0.196633
C	0.829367	1.789123	0.524343
C	-0.595082	1.811578	0.523422
H	-1.140117	2.715650	0.789528
C	-3.457290	0.703636	-1.053396
C	-4.834128	0.530768	-1.113758
C	-4.840912	-0.104631	1.216812
C	-5.570898	0.134558	0.027972
C	2.921493	0.414330	0.129770
C	3.489872	-0.870798	0.258946
C	3.800862	1.502585	-0.071868
C	4.860991	-1.068056	0.201720
C	5.174028	1.319744	-0.124705
C	5.696500	0.033023	0.013552
H	2.839701	-1.725213	0.431635
H	5.294574	-2.055606	0.307353
H	5.847633	2.153626	-0.284894
H	3.394238	2.498746	-0.213493
H	-2.919610	1.008589	-1.947879
H	-5.336088	0.707041	-2.057712
H	-2.931101	-0.121941	2.187777
H	-5.348686	-0.431995	2.116372
H	1.388918	2.676338	0.814017
N	7.155762	-0.167675	-0.047504
O	7.863722	0.825039	-0.212350
O	7.580907	-1.316211	0.070762
N	-6.945019	-0.008431	-0.014913
C	-7.631996	0.042027	-1.293045
H	-8.705333	-0.061323	-1.124282
H	-7.464339	1.004245	-1.792009
H	-7.309607	-0.759059	-1.978229
C	-7.640492	-0.596301	1.116061
H	-7.327321	-1.634864	1.312469
H	-7.469841	-0.011709	2.028115
H	-8.713299	-0.592589	0.915131

==========
ESP90_1c_NO2.out
==========

Te	0.096371	-0.860715	-0.268465
C	1.473276	0.651775	0.202850
C	2.926763	0.444880	0.132082
C	3.639746	-0.019504	1.251241
C	0.807894	1.786472	0.572816
C	-0.620344	1.780582	0.596999
C	-1.295700	0.637018	0.248904
H	-1.166340	2.664269	0.921369
C	-2.733867	0.430075	0.181984
C	-3.612672	1.505408	-0.054995
C	-3.322187	-0.837465	0.339365
C	-4.986960	1.333247	-0.109824
C	-4.694163	-1.029323	0.283819
C	-5.575160	0.058054	0.072612
C	3.630031	0.707491	-1.056543
C	5.016322	-0.208006	1.193825
C	5.006650	0.523795	-1.128186
C	5.683178	0.067124	0.001348
H	3.099175	-0.229837	2.169480
H	5.576889	-0.560729	2.051655
H	5.559642	0.727514	-2.037684
H	3.081877	1.060045	-1.925398
H	-3.204037	2.496864	-0.229982
H	-5.606806	2.198478	-0.314199
H	-2.685217	-1.699035	0.532786
H	-5.081668	-2.032985	0.412309
H	1.366705	2.676439	0.858956
N	7.150920	-0.131312	-0.067494
O	7.710953	0.121724	-1.131085
O	7.719286	-0.536673	0.943192
N	-6.944995	-0.116720	0.045833
C	-7.802114	0.983534	-0.358039
H	-8.844591	0.671127	-0.275901
H	-7.661595	1.851395	0.297365
H	-7.616391	1.304633	-1.396006
C	-7.498099	-1.459437	0.035119
H	-7.193252	-2.034317	-0.854442
H	-7.187075	-2.019536	0.925213
H	-8.587558	-1.395639	0.047191

==========
ESP90_1d.out
==========

Te	-0.030407	-0.733121	-0.704960
C	-1.373580	0.413391	0.409753
C	-2.830889	0.294556	0.265595
C	-3.570851	-0.607861	1.042941
C	-0.702105	1.209784	1.295845
C	0.720683	1.173148	1.310692
C	1.376872	0.324636	0.448366
H	1.272513	1.801537	2.002011
C	2.822335	0.200949	0.280227
C	3.440832	-0.996502	-0.130177
C	3.702226	1.283055	0.500388
C	4.816808	-1.128629	-0.292937
C	5.082799	1.175600	0.345580
C	5.649045	-0.036300	-0.049798
C	-3.540973	1.060967	-0.669097
C	-4.922014	0.944878	-0.824742
C	-4.952049	-0.742919	0.905842
C	-5.629017	0.038294	-0.032544
F	-2.885881	1.937329	-1.446081
F	-5.574171	1.694332	-1.723211
F	-6.953192	-0.080573	-0.171490
F	-5.632931	-1.611380	1.665116
F	-2.945315	-1.374433	1.949365
F	3.226283	2.490784	0.848893
F	5.871047	2.236078	0.564064
F	6.972163	-0.148145	-0.198643
F	5.344798	-2.298262	-0.675366
F	2.690104	-2.087867	-0.385760
H	-1.248259	1.857674	1.978348

==========
ESP90_2,5-Bis(pentafluorophenyl)thiophene.out
==========

S	0.027981	0.329723	-0.460899
C	1.248093	-0.350119	0.557356
C	2.676851	-0.177573	0.238933
C	3.405845	0.914505	0.726888
C	0.689476	-1.009186	1.629161
C	-0.725041	-0.973670	1.623252
C	-1.250310	-0.276806	0.549979
H	-1.342030	-1.435811	2.383823
C	-2.663352	-0.076342	0.219665
C	-3.160376	1.130238	-0.305389
C	-3.611618	-1.097885	0.417621
C	-4.506884	1.317573	-0.610954
C	-4.963513	-0.931364	0.123402
C	-5.416555	0.282465	-0.394149
C	3.361684	-1.101356	-0.560991
C	4.715452	-0.953851	-0.862816
C	4.760010	1.084722	0.439009
C	5.414723	0.144948	-0.359667
F	2.712052	-2.164341	-1.057269
F	5.347888	-1.853114	-1.627125
F	6.711801	0.296875	-0.642059
F	5.434937	2.136198	0.920265
F	2.799314	1.831201	1.494935
F	-3.228053	-2.298121	0.884392
F	-5.828550	-1.934319	0.321371
F	-6.710681	0.451638	-0.680653
F	-4.934380	2.488946	-1.098527
F	-2.330703	2.167215	-0.514251
H	1.284803	-1.497120	2.393018

==========
ESPComplex_1d.out
==========

Te	-0.031044	-0.790954	-0.641083
C	-1.375210	0.380039	0.446371
C	-2.831638	0.281591	0.283465
C	-3.534758	1.179173	-0.533147
C	-0.702600	1.225735	1.285033
C	0.720207	1.201922	1.288894
C	1.377414	0.327074	0.453414
H	1.270914	1.861243	1.951370
C	2.822216	0.210258	0.275798
C	3.446867	-0.989366	-0.119630
C	3.696992	1.302483	0.467126
C	4.821989	-1.113945	-0.294795
C	5.076659	1.202554	0.300096
C	5.648530	-0.011575	-0.079765
C	-3.577502	-0.727920	0.908473
C	-4.914398	1.088302	-0.715546
C	-4.957278	-0.840670	0.740898
C	-5.627268	0.073149	-0.074847
F	-2.874200	2.157742	-1.170572
F	-5.559295	1.962426	-1.499294
F	-6.950199	-0.022921	-0.241130
F	-5.643713	-1.811322	1.357967
F	-2.959831	-1.619457	1.699280
F	3.216893	2.513527	0.798317
F	5.858586	2.272849	0.491770
F	6.970826	-0.115970	-0.240693
F	5.354574	-2.286118	-0.662810
F	2.703049	-2.091427	-0.349101
H	-1.248174	1.901574	1.940326

==========
ESP_2.out
==========

C	1.996558	1.187771	0.477026
C	2.895239	2.199341	0.775948
C	4.278587	1.936560	0.674138
C	4.710911	0.678073	0.294411
H	4.992114	2.720362	0.903917
C	6.089647	0.263181	0.075280
C	6.507419	-1.080729	0.175207
C	7.111825	1.174511	-0.278085
C	7.819442	-1.493974	-0.033016
C	8.432367	0.785679	-0.489449
C	8.796040	-0.555090	-0.364027
F	6.834769	2.478089	-0.457943
F	9.356861	1.694399	-0.827039
F	10.061637	-0.935510	-0.563314
F	8.149792	-2.786201	0.088488
F	5.612013	-2.041352	0.488516
Te	3.043817	-0.567796	-0.026880
C	0.614205	1.228895	0.501906
C	-0.614174	1.228870	0.501626
C	-1.996533	1.187723	0.476820
C	-2.895224	2.199292	0.775721
C	-4.278571	1.936483	0.673970
H	-2.530968	3.176390	1.082679
C	-4.710886	0.677964	0.294352
H	-4.992114	2.720289	0.903706
C	-6.089636	0.263106	0.075260
C	-7.111741	1.174499	-0.278126
C	-6.507513	-1.080770	0.175262
C	-8.432319	0.785770	-0.489453
C	-7.819572	-1.493915	-0.032930
C	-8.796099	-0.554965	-0.363973
Te	-3.043782	-0.567889	-0.026958
H	2.530975	3.176413	1.082977
F	-5.612194	-2.041459	0.488615
F	-8.150030	-2.786108	0.088642
F	-10.061729	-0.935293	-0.563226
F	-9.356743	1.694555	-0.827061
F	-6.834562	2.478049	-0.458000

3.3.4.3 Donor Coordinates

==========
binding_1a.out
==========

C	1.380431	0.608516	0.144315
C	0.708514	1.790201	0.375519
C	-0.708574	1.790199	0.375533
C	-1.380441	0.608475	0.144325
H	-1.253743	2.706440	0.590232
C	-2.820903	0.416421	0.090955
C	-3.679107	1.503277	-0.190721
C	-3.409433	-0.846298	0.311728
C	-5.053959	1.340391	-0.234830
C	-4.782767	-1.023467	0.264974
C	-5.621757	0.072755	-0.006348
C	2.820896	0.416433	0.090940
C	3.409372	-0.846480	0.310728
C	3.679190	1.503475	-0.189758
C	4.782701	-1.023666	0.263976
C	5.054038	1.340570	-0.233882
C	5.621776	0.072732	-0.006379
Te	-0.000001	-0.944301	-0.164109
H	2.777984	-1.699697	0.545601
H	5.215539	-2.002902	0.441598
H	5.697977	2.185914	-0.455162
H	3.257846	2.481558	-0.396845
H	-3.257650	2.481148	-0.398591
H	-5.697861	2.185573	-0.456834
H	-2.778053	-1.699294	0.547417
H	-5.215675	-2.002539	0.443330
C	7.034849	-0.100125	-0.055174
C	-7.034836	-0.100080	-0.055164
N	8.189375	-0.241366	-0.094400
N	-8.189356	-0.241352	-0.094413
H	1.253626	2.706492	0.590195

==========
binding_1b.out
==========

C	-1.381990	0.637069	-0.143558
C	-0.712850	1.814745	-0.391705
C	0.706734	1.816415	-0.399771
C	1.380930	0.640046	-0.160193
H	1.250928	2.730172	-0.628559
C	2.824170	0.447562	-0.117381
C	3.681658	1.524183	0.193049
C	3.413877	-0.804163	-0.381359
C	5.060231	1.358990	0.221255
C	4.791637	-0.975632	-0.348081
C	5.624643	0.108751	-0.054304
C	-2.824206	0.440762	-0.085088
C	-3.411018	-0.820563	-0.306138
C	-3.684517	1.522133	0.201412
C	-4.787449	-0.997909	-0.253123
C	-5.061717	1.351332	0.248148
C	-5.622376	0.088777	0.025530
Te	0.003567	-0.909557	0.179015
H	-2.779247	-1.672649	-0.544871
H	-5.210769	-1.981208	-0.430457
H	-5.700418	2.199022	0.474756
H	-3.266160	2.501126	0.411385
H	3.259779	2.494613	0.433927
H	5.697253	2.203177	0.464906
H	2.783267	-1.650409	-0.642674
H	5.218230	-1.950111	-0.562599
C	-7.115481	-0.087449	0.029410
C	7.113016	-0.086409	0.031840
F	-7.742374	0.787196	0.860458
F	-7.493558	-1.336616	0.410848
F	-7.653869	0.112155	-1.214070
F	7.562564	-1.050032	-0.816019
F	7.504302	-0.468472	1.287464
F	7.806338	1.047285	-0.254227
H	-1.260742	2.727740	-0.614335

==========
binding_1c.out
==========

C	1.484711	0.647463	0.077334
C	0.801468	1.842901	0.213401
C	-0.609869	1.847114	0.221675
C	-1.297522	0.651045	0.092163
H	-1.146577	2.783337	0.354830
C	-2.728846	0.451570	0.062680
C	-3.619616	1.537499	-0.107409
C	-3.318426	-0.823597	0.195953
C	-4.991129	1.366465	-0.135589
C	-4.687549	-1.016110	0.171913
C	-5.576260	0.079330	0.006802
C	2.913717	0.448912	0.051689
C	3.487412	-0.846289	0.069874
C	3.808287	1.550570	0.000620
C	4.856159	-1.040849	0.045035
C	5.178243	1.369198	-0.022297
C	5.704625	0.071085	0.000408
Te	0.087514	-0.924997	-0.096515
H	2.840950	-1.719217	0.116218
H	5.277299	-2.038905	0.062929
H	5.849667	2.218642	-0.063804
H	3.418336	2.561881	-0.033882
H	-3.224707	2.540310	-0.239931
H	-5.618887	2.238501	-0.276256
H	-2.682095	-1.694720	0.342814
H	-5.073612	-2.021959	0.285057
H	1.339922	2.779541	0.338620
N	7.144691	-0.123197	-0.025712
O	7.873038	0.877865	-0.060533
O	7.583119	-1.281341	-0.011449
N	-6.932159	-0.096261	-0.016699
C	-7.817569	1.042806	-0.210000
H	-8.849603	0.692827	-0.219334
H	-7.710232	1.778585	0.598365
H	-7.617942	1.548866	-1.163926
C	-7.504299	-1.425634	0.139650
H	-7.200184	-2.095484	-0.676242
H	-7.199999	-1.881696	1.090742
H	-8.591264	-1.347507	0.131873

==========
binding_1d.out
==========

C	-1.378765	0.395907	0.371880
C	-0.709538	1.411214	1.017360
C	0.709556	1.411211	1.017365
C	1.378778	0.395906	0.371894
H	1.253212	2.195016	1.536227
C	2.826529	0.276837	0.222777
C	3.497287	-0.959924	0.258148
C	3.647644	1.403759	0.012941
C	4.875831	-1.078996	0.112446
C	5.028935	1.309088	-0.136127
C	5.651144	0.062723	-0.083846
C	-2.826524	0.276833	0.222766
C	-3.647684	1.403768	0.013108
C	-3.497265	-0.959945	0.257955
C	-5.028969	1.309082	-0.135948
C	-4.875811	-1.079031	0.112258
C	-5.651154	0.062695	-0.083842
F	-3.107061	2.631435	-0.085393
F	-5.765266	2.411294	-0.342996
F	-6.978247	-0.037312	-0.223535
F	-5.463582	-2.283313	0.168565
F	-2.799358	-2.097660	0.448411
F	3.106973	2.631394	-0.085713
F	5.765192	2.411294	-0.343344
F	6.978236	-0.037288	-0.223551
F	5.463638	-2.283255	0.168922
F	2.799388	-2.097614	0.448783
Te	0.000015	-0.951492	-0.456742
H	-1.253189	2.195020	1.536220

==========
binding_2,5-Bis(pentafluorophenyl)thiophene.out
==========

C	-1.252900	0.453981	0.408334
C	-0.705339	1.485835	1.151351
C	0.705340	1.485836	1.151353
C	1.252900	0.453981	0.408337
H	1.306046	2.207348	1.691173
C	2.671408	0.180054	0.171760
C	3.208252	-1.119523	0.154186
C	3.586735	1.225688	-0.051397
C	4.560320	-1.369476	-0.065657
C	4.943357	0.998597	-0.268568
C	5.436060	-0.305615	-0.276573
C	-2.671408	0.180055	0.171759
C	-3.586735	1.225689	-0.051401
C	-3.208251	-1.119522	0.154189
C	-4.943357	0.998596	-0.268570
C	-4.560318	-1.369476	-0.065654
C	-5.436059	-0.305615	-0.276572
F	-3.162995	2.501120	-0.089433
F	-5.776933	2.026441	-0.485717
F	-6.737569	-0.534027	-0.485291
F	-5.027216	-2.626386	-0.060226
F	-2.413739	-2.182176	0.378223
F	3.162996	2.501119	-0.089427
F	5.776933	2.026442	-0.485713
F	6.737570	-0.534025	-0.485294
F	5.027217	-2.626385	-0.060232
F	2.413743	-2.182180	0.378221
S	-0.000006	-0.521168	-0.293726
H	-1.306046	2.207347	1.691170

==========
binding_2.out
==========

C	1.997467	1.170582	0.563365
C	2.902980	2.146769	0.947831
C	4.285347	1.878778	0.827458
C	4.701829	0.651657	0.347262
H	5.009487	2.630341	1.125936
C	6.079983	0.245199	0.102064
C	6.516972	-1.087818	0.234872
C	7.072402	1.161851	-0.308338
C	7.829085	-1.485747	0.001221
C	8.391614	0.786820	-0.547166
C	8.778591	-0.543108	-0.389510
F	6.761934	2.453424	-0.521865
F	9.292963	1.697936	-0.944105
F	10.045207	-0.911215	-0.615138
F	8.187430	-2.768754	0.157786
F	5.645723	-2.046519	0.611936
Te	3.029210	-0.546348	-0.093915
C	0.614304	1.218368	0.591774
C	-0.614308	1.218409	0.591785
C	-1.997467	1.170542	0.563384
C	-2.903023	2.146744	0.947713
C	-4.285379	1.878685	0.827358
H	-2.547713	3.097769	1.336196
C	-4.701821	0.651492	0.347317
H	-5.009550	2.630267	1.125719
C	-6.079969	0.245051	0.102070
C	-7.072354	1.161843	-0.308095
C	-6.517043	-1.087968	0.234636
C	-8.391594	0.786948	-0.546957
C	-7.829189	-1.485769	0.000937
C	-8.778645	-0.542995	-0.389578
Te	-3.029137	-0.546417	-0.093941
H	2.547621	3.097732	1.336419
F	-5.645882	-2.046821	0.611527
F	-8.187612	-2.768780	0.157283
F	-10.045297	-0.910969	-0.615219
F	-9.292911	1.698203	-0.943639
F	-6.761809	2.453460	-0.521256

3.3.4.4 Complex Coordinates

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binding_1a-Cl.out
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C	1.193712	-0.968473	0.093512
C	0.476556	-2.143040	0.226965
C	-0.937321	-2.099898	0.225379
C	-1.561271	-0.875556	0.095974
H	-1.510222	-3.015336	0.362645
C	-2.995521	-0.642985	0.062505
C	-3.550134	0.610595	0.402683
C	-3.888417	-1.670837	-0.320869
C	-4.917337	0.831180	0.375033
C	-5.257629	-1.465136	-0.347407
C	-5.789693	-0.208911	0.002480
C	2.644809	-0.851632	0.061263
C	3.454804	-1.992836	-0.152473
C	3.292679	0.389318	0.235939
C	4.836277	-1.903827	-0.167796
C	4.674648	0.489831	0.215732
C	5.465233	-0.657692	0.020874
Te	-0.128876	0.668615	-0.068229
Cl	1.745978	3.556661	-0.176134
H	-5.925831	-2.266354	-0.648004
H	-3.495038	-2.636235	-0.622347
H	-5.321169	1.801555	0.646298
H	-2.894318	1.418751	0.716049
H	2.712630	1.302349	0.369113
H	2.994701	-2.959691	-0.326575
H	5.439574	-2.790870	-0.335369
H	5.148733	1.457466	0.349036
C	6.885451	-0.563200	0.003578
C	-7.196408	0.007066	-0.024654
N	-8.347409	0.181763	-0.045753
N	8.047560	-0.489307	-0.009045
H	0.987168	-3.093819	0.362613

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binding_1b-Cl.out
==========

C	-1.238523	-0.907268	-0.085699
C	-0.546070	-2.094132	-0.218303
C	0.871166	-2.079001	-0.226472
C	1.520189	-0.869132	-0.108078
H	1.425859	-3.006204	-0.361639
C	2.961608	-0.662707	-0.085336
C	3.540982	0.562987	-0.472547
C	3.834169	-1.691468	0.333240
C	4.916939	0.752990	-0.454596
C	5.210158	-1.509204	0.346387
C	5.762730	-0.286230	-0.053190
C	-2.689142	-0.756710	-0.048478
C	-3.524254	-1.877083	0.171329
C	-3.310271	0.494432	-0.224128
C	-4.905118	-1.752302	0.189325
C	-4.694603	0.622920	-0.199588
C	-5.502676	-0.498543	0.002296
Te	0.119681	0.702632	0.061362
Cl	-1.698003	3.660019	0.203285
H	5.856299	-2.317616	0.674592
H	3.422658	-2.637338	0.671141
H	5.331791	1.706693	-0.764387
H	2.901973	1.372754	-0.815651
H	-2.711813	1.394757	-0.361412
H	-3.086353	-2.854004	0.347803
H	-5.521968	-2.629341	0.362982
H	-5.139099	1.603622	-0.333635
C	-6.999677	-0.395447	-0.005966
C	7.247813	-0.076820	0.016820
F	-7.544913	-0.934126	-1.143632
F	-7.572320	-1.071784	1.033856
F	-7.447874	0.883078	0.064842
F	7.686936	0.876862	-0.847079
F	7.948839	-1.211719	-0.259473
F	7.652335	0.322290	1.264443
H	-1.076264	-3.035650	-0.345157

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binding_1c-Cl_NMe2.out
==========

C	-1.127617	-0.998198	-0.027936
C	-0.401125	-2.182077	-0.059251
C	1.006581	-2.136127	-0.056829
C	1.648206	-0.907626	-0.025243
H	1.570619	-3.066124	-0.092203
C	3.069737	-0.673823	-0.014488
C	3.609747	0.635907	-0.096946
C	3.999612	-1.745170	0.082737
C	4.971598	0.869618	-0.088963
C	5.362952	-1.524713	0.090712
C	5.855072	-0.214119	0.003755
C	-2.566120	-0.852152	-0.019338
C	-3.426539	-1.976041	-0.029802
C	-3.189479	0.414535	0.001979
C	-4.803725	-1.848016	-0.019281
C	-4.564001	0.560091	0.012756
C	-5.423175	-0.569398	0.003056
Te	0.202843	0.640953	0.010006
Cl	-1.779433	3.753356	0.018738
H	6.058586	-2.351997	0.168097
H	3.639577	-2.765062	0.162957
H	5.363058	1.877716	-0.155816
H	2.938980	1.487584	-0.178222
H	-2.591259	1.327285	0.009260
H	-3.009465	-2.978563	-0.045139
H	-5.408085	-2.747726	-0.027456
H	-4.971139	1.564561	0.028542
H	-0.907266	-3.144237	-0.088176
N	7.283358	0.019687	0.012850
N	-6.785848	-0.434797	0.014918
O	7.693910	1.188452	-0.061131
O	8.043509	-0.958669	0.094149
C	-7.391501	0.888398	0.040167
H	-7.091271	1.451176	0.934071
H	-7.110753	1.476975	-0.843513
H	-8.476412	0.782584	0.050642
C	-7.640392	-1.611533	0.000885
H	-7.475252	-2.218631	-0.899673
H	-7.465070	-2.247441	0.879374
H	-8.683225	-1.294557	0.012048

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binding_1c-Cl_NO2.out
==========

C	-1.311928	-0.970669	-0.051775
C	-0.594580	-2.154433	-0.118745
C	0.815459	-2.123344	-0.120821
C	1.462587	-0.899252	-0.055308
H	1.374827	-3.053896	-0.194122
C	2.893492	-0.671856	-0.033841
C	3.454502	0.609976	-0.217265
C	3.810719	-1.727097	0.176995
C	4.819909	0.835276	-0.201010
C	5.179505	-1.523388	0.197980
C	5.733709	-0.229852	0.009702
C	-2.749904	-0.830397	-0.038252
C	-3.599340	-1.969836	-0.072011
C	-3.372895	0.440698	0.014049
C	-4.975239	-1.847894	-0.055134
C	-4.749765	0.572118	0.030964
C	-5.555554	-0.572532	-0.003067
Te	0.037820	0.660085	0.031401
Cl	-1.842074	3.677828	0.073509
H	5.827897	-2.374758	0.369972
H	3.440365	-2.733988	0.346110
H	5.181719	1.844624	-0.356606
H	2.798398	1.459696	-0.397028
H	-2.774771	1.352627	0.041462
H	-3.171376	-2.965569	-0.109938
H	-5.610747	-2.725225	-0.081302
H	-5.206290	1.554252	0.071364
H	-1.106140	-3.112668	-0.179350
N	7.087861	-0.019315	0.034515
C	7.626992	1.311774	-0.196784
H	7.359207	1.690856	-1.193156
H	7.260899	2.027595	0.551006
H	8.714073	1.272112	-0.126163
C	8.000234	-1.138086	0.209988
H	9.024427	-0.764743	0.212062
H	7.822691	-1.654559	1.162735
H	7.902627	-1.873999	-0.600873
N	-6.999445	-0.441778	0.016473
O	-7.491142	0.695414	0.057576
O	-7.688299	-1.474098	-0.008775

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binding_1d-Br.out
==========

C	-0.961231	0.848741	0.587371
C	-0.213402	1.836872	1.168965
C	1.208291	1.736469	1.130575
C	1.761998	0.634692	0.528619
H	1.825506	2.510999	1.580993
C	3.194861	0.410060	0.341413
C	3.808292	-0.826694	0.609931
C	4.049387	1.417905	-0.145213
C	5.168819	-1.052267	0.417908
C	5.412377	1.215506	-0.347946
C	5.979230	-0.025718	-0.063878
C	-2.425921	0.810431	0.541035
C	-3.149795	1.616305	-0.345396
C	-3.168127	-0.054793	1.353720
C	-4.539159	1.565901	-0.428724
C	-4.556557	-0.121918	1.293019
C	-5.245427	0.690940	0.394653
F	-2.499267	2.457614	-1.170797
F	-5.204117	2.350214	-1.295677
F	-6.584422	0.635639	0.326650
F	-5.238482	-0.964413	2.088218
F	-2.536032	-0.856210	2.229186
F	3.554980	2.628328	-0.467869
F	6.185641	2.205838	-0.826048
F	7.291261	-0.230407	-0.252519
F	5.709536	-2.248022	0.706138
F	3.076719	-1.848845	1.095328
Te	0.251495	-0.642783	-0.259871
Br	-2.455639	-2.089894	-1.538203
H	-0.700072	2.677746	1.659616

==========
binding_1d-Cl.out
==========

C	1.171202	0.538508	-0.601464
C	0.466222	1.362623	-1.435996
C	-0.959103	1.305587	-1.416794
C	-1.555293	0.405254	-0.570172
H	-1.541510	1.953920	-2.068431
C	-2.998040	0.270421	-0.373544
C	-3.640538	-0.979762	-0.316031
C	-3.835828	1.388707	-0.195858
C	-5.009688	-1.117637	-0.103999
C	-5.206942	1.276179	0.020849
C	-5.801586	0.016505	0.065832
C	2.632393	0.485052	-0.494471
C	3.339680	1.403212	0.288642
C	3.382367	-0.513256	-1.125489
C	4.721748	1.336308	0.445575
C	4.764137	-0.601899	-0.988010
C	5.436953	0.326749	-0.195803
F	2.677567	2.376407	0.942806
F	5.371477	2.233864	1.208702
F	6.770268	0.253606	-0.057018
F	5.455269	-1.575467	-1.607393
F	2.763316	-1.434264	-1.885546
F	-3.316710	2.632070	-0.195361
F	-5.962457	2.374579	0.197710
F	-7.122263	-0.103063	0.270805
F	-5.576563	-2.336009	-0.074671
F	-2.928396	-2.110737	-0.491361
Te	-0.094262	-0.679053	0.551722
Cl	2.401525	-1.817789	1.922721
H	0.987530	2.045056	-2.105004

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binding_1d-I.out
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C	-0.723843	1.160636	0.527317
C	0.076791	2.214410	0.877641
C	1.491756	2.048474	0.833023
C	1.989705	0.826035	0.458416
H	2.149754	2.871696	1.102251
C	3.405754	0.506963	0.283572
C	3.978466	-0.684889	0.762584
C	4.282377	1.368210	-0.404197
C	5.321851	-1.002779	0.581810
C	5.629090	1.071399	-0.598651
C	6.155706	-0.119885	-0.102331
C	-2.189345	1.179472	0.502776
C	-2.891437	1.840701	-0.512725
C	-2.956158	0.511533	1.465203
C	-4.282539	1.838491	-0.575688
C	-4.347188	0.498399	1.428043
C	-5.013564	1.164419	0.401026
F	-2.217962	2.484751	-1.483957
F	-4.925362	2.478211	-1.568181
F	-6.354005	1.156956	0.352475
F	-5.051969	-0.152613	2.368566
F	-2.345339	-0.144411	2.467586
F	3.824733	2.517099	-0.936674
F	6.424309	1.920602	-1.271588
F	7.451540	-0.414055	-0.281690
F	5.823857	-2.147693	1.073248
F	3.222432	-1.566936	1.445052
Te	0.413718	-0.520676	-0.014936
I	-2.557237	-2.276823	-1.067330
H	-0.364116	3.158320	1.192492

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binding_1d-NO3.out
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C	0.949878	-0.695368	0.663536
C	0.203810	-1.659618	1.288504
C	-1.216848	-1.578246	1.224924
C	-1.776153	-0.522644	0.544187
H	-1.830016	-2.328395	1.718266
C	-3.209266	-0.326038	0.329587
C	-3.821589	0.938785	0.406224
C	-4.071289	-1.392800	0.005457
C	-5.182454	1.136909	0.189913
C	-5.435186	-1.219318	-0.216249
C	-5.999007	0.051661	-0.122439
C	2.414693	-0.654286	0.615770
C	3.140800	-1.539930	-0.190621
C	3.155567	0.285428	1.343820
C	4.530036	-1.493946	-0.278956
C	4.543826	0.351943	1.272574
C	5.234169	-0.541220	0.454522
F	2.494044	-2.460127	-0.928191
F	5.195592	-2.352939	-1.070686
F	6.572033	-0.485723	0.376530
F	5.224028	1.267026	1.984290
F	2.523997	1.155426	2.150781
F	-3.585371	-2.640591	-0.138659
F	-6.212144	-2.269267	-0.533466
F	-7.311699	0.228697	-0.331991
F	-5.716924	2.365244	0.292158
F	-3.086253	2.024648	0.718909
Te	-0.270191	0.724612	-0.275018
H	0.692044	-2.466894	1.831195
O	2.167035	2.070600	-0.929051
O	4.058250	2.001656	-2.013575
O	2.436304	0.652441	-2.576005
N	2.893367	1.568350	-1.851582

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binding_2,5-Bis(pentafluorophenyl)thiophene-Cl.out
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C	1.048900	0.655077	-0.611990
C	0.465913	1.732419	-1.256425
C	-0.944729	1.706260	-1.218930
C	-1.444954	0.600922	-0.551806
H	-1.576490	2.459839	-1.673948
C	-2.850265	0.274071	-0.299156
C	-3.365161	-1.027291	-0.433545
C	-3.770557	1.261203	0.097346
C	-4.701928	-1.333160	-0.190468
C	-5.112179	0.978430	0.341561
C	-5.583030	-0.325797	0.198684
C	2.481099	0.387720	-0.457745
C	3.360914	1.391269	-0.022968
C	3.050490	-0.866685	-0.722836
C	4.724923	1.165864	0.139213
C	4.412051	-1.112316	-0.576078
C	5.254448	-0.092917	-0.138408
F	2.893814	2.616530	0.282867
F	5.533357	2.150819	0.567166
F	6.567540	-0.319166	0.010403
F	4.919532	-2.324909	-0.850078
F	2.281358	-1.877378	-1.161874
F	-3.365019	2.530495	0.282078
F	-5.952829	1.951145	0.728604
F	-6.871710	-0.607790	0.431438
F	-5.151223	-2.588203	-0.345228
F	-2.566694	-2.032258	-0.835816
S	-0.158255	-0.391213	0.059773
Cl	2.136157	-1.562852	2.629579
H	1.045160	2.504078	-1.750027

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binding_1d-OBz.out
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Imaginary frequency: -11.53
Vibrational mode: Rotation of non-binding aryl group and facial ‘slide’ of benzoate with binding aryl group

C	0.190950	-1.107745	0.418182
C	-0.650641	-2.045847	0.956221
C	-2.056149	-1.812467	0.924690
C	-2.499407	-0.636093	0.370593
H	-2.740411	-2.548411	1.341329
C	-3.905857	-0.275114	0.201483
C	-4.391031	1.023228	0.447552
C	-4.869978	-1.198955	-0.250228
C	-5.725175	1.380790	0.272556
C	-6.208656	-0.863980	-0.437423
C	-6.644383	0.432864	-0.172436
C	1.653518	-1.235703	0.393744
C	2.344575	-1.586124	-0.772390
C	2.427253	-1.031223	1.542587
C	3.726886	-1.743422	-0.799385
C	3.813739	-1.174471	1.539241
C	4.465629	-1.539577	0.364423
F	1.666216	-1.794554	-1.914716
F	4.355837	-2.089095	-1.937332
F	5.798964	-1.686475	0.350548
F	4.527593	-0.959742	2.659131
F	1.835233	-0.681941	2.698687
F	-4.510253	-2.461191	-0.558441
F	-7.085554	-1.781600	-0.883270
F	-7.933263	0.765115	-0.345632
F	-6.136656	2.632051	0.541525
F	-3.554393	1.981839	0.893859
Te	-0.858781	0.556238	-0.308672
H	-0.247839	-2.958637	1.391914
O	1.546869	1.425014	-1.079324
O	1.938970	2.304505	0.965356
C	2.304045	1.866009	-0.148502
C	3.804163	1.816069	-0.440063
C	4.286231	1.426460	-1.696065
C	4.727155	2.121011	0.568575
C	5.657524	1.342982	-1.939758
H	3.569767	1.174330	-2.471574
C	6.098855	2.029681	0.333342
H	4.348124	2.416765	1.542362
C	6.568955	1.641448	-0.924133
H	6.016474	1.034520	-2.919183
H	6.803050	2.256191	1.130988
H	7.638000	1.566136	-1.109188

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binding_2-Br.out
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C	1.994246	1.414013	0.557262
C	2.907207	2.398772	0.901886
C	4.289136	2.118307	0.801682
C	4.686976	0.863845	0.382844
H	5.015172	2.881585	1.068400
C	6.067989	0.448589	0.166113
C	6.516003	-0.865216	0.412771
C	7.053515	1.328082	-0.333079
C	7.828409	-1.275410	0.199741
C	8.371755	0.940000	-0.555247
C	8.768448	-0.368541	-0.285672
F	6.734760	2.596565	-0.657307
F	9.265346	1.817447	-1.043651
F	10.036975	-0.750530	-0.493604
F	8.198928	-2.537903	0.470761
F	5.659617	-1.789590	0.893909
Te	2.994723	-0.359458	-0.023474
Br	0.000034	-1.860486	-0.606784
C	0.614100	1.493658	0.585372
C	-0.614102	1.493719	0.585057
C	-1.994247	1.414036	0.557075
C	-2.907215	2.398680	0.902006
C	-4.289142	2.118180	0.801871
H	-2.555197	3.368922	1.244821
C	-4.686978	0.863772	0.382868
H	-5.015178	2.881402	1.068749
C	-6.067992	0.448527	0.166143
C	-7.053606	1.328126	-0.332698
C	-6.515938	-0.865367	0.412455
C	-8.371855	0.940063	-0.554842
C	-7.828350	-1.275547	0.199436
C	-8.768474	-0.368572	-0.285613
Te	-2.994711	-0.359397	-0.023796
H	2.555179	3.369053	1.244582
F	-5.659475	-1.789856	0.893238
F	-8.198794	-2.538132	0.470128
F	-10.037011	-0.750543	-0.493518
F	-9.265528	1.817624	-1.042892
F	-6.734938	2.596720	-0.656581

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binding_2-Cl.out
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C	1.990458	1.400908	0.618163
C	2.942232	2.342882	0.975357
C	4.311529	2.017637	0.840668
C	4.656110	0.762940	0.377232
H	5.068619	2.746944	1.116279
C	6.018714	0.308856	0.123880
C	6.427613	-1.024655	0.328998
C	7.023681	1.168076	-0.371884
C	7.721864	-1.471671	0.081487
C	8.324267	0.743301	-0.628293
C	8.682544	-0.583787	-0.398662
F	6.741242	2.454237	-0.658510
F	9.237496	1.603591	-1.111373
F	9.934056	-1.001419	-0.639732
F	8.055497	-2.752201	0.313958
F	5.549942	-1.932735	0.802954
Te	2.914387	-0.389805	-0.033395
Cl	0.000344	-1.672179	-0.561884
C	0.614081	1.515726	0.666044
C	-0.614032	1.515667	0.665954
C	-1.990413	1.400830	0.618088
C	-2.942185	2.342795	0.975346
C	-4.311483	2.017563	0.840704
H	-2.630652	3.314079	1.352807
C	-4.656107	0.762894	0.377207
H	-5.068582	2.746841	1.116350
C	-6.018748	0.308817	0.123872
C	-7.023712	1.168097	-0.371785
C	-6.427644	-1.024703	0.328902
C	-8.324302	0.743356	-0.628210
C	-7.721901	-1.471690	0.081374
C	-8.682577	-0.583754	-0.398689
Te	-2.914471	-0.389863	-0.033359
H	2.630733	3.314191	1.352781
F	-5.549965	-1.932835	0.802749
F	-8.055538	-2.752235	0.313728
F	-9.934087	-1.001354	-0.639783
F	-9.237538	1.603687	-1.111196
F	-6.741275	2.454285	-0.658297

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binding_2-I.out
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C	1.997060	1.446841	0.461939
C	2.864328	2.483486	0.771947
C	4.258007	2.250823	0.724014
C	4.712838	0.990528	0.394241
H	4.949605	3.054956	0.961865
C	6.113418	0.614793	0.237414
C	6.610668	-0.645722	0.623534
C	7.066637	1.483334	-0.335775
C	7.942894	-1.017017	0.469172
C	8.403877	1.133388	-0.501405
C	8.850634	-0.122884	-0.095370
F	6.696650	2.697068	-0.788085
F	9.267713	1.995350	-1.064620
F	10.137451	-0.467399	-0.247421
F	8.363512	-2.226737	0.873901
F	5.785787	-1.549609	1.189588
Te	3.081452	-0.314013	0.002723
I	0.000051	-2.069355	-0.797007
C	0.614143	1.485935	0.466596
C	-0.614109	1.485852	0.466586
C	-1.997028	1.446628	0.461896
C	-2.864255	2.483324	0.771933
C	-4.257940	2.250731	0.724020
H	-2.467224	3.456717	1.050394
C	-4.712827	0.990451	0.394230
H	-4.949489	3.054895	0.961899
C	-6.113418	0.614760	0.237402
C	-7.066683	1.483438	-0.335513
C	-6.610661	-0.645845	0.623252
C	-8.403935	1.133539	-0.501132
C	-7.942900	-1.017095	0.468896
C	-8.850677	-0.122824	-0.095367
Te	-3.081486	-0.314140	0.002690
H	2.467351	3.456905	1.050399
F	-5.785756	-1.549887	1.189030
F	-8.363491	-2.226910	0.873366
F	-10.137506	-0.467295	-0.247413
F	-9.267803	1.995643	-1.064083
F	-6.696733	2.697280	-0.787570

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binding_2-NO3.out
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C	1.987369	-1.695342	-0.529055
C	2.970194	-2.634053	-0.799958
C	4.326308	-2.248858	-0.695978
C	4.625795	-0.945141	-0.348707
H	5.109987	-2.971559	-0.905345
C	5.970585	-0.419869	-0.137831
C	6.328809	0.904917	-0.460048
C	7.005825	-1.193361	0.430722
C	7.604281	1.421495	-0.254095
C	8.288799	-0.698024	0.646774
C	8.596993	0.616314	0.300950
F	6.772038	-2.458163	0.832005
F	9.232630	-1.477043	1.202742
F	9.831053	1.100369	0.502315
F	7.888779	2.688118	-0.598383
F	5.417402	1.733596	-1.009016
Te	2.852325	0.175791	-0.043219
C	0.613881	-1.843799	-0.569428
C	-0.614478	-1.843797	-0.570964
C	-1.987914	-1.694385	-0.531870
C	-2.971631	-2.625579	-0.824649
C	-4.327345	-2.238874	-0.719831
H	-2.696663	-3.631940	-1.132161
C	-4.625093	-0.941323	-0.349108
H	-5.112162	-2.954806	-0.947750
C	-5.970045	-0.415578	-0.139803
C	-7.009863	-1.194203	0.412783
C	-6.324065	0.913206	-0.449648
C	-8.293726	-0.699737	0.625619
C	-7.600372	1.428996	-0.246672
C	-8.597817	0.618847	0.292456
Te	-2.850748	0.167829	-0.009827
H	2.694198	-3.645723	-1.088560
F	-5.408128	1.746423	-0.983788
F	-7.881134	2.699661	-0.578951
F	-9.832659	1.102245	0.490601
F	-9.242417	-1.483753	1.166064
F	-6.779892	-2.463881	0.800583
O	0.002868	1.066827	0.338874
O	1.085359	2.926550	0.729914
O	-1.091662	2.887937	0.856824
N	-0.001125	2.309435	0.645689

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binding_2-OBz.out
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Imaginary frequency:-10.25
Vibrational mode: Symmetric twist about the acetylene

Imaginary frequency: -6.87
Vibrational mode: Symmetric bend about the acetylene

C	1.703472	-2.245575	-0.491143
C	2.689657	-3.190855	-0.724048
C	4.044371	-2.791050	-0.656077
C	4.341475	-1.468533	-0.377213
H	4.828214	-3.520473	-0.836491
C	5.677910	-0.916153	-0.193145
C	5.991239	0.430792	-0.475369
C	6.755659	-1.674145	0.318211
C	7.254629	0.980296	-0.283645
C	8.028686	-1.146714	0.515670
C	8.288208	0.188183	0.211647
F	6.576944	-2.959387	0.682586
F	9.011227	-1.916702	1.014796
F	9.512600	0.703176	0.396272
F	7.487094	2.268817	-0.584163
F	5.042418	1.256509	-0.963353
Te	2.558699	-0.350272	-0.118941
C	0.327990	-2.377890	-0.486515
C	-0.896949	-2.304283	-0.432947
C	-2.257087	-2.071537	-0.360380
C	-3.292081	-2.991217	-0.428908
C	-4.623887	-2.525661	-0.340296
H	-3.073039	-4.049562	-0.552175
C	-4.843023	-1.167394	-0.214723
H	-5.448448	-3.232401	-0.390351
C	-6.153686	-0.548955	-0.046276
C	-7.177481	-1.141045	0.724258
C	-6.484435	0.697371	-0.615568
C	-8.425992	-0.552322	0.904740
C	-7.726083	1.304006	-0.451033
C	-8.708762	0.677140	0.312703
Te	-3.000337	-0.095544	-0.184384
H	2.419783	-4.219122	-0.954067
F	-5.582821	1.350083	-1.376648
F	-7.989291	2.485622	-1.034293
F	-9.910148	1.250938	0.478325
F	-9.360366	-1.156347	1.660193
F	-6.961887	-2.309275	1.361569
C	-0.234647	1.940306	-0.183940
O	-0.278082	0.703610	0.142074
O	-1.073089	2.559049	-0.877735
C	0.973096	2.715988	0.325053
C	1.479600	2.499686	1.613629
C	1.621275	3.635005	-0.509750
C	2.607552	3.189775	2.059988
H	0.987893	1.774442	2.255653
C	2.770971	4.298620	-0.080325
H	1.220998	3.809224	-1.504733
C	3.265537	4.080985	1.208644
H	2.983204	3.020681	3.066715
H	3.282411	4.986624	-0.749802
H	4.158281	4.601871	1.546460

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