Supporting Information

Chalcogen Bonding in Solution: Interactions of Benzotelluradiazoles With Anionic and Uncharged Lewis Bases

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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, dichloromethane and toluene 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. Deuterated DMSO-d_6 was purchased from Cambridge Isotope Laboratories and deuterated THF-d_8 was purchased from Sigma Aldrich. DMSO-d_6 was dried over molecular sieves and stored in a glove box prior to use. THF-d_8 was used as received. 4,7-Dibromobenzo[c]-1,2,5-thiadiazole (**3c**) was purified by silica gel chromatography eluting with hexanes followed by recrystallization from ethanol before use. 1,2-Diamino-3,4,5,6-tetrafluorobenzene was purchased from Matrix Scientific. 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. Solvents used during synthesis were degassed with argon for 25 minutes and dried on 4 A molecular sieves. 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 DMSO-d_6 either on an Agilent DD2 500 spectrometer equipped with a 5 mm Xsens Cold Probe at 500 and 150.7 MHz, respectively, or an Agilent DD2 600 spectrometer equipped with a 5 mm OneNMR H/F[X] probe at 600 MHz. Due to the low solubility of the donors in THF-d_8, ^{1}H spectra obtained for NMR titrations were performed on an Agilent DD2 700 spectrometer equipped with a 5 mm Xsens Cold Probe at 700 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 2.50 for DMSO 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 DMSO (δ 39.52).

Infared (IR) spectra were obtained on a Perkin-Elmer Spectrum 100 instrument equipped with a single-reflection diamond/ZnSe ATR accessory, either in the solid state or as neat liquids, as indicated. Spectral features are tabulated as follows: wavenumber (cm^{-1}); intensity (s-strong, m-medium, w-weak, br-broad).

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 (DART+).

Mass spectrometry experiments were performed on a 7T Fourier transform ion cyclotron resonance (FTICR) mass spectrometer (Bruker Apex Qe, Bruker Daltonics, Billerica, MA). The telluradiazole complex was ionized and carried into the gas-phase via negative ion mode nanoelectrospray (nanoESI) ionization. The nanoESI source employs emitters pulled from borosilicate glass capillaries (Sutter, o.d. 1.0 mm, i.d. 0.75 mm) using a micropipet puller (Model P97, Sutter Instruments, Novato, CA). To generate the spray, a -1200 V potential was applied to a platinum wire inserted into the glass capillary that was placed in front of the grounded inlet to the mass spectrometer.

The vacuum system of the FT-ICR is modified to increase pressure in the first vacuum stage, which is separated from atmosphere by a heated glass capillary inlet to the mass spectrometer and contains an ion funnel, from 2.0 mbar to 4.5 mbar. The use of higher pressures provides a gentler environment for complexes, and reduces the extent of gas phase dissociation in this region of the mass spectrometer. Gaseous ions and complexes were accumulated in a storage hexapole, termed the source hexapole, for 0.5 seconds. A quadrupole mass filter (50 *m/z* isolation window) was then used to isolate the species of interest. This was done to remove unwanted salt cluster peaks which otherwise dominated the spectrum. Following mass selection, ions were accumulated for an additional 3.0 seconds in a second "collision" hexapole cell, where complex S/N was significantly improved by introduction of argon collision gas (~4.5×10^{-6} mbar, as read by an ion gauge located externally to the hexapole, corresponding

to an estimated pressure ~10^{-3} mbar[1]). Ions were then transferred into the ICR cell for analysis. The mass spectrum shown is the sum of spectra from 50 separate ion populations.

1.3 Donor Preparation

1.3.1 Methods

Selenadiazoles[2] and telluradiazoles[3] were synthesized according to previous literature procedures with slight modifications for the telluradiazole preparations. The telluradiazoles were purified by careful trituration of toluene (3 x 10 mL) and DCM (5 x 10 mL) in the glovebox to remove any unreacted diamine and triethylamine hydrochloride by-product. Trituration can be augmented by centrifugation if available in the glovebox. The solids were collected by filtration.

1.3.2 Donor Characterization

1.3.2.1 benzo[c][1,2,5]telluradiazole (2)

Telluradiazole **2** was synthesized following the modified procedure using 1,2-phenylenediamine (2.0 g, 18.5 mmol), $TeCl_4$ (1.006 g, 3.39 mmol), and Et_3N (3 mL, 21.5 mmol) to give **2** as an orange solid (95 mg, 0.410 mmol, 12 %). ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.53 - 7.44 (m, 2H), 7.28 - 7.21 (m,2H). ^{1}H NMR (700 MHz, THF-d_8) δ 7.48 (dd, *J* = 7.0, 3.3 Hz, 2H), 7.17 (dd, *J* = 7.1, 3.3 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6): δ 166.2, 128.2, 127.7. HMRS calculated for $C_6H_4N_2Te$ $[M+H]^+$ 234.95150, found 234.95165.

1.3.2.2 4,7-dibromobenzo[c][1,2,5]telluradiazole (3a)

Telluradiazole **3a** was synthesized following the modified procedure using 3,6-dibromobenzene-1,2-diamine (1.1 g, 4.14 mmol), $TeCl_4$ (236 mg, 0.796 mmol), and Et_3N (0.72 mL, 5.17 mmol) to give **3a** as a brown solid (87 mg, 0.223 mmol, 61 %). ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.56 (s, 2H). ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.56 (s, 2H). ^{1}H NMR (700 MHz, THF-d_8) δ 7.47 (s, 2H). ^{13}C NMR (126 MHz, DMSO-d_6): δ 160.8, 129.6, 123.0. HMRS calculated for $C_6H_2Br_2N_2Te$ $[M+H]^+$ 390.76936, found 390.76835.

1.3.2.3 benzo[c][1,2,5]telluradiazole-5-carbonitrile (4)

Telluradiazole **4** was synthesized following the modified procedure using 3,4-diaminobenzonitrile (1.2 g, 9.01 mmol), $TeCl_4$ (544.6 mg, 2.021 mmol), and Et_3N (1.8 mL, 12.905 mmol) to give **4** as a brown solid (182 mg, 0.709 mmol, 35 %). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.19 (d, *J* = 0.8 Hz, 1H), 7.66 (d, *J* = 9.1 Hz, 1H), 7.48 (dd, *J* = 9.1, 1.8 Hz, 1H). ^{1}H NMR (700 MHz, DMSO-d_6) δ 8.19 (s, 1H), 7.66 (d, *J* = 9.1 Hz, 1H), 7.48 (dd, *J* = 9.0, 1.8 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6): δ 165.7, 164.2, 135.0, 129.4, 126.0, 118.7, 110.4. IR (thin film, cm^{-1}): 2219 (m), 1506 (m), 1485 (m), 1300 (w), 1277 (m), 1149 (w), 952 (w), 880 (m), 803 (s), 745 (w), 711 (s), 696 (m) 680 (m). HMRS calculated for $C_7H_4N_3Te$ $[M+H]^+$ 259.94674, found 2594642.

1.3.2.4 perfluorobenzo[c][1,2,5]telluradiazole (5)

Telluradiazole **5** was synthesized following the modified procedure using 1,2-Diamino-3,4,5,6-tetrafluorobenzene (216.7 mg, 1.203 mmol), $TeCl_4$ (76.5 mg, 0.284 mmol), and Et_3N (0.26 mL, 1.864 mmol) to give **5** as a red solid (23 mg, 0.076 mmol, 27 %). ^{19}F NMR (564 MHz, DMSO-d_6) δ -149.78 – -149.85 (m, 2H), -162.38 – -162.45 (m, 2H) HMRS calculated for $C_6H_1F_4N_2Te$ $[M+H]^+$ 306.91381, found 306.91347.

1.3.3 NMR spectra

1.3.3.1 benzo[c][1,2,5]telluradiazole (2)

Figure S 1: ^{1}H NMR spectrum of **2** taken in DMSO-d_6 at 500 MHz.

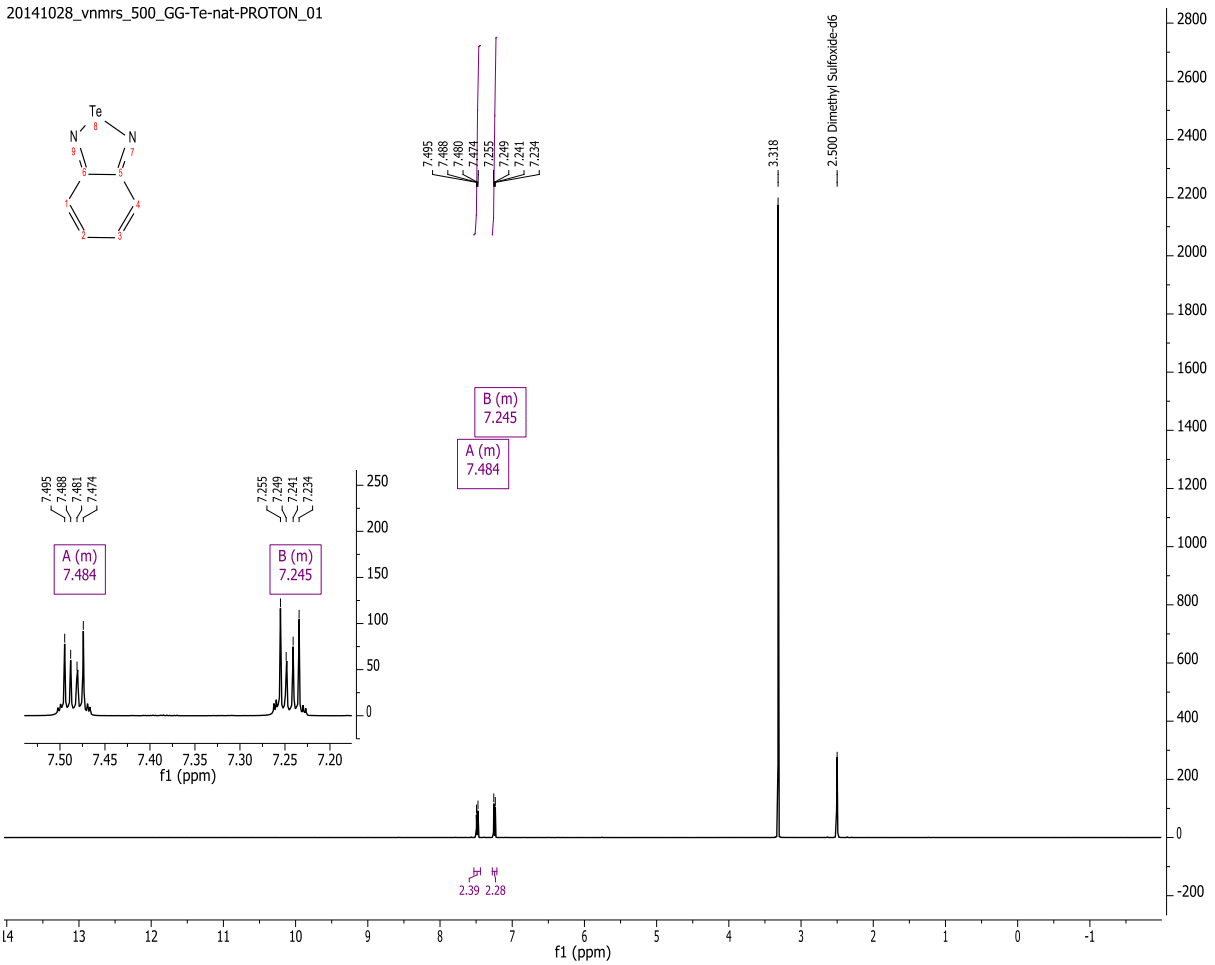


Figure S 2: ^{1}H NMR spectrum of **2** taken in THF-d_8 at 700 MHz.

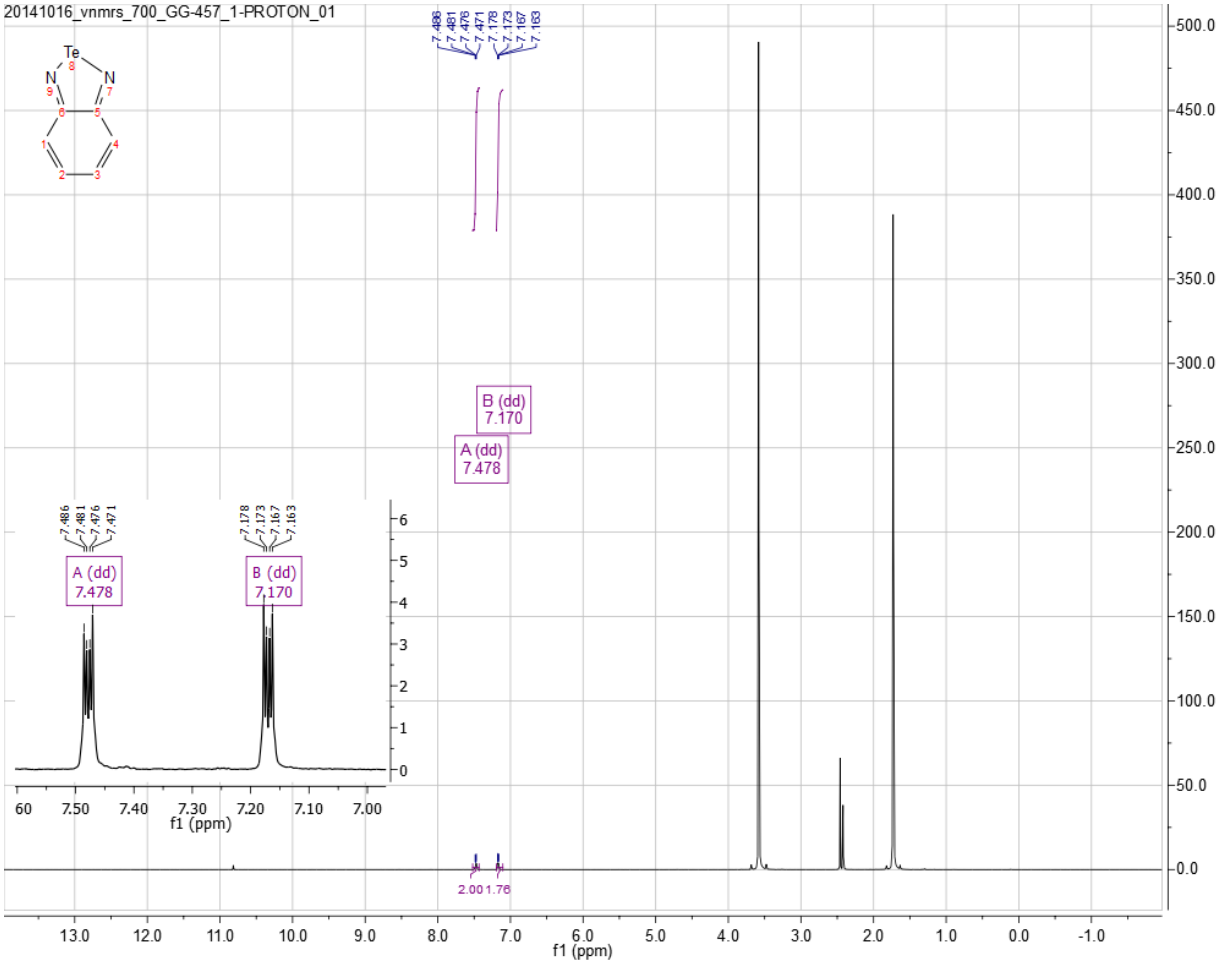
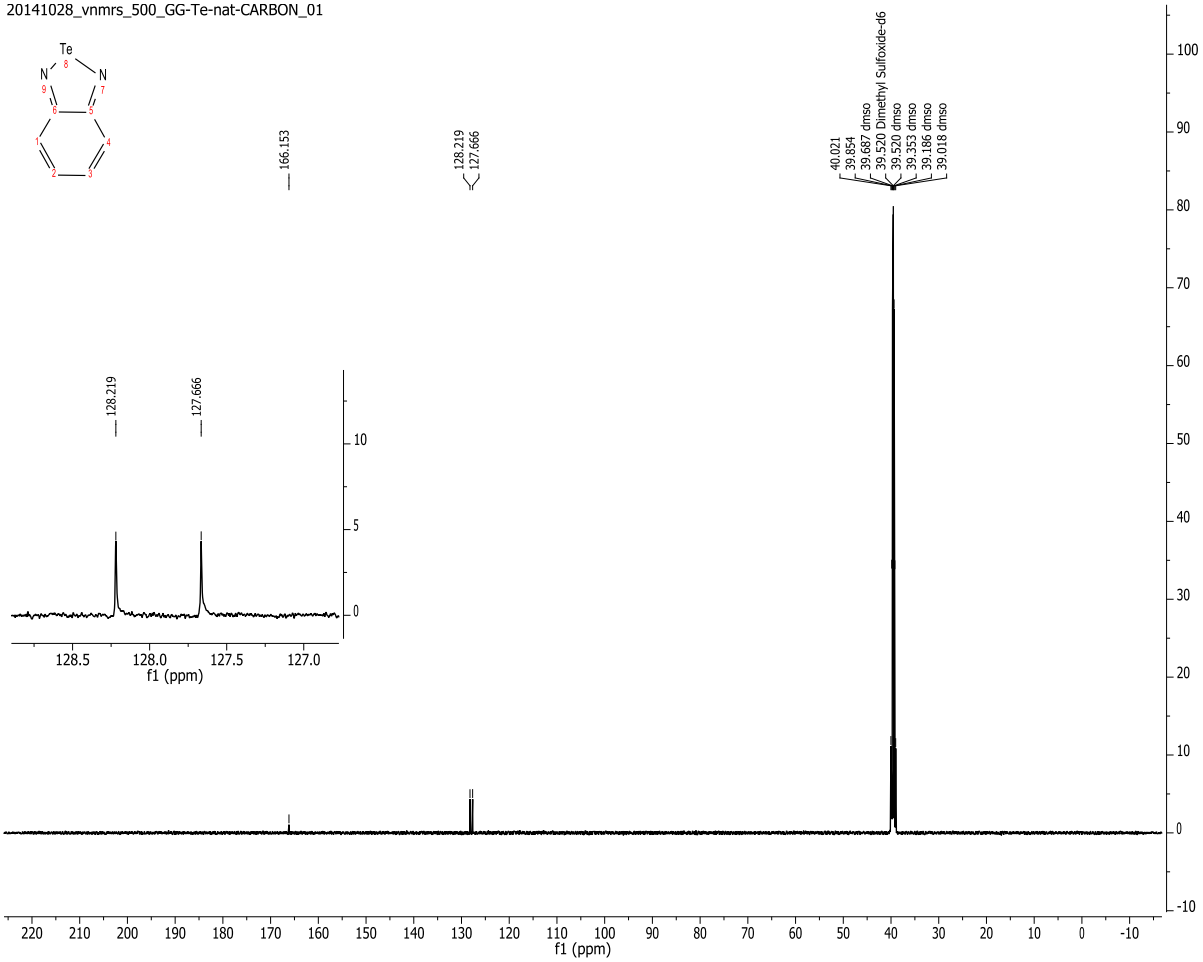


Figure S 3: ^{13}C NMR spectrum of **2** taken in DMSO-d_6 at 126 MHz



1.3.3.2 4,7-dibromobenzo[c][1,2,5]telluradiazole (3a)

Figure S 4: ^{1}H NMR spectrum of **3a** taken in DMSO-d_6 at 500 MHz

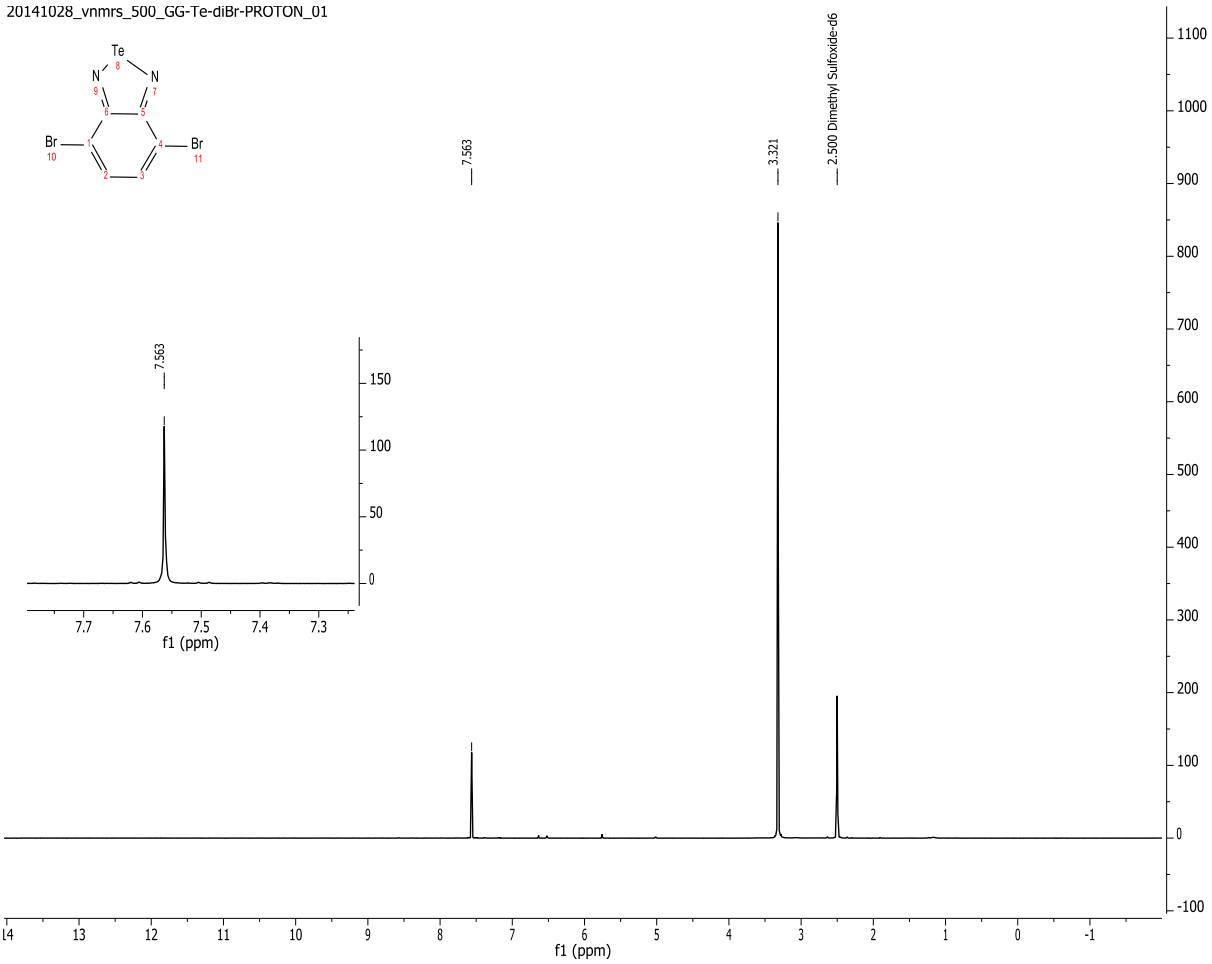


Figure S 5: ^{1}H NMR spectrum of **3a** taken in DMSO-d_6 at 600 MHz

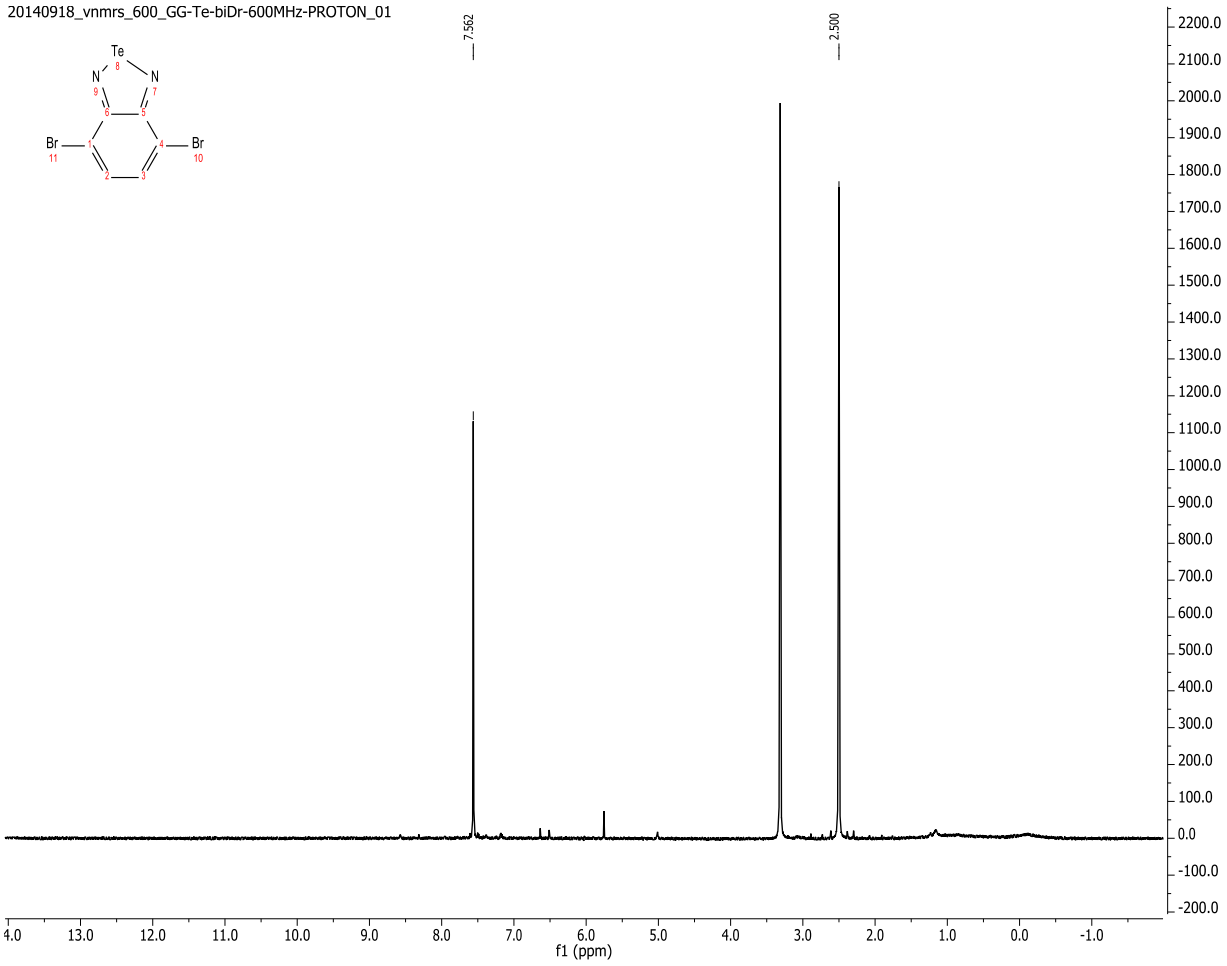


Figure S 6: ^{1}H NMR spectrum of **3a** taken in THF-d_8 at 700 MHz

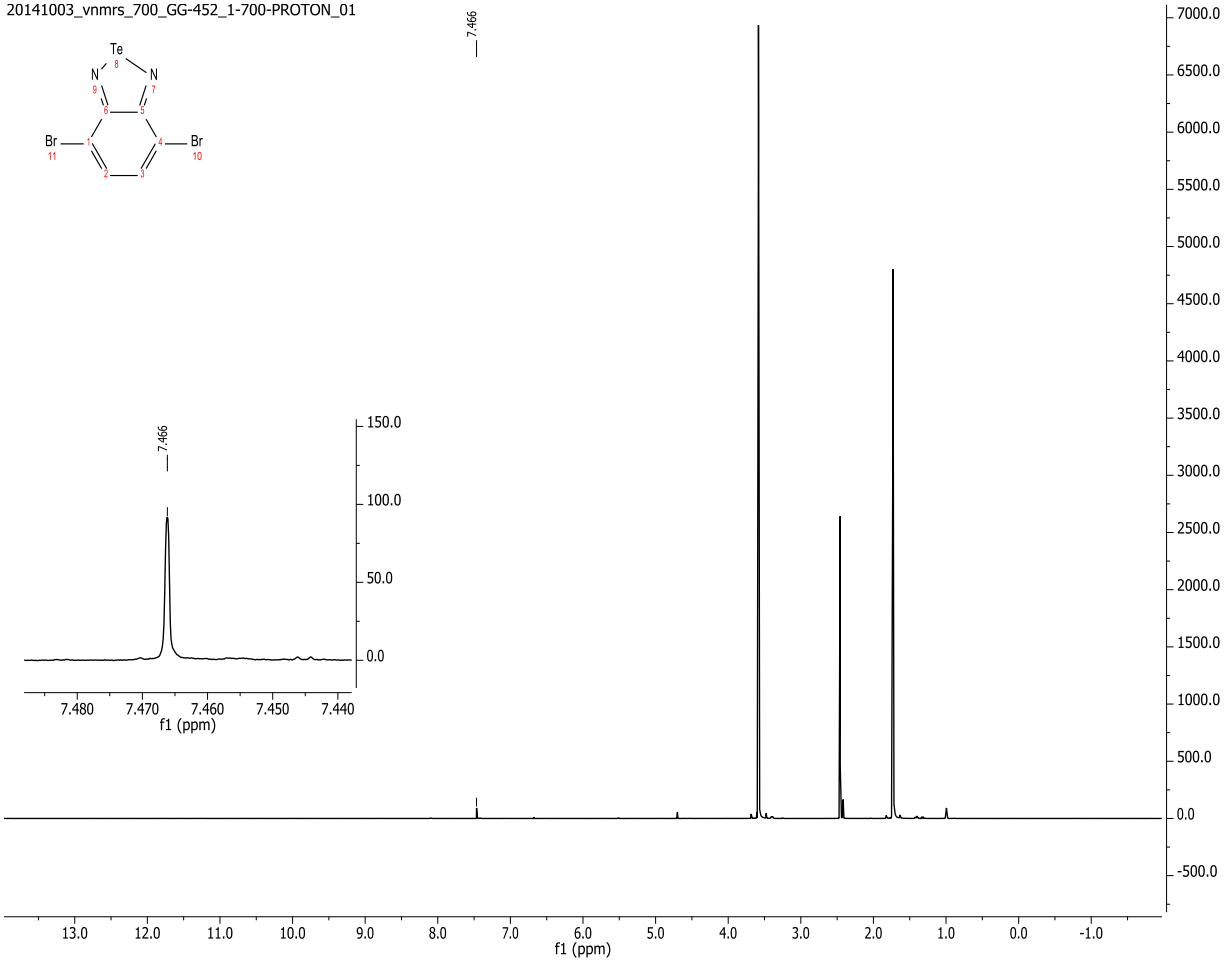
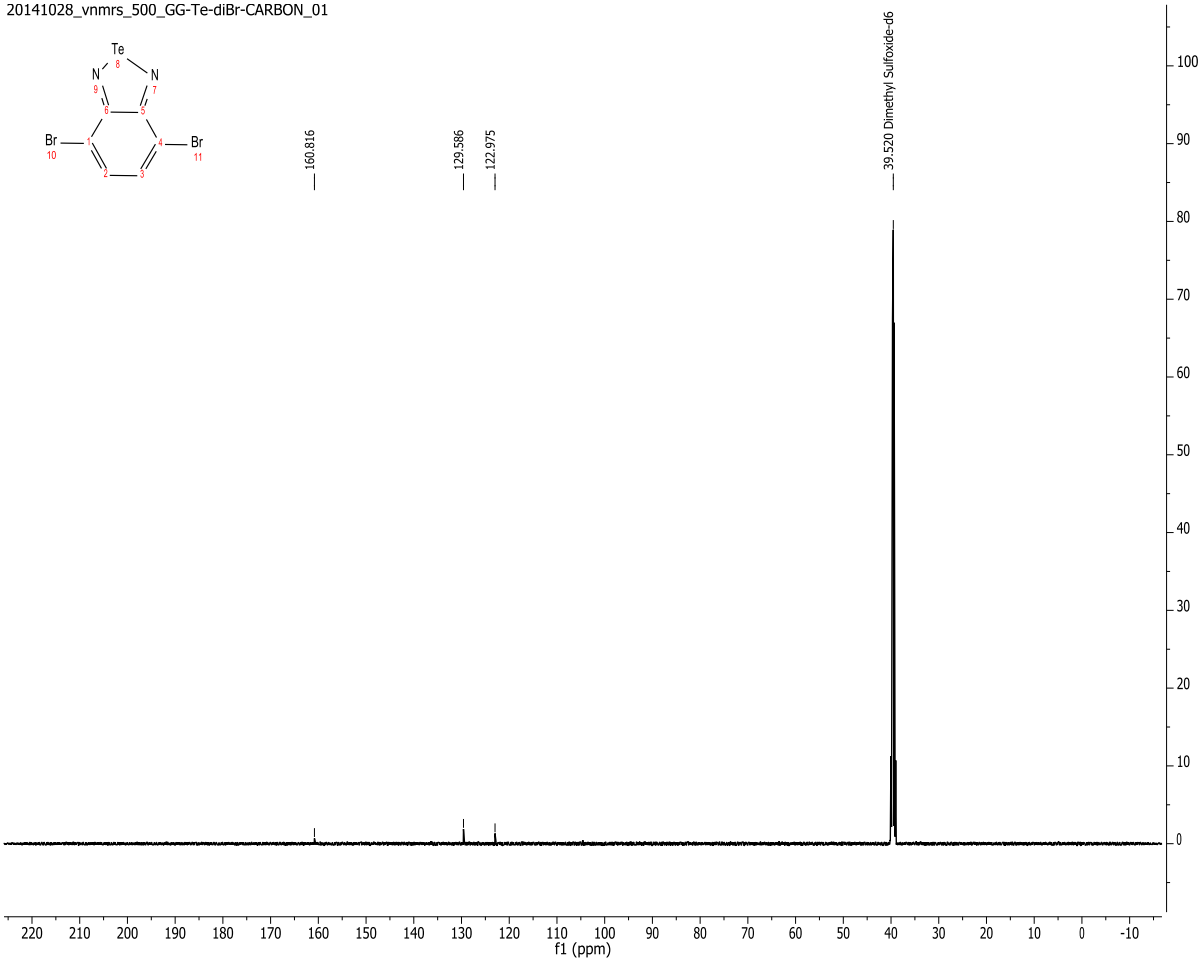


Figure S 7: ^{13}C NMR spectrum of **3a** taken in DMSO-d_6 at 126 MHz



1.3.3.3 benzo[c][1,2,5]telluradiazole-5-carbonitrile (4)

Figure S 8: ^{1}H NMR spectrum of **4** taken in DMSO-d_6 at 700 MHz

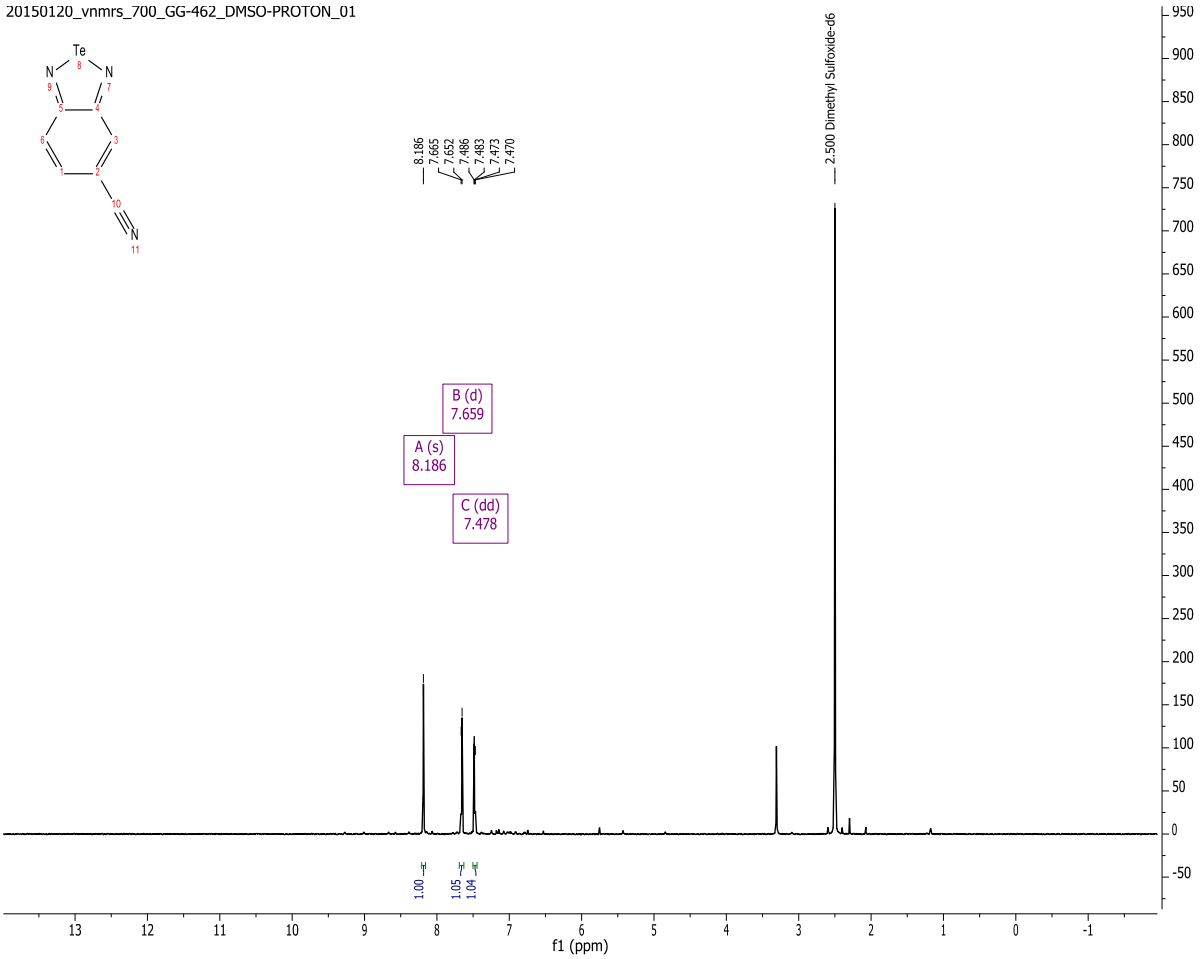


Figure S 9: ^{1}H NMR spectrum of **4** taken in DMSO-d_6 at 500 MHz

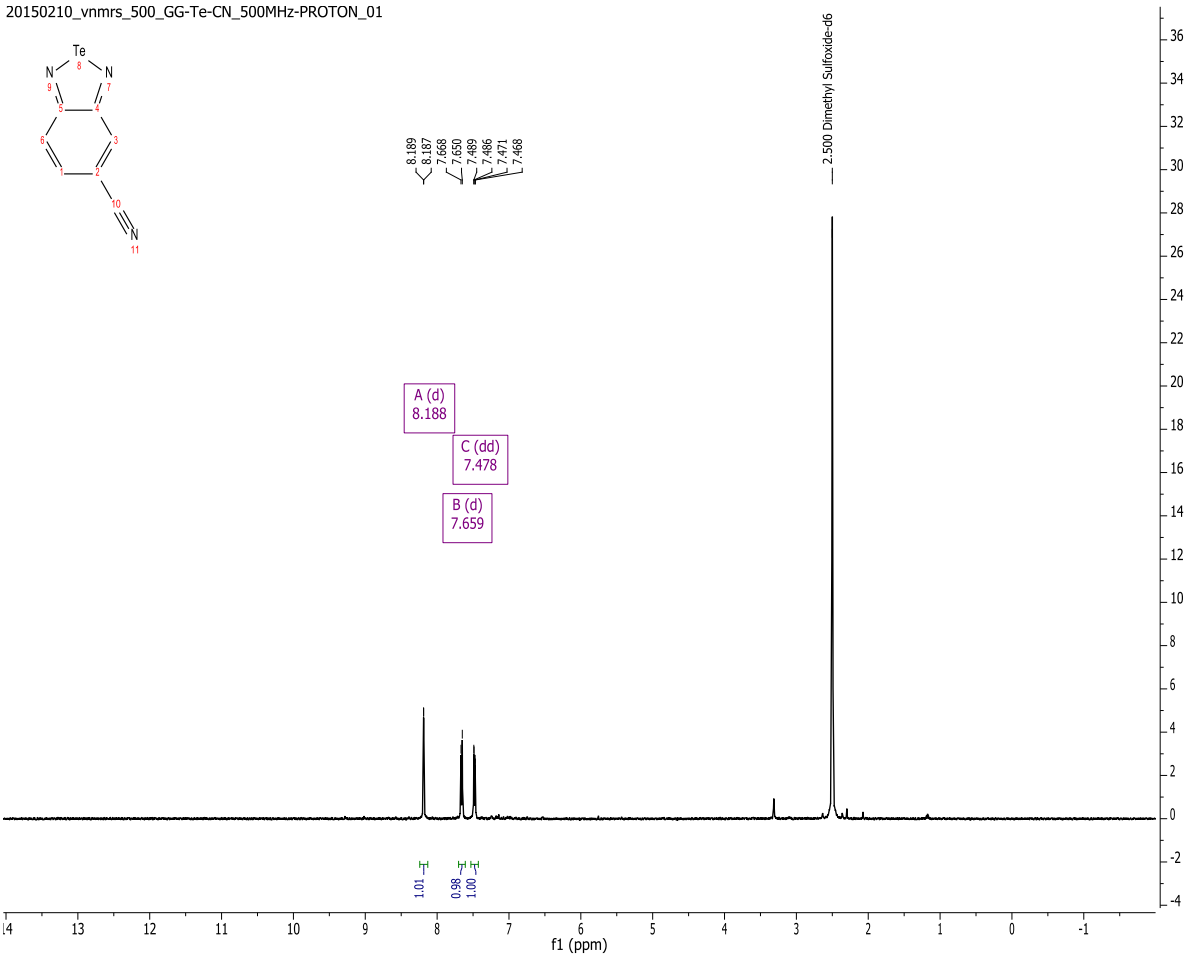
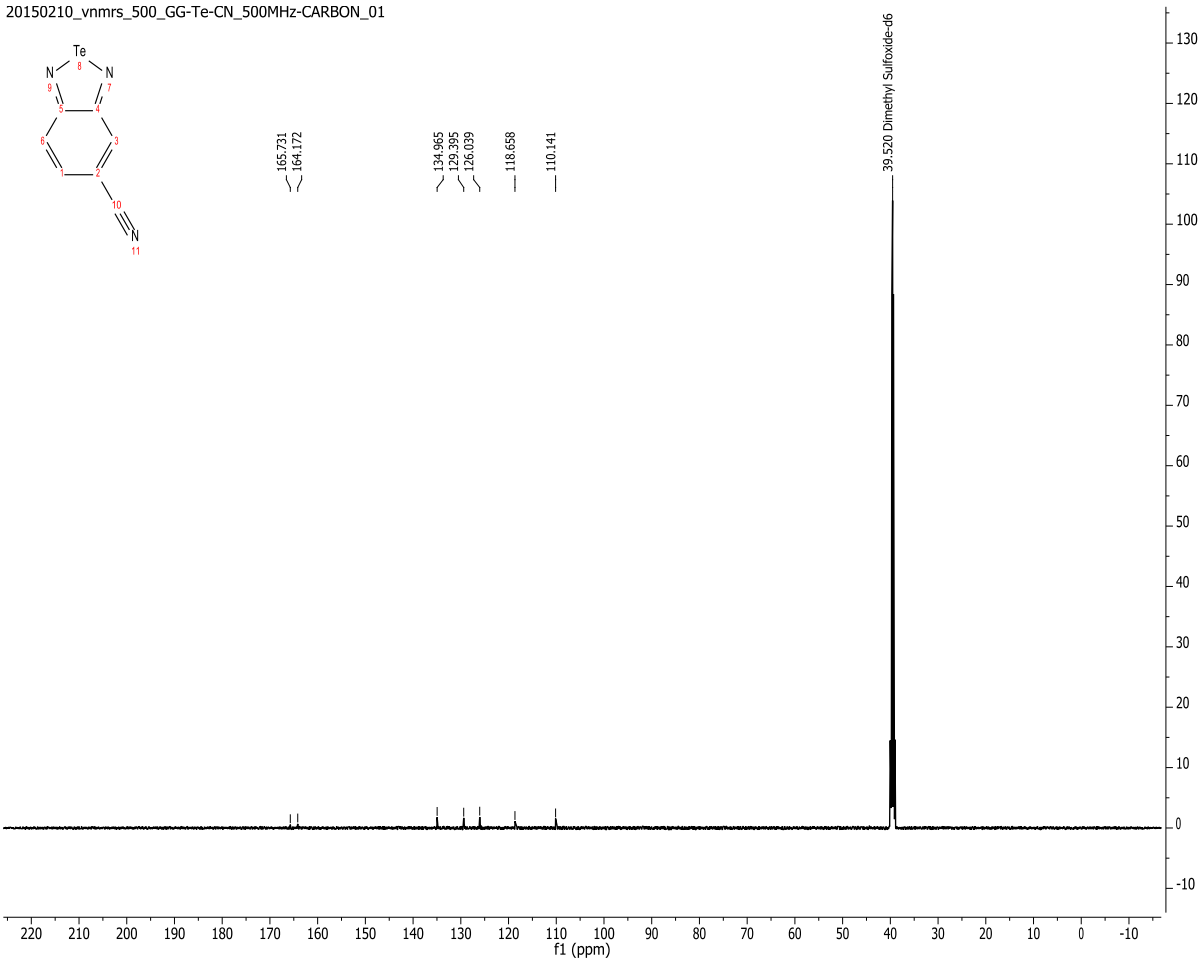
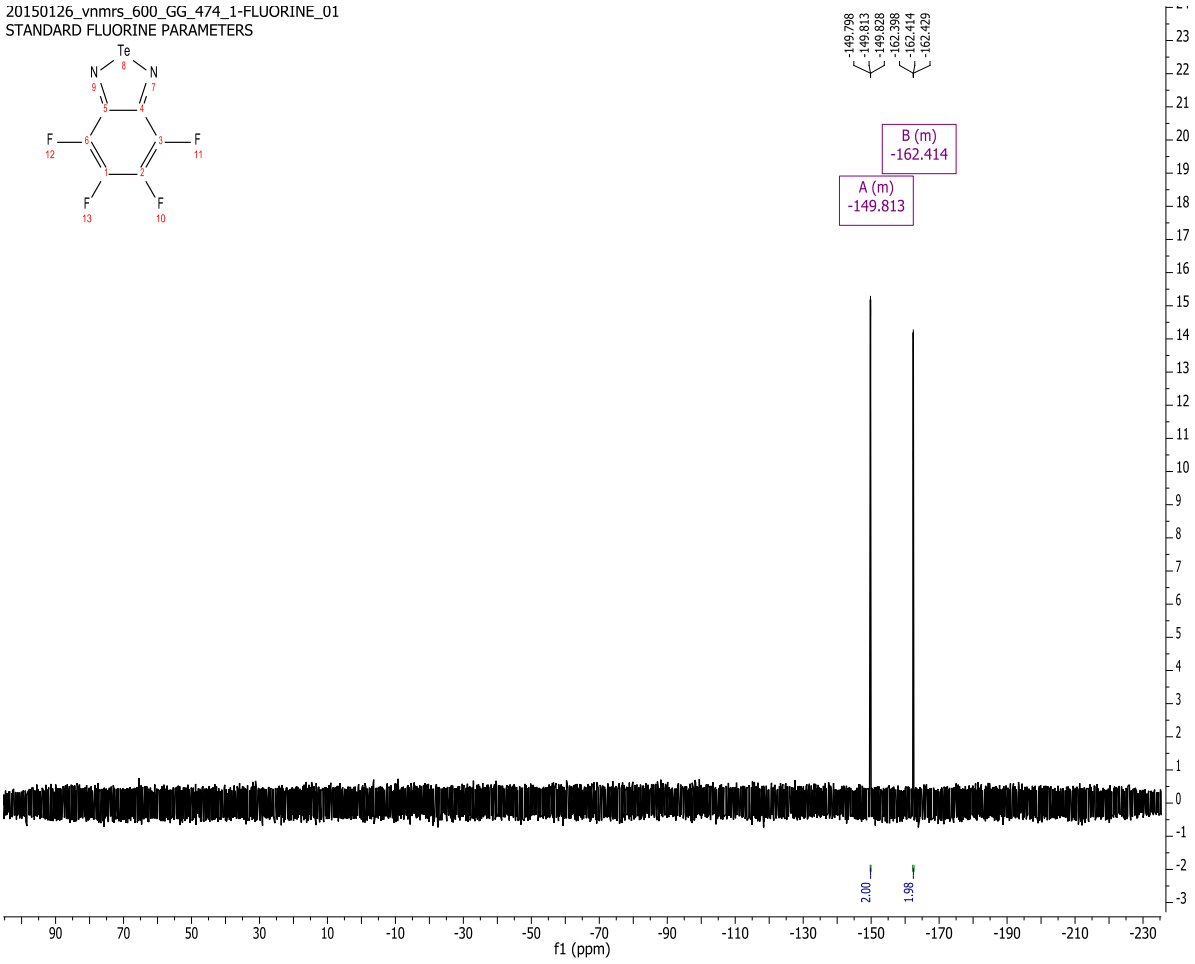


Figure S 10: ^{13}C NMR spectrum of **4** taken in DMSO-d_6 at 126 MHz



1.3.3.4 perfluorobenzo[c][1,2,5]telluradiazole (5)

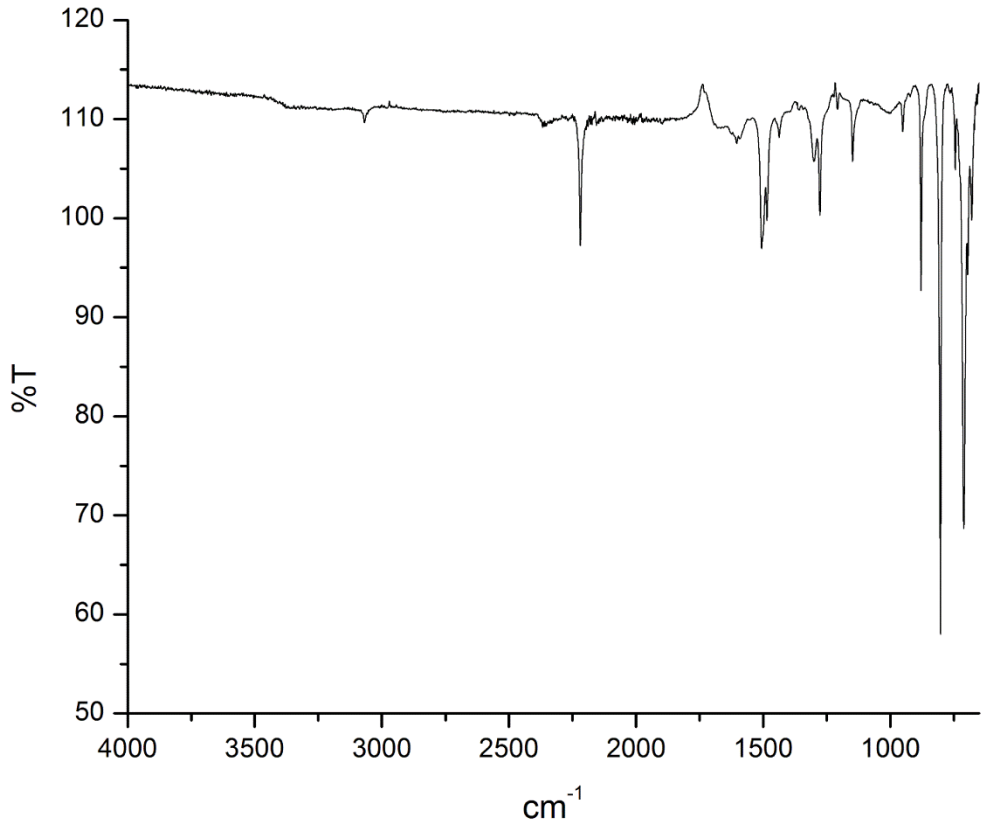
Figure S 11: ^{19}F NMR spectrum of **5** taken in DMSO-d_6 at 546 MHz



1.3.4 IR Spectra

1.3.4.1 benzo[c][1,2,5]telluradiazole-5-carbonitrile (4)

Figure S 12: IR spectrum of **4**



1.4 Diamine decomposition product characterization

1.4.1 NMR assignments

1.4.1.1 1,2-phenylenediamine

^{1}H NMR (700 MHz, THF-d_8) δ 6.52 (dd, *J* = 5.6, 3.5 Hz, 2H), 6.43 (dd, *J* = 5.7, 3.4 Hz, 2H).

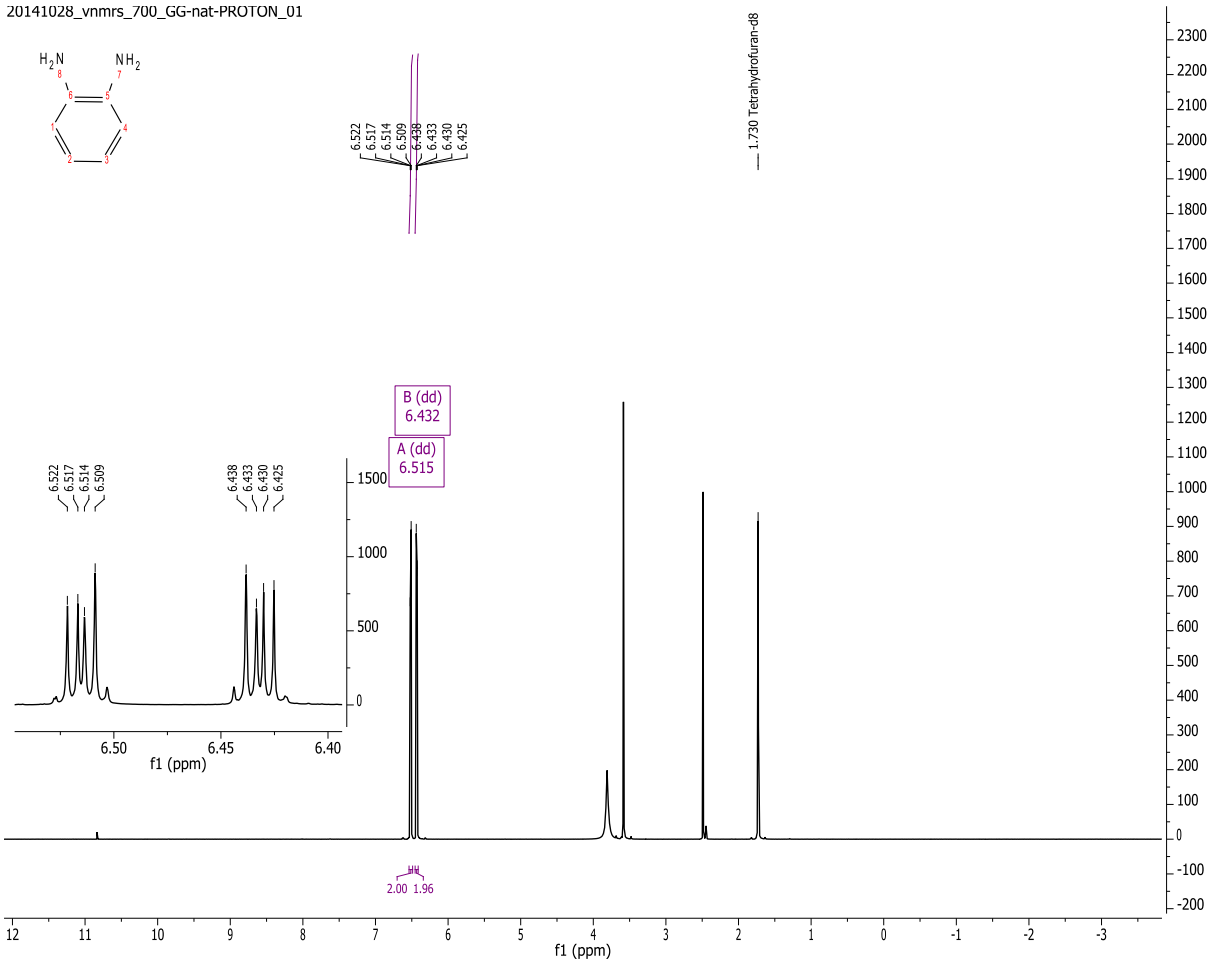
1.4.1.2 3,6-dibromobenzene-1,2-diamine

^{1}H NMR (700 MHz, THF-d_8) δ 6.68 (s, 2H).

1.4.2 NMR spectra

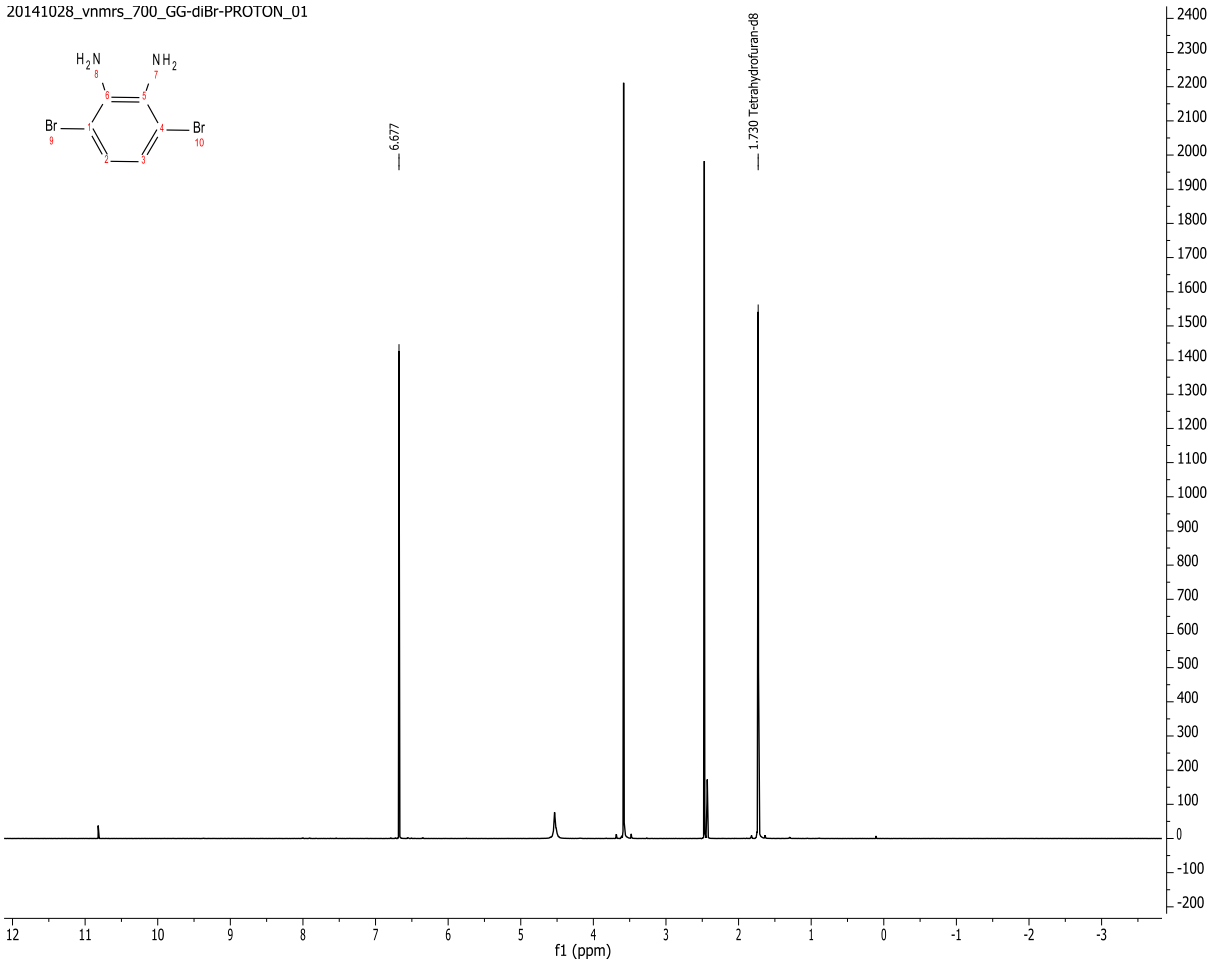
1.4.2.1 1,2-phenylenediamine

Figure S 13: ^{1}H NMR spectrum of 1,2-phenylenediamine taken in THF-d_8 at 700 MHz.



1.4.2.2 3,6-dibromobenzene-1,2-diamine

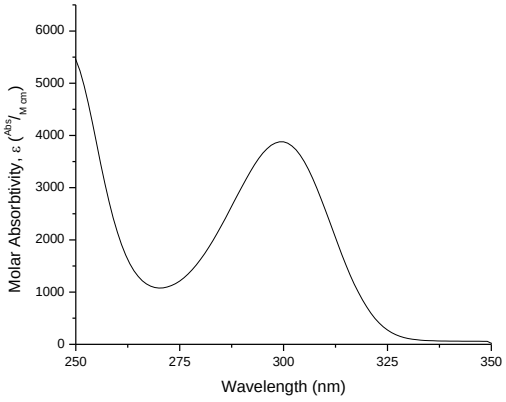
Figure S 14: ^{1}H NMR spectrum of 3,6-dibromobenzene-1,2-diamine taken in THF-d_8 at 700 MHz.



1.4.3 UV/Vis spectra

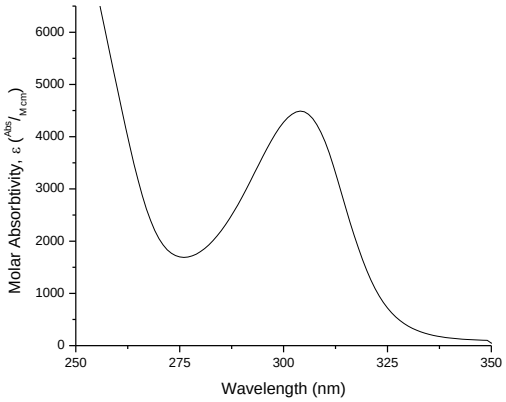
1.4.3.1 1,2-phenylenediamine

Figure S 15: UV/Vis spectrum of 1,2-phenylenediamine in THF. λ_{max} = 299 nm.



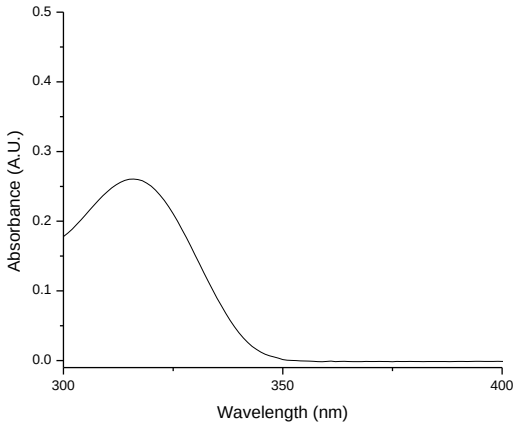
1.4.3.2 3,6-dibromobenzene-1,2-diamine

Figure S 16: UV/Vis spectrum of 3,6-dibromobenzene-1,2-diamine in THF. λ_{max} = 304 nm.



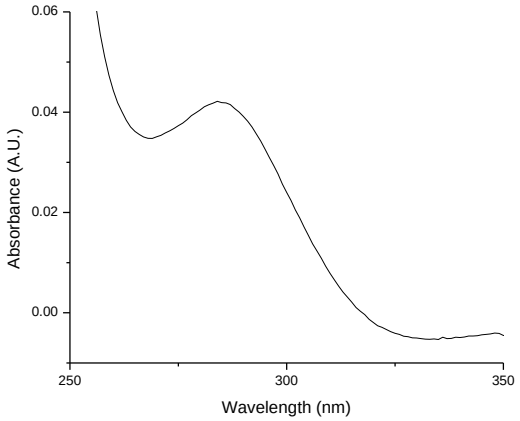
1.4.3.3 3,4-diaminobenzonitrile

Figure S 17: UV/Vis spectrum of 3,4-diaminobenzonitrile in THF. λ_{max} = 316 nm.



1.4.3.4 1,2-diamino-3,4,5,6-tetrafluorobenzene

Figure S 18: UV/Vis spectrum of 1,2-diamino-3,4,5,6-tetrafluorobenzene in THF. λ_{max} = 284 nm.



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 different samples by mixing varying ratios of the two solutions. 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.[4] NMR titrations were characterized by an upfield shift of the ^{1}H aromatic resonances. 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[5] in Origin 6.0. Stoichiometry of binding was determined using the continuous variation method (Job Plot).[4]

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

2.2 Association constant summary

In the tables below, #fits gives the number of 1:1 binding curves used to determine the association constants and the experimental error in the measurement. Pts/fit give the number of data points used for each curve. β is the complexation ratio.

Table S 1: Association constants determined for **2** with various acceptors in THF.

Acceptor	K_a (M^{-1})		
TBACl	970	±	10
TBABr	193	±	6
$TBANO_3$	15	±	1
Quinuclidine	19.0	±	0.3

Table S 2: Association constants determined for **2** with various acceptors in ACN.

Acceptor	K_a (M^{-1})		
TBACl	74	±	1
TBABr	30.1	±	0.4
TBAI	8.58	±	0.09
$TBANO_3$	<10	±	

Table S 3: Association constants determined for **3a** with various acceptors in THF.

Acceptor	K_a (M^{-1})		
TBACl	12200	±	300
TBABr	1170	±	20
$TBANO_3$	82	±	4
Quinuclidine	56	±	

Table S 4: Association constants determined for **4** with various acceptors in THF.

Acceptor	K_a (M^{-1})		
TBACl	38000	±	6000
TBABr	2200	±	200
$TBANO_3$	80	±	10*
Quinuclidine	53	±	4*

*decomposition of donor observed during titration

Table S 5: Association constants determined for **5** with various acceptors in THF.

Acceptor	K_a (M^{-1})		
TBACl	130000	±	200000
TBABr	9800	±	600
$TBANO_3$	190	±	10*
Quinuclidine	96	±	6

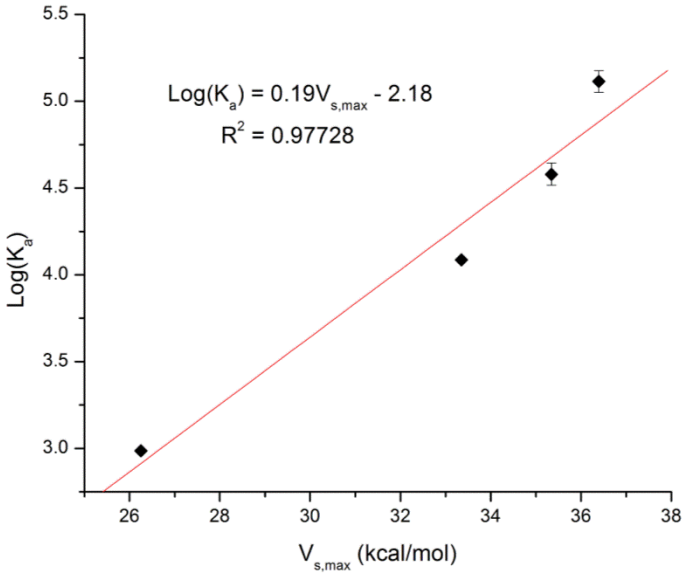
*decomposition of donor observed during titration

Table S 6: Association constants determined for **2** with TBACl in various solvents.

Solvent	K_a (M^{-1})		
THF	19.0	±	0.3
Acetone	27	±	1
ACN	40	±	2
DCM	55	±	3
Toluene	82	±	2

2.2.1 Substituent effects

Figure S 19: Plot of experimentally determined log(K_a) for the binding of Cl^- in THF versus $V_{s,max}$ calculated at the B97D3 level of theory



2.3 Associations constants determined by UV/Vis spectroscopy

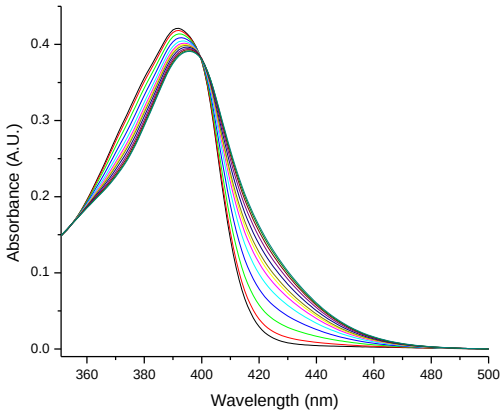
2.3.1 THF

2.3.1.1 benzo[c][1,2,5]telluradiazole (2)

2.3.1.1.1 TBACl

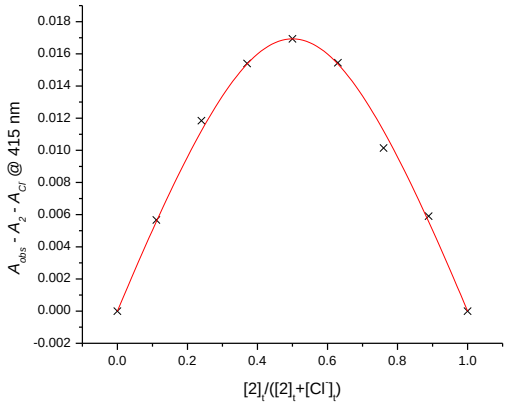
2.3.1.1.1.1 Spectrum

Figure S 20: Representative spectral change of **2** upon the addition of TBACl in THF. Titration carried out at 15.5 µM **2**, every other spectrum removed for clarity.



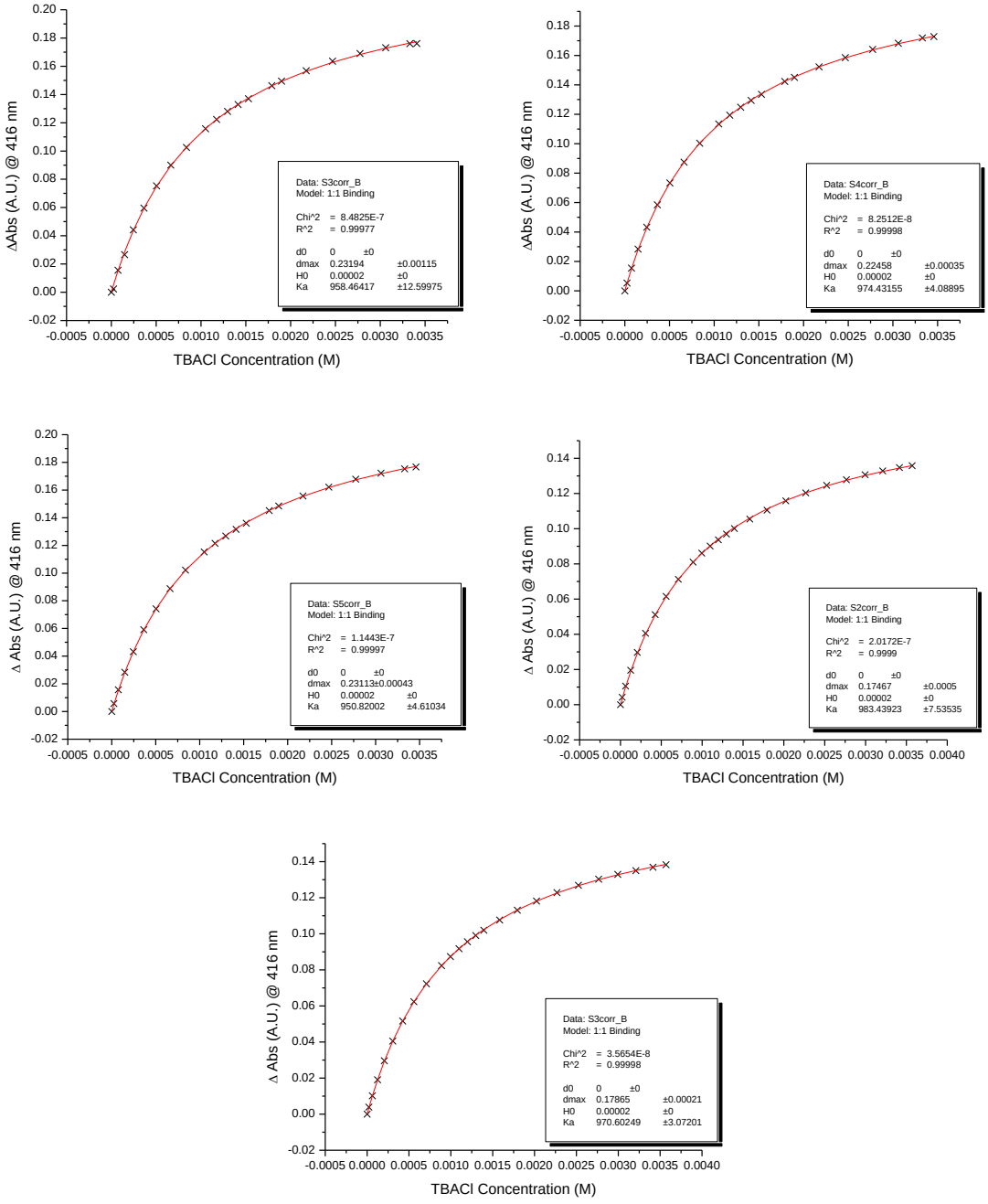
2.3.1.1.1.2 Job Plot

Figure S 21: UV/Vis Job Plot for the **2**-Cl^- complex in THF. [**2** + TBACl] = 103.6 µM.



2.3.1.1.1.3 Titrations

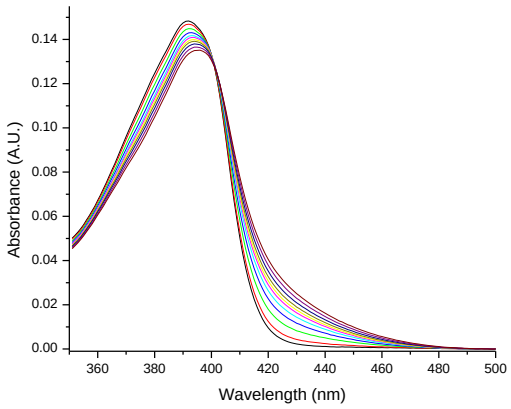
Figure S 22: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **2** in THF. From left to right: 17.3 µM **2**, K_a = 958.5 M^{-1}, 17.3 µM **2**, K_a = 974.4 M^{-1}, 17.3 µM **2**, K_a = 950.8 M^{-1}, 15.5 µM **2**, K_a = 983.4 M^{-1}, 15.5 µM **2**, K_a = 970.6 M^{-1}.



2.3.1.1.2 TBABr

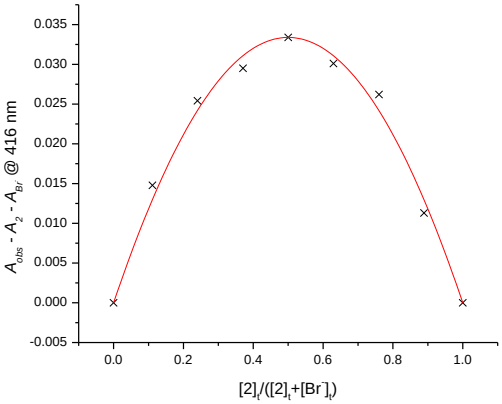
2.3.1.1.2.1 Spectrum

Figure S 23: Representative spectral change of **2** upon the addition of TBABr in THF. Titration carried out at 11.4 µM **2**, every other spectrum removed for clarity.



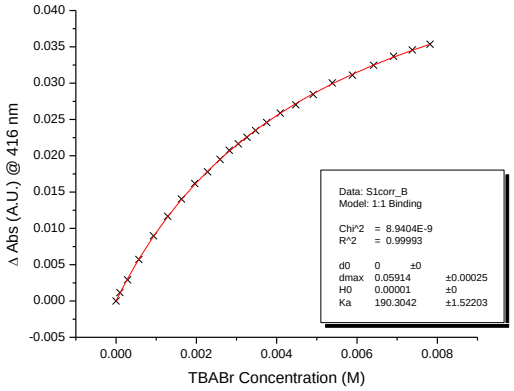
2.3.1.1.2.2 Job Plot

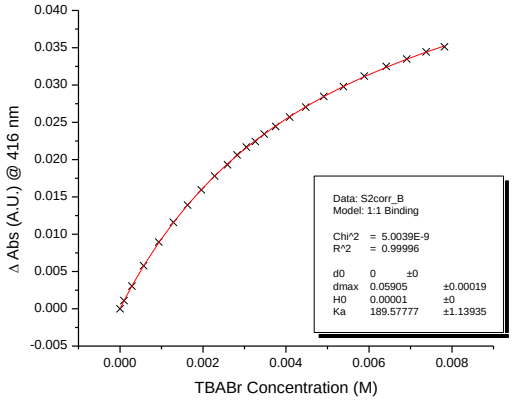
Figure S 24: UV/Vis Job Plot for the **2**-Br^- complex in THF. [**2** + TBABr] = 293 µM.

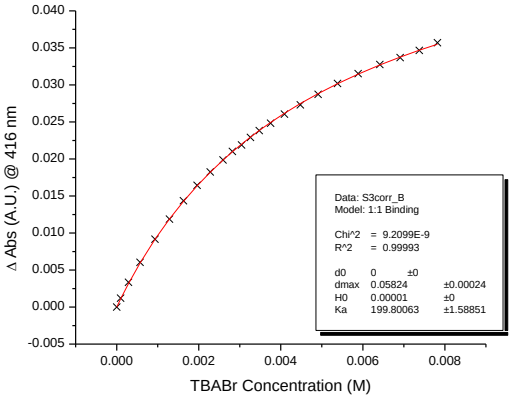


2.3.1.1.2.3 Titrations

Figure S 25: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **2** in THF. All titrations carried out at 11.4 µM **2**. From left to right: K_a = 190.3 M^{-1}, K_a = 189.6 M^{-1}, K_a = 199.8 M^{-1}.



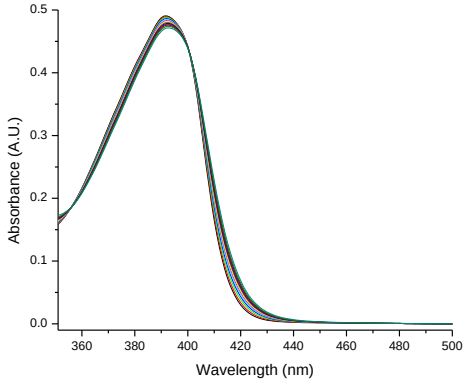




2.3.1.1.3 $TBANO_3$

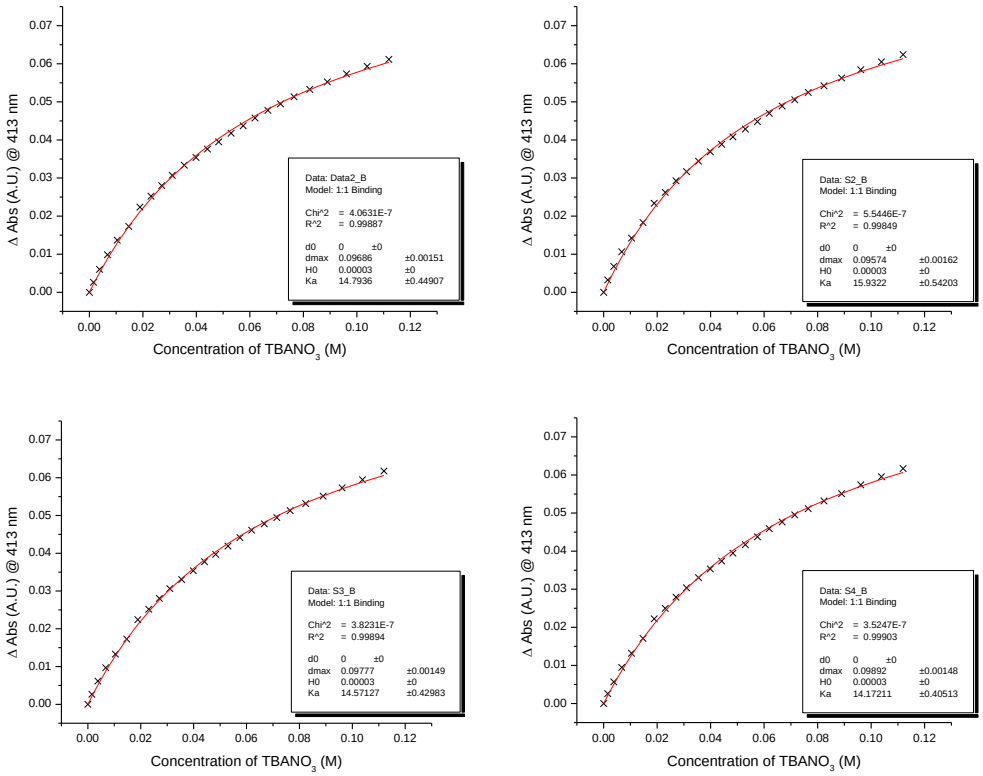
2.3.1.1.3.1 Spectrum

Figure S 26: Representative spectral change of **2** upon the addition of $TBANO_3$ in THF. Titration carried out at 20.7 µM **2**, every other spectrum removed for clarity.



2.3.1.1.3.2 Titrations

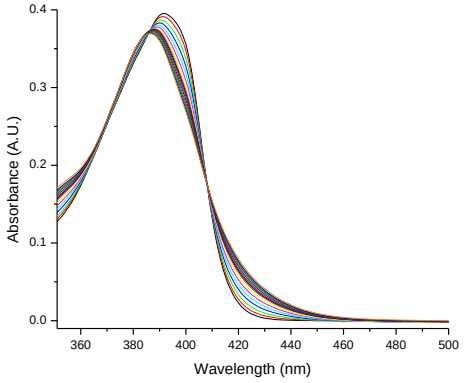
Figure S 27: Plots of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **2** in THF. All titrations carried out at 27.6 µM **2**. From left to right: K_a = 14.8 M^{-1}, K_a = 15.9 M^{-1}, K_a = 14.6 M^{-1}, K_a = 14.2 M^{-1}.



2.3.1.1.4 Quinuclidine

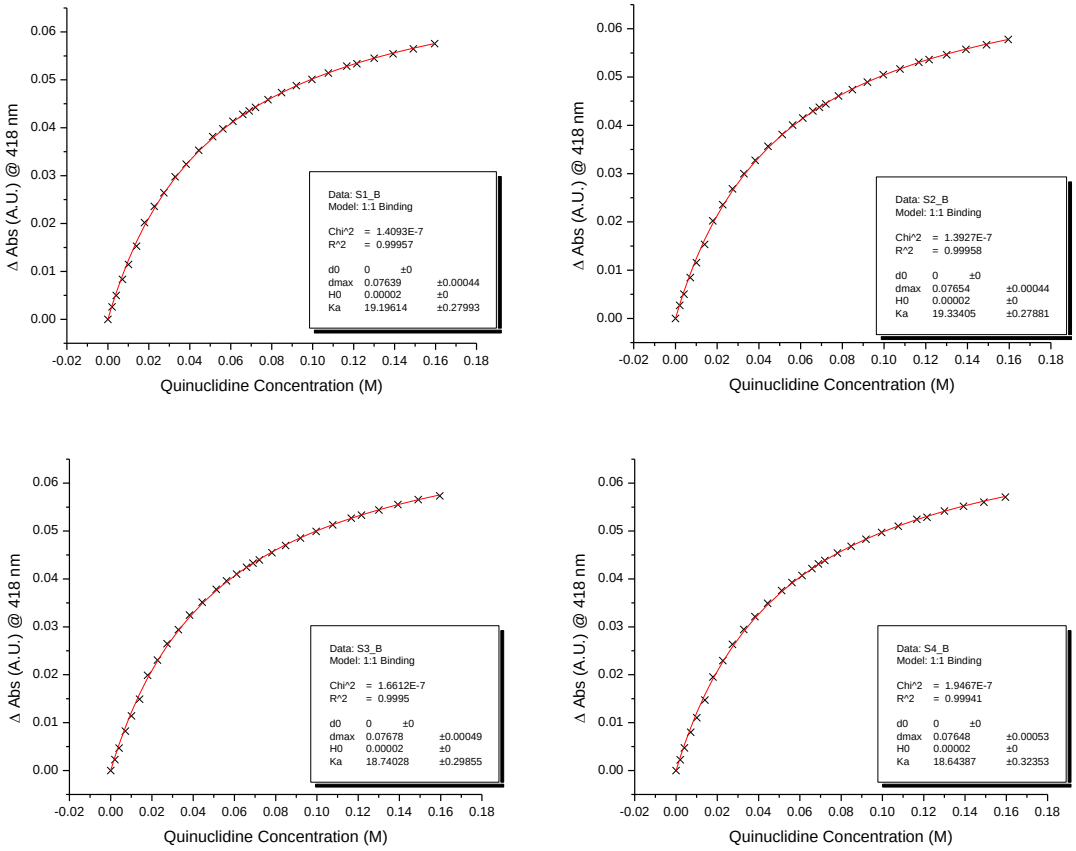
2.3.1.1.4.1 Spectrum

Figure S 28: Representative spectral change of **2** upon the addition of Quinuclidine in THF. Titration carried out at 17.3 µM **2**, every other spectrum removed for clarity.



2.3.1.1.4.2 Titrations

Figure S 29: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **2** in THF. All titrations carried out at 17.3 µM **2**. From left to right: K_a = 19.1 M^{-1}, K_a = 19.3 M^{-1}, K_a = 18.7 M^{-1}, K_a = 18.6 M^{-1}.

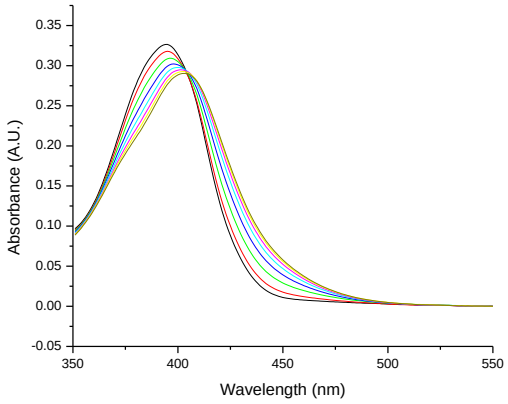


2.3.1.2 4,7-dibromobenzo[c][1,2,5]telluradiazole (3a)

2.3.1.2.1 TBACl

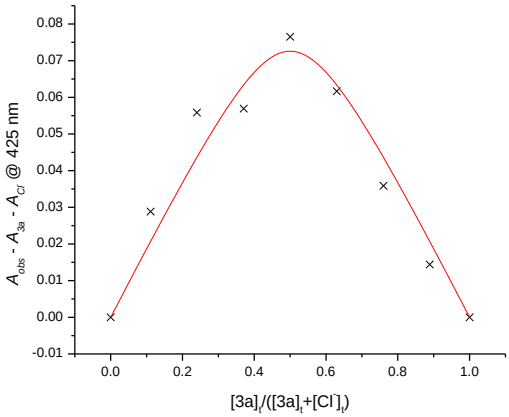
2.3.1.2.1.1 Spectrum

Figure S 30: Representative spectral change of **3a** upon the addition of TBACl in THF. Titration carried out at 14.4 µM **3a**, every other spectrum removed for clarity.



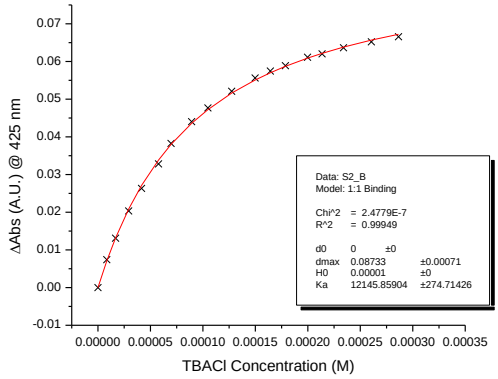
2.3.1.2.1.2 Job Plot

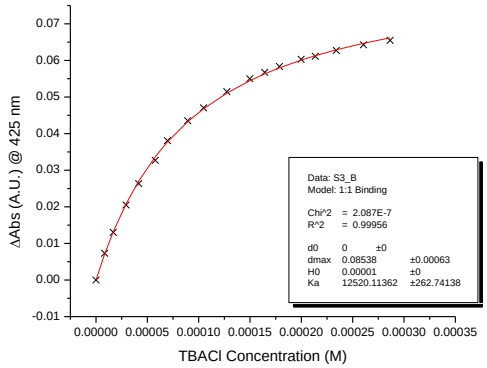
Figure S 31: UV/Vis Job Plot for the **3a**-Cl^- complex in THF. [**3a** + TBACl] = 102.6 µM.

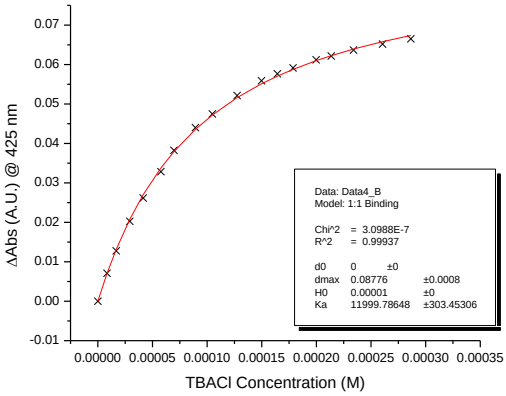


2.3.1.2.1.3 Titrations

Figure S 32: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **3a** in THF. All titrations carried out at 14.4 µM **3a**. From left to right: K_a = 12145.9 M^{-1}, K_a = 12520.1 M^{-1}, K_a = 11999.8 M^{-1}.



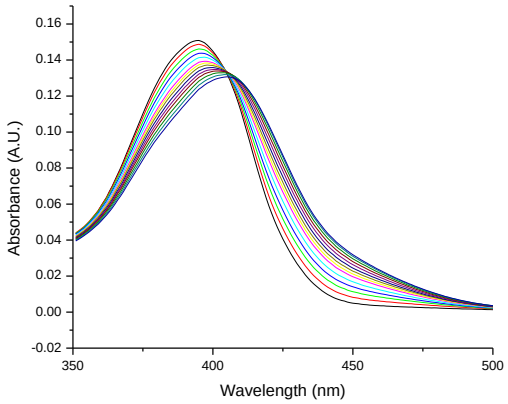




2.3.1.2.2 TBABr

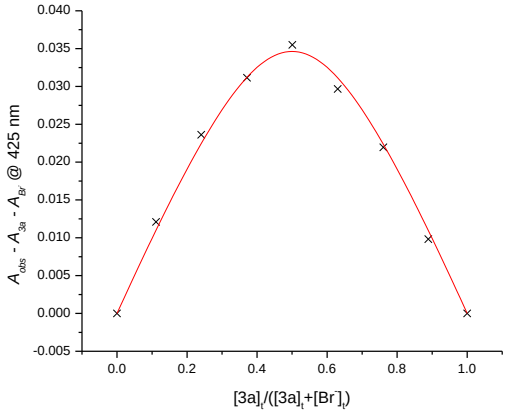
2.3.1.2.2.1 Spectrum

Figure S 33: Representative spectral change of **3a** upon the addition of TBABr in THF. Titration carried out at 12.3 µM **3a**, every other spectrum removed for clarity.



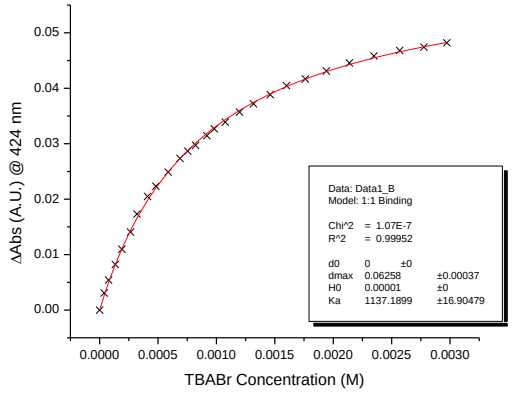
2.3.1.2.2.2 Job Plot

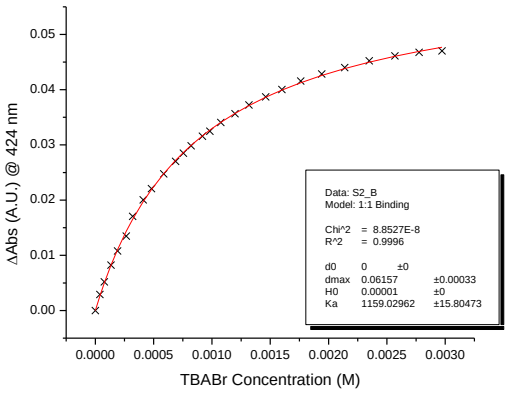
Figure S 34: UV/Vis Job Plot for the **3a**-Br^- complex in THF. [**3a** + TBABr] = 164 µM

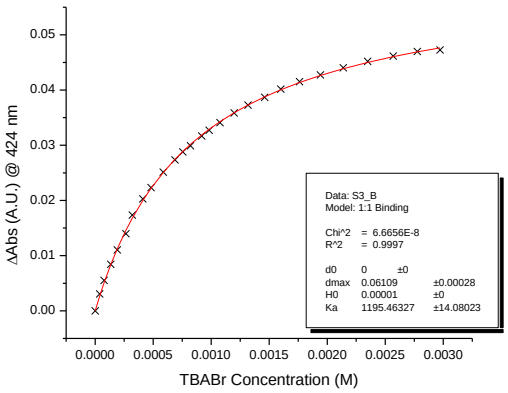


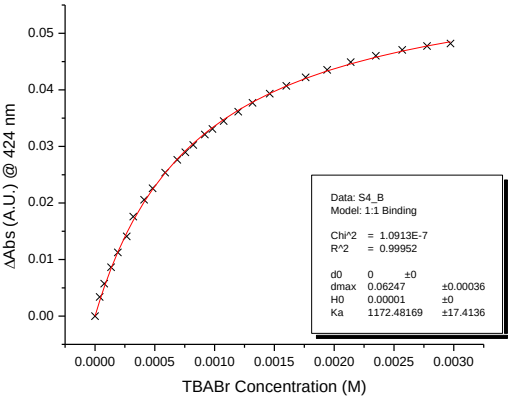
2.3.1.2.2.3 Titrations

Figure S 35: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **3a** in THF. All titrations carried out at 12.3 µM **3a**. From left to right: K_a = 1137.2 M^{-1}, K_a = 1159.0 M^{-1}, K_a = 1195.5 M^{-1}, K_a = 1172.5 M^{-1}.





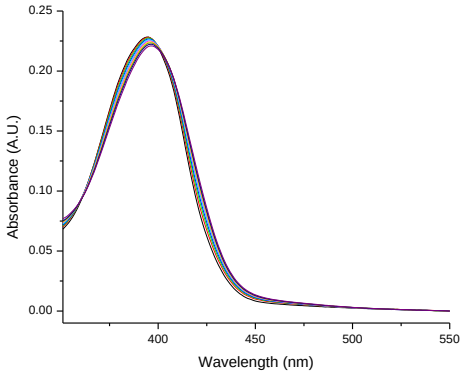




2.3.1.2.3 $TBANO_3$

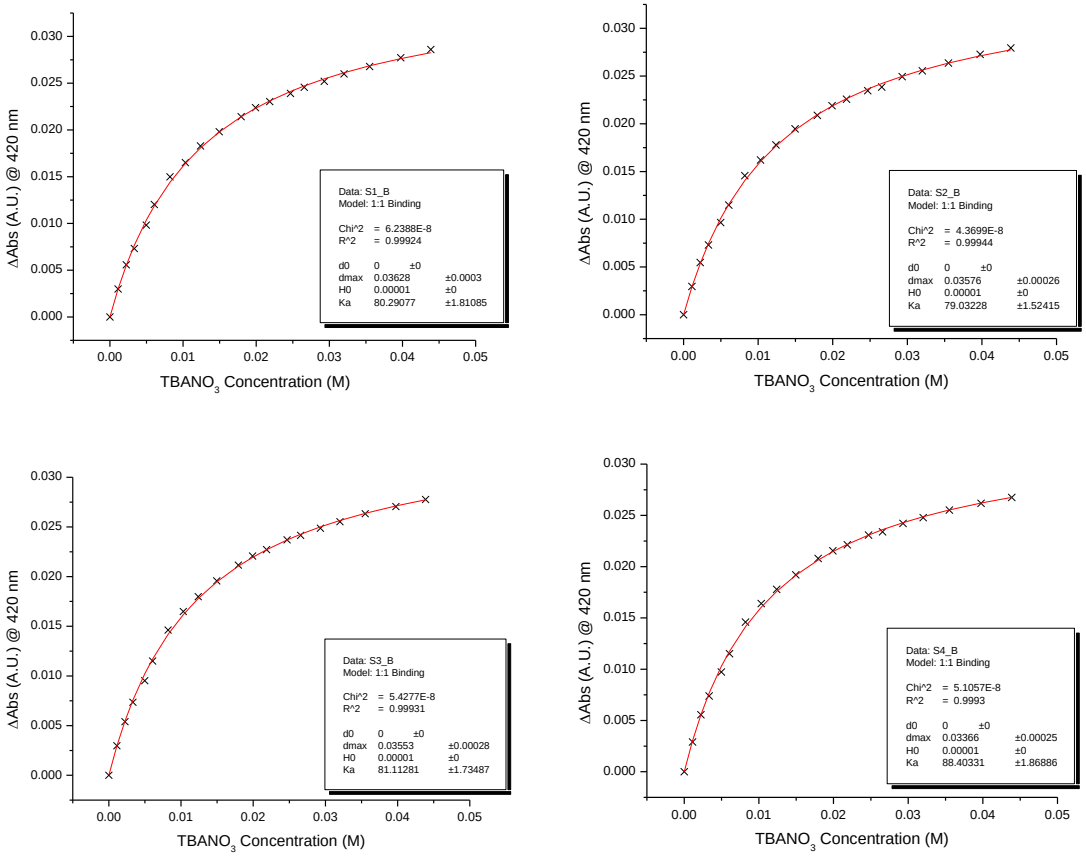
2.3.1.2.3.1 Spectrum

Figure S 36: Representative spectral change of **3a** upon the addition of $TBANO_3$ in THF. Titration carried out at 12.3 µM **3a**, every other spectrum removed for clarity.



2.3.1.2.3.2 Titrations

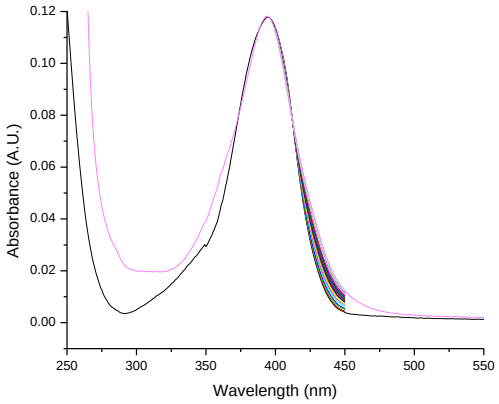
Figure S 37: Plots of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **3a** in THF. All titrations carried out at 12.3 µM **3a**. From left to right: K_a = 80.3 M^{-1}, K_a = 79.0 M^{-1}, K_a = 81.1 M^{-1}, K_a = 88.4 M^{-1}.



2.3.1.2.4 Quinuclidine

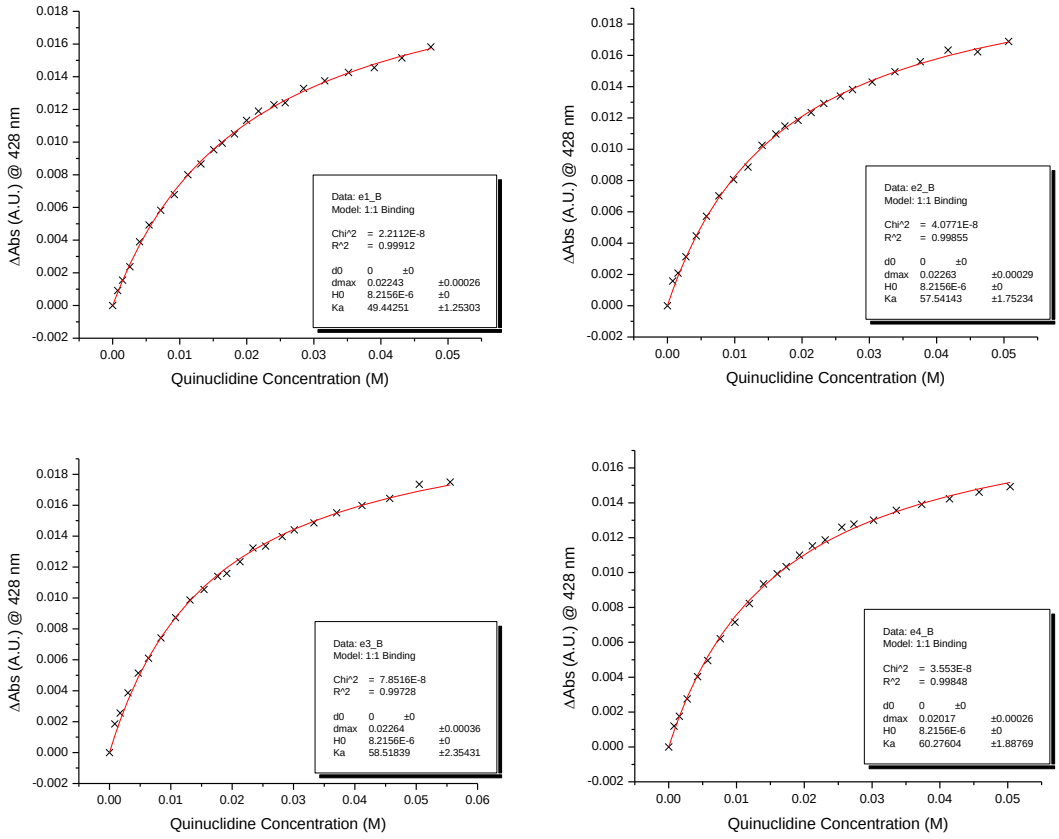
2.3.1.2.4.1 Spectrum

Figure S 38: Representative spectral change of **3a** upon the addition of Quinuclidine in THF. Titration carried out at 8.2µM **3a**.



2.3.1.2.4.2 Titrations

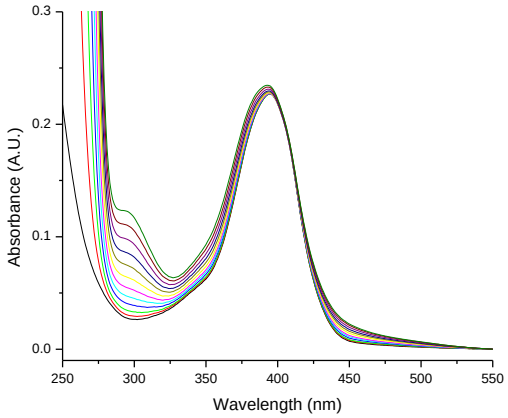
Figure S 39: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **3a** in THF carried out at 8.2 µM **3a**. K_a = 49 M^{-1}, K_a = 57 M^{-1}, K_a = 58 M^{-1}, K_a = 60 M^{-1}.



2.3.1.2.5 TBAI

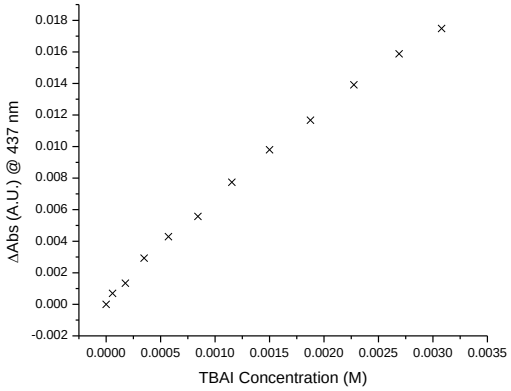
2.3.1.2.5.1 Spectrum

Figure S 40: Spectral change of **3a** upon the addition of TBAI in THF. Titration carried out at 16.4µM **3a**. Low solubility of TBAI in THF did not allow the measurement of association constants.

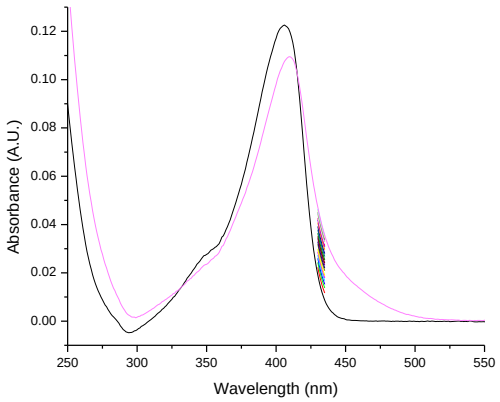


2.3.1.2.5.2 Titration

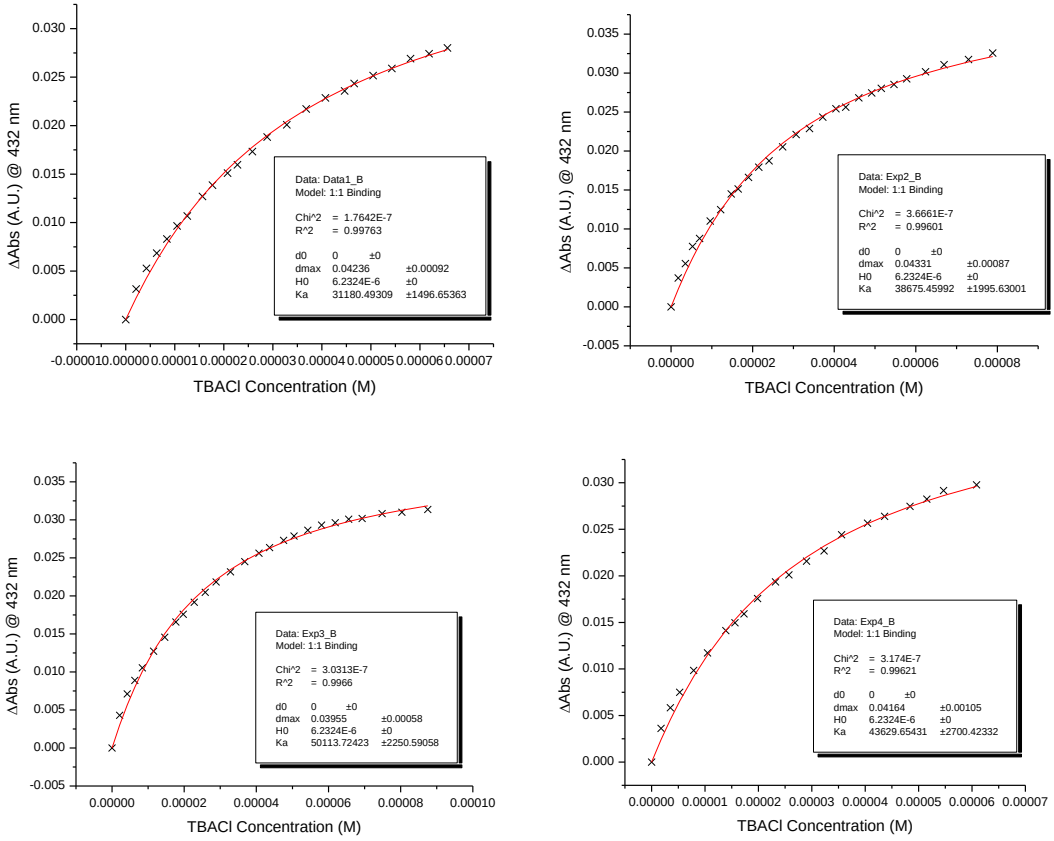
Figure S 41: Plot of ΔAbs versus TBAI concentration or the UV/Vis titration of 3a in THF. Titration carried out at 16.4µM **3a**. The low solubility of TBAI in THF precluded using the higher TBAI concentrations needed to measure association constants.



2.3.1.3 benzo[c][1,2,5]telluradiazole (4)
2.3.1.3.1 TBACl
2.3.1.3.1.1 Spectrum
Figure S 42: Spectral change of **4** upon the addition of TBACl in THF. Titration carried out at 6.2 µM **4**.



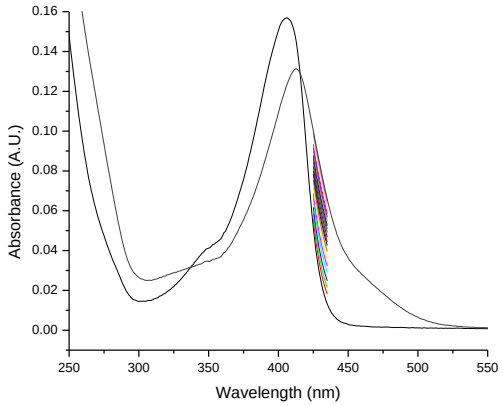
2.3.1.3.1.2 Titration
Figure S 43: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **4** in THF carried out at 6.2 µM **4**. From left to right: K_a = 31000 M^{-1}, K_a = 39000 M^{-1}, K_a = 50000 M^{-1}, K_a = 44000 M^{-1}.



2.3.1.3.2 TBABr

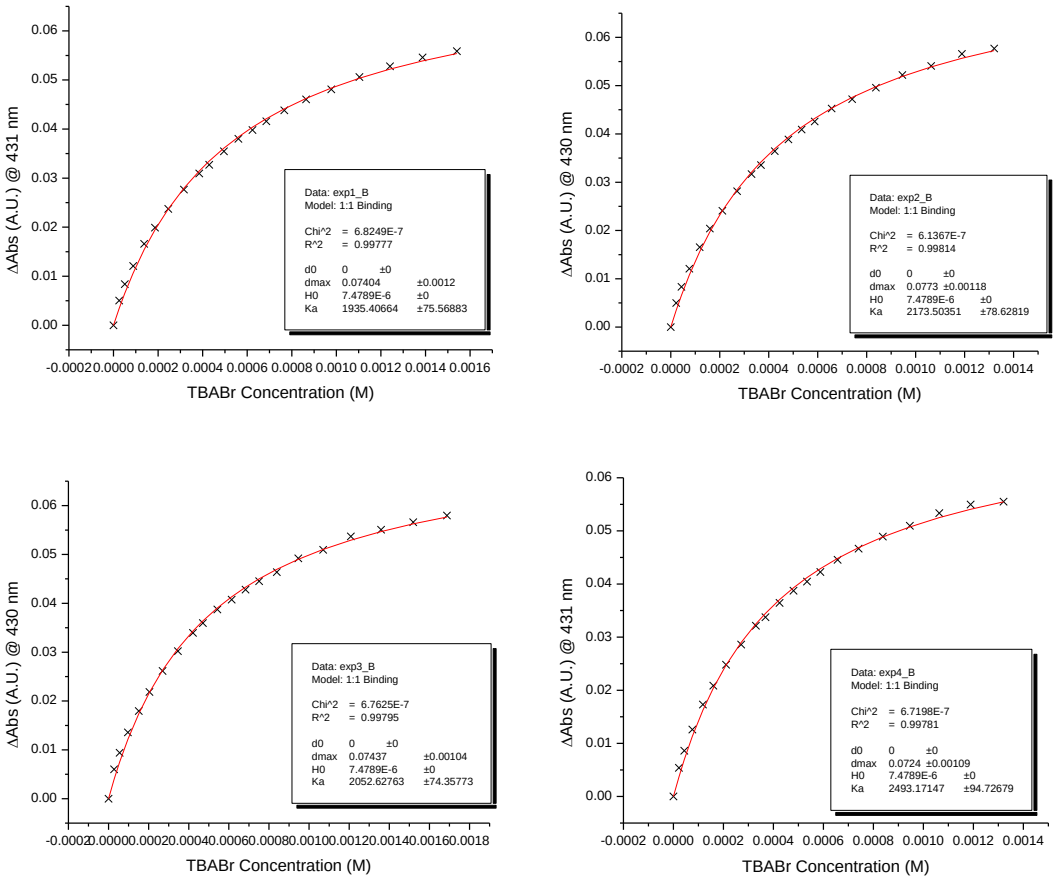
2.3.1.3.2.1 Spectrum

Figure S 44: Spectral change of **4** upon the addition of TBABr in THF. Titration carried out at 7.5 µM **4**.



2.3.1.3.2.2 Titration

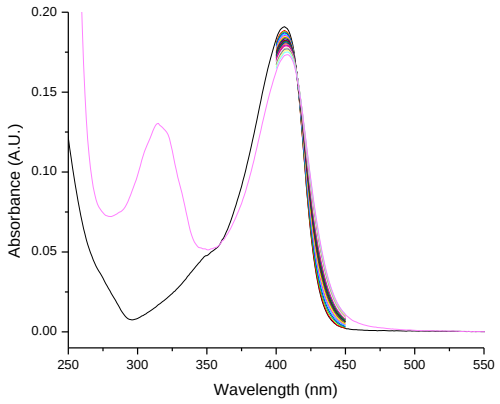
Figure S 45: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **4** in THF carried out at 7.5 µM **4**. From left to right: K_a = 1940 M^{-1}, K_a = 2170 M^{-1}, K_a = 2050 M^{-1}, K_a = 2490 M^{-1}.



2.3.1.3.3 $TBANO_3$

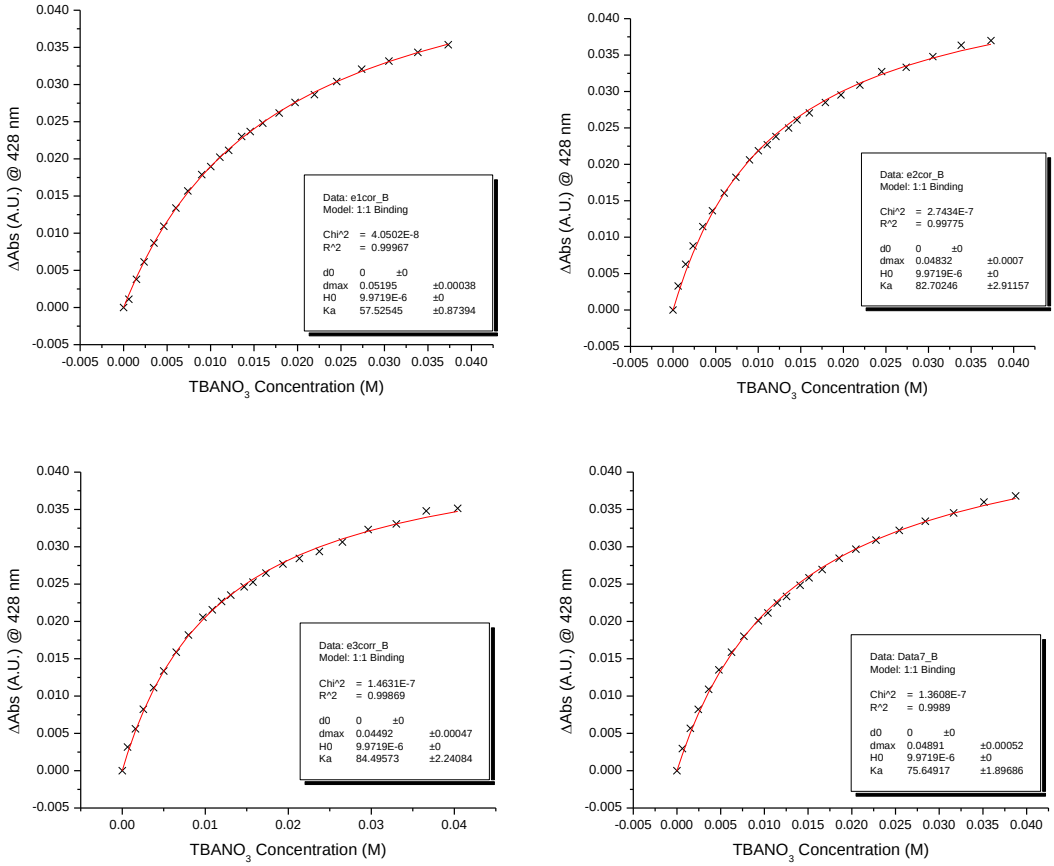
2.3.1.3.3.1 Spectrum

Figure S 46: Spectral change of **4** upon the addition of $TBANO_3$ in THF. Titration carried out at 10.0 µM **4**. Note the absorbance increase upon addition of quinuclidine, characteristic of donor decomposition to the diamine.



2.3.1.3.3.2 Titration

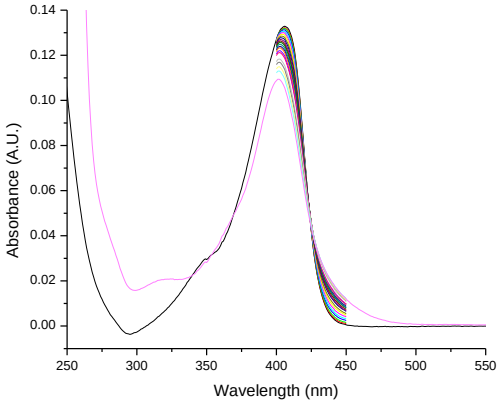
Figure S 47: Plots of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **4** in THF carried out at 10.0 µM **4**. From left to right: K_a = 57.5 M^{-1}, K_a = 83 M^{-1}, K_a = 84 M^{-1}, K_a = 76 M^{-1}.



2.3.1.3.4 Quinuclidine

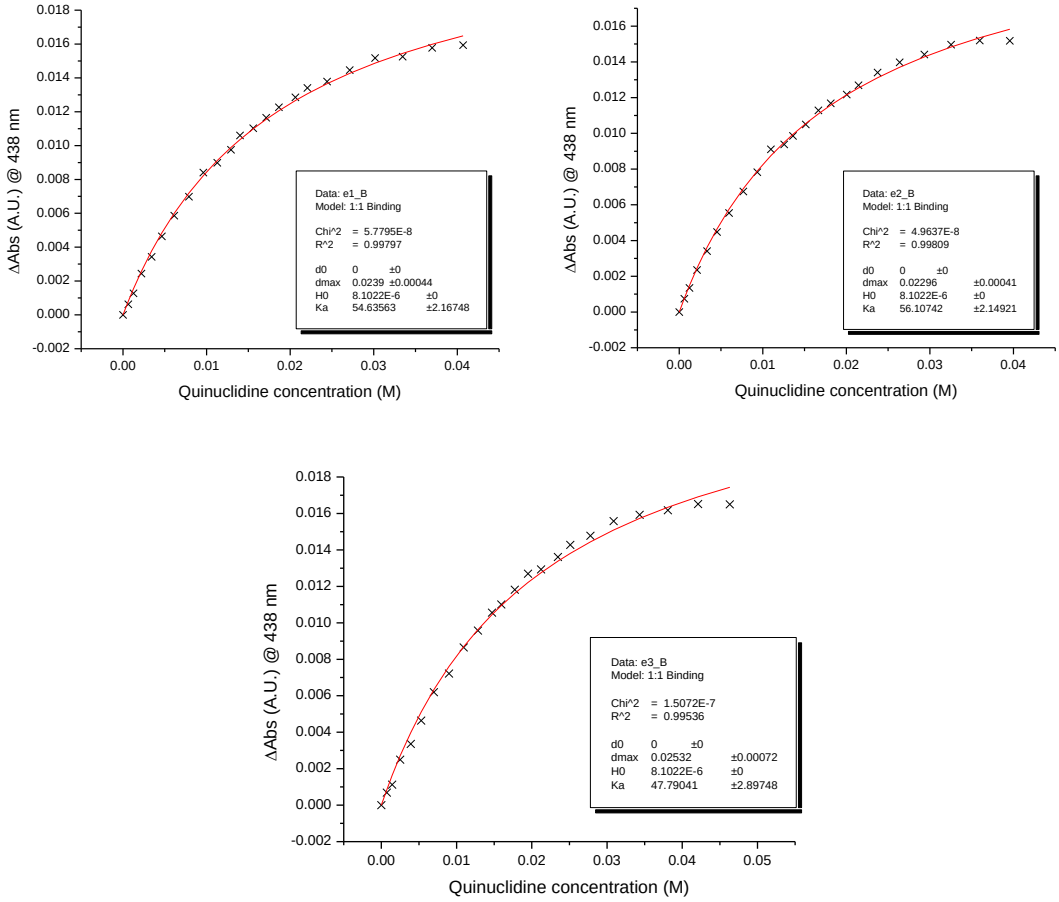
2.3.1.3.4.1 Spectrum

Figure S 48: Spectral change of **4** upon the addition of Quinuclidine in THF. Titration carried out at 8.1µM **4**. Note the absorbance decrease upon addition of quinuclidine, characteristic of donor decomposition.



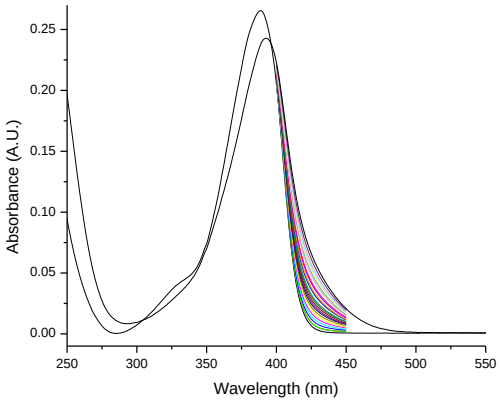
2.3.1.3.4.2 Titration

Figure S 49: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **4** in THF carried out at 8.1 µM **4**. From left to right: K_a = 55 M^{-1}, K_a = 56 M^{-1}, K_a = 48 M^{-1}.



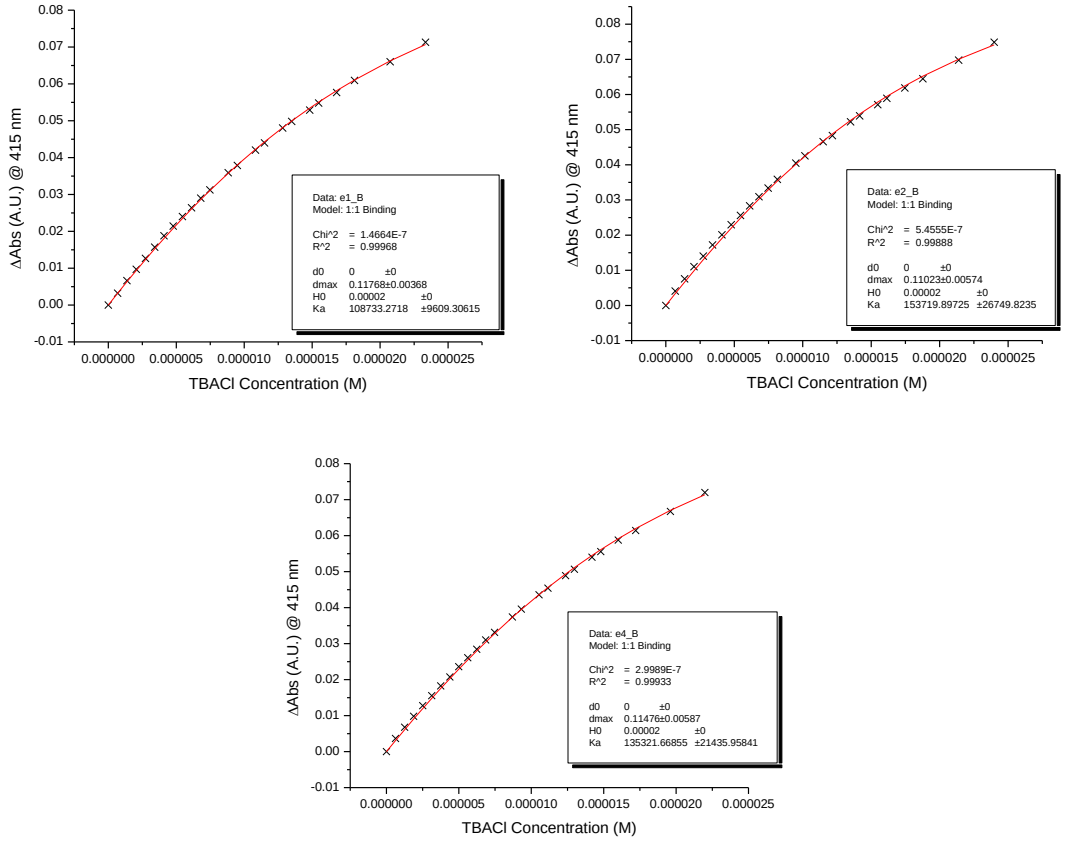
2.3.1.4 perfluoro[c][1,2,5]telluradiazole-5-carbonitrile (5)
2.3.1.4.1 TBACl
2.3.1.4.1.1 Spectrum

Figure S 50: Spectral change of **5** upon the addition of TBACl in THF. Titration carried out at 15.8µM **5**.



2.3.1.4.1.2 Titration

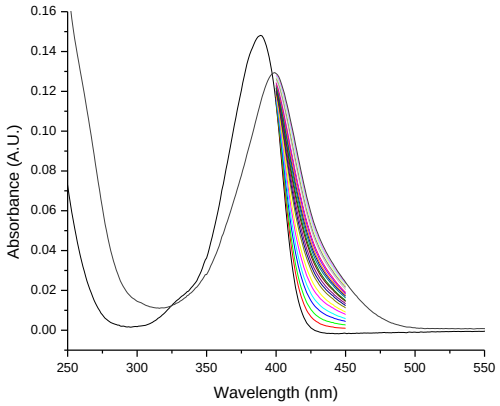
Figure S 51: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **5** in THF carried out at 15.8 µM **5**. From left to right: K_a = 110000 M^{-1}, K_a = 150000 M^{-1}, K_a = 140000 M^{-1}.



2.3.1.4.2 TBABr

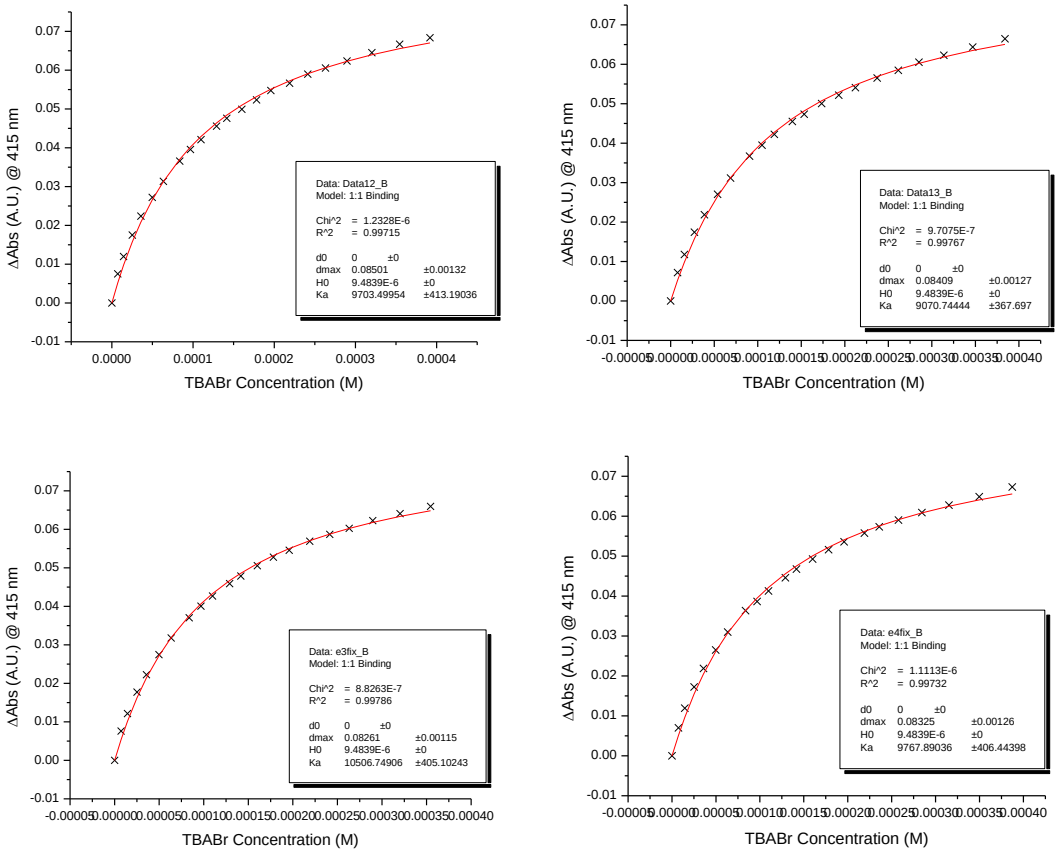
2.3.1.4.2.1 Spectrum

Figure S 52: Spectral change of **5** upon the addition of TBABr in THF. Titration carried out at 9.5 µM **5**.



2.3.1.4.2.2 Titration

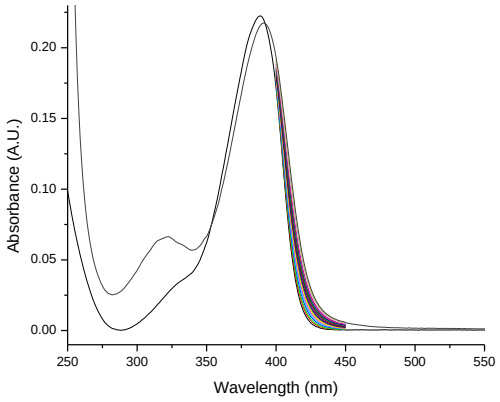
Figure S 53: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **5** in THF carried out at 9.5 µM **5**. From left to right: K_a = 9700 M^{-1}, K_a = 9100 M^{-1}, K_a = 10500 M^{-1}, K_a = 9800 M^{-1}.



2.3.1.4.3 $TBANO_3$

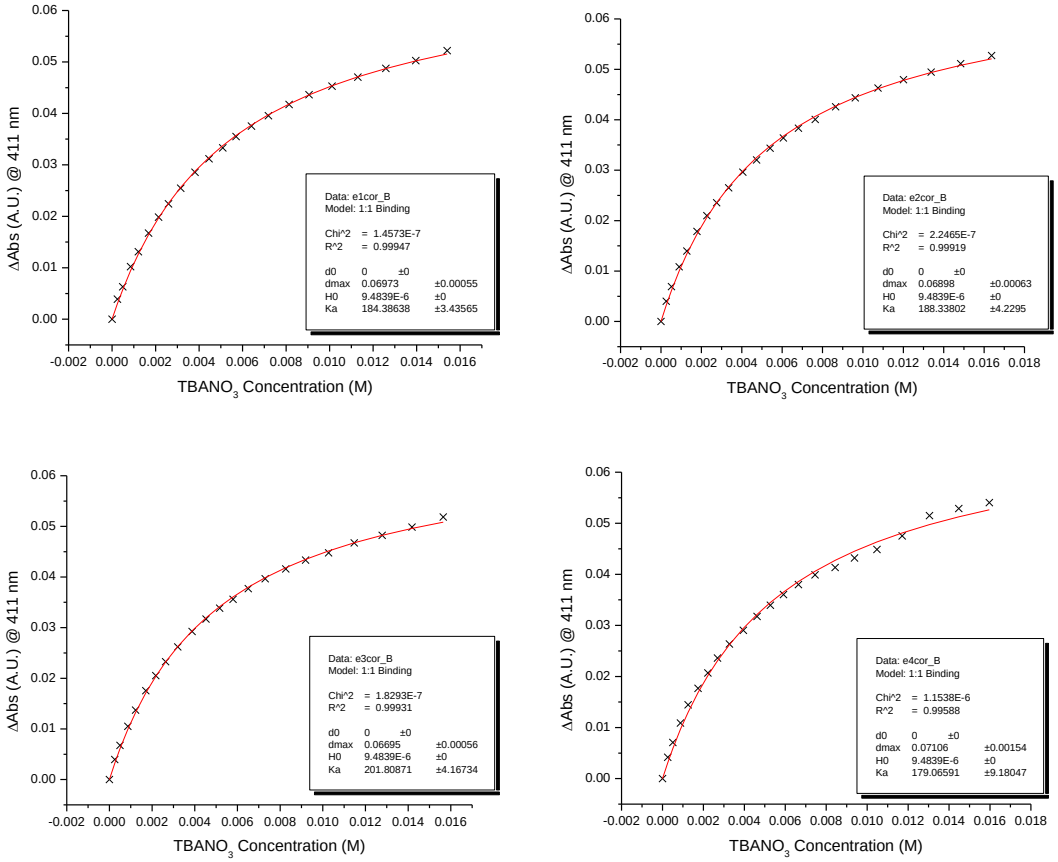
2.3.1.4.3.1 Spectrum

Figure S 54: Spectral change of **5** upon the addition of $TBANO_3$ in THF. Titration carried out at 9.4 µM **5**. Note the absorbance increase caused by decomposition to the diamine.



2.3.1.4.3.2 Titration

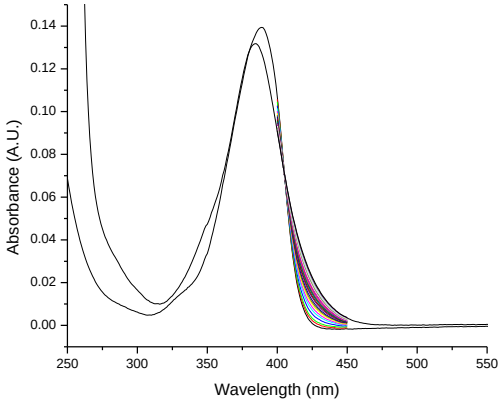
Figure S 55: Plots of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **5** in THF carried out at 9.4 µM **5**. From left to right: K_a = 184 M^{-1}, K_a = 188 M^{-1}, K_a = 202 M^{-1}, K_a = 179 M^{-1}.



2.3.1.4.4 Quinuclidine

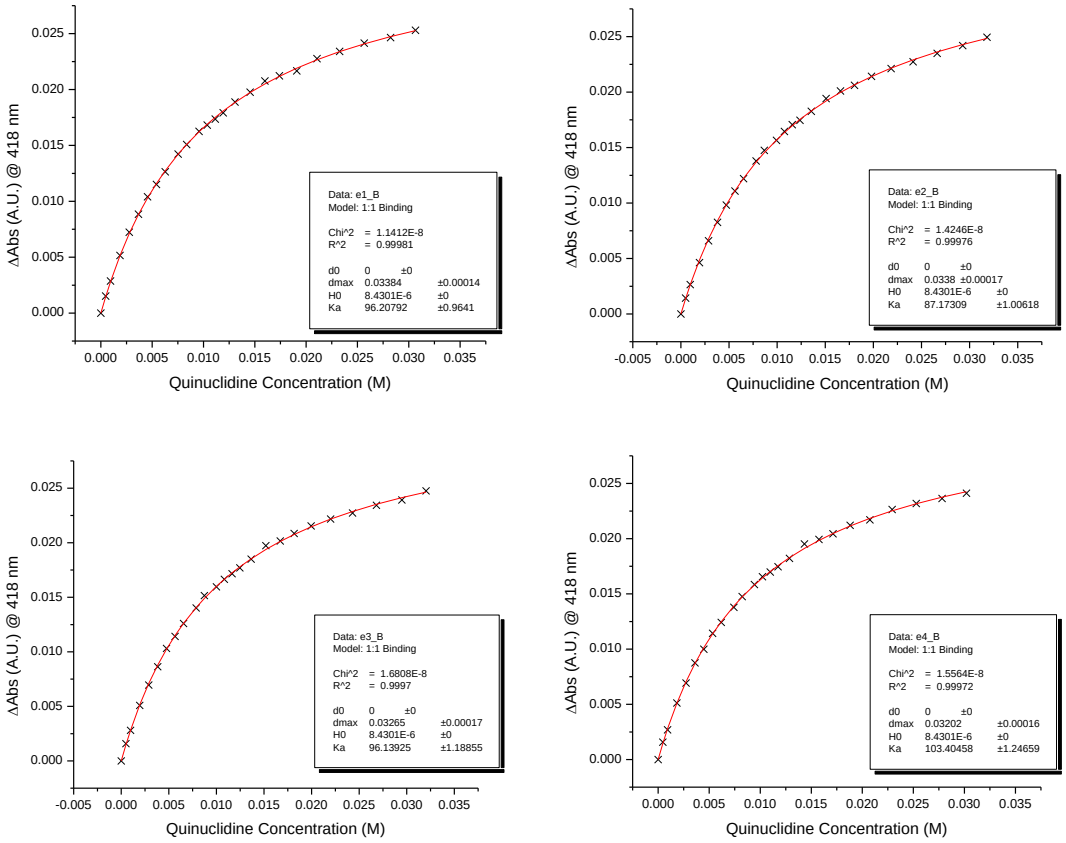
2.3.1.4.4.1 Spectrum

Figure S 56: Spectral change of **5** upon the addition of Quinuclidine in THF. Titration carried out at 8.3µM **5**



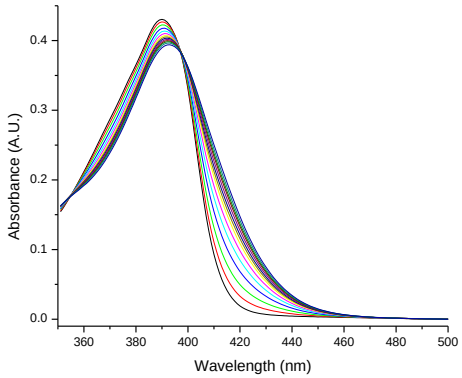
2.3.1.4.4.2 Titration

Figure S 57: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **5** in THF carried out at 8.3 µM **5**. From left to right: K_a = 96 M^{-1}, K_a = 87 M^{-1}, K_a = 96 M^{-1}, K_a = 103 M^{-1}.



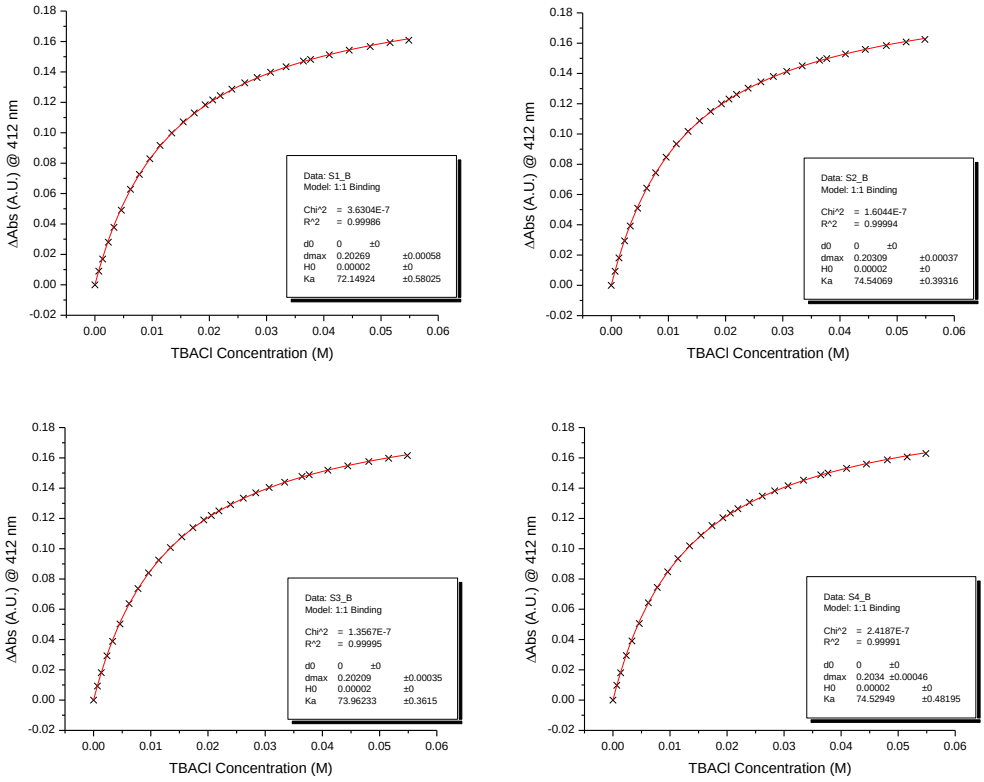
2.3.2 ACN
2.3.2.1 benzo[c][1,2,5]telluradiazole (2)
2.3.2.1.1 TBACl
2.3.2.1.1.1 Spectrum

Figure S 58: Representative spectral change of **2** upon the addition of TBACl in ACN. Titration carried out at 19.3 µM **2**, every other spectrum removed for clarity.



2.3.2.1.1.2 Titrations

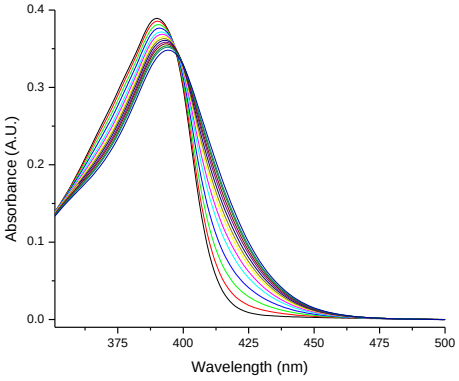
Figure S 59: Plots of ΔAbs versus TBACl concentration for the UV/Vis titration of **2** in ACN. All titrations carried out at 19.3 µM **2**. From left to right: K_a = 72.1 M^{-1}, K_a = 74.5 M^{-1}, K_a = 74.0 M^{-1}, K_a = 74.5 M^{-1}.



2.3.2.1.2 TBABr

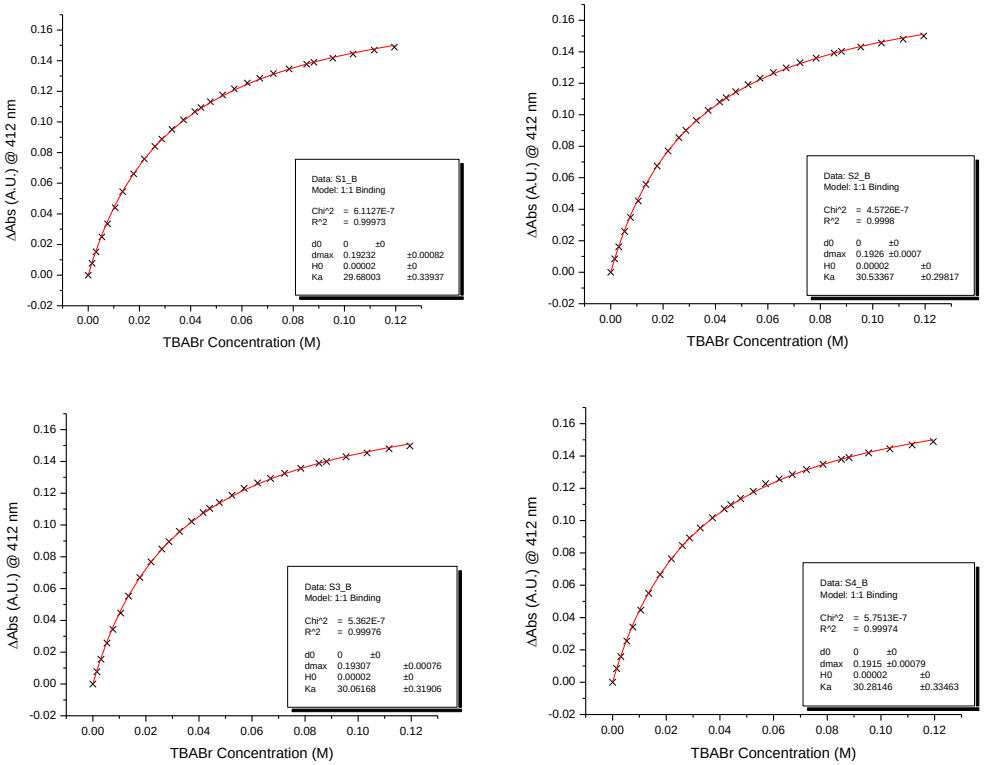
2.3.2.1.2.1 Spectrum

Figure S 60: Representative spectral change of **2** upon the addition of TBABr in ACN. Titration carried out at 20.7 µM **2**, every other spectrum removed for clarity.



2.3.2.1.2.2 Titrations

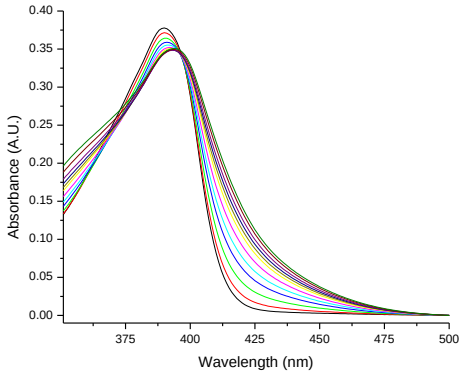
Figure S 61: Plots of ΔAbs versus TBABr concentration for the UV/Vis titration of **2** in ACN. All titrations carried out at 20.7 µM **2**. From left to right: K_a = 29.7 M^{-1}, K_a = 30.5 M^{-1}, K_a = 30.1 M^{-1}, K_a = 30.3 M^{-1}.



2.3.2.1.3 TBAI

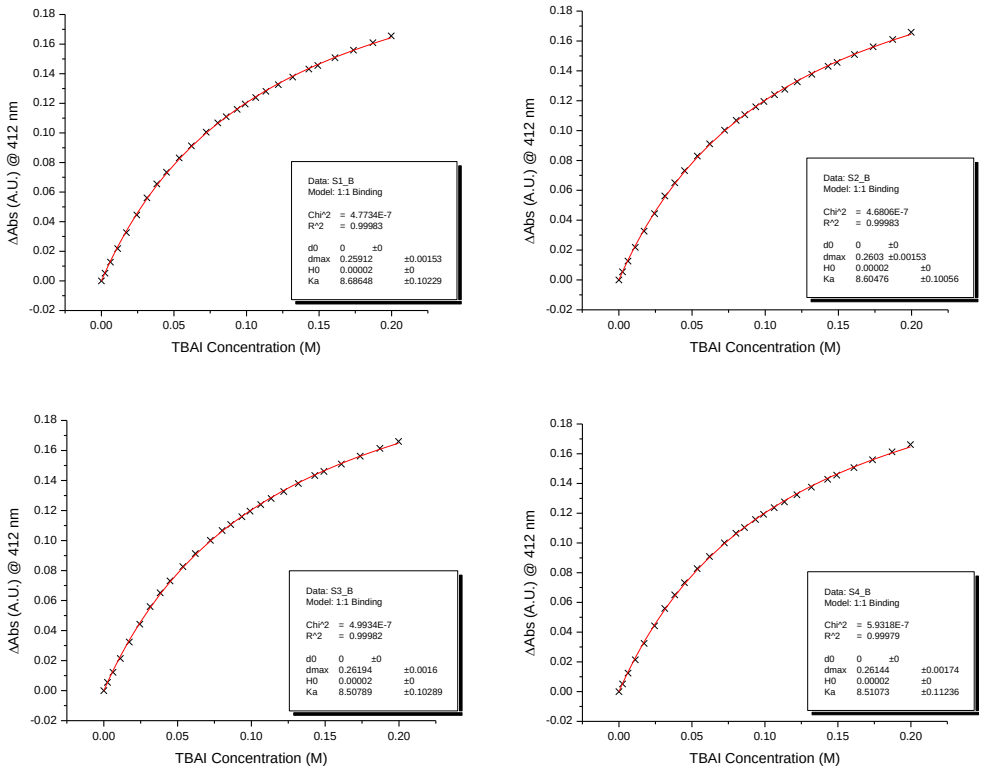
2.3.2.1.3.1 Spectrum

Figure S 62: Representative spectral change of **2** upon the addition of TBAI in ACN. Titration carried out at 19.3 µM **2**, every other spectrum removed for clarity.



2.3.2.1.3.2 Titrations

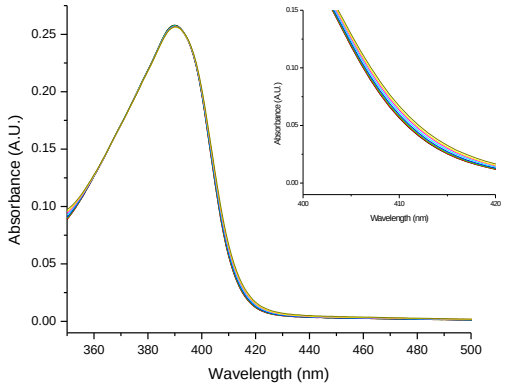
Figure S 63: Plots of ΔAbs versus TBAI concentration for the UV/Vis titration of **2** in ACN. All titrations carried out at 19.3 µM **2**. From left to right: K_a = 8.7 M^{-1}, K_a = 8.6 M^{-1}, K_a = 8.5 M^{-1}, K_a = 8.5 M^{-1}.



2.3.2.1.4 $TBANO_3$

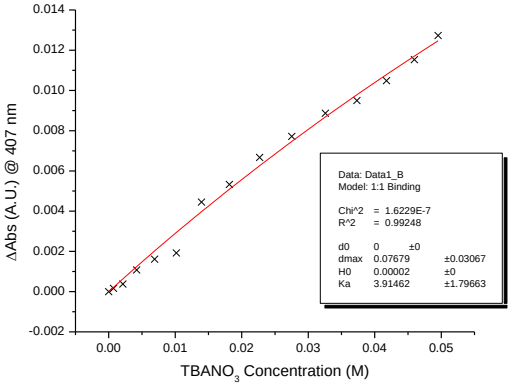
2.3.2.1.4.1 Spectrum

Figure S 64: Representative spectral change of **2** upon the addition of $TBANO_3$ in ACN. Titration carried out at 17.3 µM **2**, every other spectrum removed for clarity.



2.3.2.1.4.2 Titration

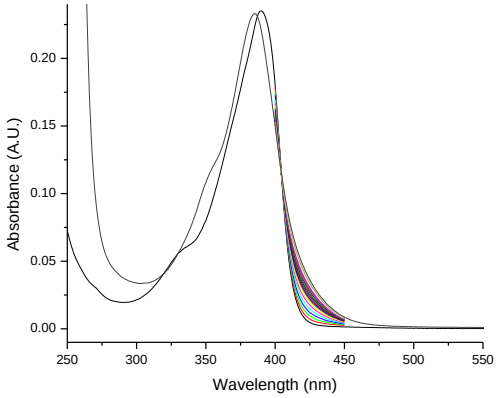
Figure S 65: Plot of ΔAbs versus $TBANO_3$ concentration for the UV/Vis titration of **2** in ACN. Titration carried out at 17.3 µM **2**. K_a = 3.9 M^{-1}, too small to measure accurately. The low solubility of $TBANO_3$ in ACN precluded using higher concentrations of $TBANO_3$,



2.3.2.1.5 Quinuclidine

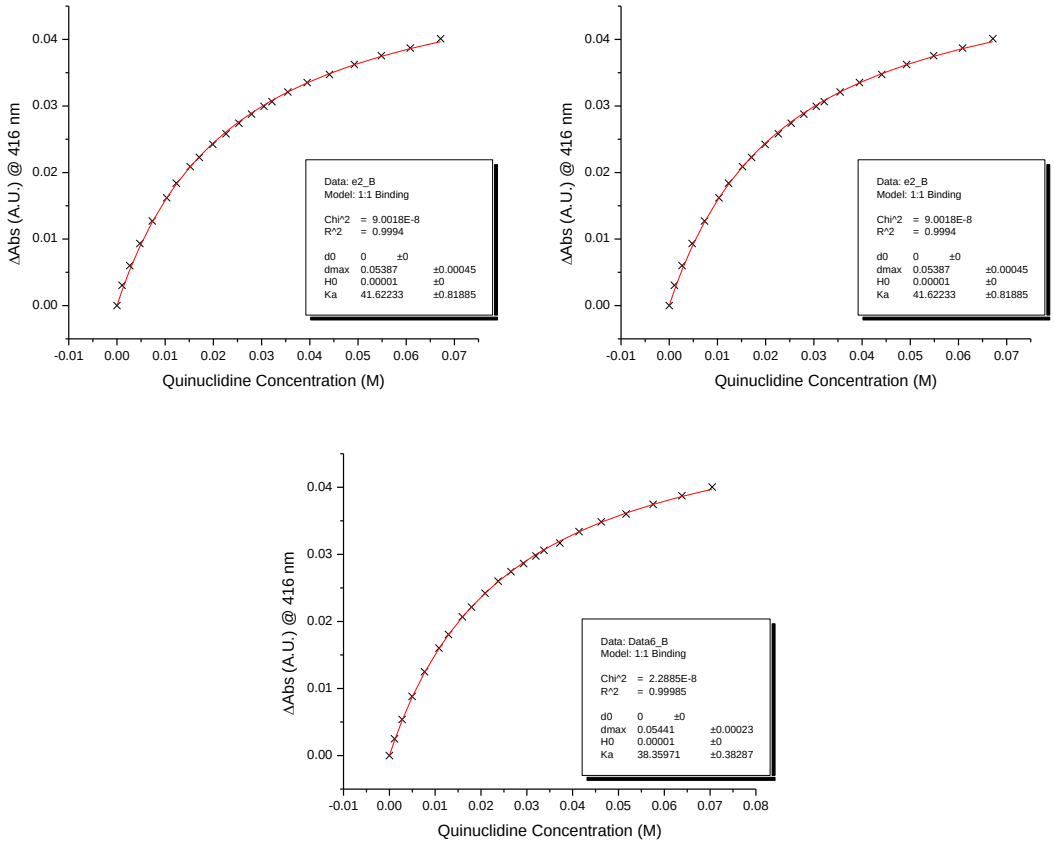
2.3.2.1.5.1 Spectrum

Figure S 66: Representative spectral change of **2** upon the addition of Quinuclidine in ACN. Titration carried out at 11.0 µM **2**.



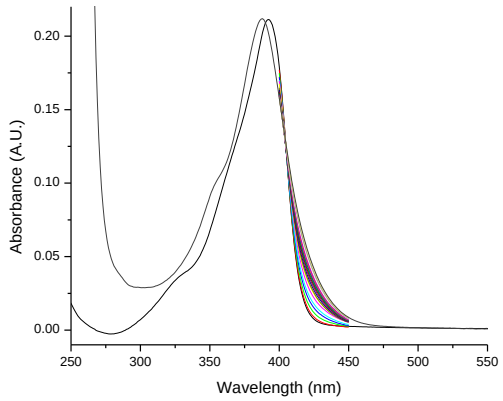
2.3.2.1.4.2 Titration

Figure S 67: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **2** in ACN. All titrations carried out at 11.0 µM **2**. From left to right: K_a = 41.6 M^{-1}, K_a = 38.4 M^{-1}, K_a = 40.6 M^{-1}.



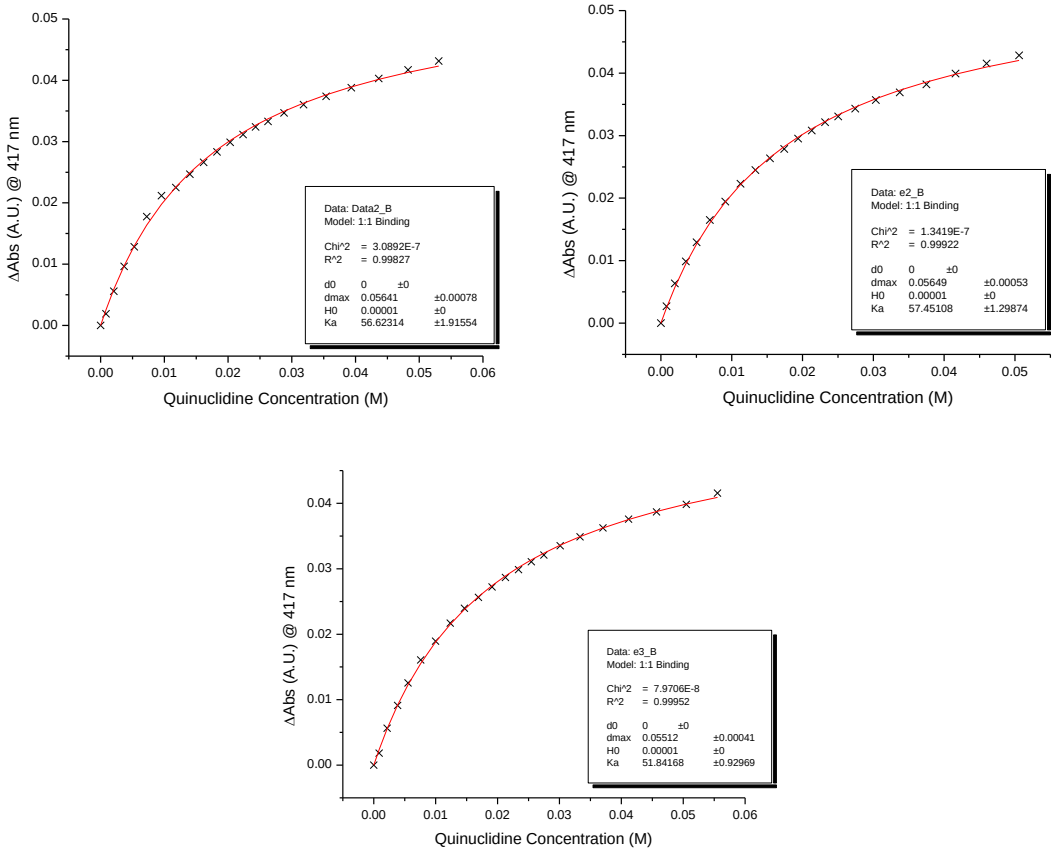
2.3.3 DCM
2.3.3.1 benzo[c][1,2,5]telluradiazole (2)
2.3.3.1.1 Quinuclidine
2.3.3.1.1.1 Spectrum

Figure S 68: Representative spectral change of **2** upon the addition of Quinuclidine in DCM. Titration carried out at 10.3 µM **2**.



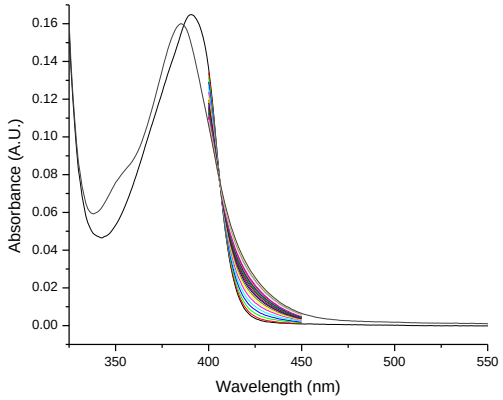
2.3.3.1.1.1 Titration

Figure S 69: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **2** in DCM. All titrations carried out at 10.3 µM **2**. From left to right: K_a = 57 M^{-1}, K_a = 57 M^{-1}, K_a = 51 M^{-1}.



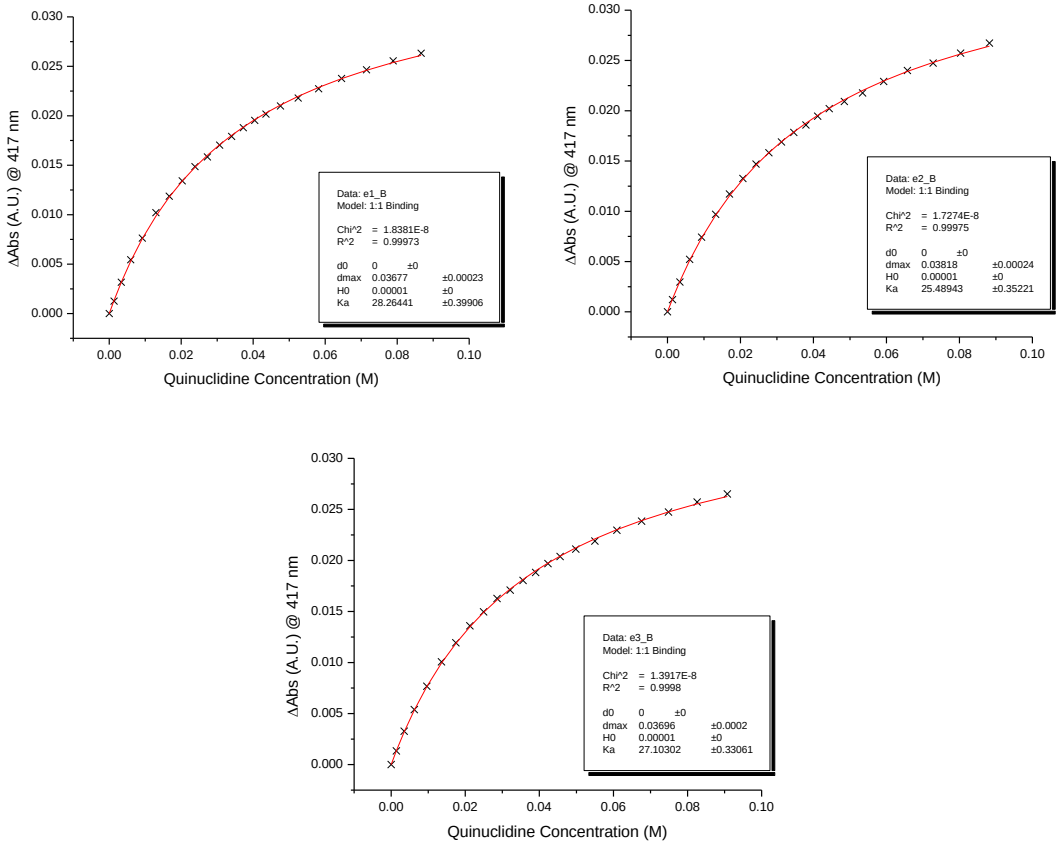
2.3.4 Acetone
2.3.4.1 benzo[c][1,2,5]telluradiazole (2)
2.3.4.1.1 Quinuclidine
2.3.4.1.1.1 Spectrum

Figure S 70: Spectral change of **2** upon the addition of Quinuclidine in Acetone. Titration carried out at 10.4 µM **2**.

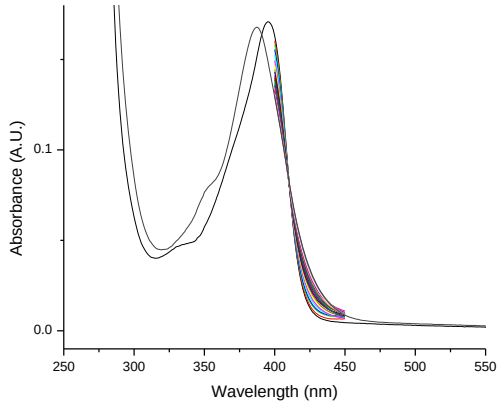


2.3.4.1.1.1 Titration

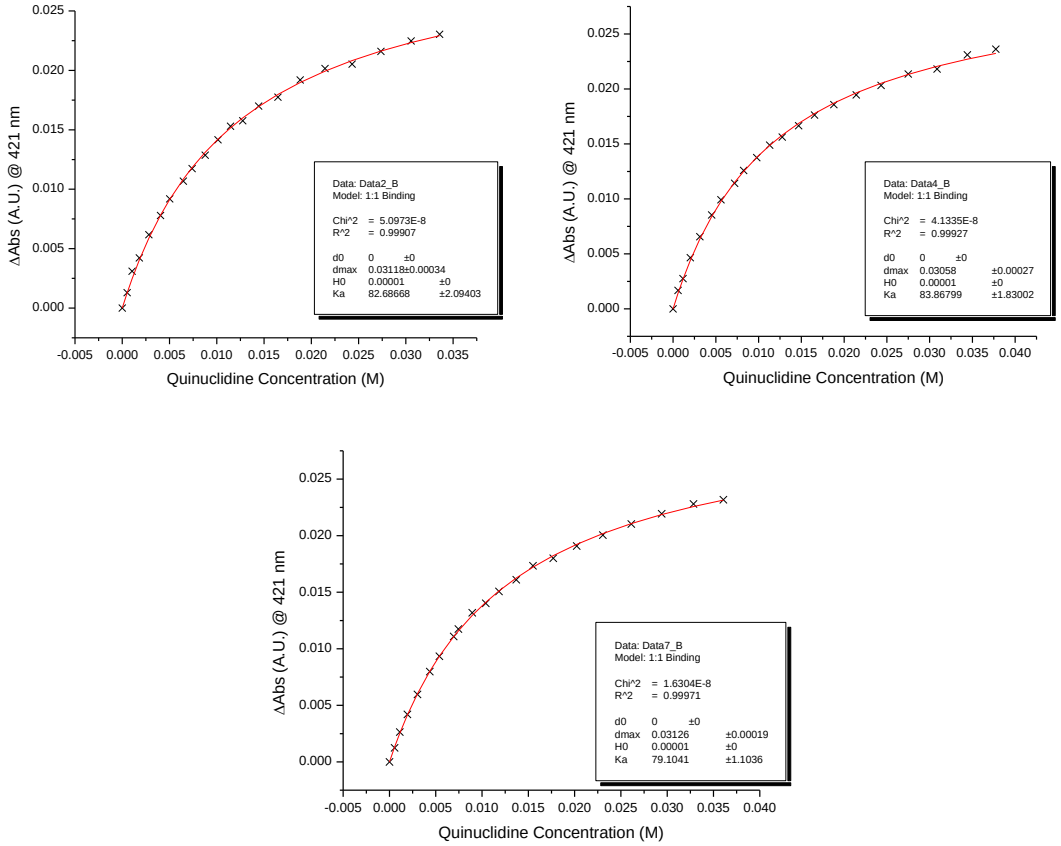
Figure S 71: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **2** in Acetone. All titrations carried out at 10.4 µM **2**. From left to right: K_a = 28.3 M^{-1}, K_a = 25.5 M^{-1}, K_a = 27.1 M^{-1}.



2.3.5 Toluene
2.3.5.1 benzo[c][1,2,5]telluradiazole (2)
2.3.5.1.1 Quinuclidine
2.3.5.1.1.1 Spectrum
Figure S 72: Spectral change of **2** upon the addition of Quinuclidine in Toluene. Titration carried out at 12.4 µM **2**.



2.3.5.1.1.1 Titration
Figure S 73: Plots of ΔAbs versus Quinuclidine concentration for the UV/Vis titration of **2** in Toluene. All titrations carried out at 12.4 µM **2**. From left to right: K_a = 83 M^{-1}, K_a = 84 M^{-1}, K_a = 79 M^{-1}.

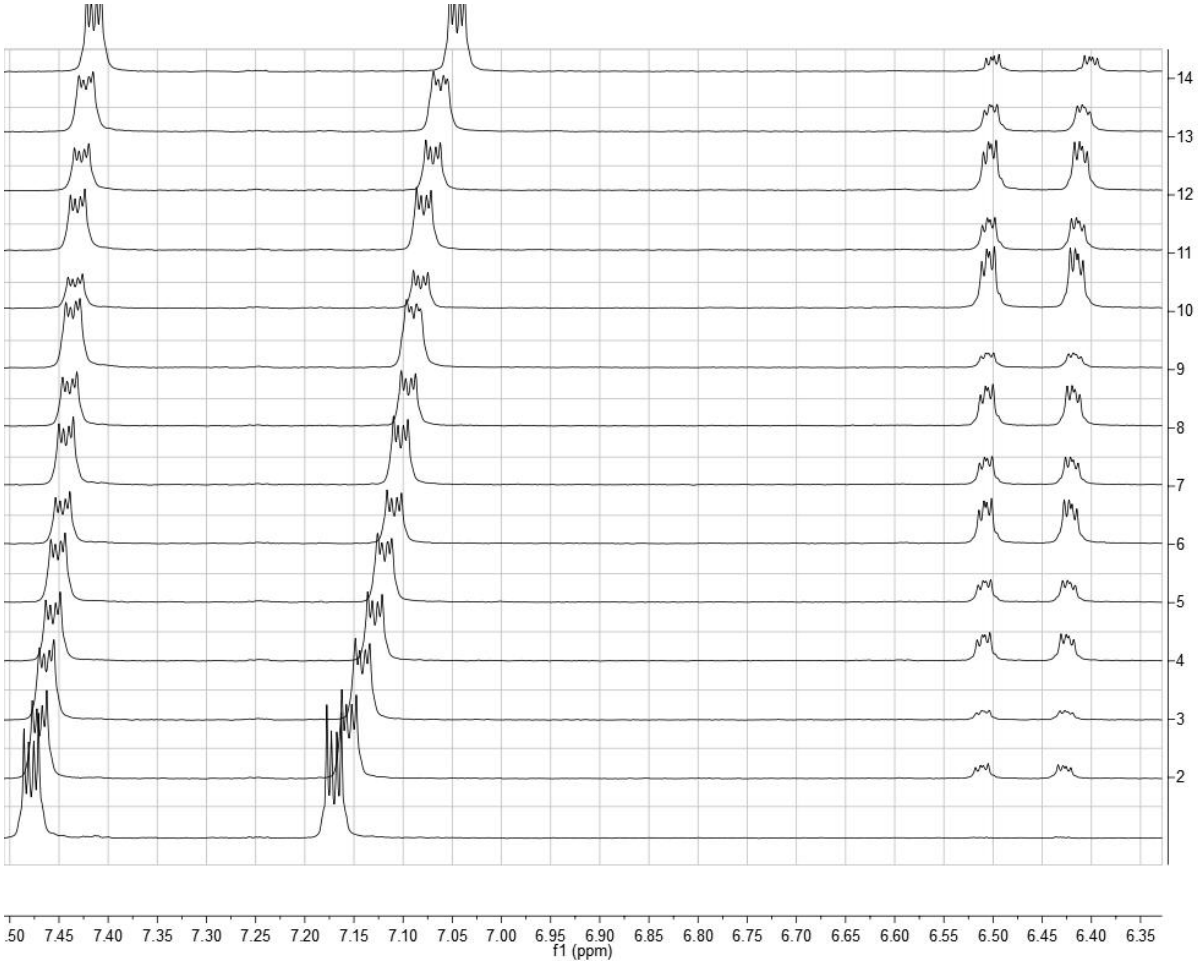


2.4 NMR Titrations with TBACl in THF-d_8

2.4.1 benzo[c][1,2,5]telluradiazole (2)

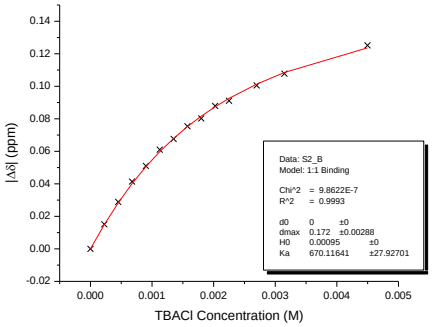
2.4.1.1 NMR Spectra

Figure S 74: NMR spectra of the titration of 959.5 µM **2** with TBACl in THF-d_8. TBACl concentration increases on the y-axis. Upfield peak shift from δ 7.47 and δ 7.16 represents donor-acceptor binding. Peak growth at δ 6.51 and δ 6.43 is that of the 1,2-phenylenediamine decomposition product. Experiments were not run in the order presented. Sample order was randomized to reduce systematic error in the fit.



2.4.1.2 Titration curve

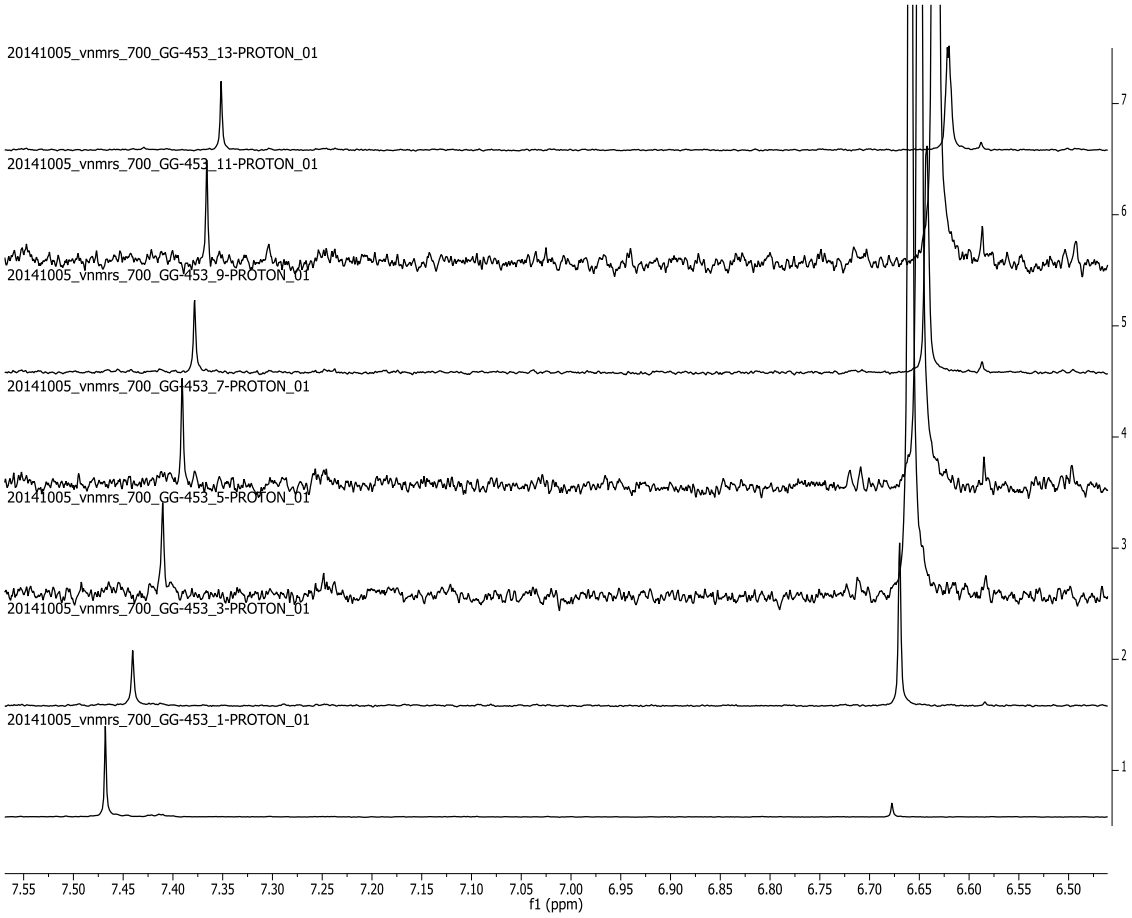
Figure S 75: Plot of |Δδ| versus TBACl concentration for the NMR titration of **2** in THF-d_8. Titration carried out at 959.5 µM **2**. K_a = 670.1 M^{-1}.



2.4.2 4,7-Dibromobenzo[c]-1,2,5-telluradiazole (3a)

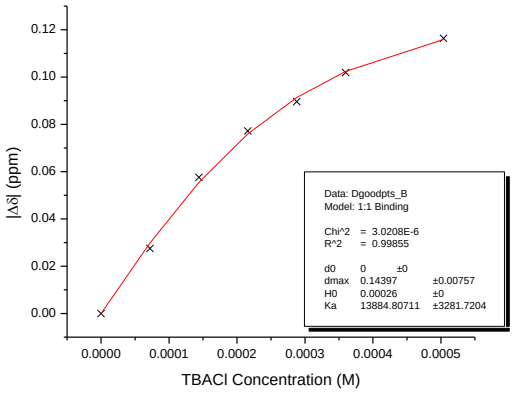
2.4.2.1 NMR Spectra

Figure S 76: NMR spectra of the titration of 256.7 µM **3a** with TBACl in THF-d_8. TBACl concentration increases on the y-axis. Upfield peak shift from δ 7.46 represents donor-acceptor binding. Peak growth at δ 6.50 is that of the 3,6-dibromobenzene-1,2-diamine decomposition product. Experiments were not run in the order presented. Sample order was randomized to reduce systematic error in the fit.



2.4.2.2 Titration curve

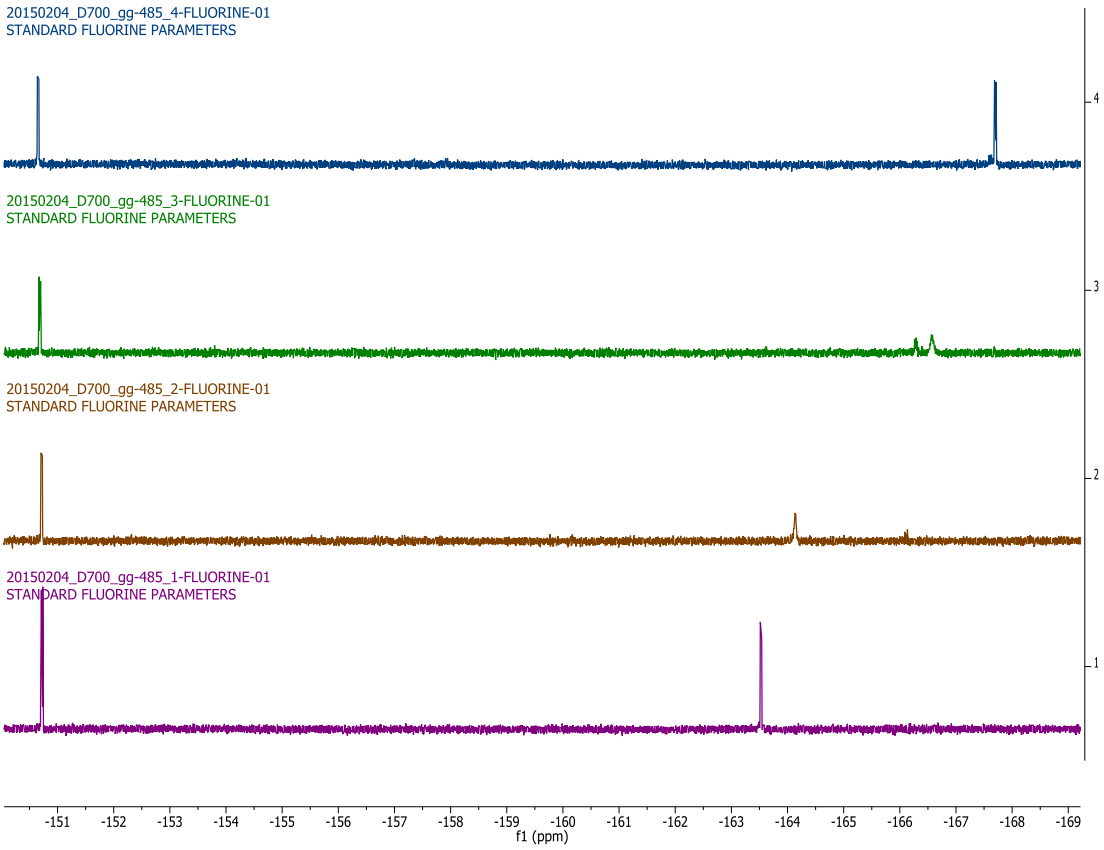
Figure S 77: Plot of |Δδ| versus TBACl concentration for the NMR titration of **3a** in THF-d_8. Titration carried out at 256.7 µM **3a**. K_a = 13884.8 M^{-1}.



2.4.3 perfluorobenzo[c][1,2,5]telluradiazole (5)

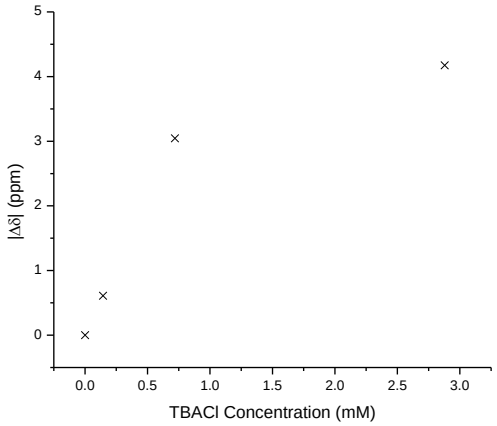
2.4.3.1 NMR Spectra

Figure S 78: ^{19}F NMR spectra of 329.3 µM **4** upon the addition of TBACl in THF-d_8. TBACl concentration increases on the y-axis. Upfield peak shift from δ -163.53 represents donor-acceptor binding. Experiments were not run in the order presented, first and last data points obtained first.



2.4.3.2 Titration curve

Figure S 79: Plot of |Δδ| versus TBACl concentration for **5** in THF-d_8. Titration carried out at 329.3 µM **5**. Data not fit to a binding isotherm.



2.5 Other acceptors tested for chalcogen bonding

2.5.1 benzo[c][1,2,5]telluradiazole (2) in ACN

Figure S 80: Spectral change of **2** upon the addition of TBA halide salts. Spectra were stable over time with no lowering of peak absorbance. Test conducted at 27.6 µM **2**.

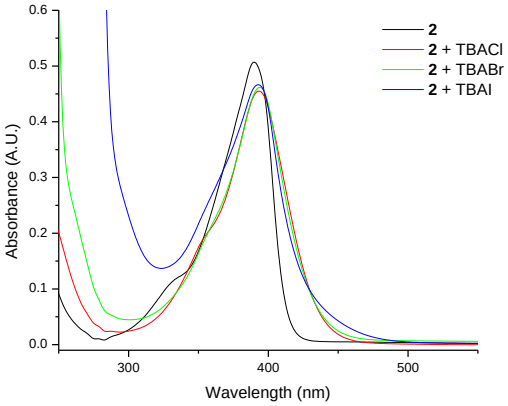
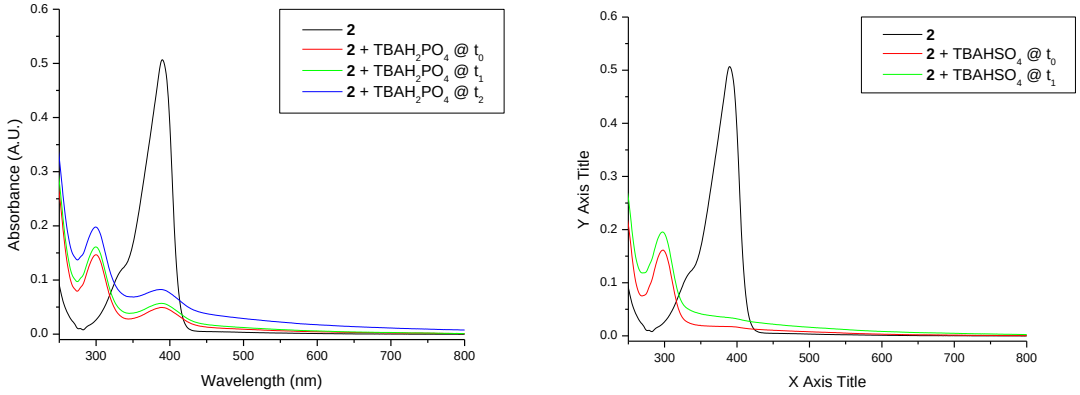


Figure S 81: Spectral change of **2** upon the addition of $TBAH_2PO_4$ (right) and $TBAHSO_4$ (left). Telluradiazole absorbance disappeared immediately after addition, followed by precipitate formation over time, increasing absorbance. Peak growth at 300 nm suggests diamine formation. Test conducted at 27.6 µM **2**.



2.5.2 benzo[c][1,2,5]telluradiazole (2) in THF

Figure S 82: TBAF titration with **2** in THF at 11.4 µM. Left: Spectral changes upon TBAF addition. Telluradiazole absorbance decreases. Right: absolute absorbance change vs. TBAF equivalents added. Data could not be fit to a 1:1 or 2:1 binding isotherm.

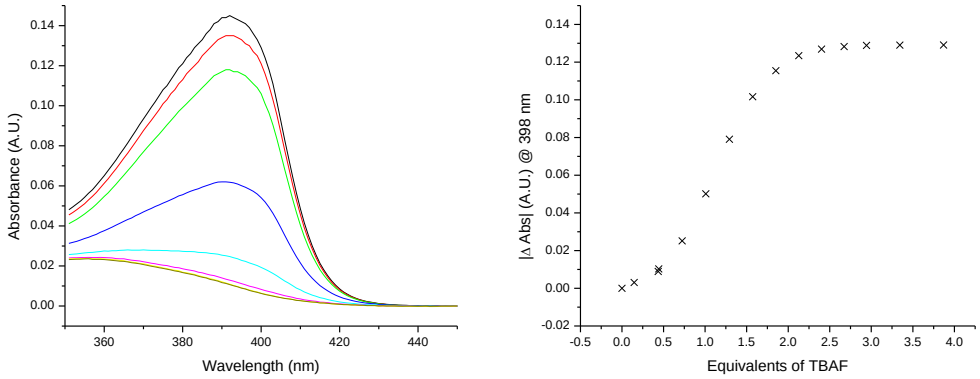
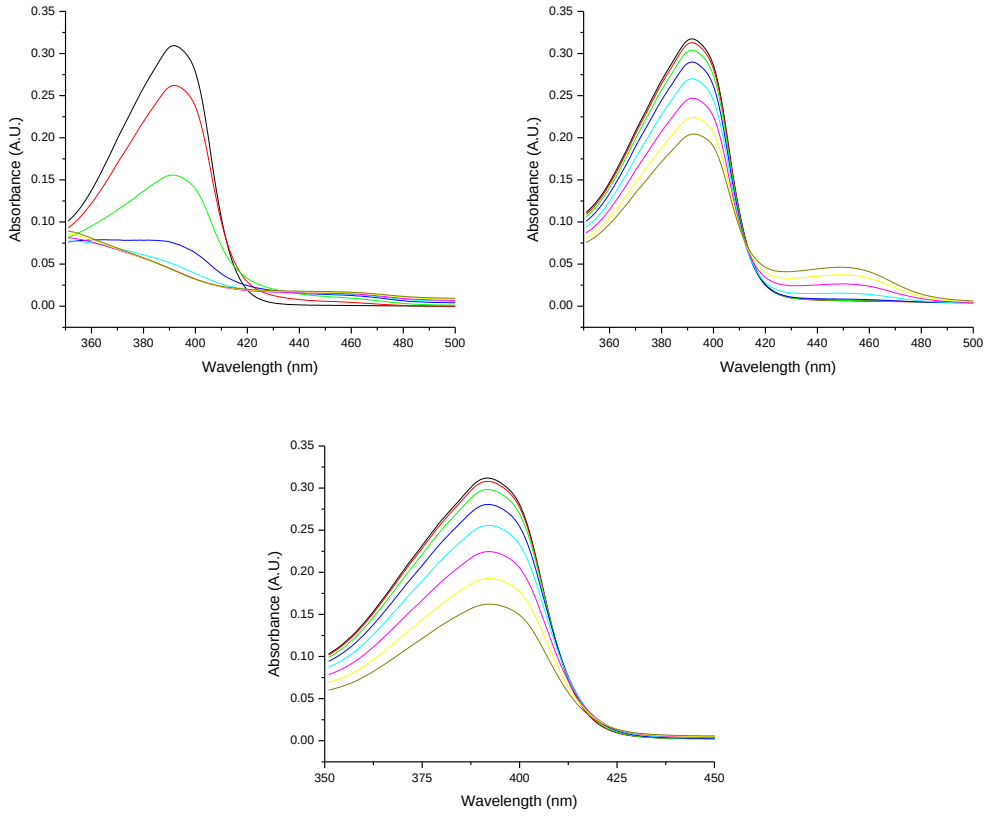
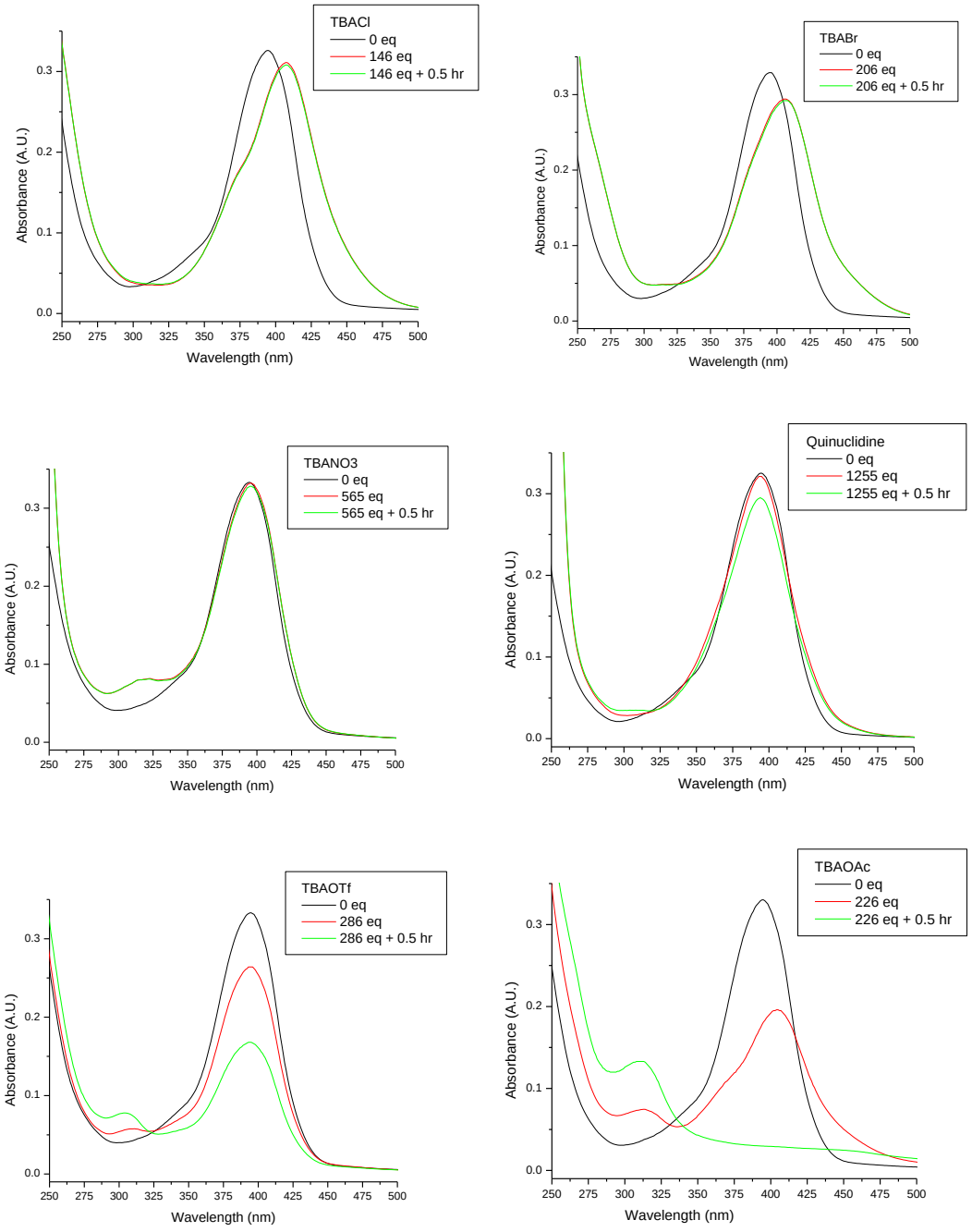


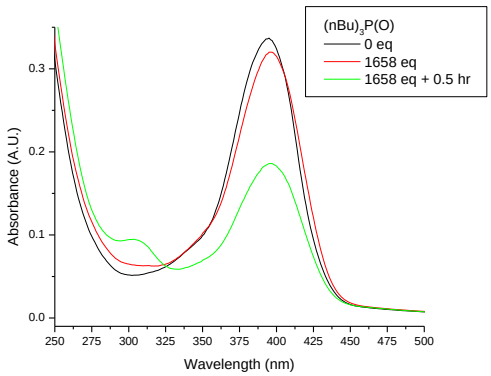
Figure S 83: Spectral changes upon the addition of TBAOAc (left), TBAOTf (right), and (nBu)$_3$P(O) (bottom middle) to **2** at 19.0 µM in THF. Data could not be fit to a 1:1 binding isotherm. ¯OAc and ¯OTf caused a time dependant decrease in absorbance (not shown).

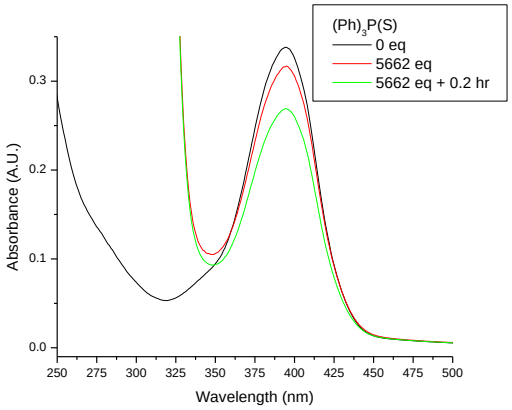


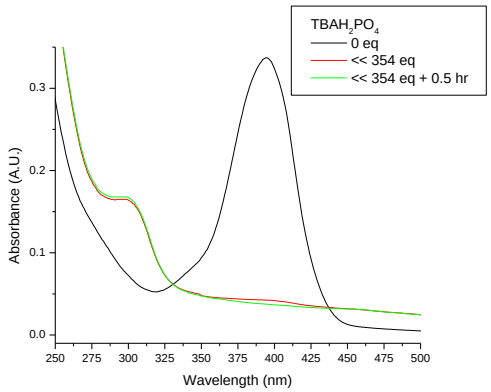
2.5.3 4,7-Dibromobenzo[c]-1,2,5-telluradiazole (3a) in THF

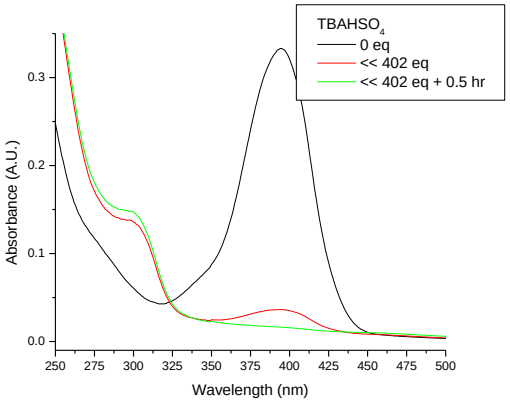
Figure S 84: Telluradiazole **3a** at 20.5 µM with various acceptors in THF. Incompatible donors show a decrease in the telluradiazole absorbance over time. The final plot shows the stability of a concentrated stock solution of **3a** over a two hour period.

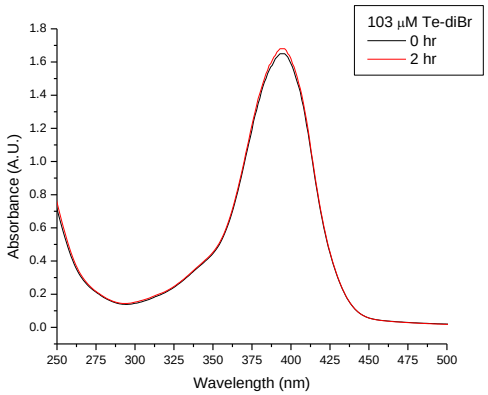



(nBu)3P(O)
0 eq
1658 eq
1658 eq + 0.5 hr
Absorbance (A.U.)
Wavelength (nm)


(Ph)3P(S)
0 eq
5662 eq
5662 eq + 0.2 hr
Absorbance (A.U.)
Wavelength (nm)


TBAH2PO4
0 eq
<< 354 eq
<< 354 eq + 0.5 hr
Absorbance (A.U.)
Wavelength (nm)


TBAHSO4
0 eq
<< 402 eq
<< 402 eq + 0.5 hr
Absorbance (A.U.)
Wavelength (nm)


103 μM Te-diBr
0 hr
2 hr
Absorbance (A.U.)
Wavelength (nm)

2.6 Anion π and halogen bonding control titrations

2.6.1 Methodology

In order to check for anion π interactions with the electron poor aromatic ring, and to make sure that halogen bonding with the bromo groups was not responsible for the observed binding, titrations were carried out on the selenium and sulfur analogues of **3a**. Titrations were performed in the same manner as those for the tellurium chalcogenadiazoles. TBACl and THF were selected as the acceptor and solvent, respectively, since they produced the largest association constants out of the conditions studied. As the chalcogen atom moves down the periodic table, from S to Te, the aromatic ring and bromine atoms become less electropositive (below).

Table S 7: Largest ESP values ($V_{s,max}$ kcal/mol) on either the π face or the bromine atoms on the 4,7-dibromobenzo[c][1,2,5]chalcogenadiazoles **3a-c**. Determined at the B97D3/Def2-TZVP level of theory.

Element	Compound	π system	Bromine
Te	**3a**	13.2	11.1
Se	**3b**	14.8	13.2
S	**3c**	17.1	14.4

2.6.2 Results

2.6.2.1 4,7-dibromobenzo[c][1,2,5]selenadiazole (3b)

Figure S 85: Spectral change upon the addition of TBACl to **3b** in THF. Titration carried out 25.3 µM **3b**. Every second titration removed for clarity. Data could not be fit to a 1:1 binding isotherm, but spectral changes are consistent with binding at a low association constant.

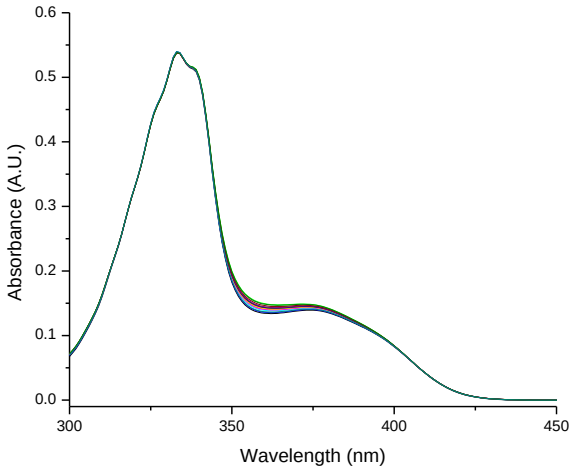
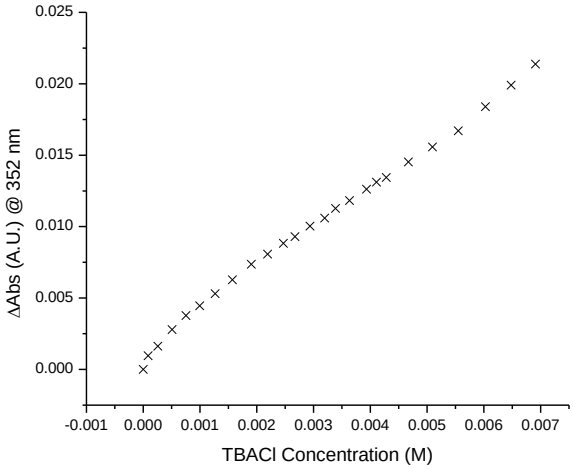


Figure S 86: Absorbance change at 352 nm during the titration of **3b** with TBACl in THF. Titration carried out 23.5 µM **3b**. Data could not be fit to a 1:1 binding isotherm.



2.6.2.2 4,7-dibromobenzo[c][1,2,5]thiadiazole (3c)

Figure S 87: Spectral change upon the addition of TBACl to **3c** in THF. Titration carried out 16.3 µM **3c**. No binding observed. Every second titration removed for clarity.

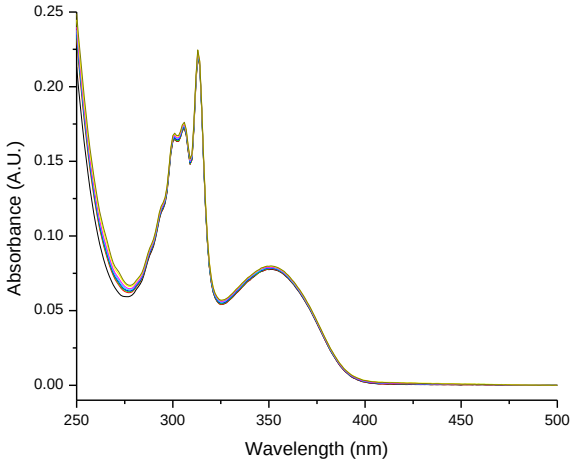
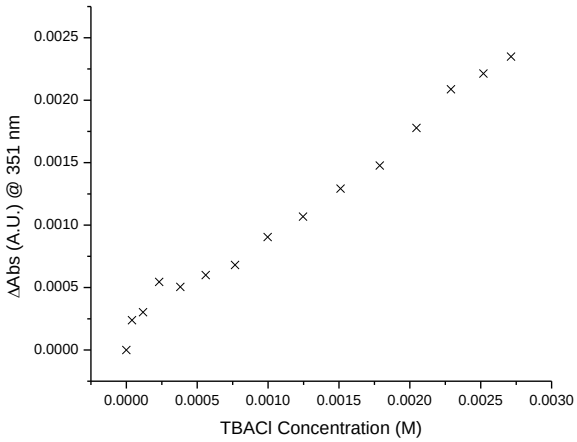


Figure S 88: Absorbance change at 351 nm during the titration of **3c** with TBACl in THF. Titration carried out 16.3 µM **3c**. Data could not be fit to a 1:1 binding isotherm. No binding observed.



3.0 Donor UV/Vis absorption concentration dependence

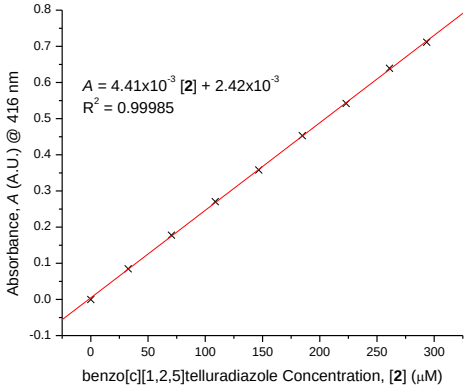
3.1 Methodology

In order to check for dimerization in solution, the absorption vs. concentration profiles were determined. A concentrated solution of the donor in THF was diluted. UV/Vis spectra were then obtained.

3.2 UV/Vis Absorption vs. concentration plots

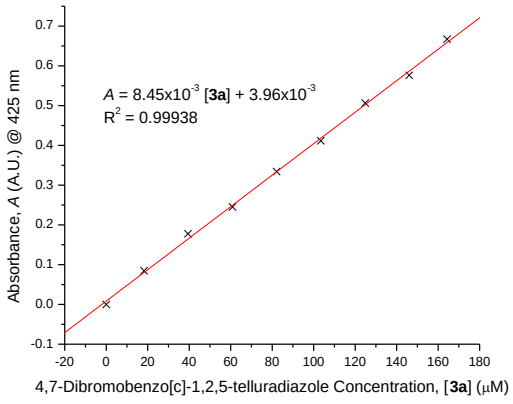
3.2.1 benzo[c][1,2,5]telluradiazole (2)

Figure S 89: Plot of absorption vs. concentration of telluradiazole **2** in THF. Linearity suggests no dimerization is occurring.



3.2.2 4,7-Dibromobenzo[c]-1,2,5-telluradiazole (3a)

Figure S 90: Plot of absorption vs. concentration of telluradiazole **3a** in THF. Linearity suggests no dimerization is occurring.



4.0 Nanospray-MS of 3a-Cl^- complex

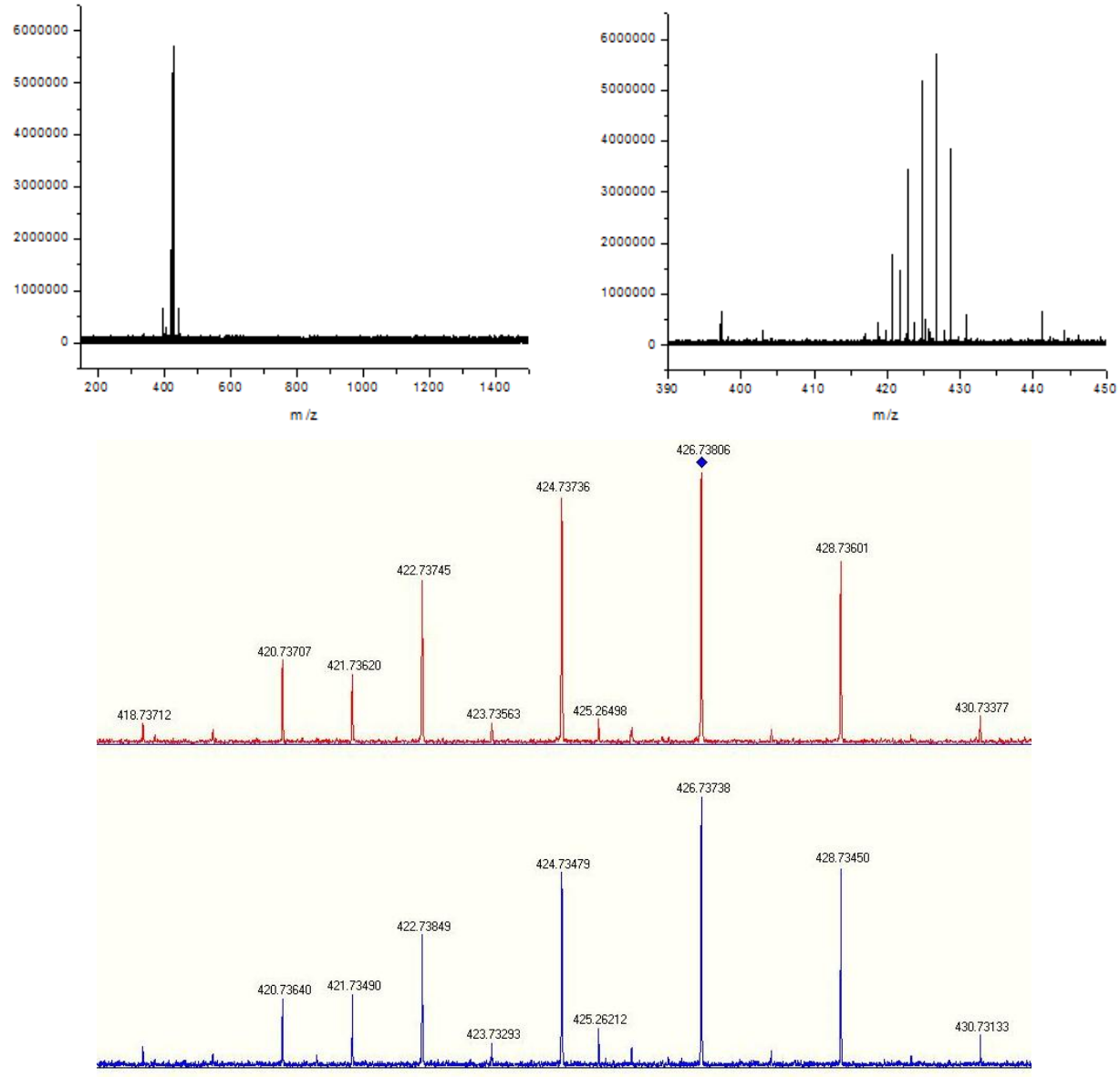
4.1 Methodology

To observe chalcogen bond formation in the gas phase, a 256.7 µM solution of **3a** was made in THF. This donor solution of **3a** was then used as solute to dissolve TBACl, at to concentration of 2.88 mM. These were then combined to form a 14.3 µM solution of TBACl (β = 0.02) which was sprayed into the MS in negative ion mode. Cl^- salt cluster formation was predominate at high TBACl concentrations. To avoid this, the telluradiazole concentration was increased to promote complex formation at lower TBACl concentrations. The non-complexed telluradiazole does not produce a signal in negative ion mode, allowing its concentration to be elevated without interfering with complex isolation.

Due to the lower association constant of **2** with Cl^-, the **2**-Cl^- complex could not be isolated. It was observed in the MS but because of the high TBACl concentrations required for observable complex formation, Cl^- salt cluster formation obscured the signal.

4.2 Spectrum of the 3a-Cl^- complex

Figure S 91: Nanospray-MS spectra of the **3a-Cl^-** complex in THF. $C_6H_2Br_2ClN_2Te$ $[M]^-$ 426.732, found 426.738



5.0 Computational Methods

5.1 Methodology

All thermodynamic calculations were performed using the Gaussian 09 program.[6] DFT calculations were carried out at the B97-D3[7] or M06-2X[8] level with and without the addition of Grimme's D3 dispersion correction[9], with all stationary points optimized using the Def2-TZVP[10] basis set. ESP surfaces were optimized and created at the B97-D3/Def2-TZVP level of theory. Vibrational frequency calculations were performed to characterize each stationary point as a minimum (no imaginary frequencies) on the potential energy surface. In some cases, there were small negative frequencies that could not be avoided during optimization. The negative vibrational modes were checked to make sure that they did not correspond to any motion along the chalcogen bond axes (bond formation or breaking). For those small frequencies which were able to be removed, the largest change in binding free energy was 0.2 kcal/mol lower in energy. All imaginary frequencies are provided along with a brief description of the vibrational mode with the 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.[11] Gas phase calculations of the complexes were carried out with and without counterpoise correction.[12] Solvation was modeled using a self-consistent reaction field by means of the PCM[13] and CPCM[14] methods. For complexes of the non-symmetrical donor **4**, which has two separate s-hole $V_{s,max}$ values, the obtained energies or Gibbs free energies of binding were Boltzmann averaged to obtain the reported binding energy.

UV/Vis spectra were computed by TD-DFT using either Gaussian 09[6] or ORCA (3.0.2)[15] for the B97D3/Def2-TZVP and RI-B2PLYP/Def2-TZVP calculations, respectively. For the double-hybrid DFT method used in ORCA, the RIJCOSX was used to speed up the calculations.[16] UV/Vis spectra were visualized using Gabedit 2.4.8.[17] All TD-DFT calculations were carried out in the gas phase.

5.1.1 2D Electrostatic Potential Maps

2D electrostatic potential maps were generated using jmol version 14.2.7[18] and the following script. Items enclose in <> should be replaced by the correct values:

isosurface delete
draw delete
load <path/filename-POTENTIAL.cube>
isosurface ID myisosurface PLANE (atomno=1) (atomno=2) (atomno=3) color absolute 0 <$V_{s,max}$ value in hartree> "<path/filename-POTENTIAL.cube>" ANGSTROMS FULLPLANE RESOLUTION 500
set meshScale 3
isosurface ID density contour increment {0,0.001,0.001} PLANE (atomno=1) (atomno=2) (atomno=3) "<path/filename-DENSITY.cube>" "
color isosurface black

5.2 Thermodynamic summary

5.2.1 Electrostatic Potentials

Table S 8: σ-hole electrostatic potentials ($V_{S,max}$)calculated at the B97D3/Def2-TZVP level of theory, presented in kcal/mol

	E=		
Compound	**Te**	**Se**	**S**
2	26.3	18.4	11.6
3	33.4	25.0	17.6
1	49.2	41.5	34.9
4	36.4	28.4	21.1
5	35.3[a]	-	-

C_6F_5I	22.3

a) The two σ-holes on **4** have differing $V_{s,max}$ values of 35.6 and 35.1 kcal/mol. The displayed value of an average of the two $V_{s,max}$ values. A Boltzmann average yields a $V_{s,max}$ of 35.4 kcal/mol. All obtained complexes which were Boltzmann averaged between these two σ-holes differed by at most 0.5 kcal/mol.

5.2.2 Complexation Energies

5.2.2.1 Gas phase with counterpoise correction

Table S 9: Gas phase counterpoise corrected complexation energies and free energies for the binding of **2** with various acceptors.

	ΔG (kcal/mol)			ΔE (kcal/mol)		
Acceptor	**B97-D3**	**M06-2X**	**M062X-D3**	**B97-D3**	**M06-2X**	**M062X-D3**
TBACl	-24.8	-22.1	-22.1	-31.6	-29.5	-29.6
TBABr	-19.8	-16.9	-17.0	-26.1	-23.9	-24.0
TBAI	-16.0	-12.2	-12.3	-21.6	-18.8	-18.9
$TBANO_3$	-14.8	-12.9	-13.0	-25.3	-24.3	-24.4
Quinuclidine	-1.5	-0.7	-1.4	-14.9	-14.0	-14.6

Table S 10: Gas phase counterpoise corrected complexation energies and free energies for the binding of **3a** with various acceptors.

	ΔG (kcal/mol)			ΔE (kcal/mol)		
Acceptor	**B97-D3**	**M06-2X**	**M062X-D3**	**B97-D3**	**M06-2X**	**M062X-D3**
TBACl	-33.4	-30.1	-30.2	-40.1	-37.3	-37.4
TBABr	-27.5	-23.5	-23.6	-34.0	-30.9	-31.0
TBAI	-22.7	-17.9	-18.0	-28.9	-25.1	-25.2
$TBANO_3$	-22.4	-19.3	-19.5	-32.8	-31.0	-31.1
Quinuclidine	-3.1	-4.7	-5.5	-18.3	-16.9	-17.6

Table S 11: Gas phase counterpoise corrected complexation energies and free energies for the binding of **4** with various acceptors.

	ΔG (kcal/mol)			ΔE (kcal/mol)		
Acceptor	**B97-D3**	**M06-2X**	**M062X-D3**	**B97-D3**	**M06-2X**	**M062X-D3**
TBACl	-34.4	-31.6	-31.6	-41.3	-38.7	-38.8
TBABr	-28.9	-25.5	-25.6	-35.4	-32.4	-32.5
TBAI	-23.6	-20.3	-20.4	-30.3	-26.8	-26.8
$TBANO_3$	-23.7	-21.0	-21.2	-34.0	-32.4	-32.6
Quinuclidine	-3.8	-2.6	-3.3	-16.8	-15.7	-16.2

Table S 12: Gas phase counterpoise corrected complexation energies and free energies for the binding of **5** with various acceptors.

	ΔG (kcal/mol)			ΔE (kcal/mol)		
Acceptor	**B97-D3**	**M06-2X**	**M062X-D3**	**B97-D3**	**M06-2X**	**M062X-D3**
TBACl	-35.0	-33.1	-33.2	-41.9	-40.5	-40.6
TBABr	-29.2	-26.9	-26.9	-35.8	-34.1	-34.2
TBAI	-24.4	-21.4	-21.5	-30.7	-28.2	-28.3
$TBANO_3$	-23.9	-22.2	-22.4	-34.6	-34.1	-34.3
Quinuclidine	-3.5		-4.9	-18.3		-18.0

5.2.2.2 PCM solvation model

5.2.2.2.1 THF

Table S 13: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** with various acceptors modeled using the PCM in THF.

				B97-D3		**M06-2X**		**M06-2X-D3**	
Acceptor	Exp				Error		Error		Error
TBACl	-4.07	±	0.01	-3.5	0.6	-2.4	1.7	-2.5	1.6
TBABr	-3.12	±	0.02	-1.2	1.9	-0.4	2.7	-0.5	2.6
TBAI	-	±	-	-0.4		0.6		0.6	
TBANO3	-1.60	±	0.04	-0.7	0.9	1.3	2.9	1.1	2.7
Quinuclidine	-1.74	±	0.01	-0.9	0.9	0.2	1.9	-0.5	1.2
Avg Error					**1.1**		**2.3**		**2.0**
Abs Avg Error					**1.1**		**2.3**		**2.0**
SSE					**5.6**		**22.2**		**18.2**
Error Variance					**1.9**		**7.4**		**6.1**
ASSE					**1.4**		**5.5**		**4.6**

Table S 14: Gibbs Free Energies of complexation (kcal/mol) for the binding of **3a** with various acceptors modeled using the PCM in THF.

				B97-D3		**M06-2X**		**M06-2X-D3**	
Acceptor	Exp				Error		Error		Error
TBACl	-5.57	±	0.01	-6.5	-0.9	-5.6	0.0	-5.1	0.4
TBABr	-4.19	±	0.01	-4.5	-0.3	-1.6	2.6	-2.3	1.9
TBAI	-	±	-	-2.3		-0.1		-0.2	
TBANO3	-2.61	±	0.03	-0.2	2.4	0.4	3.0	0.2	2.8
Quinuclidine	-2.38	±	0.05	-2.2	0.2	-0.7	1.7	-4.3	-1.9
Avg Error					**0.4**		**1.8**		**0.8**
Abs Avg Error					**1.0**		**1.8**		**1.8**
SSE					**6.9**		**18.5**		**15.3**
Error Variance					**2.3**		**6.2**		**5.1**

Table S 15: Gibbs Free Energies of complexation (kcal/mol) for the binding of **4** with various acceptors modeled using the PCM in THF.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-6.25	±	-0.09	-6.7	-0.4	-5.1	1.1	-5.2	1.0
TBABr	-4.56	±	-0.05	-3.7	0.9	-2.5	2.0	-2.6	1.9
TBAI	-	±	-	-2.5		-0.8		-0.9	
TBANO3	-2.60	±	0.07	-2.1	0.5	-0.3	2.3	-0.4	2.2
Quinuclidine	-2.35	±	0.04	-2.7	-0.4	-1.1	1.3	-1.8	0.5
Avg Error					**0.1**		**1.7**		**1.4**
Abs Avg Error					**0.5**		**1.7**		**1.4**
SSE					**1.4**		**12.3**		**9.8**
Error Variance					**0.5**		**4.1**		**3.3**

Table S 16: Gibbs Free Energies of complexation (kcal/mol) for the binding of **5** with various acceptors modeled using the PCM in THF.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-6.98	±	0.08	-7.5	-0.5	-6.2	0.7	-6.3	0.6
TBABr	-5.45	±	0.04	-4.6	0.8	-4.3	1.1	-4.4	1.0
TBAI	-	±	-	-3.4		-2.2		-2.3	
TBANO3	-3.11	±	0.03	-2.7	0.4	-1.4	3.1	-1.5	3.1
Quinuclidine	-2.70	±	0.04	-3.6	-0.9	-2.5	0.2	-3.3	-0.6
Avg Error					**0.0**		**1.0**		**0.7**
Abs Avg Error					**0.7**		**1.0**		**1.0**
SSE					**2.0**		**4.9**		**4.4**
Error Variance					**0.7**		**1.6**		**1.5**

5.2.2.2.2 ACN

Table S 17: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** with various acceptors modeled using the PCM in ACN.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-2.55	±	-0.01	-1.7	0.8	-1.0	1.5	-0.4	2.2
TBABr	-2.02	±	-0.01	0.1	2.1	0.5	2.5	-0.4	1.7
TBAI	-1.27	±	-0.01	0.6	1.9	1.5	2.8	1.4	2.7
TBANO3	-	±	-	1.9		2.7		2.5	
Quinuclidine	-2.19	±	-0.03	-0.9	1.3	-0.5	1.7	-0.3	1.9
Avg Error					**1.5**		**2.1**		**2.1**
Abs Avg Error					**1.5**		**2.1**		**2.1**
SSE					**10.2**		**19.2**		**18.5**

Error Variance	**3.4**	**6.4**	**6.2**

Table S 18: Gibbs Free Energies of complexation (kcal/mol) for the binding of **3a** with various acceptors modeled using the PCM in ACN.

				B97-D3	**M06-2X**	**M06-2X-D3**
Acceptor	Exp			Error	Error	Error
TBACl	-	±	-	-4.0	-2.9	-2.2
TBABr	-	±	-	-2.0	-0.6	-1.4
TBAI	-	±	-	-0.8	0.9	0.8
TBANO3	-	±	-	0.7	2.1	1.9
Quinuclidine	-	±	-	-3.5	-2.6	-2.6

Table S 19: Gibbs Free Energies of complexation (kcal/mol) for the binding of **4** with various acceptors modeled using the PCM in ACN.

				B97-D3	**M06-2X**	**M06-2X-D3**
Acceptor	Exp			Error	Error	Error
TBACl	-	±	-	-3.7	-2.6	-2.0
TBABr	-	±	-	-1.3	-0.7	-1.5
TBAI	-	±	-	-0.7	0.7	0.6
TBANO3	-	±	-	-0.8	1.5	1.4
Quinuclidine	-	±	-	-2.6	-1.6	-1.4

Table S 20: Gibbs Free Energies of complexation (kcal/mol) for the binding of **5** with various acceptors modeled using the PCM in ACN.

				B97-D3	**M06-2X**	**M06-2X-D3**
Acceptor	Exp			Error	Error	Error
TBACl	-	±	-	-4.5	-3.6	-2.9
TBABr	-	±	-	-2.2	-2.0	-2.9
TBAI	-	±	-	-1.3	-0.2	-0.3
TBANO3	-	±	-	-0.4	0.8	0.6
Quinuclidine	-	±	-	-4.5	-2.9	-2.7

5.2.2.3 CPCM solvation model

5.2.2.3.1 THF

Table S 21: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** with various acceptors modeled using the CPCM in THF.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-4.07	±	0.01	-4.0	0.0	-2.9	1.2	-2.9	1.1
TBABr	-3.12	±	0.02	-1.7	1.4	-1.0	2.1	-1.1	2.0
TBAI	-	±	-	-0.9		0.5		0.4	
TBANO3	-1.60	±	0.04	0.4	2.0	1.3	2.9	1.2	2.8
Quinuclidine	-1.74	±	0.01	0.3	2.0	0.2	2.0	-0.1	1.6
Avg Error					**1.4**		**2.1**		**1.9**
Abs Avg Error					**1.4**		**2.1**		**1.9**
SSE					**9.9**		**18.4**		**15.8**
Error Variance					**3.3**		**6.1**		**5.3**

Table S 22: Gibbs Free Energies of complexation (kcal/mol) for the binding of **3a** with various acceptors modeled using the CPCM in THF.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-5.57	±	0.01	-7.1	-1.5	-5.5	0.1	-5.6	0.0
TBABr	-4.19	±	0.01	-4.4	-0.2	-2.7	1.5	-2.8	1.4
TBAI	-	±	-	-2.8		-0.7		-0.8	
TBANO3	-2.61	±	0.03	-1.5	1.1	0.0	2.6	-0.2	2.4
Quinuclidine	-2.38	±	0.05	-1.5	0.9	-1.5	0.9	-3.3	-0.9
Avg Error					**0.1**		**1.3**		**0.7**
Abs Avg Error					**0.9**		**1.3**		**1.2**
SSE					**4.3**		**9.6**		**8.5**
Error Variance					**1.4**		**3.2**		**2.8**

Table S 23: Gibbs Free Energies of complexation (kcal/mol) for the binding of **4** with various acceptors modeled using the CPCM in THF.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-6.25	±	0.09	-7.1	-0.8	-5.5	0.7	-5.6	0.6
TBABr	-4.56	±	0.05	-4.2	0.4	-3.0	1.6	-3.1	1.5
TBAI	-	±	-	-3.1		-1.2		-1.3	
TBANO3	-2.60	±	0.07	-2.2	0.4	-0.5	2.1	-0.6	2.0
Quinuclidine	-2.35	±	0.04	-1.5	0.8	-1.0	1.3	-1.4	1.0
Avg Error					**0.2**		**1.4**		**1.3**
Abs Avg Error					**0.6**		**1.4**		**1.3**
SSE					**1.6**		**9.2**		**7.3**
Error Variance					**0.5**		**3.1**		**2.4**

Table S 24: Gibbs Free Energies of complexation (kcal/mol) for the binding of **5** with various acceptors modeled using the CPCM in THF.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-6.98	±	0.08	-7.7	-0.8	-6.5	0.5	-6.6	0.4
TBABr	-5.45	±	0.04	-5.0	0.5	-4.0	1.4	-4.1	1.3
TBAI	-	±	-	-3.5		-2.0		-2.0	
TBANO3	-3.11	±	0.03	-2.7	0.4	-1.4	1.7	-1.5	1.6
Quinuclidine	-2.70	±	0.04	-3.2	-0.5	-2.2	0.5	-2.6	0.1
Avg Error					**-0.1**		**1.0**		**0.8**
Abs Avg Error					**0.5**		**1.0**		**0.8**
SSE					**1.2**		**5.5**		**4.4**
Error Variance					**0.4**		**1.8**		**1.5**

5.2.2.3.2 ACN

Table S 25: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** with various acceptors modeled using the CPCM in ACN.

				B97-D3		M06-2X		M06-2X-D3	
Acceptor	Exp				Error		Error		Error
TBACl	-2.55	±	0.01	-1.9	0.6	-1.1	1.4	-1.2	1.3
TBABr	-2.02	±	0.01	-0.1	2.0	0.3	2.3	0.2	2.3
TBAI	-1.27	±	0.01	0.4	1.7	1.5	2.8	1.4	2.7
TBANO3	-	±	-	1.6		2.6		2.4	
Quinuclidine	-2.19	±	0.03	-0.8	1.4	0.4	2.6	-0.2	2.0
Avg Error					**1.4**		**2.3**		**2.1**
Abs Avg Error					**1.4**		**2.3**		**2.1**
SSE					**8.9**		**21.9**		**18.0**
Error Variance					**3.0**		**7.3**		**6.0**

Table S 26: Gibbs Free Energies of complexation (kcal/mol) for the binding of **3a** with various acceptors modeled using the CPCM in ACN.

				B97-D3	M06-2X	M06-2X-D3
Acceptor	Exp			Error	Error	Error
TBACl	-	±	-	-4.2	-3.0	-3.1
TBABr	-	±	-	-2.0	-0.8	-0.9
TBAI	-	±	-	-1.0	0.7	0.6
TBANO3	-	±	-	0.7	1.9	1.7
Quinuclidine	-	±	-	-2.4	-1.2	-1.9

Table S 27: Gibbs Free Energies of complexation (kcal/mol) for the binding of **4** with various acceptors modeled using the CPCM in ACN.

Acceptor	Exp			B97-D3 Error	M06-2X Error	M06-2X-D3 Error
TBACl	-	±	-	-3.8	-3.6	-2.8
TBABr	-	±	-	-1.5	0.1	-0.9
TBAI	-	±	-	-0.9	0.5	0.4
TBANO3	-	±	-	-0.3	1.5	1.4
Quinuclidine	-	±	-	-2.6	-0.7	-1.3

Table S 28: Gibbs Free Energies of complexation (kcal/mol) for the binding of **5** with various acceptors modeled using the CPCM in ACN.

Acceptor	Exp			B97-D3 Error	M06-2X Error	M06-2X-D3 Error
TBACl	-	±	-	-4.6	-3.7	-3.7
TBABr	-	±	-	-2.3	-1.8	-1.9
TBAI	-	±	-	-1.4	-0.2	-0.3
TBANO3	-	±	-	-0.5	0.8	0.7
Quinuclidine	-	±	-	-4.1	-1.9	-2.6

5.2.2.4 Summary of errors by method

Table S 29: Sum of Squared Errors (SSE) of the Gibbs Free Energies of binding for methods and solvation models used.

Compound	**2**				**3a**		**4**		**5**	
Solvation Model	*PCM*		*CPCM*		*PCM*	*CPCM*	*PCM*	*CPCM*	*PCM*	*CPCM*
Solvent	THF	ACN	THF	ACN	THF	THF	THF	THF	THF	THF
B97-D3	5.6	10.2	9.9	8.9	6.9	4.3	1.4	1.6	2.0	1.2
M06-2X	22.2	19.2	18.4	21.9	18.5	9.6	12.3	9.2	4.9	5.5
M06-2X-D3	18.2	18.5	15.8	18.0	15.3	8.5	9.8	7.3	4.4	4.4

5.2.2.5 Graphical representation of computational results

5.2.2.5.1 PCM solvation model

Figure S 92: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** (top left), **3a** (top right), **4** (bottom left), and **5** (bottom right) with various acceptors modeled using the PCM method in THF.

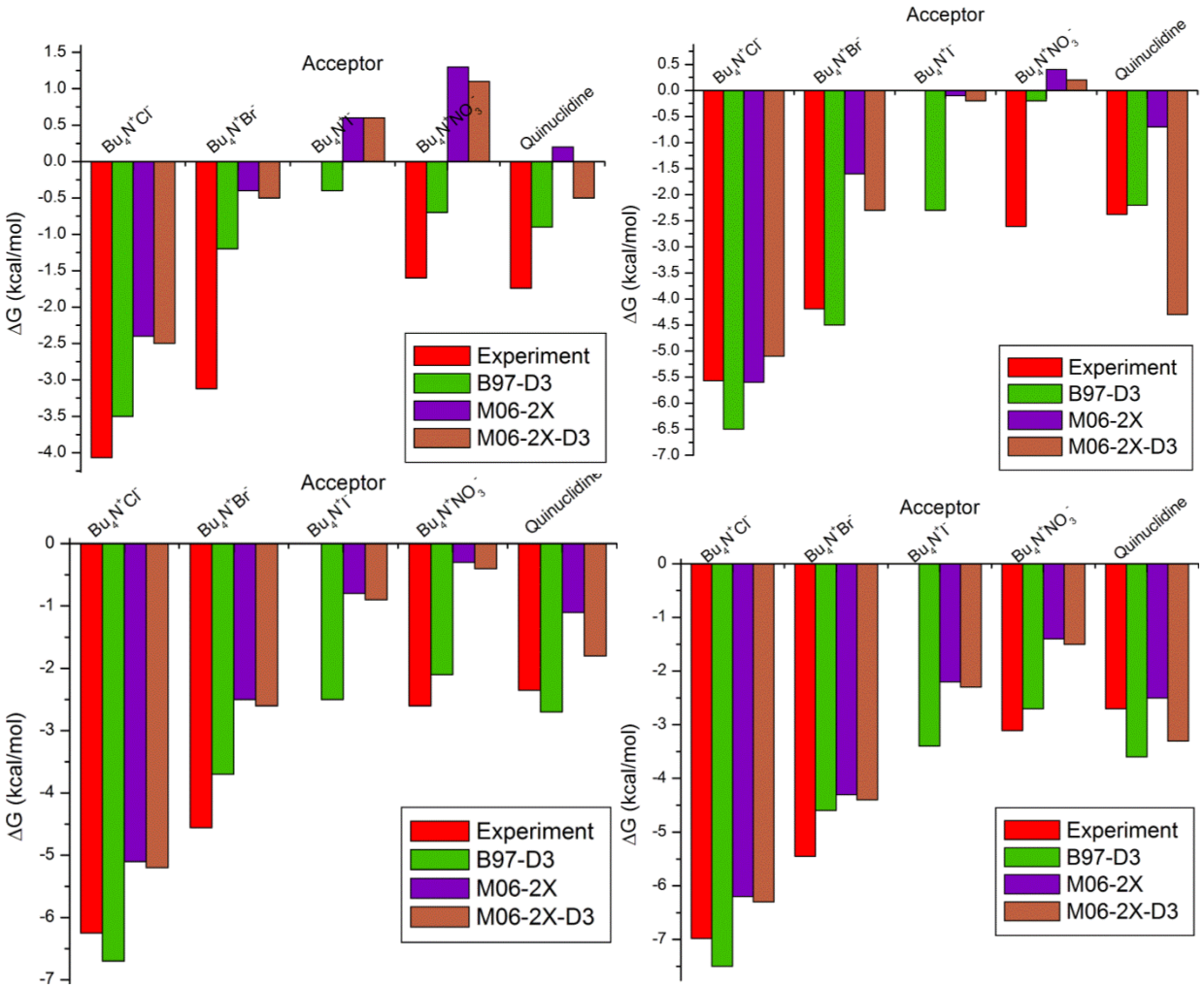
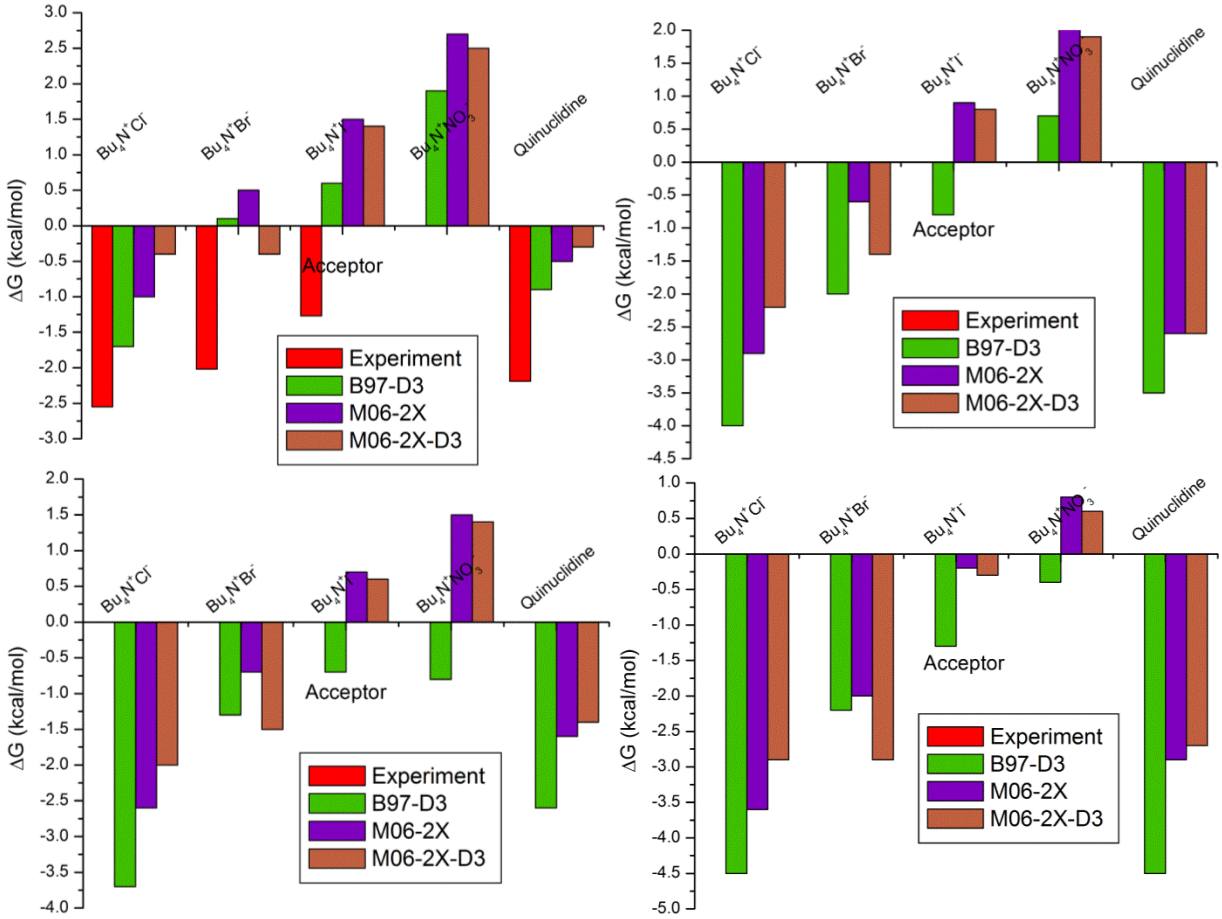


Figure S 93: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** (top left), **3a** (top right), **4** (bottom left), and **5** (bottom right) with various acceptors modeled using the PCM method in ACN.



5.2.2.5.1 CPCM solvation model

Figure S 94: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** (top left), **3a** (top right), **4** (bottom left), and **5** (bottom right) with various acceptors modeled using the CPCM method in THF.

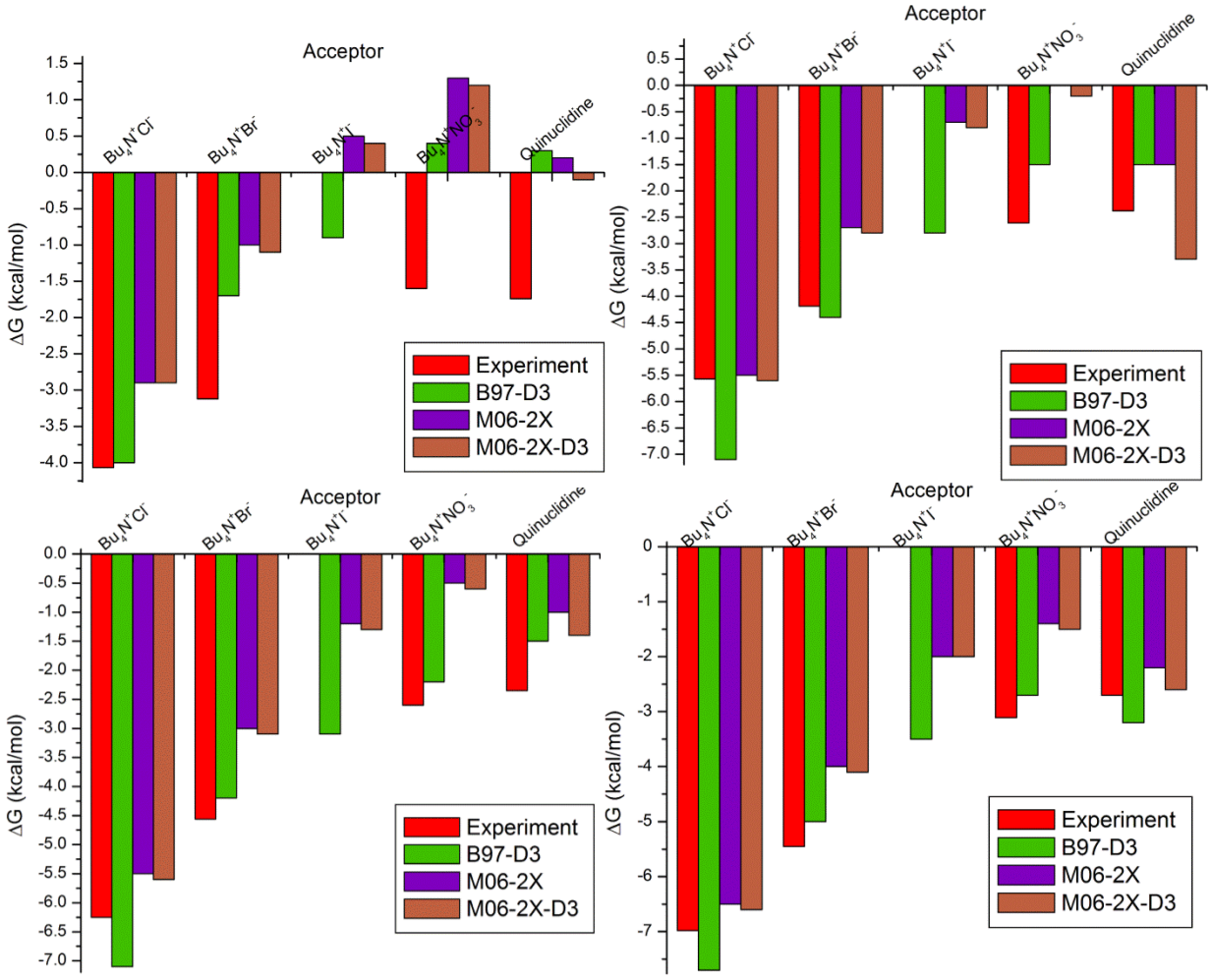
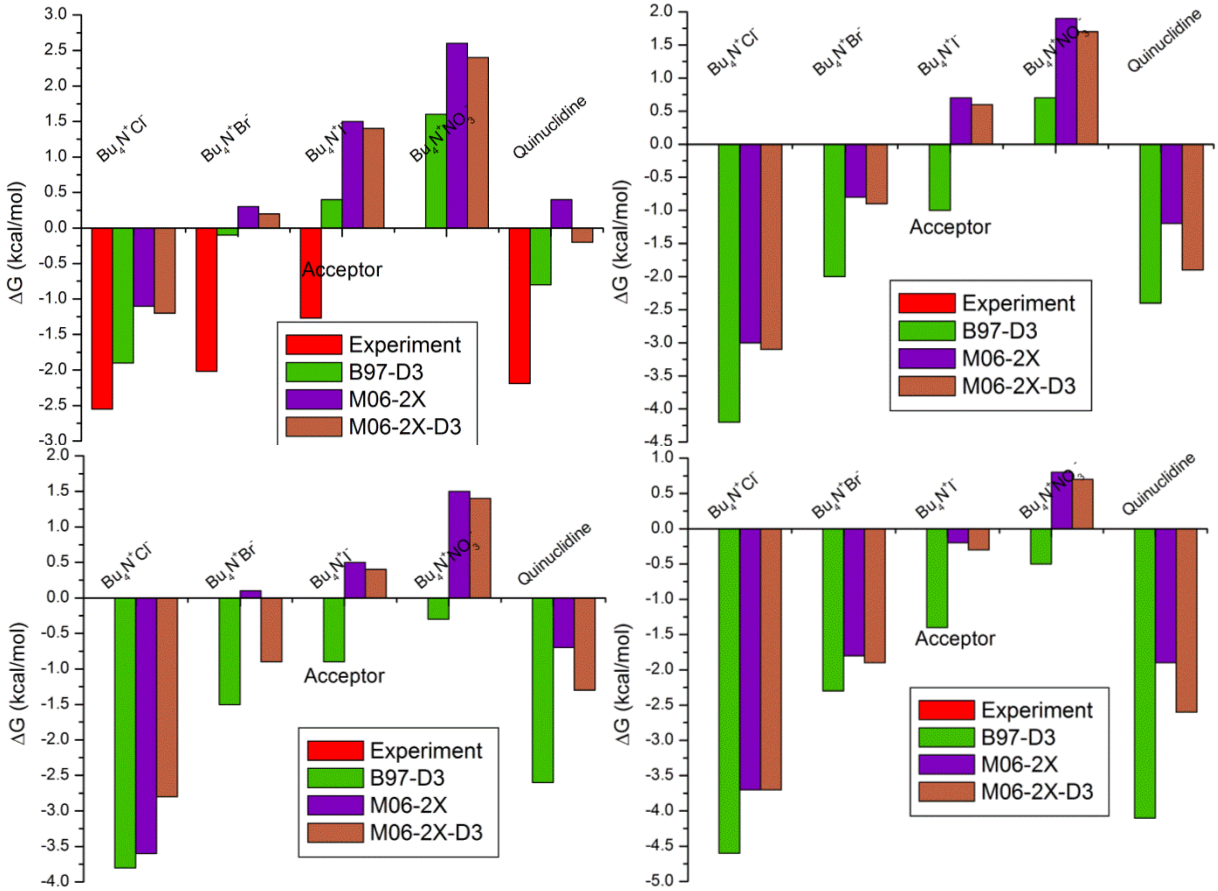


Figure S 95: Gibbs Free Energies of complexation (kcal/mol) for the binding of **2** (top left), **3a** (top right), **4** (bottom left), and **5** (bottom right) with various acceptors modeled using the CPCM method in ACN.



5.3 TD-DFT UV/Vis spectrum determination

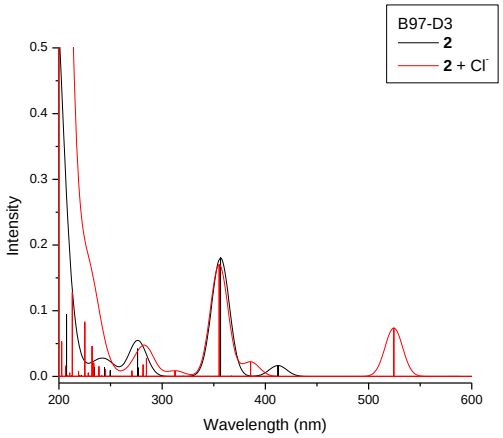
5.3.1 Methodology

To probe the spectral changes observed experimentally upon complex and chalcogen bond formation, UV/Vis spectra were calculated for **2** and [**2-Cl**]$^-$. The B97D3 method used for the thermodynamic calculations was used, as well as the double hybrid method, B2PLYP, which is better suited for the calculation of UV/Vis spectra of this system.[19] Gaussian 09 is unable to perform the TD-DFT calculations accurately for the double hybrid method, as a result he ORCA program was used. Due to the differences in solvation models between the two programs, gas phase calculations were carried out for a more direct comparison between the methods.

5.3.2 Results

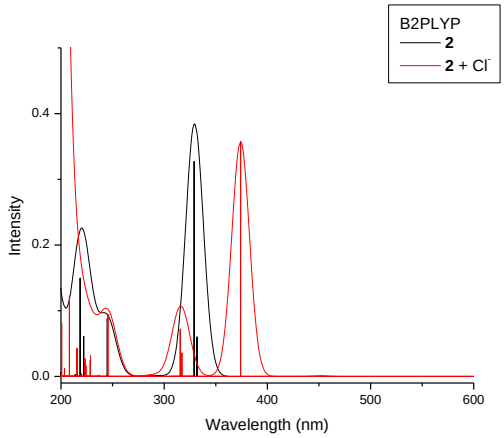
5.3.2.1 B97-D3

Figure S 96: Calculated UV/Vis spectra of **2** and [**2-Cl**]$^-$ in the gas phase at the B97D3/Def2-TZVP level of theory as calculated in Gaussian 09. A red shift in λ_{max} is observed in [**2-Cl**]$^-$ vs **2**.



5.3.2.2 B2PLYP

Figure S 97: Calculated UV/Vis spectra of **2** and [**2-Cl**]$^-$ in the gas phase at the B2pLYP/Def2-TZVP level of theory as calculated in ORCA 3.0.2. A red shift in λ_{max} is observed in [**2-Cl**]$^-$ vs **2**.



5.4 Optimized geometries

5.4.1 Structure nomenclature

5.4.1.1 Thermodynamics

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

<method>-<solvation>-<solvent>_<type>-<structure>.out

Where:

<method>	: B97D3, M062X, M062XD3
<solvation>	: PCM, CPCM, null
<solvent>	: THF, ACN, null
<type>	: donor, acceptor, complex
<structure>	: The name of the compound being modeled. Most are obvious except for Te-nat (**2**), Te-diBr (**3a**), Te-CN (**4**), and Te-F4 (**5**). Complexes contain an additional structure, separated by a -. Compounds of Te-CN also contain an extra tag, opp or same, denoting whether the complex has the acceptor on the opposite or same side of the ring as the cyano group

Examples:

The M06-2X model of the **2**-Cl^- complex in THF modeled by the PCM method would be called:

M062X-PCM-THF_complex-Te-nat-Cl.out

The B970D3 model in the gas phase of NO_3^- would be called:

B97D3-null-null_acceptor-NO3.out

5.4.1.2 Electrostatic Potentials (ESP)

All optimized structures used for modeling ESP are reported using the following filename format:

<element>_<diazole>.out

Where:

<element>	: S, Se, Te
<diazole>	: nat, diBr, zib, CN, F4.

nat, diBr, zib, CN, and F4 represent compounds of type **2**, **3**, **1**, **4**, and **5** respectively.

The only exception to this naming convention is iodoperflourbenzene, which is tabled as C6F5I.out

5.4.2.3 TD-DFT calculations

All optimized structures used for modeling UV/Vis spectra by TD-DFT are reported using the following filename format:

<method>_<structure>.out

Where:

<method>	: B97D3 or B2PLYP
<structure>	: donor or complex

5.4.2 ESP geometries

==========
D3-ESP_S-zib.out
==========

C	0.000074	-0.142391	0.722068
C	0.000074	-0.142391	-0.722068
N	-0.000041	1.081660	1.249243
N	-0.000041	1.081660	-1.249243
S	0.000118	2.137599	-0.000000
C	-0.000041	-1.308383	-1.538184
C	-0.000041	-1.308383	1.538184
N	-0.000123	-2.281110	-2.172013
N	-0.000123	-2.281110	2.172013

==========
D3-ESP_S-diBr.out
==========

C	0.710657	-1.797765	0.000079
C	-0.710656	-1.797765	0.000080
C	-1.430429	-0.625681	0.000032
C	1.430429	-0.625681	0.000032
H	1.232072	-2.749560	0.000068
H	-1.232071	-2.749560	0.000068
C	0.728444	0.608758	0.000037
C	-0.728444	0.608758	0.000037
N	1.256471	1.844649	-0.000207
N	-1.256472	1.844649	-0.000207
S	-0.000000	2.872620	0.000408
Br	3.326320	-0.635880	-0.000079
Br	-3.326319	-0.635881	-0.000079

==========
D3-ESP_S-nat.out
==========

C	2.411159	-0.713043	0.000006
C	2.411158	0.713045	0.000006
C	1.241853	1.438071	0.000004
C	1.241855	-1.438071	0.000004
H	3.364917	-1.234356	0.000009
H	3.364915	1.234360	0.000009
H	1.236661	2.523588	0.000005
H	1.236665	-2.523588	0.000005
C	0.016037	-0.725747	0.000001
C	0.016036	0.725746	0.000001
N	-1.224354	-1.259701	0.000001
N	-1.224356	1.259700	0.000002
S	-2.255673	-0.000000	-0.000012

==========
D3-ESP_Se- zib.out
==========

C	-0.000154	-0.625987	0.730312
C	-0.000154	-0.625987	-0.730312
N	0.000598	0.555260	1.318886
N	0.000598	0.555260	-1.318886
Se	-0.000521	1.795716	0.000000
C	0.000234	-1.823447	-1.507804
C	0.000234	-1.823447	1.507804
N	0.000598	-2.816770	-2.109196
N	0.000598	-2.816770	2.109196

==========
D3-ESP_Se-diBr.out
==========

C	-0.712379	-2.155593	-0.000002
C	0.712379	-2.155593	-0.000002
C	1.428839	-0.986931	-0.000003
C	-1.428839	-0.986931	-0.000002
H	-1.233506	-3.107556	0.000001
H	1.233506	-3.107556	0.000001
C	-0.737478	0.264845	-0.000008
C	0.737478	0.264845	-0.000009
N	-1.326083	1.457853	-0.000007
N	1.326083	1.457853	-0.000006
Se	0.000000	2.672532	0.000004
Br	-3.326565	-1.007553	0.000002
Br	3.326565	-1.007554	0.000002

==========
D3-ESP_Se-nat.out
==========

C	-2.929958	-0.715185	-0.000007
C	-2.929958	0.715184	-0.000007
C	-1.763505	1.435393	-0.000005
C	-1.763505	-1.435393	-0.000005
H	-3.883497	-1.237105	-0.000011
H	-3.883498	1.237104	-0.000011
H	-1.756920	2.521010	-0.000007
H	-1.756919	-2.521010	-0.000007
C	-0.520771	-0.733812	-0.000002
C	-0.520772	0.733812	-0.000001
N	0.674297	-1.330466	-0.000003
N	0.674296	1.330466	-0.000006
Se	1.894456	0.000000	0.000008

==========
D3-ESP_Te- zib.out
==========

C	-0.000007	-1.012622	0.737839
C	-0.000007	-1.012622	-0.737839
N	0.000007	0.131241	1.381895
N	0.000007	0.131241	-1.381895
Te	-0.000001	1.589345	-0.000000
C	-0.000001	-2.239026	-1.478118
C	-0.000001	-2.239026	1.478118
N	0.000002	-3.247397	-2.054528
N	0.000002	-3.247397	2.054528

==========
D3-ESP_Te-diBr.out
==========

C	-0.713068	-2.483835	0.000002
C	0.713044	-2.483843	0.000002
C	1.425890	-1.316366	0.000026
C	-1.425904	-1.316351	0.000026
H	-1.235101	-3.435267	0.000012
H	1.235066	-3.435281	0.000012
C	-0.746285	-0.048825	0.000026
C	0.746285	-0.048833	0.000028
N	-1.387998	1.108316	0.000146
N	1.388005	1.108303	0.000144
Te	0.000013	2.539422	-0.000168
Br	-3.326023	-1.350095	0.000086
Br	3.326010	-1.350117	0.000086

==========
D3-ESP_Te-nat.out
==========

C	-3.345430	-0.716150	-0.000004
C	-3.345380	0.716169	-0.000005
C	-2.179751	1.431632	0.000000
C	-2.179836	-1.431622	0.000000
H	-4.298512	-1.239289	-0.000005
H	-4.298429	1.239384	-0.000006
H	-2.171487	2.517456	0.000003
H	-2.171488	-2.517461	0.000003
C	-0.922047	-0.742012	-0.000001
C	-0.922003	0.741942	0.000002
N	0.235694	-1.394252	0.000015
N	0.235685	1.394340	0.000014
Te	1.673210	-0.000009	-0.000003

==========
D3-ESP_S-F4.out
==========

C	1.645945	0.714539	-0.000004
C	1.645945	-0.714539	-0.000004
C	0.472812	-1.434868	-0.000001
C	0.472812	1.434868	-0.000001
C	-0.754837	0.727466	0.000002
C	-0.754837	-0.727466	0.000002
N	-1.989938	1.258017	0.000005
N	-1.989938	-1.258018	0.000005
S	-3.021222	0.000000	0.000007
F	0.495244	2.771376	-0.000001
F	2.828736	1.336924	-0.000007
F	2.828736	-1.336924	-0.000007
F	0.495244	-2.771376	-0.000001

==========
D3-ESP_Se-F4.out
==========

C	-2.139714	0.716634	0.000005
C	-2.139714	-0.716634	0.000005
C	-0.970035	-1.433257	0.000002
C	-0.970035	1.433257	0.000002
C	0.274105	0.735826	-0.000001
C	0.274105	-0.735826	-0.000001
N	1.465510	1.328128	-0.000003
N	1.465510	-1.328128	-0.000003
Se	2.683517	0.000000	-0.000006
F	-0.993996	2.770283	0.000002
F	-3.324282	1.335817	0.000007
F	-3.324282	-1.335817	0.000007
F	-0.993996	-2.770283	0.000002

==========
D3-ESP_Te-CN.out
==========

C	-2.630065	1.349768	0.000005
C	-2.865123	-0.072843	0.000007
C	-1.821164	-0.972934	0.000005
C	-1.363271	1.855596	0.000003
C	-0.234686	0.969645	0.000002
C	-0.476373	-0.491872	0.000001
N	1.012953	1.423911	-0.000005
N	0.559758	-1.326903	-0.000010
Te	2.202027	-0.187970	-0.000003
H	-1.998465	-2.043080	0.000003
H	-3.489958	2.012450	0.000004
H	-1.180217	2.925522	0.000001
C	-4.213559	-0.543305	0.000007
N	-5.317186	-0.909123	0.000006

==========
D3-ESP_Te-F4.out
==========

C	2.560287	-0.717335	0.000005
C	2.560287	0.717335	0.000005
C	1.391984	1.430349	0.000002
C	1.391984	-1.430349	0.000002
C	0.133169	-0.744235	-0.000001
C	0.133169	0.744235	-0.000001
N	-1.021598	-1.390830	-0.000003
N	-1.021598	1.390830	-0.000003
Te	-2.456068	0.000000	-0.000004
F	1.420152	-2.768210	0.000001
F	3.746105	-1.335757	0.000009
F	3.746105	1.335757	0.000009
F	1.420152	2.768210	0.000002

5.4.3 Telluradiazole complexation structures

5.4.3.1 B97-D3 geometries

5.4.3.1.1 Gas phase

==========
B97D3-null-null_acceptor-NO3.out
==========

O	1.214371	-0.352044	0.000003
O	-0.302346	1.227644	0.000026
O	-0.912103	-0.875653	-0.000042
N	0.000088	0.000061	0.000015

==========
B97D3-null-null_acceptor-quin.out
==========

C	-0.799546	-0.627939	1.233615
C	1.292015	0.000684	0.002399
C	0.759786	-0.649978	1.291084
H	-1.215675	-0.070291	2.080532
H	-1.208530	-1.643933	1.278769
H	1.127927	-0.100057	2.165867
H	1.135031	-1.677425	1.373043
C	-0.798140	1.382856	-0.075377
H	-1.211442	1.838290	-0.982769
H	-1.208739	1.929970	0.781058
C	0.761332	1.442587	-0.080505
H	1.132381	1.925046	-0.993170
H	1.134664	2.027540	0.769022
H	2.387561	0.001264	0.004502
C	0.764571	-0.791615	-1.206497
H	1.141152	-0.348963	-2.136838
H	1.134917	-1.823484	-1.167075
C	-0.795036	-0.755977	-1.162464
H	-1.202670	-0.287339	-2.065712
H	-1.209389	-1.769135	-1.104854
N	-1.292442	-0.000742	-0.002273

==========
B97D3-null-null_complex-Te-diBr-Br.out
==========

C	-2.490369	2.130821	0.000068
C	-3.310320	0.965856	0.000119
C	-2.747150	-0.282190	0.000031
C	-1.124132	2.028187	-0.000070
H	-2.961891	3.108605	0.000090
H	-4.389942	1.079294	0.000182
C	-0.461905	0.753785	-0.000126
C	-1.321797	-0.477767	-0.000063
N	0.848951	0.624328	-0.000458
N	-0.719287	-1.641910	-0.000281
Te	1.319372	-1.341752	-0.000062
Br	4.145807	-0.604211	0.000479
Br	-3.890378	-1.826093	0.000005
Br	-0.067689	3.630136	-0.000245

==========
B97D3-null-null_complex-Te-diBr-Cl.out
==========

C	-1.707004	2.394054	-0.000385
C	-2.710599	1.383078	-0.000419
C	-2.363905	0.058428	-0.000177
C	-0.377525	2.062797	-0.000111
H	-2.007683	3.437091	-0.000490
H	-3.755837	1.676075	-0.000563
C	0.062843	0.696247	0.000082
C	-0.992058	-0.375447	0.000013
N	1.332660	0.348871	0.000703
N	-0.589567	-1.621496	0.000445
Te	1.475706	-1.668389	0.000185
Cl	4.180605	-1.391213	-0.000684
Br	0.932351	3.468160	0.000104
Br	-3.752798	-1.271384	-0.000074

==========
B97D3-null-null_complex-Te-diBr-I.out
==========

C	-2.959111	2.055671	0.000000
C	-3.732338	0.859072	0.000015
C	-3.121252	-0.366117	0.000008
C	-1.589988	2.008095	-0.000021
H	-3.469291	3.013812	0.000003
H	-4.815559	0.929849	0.000029
C	-0.879184	0.759789	-0.000026
C	-1.689261	-0.503508	-0.000011
N	0.436022	0.682049	-0.000058
N	-1.044030	-1.645563	-0.000029
Te	0.978566	-1.264864	-0.000032
I	4.026621	-0.370052	0.000062
Br	-0.596338	3.647783	-0.000048
Br	-4.201622	-1.953252	0.000023

B97D3-null-null_complex-Te-diBr-NO3.out

C	2.755717	1.844031	0.000140
C	3.396005	0.570578	0.000155
C	2.658226	-0.582056	0.000077
C	1.390186	1.944169	0.000049
H	3.366561	2.741279	0.000200
H	4.480549	0.525569	0.000227
C	0.548376	0.779317	-0.000034
C	1.219435	-0.563999	-0.000019
N	-0.766691	0.838270	-0.000133
N	0.452657	-1.628304	-0.000097
Te	-1.504402	-1.039719	-0.000221
O	-3.648863	0.243213	0.000156
O	-5.806018	-0.063916	0.000386
O	-4.472818	-1.794618	0.000052
N	-4.673134	-0.558222	0.000179
Br	0.578618	3.681377	0.000030
Br	3.561551	-2.275473	0.000099

B97D3-null-null_complex-Te-diBr-quin.out

Imaginary Frequency : -25.57
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis
Imaginary Frequency : -9.85
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	2.873759	2.313242	0.000024
C	3.829331	1.251330	0.000044
C	3.435890	-0.057670	0.000029
C	1.532151	2.055855	-0.000009
H	3.230985	3.338102	0.000036
H	4.885361	1.501207	0.000073
C	1.038461	0.705624	-0.000032
C	2.037680	-0.413494	-0.000018
N	-0.241918	0.415386	-0.000058
N	1.586136	-1.644279	-0.000049
Te	-0.444229	-1.592128	-0.000071
C	-3.194097	0.087942	-1.209773
C	-5.392053	0.076575	0.000087
C	-4.663097	0.594422	-1.250584
H	-2.474102	0.908248	-1.185206
H	-2.959502	-0.534601	-2.079871
H	-4.690146	1.689597	-1.273109
H	-5.171424	0.238456	-2.154132
C	-3.193900	0.088301	1.209596
H	-2.959286	-0.534032	2.079838
H	-2.473817	0.908522	1.184732
C	-4.662850	0.594928	1.250406
H	-5.171058	0.239423	2.154201
H	-4.689798	1.690116	1.272429
H	-6.432046	0.419274	0.000120
C	-5.344808	-1.460164	0.000392
H	-5.863151	-1.852205	0.882748
H	-5.863423	-1.852572	-0.881640
C	-3.853587	-1.902398	0.000250
H	-3.614335	-2.504322	0.883924
H	-3.614560	-2.504496	-0.883366
N	-2.952020	-0.733487	0.000013
Br	0.276996	3.496568	-0.000026
Br	4.738934	-1.446007	0.000058

B97D3-null-null_complex-Te-nat-Br.out

C	-4.005853	1.565271	0.000026
C	-4.490011	0.219901	0.000058
C	-3.623717	-0.843794	0.000023
C	-2.661108	1.836642	-0.000040
H	-4.723014	2.384785	0.000046
H	-5.565202	0.046210	0.000102
H	-3.983833	-1.870479	0.000037
H	-2.285294	2.857096	-0.000076
C	-1.703494	0.766873	-0.000073
C	-2.202174	-0.631941	-0.000037
N	-0.400155	1.003697	-0.000173
N	-1.316397	-1.612066	-0.000107
Te	0.566501	-0.776426	-0.000121
Br	3.178094	0.678212	0.000240

B97D3-null-null_complex-Te-nat-Cl.out

C	-3.670486	1.300629	0.000007
C	-4.013162	-0.087546	0.000012
C	-3.040829	-1.055504	0.000025
C	-2.360469	1.708752	0.000016
H	-4.468414	2.041913	0.000004
H	-5.064665	-0.372015	0.000012
H	-3.292774	-2.114158	0.000037
H	-2.092889	2.762961	0.000022
C	-1.296204	0.744703	0.000023
C	-1.648052	-0.699375	0.000025
N	-0.025082	1.115016	0.000062
N	-0.665029	-1.579920	0.000060
Te	1.127783	-0.555497	-0.000013
Cl	3.369412	1.079500	-0.000053

B97D3-null-null_complex-Te-nat-I.out

C	-4.341822	1.730777	-0.000001
C	-4.909221	0.418023	0.000007
C	-4.112239	-0.698076	0.000008
C	-2.983314	1.917977	-0.000006
H	-5.006712	2.593034	-0.000004
H	-5.993043	0.312029	0.000013
H	-4.535620	-1.700126	0.000015
H	-2.544017	2.912556	-0.000012
C	-2.095260	0.789779	-0.000002
C	-2.680532	-0.574342	0.000002
N	-0.779525	0.943388	-0.000003
N	-1.859979	-1.610413	0.000002
Te	0.068238	-0.894928	-0.000003
I	3.013998	0.482700	0.000002

B97D3-null-null_complex-Te-nat-NO3.out

C	4.141653	1.397578	0.000026
C	4.518339	0.017441	-0.000012
C	3.572383	-0.975056	-0.000032
C	2.823347	1.774290	0.000044
H	4.921759	2.157210	0.000043
H	5.576470	-0.239912	-0.000024
H	3.850562	-2.026742	-0.000060
H	2.529189	2.821171	0.000076
C	1.784115	0.782897	0.000025
C	2.172543	-0.650491	-0.000017
N	0.502540	1.116262	0.000049
N	1.212492	-1.559043	-0.000029
Te	-0.586645	-0.590511	-0.000015
O	-2.487863	1.111681	-0.000003
O	-4.662622	1.255305	0.000034
O	-3.712417	-0.712315	0.000015
N	-3.649817	0.539567	0.000006

B97D3-null-null_complex-Te-nat-quin.out

Imaginary Frequency : -18.55
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	4.273252	2.169566	0.000163
C	5.064252	0.973938	-0.000757
C	4.482530	-0.263006	-0.001064
C	2.906547	2.123433	0.000757
H	4.779843	3.132044	0.000387
H	6.148096	1.063301	-0.001200
H	5.073663	-1.174540	-0.001743
H	2.305241	3.028459	0.001462
C	2.230166	0.855716	0.000442
C	3.050210	-0.387601	-0.000497
N	0.912222	0.766530	0.000944
N	2.432194	-1.552635	-0.000652
Te	0.432568	-1.205153	0.000363
C	-2.155575	0.793129	-1.208292
C	-4.345549	0.989578	-0.001108
C	-3.568961	1.441345	-1.249329
H	-1.357016	1.538151	-1.188995
H	-1.984515	0.149089	-2.077502
H	-3.491866	2.534541	-1.266224
H	-4.108357	1.140590	-2.155087
C	-2.157096	0.793589	1.208945
H	-1.982712	0.151189	2.078693
H	-1.361409	1.541637	1.188034
C	-3.572739	1.436980	1.250992
H	-4.112914	1.129237	2.153945
H	-3.499153	2.530286	1.274372
H	-5.349038	1.428242	-0.001868
C	-4.441383	-0.545814	-0.003871
H	-4.997930	-0.888460	0.875924
H	-4.991847	-0.885504	-0.888636
C	-2.998004	-1.123032	0.000239
H	-2.816786	-1.743456	0.884939
H	-2.813036	-1.746612	-0.881472
N	-1.992941	-0.043492	0.000617

B97D3-null-null_donor-Te-diBr.out

C	-0.713068	-2.483835	0.000002
C	0.713044	-2.483843	0.000002
C	1.425890	-1.316366	0.000026
C	-1.425904	-1.316351	0.000026
H	-1.235102	-3.435267	0.000012
H	1.235065	-3.435281	0.000012
C	-0.746285	-0.048825	0.000026
C	0.746285	-0.048833	0.000028
N	-1.387998	1.108316	0.000146
N	1.388005	1.108303	0.000144
Te	0.000013	2.539422	-0.000168
Br	-3.326023	-1.350095	0.000086
Br	3.326010	-1.350118	0.000086

B97D3-null-null_donor-Te-nat.out

C	-3.345430	0.716150	0.000004
C	-3.345380	-0.716169	0.000005
C	-2.179751	-1.431632	-0.000000
C	-2.179836	1.431622	0.000000
H	-4.298512	1.239289	0.000005
H	-4.298429	-1.239384	0.000006
H	-2.171487	-2.517456	-0.000003
H	-2.171488	2.517461	-0.000003
C	-0.922047	0.742012	0.000001
C	-0.922003	-0.741942	-0.000002
N	0.235694	1.394252	-0.000015
N	0.235685	-1.394340	-0.000014
Te	1.673210	0.000009	0.000003

B97D3-null-null_complex-Te-CN-Br-opp.out

C	-3.460678	1.604063	-0.000040
C	-3.956304	0.252497	-0.000039
C	-3.085572	-0.824654	0.000086
C	-2.116990	1.857209	0.000072
H	-4.179943	2.418521	-0.000095
H	-3.460810	-1.843984	0.000121
H	-1.736244	2.875236	0.000118
C	-1.165729	0.781276	0.000155
C	-1.672709	-0.614580	0.000163
N	0.136141	1.008585	0.000449
N	-0.791163	-1.600853	0.000373
Te	1.095314	-0.779557	0.000234
Br	3.645270	0.672478	-0.000527
C	-5.365306	0.036512	-0.000120
N	-6.519845	-0.122510	-0.000183

B97D3-null-null_complex-Te-CN-Cl-opp.out

C	3.056796	1.509783	-0.000001
C	3.465150	0.129375	0.000007
C	2.526465	-0.889523	0.000022
C	1.731611	1.847633	-0.000001
H	3.826365	2.276983	0.000002
H	2.835786	-1.930891	0.000039
H	1.417223	2.888232	0.000008
C	0.712505	0.835493	-0.000001
C	1.129553	-0.590834	0.000018
N	-0.571492	1.145675	0.000065
N	0.186029	-1.516418	0.000065
Te	-1.649468	-0.577004	-0.000018
Cl	-3.910457	0.955735	-0.000034
C	4.857110	-0.176901	0.000017
N	5.999115	-0.410368	0.000027

B97D3-null-null_complex-Te-CN-I-opp.out

C	-3.840748	1.677675	-0.000240
C	-4.397218	0.349791	0.000200
C	-3.577059	-0.765857	0.000322
C	-2.487347	1.870005	-0.000553
H	-4.522493	2.523696	-0.000350
H	-3.998012	-1.767038	0.000628
H	-2.060531	2.869441	-0.000922
C	-1.586421	0.751492	-0.000435
C	-2.156258	-0.619088	0.000099
N	-0.275443	0.918678	-0.000859
N	-1.322683	-1.646898	0.000172
Te	0.596870	-0.912804	-0.000304
I	3.447446	0.519532	0.000315
C	-5.814695	0.197341	0.000495
N	-6.975067	0.090558	0.000745

B97D3-null-null_complex-Te-CN-Br-same.out

C	-3.757224	0.584775	-0.000065
C	-3.968531	-0.839314	-0.000003
C	-2.907420	-1.701429	0.000029
C	-2.478808	1.117690	-0.000090
H	-4.990181	-1.209652	0.000011
H	-3.059038	-2.778177	0.000070
H	-2.321689	2.192139	-0.000143
C	-1.341470	0.255877	-0.000051
C	-1.554898	-1.213796	0.000011
N	-0.108159	0.745530	-0.000102
N	-0.495136	-1.996976	0.000027
Te	1.190871	-0.803206	0.000011
Br	3.398223	1.129029	0.000075
C	-4.893650	1.445552	-0.000107
N	-5.836729	2.130055	-0.000140

B97D3-null-null_complex-Te-CN-Cl-same.out

C	3.349245	0.366612	0.000029
C	3.396996	-1.072341	0.000115
C	2.244160	-1.807535	0.000105
C	2.139078	1.041101	-0.000062
H	4.369827	-1.556786	0.000172
H	2.272432	-2.894678	0.000154
H	2.105632	2.126575	-0.000150
C	0.910613	0.315328	-0.000057
C	0.954802	-1.170372	0.000029
N	-0.257997	0.942831	-0.000222
N	-0.187348	-1.824949	-0.000023
Te	-1.732158	-0.443217	-0.000036
Cl	-3.536033	1.605062	0.000138
C	4.575578	1.093025	0.000012
N	5.590211	1.666577	0.000004

B97D3-null-null_complex-Te-CN-I-same.out

C	-4.128977	0.757025	0.000054
C	-4.453720	-0.645766	0.000484
C	-3.466079	-1.590719	0.000553
C	-2.812436	1.185584	-0.000348
H	-5.501706	-0.933047	0.000749
H	-3.703759	-2.651648	0.000855
H	-2.569033	2.243727	-0.000682
C	-1.748184	0.234616	-0.000326
C	-2.079021	-1.212651	0.000245
N	-0.479433	0.623092	-0.000707
N	-1.087959	-2.081901	0.000254
Te	0.686955	-1.028604	-0.000245
I	3.261797	0.852964	0.000203
C	-5.193329	1.705651	0.000028
N	-6.080027	2.461502	0.000019

B97D3-null-null_complex-Te-CN-NO3-opp.out

C	3.560802	1.540453	-0.000032
C	3.975332	0.161107	-0.000093
C	3.044389	-0.862672	-0.000022
C	2.235151	1.873062	0.000103
H	4.327440	2.310352	-0.000040
H	3.358515	-1.902357	-0.000013
H	1.915589	2.911889	0.000215
C	1.221624	0.854905	0.000143
C	1.646566	-0.567568	0.000062
N	-0.065638	1.153479	0.000503
N	0.708711	-1.501494	0.000325
Te	-1.113235	-0.581495	-0.000021
O	-3.004314	1.062794	-0.000563
O	-5.181393	1.159168	-0.000256
O	-4.190824	-0.787697	0.000548
N	-4.159294	0.463790	-0.000165
C	5.369857	-0.137315	-0.000160
N	6.512876	-0.362648	-0.000219

B97D3-null-null_complex-Te-CN-NO3-same.out

C	3.820343	0.538141	-0.000088
C	3.963170	-0.895085	-0.000197
C	2.863062	-1.705815	-0.000112
C	2.570622	1.132398	0.000098
H	4.965932	-1.313564	-0.000283
H	2.962990	-2.788442	-0.000119
H	2.465220	2.213115	0.000256
C	1.392641	0.325521	0.000140
C	1.536509	-1.152043	0.000020
N	0.182350	0.868908	0.000609
N	0.439876	-1.884646	0.000353
Te	-1.175415	-0.624956	-0.000017
O	-2.728687	1.345542	-0.000598
O	-4.852586	1.833565	-0.000252
O	-4.229755	-0.260175	0.000573
N	-3.972734	0.965409	-0.000211
C	4.997579	1.343275	-0.000084
N	5.972239	1.981297	-0.000096

B97D3-null-null_complex-Te-CN-Quin-opp.out

Imaginary Frequency : -29.77
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.915130	1.873299	-0.004472
C	4.632624	0.621062	0.001820
C	3.965221	-0.584262	0.004335
C	2.551835	1.904741	-0.007885
H	4.490249	2.794349	-0.006412
H	4.504207	-1.526143	0.009056
H	2.010984	2.846645	-0.012582
C	1.796003	0.682372	-0.005164
C	2.533848	-0.609207	0.000717
N	0.476561	0.676145	-0.007726
N	1.842789	-1.733785	0.002496
Te	-0.129369	-1.260110	-0.002383
C	-2.591210	0.867360	-1.210424
C	-4.764763	1.162293	0.005735
C	-3.969666	1.586571	-1.240077
H	-1.756351	1.571507	-1.198833
H	-2.460633	0.214361	-2.079891
H	-3.836514	2.674290	-1.245943
H	-4.525084	1.323404	-2.147603
C	-2.584729	0.866329	1.209542
H	-2.431812	0.216680	2.077862
H	-1.759712	1.581682	1.184513
C	-3.972013	1.566956	1.259501
H	-4.522355	1.274634	2.161221
H	-3.852442	2.655744	1.291999
H	-5.747462	1.645194	0.008591
C	-4.929677	-0.367238	-0.006588
H	-5.505525	-0.690179	0.867958
H	-5.489874	-0.676564	-0.896165
C	-3.515035	-1.010960	0.001410
H	-3.363190	-1.634590	0.889319
H	-3.358031	-1.645811	-0.877634
N	-2.461135	0.023801	-0.001090
C	6.060143	0.651701	0.005474
N	7.222425	0.695902	0.008449

B97D3-null-null_complex-Te-CN-Quin-same.out

Imaginary Frequency : -38.35
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	4.204396	1.126941	-0.000281
C	4.760639	-0.204632	0.003520
C	3.951467	-1.301953	0.004000
C	2.841918	1.336315	-0.003992
H	5.841318	-0.309730	0.006124
H	4.362608	-2.307156	0.006973
H	2.430032	2.340374	-0.006750
C	1.950516	0.218110	-0.003370
C	2.520710	-1.155613	0.000913
N	0.638039	0.379860	-0.005611
N	1.693050	-2.180426	0.002094
Te	-0.207171	-1.458317	-0.001091
C	-2.361791	0.963727	-1.219242
C	-4.462590	1.593414	0.001614
C	-3.621412	1.873847	-1.255058
H	-1.434829	1.541082	-1.218229
H	-2.330258	0.288736	-2.081113
H	-3.331181	2.930263	-1.281886
H	-4.215120	1.678310	-2.155301
C	-2.339575	0.993541	1.198782
H	-2.277551	0.341184	2.076244
H	-1.419044	1.579587	1.158539
C	-3.607804	1.891071	1.245041
H	-4.188424	1.695206	2.153790
H	-3.327861	2.950431	1.261873
H	-5.362182	2.217462	0.002168
C	-4.851498	0.105250	0.014255
H	-5.459973	-0.117263	0.898026
H	-5.459473	-0.131797	-0.866153
C	-3.546003	-0.740433	0.021998
H	-3.482567	-1.369753	0.916681
H	-3.492790	-1.402116	-0.849800
N	-2.349283	0.124520	0.000192
C	5.095898	2.242303	0.000317
N	5.834047	3.141239	0.001116

==========
B97D3-null-null_complex-Te-F4-Br.out
==========

C	-3.277443	1.188755	-0.000045
C	-3.675873	-0.183351	-0.000010
C	-2.745662	-1.187256	-0.000003
C	-1.954509	1.544520	-0.000077
C	-0.927078	0.543311	-0.000053
C	-1.339308	-0.891079	-0.000007
N	0.354023	0.854426	-0.000146
N	-0.397333	-1.805229	-0.000040
Te	1.439514	-0.857966	0.000055
Br	3.867361	0.762792	0.000044
F	-4.252591	2.126350	-0.000076
F	-1.627052	2.852360	-0.000143
F	-5.002413	-0.453294	-0.000001
F	-3.161272	-2.471779	0.000008

==========
B97D3-null-null_complex-Te-F4-Cl.out
==========

C	2.912028	1.032888	-0.000077
C	3.188824	-0.368547	-0.000131
C	2.173929	-1.286880	-0.000093
C	1.625238	1.503197	0.000010
C	0.513262	0.597078	0.000036
C	0.798366	-0.870012	-0.000011
N	-0.735115	1.019036	0.000186
N	-0.221419	-1.694557	0.000075
Te	-1.972404	-0.589143	0.000053
Cl	-4.066057	1.145373	-0.000003
F	3.966245	1.881887	-0.000092
F	1.415457	2.836092	0.000081
F	4.487421	-0.753920	-0.000192
F	2.476856	-2.603349	-0.000121

==========
B97D3-null-null_complex-Te-F4-I.out
==========

C	-3.634048	1.295254	-0.000167
C	-4.110391	-0.052086	-0.000105
C	-3.239786	-1.108065	-0.000010
C	-2.293162	1.575052	-0.000135
C	-1.325307	0.515946	-0.000020
C	-1.818911	-0.892466	0.000032
N	-0.028504	0.752591	-0.000036
N	-0.932523	-1.861303	0.000107
Te	0.953158	-1.019383	0.000194
I	3.703355	0.565077	-0.000047
F	-4.553392	2.286423	-0.000283
F	-1.890149	2.860673	-0.000219
F	-5.449276	-0.245478	-0.000158
F	-3.727767	-2.366286	0.000036

==========
B97D3-null-null_complex-Te-F4-NO3.out
==========

C	3.357282	1.102879	-0.000007
C	3.668769	-0.292666	0.000083
C	2.678818	-1.237283	0.000082
C	2.060264	1.541627	-0.000075
C	0.971735	0.606040	-0.000040
C	1.294382	-0.851947	0.000026
N	-0.287908	0.991969	-0.000150
N	0.296146	-1.705371	-0.000007
Te	-1.463589	-0.656802	-0.000049
O	-3.213472	1.116959	-0.000225
O	-5.376636	1.375452	0.000074
O	-4.534025	-0.640340	0.000440
N	-4.409659	0.605528	0.000037
F	4.389679	1.975197	-0.000024
F	1.814444	2.866379	-0.000168
F	4.974637	-0.643969	0.000127
F	3.012589	-2.544232	0.000138

==========
B97D3-null-null_complex-Te-F4-Quin.out
==========

Imaginary Frequency : -22.82
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis
Imaginary Frequency : -21.18
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	-3.672814	1.567457	0.000039
C	-4.347609	0.300323	-0.000110
C	-3.649718	-0.874946	0.000043
C	-2.307777	1.648000	0.000260
C	-1.512098	0.454790	0.000380
C	-2.211192	-0.867419	0.000322
N	-0.198058	0.487836	0.000282
N	-1.483548	-1.957812	0.000093
Te	0.479851	-1.421384	0.000037
C	2.810331	0.802311	1.214590
C	4.963746	1.226649	0.000213
C	4.147386	1.594110	1.249908
H	1.939637	1.461138	1.204626
H	2.713702	0.138095	2.079825
H	3.954345	2.672578	1.266559
H	4.717027	1.352898	2.154713
C	2.803846	0.814931	-1.206893
H	2.690632	0.161788	-2.078525
H	1.939236	1.481175	-1.178906
C	4.147373	1.595349	-1.249113
H	4.713301	1.345163	-2.153862
H	3.963055	2.675230	-1.270699
H	5.917538	1.764329	0.000504
C	5.214912	-0.290503	-0.000637
H	5.803985	-0.573667	-0.880177
H	5.795403	-0.575592	0.884023
C	3.838635	-1.014947	-0.008389
H	3.721049	-1.643083	-0.898274
H	3.719946	-1.660125	0.869124
N	2.726793	-0.041059	-0.000346
F	-4.431388	2.672885	-0.000197
F	-1.707552	2.850682	0.000291
F	-5.688841	0.314471	-0.000432
F	-4.306394	-2.043299	-0.000188

==========
B97D3-null-null_donor-Te-CN.out
==========

C	-2.630104	1.349482	-0.000001
C	-2.865351	-0.073440	-0.000001
C	-1.820935	-0.973314	-0.000002
C	-1.363446	1.855422	-0.000002
H	-3.490278	2.011846	-0.000002
H	-1.998250	-2.043510	-0.000003
H	-1.180576	2.925412	-0.000003
C	-0.234716	0.969745	-0.000002
C	-0.476156	-0.492363	-0.000002
N	1.012540	1.424146	-0.000006
N	0.559551	-1.327167	-0.000006
Te	2.202270	-0.187853	0.000003
C	-4.213866	-0.543394	-0.000002
N	-5.318020	-0.908151	-0.000002

==========
B97D3-null-null_donor-Te-F4.out
==========

C	-0.000002	-2.560287	0.717335
C	-0.000002	-2.560287	-0.717335
C	-0.000002	-1.391984	-1.430349
C	-0.000002	-1.391984	1.430349
C	-0.000001	-0.133169	0.744235
C	-0.000001	-0.133169	-0.744235
N	-0.000000	1.021598	1.390830
N	-0.000000	1.021598	-1.390830
Te	0.000002	2.456068	0.000000
F	-0.000003	-1.420152	2.768210
F	-0.000001	-3.746105	1.335757
F	-0.000001	-3.746105	-1.335757
F	-0.000003	-1.420152	-2.768210

5.4.3.1.2 PCM

==========
B97D3-PCM-ACN_acceptor-NO3.out
==========

O	1.188960	0.422540	0.000002
O	-0.960492	0.818236	0.000025
O	-0.228484	-1.240900	-0.000043
N	0.000018	0.000141	0.000018

==========
B97D3-PCM-ACN_acceptor-quin.out
==========

C	-0.794108	-1.166843	0.753180
C	1.291547	0.001392	-0.001355
C	0.764068	-1.212999	0.781158
H	-1.201649	-1.109449	1.769006
H	-1.203527	-2.068584	0.283584
H	1.136601	-1.183152	1.812153
H	1.134926	-2.139460	0.326365
C	-0.797259	1.233697	0.634141
H	-1.207208	2.083373	0.076227
H	-1.206611	1.277331	1.649955
C	0.761010	1.285028	0.659729
H	1.130852	2.164193	0.118423
H	1.131956	1.355311	1.689374
H	2.386966	0.002629	-0.002468
C	0.760359	-0.069263	-1.443118
H	1.128780	0.788203	-2.019050
H	1.132320	-0.976727	-1.933934
C	-0.797692	-0.069545	-1.384957
H	-1.209320	0.787703	-1.929942
H	-1.205825	-0.978316	-1.842000
N	-1.296544	-0.001694	0.001377

==========
B97D3-PCM-ACN_complex-Te-diBr-Br.out
==========

C	2.429561	2.190345	-0.000067
C	3.287340	1.050692	-0.000066
C	2.769702	-0.215027	0.000062
C	1.069145	2.046943	0.000078
H	2.877185	3.178692	-0.000196
H	4.360998	1.206744	-0.000161
C	0.453579	0.748537	0.000229
C	1.349659	-0.447107	0.000199
N	-0.854435	0.568490	0.000376
N	0.788783	-1.637859	0.000282
Te	-1.229259	-1.410164	0.000341
Br	-4.216746	-0.618006	-0.000827
Br	3.948390	-1.723005	0.000092
Br	-0.046247	3.603366	0.000032

==========
B97D3-PCM-ACN_complex-Te-diBr-Cl.out
==========

C	1.639740	2.433748	0.000383
C	2.672296	1.449691	0.000359
C	2.367934	0.116416	0.000198
C	0.321273	2.069121	0.000220
H	1.919785	3.481935	0.000530
H	3.705772	1.779814	0.000480
C	-0.074586	0.688031	-0.000015
C	1.005104	-0.346424	0.000045
N	-1.334660	0.296648	-0.000068
N	0.640985	-1.609796	-0.000210
Te	-1.392717	-1.717756	-0.000362
Cl	-4.243152	-1.406033	-0.000096
Br	-1.032742	3.425160	0.000260
Br	3.781155	-1.176799	0.000147

==========
B97D3-PCM-ACN_complex-Te-diBr-I.out
==========

C	2.879258	2.140193	-0.000038
C	3.705906	0.977510	-0.000057
C	3.155569	-0.274321	0.000026
C	1.515706	2.033912	0.000068
H	3.353712	3.115953	-0.000064
H	4.783323	1.105068	-0.000101
C	0.866977	0.751645	0.000122
C	1.729682	-0.467115	0.000085
N	-0.445242	0.606458	0.000365
N	1.138641	-1.644100	0.000294
Te	-0.870986	-1.360139	0.000052
I	-4.084810	-0.384155	-0.000333
Br	0.440521	3.617115	0.000186
Br	4.293102	-1.812573	0.000080

==========
B97D3-PCM-ACN_complex-Te-diBr-NO3.out
==========

C	2.679050	1.935350	-0.000017
C	3.375124	0.690223	-0.000054
C	2.692131	-0.494272	-0.000050
C	1.312123	1.977041	0.000021
H	3.256388	2.853914	-0.000021
H	4.459993	0.700781	-0.000087
C	0.525963	0.773588	0.000025
C	1.253734	-0.533123	-0.000006
N	-0.793312	0.769688	0.000054
N	0.535278	-1.635926	0.000003
Te	-1.427974	-1.141001	0.000049
O	-3.668208	0.175927	0.000079
O	-5.833446	-0.049077	-0.000030
O	-4.566677	-1.826167	-0.000147
N	-4.708949	-0.583126	-0.000021
Br	0.419796	3.671449	0.000065
Br	3.660920	-2.145031	-0.000106

==========
B97D3-PCM-ACN_complex-Te-diBr-quin.out
==========

Imaginary Frequency : -35.63
Vibrational Mode : Quinuclidine rotational about Te-N(quin) axis
Imaginary Frequency : -32.30
Vibrational Mode : Quinuclidine rotational about Te-N(quin) axis

C	2.977815	2.251435	0.000287
C	3.889317	1.151791	0.000427
C	3.435144	-0.136837	0.000252
C	1.627289	2.043824	-0.000004
H	3.379403	3.259297	0.000417
H	4.953952	1.360751	0.000669
C	1.073270	0.717117	-0.000168
C	2.026177	-0.441364	-0.000084
N	-0.218559	0.476750	-0.000363
N	1.519114	-1.650298	-0.000317
Te	-0.524142	-1.518429	-0.000611
C	-3.233912	0.142847	-1.212608
C	-5.427256	0.036244	0.000938
C	-4.723066	0.582808	-1.250997
H	-2.553998	0.996686	-1.189364
H	-2.973633	-0.470255	-2.080932
H	-4.796818	1.675484	-1.275054
H	-5.212492	0.200128	-2.153213
C	-3.233696	0.139926	1.214314
H	-2.981203	-0.478781	2.080969
H	-2.548154	0.989408	1.197721
C	-4.720121	0.589364	1.248322
H	-5.211855	0.217779	2.153887
H	-4.787399	1.682657	1.262476
H	-6.480410	0.334395	0.001389
C	-5.313633	-1.496685	0.004852
H	-5.807784	-1.907402	0.891820
H	-5.816535	-1.912998	-0.874530
C	-3.808211	-1.878537	-0.001579
H	-3.541111	-2.470447	0.879735
H	-3.546906	-2.463619	-0.889141
N	-2.953941	-0.666396	-0.000146
Br	0.434613	3.543363	-0.000226
Br	4.689369	-1.582985	0.000426

==========
B97D3-PCM-ACN_complex-Te-nat-Br.out
==========

C	3.948292	1.662341	-0.000016
C	4.479857	0.332699	-0.000171
C	3.656975	-0.762122	-0.000210
C	2.597853	1.891052	0.000127
H	4.637832	2.502988	-0.000016
H	5.558902	0.199481	-0.000279
H	4.057519	-1.772559	-0.000339
H	2.193184	2.899638	0.000228
C	1.682292	0.784983	0.000176
C	2.230696	-0.592604	-0.000069
N	0.367136	0.963690	0.000179
N	1.380154	-1.608945	-0.000063
Te	-0.506990	-0.856857	0.000079
Br	-3.254022	0.724163	-0.000101

==========
B97D3-PCM-ACN_complex-Te-nat-Cl.out
==========

C	-3.634952	1.360824	0.000122
C	-4.005502	-0.022251	0.000173
C	-3.058138	-1.011468	0.000182
C	-2.320628	1.746967	0.000087
H	-4.418866	2.114343	0.000138
H	-5.061245	-0.282470	0.000223
H	-3.336704	-2.062308	0.000246
H	-2.038850	2.796712	0.000080
C	-1.279523	0.757676	0.000089
C	-1.661097	-0.675845	0.000125
N	0.004172	1.091718	0.000139
N	-0.695039	-1.581253	0.000219
Te	1.096345	-0.611986	-0.000097
Cl	3.437695	1.161667	-0.000166

==========
B97D3-PCM-ACN_complex-Te-nat-I.out
==========

C	-4.292834	1.839080	0.000033
C	-4.912085	0.547893	-0.000055
C	-4.165185	-0.599837	0.000045
C	-2.930387	1.977127	0.000219
H	-4.924739	2.723738	-0.000013
H	-5.997575	0.487048	-0.000167
H	-4.632645	-1.580963	0.000019
H	-2.458867	2.956055	0.000328
C	-2.091615	0.811969	0.000291
C	-2.730963	-0.525152	0.000196
N	-0.766995	0.901366	0.000581
N	-1.953223	-1.599050	0.000417
Te	-0.022865	-0.974282	0.000264
I	3.112882	0.502907	-0.000476

==========
B97D3-PCM-ACN_complex-Te-nat-NO3.out
==========

C	4.103860	1.472897	-0.000241
C	4.517980	0.101975	-0.000385
C	3.603294	-0.917193	-0.000272
C	2.778395	1.817823	0.000010
H	4.863918	2.250395	-0.000306
H	5.581438	-0.124292	-0.000556
H	3.915294	-1.958447	-0.000349
H	2.463496	2.858025	0.000152
C	1.769357	0.795695	0.000094
C	2.196948	-0.624729	-0.000047
N	0.474828	1.086601	0.000444
N	1.260718	-1.562629	0.000138
Te	-0.550280	-0.654593	0.000246
O	-2.532382	1.125462	-0.000333
O	-4.700712	1.329489	-0.000571
O	-3.804028	-0.660822	-0.000088
N	-3.697205	0.587645	-0.000406

==========
B97D3-PCM-ACN_complex-Te-nat-quin.out
==========

Imaginary Frequency : -17.45
Vibrational Mode : Quinuclidine rotational about Te-N(quin) axis

C	4.340173	2.109345	0.000023
C	5.100465	0.894014	-0.000088
C	4.486125	-0.328593	-0.000132
C	2.971615	2.095710	0.000084
H	4.870419	3.058587	0.000058
H	6.185991	0.955815	-0.000134
H	5.060239	-1.251654	-0.000213
H	2.396118	3.017695	0.000170
C	2.263712	0.844807	0.000046
C	3.050569	-0.418605	-0.000057
N	0.943143	0.787328	0.000105
N	2.394325	-1.563511	-0.000075
Te	0.387872	-1.163343	0.000045
C	-2.148849	0.811549	-1.211876
C	-4.340139	0.958401	-0.000116
C	-3.576446	1.424310	-1.250206
H	-1.372700	1.579460	-1.191704
H	-1.963715	0.171408	-2.080237
H	-3.522902	2.518419	-1.270171
H	-4.107299	1.104360	-2.153629
C	-2.149126	0.811303	1.212116
H	-1.964000	0.171045	2.080391
H	-1.373112	1.579356	1.192188
C	-3.576825	1.423841	1.250376
H	-4.107861	1.103384	2.153513
H	-3.523441	2.517947	1.270877
H	-5.352185	1.375781	-0.000191
C	-4.403486	-0.577436	-0.000411
H	-4.946786	-0.930577	0.882735
H	-4.946361	-0.930249	-0.883950
C	-2.951056	-1.126986	-0.000157
H	-2.755665	-1.742468	0.883995
H	-2.755341	-1.742429	-0.884266
N	-1.964773	-0.022674	0.000057

==========
B97D3-PCM-ACN_donor-Te-diBr.out
==========

C	-0.712842	-2.489149	0.000002
C	0.712821	-2.489156	0.000002
C	1.419292	-1.317926	0.000016
C	-1.419304	-1.317914	0.000016
H	-1.231844	-3.441790	0.000010
H	1.231813	-3.441801	0.000010
C	-0.744282	-0.050087	0.000014
C	0.744282	-0.050093	0.000015
N	-1.382097	1.111650	0.000091
N	1.382104	1.111638	0.000091
Te	0.000011	2.545483	-0.000108
Br	-3.326702	-1.353684	0.000056
Br	3.326691	-1.353704	0.000057

==========
B97D3-PCM-ACN_donor-Te-nat.out
==========

C	-3.351627	0.715862	0.000007
C	-3.351574	-0.715884	0.000007
C	-2.183917	-1.430770	-0.000000
C	-2.184007	1.430761	0.000000
H	-4.304257	1.239128	0.000008
H	-4.304172	-1.239226	0.000008
H	-2.180447	-2.516939	-0.000004
H	-2.180457	2.516948	-0.000004
C	-0.927155	0.740769	-0.000001
C	-0.927103	-0.740677	-0.000002
N	0.235961	1.388625	-0.000023
N	0.235938	-1.388738	-0.000021
Te	1.677276	0.000010	0.000004

==========
B97D3-PCM-THF_acceptor-NO3.out
==========

O	-0.160844	-1.251599	0.000019
O	1.164891	0.486615	0.000042
O	-1.004184	0.764965	-0.000026
N	0.000156	0.000021	-0.000040

==========
B97D3-PCM-THF_acceptor-quin.out
==========

C	-0.802315	-0.265573	-1.358581
C	1.290930	0.001912	-0.004830
C	0.756448	-0.285984	-1.418234
H	-1.218927	-1.225416	-1.684860
H	-1.208620	0.511296	-2.016146
H	1.120878	-1.261451	-1.762384
H	1.130627	0.468262	-2.120729
C	-0.791594	-1.047607	0.913567
H	-1.203447	-0.852386	1.910462
H	-1.195765	-2.007790	0.572911
C	0.766912	-1.082284	0.951969
H	1.136522	-0.893981	1.967224
H	1.143662	-2.065684	0.645244
H	2.386389	0.003171	-0.009484
C	0.762233	1.370221	0.456857
H	1.142485	1.598263	1.459848
H	1.124478	2.156840	-0.216031
C	-0.795837	1.310918	0.454111
H	-1.196489	1.494218	1.457496
H	-1.214920	2.073267	-0.212512
N	-1.295362	-0.001176	0.005688

==========
B97D3-PCM-THF_complex-Te-diBr-Br.out
==========

C	2.447157	2.174405	-0.000079
C	3.294524	1.027263	0.000281
C	2.763677	-0.233158	0.000109
C	1.084940	2.043790	-0.000473
H	2.902725	3.159243	0.000039
H	4.369914	1.171892	0.000775
C	0.455803	0.751690	-0.000623
C	1.341906	-0.452760	-0.000572
N	-0.853614	0.585024	-0.000683
N	0.770492	-1.637162	-0.001089
Te	-1.250256	-1.391377	-0.000988
Br	-4.199101	-0.614587	0.001714
Br	3.926672	-1.754523	0.001075
Br	-0.013443	3.612483	-0.000757

==========
B97D3-PCM-THF_complex-Te-diBr-Cl.out
==========

C	1.661581	2.421844	-0.000124
C	2.685046	1.428749	-0.000141
C	2.367391	0.098372	-0.000062
C	0.339497	2.069020	-0.000024
H	1.949856	3.467902	-0.000163
H	3.722019	1.748173	-0.000195
C	-0.070315	0.691872	0.000060
C	1.000893	-0.353401	0.000014
N	-1.333944	0.314122	0.000264
N	0.624573	-1.612022	0.000211
Te	-1.415281	-1.701557	0.000095
Cl	-4.231583	-1.404065	-0.000318
Br	-1.000800	3.439029	0.000035
Br	3.769963	-1.208156	-0.000059

==========
B97D3-PCM-THF_complex-Te-diBr-I.out
==========

C	2.889227	2.126275	-0.000025
C	3.707076	0.957812	0.000008
C	3.146243	-0.289607	-0.000035
C	1.524496	2.030228	-0.000098
H	3.369683	3.099201	0.000033
H	4.785723	1.075748	0.000079
C	0.865034	0.753104	-0.000161
C	1.719136	-0.473143	-0.000134
N	-0.447815	0.619532	-0.000145
N	1.118900	-1.644283	-0.000197
Te	-0.894449	-1.344178	-0.000195
I	-4.061358	-0.382362	0.000311
Br	0.463830	3.623338	-0.000072
Br	4.273401	-1.836689	0.000032

==========
B97D3-PCM-THF_complex-Te-diBr-NO3.out
==========

Imaginary Frequency : -12.66
Vibrational Mode : Out of plane bend of NO_3 oxygen atoms about Te-N(NO_3) axis

C	-2.713278	1.898862	-0.000022
C	-3.386378	0.641477	-0.000007
C	-2.681186	-0.530149	-0.000004
C	-1.346986	1.965281	-0.000032
H	-3.306090	2.807640	-0.000021
H	-4.471341	0.630638	0.000005
C	-0.538456	0.776557	-0.000026
C	-1.242323	-0.543725	-0.000015
N	0.780396	0.798295	0.000002
N	-0.504244	-1.632884	-0.000010
Te	1.452170	-1.100611	-0.000013
O	3.685743	0.211610	0.000157
O	5.845472	-0.063727	0.000183
O	4.537543	-1.811290	-0.000124
N	4.710371	-0.571214	0.000044
Br	-0.485907	3.675906	-0.000042
Br	-3.620935	-2.199004	0.000024

==========
B97D3-PCM-THF_complex-Te-diBr-quin.out
==========

Imaginary Frequency : -31.50
Vibrational Mode : Quinuclidine rotational about Te-N(quin) axis
Imaginary Frequency : -25.88
Vibrational Mode : Quinuclidine rotational about Te-N(quin) axis

C	2.962441	2.260710	-0.000002
C	3.880326	1.166232	-0.000003
C	3.434738	-0.125406	-0.000002
C	1.613049	2.046290	-0.000000
H	3.357764	3.271127	-0.000003
H	4.943890	1.380853	-0.000005
C	1.067306	0.716136	0.000001
C	2.027129	-0.437000	0.000001
N	-0.222916	0.468973	0.000002
N	1.528508	-1.649194	0.000002
Te	-0.512695	-1.528926	0.000005
C	-3.226711	0.133267	-1.213097
C	-5.420891	0.041038	-0.000007
C	-4.711887	0.587071	-1.249570
H	-2.537829	0.979900	-1.193399
H	-2.973782	-0.484261	-2.080649
H	-4.776069	1.680503	-1.268301
H	-5.205318	0.214029	-2.153762
C	-3.226712	0.133287	1.213085
H	-2.973745	-0.484210	2.080648
H	-2.537857	0.979941	1.193351
C	-4.711903	0.587045	1.249578
H	-5.205323	0.213952	2.153754
H	-4.776116	1.680474	1.268352
H	-6.472435	0.345062	-0.000009
C	-5.316052	-1.492723	-0.000023
H	-5.817509	-1.903513	0.882904
H	-5.817464	-1.903487	-0.882987
C	-3.812329	-1.882611	0.000011
H	-3.551209	-2.473083	0.884309
H	-3.551179	-2.473123	-0.884252
N	-2.951961	-0.676112	0.000001
Br	0.411368	3.537577	0.000002
Br	4.695143	-1.564026	-0.000003

==========
B97D3-PCM-THF_complex-Te-nat-Br.out
==========

C	3.952008	1.644386	0.000009
C	4.475744	0.311983	-0.000081
C	3.645703	-0.777857	-0.000105
C	2.602517	1.879909	0.000053
H	4.645995	2.481707	0.000051
H	5.554247	0.172120	-0.000127
H	4.039732	-1.791005	-0.000157
H	2.201818	2.890142	0.000149
C	1.680053	0.779454	0.000011
C	2.219984	-0.601661	-0.000037
N	0.367081	0.968433	0.000123
N	1.362861	-1.611407	-0.000099
Te	-0.524647	-0.844614	0.000056
Br	-3.220738	0.721444	-0.000060

==========
B97D3-PCM-THF_complex-Te-nat-Cl.out
==========

C	-3.639109	1.347315	0.000125
C	-4.003992	-0.036926	0.000130
C	-3.051845	-1.021986	0.000089
C	-2.325851	1.738024	0.000104
H	-4.425942	2.098198	0.000124
H	-5.058884	-0.301921	0.000156
H	-3.325585	-2.074317	0.000093
H	-2.047003	2.788699	0.000061
C	-1.280018	0.753498	0.000162
C	-1.655552	-0.682157	0.000104
N	0.001086	1.094838	-0.000009
N	-0.685541	-1.582023	0.000128
Te	1.106093	-0.601149	-0.000041
Cl	3.404114	1.151339	-0.000202

==========
B97D3-PCM-THF_complex-Te-nat-I.out
==========

C	-4.306853	1.813680	0.000342
C	-4.913574	0.517059	-0.000111
C	-4.154767	-0.623312	-0.000545
C	-2.945404	1.963592	0.000356
H	-4.946550	2.693032	0.000525
H	-5.998673	0.445205	-0.000256
H	-4.612214	-1.609292	-0.001066
H	-2.481295	2.946004	0.000527
C	-2.094969	0.807051	0.000044
C	-2.721232	-0.536248	-0.000395
N	-0.771900	0.912191	-0.000415
N	-1.932507	-1.601571	-0.001324
Te	-0.004600	-0.954980	0.000463
I	3.094897	0.497335	-0.000184

==========
B97D3-PCM-THF_complex-Te-nat-NO3.out
==========

C	4.110207	1.456514	-0.000262
C	4.516271	0.083473	-0.000365
C	3.595090	-0.930117	-0.000266
C	2.786427	1.808597	-0.000066
H	4.874660	2.230035	-0.000338
H	5.578565	-0.149492	-0.000519
H	3.900149	-1.973605	-0.000340
H	2.476329	2.850345	0.000020
C	1.770807	0.792766	0.000039
C	2.190109	-0.630419	-0.000058
N	0.478817	1.092718	0.000251
N	1.248464	-1.562024	0.000060
Te	-0.559528	-0.641357	0.000294
O	-2.516794	1.122323	0.000026
O	-4.685950	1.316180	-0.000579
O	-3.780945	-0.670575	-0.000550
N	-3.681311	0.578589	-0.000226

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B97D3-PCM-THF_complex-Te-nat-quin.out

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Imaginary Frequency : -22.01

Vibrational Mode : Quinuclidine rotational about Te-N(quin) axis

C	4.329559	2.118614	0.000030
C	5.094567	0.906212	-0.000143
C	4.485237	-0.318589	-0.000205
C	2.961290	2.100172	0.000144
H	4.856286	3.069907	0.000073
H	6.179909	0.972196	-0.000227
H	5.061717	-1.240039	-0.000337
H	2.381763	3.019562	0.000280
C	2.258094	0.846661	0.000081
C	3.050117	-0.413862	-0.000107
N	0.937993	0.784485	0.000188
N	2.399923	-1.561962	-0.000143
Te	0.394854	-1.169842	0.000076
C	-2.149652	0.808416	-1.211400
C	-4.340742	0.963533	-0.000223
C	-3.574896	1.427196	-1.249932
H	-1.369493	1.572236	-1.191866
H	-1.967018	0.167538	-2.079873
H	-3.517388	2.521182	-1.269332
H	-4.107324	1.110652	-2.153769
C	-2.149976	0.808464	1.211555
H	-1.966340	0.168001	2.080121
H	-1.370603	1.573075	1.191525
C	-3.575817	1.425871	1.250536
H	-4.108349	1.107312	2.153606
H	-3.519299	2.519870	1.271813
H	-5.351419	1.384403	-0.000371
C	-4.409360	-0.572264	-0.001049
H	-4.955027	-0.923861	0.881386
H	-4.953418	-0.922938	-0.884846
C	-2.958361	-1.126359	0.000023
H	-2.765397	-1.742605	0.884345
H	-2.764401	-1.743427	-0.883512
N	-1.968915	-0.026193	0.000123

==========

B97D3-PCM-THF_donor-Te-diBr.out

==========

C	-0.712916	-2.488351	0.000002
C	0.712895	-2.488357	0.000002
C	1.420425	-1.317755	0.000017
C	-1.420437	-1.317743	0.000017
H	-1.232601	-3.440688	0.000011
H	1.232570	-3.440700	0.000011
C	-0.744623	-0.049998	0.000016
C	0.744622	-0.050004	0.000016
N	-1.383191	1.110848	0.000097
N	1.383198	1.110836	0.000097
Te	0.000011	2.544122	-0.000115
Br	-3.326601	-1.352726	0.000060
Br	3.326590	-1.352746	0.000060

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B97D3-PCM-THF_donor-Te-nat.out

==========

C	-3.350440	-0.715926	-0.000006
C	-3.350387	0.715948	-0.000006
C	-2.183177	1.431012	-0.000000
C	-2.183265	-1.431003	-0.000000
H	-4.303147	-1.239179	-0.000007
H	-4.303062	1.239276	-0.000008
H	-2.178806	2.517115	0.000004
H	-2.178814	-2.517123	0.000004
C	-0.926248	-0.741031	-0.000000
C	-0.926198	0.740943	0.000002
N	0.235880	-1.389657	0.000021
N	0.235859	1.389766	0.000020
Te	1.676537	-0.000010	-0.000004

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B97D3-PCM-ACN_complex-Te-CN-Br-opp.out

==========

C	3.429388	1.645468	-0.000065
C	3.948889	0.302143	-0.000090
C	3.109896	-0.795635	0.000088
C	2.082807	1.872737	0.000128
H	4.130162	2.474413	-0.000141
H	3.508748	-1.805092	0.000150
H	1.687434	2.884287	0.000214
C	1.159108	0.773535	0.000231
C	1.694090	-0.607128	0.000215
N	-0.152499	0.962359	0.000599
N	0.835592	-1.618469	0.000623
Te	-1.044241	-0.851485	-0.000104
Br	-3.718496	0.734267	-0.000078
C	5.362133	0.112486	-0.000218
N	6.517433	-0.029230	-0.000342

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B97D3-PCM-ACN_complex-Te-CN-Br-same.out

==========

C	-3.738765	0.635938	-0.000131
C	-3.986884	-0.782784	-0.000090
C	-2.948822	-1.670081	-0.000147
C	-2.454644	1.146304	-0.000228
H	-5.014950	-1.131227	-0.000055
H	-3.130219	-2.741117	-0.000168
H	-2.277425	2.216953	-0.000326
C	-1.340394	0.254163	-0.000252
C	-1.589601	-1.205523	-0.000184
N	-0.090458	0.706730	-0.000565
N	-0.546149	-2.019014	-0.000395
Te	1.143594	-0.884924	-0.000148
Br	3.464832	1.192317	0.000660
C	-4.852023	1.526926	-0.000149
N	-5.770054	2.242377	-0.000153

B97D3-PCM-ACN_complex-Te-CN-Cl-opp.out

C	3.033090	1.535545	0.000194
C	3.452748	0.157889	0.000088
C	2.534710	-0.875230	-0.000026
C	1.706455	1.860315	0.000204
H	3.792442	2.311315	0.000269
H	2.859212	-1.911142	-0.000108
H	1.386658	2.898417	0.000279
C	0.704010	0.832166	0.000093
C	1.135985	-0.584742	-0.000059
N	-0.589371	1.117393	0.000090
N	0.203136	-1.526716	-0.000193
Te	-1.619888	-0.623632	-0.000159
Cl	-3.971970	1.044959	0.000250
C	4.848186	-0.134399	0.000098
N	5.990266	-0.359714	0.000106

B97D3-PCM-ACN_complex-Te-CN-Cl-same.out

C	3.332854	0.387349	0.000010
C	3.398593	-1.051219	-0.000058
C	2.255666	-1.798969	-0.000048
C	2.123240	1.056203	0.000070
H	4.374152	-1.527445	-0.000104
H	2.300347	-2.884493	-0.000091
H	2.083624	2.140905	0.000125
C	0.904389	0.313418	0.000038
C	0.965384	-1.166808	0.000013
N	-0.277232	0.921494	0.000125
N	-0.174016	-1.837167	0.000029
Te	-1.711107	-0.495203	-0.000008
Cl	-3.567718	1.713431	-0.000055
C	4.549684	1.130557	0.000014
N	5.550073	1.725681	0.000012

B97D3-PCM-ACN_complex-Te-CN-I-opp.out

C	-3.808795	1.727446	0.000012
C	-4.396205	0.412299	0.000012
C	-3.615064	-0.727120	0.000034
C	-2.452620	1.886070	0.000094
H	-4.466357	2.591011	-0.000003
H	-4.064411	-1.715071	0.000064
H	-2.005932	2.875915	0.000138
C	-1.586888	0.740899	0.000262
C	-2.191682	-0.609975	0.000061
N	-0.266873	0.861628	0.000264
N	-1.387489	-1.665909	0.000260
Te	0.525400	-0.995041	0.000323
I	3.525609	0.562017	-0.000418
C	-5.817478	0.295209	-0.000048
N	-6.978347	0.212055	-0.000157

B97D3-PCM-ACN_complex-Te-CN-I-same.out

C	-4.107150	0.831324	-0.000028
C	-4.482015	-0.559424	-0.000784
C	-3.529071	-1.537364	-0.000876
C	-2.782467	1.223332	0.000601
H	-5.537284	-0.813607	-0.001262
H	-3.806961	-2.587397	-0.001448
H	-2.508106	2.273266	0.001087
C	-1.753960	0.233414	0.000469
C	-2.133694	-1.197027	-0.000180
N	-0.467910	0.570481	0.000965
N	-1.169860	-2.104544	-0.000386
Te	0.612662	-1.127867	0.000337
I	3.337680	0.893005	-0.000281
C	-5.135617	1.819316	-0.000028
N	-5.984985	2.614943	-0.000017

B97D3-PCM-ACN_complex-Te-CN-NO3-opp.out

C	3.542809	1.571308	0.000073
C	3.973005	0.196486	0.000130
C	3.063828	-0.843498	0.000057
C	2.214145	1.886897	-0.000057
H	4.296907	2.352121	0.000104
H	3.395068	-1.877160	0.000067
H	1.886976	2.922627	-0.000137
C	1.219124	0.851247	-0.000111
C	1.663519	-0.561923	-0.000048
N	-0.077680	1.123644	-0.000352
N	0.739889	-1.514177	-0.000235
Te	-1.078961	-0.631486	-0.000127
O	-3.059357	1.090109	-0.000010
O	-5.232918	1.223721	0.000416
O	-4.273146	-0.736723	0.000380
N	-4.209548	0.513756	0.000096
C	5.370755	-0.085845	0.000223
N	6.514092	-0.303964	0.000303

B97D3-PCM-ACN_complex-Te-CN-NO3-same.out

Imaginary Frequency : -8.83
Vibrational Mode : NO_3 out of plane bend

C	-3.802956	0.581906	-0.000002
C	-3.979821	-0.847764	-0.000001
C	-2.899049	-1.682213	0.000001
C	-2.546081	1.155604	-0.000001
H	-4.989242	-1.246881	-0.000001
H	-3.027154	-2.760908	0.000003
H	-2.422310	2.233846	-0.000003
C	-1.388044	0.320302	0.000001
C	-1.564837	-1.150500	0.000002
N	-0.162121	0.832937	0.000002
N	-0.481375	-1.910100	0.000003
Te	1.145164	-0.699028	0.000003
O	2.763614	1.371629	0.000013
O	4.866618	1.936403	0.000012
O	4.317876	-0.176146	-0.000037
N	4.005448	1.036234	-0.000004
C	-4.959755	1.415981	-0.000005
N	-5.912152	2.084989	-0.000007

B97D3-PCM-ACN_complex-Te-CN-Quin-opp.out

Imaginary Frequency : -29.00
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.954490	1.854683	-0.003432
C	4.648222	0.590606	0.001334
C	3.963523	-0.607624	0.003053
C	2.590765	1.902872	-0.006130
H	4.540123	2.768634	-0.004791
H	4.492663	-1.555410	0.006685
H	2.066935	2.854378	-0.009670
C	1.817787	0.691408	-0.004121
C	2.532960	-0.610928	0.000223
N	0.497527	0.703384	-0.006073
N	1.817021	-1.721353	0.001581
Te	-0.160457	-1.212972	-0.001897
C	-2.589668	0.873163	-1.215586
C	-4.768049	1.109339	0.004655
C	-3.968172	1.589658	-1.216940
H	-1.759111	1.582043	-1.227000
H	-2.479660	0.212723	-2.081403
H	-3.834633	2.676092	-1.170747
H	-4.515425	1.364312	-2.138715
C	-2.581314	0.879035	1.210631
H	-2.375803	0.245982	2.079456
H	-1.802852	1.643370	1.162821
C	-4.004221	1.498793	1.280415
H	-4.540103	1.131690	2.162651
H	-3.940784	2.589127	1.363858
H	-5.762800	1.566035	0.006970
C	-4.890534	-0.422170	-0.053831
H	-5.494804	-0.785389	0.784247
H	-5.396359	-0.720911	-0.978373
C	-3.463791	-1.030099	0.006042
H	-3.317755	-1.619371	0.916928
H	-3.270915	-1.684652	-0.850199
N	-2.433312	0.035528	-0.000856
C	6.074477	0.590811	0.004431
N	7.238223	0.603672	0.006986

B97D3-PCM-ACN_complex-Te-CN-Quin-same.out

Imaginary Frequency : -33.73
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	4.246485	1.080935	-0.000052
C	4.779227	-0.258991	0.010552
C	3.945586	-1.339090	0.012291
C	2.886728	1.319172	-0.009333
H	5.856902	-0.388877	0.017301
H	4.342909	-2.350095	0.020436
H	2.495030	2.331413	-0.017068
C	1.975789	0.218385	-0.007352
C	2.517880	-1.164855	0.003830
N	0.665248	0.405151	-0.013567
N	1.662622	-2.167910	0.006080
Te	-0.235740	-1.402243	-0.003980
C	-2.379062	0.973661	-1.230205
C	-4.488428	1.536283	0.008079
C	-3.664013	1.846418	-1.251809
H	-1.471477	1.580668	-1.246173
H	-2.342831	0.292749	-2.086223
H	-3.402530	2.910092	-1.274173
H	-4.255445	1.634511	-2.149188
C	-2.338298	1.019332	1.194163
H	-2.242020	0.374309	2.072987
H	-1.445475	1.645444	1.139877
C	-3.640351	1.864461	1.247460
H	-4.206745	1.639687	2.157917
H	-3.400292	2.933188	1.265182
H	-5.408625	2.128883	0.012386
C	-4.825758	0.036742	0.022769
H	-5.425072	-0.205438	0.906979
H	-5.421023	-0.222624	-0.859421
C	-3.495441	-0.766272	0.034337
H	-3.405468	-1.379883	0.936554
H	-3.422174	-1.433011	-0.831070
N	-2.325782	0.143235	-0.002591
C	5.155073	2.180332	-0.000038
N	5.906527	3.069027	0.000434

B97D3-PCM-ACN_complex-Te-F4-Br.out

C	-3.259244	1.232123	-0.000072
C	-3.684533	-0.133959	-0.000038
C	-2.774880	-1.154590	0.000014
C	-1.931249	1.560947	-0.000055
C	-0.926952	0.539338	0.000021
C	-1.366575	-0.880913	0.000059
N	0.364649	0.817546	-0.000044
N	-0.443050	-1.819951	0.000029
Te	1.385916	-0.924937	0.000266
Br	3.944023	0.801268	-0.000280
F	-4.209554	2.182688	-0.000163
F	-1.567903	2.858409	-0.000128
F	-5.006962	-0.377299	-0.000098
F	-3.204366	-2.431409	0.000003

B97D3-PCM-ACN_complex-Te-F4-Cl.out

C	2.893794	1.060751	0.000091
C	3.187462	-0.339388	0.000110
C	2.184905	-1.268982	-0.000018
C	1.602885	1.513549	-0.000069
C	0.505838	0.592424	-0.000164
C	0.808006	-0.864521	-0.000120
N	-0.752141	0.992797	-0.000478
N	-0.202619	-1.706849	-0.000384
Te	-1.945200	-0.639831	-0.000076
Cl	-4.099264	1.228509	0.000587
F	3.930392	1.917555	0.000152
F	1.364207	2.840500	-0.000162
F	4.481598	-0.707608	0.000192
F	2.493124	-2.581346	-0.000066

B97D3-PCM-ACN_complex-Te-F4-I.out

C	-3.609713	1.348881	-0.000138
C	-4.120819	0.012161	-0.000114
C	-3.278351	-1.064639	-0.000081
C	-2.263752	1.593222	-0.000124
C	-1.327114	0.509221	-0.000087
C	-1.855835	-0.880088	-0.000073
N	-0.020414	0.704259	-0.000046
N	-0.994988	-1.877607	-0.000023
Te	0.884849	-1.099056	-0.000016
I	3.770847	0.592135	0.000174
F	-4.497849	2.357124	-0.000162
F	-1.817518	2.864000	-0.000135
F	-5.455471	-0.146574	-0.000119
F	-3.787575	-2.311367	-0.000053

B97D3-PCM-ACN_complex-Te-F4-NO3.out

C	3.331235	1.147651	-0.000028
C	3.673929	-0.241898	0.000040
C	2.705710	-1.207200	0.000048
C	2.025764	1.555145	-0.000086
C	0.962245	0.594880	-0.000060
C	1.316106	-0.850421	0.000004
N	-0.309226	0.948232	-0.000130
N	0.336128	-1.730102	-0.000035
Te	-1.430839	-0.730192	0.000020
O	-3.231982	1.128061	0.000388
O	-5.381666	1.473066	0.000164
O	-4.619691	-0.572027	-0.000457
N	-4.435190	0.665267	0.000052
F	4.337159	2.039119	-0.000053
F	1.739183	2.871770	-0.000173
F	4.979442	-0.563327	0.000076
F	3.059595	-2.507068	0.000090

B97D3-PCM-ACN_complex-Te-F4-Quin.out

Imaginary Frequency : -29.94
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.720082	1.529623	0.000000
C	4.366447	0.250752	-0.000000
C	3.640878	-0.906696	-0.000001
C	2.357294	1.635069	0.000000
C	1.535018	0.461119	0.000000
C	2.204551	-0.873400	-0.000000
N	0.221614	0.520837	0.000001
N	1.448911	-1.945084	-0.000000
Te	-0.519770	-1.363972	0.000001
C	-2.811102	0.828687	-1.213821
C	-4.979370	1.175785	-0.000001
C	-4.176114	1.568876	-1.249835
H	-1.968368	1.522431	-1.193558
H	-2.686123	0.173344	-2.081171
H	-4.021024	2.653040	-1.269486
H	-4.733627	1.299707	-2.153497
C	-2.811102	0.828689	1.213819
H	-2.686098	0.173354	2.081171
H	-1.968381	1.522449	1.193541
C	-4.176126	1.568854	1.249849
H	-4.733640	1.299648	2.153499
H	-4.021055	2.653019	1.269533
H	-5.948781	1.683897	-0.000001
C	-5.183208	-0.347659	-0.000015
H	-5.755824	-0.650039	0.883209
H	-5.755796	-0.650025	-0.883263
C	-3.788713	-1.030622	0.000002
H	-3.650672	-1.660789	0.884413
H	-3.650659	-1.660808	-0.884394
N	-2.703516	-0.019510	0.000000
F	4.501579	2.622321	0.000000
F	1.782634	2.854007	0.000001
F	5.710453	0.232766	-0.000001
F	4.277312	-2.093630	-0.000001

B97D3-PCM-ACN_donor-Te-CN.out

C	-2.635784	1.353481	0.000003
C	-2.866552	-0.067936	0.000003
C	-1.822344	-0.970952	0.000004
C	-1.366546	1.856250	0.000004
H	-3.493026	2.018949	0.000004
H	-2.002282	-2.040749	0.000007
H	-1.187967	2.926954	0.000006
C	-0.239911	0.969621	0.000004
C	-0.480057	-0.488735	0.000004
N	1.012300	1.418747	0.000012
N	0.561634	-1.321280	0.000012
Te	2.203637	-0.188245	-0.000007
C	-4.211638	-0.544305	0.000004
N	-5.312345	-0.920461	0.000004

B97D3-PCM-ACN_donor-Te-F4.out

C	-0.000001	-2.563569	0.715835
C	-0.000001	-2.563569	-0.715835
C	-0.000001	-1.393940	-1.425168
C	-0.000001	-1.393940	1.425168
C	-0.000001	-0.136017	0.741655
C	-0.000001	-0.136017	-0.741655
N	-0.000001	1.022631	1.384593
N	-0.000001	1.022631	-1.384593
Te	0.000002	2.459938	-0.000000
F	-0.000001	-1.422316	2.767715
F	-0.000002	-3.750535	1.338271
F	-0.000002	-3.750535	-1.338271
F	-0.000001	-1.422316	-2.767715

B97D3-PCM-THF_complex-Te-CN-Br-opp.out

C	-3.428759	1.637581	-0.000108
C	-3.944957	0.293092	0.000056
C	-3.101699	-0.802252	0.000060
C	-2.082568	1.868102	-0.000293
H	-4.132196	2.464554	-0.000057
H	-3.497793	-1.812949	0.000196
H	-1.688021	2.880094	-0.000376
C	-1.155405	0.771700	-0.000321
C	-1.686161	-0.611297	-0.000125
N	0.154425	0.966473	-0.000328
N	-0.822905	-1.617879	-0.000186
Te	1.058150	-0.841538	-0.000057
Br	3.688814	0.729534	0.000186
C	-5.357638	0.100686	0.000254
N	-6.513110	-0.041605	0.000450

B97D3-PCM-THF_complex-Te-CN-Cl-opp.out

C	3.037833	1.529631	0.000054
C	3.454196	0.151085	0.000026
C	2.531687	-0.878795	-0.000062
C	1.711738	1.857884	0.000005
H	3.799579	2.303314	0.000059
H	2.852832	-1.915969	-0.000157
H	1.393840	2.896720	-0.000046
C	0.705357	0.833247	-0.000020
C	1.133558	-0.585620	-0.000061
N	-0.586104	1.124037	-0.000355
N	0.197671	-1.523520	-0.000341
Te	-1.627299	-0.612476	-0.000002
Cl	-3.951577	1.024065	0.000341
C	4.848571	-0.145450	-0.000009
N	5.990211	-0.374272	-0.000041

B97D3-PCM-THF_complex-Te-CN-I-opp.out

C	-3.812306	1.716349	0.000002
C	-4.392597	0.398141	-0.000018
C	-3.603402	-0.736343	-0.000085
C	-2.456772	1.882229	0.000019
H	-4.475150	2.576111	0.000026
H	-4.046889	-1.727043	-0.000099
H	-2.014209	2.873936	0.000040
C	-1.583483	0.742650	0.000077
C	-2.180548	-0.612396	-0.000097
N	-0.265176	0.873634	0.000028
N	-1.369483	-1.662059	-0.000080
Te	0.544361	-0.977417	0.000041
I	3.500745	0.553912	-0.000022
C	-5.812936	0.272807	0.000007
N	-6.973588	0.183385	0.000004

B97D3-PCM-THF_complex-Te-CN-Br-same.out

C	-3.740520	0.623851	-0.000078
C	-3.980507	-0.796276	-0.000126
C	-2.937541	-1.677914	-0.000144
C	-2.457726	1.139149	-0.000018
H	-5.007146	-1.149545	-0.000198
H	-3.112685	-2.750104	-0.000229
H	-2.285351	2.210575	-0.000044
C	-1.338565	0.253618	0.000057
C	-1.579927	-1.207943	-0.000050
N	-0.092211	0.714391	-0.000109
N	-0.532539	-2.014368	-0.000147
Te	1.155669	-0.867680	0.000160
Br	3.443772	1.180968	-0.000047
C	-4.859366	1.508536	-0.000147
N	-5.783352	2.216608	-0.000200

B97D3-PCM-THF_complex-Te-CN-Cl-same.out

C	3.333766	0.380086	-0.000069
C	3.394981	-1.058606	-0.000114
C	2.249632	-1.803123	-0.000059
C	2.124891	1.051276	-0.000044
H	4.369602	-1.537259	-0.000174
H	2.290985	-2.888995	-0.000090
H	2.087264	2.136217	0.000020
C	0.903626	0.312472	-0.000115
C	0.959879	-1.168922	-0.000014
N	-0.274742	0.925396	0.000054
N	-0.181108	-1.834302	-0.000013
Te	-1.718731	-0.482230	-0.000024
Cl	-3.541066	1.692437	0.000246
C	4.553065	1.118911	-0.000041
N	5.556597	1.709195	-0.000036

B97D3-PCM-THF_complex-Te-CN-I-same.out

C	-4.108741	0.812684	0.000031
C	-4.472142	-0.581092	0.000160
C	-3.511105	-1.551326	0.000188
C	-2.786393	1.214064	-0.000084
H	-5.525682	-0.843235	0.000244
H	-3.779963	-2.603919	0.000288
H	-2.519665	2.266117	-0.000208
C	-1.749467	0.232818	-0.000076
C	-2.117770	-1.201439	0.000122
N	-0.467262	0.581836	-0.000187
N	-1.146848	-2.099775	0.000080
Te	0.633181	-1.105575	-0.000088
I	3.312792	0.885863	0.000063
C	-5.145919	1.791373	-0.000015
N	-6.004300	2.577610	-0.000041

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B97D3-PCM-THF_complex-Te-CN-NO3-opp.out
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C	3.548648	1.563565	-0.000105
C	3.973471	0.187174	-0.000099
C	3.058773	-0.848402	-0.000026
C	2.221083	1.884765	-0.000035
H	4.306319	2.341132	-0.000149
H	3.384949	-1.883845	-0.000005
H	1.897295	2.921675	-0.000019
C	1.220817	0.853880	0.000035
C	1.659513	-0.561585	0.000031
N	-0.074052	1.133145	0.000170
N	0.731719	-1.509141	0.000161
Te	-1.085722	-0.617351	0.000087
O	-3.051779	1.084573	0.000014
O	-5.226183	1.200766	-0.000219
O	-4.251879	-0.752636	-0.000188
N	-4.199712	0.498502	-0.000014
C	5.369953	-0.101224	-0.000150
N	6.512642	-0.323560	-0.000194

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B97D3-PCM-THF_complex-Te-CN-NO3-same.out
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C	3.808054	0.570723	0.006180
C	3.976247	-0.859973	0.010942
C	2.890387	-1.688041	0.008472
C	2.553711	1.150651	-0.001607
H	4.983741	-1.264468	0.016693
H	3.011163	-2.767664	0.012164
H	2.435164	2.229500	-0.005188
C	1.390453	0.322622	-0.004972
C	1.558680	-1.149652	0.001124
N	0.168377	0.843389	-0.012883
N	0.471344	-1.902403	-0.000175
Te	-1.150732	-0.679654	-0.011004
O	-2.762431	1.365939	-0.041203
O	-4.871383	1.905524	0.006460
O	-4.296852	-0.199277	0.069570
N	-4.001609	1.016336	0.012657
C	4.970246	1.397095	0.009908
N	5.928553	2.057908	0.013211

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B97D3-PCM-THF_complex-Te-CN-Quin-opp.out
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Imaginary Frequency : -29.19
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.948993	1.856956	-0.004932
C	4.645792	0.594291	0.001968
C	3.963293	-0.604683	0.004595
C	2.585380	1.903366	-0.008705
H	4.533570	2.771668	-0.007029
H	4.493341	-1.551896	0.009828
H	2.059337	2.853626	-0.013855
C	1.814329	0.690591	-0.005731
C	2.532530	-0.610570	0.000563
N	0.494265	0.700421	-0.008490
N	1.820164	-1.722877	0.002466
Te	-0.156075	-1.219156	-0.002748
C	-2.590232	0.873515	-1.214327
C	-4.767519	1.116405	0.006564
C	-3.965712	1.596202	-1.214093
H	-1.755805	1.577832	-1.225704
H	-2.483482	0.213757	-2.081225
H	-3.827845	2.682027	-1.165427
H	-4.514370	1.376287	-2.136445
C	-2.581224	0.875789	1.211066
H	-2.377155	0.240813	2.078977
H	-1.799329	1.636680	1.164437
C	-4.001957	1.500617	1.282956
H	-4.539215	1.134224	2.164751
H	-3.935083	2.590595	1.368878
H	-5.760685	1.576617	0.009801
C	-4.895548	-0.414732	-0.054659
H	-5.501814	-0.777195	0.782429
H	-5.402924	-0.710109	-0.979532
C	-3.470553	-1.027586	0.004247
H	-3.326447	-1.619163	0.914155
H	-3.280020	-1.682178	-0.852685
N	-2.436860	0.033743	-0.001277
C	6.072347	0.598541	0.006235
N	7.235905	0.615904	0.009739

==========
B97D3-PCM-THF_complex-Te-CN-Quin-same.out
==========

Imaginary Frequency : -28.59
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	4.239596	1.087739	-0.000254
C	4.775839	-0.250998	0.013178
C	3.945875	-1.333671	0.015227
C	2.879533	1.321817	-0.012322
H	5.854008	-0.377116	0.021896
H	4.344878	-2.343908	0.025569
H	2.484692	2.332786	-0.022114
C	1.971351	0.218416	-0.009898
C	2.517681	-1.163576	0.004459
N	0.660687	0.401641	-0.017691
N	1.666733	-2.169948	0.007528
Te	-0.231698	-1.410869	-0.004769
C	-2.384903	0.960489	-1.236518
C	-4.483835	1.545217	0.009269
C	-3.662659	1.843971	-1.255646
H	-1.471717	1.558584	-1.265819
H	-2.361470	0.271674	-2.086862
H	-3.392874	2.905494	-1.282933
H	-4.260050	1.634700	-2.149767
C	-2.328979	1.027189	1.186163
H	-2.225888	0.389864	2.070003
H	-1.434713	1.649883	1.118822
C	-3.628810	1.875654	1.243384
H	-4.191724	1.655900	2.157326
H	-3.386431	2.943944	1.256750
H	-5.400982	2.142574	0.013945
C	-4.828809	0.047324	0.033826
H	-5.429286	-0.186264	0.919633
H	-5.426442	-0.214506	-0.846139
C	-3.502009	-0.761832	0.049801
H	-3.411263	-1.365384	0.958899
H	-3.435472	-1.439978	-0.807477
N	-2.328661	0.140585	-0.002468
C	5.145791	2.189527	0.000234
N	5.895397	3.079628	0.001317

==========
B97D3-PCM-THF_complex-Te-F4-Br.out
==========

C	-3.266940	1.219515	-0.000052
C	-3.683583	-0.148723	0.000041
C	-2.767152	-1.163494	0.000097
C	-1.940822	1.557370	-0.000115
C	-0.928781	0.542654	-0.000101
C	-1.360081	-0.881288	0.000056
N	0.360408	0.830451	-0.000106
N	-0.430787	-1.813324	0.000063
Te	1.397064	-0.905078	-0.000049
Br	3.931842	0.787966	0.000094
F	-4.224415	2.164966	-0.000087
F	-1.589030	2.857737	-0.000201
F	-5.005941	-0.400853	0.000098
F	-3.190055	-2.443058	0.000189

==========
B97D3-PCM-THF_complex-Te-F4-Cl.out
==========

C	2.897700	1.053383	0.000083
C	3.186922	-0.347133	0.000061
C	2.180980	-1.273439	0.000084
C	1.607974	1.510802	0.000099
C	0.507021	0.593706	0.000245
C	0.804834	-0.865161	0.000192
N	-0.748775	0.999742	0.000049
N	-0.208417	-1.703108	0.000175
Te	-1.951708	-0.627169	0.000014
Cl	-4.086373	1.208635	-0.000242
F	3.938158	1.907901	-0.000087
F	1.376490	2.838705	-0.000094
F	4.481375	-0.720101	-0.000074
F	2.486745	-2.586885	-0.000052

==========
B97D3-PCM-THF_complex-Te-F4-I.out
==========

C	-3.616920	1.333953	-0.000118
C	-4.117791	-0.006194	-0.000097
C	-3.267184	-1.076784	-0.000016
C	-2.272589	1.588881	-0.000037
C	-1.327002	0.511895	0.000042
C	-1.845513	-0.882539	-0.000020
N	-0.022779	0.718266	0.000643
N	-0.977010	-1.872061	0.000362
Te	0.902404	-1.076793	0.000107
I	3.753179	0.584449	-0.000240
F	-4.514069	2.336025	-0.000033
F	-1.838070	2.863540	0.000118
F	-5.452691	-0.174842	-0.000028
F	-3.768832	-2.327080	0.000119

==========
B97D3-PCM-THF_complex-Te-F4-NO3.out
==========

C	3.335023	1.139709	0.000226
C	3.672170	-0.251048	0.000234
C	2.700424	-1.213195	0.000076
C	2.030994	1.552526	0.000067
C	0.963697	0.595804	-0.000065
C	1.311614	-0.851599	-0.000080
N	-0.305466	0.955133	-0.000198
N	0.327836	-1.726289	-0.000284
Te	-1.437338	-0.716223	-0.000283
O	-3.226651	1.130008	0.000368
O	-5.379834	1.451939	0.000653
O	-4.597446	-0.585350	-0.000278
N	-4.427011	0.654369	0.000246
F	4.345597	2.027793	0.000365
F	1.750096	2.870014	0.000045
F	4.977803	-0.577487	0.000378
F	3.051169	-2.514189	0.000064

==========
B97D3-PCM-THF_complex-Te-F4-Quin.out
==========

Imaginary Frequency : -33.96
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis
Imaginary Frequency : -12.64
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	3.714410	1.533637	0.000008
C	4.363810	0.255721	-0.000081
C	3.641205	-0.903718	-0.000085
C	2.351365	1.637233	0.000103
C	1.531569	0.461280	0.000120
C	2.204466	-0.872340	0.000015
N	0.218206	0.518297	0.000168
N	1.452282	-1.946074	0.000013
Te	-0.514783	-1.370434	0.000082
C	-2.810348	0.826817	-1.213511
C	-4.977763	1.180774	-0.000128
C	-4.170624	1.576172	-1.246852
H	-1.962308	1.514103	-1.196059
H	-2.691654	0.170079	-2.080863
H	-4.008975	2.659512	-1.259884
H	-4.729123	1.316794	-2.152874
C	-2.810247	0.827213	1.213192
H	-2.681962	0.172745	2.080884
H	-1.967335	1.520624	1.190150
C	-4.175738	1.566692	1.252859
H	-4.734510	1.292325	2.154313
H	-4.021414	2.650814	1.279678
H	-5.945772	1.691653	-0.000159
C	-5.186076	-0.342208	-0.006324
H	-5.765639	-0.646057	0.871944
H	-5.754536	-0.639914	-0.893936
C	-3.793039	-1.028688	0.000232
H	-3.659057	-1.656449	0.887194
H	-3.654070	-1.663197	-0.881165
N	-2.705682	-0.021425	-0.000027
F	4.493875	2.627367	-0.000021
F	1.774641	2.854534	0.000165
F	5.707490	0.241440	-0.000169
F	4.278827	-2.088627	-0.000179

==========
B97D3-PCM-THF_donor-Te-CN.out
==========

C	-2.634749	1.352870	0.000003
C	-2.866194	-0.068775	0.000003
C	-1.822158	-0.971379	0.000005
C	-1.365968	1.856191	0.000004
H	-3.492414	2.017911	0.000004
H	-2.001618	-2.041234	0.000007
H	-1.186658	2.926741	0.000007
C	-0.239011	0.969659	0.000004
C	-0.479416	-0.489287	0.000005
N	1.012396	1.419666	0.000013
N	0.561244	-1.322288	0.000012
Te	2.203343	-0.188201	-0.000008
C	-4.211941	-0.544150	0.000004
N	-5.313143	-0.918483	0.000005

==========
B97D3-PCM-THF_donor-Te-F4.out
==========

C	-0.000001	-2.562944	0.716112
C	-0.000001	-2.562944	-0.716112
C	-0.000001	-1.393565	-1.426121
C	-0.000001	-1.393565	1.426121
C	-0.000001	-0.135476	0.742143
C	-0.000001	-0.135476	-0.742143
N	-0.000001	1.022480	1.385722
N	-0.000001	1.022480	-1.385722
Te	0.000002	2.459198	-0.000000
F	-0.000001	-1.421888	2.767792
F	-0.000002	-3.749733	1.337757
F	-0.000002	-3.749733	-1.337757
F	-0.000001	-1.421888	-2.767792

5.4.3.1.3 CPCM

==========
B97D3-CPCM-ACN_acceptor-NO3.out
==========

O	0.710699	1.042602	0.000002
O	-1.258382	0.094028	0.000025
O	0.547758	-1.136730	-0.000043
N	-0.000086	0.000114	0.000017

==========
B97D3-CPCM-ACN_acceptor-quin.out
==========

C	-0.797114	0.576497	-1.261616
C	1.291396	0.000285	-0.000477
C	0.761045	0.598915	-1.314462
H	-1.207590	-0.018176	-2.085765
H	-1.205620	1.589728	-1.349540
H	1.130466	0.015318	-2.166278
H	1.132248	1.623802	-1.434437
C	-0.795635	-1.381784	0.131587
H	-1.206075	-1.799400	1.058083
H	-1.203441	-1.964629	-0.702316
C	0.762417	-1.437174	0.138801
H	1.132519	-1.882528	1.070151
H	1.134301	-2.053913	-0.688290
H	2.386822	0.000692	-0.000889
C	0.761986	0.839395	1.174797
H	1.134611	0.431869	2.122212
H	1.131014	1.868913	1.093745
C	-0.796248	0.804405	1.130895
H	-1.203782	0.374333	2.052971
H	-1.207028	1.815310	1.028015
N	-1.296504	-0.000651	0.000741

==========
B97D3-CPCM-ACN_complex-Te-diBr-Br.out
==========

C	2.425176	2.193785	-0.000039
C	3.285247	1.055905	-0.000050
C	2.770614	-0.211111	0.000039
C	1.065177	2.047202	0.000046
H	2.870655	3.183081	-0.000106
H	4.358528	1.214408	-0.000127
C	0.452837	0.747398	0.000124
C	1.351007	-0.446504	0.000149
N	-0.854730	0.564650	0.000197
N	0.791941	-1.638344	0.000242
Te	-1.226443	-1.414064	0.000283
Br	-4.217587	-0.618910	-0.000609
Br	3.954203	-1.715386	0.000002
Br	-0.054187	3.600857	0.000059

==========
B97D3-CPCM-ACN_complex-Te-diBr-Cl.out
==========

C	1.634066	2.436681	0.000285
C	2.668861	1.454947	0.000179
C	2.367726	0.120940	0.000042
C	0.316548	2.068827	0.000277
H	1.911792	3.485475	0.000361
H	3.701529	1.787529	0.000189
C	-0.075838	0.686783	0.000205
C	1.006036	-0.345228	0.000016
N	-1.334889	0.292297	0.000083
N	0.644734	-1.609511	-0.000086
Te	-1.388739	-1.721856	-0.000163
Cl	-4.240193	-1.406340	-0.000454
Br	-1.041080	3.421494	0.000362
Br	3.784254	-1.168520	-0.000087

==========
B97D3-CPCM-ACN_complex-Te-diBr-I.out
==========

C	2.877676	2.141862	-0.000016
C	3.705317	0.979864	-0.000063
C	3.156208	-0.272510	-0.000003
C	1.514278	2.034186	0.000091
H	3.351342	3.117988	-0.000029
H	4.782589	1.108487	-0.000115
C	0.866853	0.751364	0.000126
C	1.730476	-0.466632	0.000069
N	-0.445239	0.604975	0.000356
N	1.140264	-1.644119	0.000228
Te	-0.869323	-1.361895	0.000113
I	-4.085762	-0.384484	-0.000365
Br	0.437128	3.616129	0.000236
Br	4.295620	-1.809416	0.000000

==========
B97D3-CPCM-ACN_complex-Te-diBr-NO3.out
==========

C	2.676353	1.938208	0.000038
C	3.374156	0.694026	-0.000003
C	2.692785	-0.491400	-0.000029
C	1.309390	1.977889	0.000050
H	3.252482	2.857518	0.000057
H	4.458998	0.706211	-0.000015
C	0.524945	0.773411	0.000025
C	1.254481	-0.532254	-0.000016
N	-0.794327	0.767519	0.000040
N	0.537450	-1.636022	-0.000034
Te	-1.426410	-1.143992	-0.000021
O	-3.666100	0.173556	-0.000030
O	-5.831601	-0.048814	0.000022
O	-4.566893	-1.827382	0.000052
N	-4.707729	-0.584301	0.000023
Br	0.414437	3.671051	0.000097
Br	3.663797	-2.140898	-0.000094

==========
B97D3-CPCM-ACN_complex-Te-diBr-quin.out
==========

Imaginary Frequency : -34.35
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis
Imaginary Frequency : -31.03
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	-2.976797	2.251991	-0.000230
C	-3.888761	1.152773	-0.000356
C	-3.435085	-0.136034	-0.000209
C	-1.626357	2.043777	0.000059
H	-3.377993	3.260003	-0.000386
H	-4.953279	1.362279	-0.000584
C	-1.072869	0.716849	0.000239
C	-2.026256	-0.441119	0.000102
N	0.218878	0.475639	0.000446
N	-1.519550	-1.650261	0.000269
Te	0.523786	-1.519545	0.000540
C	3.233202	0.142061	1.212725
C	5.426549	0.037401	-0.000827
C	4.722772	0.580437	1.252891
H	2.554426	0.996786	1.187926
H	2.971024	-0.470212	2.081055
H	4.797591	1.672942	1.280863
H	5.211745	0.193888	2.153700
C	3.232910	0.139941	-1.214002
H	2.982423	-0.479097	-2.080999
H	2.545704	0.988101	-1.197619
C	4.718377	0.592636	-1.246693
H	5.210865	0.224496	-2.153240
H	4.783437	1.686105	-1.257704
H	6.479456	0.336435	-0.001208
C	5.314309	-1.495577	-0.008144
H	5.806546	-1.903580	-0.897426
H	5.819691	-1.913622	0.868977
C	3.809351	-1.878669	0.001142
H	3.541248	-2.471683	-0.879103
H	3.549932	-2.463049	0.889692
N	2.954132	-0.667409	0.000104
Br	-0.433381	3.543132	0.000175
Br	-4.690104	-1.581648	-0.000402

==========
B97D3-CPCM-ACN_complex-Te-nat-Br.out
==========

C	3.947183	1.664229	-0.000078
C	4.479674	0.334936	-0.000465
C	3.657603	-0.760491	-0.000463
C	2.596588	1.892009	0.000303
H	4.636134	2.505332	-0.000073
H	5.558790	0.202474	-0.000739
H	4.058949	-1.770621	-0.000734
H	2.191302	2.900369	0.000611
C	1.681866	0.785267	0.000272
C	2.231209	-0.591956	-0.000107
N	0.366574	0.962793	0.000660
N	1.381449	-1.608964	-0.000012
Te	-0.506042	-0.858402	0.000153
Br	-3.255196	0.725103	-0.000237

==========
B97D3-CPCM-ACN_complex-Te-nat-Cl.out
==========

C	-3.635536	1.361381	0.000049
C	-4.006129	-0.021686	0.000060
C	-3.058770	-1.010917	0.000111
C	-2.321186	1.747508	0.000097
H	-4.419415	2.114902	0.000027
H	-5.061851	-0.281893	0.000045
H	-3.337317	-2.061745	0.000143
H	-2.039458	2.797251	0.000119
C	-1.280164	0.758201	0.000140
C	-1.661804	-0.675206	0.000133
N	0.003666	1.092040	0.000273
N	-0.695850	-1.580841	0.000261
Te	1.095312	-0.612211	0.000021
Cl	3.442861	1.160729	-0.000511

B97D3-CPCM-ACN_complex-Te-nat-I.out

C	-4.287666	1.842447	0.000043
C	-4.908913	0.552181	-0.000029
C	-4.163783	-0.596703	0.000054
C	-2.924995	1.978487	0.000196
H	-4.918295	2.727999	0.000014
H	-5.994483	0.493046	-0.000116
H	-4.632703	-1.577142	0.000042
H	-2.452172	2.956851	0.000296
C	-2.088047	0.811965	0.000249
C	-2.729452	-0.524155	0.000171
N	-0.763279	0.898963	0.000520
N	-1.953352	-1.599223	0.000373
Te	-0.021921	-0.977841	0.000202
I	3.108889	0.504971	-0.000398

B97D3-CPCM-ACN_complex-Te-nat-NO3.out

C	4.106046	1.471207	0.000107
C	4.519078	0.099961	0.000094
C	3.603540	-0.918479	0.000040
C	2.780819	1.817147	0.000065
H	4.866725	2.248080	0.000146
H	5.582348	-0.127114	0.000124
H	3.914709	-1.959968	0.000026
H	2.466773	2.857600	0.000066
C	1.771045	0.795829	0.000014
C	2.197491	-0.624844	0.000000
N	0.476631	1.087538	-0.000067
N	1.260480	-1.562086	-0.000061
Te	-0.549649	-0.652918	-0.000094
O	-2.537845	1.128474	-0.000066
O	-4.707139	1.323305	0.000133
O	-3.801817	-0.663096	0.000273
N	-3.700326	0.585794	0.000112

B97D3-CPCM-ACN_complex-Te-nat-quin.out

Imaginary Frequency : -14.56
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	4.340853	2.108790	0.000190
C	5.100847	0.893281	-0.001320
C	4.486176	-0.329195	-0.001770
C	2.972257	2.095450	0.001201
H	4.871304	3.057905	0.000529
H	6.186376	0.954813	-0.002094
H	5.060162	-1.252339	-0.002890
H	2.397058	3.017628	0.002342
C	2.264085	0.844718	0.000732
C	3.050603	-0.418834	-0.000707
N	0.943443	0.787467	0.001586
N	2.393959	-1.563557	-0.000900
Te	0.387449	-1.162981	0.000600
C	-2.148782	0.809717	-1.212807
C	-4.340064	0.958192	-0.001301
C	-3.574499	1.426862	-1.249221
H	-1.370276	1.575341	-1.196262
H	-1.967790	0.166842	-2.080016
H	-3.517727	2.520894	-1.264429
H	-4.105738	1.112280	-2.154281
C	-2.149111	0.813301	1.211302
H	-1.959897	0.175640	2.080586
H	-1.375843	1.584031	1.187849
C	-3.578767	1.421140	1.251354
H	-4.109257	1.095233	2.152864
H	-3.528720	2.515293	1.276347
H	-5.352168	1.375435	-0.002066
C	-4.403196	-0.577648	-0.004907
H	-4.951011	-0.932731	0.874647
H	-4.941348	-0.928610	-0.892071
C	-2.950748	-1.127042	0.002016
H	-2.757855	-1.738416	0.889528
H	-2.752379	-1.746399	-0.878757
N	-1.964572	-0.022518	0.000519

B97D3-CPCM-ACN_donor-Te-diBr.out

C	-0.712835	-2.489154	0.000002
C	0.712813	-2.489160	0.000002
C	1.419226	-1.317906	0.000016
C	-1.419238	-1.317894	0.000016
H	-1.231718	-3.441852	0.000010
H	1.231686	-3.441864	0.000010
C	-0.744261	-0.050053	0.000014
C	0.744260	-0.050060	0.000015
N	-1.381998	1.111763	0.000091
N	1.382005	1.111751	0.000090
Te	0.000011	2.545647	-0.000108
Br	-3.326717	-1.353835	0.000056
Br	3.326705	-1.353856	0.000056

B97D3-CPCM-ACN_donor-Te-nat.out

C	-3.351729	0.715859	0.000007
C	-3.351676	-0.715881	0.000007
C	-2.183970	-1.430741	-0.000000
C	-2.184060	1.430732	0.000001
H	-4.304355	1.239119	0.000008
H	-4.304269	-1.239218	0.000008
H	-2.180586	-2.516913	-0.000004
H	-2.180595	2.516922	-0.000004
C	-0.927223	0.740742	-0.000001
C	-0.927171	-0.740650	-0.000002
N	0.235971	1.388534	-0.000023
N	0.235948	-1.388648	-0.000021
Te	1.677334	0.000010	0.000004

B97D3-CPCM-THF_acceptor-NO3.out

O	0.630960	1.093022	0.000002
O	-1.262161	-0.000212	0.000025
O	0.631274	-1.092902	-0.000042
N	-0.000083	0.000105	0.000017

B97D3-CPCM-THF_acceptor-quin.out

C	-0.788729	-1.373068	0.224778
C	1.291948	0.006455	-0.003909
C	0.769907	-1.417061	0.255654
H	-1.208785	-1.738954	1.168719
H	-1.181006	-2.006485	-0.578995
H	1.130783	-1.774354	1.227759
H	1.155720	-2.103011	-0.508095
C	-0.797630	0.873658	1.076645
H	-1.227575	1.869500	0.919688
H	-1.186577	0.492342	2.027814
C	0.760393	0.937428	1.099072
H	1.111578	1.961292	0.922570
H	1.149490	0.621987	2.074574
H	2.387360	0.012240	-0.007308
C	0.754973	0.490867	-1.361714
H	1.133964	1.497187	-1.576805
H	1.111644	-0.170515	-2.160566
C	-0.803283	0.487866	-1.294509
H	-1.202828	1.498177	-1.439131
H	-1.227411	-0.149957	-2.078470
N	-1.295976	-0.006617	0.004592

B97D3-CPCM-THF_complex-Comp_Te-nat-I.out

C	-4.292816	1.823026	0.000027
C	-4.905051	0.528742	-0.000025
C	-4.151187	-0.614803	0.000025
C	-2.930787	1.967749	0.000128
H	-4.929227	2.704677	0.000005
H	-5.990383	0.461663	-0.000088
H	-4.612693	-1.598926	0.000007
H	-2.463614	2.948897	0.000191
C	-2.085258	0.807324	0.000164
C	-2.717180	-0.533375	0.000108
N	-0.761779	0.905336	0.000327
N	-1.933024	-1.601804	0.000216
Te	-0.002190	-0.964957	0.000166
I	3.084285	0.503108	-0.000285

B97D3-CPCM-THF_complex-Te-diBr-Cl.out

C	1.643115	2.431555	0.000272
C	2.673893	1.445980	0.000256
C	2.366580	0.113126	0.000113
C	0.324000	2.068256	0.000132
H	1.923696	3.479653	0.000419
H	3.708297	1.773383	0.000371
C	-0.074642	0.688050	-0.000069
C	1.003634	-0.349221	-0.000053
N	-1.335044	0.300000	-0.000149
N	0.636295	-1.610818	-0.000187
Te	-1.402709	-1.714853	-0.000328
Cl	-4.220495	-1.405767	0.000096
Br	-1.027626	3.427650	0.000253
Br	3.779884	-1.181747	0.000121

B97D3-CPCM-THF_complex-Te-diBr-I.out

C	2.888250	2.129087	0.000045
C	3.707531	0.961521	0.000111
C	3.148667	-0.286764	-0.000003
C	1.523834	2.030713	-0.000134
H	3.367759	3.102427	0.000089
H	4.785901	1.081336	0.000208
C	0.866554	0.752804	-0.000217
C	1.721782	-0.472195	-0.000139
N	-0.446136	0.617187	-0.000569
N	1.122461	-1.644091	-0.000391
Te	-0.889998	-1.346787	-0.000270
I	-4.067643	-0.382863	0.000651
Br	0.459218	3.621348	-0.000332
Br	4.278992	-1.831684	-0.000010

B97D3-CPCM-THF_complex-Te-diBr-Br.out

C	2.433891	2.185189	-0.000013
C	3.288221	1.043286	-0.000015
C	2.766433	-0.221066	0.000034
C	1.072909	2.044859	0.000031
H	2.883170	3.172841	-0.000055
H	4.362513	1.195388	-0.000046
C	0.453510	0.748420	0.000071
C	1.345939	-0.450774	0.000090
N	-0.854595	0.573517	0.000116
N	0.780074	-1.638503	0.000145
Te	-1.241752	-1.403084	0.000141
Br	-4.200892	-0.617815	-0.000362
Br	3.944061	-1.731461	0.000039
Br	-0.037979	3.604921	0.000031

B97D3-CPCM-THF_complex-Te-diBr-NO3.out

C	2.688170	1.924290	0.000037
C	3.377265	0.675516	-0.000000
C	2.687155	-0.505086	-0.000026
C	1.321235	1.973104	0.000046
H	3.269695	2.840252	0.000056
H	4.462231	0.679062	-0.000009
C	0.528167	0.774239	0.000020
C	1.248599	-0.536912	-0.000017
N	-0.790737	0.778348	0.000032
N	0.523702	-1.634913	-0.000036
Te	-1.439219	-1.127913	-0.000024
O	-3.660575	0.184770	-0.000006
O	-5.824450	-0.053101	0.000038
O	-4.547869	-1.823270	0.000029
N	-4.698839	-0.581199	0.000028
Br	0.438505	3.672766	0.000088
Br	3.648015	-2.161383	-0.000083

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B97D3-CPCM-THF_complex-Te-diBr-quin.out
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Imaginary Frequency : -33.71
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis
Imaginary Frequency : -29.73
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	2.966360	2.258436	-0.000007
C	3.882814	1.162850	-0.000011
C	3.435323	-0.128135	-0.000007
C	1.616699	2.045584	0.000002
H	3.363144	3.268246	-0.000012
H	4.946574	1.376328	-0.000019
C	1.069090	0.716220	0.000008
C	2.027349	-0.437882	0.000003
N	-0.221575	0.470072	0.000015
N	1.526632	-1.649398	0.000009
Te	-0.514635	-1.527061	0.000017
C	-3.229910	0.135970	-1.212905
C	-5.424049	0.040038	-0.000025
C	-4.715946	0.587010	-1.249695
H	-2.543314	0.984511	-1.192138
H	-2.975483	-0.480351	-2.080810
H	-4.782174	1.680311	-1.268948
H	-5.208402	0.212109	-2.153624
C	-3.229923	0.136016	1.212874
H	-2.975075	-0.480084	2.080813
H	-2.543629	0.984795	1.191828
C	-4.716108	0.586542	1.249942
H	-5.208442	0.210956	2.153654
H	-4.782687	1.679808	1.269831
H	-6.476008	0.342624	-0.000036
C	-5.317058	-1.493479	-0.000306
H	-5.817939	-1.905057	0.882572
H	-5.817465	-1.904677	-0.883631
C	-3.812985	-1.881180	0.000023
H	-3.551192	-2.471001	0.884452
H	-3.550881	-2.471289	-0.884123
N	-2.954145	-0.673524	0.000002
Br	0.417499	3.539239	0.000006
Br	4.694435	-1.568326	-0.000013

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B97D3-CPCM-THF_complex-Te-nat-Br.out
==========

C	3.956451	1.644664	-0.000093
C	4.479548	0.311988	-0.000412
C	3.649001	-0.777468	-0.000389
C	2.607046	1.881126	0.000241
H	4.650995	2.481435	-0.000083
H	5.557904	0.171595	-0.000637
H	4.042768	-1.790740	-0.000591
H	2.207682	2.891931	0.000523
C	1.684100	0.781165	0.000228
C	2.223511	-0.600065	-0.000093
N	0.370810	0.969763	0.000647
N	1.366027	-1.609795	0.000071
Te	-0.519887	-0.843436	0.000114
Br	-3.233744	0.718177	-0.000202

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B97D3-CPCM-THF_complex-Te-nat-Cl.out
==========

C	-3.640069	1.349595	0.000083
C	-4.005540	-0.034532	0.000111
C	-3.053740	-1.020000	0.000107
C	-2.326603	1.739766	0.000055
H	-4.426478	2.100793	0.000097
H	-5.060442	-0.299093	0.000145
H	-3.327848	-2.072167	0.000140
H	-2.047503	2.790305	0.000048
C	-1.281449	0.754772	0.000048
C	-1.657541	-0.680344	0.000066
N	0.000158	1.094999	0.000060
N	-0.687917	-1.581030	0.000094
Te	1.103356	-0.602567	-0.000058
Cl	3.417162	1.150606	-0.000079

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B97D3-CPCM-THF_complex-Te-nat-NO3.out
==========

C	4.111535	1.457131	-0.000058
C	4.517652	0.084072	-0.000176
C	3.596409	-0.929565	-0.000142
C	2.787655	1.809068	0.000091
H	4.875864	2.230671	-0.000059
H	5.579888	-0.148784	-0.000266
H	3.901666	-1.972933	-0.000202
H	2.477716	2.850818	0.000213
C	1.772399	0.793160	0.000100
C	2.191577	-0.629709	-0.000022
N	0.480126	1.092466	0.000338
N	1.249843	-1.561527	0.000089
Te	-0.557670	-0.641497	0.000057
O	-2.524511	1.126415	-0.000389
O	-4.694629	1.311337	-0.000210
O	-3.781287	-0.671421	0.000280
N	-3.686575	0.577991	-0.000265

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B97D3-CPCM-THF_complex-Te-nat-quin.out
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Imaginary Frequency : -14.36
Vibrational Mode : Quinuclidine rotation about Te-N(quin) axis

C	4.332211	2.116467	0.000184
C	5.096072	0.903342	-0.001350
C	4.485472	-0.320944	-0.001799
C	2.963812	2.099197	0.001227
H	4.859761	3.067255	0.000516
H	6.181430	0.968292	-0.002145
H	5.061434	-1.242735	-0.002936
H	2.385410	3.019319	0.002387
C	2.259535	0.846333	0.000757
C	3.050271	-0.414784	-0.000714
N	0.939207	0.785071	0.001637
N	2.398533	-1.562132	-0.000917
Te	0.393265	-1.168443	0.000606
C	-2.149565	0.807453	-1.212335
C	-4.340700	0.962318	-0.001304
C	-3.573685	1.428725	-1.249301
H	-1.368410	1.570372	-1.195638
H	-1.969904	0.164333	-2.079732
H	-3.514182	2.522663	-1.264744
H	-4.106078	1.115946	-2.154427
C	-2.149904	0.810986	1.210852
H	-1.962309	0.172930	2.080289
H	-1.373774	1.578839	1.187458
C	-3.577850	1.423288	1.251257
H	-4.109574	1.099620	2.152966
H	-3.524850	2.517363	1.276087
H	-5.351722	1.382360	-0.002066
C	-4.408040	-0.573513	-0.004753
H	-4.957110	-0.926982	0.874785
H	-4.947719	-0.923054	-0.891666
C	-2.956725	-1.126497	0.001979
H	-2.765388	-1.738866	0.889268
H	-2.760084	-1.746663	-0.878739
N	-1.968049	-0.025253	0.000514

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B97D3-CPCM-THF_donor-Te-diBr.out
==========

C	-0.712893	-2.488409	0.000002
C	0.712870	-2.488416	0.000002
C	1.420169	-1.317713	0.000017
C	-1.420181	-1.317699	0.000016
H	-1.232158	-3.440951	0.000010
H	1.232124	-3.440964	0.000010
C	-0.744535	-0.049915	0.000015
C	0.744535	-0.049922	0.000016
N	-1.382816	1.111220	0.000095
N	1.382824	1.111208	0.000094
Te	0.000012	2.544682	-0.000112
Br	-3.326654	-1.353219	0.000058
Br	3.326642	-1.353241	0.000058

==========
B97D3-CPCM-THF_donor-Te-nat.out
==========

C	-3.350820	0.715915	0.000007
C	-3.350767	-0.715938	0.000007
C	-2.183380	-1.430912	-0.000000
C	-2.183469	1.430903	0.000000
H	-4.303508	1.239151	0.000008
H	-4.303422	-1.239249	0.000008
H	-2.179345	-2.517027	-0.000004
H	-2.179354	2.517036	-0.000004
C	-0.926507	0.740933	-0.000000
C	-0.926456	-0.740844	-0.000002
N	0.235917	1.389311	-0.000022
N	0.235896	-1.389422	-0.000020
Te	1.676756	0.000010	0.000004

==========
B97D3-CPCM-ACN_complex-Te-CN-Br-opp.out
==========

C	-3.429919	1.645205	-0.000047
C	-3.949149	0.301806	-0.000103
C	-3.110076	-0.795980	-0.000105
C	-2.083397	1.872849	0.000006
H	-4.130900	2.473999	-0.000048
H	-3.508806	-1.805490	-0.000148
H	-1.688339	2.884548	0.000048
C	-1.159736	0.773728	0.000001
C	-1.694395	-0.607008	-0.000056
N	0.152063	0.962372	0.000051
N	-0.834905	-1.617817	-0.000050
Te	1.042944	-0.850437	0.000009
Br	3.720934	0.732808	0.000108
C	-5.362374	0.112202	-0.000154
N	-6.517652	-0.029617	-0.000194

==========
B97D3-CPCM-ACN_complex-Te-CN-Br-same.out
==========

C	-3.739635	0.636410	-0.000120
C	-3.987727	-0.782341	-0.000143
C	-2.949690	-1.669639	-0.000118
C	-2.455469	1.146777	-0.000074
H	-5.015768	-1.130805	-0.000179
H	-3.131214	-2.740652	-0.000136
H	-2.278388	2.217500	-0.000058
C	-1.341281	0.254564	-0.000049
C	-1.590529	-1.205055	-0.000070
N	-0.091242	0.706901	-0.000005
N	-0.547128	-2.018696	-0.000046
Te	1.142569	-0.885098	0.000020
Br	3.468018	1.191729	0.000149
C	-4.853034	1.527451	-0.000147
N	-5.770872	2.243160	-0.000169

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B97D3-CPCM-ACN_complex-Te-CN-Cl-opp.out
==========

C	3.034054	1.535755	0.000075
C	3.453424	0.158044	0.000017
C	2.535279	-0.874924	-0.000028
C	1.707466	1.860769	0.000097
H	3.793517	2.311388	0.000103
H	2.859525	-1.910884	-0.000068
H	1.387959	2.898943	0.000138
C	0.704898	0.832793	0.000052
C	1.136658	-0.584075	-0.000032
N	-0.588548	1.118098	0.000069
N	0.203748	-1.526089	-0.000072
Te	-1.618800	-0.623223	-0.000062
Cl	-3.978172	1.042555	0.000112
C	4.848814	-0.134576	0.000010
N	5.990793	-0.360296	0.000002

B97D3-CPCM-ACN_complex-Te-CN-Cl-same.out

C	3.332839	0.387798	0.000014
C	3.398801	-1.050769	-0.000042
C	2.255950	-1.798604	-0.000046
C	2.123171	1.056547	0.000060
H	4.374390	-1.526887	-0.000070
H	2.300645	-2.884115	-0.000079
H	2.083517	2.141222	0.000107
C	0.904411	0.313647	0.000034
C	0.965701	-1.166495	-0.000008
N	-0.277436	0.921387	0.000110
N	-0.173563	-1.837172	0.000005
Te	-1.710739	-0.496070	-0.000018
Cl	-3.569132	1.714821	-0.000017
C	4.549577	1.131142	0.000026
N	5.549915	1.726337	0.000034

B97D3-CPCM-ACN_complex-Te-CN-I-opp.out

C	-3.808783	1.728179	-0.000136
C	-4.396548	0.413187	0.000027
C	-3.615871	-0.726474	0.000053
C	-2.452553	1.886464	-0.000227
H	-4.466102	2.591900	-0.000181
H	-4.065381	-1.714349	0.000176
H	-2.005723	2.876283	-0.000355
C	-1.587247	0.740963	-0.000109
C	-2.192435	-0.609673	-0.000036
N	-0.267101	0.860892	-0.000266
N	-1.388685	-1.665964	0.000055
Te	0.524206	-0.996081	-0.000102
I	3.527319	0.562435	0.000141
C	-5.817878	0.296620	0.000138
N	-6.978720	0.213321	0.000197

B97D3-CPCM-ACN_complex-Te-CN-I-same.out

C	-4.106004	0.832165	-0.000014
C	-4.481597	-0.558387	-0.000462
C	-3.529137	-1.536804	-0.000513
C	-2.781125	1.223489	0.000380
H	-5.536974	-0.812045	-0.000754
H	-3.807620	-2.586668	-0.000854
H	-2.506249	2.273272	0.000668
C	-1.753175	0.233048	0.000323
C	-2.133611	-1.197142	-0.000103
N	-0.466913	0.569329	0.000617
N	-1.170198	-2.105144	-0.000208
Te	0.612777	-1.129616	0.000187
I	3.336531	0.894233	-0.000167
C	-5.133875	1.820778	-0.000033
N	-5.982680	2.616996	-0.000044

B97D3-CPCM-ACN_complex-Te-CN-NO3-opp.out

C	3.541155	1.572503	0.000064
C	3.972518	0.198058	0.000120
C	3.064342	-0.842815	0.000053
C	2.212207	1.886813	-0.000061
H	4.294513	2.354009	0.000092
H	3.396654	-1.876108	0.000065
H	1.884070	2.922228	-0.000138
C	1.218270	0.850207	-0.000109
C	1.663772	-0.562521	-0.000046
N	-0.078771	1.121359	-0.000337
N	0.740837	-1.515528	-0.000220
Te	-1.078680	-0.634234	-0.000117
O	-3.057548	1.090899	0.000002
O	-5.230807	1.229525	0.000402
O	-4.275568	-0.733098	0.000347
N	-4.209009	0.517150	0.000082
C	5.370558	-0.082810	0.000210
N	6.514170	-0.299432	0.000286

B97D3-CPCM-ACN_complex-Te-CN-NO3-same.out

C	3.800271	0.583297	-0.000005
C	3.978959	-0.845993	0.000046
C	2.899101	-1.681683	0.000039
C	2.542933	1.155876	-0.000063
H	4.988828	-1.243908	0.000076
H	3.028434	-2.760256	0.000061
H	2.417972	2.234000	-0.000117
C	1.385852	0.319144	-0.000060
C	1.564353	-1.151251	-0.000004
N	0.159230	0.830216	-0.000172
N	0.481542	-1.911954	-0.000068
Te	-1.146220	-0.702794	-0.000013
O	-2.756052	1.371322	0.000082
O	-4.856430	1.945614	0.000159
O	-4.317188	-0.169279	0.000045
N	-3.999386	1.041467	0.000078
C	4.956051	1.418863	-0.000016
N	5.907248	2.089508	-0.000021

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B97D3-CPCM-ACN_complex-Te-CN-Quin-opp.out

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Imaginary Frequency : -28.53
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.954537	1.854687	-0.002506
C	4.648252	0.590616	0.000924
C	3.963567	-0.607635	0.002084
C	2.590798	1.902820	-0.004506
H	4.540105	2.768668	-0.003424
H	4.492775	-1.555385	0.004714
H	2.067040	2.854372	-0.007040
C	1.817866	0.691341	-0.003085
C	2.533010	-0.610952	0.000026
N	0.497572	0.703237	-0.004508
N	1.816966	-1.721351	0.001050
Te	-0.160643	-1.213007	-0.001346
C	-2.589125	0.872707	-1.215823
C	-4.767941	1.109358	0.003454
C	-3.967279	1.589829	-1.217562
H	-1.758344	1.581335	-1.227574
H	-2.479454	0.211732	-2.081261
H	-3.833234	2.676182	-1.170817
H	-4.514134	1.364995	-2.139689
C	-2.581645	0.879754	1.210394
H	-2.375716	0.247391	2.079601
H	-1.803764	1.644648	1.161963
C	-4.004949	1.498646	1.279778
H	-4.541049	1.130731	2.161549
H	-3.942116	2.588974	1.363753
H	-5.762700	1.566046	0.005193
C	-4.890318	-0.422137	-0.055425
H	-5.495722	-0.785565	0.781732
H	-5.394729	-0.720671	-0.980809
C	-3.463675	-1.030038	0.006455
H	-3.318542	-1.618177	0.918184
H	-3.270014	-1.685522	-0.848876
N	-2.433145	0.035628	-0.000630
C	6.074502	0.590802	0.003271
N	7.238243	0.603602	0.005218

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B97D3-CPCM-ACN_complex-Te-CN-Quin-same.out

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Imaginary Frequency : -38.12
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	4.246635	1.080771	-0.000011
C	4.779358	-0.259168	0.003329
C	3.945638	-1.339235	0.003877
C	2.886852	1.319108	-0.002936
H	5.857027	-0.389166	0.005456
H	4.343045	-2.350246	0.006444
H	2.495235	2.331403	-0.005372
C	1.975918	0.218337	-0.002322
C	2.517926	-1.164880	0.001229
N	0.665294	0.405095	-0.004295
N	1.662515	-2.167878	0.001952
Te	-0.235939	-1.402133	-0.001263
C	-2.364378	0.990465	-1.217736
C	-4.488386	1.536241	0.002787
C	-3.655493	1.853628	-1.249673
H	-1.461538	1.604543	-1.208266
H	-2.307131	0.322551	-2.082743
H	-3.401464	2.919137	-1.269463
H	-4.238175	1.637800	-2.151879
C	-2.352221	1.002951	1.207212
H	-2.276394	0.345058	2.078436
H	-1.454132	1.623216	1.177009
C	-3.648811	1.857249	1.249833
H	-4.224138	1.635800	2.155439
H	-3.401598	2.924326	1.270108
H	-5.408602	2.128839	0.004341
C	-4.825834	0.036668	0.006091
H	-5.424060	-0.211996	0.889281
H	-5.422198	-0.216005	-0.877260
C	-3.495630	-0.766655	0.009534
H	-3.411864	-1.399377	0.899077
H	-3.416578	-1.414764	-0.869338
N	-2.325676	0.143220	-0.001051
C	5.155190	2.180193	-0.000011
N	5.906551	3.068954	0.000131

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B97D3-CPCM-ACN_complex-Te-F4-Br.out

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C	-3.255595	1.234748	-0.000102
C	-3.683144	-0.130684	-0.000103
C	-2.775315	-1.152990	-0.000019
C	-1.927033	1.561059	-0.000010
C	-0.924866	0.537580	0.000095
C	-1.366553	-0.881891	0.000077
N	0.367069	0.813544	0.000187
N	-0.444298	-1.822212	0.000174
Te	1.385964	-0.929802	0.000301
Br	3.939021	0.805944	-0.000401
F	-4.204107	2.186982	-0.000191
F	-1.560633	2.857793	-0.000010
F	-5.005903	-0.371751	-0.000195
F	-3.207159	-2.429090	-0.000024

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B97D3-CPCM-ACN_complex-Te-F4-Cl.out

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C	2.893559	1.060818	0.000074
C	3.187238	-0.339360	-0.000029
C	2.184739	-1.268975	-0.000037
C	1.602665	1.513622	0.000174
C	0.505671	0.592487	0.000165
C	0.807852	-0.864614	0.000035
N	-0.752343	0.992548	0.000375
N	-0.202624	-1.707031	0.000157
Te	-1.945481	-0.640325	-0.000064
Cl	-4.097620	1.229948	-0.000289
F	3.930252	1.917416	0.000115
F	1.364114	2.840816	0.000317
F	4.481364	-0.707396	-0.000086
F	2.493046	-2.581360	-0.000099

B97D3-CPCM-ACN_complex-Te-F4-I.out

C	-3.608493	1.350790	-0.000192
C	-4.120955	0.014584	-0.000152
C	-3.279584	-1.063074	-0.000142
C	-2.262280	1.593549	-0.000233
C	-1.326798	0.508692	-0.000253
C	-1.856922	-0.880212	-0.000158
N	-0.019939	0.702017	-0.000384
N	-0.996986	-1.878471	-0.000226
Te	0.883267	-1.102008	-0.000247
I	3.772084	0.593353	0.000582
F	-4.495299	2.360080	-0.000223
F	-1.814565	2.863990	-0.000298
F	-5.455647	-0.142986	-0.000136
F	-3.790233	-2.309314	-0.000119

B97D3-CPCM-ACN_complex-Te-F4-NO3.out

C	3.331298	1.147783	-0.000060
C	3.674079	-0.241685	0.000000
C	2.705815	-1.206870	0.000031
C	2.025817	1.555214	-0.000091
C	0.962185	0.595117	-0.000047
C	1.316255	-0.850113	0.000015
N	-0.309449	0.948266	-0.000098
N	0.336442	-1.730001	0.000002
Te	-1.430612	-0.730795	0.000065
O	-3.232010	1.126883	0.000355
O	-5.381207	1.474943	0.000063
O	-4.621909	-0.571244	-0.000437
N	-4.435814	0.665709	0.000019
F	4.337104	2.039301	-0.000105
F	1.739522	2.871994	-0.000169
F	4.979538	-0.563158	0.000010
F	3.059600	-2.506782	0.000068

B97D3-CPCM-ACN_complex-Te-F4-Quin.out

Imaginary Frequency : -28.38
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.719405	1.530232	0.000000
C	4.366216	0.251648	-0.000000
C	3.641103	-0.906068	-0.000000
C	2.356597	1.634944	0.000000
C	1.534888	0.460649	0.000000
C	2.204795	-0.873567	-0.000000
N	0.221448	0.519905	0.000000
N	1.449396	-1.945528	0.000000
Te	-0.519653	-1.364882	0.000000
C	-2.810695	0.828279	-1.213841
C	-4.978666	1.177007	-0.000001
C	-4.175120	1.569528	-1.249819
H	-1.967523	1.521497	-1.193603
H	-2.686299	0.172824	-2.081174
H	-4.019157	2.653577	-1.269358
H	-4.732798	1.300787	-2.153501
C	-2.810695	0.828280	1.213840
H	-2.686299	0.172826	2.081174
H	-1.967524	1.521499	1.193603
C	-4.175121	1.569529	1.249818
H	-4.732799	1.300788	2.153499
H	-4.019158	2.653578	1.269356
H	-5.947699	1.685852	-0.000001
C	-5.183610	-0.346288	-0.000000
H	-5.756387	-0.648193	0.883283
H	-5.756386	-0.648194	-0.883283
C	-3.789645	-1.030355	0.000001
H	-3.652158	-1.660562	0.884438
H	-3.652158	-1.660563	-0.884437
N	-2.703628	-0.020004	0.000000
F	4.500391	2.623274	0.000000
F	1.781195	2.853605	0.000001
F	5.710215	0.234075	-0.000000
F	4.278319	-2.092662	-0.000000

B97D3-CPCM-ACN_donor-Te-CN.out

C	-2.635863	1.353511	0.000003
C	-2.866587	-0.067893	0.000003
C	-1.822373	-0.970918	0.000004
C	-1.366601	1.856257	0.000004
H	-3.493094	2.018977	0.000004
H	-2.002373	-2.040705	0.000006
H	-1.188101	2.926983	0.000006
C	-0.239982	0.969621	0.000004
C	-0.480112	-0.488690	0.000004
N	1.012286	1.418676	0.000012
N	0.561655	-1.321187	0.000012
Te	2.203673	-0.188249	-0.000007
C	-4.211636	-0.544319	0.000004
N	-5.312298	-0.920593	0.000004

B97D3-CPCM-ACN_donor-Te-F4.out

C	-0.000001	-2.563609	0.715814
C	-0.000001	-2.563609	-0.715814
C	-0.000001	-1.393972	-1.425087
C	-0.000001	-1.393972	1.425087
C	-0.000001	-0.136066	0.741619
C	-0.000001	-0.136066	-0.741619
N	-0.000001	1.022627	1.384505
N	-0.000001	1.022627	-1.384505
Te	0.000002	2.459986	-0.000000
F	-0.000001	-1.422340	2.767711
F	-0.000002	-3.750564	1.338341
F	-0.000002	-3.750564	-1.338341
F	-0.000001	-1.422340	-2.767711

B97D3-CPCM-THF_complex-Te-CN-Br-opp.out

C	-3.434901	1.637600	-0.000073
C	-3.949320	0.292472	-0.000089
C	-3.104648	-0.801667	-0.000057
C	-2.088952	1.870104	-0.000026
H	-4.139309	2.463667	-0.000091
H	-3.499236	-1.812932	-0.000065
H	-1.696762	2.883022	-0.000005
C	-1.160332	0.775040	0.000003
C	-1.689582	-0.608284	-0.000018
N	0.149841	0.970553	0.000061
N	-0.825488	-1.614417	0.000045
Te	1.053222	-0.837337	0.000039
Br	3.704307	0.722111	0.000027
C	-5.361676	0.097554	-0.000135
N	-6.516708	-0.048001	-0.000173

B97D3-CPCM-THF_complex-Te-CN-Cl-opp.out

C	3.037846	1.530457	0.000079
C	3.454412	0.152024	0.000012
C	2.532501	-0.878301	-0.000038
C	1.711655	1.858207	0.000102
H	3.799314	2.304314	0.000112
H	2.854033	-1.915246	-0.000082
H	1.393555	2.896919	0.000147
C	0.705919	0.833180	0.000033
C	1.134349	-0.585323	-0.000050
N	-0.585788	1.123236	0.000062
N	0.198747	-1.523741	-0.000107
Te	-1.625790	-0.613988	-0.000100
Cl	-3.957971	1.026402	0.000257
C	4.848966	-0.143803	0.000009
N	5.990727	-0.371792	0.000009

B97D3-CPCM-THF_complex-Te-CN-I-opp.out

C	-3.812783	1.718639	-0.000065
C	-4.394307	0.400962	0.000026
C	-3.606492	-0.734379	0.000031
C	-2.457112	1.883451	-0.000109
H	-4.474736	2.578993	-0.000079
H	-4.050882	-1.724698	0.000105
H	-2.014315	2.875180	-0.000166
C	-1.585230	0.742759	-0.000025
C	-2.183591	-0.611454	-0.000033
N	-0.266579	0.871238	-0.000099
N	-1.373708	-1.662260	0.000046
Te	0.539955	-0.980833	-0.000059
I	3.507537	0.555251	0.000061
C	-5.814885	0.277147	0.000094
N	-6.975546	0.188559	0.000120

B97D3-CPCM-THF_complex-Te-CN-Br-same.out

C	-3.741306	0.626070	0.000100
C	-3.982659	-0.793734	0.000541
C	-2.940252	-1.676275	0.000546
C	-2.458577	1.141197	-0.000328
H	-5.009391	-1.146501	0.000818
H	-3.116423	-2.748345	0.000819
H	-2.285426	2.212645	-0.000723
C	-1.340097	0.254433	-0.000286
C	-1.582537	-1.206798	0.000184
N	-0.092951	0.713560	-0.000917
N	-0.535500	-2.014464	0.000001
Te	1.152837	-0.870154	-0.000186
Br	3.450409	1.181602	0.000298
C	-4.859098	1.511168	0.000036
N	-5.782039	2.220585	-0.000000

B97D3-CPCM-THF_complex-Te-CN-Cl-same.out

C	3.334451	0.381883	-0.000006
C	3.396353	-1.056796	-0.000100
C	2.251195	-1.801525	-0.000086
C	2.125424	1.052790	0.000087
H	4.371014	-1.535178	-0.000163
H	2.292513	-2.887340	-0.000143
H	2.087773	2.137620	0.000162
C	0.904479	0.313620	0.000064
C	0.961653	-1.167380	0.000003
N	-0.274710	0.925461	0.000195
N	-0.178987	-1.833839	0.000040
Te	-1.716600	-0.484659	0.000025
Cl	-3.551317	1.694243	-0.000143
C	4.553451	1.121179	-0.000009
N	5.556876	1.711581	-0.000017

B97D3-CPCM-THF_complex-Te-CN-I-same.out

C	-4.106692	0.815721	-0.000022
C	-4.472313	-0.577431	0.000151
C	-3.512755	-1.549164	0.000157
C	-2.783735	1.215046	-0.000139
H	-5.526157	-0.838065	0.000250
H	-3.783486	-2.601222	0.000288
H	-2.515497	2.266630	-0.000246
C	-1.748607	0.232171	-0.000039
C	-2.118997	-1.201233	-0.000003
N	-0.465542	0.578650	-0.000167
N	-1.149334	-2.101172	0.000087
Te	0.631612	-1.110697	-0.000181
I	3.312909	0.888760	0.000178
C	-5.141997	1.796371	-0.000032
N	-5.998307	2.584774	-0.000032

B97D3-CPCM-THF_complex-Te-CN-NO3-opp.out

C	3.544084	1.566857	-0.000105
C	3.972051	0.191494	-0.000107
C	3.060195	-0.846608	-0.000033
C	2.215713	1.884470	-0.000027
H	4.299730	2.346309	-0.000149
H	3.389403	-1.880991	-0.000016
H	1.889218	2.920488	-0.000005
C	1.218528	0.850896	0.000039
C	1.660209	-0.563305	0.000031
N	-0.077052	1.126642	0.000180
N	0.734271	-1.512942	0.000169
Te	-1.084961	-0.624991	0.000097
O	-3.047007	1.087504	-0.000013
O	-5.220770	1.216357	-0.000269
O	-4.257814	-0.742513	-0.000160
N	-4.198082	0.508045	-0.000007
C	5.369345	-0.092722	-0.000165
N	6.512811	-0.310827	-0.000214

B97D3-CPCM-THF_complex-Te-CN-NO3-same.out

C	3.802651	0.575621	-0.000011
C	3.975602	-0.854343	0.000034
C	2.892395	-1.685989	0.000031
C	2.546654	1.151942	-0.000058
H	4.984290	-1.255644	0.000058
H	3.017136	-2.765232	0.000051
H	2.424923	2.230499	-0.000106
C	1.386253	0.319880	-0.000052
C	1.559087	-1.151525	-0.000003
N	0.162156	0.836123	-0.000146
N	0.473660	-1.907458	-0.000054
Te	-1.151757	-0.690230	-0.000007
O	-2.748181	1.367081	0.000070
O	-4.851801	1.928994	0.000141
O	-4.301402	-0.183045	0.000042
N	-3.991917	1.029877	0.000064
C	4.961996	1.406100	-0.000023
N	5.917282	2.071172	-0.000031

B97D3-CPCM-THF_complex-Te-CN-Quin-opp.out

Imaginary Frequency : -28.54
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.949817	1.856751	-0.002637
C	4.646309	0.593927	0.000979
C	3.963640	-0.604971	0.002228
C	2.586191	1.903240	-0.004714
H	4.534396	2.771419	-0.003654
H	4.493752	-1.552150	0.004976
H	2.060576	2.853762	-0.007396
C	1.815019	0.690556	-0.003197
C	2.532869	-0.610642	0.000079
N	0.494883	0.700417	-0.004624
N	1.819909	-1.722637	0.000969
Te	-0.156752	-1.218698	-0.001379
C	-2.589305	0.871848	-1.215197
C	-4.767865	1.115376	0.003201
C	-3.965718	1.592643	-1.218202
H	-1.756188	1.577759	-1.226745
H	-2.480578	0.210554	-2.080630
H	-3.829221	2.678777	-1.172589
H	-4.513277	1.368782	-2.140241
C	-2.582400	0.878817	1.210350
H	-2.379353	0.245467	2.079618
H	-1.801115	1.640328	1.163165
C	-4.003480	1.503362	1.279173
H	-4.541319	1.139058	2.161484
H	-3.936895	2.593611	1.361857
H	-5.761356	1.574934	0.004662
C	-4.894723	-0.415932	-0.054501
H	-5.500811	-0.776898	0.783329
H	-5.401301	-0.713665	-0.979050
C	-3.469405	-1.027643	0.006453
H	-3.325567	-1.617256	0.917576
H	-3.277762	-1.683360	-0.849288
N	-2.436265	0.034559	-0.000288
C	6.072836	0.597918	0.003392
N	7.236384	0.614757	0.005402

B97D3-CPCM-THF_complex-Te-CN-Quin-same.out

Imaginary Frequency : -38.08
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	4.241309	1.086625	-0.000026
C	4.776953	-0.252332	-0.000017
C	3.946312	-1.334572	-0.000030
C	2.881282	1.321518	-0.000068
H	5.855025	-0.379205	0.000011
H	4.345283	-2.344912	-0.000007
H	2.487197	2.332826	-0.000066
C	1.972675	0.218538	-0.000086
C	2.518218	-1.163570	-0.000035
N	0.661843	0.402180	-0.000100
N	1.666304	-2.169363	0.000074
Te	-0.232088	-1.409413	0.000017
C	-2.357881	0.994700	-1.212403
C	-4.485701	1.543188	0.000247
C	-3.648114	1.859131	-1.249580
H	-1.454281	1.607374	-1.192881
H	-2.294221	0.331546	-2.080739
H	-3.393200	2.924454	-1.269426
H	-4.228343	1.643724	-2.153575
C	-2.357080	0.995094	1.211649
H	-2.291920	0.332349	2.080185
H	-1.453957	1.608424	1.190825
C	-3.647857	1.858676	1.250010
H	-4.227658	1.642171	2.154021
H	-3.393571	2.924130	1.270638
H	-5.403589	2.139470	0.000437
C	-4.829132	0.044793	0.000026
H	-5.428015	-0.203539	0.882976
H	-5.427583	-0.203352	-0.883273
C	-3.501646	-0.763440	0.000281
H	-3.422628	-1.404196	0.884660
H	-3.422802	-1.405035	-0.883507
N	-2.328652	0.141224	-0.000243
C	5.147882	2.188074	0.000040
N	5.897579	3.078057	0.000099

==========
B97D3-CPCM-THF_complex-Te-F4-Br.out
==========

C	-3.258671	1.226131	-0.000088
C	-3.680762	-0.140575	-0.000077
C	-2.768792	-1.159383	0.000002
C	-1.931205	1.557820	-0.000018
C	-0.924429	0.538345	0.000077
C	-1.360595	-0.883546	0.000084
N	0.365685	0.820546	0.000133
N	-0.434393	-1.819039	0.000144
Te	1.396580	-0.916981	0.000302
Br	3.922005	0.799162	-0.000405
F	-4.211988	2.175469	-0.000177
F	-1.571654	2.856447	-0.000038
F	-5.003982	-0.387051	-0.000158
F	-3.197340	-2.437195	0.000000

==========
B97D3-CPCM-THF_complex-Te-F4-Cl.out
==========

C	2.896351	1.055015	0.000214
C	3.186582	-0.345454	0.000240
C	2.181650	-1.272646	0.000032
C	1.606402	1.511219	-0.000023
C	0.506515	0.593000	-0.000152
C	0.805172	-0.865678	-0.000142
N	-0.749686	0.997155	-0.000515
N	-0.207438	-1.704389	-0.000430
Te	-1.951685	-0.630545	-0.000235
Cl	-4.083505	1.215885	0.000746
F	3.936314	1.909837	0.000337
F	1.373057	2.839374	-0.000133
F	4.481229	-0.716988	0.000390
F	2.488406	-2.585981	-0.000022

==========
B97D3-CPCM-THF_complex-Te-F4-I.out
==========

C	-3.611919	1.339794	-0.000217
C	-4.117258	0.001270	-0.000168
C	-3.270177	-1.072048	-0.000145
C	-2.266837	1.589807	-0.000252
C	-1.325119	0.509787	-0.000272
C	-1.847969	-0.882550	-0.000163
N	-0.020026	0.711307	-0.000314
N	-0.982446	-1.875045	-0.000185
Te	0.898364	-1.086460	-0.000264
I	3.754444	0.588846	0.000590
F	-4.505039	2.345251	-0.000230
F	-1.827375	2.863028	-0.000293
F	-5.452506	-0.163325	-0.000135
F	-3.775913	-2.320857	-0.000096

==========
B97D3-CPCM-THF_complex-Te-F4-NO3.out
==========

C	3.335207	1.140165	-0.000054
C	3.672648	-0.250312	-0.000022
C	2.700740	-1.212031	0.000008
C	2.031141	1.552758	-0.000058
C	0.963437	0.596659	-0.000018
C	1.312119	-0.850464	0.000012
N	-0.306320	0.955224	-0.000035
N	0.328916	-1.725890	0.000004
Te	-1.436574	-0.718405	0.000064
O	-3.226540	1.126096	0.000333
O	-5.378079	1.458606	0.000072
O	-4.605088	-0.582573	-0.000469
N	-4.428987	0.656015	0.000006
F	4.345381	2.028425	-0.000096
F	1.751305	2.870825	-0.000105
F	4.978084	-0.576922	-0.000030
F	3.051064	-2.513222	0.000026

==========
B97D3-CPCM-THF_complex-Te-F4-Quin.out
==========

Imaginary Frequency : -28.13
Vibrational Mode : Quinuclidine rotation about Te-N(quin)axis

C	3.713358	1.534917	0.000000
C	4.363655	0.257654	-0.000000
C	3.641961	-0.902275	-0.000000
C	2.350303	1.636797	0.000000
C	1.531759	0.460161	0.000000
C	2.205332	-0.872701	-0.000000
N	0.218275	0.516182	0.000000
N	1.453468	-1.946979	0.000000
Te	-0.514549	-1.372220	0.000000
C	-2.809906	0.826164	-1.213411
C	-4.976745	1.183218	-0.000000
C	-4.171584	1.572752	-1.249821
H	-1.963691	1.515647	-1.193209
H	-2.687690	0.170344	-2.080908
H	-4.011767	2.656272	-1.269411
H	-4.730510	1.306644	-2.153620
C	-2.809905	0.826164	1.213410
H	-2.687694	0.170344	2.080908
H	-1.963689	1.515645	1.193210
C	-4.171582	1.572756	1.249818
H	-4.730508	1.306655	2.153619
H	-4.011762	2.656277	1.269402
H	-5.943974	1.695610	-0.000000
C	-5.187299	-0.339455	0.000003
H	-5.761591	-0.639235	0.883136
H	-5.761595	-0.639238	-0.883126
C	-3.795366	-1.028236	0.000000
H	-3.660109	-1.659335	0.884303
H	-3.660111	-1.659333	-0.884304
N	-2.706241	-0.022454	-0.000000
F	4.491655	2.629419	0.000000
F	1.771783	2.853515	0.000000
F	5.707304	0.244118	-0.000000
F	4.281352	-2.086559	-0.000000

==========
B97D3-CPCM-THF_donor-Te-CN.out
==========

C	-2.635053	1.352971	0.000003
C	-2.866321	-0.068630	0.000003
C	-1.822270	-0.971272	0.000005
C	-1.366181	1.856204	0.000004
H	-3.492676	2.018004	0.000004
H	-2.001971	-2.041089	0.000007
H	-1.187163	2.926832	0.000006
C	-0.239289	0.969649	0.000004
C	-0.479629	-0.489132	0.000004
N	1.012331	1.419392	0.000013
N	0.561326	-1.321936	0.000012
Te	2.203483	-0.188209	-0.000007
C	-4.211933	-0.544203	0.000004
N	-5.312979	-0.918939	0.000005

==========
B97D3-CPCM-THF_donor-Te-F4.out
==========

C	-0.000001	-2.563090	0.716035
C	-0.000001	-2.563090	-0.716035
C	-0.000001	-1.393689	-1.425819
C	-0.000001	-1.393689	1.425819
C	-0.000001	-0.135671	0.742003
C	-0.000001	-0.135671	-0.742003
N	-0.000001	1.022459	1.385379
N	-0.000001	1.022459	-1.385379
Te	0.000002	2.459380	-0.000000
F	-0.000001	-1.421964	2.767785
F	-0.000002	-3.749857	1.337975
F	-0.000002	-3.749857	-1.337975
F	-0.000001	-1.421964	-2.767785

5.4.3.2 M06-2X geometries

5.4.3.2.1 Gas phase

==========
M062X-null-null_acceptor-NO3.out
==========

O	0.856080	-0.903990	0.000001
O	0.354895	1.193271	0.000024
O	-1.211015	-0.289346	-0.000043
N	0.000045	0.000074	0.000019

==========
M062X-null-null_acceptor-quin.out
==========

C	-0.793560	-0.710441	-1.177407
C	1.287445	-0.004526	-0.001014
C	0.749312	-0.874888	-1.141693
H	-1.290731	-1.681154	-1.221359
H	-1.105584	-0.145956	-2.058545
H	1.026388	-1.917918	-0.970100
H	1.195467	-0.574376	-2.091819
C	-0.791076	-0.661384	1.207273
H	-1.283317	-0.213335	2.072209
H	-1.106923	-1.705515	1.159007
C	0.752624	-0.554318	1.325247
H	1.036022	0.114577	2.141518
H	1.195589	-1.529303	1.538172
H	2.378070	-0.008498	-0.001927
C	0.758304	1.421801	-0.185711
H	1.206685	2.092019	0.550476
H	1.039159	1.793105	-1.174236
C	-0.784901	1.379764	-0.027722
H	-1.095578	1.862347	0.901165
H	-1.277882	1.906483	-0.846724
N	-1.283751	0.004497	0.001189

==========
M062X-null-null_complex-Te-diBr-Br.out
==========

C	-2.402165	2.171736	0.000006
C	-3.258363	1.022409	-0.000006
C	-2.740895	-0.225244	-0.000008
C	-1.057013	2.040020	0.000047
H	-2.849177	3.156317	-0.000025
H	-4.329750	1.169015	-0.000008
C	-0.431710	0.738956	0.000088
C	-1.313413	-0.453243	0.000011
N	0.854747	0.562119	0.000169
N	-0.740978	-1.613467	0.000052
Te	1.266581	-1.371022	0.000088
Br	4.064193	-0.629117	-0.000191
Br	-3.887029	-1.730782	-0.000031
Br	0.044028	3.575883	0.000025

==========
M062X-null-null_complex-Te-diBr-Cl.out
==========

C	-1.603254	2.430632	0.000031
C	-2.647284	1.448520	0.000036
C	-2.355371	0.129802	0.000024
C	-0.302556	2.063900	0.000005
H	-1.870817	3.478493	0.000034
H	-3.676673	1.779877	0.000057
C	0.086237	0.674416	-0.000024
C	-0.990481	-0.346938	0.000023
N	1.321269	0.276646	-0.000035
N	-0.627367	-1.586962	-0.000012
Te	1.401077	-1.700120	-0.000044
Cl	4.068264	-1.428312	0.000111
Br	1.053320	3.383978	-0.000013
Br	-3.751894	-1.149710	0.000016

M062X-null-null_complex-Te-diBr-I.out

C	-2.880893	2.089123	0.000009
C	-3.682788	0.900681	0.000015
C	-3.109945	-0.322521	0.000007
C	-1.531400	2.020432	-0.000005
H	-3.374328	3.051333	0.000013
H	-4.759787	0.997581	0.000021
C	-0.848345	0.748457	-0.000012
C	-1.673499	-0.482723	-0.000003
N	0.445193	0.631527	-0.000039
N	-1.050169	-1.617556	-0.000021
Te	0.937174	-1.281729	-0.000010
I	3.960651	-0.387087	0.000022
Br	-0.497338	3.600474	-0.000019
Br	-4.186016	-1.877670	0.000010

M062X-null-null_complex-Te-diBr-NO3.out

C	2.630313	1.941834	0.000107
C	3.335877	0.693790	-0.000081
C	2.670219	-0.481135	-0.000149
C	1.279961	1.978670	0.000219
H	3.198035	2.862255	0.000178
H	4.417074	0.705730	-0.000148
C	0.498748	0.763897	0.000123
C	1.225277	-0.529820	-0.000071
N	-0.798787	0.747101	0.000271
N	0.512402	-1.609872	-0.000096
Te	-1.436716	-1.120920	-0.000081
O	-3.521257	0.130483	-0.000099
O	-5.660181	-0.088553	-0.000155
O	-4.408470	-1.839679	-0.000170
N	-4.559444	-0.613195	-0.000166
Br	0.369095	3.633050	0.000537
Br	3.627814	-2.112187	-0.000347

M062X-null-null_complex-Te-diBr-quin.out

C	2.837121	2.306364	0.000316
C	3.799524	1.236487	-0.000468
C	3.414456	-0.054733	-0.000863
C	1.512643	2.060113	0.000814
H	3.198434	3.325613	0.000209
H	4.851136	1.488832	-0.001063
C	1.016098	0.701795	0.001517
C	2.007875	-0.407779	0.000362
N	-0.241740	0.403420	0.002588
N	1.554334	-1.615863	0.000529
Te	-0.443366	-1.569720	0.003481
C	-3.169139	0.045753	-1.233838
C	-5.339562	0.034232	-0.008611
C	-4.581925	0.672592	-1.177098
H	-2.392165	0.801240	-1.347775
H	-3.078948	-0.657683	-2.064581
H	-4.515599	1.752292	-1.027822
H	-5.111934	0.505825	-2.116105
C	-3.144696	0.169843	1.163985
H	-2.748913	-0.321060	2.055218
H	-2.566188	1.080398	1.008910
C	-4.658591	0.456699	1.297586
H	-5.088320	-0.099459	2.133948
H	-4.827881	1.516600	1.492193
H	-6.383975	0.346466	-0.013463
C	-5.236736	-1.489219	-0.138521
H	-5.873349	-1.982442	0.597421
H	-5.580951	-1.800794	-1.127010
C	-3.757534	-1.883577	0.075049
H	-3.606302	-2.341282	1.055401
H	-3.422722	-2.602393	-0.676993
N	-2.885284	-0.702795	0.003984
Br	0.262337	3.472009	0.000643
Br	4.680930	-1.445480	-0.002944

M062X-null-null_complex-Te-nat-Cl.out

C	-3.613720	1.313838	-0.000167
C	-3.969142	-0.080508	-0.000138
C	-3.020291	-1.045899	-0.000044
C	-2.319368	1.708816	-0.000110
H	-4.406291	2.053164	-0.000242
H	-5.019322	-0.349535	-0.000185
H	-3.275912	-2.098733	-0.000017
H	-2.038421	2.754787	-0.000132
C	-1.259670	0.731019	-0.000022
C	-1.618717	-0.698430	0.000014
N	-0.001271	1.069554	0.000059
N	-0.647233	-1.561954	0.000089
Te	1.120054	-0.564528	0.000080
Cl	3.284831	1.109974	-0.000106

M062X-null-null_complex-Te-nat-I.out

C	-4.251340	1.759996	0.000026
C	-4.842642	0.447672	-0.000007
C	-4.077025	-0.667420	0.000026
C	-2.908917	1.927271	0.000093
H	-4.904384	2.624667	0.000014
H	-5.923131	0.364246	-0.000046
H	-4.509496	-1.660330	0.000021
H	-2.451726	2.908579	0.000135
C	-2.035579	0.780174	0.000119
C	-2.637762	-0.563974	0.000079
N	-0.736267	0.893399	0.000234
N	-1.833888	-1.587581	0.000171
Te	0.062514	-0.917316	0.000115
I	2.963183	0.494722	-0.000207

M062X-null-null_complex-Te-nat-NO3.out

C	4.054986	1.437162	-0.000009
C	4.459854	0.055851	0.000025
C	3.547853	-0.943298	0.000024
C	2.748516	1.787337	-0.000042
H	4.821063	2.203732	-0.000021
H	5.518825	-0.174670	0.000041
H	3.840955	-1.986052	0.000039
H	2.430470	2.822404	-0.000078
C	1.724433	0.771490	-0.000036
C	2.135801	-0.643602	-0.000002
N	0.453480	1.060164	-0.000109
N	1.197433	-1.545040	-0.000026
Te	-0.587391	-0.622093	-0.000018
O	-2.390970	1.085220	0.000022
O	-4.529146	1.322287	0.000099
O	-3.672960	-0.652931	0.000075
N	-3.558204	0.578754	0.000085

M062X-null-null_complex-Te-nat-quin.out

C	4.201877	2.167013	0.000429
C	5.004571	0.967104	-0.009728
C	4.440545	-0.258014	-0.011925
C	2.853825	2.118322	0.008656
H	4.707081	3.124896	0.001294
H	6.082566	1.068166	-0.015744
H	5.030924	-1.164765	-0.019374
H	2.246655	3.014023	0.015969
C	2.180288	0.840887	0.006740
C	3.001359	-0.391811	-0.004082
N	0.885559	0.731020	0.012437
N	2.386537	-1.533650	-0.006762
Te	0.417508	-1.201791	0.003816
C	-2.115874	0.771633	-1.213812
C	-4.288818	0.984266	-0.010391
C	-3.456895	1.543142	-1.168989
H	-1.259719	1.440879	-1.291813
H	-2.080586	0.085660	-2.063031
H	-3.282234	2.610199	-1.015465
H	-3.993627	1.434608	-2.112843
C	-2.107378	0.827400	1.186532
H	-1.802161	0.258447	2.066868
H	-1.406511	1.654323	1.075048
C	-3.572764	1.312106	1.303782
H	-4.081226	0.816088	2.133677
H	-3.605717	2.385116	1.498602
H	-5.290101	1.415609	-0.016679
C	-4.364711	-0.539359	-0.157267
H	-5.049158	-0.961673	0.580026
H	-4.753264	-0.795657	-1.145274
C	-2.938980	-1.107844	0.034414
H	-2.840240	-1.618735	0.994983
H	-2.688201	-1.829451	-0.746843
N	-1.938834	-0.033605	0.005188

M062X-null-null_complex-nat-Br.out

C	-3.922465	1.592859	-0.000055
C	-4.429735	0.246239	-0.000040
C	-3.594143	-0.817930	0.000022
C	-2.592864	1.844383	-0.000008
H	-4.628699	2.414834	-0.000088
H	-5.502877	0.094656	-0.000065
H	-3.963736	-1.836058	0.000053
H	-2.199020	2.852889	-0.000002
C	-1.647832	0.755355	0.000045
C	-2.163755	-0.625140	0.000052
N	-0.358902	0.951275	0.000131
N	-1.295000	-1.593199	0.000162
Te	0.563634	-0.801316	0.000062
Br	3.104784	0.704599	-0.000151

M062X-null-null_donor-Te-diBr.out

C	-0.718297	-2.467400	0.000008
C	0.718286	-2.467404	0.000008
C	1.425363	-1.319020	-0.000013
C	-1.425369	-1.319012	-0.000013
H	-1.234329	-3.417790	0.000002
H	1.234312	-3.417796	0.000003
C	-0.742291	-0.044489	-0.000016
C	0.742292	-0.044493	-0.000016
N	-1.360659	1.099744	-0.000115
N	1.360661	1.099739	-0.000115
Te	0.000006	2.513923	0.000116
Br	-3.303768	-1.333050	-0.000059
Br	3.303762	-1.333061	-0.000059

M062X-null-null_donor-Te-nat.out

C	-3.317288	0.721150	0.000000
C	-3.317239	-0.721205	0.000000
C	-2.169414	-1.430054	-0.000000
C	-2.169501	1.430036	0.000000
H	-4.269241	1.236684	0.000000
H	-4.269156	-1.236817	0.000000
H	-2.156938	-2.511518	-0.000000
H	-2.157030	2.511507	0.000000
C	-0.903963	0.739037	0.000001
C	-0.903906	-0.738985	-0.000001
N	0.240633	1.366316	-0.000001
N	0.240685	-1.366312	-0.000000
Te	1.657135	0.000005	0.000000

M062X-null-null_complex-Te-CN-Br-opp.out

C	-3.393764	1.610361	-0.000140
C	-3.897657	0.257918	-0.000125
C	-3.059851	-0.816048	-0.000053
C	-2.064283	1.850847	-0.000079
H	-4.108254	2.423105	-0.000212
H	-3.441203	-1.828829	-0.000036
H	-1.670024	2.858699	-0.000106
C	-1.122907	0.760203	0.000009
C	-1.638562	-0.618157	0.000025
N	0.166085	0.951845	0.000008
N	-0.769989	-1.589476	0.000050
Te	1.087935	-0.800471	0.000210
Br	3.573008	0.702967	-0.000184
C	-5.317920	0.058160	-0.000170
N	-6.458778	-0.084089	-0.000190

M062X-null-null_complex-Te-CN-Br-same.out

C	-3.693050	0.588475	-0.000081
C	-3.919053	-0.836804	-0.000032
C	-2.877974	-1.697393	-0.000034
C	-2.436666	1.115390	-0.000121
H	-4.941028	-1.192829	-0.000008
H	-3.030083	-2.769229	-0.000011
H	-2.270997	2.184613	-0.000188
C	-1.298854	0.243062	-0.000095
C	-1.519810	-1.212200	-0.000058
N	-0.075511	0.702302	-0.000202
N	-0.469063	-1.977716	-0.000118
Te	1.185985	-0.818173	-0.000002
Br	3.321659	1.155230	0.000192
C	-4.836390	1.454607	-0.000115
N	-5.769194	2.126642	-0.000137

M062X-null-null_complex-Te-CN-Cl-opp.out

C	3.010141	1.510953	0.000122
C	3.419857	0.127454	0.000005
C	2.509419	-0.886318	-0.000017
C	1.699822	1.841240	0.000222
H	3.778372	2.273275	0.000165
H	2.820998	-1.922937	-0.000070
H	1.375437	2.873960	0.000353
C	0.685008	0.818171	0.000176
C	1.104334	-0.592711	0.000032
N	-0.587136	1.098035	0.000425
N	0.170517	-1.500097	0.000115
Te	-1.636580	-0.582535	-0.000018
Cl	-3.830912	0.983120	-0.000334
C	4.822965	-0.169037	-0.000045
N	5.951416	-0.389944	-0.000086

M062X-null-null_complex-Te-CN-Cl-same.out

C	3.299059	0.363532	-0.000016
C	3.354593	-1.078647	-0.000001
C	2.218376	-1.809459	0.000088
C	2.112859	1.034396	0.000048
H	4.327186	-1.553412	-0.000024
H	2.242914	-2.891876	0.000142
H	2.074952	2.115770	0.000079
C	0.880027	0.303490	0.000103
C	0.925468	-1.168483	0.000124
N	-0.279023	0.905685	0.000336
N	-0.209013	-1.800434	0.000337
Te	-1.722562	-0.445652	0.000107
Cl	-3.433611	1.633950	-0.000688
C	4.534883	1.091065	-0.000051
N	5.537746	1.653452	-0.000078

M062X-null-null_complex-Te-CN-I-opp.out

C	-3.765284	1.686040	-0.000361
C	-4.331260	0.357961	-0.000199
C	-3.545310	-0.753748	-0.000058
C	-2.426405	1.865026	-0.000360
H	-4.441294	2.530870	-0.000485
H	-3.972456	-1.748000	0.000056
H	-1.985803	2.853436	-0.000494
C	-1.537158	0.731406	-0.000177
C	-2.116467	-0.620683	-0.000039
N	-0.240241	0.862449	-0.000220
N	-1.296008	-1.633623	0.000077
Te	0.589603	-0.934504	0.000118
I	3.390907	0.537829	0.000108
C	-5.759395	0.223173	-0.000194
N	-6.905210	0.130879	-0.000226

M062X-null-null_complex-Te-CN-I-same.out

C	-4.057213	0.763361	-0.000293
C	-4.399863	-0.639016	-0.000076
C	-3.434450	-1.583842	-0.000002
C	-2.762336	1.183700	-0.000417
H	-5.447924	-0.909111	-0.000011
H	-3.675671	-2.639174	0.000113
H	-2.506675	2.235075	-0.000583
C	-1.701720	0.218770	-0.000325
C	-2.040498	-1.212677	-0.000104
N	-0.445139	0.576517	-0.000527
N	-1.057419	-2.064623	-0.000122
Te	0.682241	-1.043453	-0.000013
I	3.203054	0.867393	0.000342
C	-5.124143	1.722246	-0.000367
N	-5.995559	2.471772	-0.000417

M062X-null-null_complex-Te-CN-NO3-opp.out

C	3.486793	1.553897	0.000011
C	3.915453	0.175316	0.000010
C	3.021357	-0.851233	0.000010
C	2.173204	1.867577	0.000010
H	4.245198	2.325889	0.000018
H	3.346878	-1.883338	0.000017
H	1.834865	2.895633	0.000020
C	1.172608	0.829929	0.000005
C	1.612603	-0.574587	0.000003
N	-0.104186	1.088529	0.000037
N	0.692942	-1.497956	0.000029
Te	-1.109376	-0.613999	-0.000048
O	-2.900041	1.037823	-0.000233
O	-5.040523	1.248309	0.000006
O	-4.161614	-0.716545	0.000369
N	-4.065784	0.515445	0.000040
C	5.323385	-0.100055	0.000019
N	6.454971	-0.302020	0.000027

M062X-null-null_complex-Te-CN-NO3-same.out

C	3.747107	0.554824	-0.000152
C	3.915066	-0.878937	-0.000186
C	2.840688	-1.696770	-0.000087
C	2.514180	1.132956	-0.000016
H	4.921810	-1.275655	-0.000276
H	2.949106	-2.773860	-0.000091
H	2.392378	2.208033	0.000032
C	1.340994	0.307412	0.000070
C	1.503830	-1.155530	0.000030
N	0.136408	0.812669	0.000281
N	0.422867	-1.878128	0.000190
Te	-1.174936	-0.662689	0.000156
O	-2.617340	1.309422	0.000222
O	-4.674578	1.935761	-0.000127
O	-4.198669	-0.163562	-0.000541
N	-3.862324	1.026059	-0.000245
C	4.924124	1.375137	-0.000245
N	5.880501	2.012800	-0.000327

M062X-null-null_complex-Te-CN-Quin-opp.out

C	3.855218	1.864007	0.008439
C	4.572794	0.605805	-0.002723
C	3.927933	-0.586284	-0.005912
C	2.508974	1.897064	0.015649
H	4.434040	2.777991	0.010439
H	4.465455	-1.524746	-0.014416
H	1.964327	2.831636	0.023685
C	1.752334	0.667114	0.011704
C	2.487374	-0.615965	0.001014
N	0.453476	0.641663	0.015124
N	1.799623	-1.716331	-0.003362
Te	-0.141979	-1.254567	0.003785
C	-2.543331	0.849163	-1.215744
C	-4.703632	1.157568	-0.011895
C	-3.843904	1.685851	-1.164486
H	-1.655469	1.475402	-1.297146
H	-2.546340	0.162597	-2.065239
H	-3.616535	2.741270	-1.000637
H	-4.383292	1.612906	-2.110029
C	-2.532257	0.902657	1.185866
H	-2.247118	0.322837	2.065811
H	-1.800104	1.701614	1.071400
C	-3.976800	1.444064	1.306187
H	-4.504918	0.960837	2.131215
H	-3.966137	2.515364	1.511631
H	-5.684252	1.633622	-0.017794
C	-4.846980	-0.360509	-0.169674
H	-5.556198	-0.757306	0.558039
H	-5.236563	-0.592728	-1.163121
C	-3.451366	-0.993412	0.032245
H	-3.381097	-1.502750	0.996166
H	-3.231013	-1.730452	-0.743867
N	-2.401641	0.035021	0.003260
C	6.007973	0.646634	-0.011467
N	7.154559	0.700626	-0.019047

M062X-null-null_complex-Te-CN-Quin-same.out

C	4.132720	1.120139	-0.000647
C	4.701516	-0.212133	0.005862
C	3.909729	-1.301081	0.006234
C	2.793507	1.331681	-0.007062
H	5.779219	-0.304764	0.010536
H	4.318008	-2.302803	0.011242
H	2.377932	2.330102	-0.011694
C	1.899246	0.204424	-0.005805
C	2.471733	-1.158338	0.000892
N	0.606289	0.344815	-0.009183
N	1.649065	-2.160004	0.002486
Te	-0.221038	-1.461265	-0.001507
C	-2.338623	0.920897	-1.241826
C	-4.388598	1.602661	0.001190
C	-3.479637	1.962816	-1.179233
H	-1.364459	1.389917	-1.376570
H	-2.486849	0.217284	-2.064088
H	-3.074691	2.967376	-1.040427
H	-4.045702	1.966900	-2.111868
C	-2.248950	1.052005	1.153413
H	-2.012530	0.469878	2.046255
H	-1.419029	1.736932	0.983355
C	-3.596603	1.795338	1.299412
H	-4.169196	1.400383	2.141786
H	-3.426383	2.855512	1.491886
H	-5.282485	2.226204	0.001158
C	-4.767465	0.122296	-0.116651
H	-5.521772	-0.142794	0.625627
H	-5.197893	-0.071358	-1.101576
C	-3.483922	-0.714022	0.093877
H	-3.473987	-1.184634	1.079675
H	-3.398350	-1.509523	-0.650367
N	-2.286305	0.133574	0.001843
C	5.029614	2.241549	0.000634
N	5.757604	3.129011	0.002237

M062X-null-null_complex-Te-CN.out

C	-2.604111	1.350623	-0.000002
C	-2.835325	-0.077901	-0.000002
C	-1.815469	-0.971444	-0.000003
C	-1.354376	1.853671	-0.000003
H	-3.466261	2.003888	-0.000002
H	-1.990534	-2.038336	-0.000004
H	-1.167251	2.918675	-0.000004
C	-0.220108	0.963885	-0.000002
C	-0.461138	-0.490845	-0.000003
N	1.012792	1.392988	-0.000007
N	0.564646	-1.300220	-0.000007
Te	2.182279	-0.187251	0.000004
C	-4.193548	-0.544181	-0.000002
N	-5.284586	-0.899918	-0.000002

M062X-null-null_complex-Te-F4-Br.out

C	-3.214999	1.199353	-0.000074
C	-3.628290	-0.175346	-0.000097
C	-2.727894	-1.176514	0.000014
C	-1.912145	1.542211	0.000063
C	-0.891604	0.524520	0.000153
C	-1.312682	-0.891665	0.000119
N	0.374381	0.804218	0.000410
N	-0.385692	-1.792106	0.000322
Te	1.428557	-0.875405	0.000150
Br	3.783338	0.784691	-0.000357
F	-4.183204	2.120962	-0.000145
F	-1.563734	2.825129	0.000134
F	-4.944805	-0.410672	-0.000190
F	-3.141248	-2.442448	0.000035

M062X-null-null_complex-Te-F4-Cl.out

C	2.864546	1.039384	0.000356
C	3.150840	-0.367246	0.000110
C	2.162275	-1.281672	-0.000107
C	1.598094	1.499446	0.000379
C	0.488677	0.580296	0.000149
C	0.778503	-0.869825	-0.000099
N	-0.745762	0.975702	0.000176
N	-0.228001	-1.678978	-0.000284
Te	-1.956845	-0.597171	-0.000203
Cl	-3.960037	1.175846	-0.000127
F	3.913170	1.869404	0.000568
F	1.369632	2.810068	0.000620
F	4.440803	-0.722768	0.000112
F	2.458095	-2.580686	-0.000331

M062X-null-null_complex-Te-F4-I.out

C	-3.558887	1.308104	-0.000041
C	-4.052841	-0.040307	0.000054
C	-3.213527	-1.092818	0.000131
C	-2.238347	1.574382	-0.000050
C	-1.279933	0.497914	-0.000030
C	-1.784779	-0.890384	0.000051
N	0.000900	0.701499	0.000213
N	-0.913960	-1.846418	0.000303
Te	0.944247	-1.041676	-0.000284
I	3.628699	0.580294	0.000130
F	-4.470562	2.284526	-0.000015
F	-1.814004	2.833276	-0.000018
F	-5.379957	-0.197974	0.000135
F	-3.697764	-2.332640	0.000298

==========
M062X-null-null_complex-Te-F4-NO3.out
==========

C	3.285678	1.125767	0.000027
C	3.620984	-0.271042	-0.000056
C	2.666570	-1.220830	-0.000083
C	2.004665	1.541617	0.000102
C	0.928781	0.582433	0.000108
C	1.270073	-0.855920	-0.000043
N	-0.319505	0.930810	0.000127
N	0.293169	-1.702846	0.000010
Te	-1.454584	-0.692147	0.000038
O	-3.094957	1.078902	-0.000543
O	-5.211661	1.458007	-0.000254
O	-4.490783	-0.570310	0.000546
N	-4.299456	0.650033	-0.000126
F	4.304392	1.989719	0.000052
F	1.727609	2.841463	0.000166
F	4.921209	-0.579036	-0.000123
F	3.006527	-2.507619	-0.000138

==========
M062X-null-null_donor-Te-F4.out
==========

C	-0.000001	-2.534511	0.720830
C	-0.000001	-2.534511	-0.720830
C	-0.000001	-1.388809	-1.427352
C	-0.000001	-1.388809	1.427352
C	-0.000001	-0.123639	0.739716
C	-0.000001	-0.123639	-0.739716
N	-0.000005	1.016757	1.363279
N	-0.000005	1.016757	-1.363279
Te	0.000004	2.432818	0.000000
F	-0.000003	-1.404006	2.750160
F	-0.000001	-3.716974	1.315348
F	-0.000001	-3.716974	-1.315348
F	-0.000003	-1.404006	-2.750160

5.4.3.2.2 PCM

==========
M062X-PCM-ACN_acceptor-NO3.out
==========

O	-0.231740	-1.220875	-0.000030
O	1.173944	0.409936	-0.000007
O	-0.942306	0.810955	-0.000074
N	0.000118	-0.000019	0.000126

==========
M062X-PCM-ACN_acceptor-quin.out
==========

C	-0.801512	-0.944981	0.998878
C	1.286515	0.010529	0.020929
C	0.746221	-0.920722	1.110117
H	-1.263305	-0.675423	1.950566
H	-1.157048	-1.942332	0.733276
H	1.059674	-0.562128	2.092918
H	1.158885	-1.923114	0.981819
C	-0.808710	1.339040	0.295555
H	-1.250058	2.031878	-0.423046
H	-1.191626	1.604078	1.282955
C	0.740808	1.421063	0.263510
H	1.077304	2.088899	-0.532575
H	1.127830	1.815125	1.205265
H	2.376901	0.019619	0.039316
C	0.782872	-0.482822	-1.338715
H	1.194309	0.137022	-2.137844
H	1.124516	-1.505790	-1.511088
C	-0.767627	-0.412519	-1.331207
H	-1.127795	0.309161	-2.066615
H	-1.202279	-1.381572	-1.583267
N	-1.285530	-0.010422	-0.020869

==========
M062X-PCM-ACN_complex-Te-diBr-Br.out
==========

C	2.352264	2.222651	-0.000093
C	3.243267	1.096946	-0.000134
C	2.768589	-0.165351	-0.000031
C	1.013323	2.056181	0.000084
H	2.779009	3.216101	-0.000240
H	4.308268	1.283515	-0.000293
C	0.429223	0.734565	0.000294
C	1.346455	-0.427683	0.000144
N	-0.852080	0.511053	0.000360
N	0.813436	-1.610893	0.000225
Te	-1.167723	-1.437022	0.000292
Br	-4.184260	-0.634844	-0.000394
Br	3.948390	-1.638798	-0.000142
Br	-0.135957	3.554229	-0.000045

==========
M062X-PCM-ACN_complex-Te-diBr-Cl.out
==========

C	1.538242	2.464755	0.000062
C	2.609461	1.508533	0.000047
C	2.359926	0.182972	-0.000015
C	0.249134	2.067928	0.000014
H	1.787548	3.517069	0.000119
H	3.626275	1.875874	0.000066
C	-0.097565	0.665571	0.000071
C	1.004793	-0.323841	-0.000026
N	-1.320732	0.227342	0.000019
N	0.678265	-1.578061	-0.000026
Te	-1.314460	-1.747361	-0.000068
Cl	-4.167585	-1.433312	0.000156
Br	-1.146914	3.340494	-0.000034
Br	3.784067	-1.057760	0.000030

M062X-PCM-ACN_complex-Te-diBr-I.out

C	2.819858	2.165639	-0.000016
C	3.673486	1.010860	0.000017
C	3.159303	-0.236173	0.000102
C	1.476359	2.043010	0.000033
H	3.279191	3.144468	-0.000048
H	4.743878	1.162945	0.000004
C	0.851792	0.740420	0.000101
C	1.729743	-0.450669	0.000122
N	-0.436300	0.558060	0.000247
N	1.160347	-1.618042	0.000327
Te	-0.807920	-1.377118	0.000043
I	-4.085874	-0.393733	-0.000348
Br	0.372177	3.573745	0.000074
Br	4.290924	-1.746548	0.000213

M062X-PCM-ACN_complex-Te-diBr-NO3.out

C	2.564774	2.017748	0.000158
C	3.318940	0.795378	0.000107
C	2.702581	-0.404395	0.000009
C	1.216056	2.005834	0.000113
H	3.104779	2.954564	0.000258
H	4.398302	0.857550	0.000177
C	0.483369	0.759920	0.000001
C	1.259821	-0.502202	-0.000065
N	-0.814043	0.686848	0.000026
N	0.591763	-1.614228	-0.000075
Te	-1.354992	-1.210774	-0.000307
O	-3.594823	0.100158	-0.000185
O	-5.735274	-0.091798	0.000176
O	-4.504079	-1.855455	0.000481
N	-4.627878	-0.625481	0.000121
Br	0.239607	3.621837	0.000229
Br	3.712045	-2.000088	0.000038

M062X-PCM-ACN_complex-Te-diBr-quin.out

C	2.931549	2.247957	0.002054
C	3.852355	1.142863	0.001944
C	3.412381	-0.130280	0.000191
C	1.598921	2.048224	0.000307
H	3.334492	3.251298	0.003409
H	4.911975	1.358638	0.003079
C	1.046346	0.711202	-0.000307
C	1.994722	-0.434619	-0.000481
N	-0.222476	0.458282	-0.000544
N	1.489637	-1.622671	-0.000791
Te	-0.520340	-1.503163	0.000567
C	-3.206108	0.070105	-1.247882
C	-5.362711	0.007009	-0.002748
C	-4.631736	0.662510	-1.178559
H	-2.451027	0.842952	-1.389287
H	-3.113068	-0.647661	-2.065277
H	-4.590307	1.743545	-1.031161
H	-5.162284	0.477703	-2.113317
C	-3.167052	0.234535	1.152743
H	-2.743170	-0.225407	2.047026
H	-2.632697	1.167247	0.974319
C	-4.689114	0.459537	1.297033
H	-5.085349	-0.114081	2.137442
H	-4.896423	1.512462	1.491094
H	-6.416350	0.284820	-0.004304
C	-5.208594	-1.512712	-0.124590
H	-5.829215	-2.023850	0.611996
H	-5.534430	-1.839980	-1.113815
C	-3.721501	-1.857983	0.100544
H	-3.558303	-2.285146	1.092023
H	-3.363431	-2.582493	-0.634504
N	-2.884286	-0.647279	0.002061
Br	0.408845	3.515027	-0.000457
Br	4.631452	-1.571142	-0.000822

M062X-PCM-ACN_complex-Te-nat-Br.out

C	3.868953	1.710466	-0.000016
C	4.432564	0.383264	0.000279
C	3.647804	-0.716118	0.000393
C	2.533078	1.912325	-0.000206
H	4.542949	2.557635	-0.000018
H	5.510172	0.279492	0.000462
H	4.063127	-1.715768	0.000646
H	2.105679	2.906632	-0.000338
C	1.636573	0.782204	-0.000293
C	2.211867	-0.575471	0.000057
N	0.337421	0.913131	-0.000266
N	1.386981	-1.585073	0.000099
Te	-0.475585	-0.891038	-0.000125
Br	-3.244211	0.743701	0.000160

M062X-PCM-ACN_complex-Te-nat-Cl.out

C	-3.579539	1.382707	-0.000020
C	-3.966001	-0.006098	0.000008
C	-3.044410	-0.994162	0.000088
C	-2.280815	1.755250	0.000013
H	-4.357931	2.135451	-0.000035
H	-5.021307	-0.248295	-0.000028
H	-3.328167	-2.039086	0.000090
H	-1.985502	2.796797	0.000057
C	-1.244361	0.751074	-0.000115
C	-1.637497	-0.670048	0.000015
N	0.025793	1.050954	0.000022
N	-0.687112	-1.561155	0.000019
Te	1.078139	-0.627033	-0.000017
Cl	3.398510	1.189406	0.000035

==========
M062X-PCM-ACN_complex-Te-nat-I.out
==========

C	-4.191632	1.903990	0.000123
C	-4.853063	0.623161	0.000066
C	-4.154749	-0.533089	0.000040
C	-2.844557	2.004689	0.000117
H	-4.800164	2.799376	0.000134
H	-5.935366	0.601683	0.000059
H	-4.646193	-1.497473	-0.000002
H	-2.341913	2.963158	0.000134
C	-2.036771	0.809774	0.000063
C	-2.712171	-0.500962	0.000091
N	-0.731097	0.841518	0.000084
N	-1.968100	-1.572748	-0.000011
Te	-0.063385	-1.018127	0.000057
I	3.107013	0.516020	-0.000128

==========
M062X-PCM-ACN_complex-Te-nat-NO3.out
==========

C	4.017990	1.524566	0.000157
C	4.465879	0.154232	0.000245
C	3.589999	-0.874145	0.000179
C	2.704332	1.839972	0.000003
H	4.762212	2.311082	0.000205
H	5.530795	-0.040660	0.000365
H	3.920160	-1.905165	0.000242
H	2.363210	2.867275	-0.000079
C	1.713429	0.790613	-0.000057
C	2.170677	-0.611927	0.000045
N	0.430731	1.031103	-0.000197
N	1.261683	-1.546214	-0.000030
Te	-0.536003	-0.694924	-0.000217
O	-2.483951	1.122824	-0.000015
O	-4.619280	1.376587	0.000521
O	-3.776275	-0.602417	0.000360
N	-3.641274	0.627641	0.000255

==========
M062X-PCM-ACN_complex-Te-nat-quin.out
==========

C	4.259375	2.113564	-0.000251
C	5.034354	0.895220	-0.005169
C	4.441856	-0.317530	-0.005980
C	2.909689	2.094285	0.004387
H	4.786664	3.059226	-0.000492
H	6.114303	0.971919	-0.008416
H	5.017871	-1.234166	-0.009716
H	2.325788	3.005778	0.007830
C	2.207398	0.831622	0.004070
C	2.999284	-0.419727	-0.001910
N	0.910162	0.749716	0.007154
N	2.350438	-1.543381	-0.003792
Te	0.373379	-1.166450	0.001993
C	-2.108060	0.781403	-1.219938
C	-4.277128	0.961312	-0.007553
C	-3.451992	1.543198	-1.159137
H	-1.260569	1.459046	-1.315579
H	-2.082846	0.088767	-2.063595
H	-3.281833	2.608274	-0.989186
H	-3.987170	1.442503	-2.104204
C	-2.093074	0.847068	1.185977
H	-1.766669	0.291222	2.066814
H	-1.423423	1.697806	1.063577
C	-3.569504	1.289096	1.310508
H	-4.061463	0.765583	2.132805
H	-3.627295	2.357888	1.520400
H	-5.284881	1.376129	-0.012462
C	-4.325958	-0.561300	-0.166755
H	-5.009760	-1.001420	0.559934
H	-4.694332	-0.817099	-1.162168
C	-2.896140	-1.109087	0.041167
H	-2.796308	-1.603768	1.009556
H	-2.630480	-1.835002	-0.730641
N	-1.908299	-0.016624	0.004554

==========
M062X-PCM-ACN_donor-Te-diBr.out
==========

C	-0.717748	-2.472781	0.000010
C	0.717735	-2.472785	0.000010
C	1.418847	-1.320314	-0.000016
C	-1.418854	-1.320307	-0.000016
H	-1.230977	-3.424467	0.000000
H	1.230960	-3.424474	0.000000
C	-0.740010	-0.045993	-0.000018
C	0.740011	-0.045997	-0.000018
N	-1.354927	1.103167	-0.000152
N	1.354930	1.103161	-0.000151
Te	0.000006	2.521229	0.000153
Br	-3.303083	-1.337568	-0.000079
Br	3.303076	-1.337580	-0.000079

==========
M062X-PCM-ACN_donor-Te-nat.out
==========

C	-3.323722	0.720812	0.000001
C	-3.323675	-0.720860	0.000001
C	-2.173895	-1.429267	0.000000
C	-2.173979	1.429252	0.000000
H	-4.275618	1.236165	0.000001
H	-4.275540	-1.236285	0.000001
H	-2.166358	-2.511193	-0.000001
H	-2.166422	2.511189	-0.000000
C	-0.909603	0.737715	0.000000
C	-0.909543	-0.737632	-0.000001
N	0.240223	1.360874	-0.000005
N	0.240242	-1.360913	-0.000004
Te	1.661677	0.000005	0.000001

==========
M062X-PCM-THF_acceptor-NO3.out
==========

O	1.183129	0.381956	0.000030
O	-0.922448	0.833409	0.000053
O	-0.260697	-1.215485	-0.000014
N	0.000017	0.000138	-0.000080

==========
M062X-PCM-THF_acceptor-quin.out
==========

C	-0.791239	-0.442406	1.304245
C	1.286532	0.001500	0.003055
C	0.749401	-0.295175	1.406960
H	-1.292544	0.142206	2.077677
H	-1.091601	-1.484088	1.435252
H	1.017316	0.519830	2.083454
H	1.199874	-1.207783	1.801771
C	-0.788899	1.351251	-0.272577
H	-1.285597	1.728772	-1.168028
H	-1.093578	1.984985	0.562905
C	0.752116	1.365841	-0.444186
H	1.024676	1.543621	-1.487101
H	1.200391	2.164495	0.149951
H	2.377012	0.002945	0.005877
C	0.756155	-1.067959	-0.956590
H	1.209432	-0.953322	-1.943089
H	1.026861	-2.060158	-0.587805
C	-0.783890	-0.911418	-1.037569
H	-1.083217	-0.504683	-2.005700
H	-1.281897	-1.875378	-0.919910
N	-1.286884	-0.001605	-0.003613

==========
M062X-PCM-THF_complex-Te-diBr-Br.out
==========

C	2.380973	2.199920	0.000014
C	3.255854	1.062034	0.000090
C	2.761706	-0.193093	0.000089
C	1.039267	2.052323	-0.000073
H	2.820537	3.187794	0.000048
H	4.323695	1.231603	0.000154
C	0.435508	0.739527	-0.000066
C	1.336398	-0.435383	-0.000013
N	-0.848966	0.535742	-0.000117
N	0.786726	-1.609994	0.000037
Te	-1.196606	-1.407949	-0.000043
Br	-4.166543	-0.631196	-0.000017
Br	3.919038	-1.685157	0.000234
Br	-0.088017	3.566688	-0.000150

==========
M062X-PCM-THF_complex-Te-diBr-Cl.out
==========

C	1.558124	2.455658	0.000491
C	2.621505	1.491163	0.000360
C	2.359819	0.167635	0.000110
C	0.265453	2.068960	0.000386
H	1.814137	3.506367	0.000646
H	3.641772	1.849006	0.000443
C	-0.093506	0.669907	0.000138
C	1.000837	-0.328517	0.000023
N	-1.320451	0.243567	0.000148
N	0.663022	-1.578832	-0.000329
Te	-1.336627	-1.731974	-0.000275
Cl	-4.147592	-1.437003	-0.000250
Br	-1.119422	3.353678	0.000423
Br	3.773317	-1.086981	-0.000147

==========
M062X-PCM-THF_complex-Te-diBr-I.out
==========

C	2.833298	2.147692	0.000066
C	3.674515	0.984316	0.000055
C	3.146079	-0.257045	0.000025
C	1.488198	2.038951	0.000021
H	3.301703	3.122236	0.000133
H	4.746718	1.123522	0.000099
C	0.849362	0.743122	-0.000107
C	1.714552	-0.457398	0.000001
N	-0.440470	0.576312	0.000040
N	1.132150	-1.617548	-0.000108
Te	-0.838984	-1.354086	-0.000240
I	-4.051444	-0.392888	0.000111
Br	0.401317	3.581606	0.000143
Br	4.262326	-1.779303	0.000042

==========
M062X-PCM-THF_complex-Te-diBr-NO3.out
==========

C	2.577507	2.002164	0.000279
C	3.321612	0.774356	0.000363
C	2.695167	-0.420506	0.000210
C	1.228299	2.000919	0.000031
H	3.123647	2.935451	0.000352
H	4.401542	0.826250	0.000507
C	0.485317	0.760994	-0.000123
C	1.251735	-0.507527	0.000012
N	-0.812579	0.699560	-0.000591
N	0.574374	-1.613433	-0.000322
Te	-1.372045	-1.192562	-0.000214
O	-3.577676	0.107031	0.000770
O	-5.717308	-0.092805	0.000691
O	-4.480062	-1.852595	-0.000392
N	-4.610223	-0.623011	0.000513
Br	0.266127	3.625110	-0.000225
Br	3.693950	-2.023559	0.000221

M062X-PCM-THF_complex-Te-diBr-quin.out

C	2.901485	2.268113	-0.003777
C	3.835333	1.173464	-0.005579
C	3.412293	-0.105559	-0.003092
C	1.571866	2.051644	0.000569
H	3.291796	3.276429	-0.006138
H	4.892257	1.401135	-0.009121
C	1.037328	0.707800	0.003442
C	1.998636	-0.427177	0.001522
N	-0.228196	0.441332	0.006268
N	1.508683	-1.621100	0.003694
Te	-0.500734	-1.523933	0.007527
C	-3.177694	0.087496	-1.231391
C	-5.350934	0.017821	-0.011995
C	-4.605500	0.678168	-1.175745
H	-2.420309	0.863900	-1.332532
H	-3.065699	-0.604567	-2.068296
H	-4.567117	1.758556	-1.024082
H	-5.126701	0.497415	-2.116505
C	-3.163995	0.186959	1.172550
H	-2.767863	-0.310381	2.059433
H	-2.602485	1.110164	1.032268
C	-4.682833	0.446724	1.298296
H	-5.104041	-0.121109	2.130265
H	-4.869036	1.503054	1.495142
H	-6.401105	0.308167	-0.017486
C	-5.216292	-1.501882	-0.150835
H	-5.838850	-2.012183	0.584696
H	-5.554351	-1.814089	-1.140703
C	-3.730485	-1.870367	0.057511
H	-3.568600	-2.336521	1.031509
H	-3.381978	-2.569417	-0.705943
N	-2.880372	-0.667109	0.002067
Br	0.357646	3.497847	0.002697
Br	4.652246	-1.528050	-0.005468

M062X-PCM-THF_complex-Te-nat-Br.out

C	3.874454	1.683773	-0.000042
C	4.425907	0.351960	-0.000308
C	3.630540	-0.740186	-0.000290
C	2.540067	1.896230	0.000261
H	4.555335	2.525613	-0.000125
H	5.502666	0.237984	-0.000575
H	4.036689	-1.743653	-0.000516
H	2.119312	2.893306	0.000392
C	1.633254	0.774364	0.000409
C	2.195499	-0.588378	0.000009
N	0.336315	0.919836	0.000103
N	1.360283	-1.588674	-0.000071
Te	-0.501332	-0.873474	0.000100
Br	-3.194836	0.740649	-0.000138

M062X-PCM-THF_complex-Te-nat-Cl.out

C	-3.588392	1.362448	0.000014
C	-3.965260	-0.028583	-0.000113
C	-3.036079	-1.009897	-0.000164
C	-2.291736	1.742888	0.000084
H	-4.371626	2.110346	0.000110
H	-5.018940	-0.278668	-0.000124
H	-3.311908	-2.057075	-0.000202
H	-2.002173	2.786134	0.000280
C	-1.247973	0.746142	-0.000030
C	-1.630901	-0.677475	-0.000185
N	0.019088	1.056634	0.000276
N	-0.673821	-1.560372	-0.000158
Te	1.089734	-0.609939	0.000104
Cl	3.363744	1.168771	-0.000230

M062X-PCM-THF_complex-Te-nat-I.out

C	-4.219390	1.867846	0.000131
C	-4.861681	0.577668	-0.000085
C	-4.145526	-0.567874	-0.000183
C	-2.873639	1.987439	0.000212
H	-4.840501	2.754705	0.000184
H	-5.943704	0.539521	-0.000164
H	-4.621841	-1.539885	-0.000351
H	-2.383588	2.952360	0.000332
C	-2.048038	0.804908	0.000179
C	-2.703590	-0.515204	0.000016
N	-0.743274	0.858116	0.000195
N	-1.942897	-1.574835	-0.000119
Te	-0.044355	-0.989468	-0.000023
I	3.094538	0.506301	-0.000018

M062X-PCM-THF_complex-Te-nat-NO3.out

C	4.026312	1.505849	0.000204
C	4.464742	0.132743	0.000092
C	3.581490	-0.889641	0.000080
C	2.714489	1.829226	0.000311
H	4.775571	2.287764	0.000148
H	5.528460	-0.069566	-0.000019
H	3.904194	-1.923146	-0.000039
H	2.378431	2.858286	0.000329
C	1.716415	0.786543	0.000238
C	2.163531	-0.618876	0.000165
N	0.436154	1.037154	0.000029
N	1.247674	-1.545917	-0.000032
Te	-0.546187	-0.679117	-0.000182
O	-2.468437	1.119411	-0.001100
O	-4.605190	1.360483	0.000073
O	-3.751410	-0.614041	0.001143
N	-3.624758	0.617168	0.000225

M062X-PCM-THF_complex-Te-nat-quin.out

C	4.249542	2.122547	-0.000450
C	5.029179	0.907240	-0.004075
C	4.441431	-0.307607	-0.004497
C	2.900096	2.098427	0.003322
H	4.773148	3.070309	-0.000908
H	6.108873	0.987893	-0.006630
H	5.019737	-1.222681	-0.007229
H	2.312251	3.007299	0.005868
C	2.202534	0.833262	0.003394
C	2.999385	-0.415083	-0.001316
N	0.905731	0.746874	0.005763
N	2.356322	-1.541876	-0.002919
Te	0.380869	-1.172385	0.001464
C	-2.109185	0.782129	-1.217791
C	-4.278867	0.965563	-0.006367
C	-3.452810	1.545149	-1.158500
H	-1.260307	1.458602	-1.308797
H	-2.081790	0.092498	-2.063907
H	-3.282083	2.610404	-0.990050
H	-3.988363	1.444322	-2.103440
C	-2.095199	0.840533	1.187666
H	-1.773659	0.279493	2.067033
H	-1.418691	1.686506	1.070334
C	-3.569361	1.291395	1.311240
H	-4.064856	0.772578	2.134494
H	-3.621824	2.360857	1.519396
H	-5.285480	1.383366	-0.010535
C	-4.332714	-0.557035	-0.165744
H	-5.016123	-0.995028	0.562731
H	-4.705720	-0.811354	-1.159887
C	-2.903460	-1.109123	0.036970
H	-2.803239	-1.609390	1.002552
H	-2.640939	-1.832121	-0.738714
N	-1.913418	-0.019842	0.004079

M062X-PCM-THF_donor-Te-diBr.out

C	-0.717862	-2.471913	0.000009
C	0.717849	-2.471917	0.000009
C	1.419935	-1.320141	-0.000015
C	-1.419942	-1.320133	-0.000015
H	-1.231747	-3.423281	0.000001
H	1.231729	-3.423288	0.000001
C	-0.740428	-0.045734	-0.000018
C	0.740429	-0.045739	-0.000018
N	-1.355999	1.102476	-0.000145
N	1.356001	1.102470	-0.000145
Te	0.000007	2.519839	0.000146
Br	-3.303124	-1.336655	-0.000076
Br	3.303118	-1.336666	-0.000075

M062X-PCM-THF_donor-Te-nat.out

C	-3.322499	0.720891	0.000001
C	-3.322453	-0.720940	0.000001
C	-2.173112	-1.429503	0.000000
C	-2.173195	1.429488	0.000000
H	-4.274394	1.236300	0.000001
H	-4.274316	-1.236422	0.000001
H	-2.164637	-2.511348	-0.000000
H	-2.164706	2.511343	-0.000000
C	-0.908599	0.738000	0.000000
C	-0.908541	-0.737924	-0.000001
N	0.240251	1.361873	-0.000004
N	0.240276	-1.361903	-0.000003
Te	1.660860	0.000005	0.000001

M062X-PCM-ACN_complex-Te-CN-Br-opp.out

C	-3.371285	1.659102	-0.000039
C	-3.902594	0.315419	0.000147
C	-3.098888	-0.779722	0.000225
C	-2.039396	1.873315	-0.000114
H	-4.066532	2.487573	-0.000129
H	-3.504479	-1.782572	0.000377
H	-1.630667	2.874909	-0.000278
C	-1.125662	0.758439	0.000089
C	-1.673565	-0.606007	0.000187
N	0.171516	0.910090	-0.000108
N	-0.831758	-1.604032	0.000366
Te	1.015300	-0.877378	0.000046
Br	3.701187	0.759264	-0.000299
C	-5.327276	0.144795	0.000233
N	-6.468828	0.019292	0.000276

M062X-PCM-ACN_complex-Te-CN-Br-same.out

C	-3.678332	0.662024	-0.000051
C	-3.953297	-0.756309	0.000140
C	-2.944267	-1.651580	0.000237
C	-2.412502	1.155692	-0.000140
H	-4.985091	-1.080988	0.000202
H	-3.136432	-2.716317	0.000380
H	-2.217432	2.219533	-0.000285
C	-1.304738	0.242662	-0.000040
C	-1.573944	-1.203125	0.000158
N	-0.063461	0.655322	-0.000113
N	-0.548573	-2.009363	0.000234
Te	1.116611	-0.924041	0.000081
Br	3.438507	1.229486	-0.000134
C	-4.790610	1.568812	-0.000150
N	-5.691739	2.280728	-0.000226

M062X-PCM-ACN_complex-Te-CN-Cl-opp.out

C	2.985970	1.542281	-0.000052
C	3.410883	0.161566	-0.000035
C	2.523699	-0.867804	0.000011
C	1.674628	1.858782	-0.000020
H	3.743633	2.314426	-0.000053
H	2.852042	-1.898691	0.000050
H	1.344101	2.889073	0.000017
C	0.676584	0.818258	0.000002
C	1.115126	-0.585089	0.000019
N	-0.603877	1.071200	0.000215
N	0.196052	-1.511358	0.000148
Te	-1.596763	-0.638327	-0.000033
Cl	-3.936339	1.082022	-0.000009
C	4.818317	-0.117382	-0.000025
N	5.947599	-0.326962	-0.000009

M062X-PCM-ACN_complex-Te-CN-Cl-same.out

C	3.284076	0.391376	0.000075
C	3.360763	-1.051153	-0.000011
C	2.237167	-1.797620	-0.000040
C	2.097742	1.054627	0.000145
H	4.337974	-1.514904	-0.000034
H	2.280515	-2.878822	-0.000074
H	2.052029	2.135396	0.000231
C	0.874231	0.303950	0.000108
C	0.940719	-1.165003	-0.000012
N	-0.297393	0.884493	0.000252
N	-0.187290	-1.816860	0.000059
Te	-1.695936	-0.509525	-0.000067
Cl	-3.493111	1.761653	-0.000125
C	4.509005	1.138729	0.000114
N	5.495946	1.726095	0.000145

M062X-PCM-ACN_complex-Te-CN-I-opp.out

C	-3.748114	1.748787	0.000443
C	-4.353882	0.436995	-0.000197
C	-3.614086	-0.702200	-0.000525
C	-2.406463	1.887793	0.000754
H	-4.395093	2.615401	0.000650
H	-4.075394	-1.680664	-0.001029
H	-1.941181	2.864375	0.001210
C	-1.557929	0.723027	0.000514
C	-2.181174	-0.608089	-0.000187
N	-0.253736	0.800605	0.000680
N	-1.398993	-1.654694	-0.000537
Te	0.479618	-1.031453	0.000397
I	3.536977	0.580757	-0.000346
C	-5.786272	0.348490	-0.000537
N	-6.933093	0.289443	-0.000821

M062X-PCM-ACN_complex-Te-CN-I-same.out

C	-4.044321	0.867635	-0.000002
C	-4.452701	-0.518175	0.000036
C	-3.534252	-1.506309	0.000027
C	-2.737464	1.237686	-0.000017
H	-5.510740	-0.742475	0.000069
H	-3.828250	-2.547583	0.000062
H	-2.439602	2.277569	-0.000036
C	-1.722683	0.222253	0.000016
C	-2.127363	-1.190424	-0.000024
N	-0.447412	0.514005	-0.000030
N	-1.184647	-2.093322	0.000048
Te	0.571169	-1.170733	-0.000018
I	3.335741	0.910177	0.000011
C	-5.062675	1.879061	-0.000003
N	-5.886182	2.679440	-0.000010

M062X-PCM-ACN_complex-Te-CN-NO3-opp.out

C	3.464816	1.593870	0.000059
C	3.916216	0.221236	0.000102
C	3.049774	-0.824825	0.000044
C	2.147915	1.886131	-0.000044
H	4.207866	2.380023	0.000089
H	3.396484	-1.849538	0.000057
H	1.798649	2.910124	-0.000100
C	1.168905	0.827052	-0.000087
C	1.636374	-0.568033	-0.000044
N	-0.116591	1.053385	-0.000255
N	0.737302	-1.513962	-0.000165
Te	-1.064584	-0.680595	-0.000116
O	-2.980906	1.080629	-0.000114
O	-5.116644	1.325982	0.000316
O	-4.267038	-0.650023	0.000451
N	-4.139445	0.579754	0.000088
C	5.328585	-0.031897	0.000187
N	6.461099	-0.222546	0.000258

M062X-PCM-ACN_complex-Te-CN-NO3-same.out

C	3.726771	0.609352	-0.000061
C	3.935765	-0.820156	-0.000069
C	2.886167	-1.667116	-0.000029
C	2.485684	1.162116	-0.000015
H	4.951229	-1.192274	-0.000090
H	3.028682	-2.739655	-0.000013
H	2.340305	2.233932	0.000013
C	1.335375	0.302060	0.000014
C	1.537841	-1.155256	0.000005
N	0.115250	0.770419	0.000136
N	0.475340	-1.910394	0.000110
Te	-1.138990	-0.751668	0.000016
O	-2.671277	1.370637	-0.000068
O	-4.716047	2.034957	0.000033
O	-4.274743	-0.070417	0.000048
N	-3.905472	1.110035	-0.000088
C	4.879867	1.463784	-0.000074
N	5.811877	2.134883	-0.000085

M062X-PCM-ACN_complex-Te-CN-Quin-opp.out

C	3.889085	1.848641	0.005263
C	4.584605	0.579695	-0.002002
C	3.925272	-0.606317	-0.004053
C	2.542347	1.896577	0.010392
H	4.476957	2.756581	0.006195
H	4.454288	-1.550025	-0.009596
H	2.013382	2.840381	0.015563
C	1.770571	0.676312	0.008227
C	2.485327	-0.615749	0.000636
N	0.470373	0.666333	0.010733
N	1.775652	-1.703965	-0.002355
Te	-0.171618	-1.213518	0.002654
C	-2.539840	0.852399	-1.219522
C	-4.702059	1.114110	-0.009336
C	-3.852679	1.666489	-1.157818
H	-1.665954	1.496370	-1.310140
H	-2.540233	0.162623	-2.065854
H	-3.640734	2.723415	-0.984577
H	-4.389673	1.589476	-2.103957
C	-2.525800	0.909766	1.187636
H	-2.222701	0.338880	2.067041
H	-1.822525	1.733200	1.067955
C	-3.983869	1.408911	1.310971
H	-4.496664	0.902080	2.130885
H	-3.999110	2.478241	1.524858
H	-5.692436	1.568763	-0.014268
C	-4.811200	-0.405276	-0.174314
H	-5.513685	-0.820667	0.548931
H	-5.186645	-0.642354	-1.171649
C	-3.406159	-1.010320	0.035504
H	-3.328061	-1.510442	1.003091
H	-3.169089	-1.745032	-0.737222
N	-2.374457	0.042632	0.003141
C	6.019651	0.591531	-0.007774
N	7.167792	0.615120	-0.012681

M062X-PCM-ACN_complex-Te-CN-Quin-same.out

C	4.168225	1.074966	-0.000352
C	4.714287	-0.265513	0.009252
C	3.899607	-1.338619	0.010026
C	2.832298	1.314320	-0.009024
H	5.789530	-0.382150	0.015820
H	4.295630	-2.345576	0.017277
H	2.435639	2.320712	-0.015962
C	1.919233	0.203350	-0.007042
C	2.464502	-1.168730	0.002114
N	0.628063	0.367570	-0.011784
N	1.615386	-2.149900	0.003554
Te	-0.254296	-1.409483	-0.002915
C	-2.344359	0.919776	-1.252550
C	-4.398344	1.560077	0.003981
C	-3.503991	1.938553	-1.181458
H	-1.383062	1.408740	-1.406644
H	-2.492265	0.204514	-2.064060
H	-3.116804	2.950152	-1.044308
H	-4.073834	1.927917	-2.111280
C	-2.238583	1.075410	1.146524
H	-1.978837	0.506998	2.041291
H	-1.435647	1.787850	0.962015
C	-3.606240	1.777749	1.297686
H	-4.160483	1.365086	2.143277
H	-3.463002	2.842287	1.486595
H	-5.306997	2.161310	0.005244
C	-4.739653	0.070709	-0.107120
H	-5.485702	-0.211219	0.636660
H	-5.160638	-0.139554	-1.092343
C	-3.438854	-0.733029	0.111151
H	-3.412591	-1.185790	1.104394
H	-3.337592	-1.536039	-0.622379
N	-2.258962	0.144992	0.000597
C	5.081933	2.181699	0.000251
N	5.822612	3.059277	0.001259

M062X-PCM-ACN_complex-Te-CN.out

C	-2.609866	1.354508	-0.000002
C	-2.836750	-0.072392	-0.000002
C	-1.816985	-0.968870	-0.000003
C	-1.357507	1.854463	-0.000003
H	-3.469379	2.010830	-0.000002
H	-1.994518	-2.035574	-0.000004
H	-1.174722	2.920392	-0.000004
C	-0.225696	0.963774	-0.000003
C	-0.465348	-0.487042	-0.000003
N	1.012038	1.388173	-0.000008
N	0.565725	-1.294865	-0.000008
Te	2.184217	-0.187681	0.000005
C	-4.191970	-0.545524	-0.000002
N	-5.280037	-0.911845	-0.000002

M062X-PCM-ACN_complex-Te-F4-Br.out

C	-3.192849	1.252799	-0.000024
C	-3.639900	-0.113323	-0.000118
C	-2.765320	-1.135062	0.000084
C	-1.883757	1.563414	0.000232
C	-0.891242	0.521273	0.000337
C	-1.347620	-0.880341	0.000348
N	0.385286	0.762377	0.000487
N	-0.445323	-1.811042	0.000375
Te	1.361552	-0.958265	0.000320
Br	3.883506	0.830214	-0.000699
F	-4.132551	2.192675	-0.000258
F	-1.492160	2.834110	0.000296
F	-4.953834	-0.316287	-0.000390
F	-3.196900	-2.392678	-0.000023

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M062X-PCM-ACN_complex-Te-F4-Cl.out
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C	2.847189	1.070544	-0.000001
C	3.151425	-0.334577	-0.000054
C	2.176373	-1.261169	-0.000057
C	1.576756	1.513002	0.000044
C	0.482719	0.578689	0.000029
C	0.791056	-0.863584	-0.000016
N	-0.760355	0.952666	0.000068
N	-0.204575	-1.691650	-0.000027
Te	-1.921980	-0.652441	0.000039
Cl	-4.027345	1.258577	-0.000063
F	3.879032	1.909037	0.000010
F	1.317358	2.817793	0.000107
F	4.438218	-0.671289	-0.000107
F	2.477531	-2.557033	-0.000112

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M062X-PCM-ACN_complex-Te-F4-I.out
==========

C	-3.549420	1.373901	-0.000166
C	-4.084235	0.039022	0.000005
C	-3.277665	-1.037114	-0.000174
C	-2.223028	1.599864	-0.000633
C	-1.300502	0.495982	-0.000727
C	-1.847408	-0.872590	-0.000413
N	-0.010325	0.653332	-0.000744
N	-1.008785	-1.862205	-0.000540
Te	0.840996	-1.131781	-0.000542
I	3.762765	0.601653	0.001054
F	-4.425909	2.372114	0.000016
F	-1.750111	2.841859	-0.000920
F	-5.407700	-0.078663	0.000340
F	-3.786394	-2.265007	-0.000109

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M062X-PCM-ACN_complex-Te-F4-NO3.out
==========

C	3.265743	1.169139	-0.000019
C	3.629825	-0.221848	0.000121
C	2.695792	-1.189634	0.000160
C	1.977942	1.557566	-0.000106
C	0.924216	0.577033	-0.000126
C	1.295386	-0.850594	0.000052
N	-0.334320	0.894705	-0.000079
N	0.337464	-1.723067	0.000057
Te	-1.413318	-0.763946	-0.000212
O	-3.154541	1.110816	0.000224
O	-5.263349	1.526556	0.000431
O	-4.575822	-0.511297	0.000142
N	-4.352045	0.703707	0.000178
F	4.260982	2.050115	-0.000002
F	1.663690	2.849606	-0.000167
F	4.929347	-0.502164	0.000225
F	3.051660	-2.470982	0.000285

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M062X-PCM-ACN_complex-Te-F4-Quin.out
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C	3.662496	1.522954	0.000099
C	4.313644	0.238156	-0.002800
C	3.606976	-0.904358	-0.002647
C	2.322728	1.631945	0.003410
C	1.497795	0.451147	0.004126
C	2.163520	-0.871941	0.000460
N	0.205633	0.496192	0.006021
N	1.414047	-1.920996	-0.000320
Te	-0.524842	-1.355358	0.002700
C	-2.776177	0.792976	-1.229812
C	-4.914288	1.167003	-0.006933
C	-4.046589	1.670737	-1.163939
H	-1.872658	1.392022	-1.336738
H	-2.819110	0.093246	-2.066779
H	-3.781586	2.716831	-0.998451
H	-4.592581	1.614695	-2.106282
C	-2.741064	0.878850	1.177673
H	-2.452122	0.307246	2.061111
H	-2.006122	1.670926	1.039435
C	-4.175766	1.438132	1.307403
H	-4.703215	0.957080	2.133512
H	-4.144383	2.508055	1.515860
H	-5.882472	1.666928	-0.010425
C	-5.093666	-0.346928	-0.160202
H	-5.813942	-0.725672	0.565508
H	-5.478433	-0.574436	-1.156155
C	-3.718557	-1.013919	0.055870
H	-3.659558	-1.499570	1.032028
H	-3.519636	-1.772375	-0.704443
N	-2.638134	-0.009677	0.002318
F	4.449466	2.593202	-0.001022
F	1.742452	2.828687	0.005604
F	5.642923	0.241316	-0.005790
F	4.225209	-2.081374	-0.005566

M062X-PCM-ACN_donor-Te-F4.out

C	-0.000001	-2.538479	0.719039
C	-0.000001	-2.538479	-0.719039
C	-0.000001	-1.390672	-1.421382
C	-0.000001	-1.390672	1.421382
C	-0.000001	-0.126864	0.736614
C	-0.000001	-0.126864	-0.736614
N	-0.000006	1.017794	1.357828
N	-0.000006	1.017794	-1.357828
Te	0.000004	2.437081	0.000000
F	-0.000003	-1.406793	2.748817
F	-0.000001	-3.721270	1.319004
F	-0.000001	-3.721270	-1.319004
F	-0.000003	-1.406793	-2.748817

M062X-PCM-THF_complex-Te-CN-Br-opp.out

C	-3.371279	1.648451	0.000029
C	-3.897124	0.302831	-0.000042
C	-3.087469	-0.788701	-0.000142
C	-2.039969	1.867380	0.000032
H	-4.070227	2.473949	0.000084
H	-3.489140	-1.793197	-0.000184
H	-1.633199	2.869765	0.000078
C	-1.121330	0.756606	0.000072
C	-1.662640	-0.610550	-0.000117
N	0.174065	0.916364	0.000039
N	-0.814891	-1.602890	-0.000071
Te	1.034396	-0.863561	0.000056
Br	3.660919	0.752568	-0.000050
C	-5.320971	0.127314	-0.000004
N	-6.462530	0.000068	0.000015

M062X-PCM-THF_complex-Te-CN-Br-same.out

C	-3.685205	0.641383	-0.000024
C	-3.945507	-0.779435	0.000058
C	-2.926823	-1.663935	0.000124
C	-2.423406	1.146927	-0.000042
H	-4.974149	-1.114163	0.000062
H	-3.106723	-2.730868	0.000182
H	-2.238710	2.212566	-0.000114
C	-1.305965	0.246047	0.000025
C	-1.560793	-1.202452	0.000113
N	-0.069495	0.672349	-0.000029
N	-0.527304	-1.996854	0.000172
Te	1.131581	-0.891860	0.000098
Br	3.417928	1.203040	-0.000173
C	-4.807902	1.534977	-0.000098
N	-5.719842	2.233324	-0.000157

M062X-PCM-THF_complex-Te-CN-Cl-opp.out

C	2.991160	1.535015	0.000312
C	3.412227	0.153451	0.000491
C	2.520356	-0.872865	0.000299
C	1.680316	1.854777	-0.000008
H	3.751244	2.304911	0.000435
H	2.845803	-1.904846	0.000409
H	1.351112	2.885594	-0.000175
C	0.679033	0.817543	-0.000096
C	1.112602	-0.587181	0.000008
N	-0.599669	1.076551	-0.000275
N	0.189103	-1.508751	-0.000113
Te	-1.605520	-0.625462	-0.000370
Cl	-3.912377	1.060008	0.000097
C	4.818887	-0.129066	0.000884
N	5.947965	-0.340918	0.001189

M062X-PCM-THF_complex-Te-CN-Cl-same.out

C	3.284926	0.382264	-0.000066
C	3.356096	-1.060357	0.000008
C	2.229464	-1.802833	0.000033
C	2.099686	1.048453	-0.000090
H	4.331925	-1.527275	0.000084
H	2.268890	-2.884326	0.000167
H	2.056505	2.129437	-0.000079
C	0.873573	0.302460	-0.000022
C	0.934103	-1.167166	-0.000061
N	-0.294583	0.888691	0.000206
N	-0.196356	-1.812967	0.000204
Te	-1.704772	-0.493514	-0.000052
Cl	-3.461052	1.735684	0.000045
C	4.512703	1.124477	-0.000020
N	5.503140	1.706338	0.000026

M062X-PCM-THF_complex-Te-CN-I-opp.out

C	-3.752174	1.732904	0.000050
C	-4.346864	0.416185	-0.000035
C	-3.595556	-0.716000	-0.000081
C	-2.411456	1.882883	0.000097
H	-4.407014	2.593704	0.000061
H	-4.048254	-1.698518	-0.000142
H	-1.953124	2.862673	0.000156
C	-1.552076	0.726106	0.000070
C	-2.163544	-0.610530	-0.000028
N	-0.249329	0.817696	0.000110
N	-1.370845	-1.648400	-0.000057
Te	0.506838	-1.005765	0.000052
I	3.499357	0.569128	-0.000047
C	-5.778214	0.314539	-0.000068
N	-6.924658	0.245217	-0.000098

M062X-PCM-THF_complex-Te-CN-I-same.out

C	-4.046849	0.839983	-0.000046
C	-4.438056	-0.550673	-0.000188
C	-3.507314	-1.527607	-0.000211
C	-2.743715	1.224476	0.000080
H	-5.493539	-0.787421	-0.000276
H	-3.788015	-2.572686	-0.000299
H	-2.457552	2.267755	0.000285
C	-1.716623	0.221620	0.000059
C	-2.103833	-1.196040	-0.000196
N	-0.445794	0.530539	0.000123
N	-1.149692	-2.085752	-0.000099
Te	0.599515	-1.138146	0.000113
I	3.300909	0.899921	-0.000069
C	-5.078534	1.837510	0.000052
N	-5.915124	2.624435	0.000082

M062X-PCM-THF_complex-Te-CN-NO3-opp.out

C	3.469128	1.585112	0.000111
C	3.914816	0.210784	0.000153
C	3.042200	-0.830752	0.000057
C	2.153242	1.883103	-0.000026
H	4.216018	2.367731	0.000171
H	3.383843	-1.857333	0.000068
H	1.807433	2.908358	-0.000082
C	1.168768	0.828983	-0.000106
C	1.630000	-0.568324	-0.000066
N	-0.115007	1.062634	-0.000306
N	0.726155	-1.509159	-0.000228
Te	-1.074945	-0.665419	-0.000190
O	-2.958954	1.067661	-0.000207
O	-5.094785	1.310376	0.000359
O	-4.243749	-0.665124	0.000703
N	-4.119604	0.564852	0.000216
C	5.325914	-0.048767	0.000278
N	6.457786	-0.244203	0.000383

M062X-PCM-THF_complex-Te-CN-NO3-same.out

C	3.725176	0.601072	-0.004211
C	3.928828	-0.828982	0.021154
C	2.876157	-1.672462	0.026952
C	2.484572	1.155907	-0.022907
H	4.943462	-1.203501	0.035622
H	3.014453	-2.745422	0.046099
H	2.341532	2.227860	-0.040946
C	1.331695	0.300164	-0.015059
C	1.529037	-1.157617	0.009296
N	0.113845	0.773782	-0.024976
N	0.463897	-1.908083	0.016073
Te	-1.148790	-0.740821	-0.001634
O	-2.643193	1.351139	0.035140
O	-4.680731	2.035727	0.057399
O	-4.261842	-0.069791	-0.080400
N	-3.882553	1.104142	0.003774
C	4.881155	1.451202	-0.007470
N	5.816820	2.117507	-0.009078

M062X-PCM-THF_complex-Te-CN-Quin-opp.out

C	3.883134	1.851098	0.004359
C	4.582157	0.583655	-0.001669
C	3.925315	-0.603336	-0.003225
C	2.536551	1.896778	0.008834
H	4.469774	2.759890	0.004937
H	4.455555	-1.546305	-0.007852
H	2.004881	2.839010	0.013124
C	1.766987	0.674890	0.007201
C	2.485096	-0.616017	0.000754
N	0.467220	0.662646	0.009241
N	1.779122	-1.706008	-0.002019
Te	-0.167250	-1.220293	0.002174
C	-2.540849	0.850024	-1.219754
C	-4.701170	1.122085	-0.008352
C	-3.851140	1.668605	-1.159229
H	-1.664287	1.490230	-1.311003
H	-2.543102	0.159517	-2.065609
H	-3.635860	2.725370	-0.988958
H	-4.389615	1.591638	-2.104596
C	-2.524519	0.909010	1.186864
H	-2.224627	0.336447	2.066346
H	-1.814872	1.726974	1.067581
C	-3.979685	1.417225	1.310195
H	-4.494860	0.916753	2.132601
H	-3.989202	2.487379	1.520417
H	-5.689772	1.580701	-0.012821
C	-4.816961	-0.397345	-0.169868
H	-5.519711	-0.808312	0.555735
H	-5.196649	-0.634763	-1.165592
C	-3.413413	-1.007578	0.037073
H	-3.335325	-1.508716	1.004271
H	-3.180525	-1.743222	-0.736142
N	-2.378382	0.040887	0.003118
C	6.017295	0.600282	-0.006685
N	7.165242	0.629103	-0.010978

M062X-PCM-THF_complex-Te-CN-Quin-same.out

C	4.162720	1.081333	-0.000313
C	4.711977	-0.258059	0.010616
C	3.900558	-1.333421	0.011557
C	2.826367	1.316815	-0.010058
H	5.787622	-0.371243	0.018030
H	4.297964	-2.339737	0.019794
H	2.426865	2.322026	-0.017961
C	1.915855	0.203546	-0.007811
C	2.464988	-1.167408	0.002572
N	0.624580	0.364625	-0.013206
N	1.619816	-2.151568	0.004174
Te	-0.249599	-1.416932	-0.003404
C	-2.343785	0.920041	-1.251209
C	-4.396287	1.566692	0.004833
C	-3.500307	1.942585	-1.180286
H	-1.380449	1.405649	-1.403022
H	-2.492498	0.206643	-2.064344
H	-3.110021	2.952944	-1.042705
H	-4.070100	1.934975	-2.110229
C	-2.238752	1.071475	1.147361
H	-1.981887	0.500636	2.041482
H	-1.431461	1.779472	0.964804
C	-3.603261	1.780214	1.298746
H	-4.159871	1.370245	2.144193
H	-3.455692	2.844064	1.488331
H	-5.302670	2.171409	0.006558
C	-4.743531	0.078666	-0.107279
H	-5.490492	-0.200798	0.636601
H	-5.166759	-0.128906	-1.092175
C	-3.445233	-0.730239	0.108828
H	-3.420644	-1.185905	1.100908
H	-3.347037	-1.532204	-0.626412
N	-2.262676	0.143083	0.000370
C	5.074138	2.190167	0.000157
N	5.813077	3.069110	0.001075

M062X-PCM-THF_complex-Te-CN.out

C	-2.608796	1.353944	-0.000002
C	-2.836374	-0.073256	-0.000002
C	-1.816775	-0.969377	-0.000004
C	-1.356908	1.854417	-0.000003
H	-3.468702	2.009834	-0.000002
H	-1.993853	-2.036121	-0.000005
H	-1.173346	2.920159	-0.000004
C	-0.224690	0.963824	-0.000003
C	-0.464611	-0.487727	-0.000004
N	1.012173	1.389009	-0.000009
N	0.565450	-1.295860	-0.000008
Te	2.183833	-0.187619	0.000005
C	-4.192186	-0.545189	-0.000002
N	-5.280678	-0.909935	-0.000002

M062X-PCM-THF_complex-Te-F4-Br.out

C	-3.206995	1.233405	-0.000085
C	-3.639860	-0.136677	-0.000015
C	-2.753974	-1.148690	0.000044
C	-1.901028	1.558578	-0.000059
C	-0.895793	0.527568	0.000014
C	-1.338560	-0.879088	0.000031
N	0.377899	0.782966	0.000004
N	-0.427204	-1.799745	0.000061
Te	1.376270	-0.927104	0.000223
Br	3.871414	0.808381	-0.000303
F	-4.157856	2.163902	-0.000130
F	-1.527462	2.834251	-0.000086
F	-4.952890	-0.353792	-0.000030
F	-3.173250	-2.410704	0.000128

M062X-PCM-THF_complex-Te-F4-Cl.out

C	2.850806	1.063252	0.000105
C	3.150623	-0.342373	-0.000027
C	2.172454	-1.266074	-0.000035
C	1.581399	1.509764	0.000202
C	0.484034	0.578793	0.000297
C	0.787733	-0.864848	0.000167
N	-0.756901	0.958548	0.000048
N	-0.210950	-1.688320	0.000026
Te	-1.929650	-0.639169	0.000133
Cl	-4.009005	1.238884	-0.000403
F	3.886391	1.899398	-0.000055
F	1.327332	2.815183	0.000088
F	4.437748	-0.683642	-0.000267
F	2.471592	-2.562817	-0.000302

M062X-PCM-THF_complex-Te-F4-I.out

C	-3.563698	1.350400	0.000131
C	-4.081410	0.009302	0.001222
C	-3.261169	-1.056653	0.000837
C	-2.240072	1.593580	-0.001324
C	-1.302826	0.501198	-0.001369
C	-1.832481	-0.874662	-0.000455
N	-0.015407	0.676297	-0.002166
N	-0.980935	-1.852334	-0.000355
Te	0.865263	-1.095485	-0.001302
I	3.740921	0.588338	0.001257
F	-4.454160	2.337899	0.000638
F	-1.785011	2.841762	-0.002404
F	-5.404570	-0.125112	0.002636
F	-3.756055	-2.290486	0.001851

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M062X-PCM-THF_complex-Te-F4-NO3.out
==========

C	3.270365	1.159507	0.001818
C	3.627781	-0.232978	0.007349
C	2.689077	-1.196166	0.006744
C	1.984272	1.554782	-0.004300
C	0.925395	0.579453	-0.005232
C	1.290225	-0.850180	0.000663
N	-0.331343	0.903408	-0.010584
N	0.327950	-1.717116	0.000193
Te	-1.420274	-0.748554	-0.008521
O	-3.148457	1.113880	-0.015300
O	-5.261962	1.502730	0.038573
O	-4.549717	-0.526519	0.005950
N	-4.342415	0.691923	0.010207
F	4.270320	2.036570	0.003090
F	1.678274	2.848387	-0.009282
F	4.926792	-0.520328	0.013066
F	3.039424	-2.479067	0.011831

==========
M062X-PCM-THF_complex-Te-F4-Quin.out
==========

C	-3.658455	1.526240	-0.000037
C	-4.312121	0.242209	0.002070
C	-3.607777	-0.901917	0.001938
C	-2.318418	1.633898	-0.002603
C	-1.495425	0.451473	-0.003335
C	-2.163980	-0.870955	-0.000382
N	-0.203323	0.494290	-0.004787
N	-1.417427	-1.921730	0.000408
Te	0.519815	-1.360297	-0.001913
C	2.777838	0.792251	1.229361
C	4.915093	1.169671	0.005520
C	4.048407	1.670255	1.164696
H	1.873906	1.390916	1.334828
H	2.819526	0.092890	2.066834
H	3.783269	2.716784	1.002298
H	4.595748	1.612546	2.106241
C	2.741062	0.877789	-1.177259
H	2.453574	0.305109	-2.060553
H	2.002750	1.666776	-1.039468
C	4.174110	1.441817	-1.307321
H	4.702529	0.964957	-2.135341
H	4.139829	2.512177	-1.513172
H	5.882558	1.671110	0.008328
C	5.097387	-0.344244	0.156205
H	5.816513	-0.720820	-0.571892
H	5.486098	-0.572446	1.150545
C	3.722207	-1.012863	-0.056281
H	3.661945	-1.500438	-1.031549
H	3.525359	-1.770765	0.705280
N	2.641144	-0.010691	-0.002185
F	-4.443851	2.597293	0.000947
F	-1.736694	2.829394	-0.004060
F	-5.641130	0.248487	0.004291
F	-4.226802	-2.077418	0.004114

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M062X-PCM-THF_donor-Te-F4.out
==========

C	-0.000001	-2.537762	0.719371
C	-0.000001	-2.537762	-0.719371
C	-0.000001	-1.390357	-1.422484
C	-0.000001	-1.390357	1.422484
C	-0.000001	-0.126299	0.737170
C	-0.000001	-0.126299	-0.737170
N	-0.000005	1.017573	1.358773
N	-0.000005	1.017573	-1.358773
Te	0.000004	2.436341	0.000000
F	-0.000003	-1.406263	2.749049
F	-0.000001	-3.720556	1.318246
F	-0.000001	-3.720556	-1.318246
F	-0.000003	-1.406263	-2.749049

5.4.3.2.3 CPCM

==========
M062X-CPCM-ACN_acceptor-NO3.out
==========

O	-0.247233	-1.217812	-0.000061
O	1.178919	0.394947	-0.000038
O	-0.931799	0.822811	-0.000106
N	0.000129	0.000062	0.000235

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M062X-CPCM-ACN_acceptor-quin.out
==========

C	-0.786901	-0.715174	-1.180171
C	1.286905	-0.003224	0.003279
C	0.753114	-0.887369	-1.128365
H	-1.286860	-1.684098	-1.229938
H	-1.084694	-0.146501	-2.063544
H	1.020510	-1.929383	-0.937603
H	1.205593	-0.602781	-2.080085
C	-0.792831	-0.659715	1.208199
H	-1.291188	-0.215771	2.071825
H	-1.096939	-1.707144	1.156487
C	0.747618	-0.538205	1.333594
H	1.018249	0.145698	2.141548
H	1.194055	-1.507487	1.563600
H	2.377371	-0.006274	0.005964
C	0.756866	1.419528	-0.199881
H	1.207183	2.100219	0.525025
H	1.031074	1.774959	-1.196019
C	-0.784076	1.381090	-0.033679
H	-1.086317	1.861547	0.899070
H	-1.277840	1.910796	-0.850298
N	-1.287767	0.003520	-0.003412

M062X-CPCM-ACN_complex-Te-diBr-Br.out

C	2.341088	2.230227	-0.000093
C	3.237462	1.108821	-0.000086
C	2.769161	-0.155873	0.000001
C	1.003076	2.057083	-0.000001
H	2.762927	3.225754	-0.000202
H	4.301508	1.300814	-0.000179
C	0.425741	0.732587	0.000158
C	1.348292	-0.425387	0.000108
N	-0.854322	0.502691	0.000134
N	0.820521	-1.611095	0.000201
Te	-1.161412	-1.446235	0.000220
Br	-4.180062	-0.636700	-0.000242
Br	3.956853	-1.622952	-0.000013
Br	-0.153458	3.549701	-0.000143

M062X-CPCM-ACN_complex-Te-diBr-Cl.out

C	1.535687	2.465677	0.000323
C	2.607788	1.510469	0.000283
C	2.359659	0.184697	0.000156
C	0.247089	2.067465	0.000246
H	1.784145	3.518187	0.000385
H	3.624200	1.878879	0.000349
C	-0.098168	0.664734	0.000133
C	1.005085	-0.323700	0.000091
N	-1.320814	0.225211	-0.000010
N	0.679690	-1.578228	-0.000034
Te	-1.312845	-1.749447	-0.000312
Cl	-4.166660	-1.431819	-0.000095
Br	-1.150228	3.338686	0.000198
Br	3.785595	-1.053824	0.000088

M062X-CPCM-ACN_complex-Te-diBr-I.out

C	2.818326	2.167119	0.000043
C	3.672953	1.013078	0.000042
C	3.159957	-0.234434	-0.000007
C	1.474991	2.043141	-0.000014
H	3.276819	3.146328	-0.000033
H	4.743184	1.166183	-0.000034
C	0.851702	0.740028	0.000025
C	1.730584	-0.450295	0.000060
N	-0.436228	0.556375	-0.000423
N	1.161995	-1.618152	-0.000371
Te	-0.806250	-1.379087	0.000485
I	-4.087156	-0.393738	-0.000004
Br	0.369256	3.572798	-0.000324
Br	4.293396	-1.743405	-0.000255

M062X-CPCM-ACN_complex-Te-diBr-NO3.out

C	2.565237	2.018017	0.000307
C	3.319397	0.795717	0.000352
C	2.703090	-0.404158	0.000160
C	1.216487	2.005810	0.000069
H	3.105091	2.954909	0.000420
H	4.398748	0.857904	0.000502
C	0.484220	0.759844	-0.000109
C	1.260439	-0.502013	-0.000049
N	-0.813321	0.686602	-0.000507
N	0.592313	-1.614245	-0.000398
Te	-1.354217	-1.210887	-0.000221
O	-3.598119	0.100823	0.000569
O	-5.738483	-0.092514	0.000620
O	-4.505822	-1.855221	-0.000142
N	-4.630624	-0.625415	0.000403
Br	0.239339	3.621401	-0.000102
Br	3.712748	-1.999667	0.000139

M062X-CPCM-ACN_complex-Te-diBr-quin.out

C	2.930760	2.248511	0.003069
C	3.852002	1.143796	0.003646
C	3.412505	-0.129523	0.001164
C	1.598212	2.048202	0.000298
H	3.333366	3.251980	0.004775
H	4.911512	1.360083	0.005850
C	1.046206	0.710946	-0.000839
C	1.994996	-0.434408	-0.001058
N	-0.222545	0.457287	-0.001622
N	1.490225	-1.622677	-0.002685
Te	-0.519795	-1.504175	-0.002131
C	-3.206812	0.070061	-1.246763
C	-5.362596	0.008244	0.000102
C	-4.632354	0.662642	-1.176776
H	-2.451774	0.842994	-1.388056
H	-3.113899	-0.647181	-2.064528
H	-4.590710	1.743797	-1.030319
H	-5.163662	0.477007	-2.110941
C	-3.165766	0.233077	1.153999
H	-2.742426	-0.228353	2.047781
H	-2.630193	1.165226	0.976336
C	-4.687415	0.460587	1.299084
H	-5.083974	-0.111821	2.140157
H	-4.892926	1.514001	1.492418
H	-6.415979	0.287061	-0.000528
C	-5.210103	-1.511604	-0.121094
H	-5.829599	-2.021560	0.617263
H	-5.538281	-1.839336	-1.109376
C	-3.722813	-1.858304	0.101098
H	-3.558214	-2.286673	1.091783
H	-3.367254	-2.582246	-0.635625
N	-2.884598	-0.648203	0.002549
Br	0.407705	3.514820	-0.001400
Br	4.632319	-1.569851	0.001131

M062X-CPCM-ACN_complex-Te-nat-Br.out

C	3.868130	1.712294	0.000024
C	4.432615	0.385396	-0.000098
C	3.648622	-0.714493	-0.000172
C	2.532141	1.913379	0.000067
H	4.541695	2.559791	0.000059
H	5.510285	0.282441	-0.000121
H	4.064606	-1.713885	-0.000250
H	2.104224	2.907515	0.000138
C	1.636381	0.782599	0.000102
C	2.212573	-0.574729	-0.000070
N	0.337192	0.912405	0.000100
N	1.388424	-1.584861	-0.000034
Te	-0.474482	-0.892528	0.000055
Br	-3.245996	0.744460	-0.000064

M062X-CPCM-ACN_complex-Te-nat-Cl.out

C	-3.578024	1.385095	0.000007
C	-3.965718	-0.003354	-0.000032
C	-3.045086	-0.992368	-0.000061
C	-2.278927	1.756372	0.000020
H	-4.355631	2.138632	0.000028
H	-5.021230	-0.244575	-0.000043
H	-3.330134	-2.036917	-0.000084
H	-1.982684	2.797639	0.000045
C	-1.243621	0.751163	0.000066
C	-1.637886	-0.669544	-0.000031
N	0.026927	1.049680	0.000013
N	-0.688255	-1.561623	-0.000020
Te	1.077523	-0.629259	0.000022
Cl	3.399021	1.193301	-0.000050

M062X-CPCM-ACN_complex-Te-nat-I.out

C	-4.185543	1.907763	0.000059
C	-4.849268	0.628160	0.000081
C	-4.152989	-0.529367	0.000076
C	-2.838270	2.006038	0.000031
H	-4.792413	2.804267	0.000065
H	-5.931592	0.608589	0.000100
H	-4.646160	-1.492874	0.000087
H	-2.334053	2.963690	0.000024
C	-2.032633	0.809674	0.000018
C	-2.710369	-0.499837	0.000039
N	-0.726877	0.838982	-0.000008
N	-1.968239	-1.573002	0.000053
Te	-0.062402	-1.022060	-0.000072
I	3.102441	0.518245	0.000025

M062X-CPCM-ACN_complex-Te-nat-NO3.out

C	4.017133	1.525155	0.000062
C	4.465396	0.154951	0.000120
C	3.589654	-0.873541	0.000116
C	2.703371	1.840313	-0.000000
H	4.761189	2.311817	0.000077
H	5.530335	-0.039749	0.000180
H	3.919962	-1.904513	0.000174
H	2.362292	2.867623	-0.000032
C	1.712590	0.790865	-0.000024
C	2.170337	-0.611550	0.000044
N	0.429749	1.031021	-0.000022
N	1.261703	-1.546167	0.000066
Te	-0.536327	-0.695878	-0.000145
O	-2.480915	1.120424	-0.000042
O	-4.615492	1.380494	0.000281
O	-3.778246	-0.600986	0.000249
N	-3.639799	0.628553	0.000146

M062X-CPCM-ACN_complex-Te-nat-quin.out

C	4.260000	2.113019	-0.000223
C	5.034685	0.894482	-0.005455
C	4.441870	-0.318137	-0.006338
C	2.910286	2.094051	0.004644
H	4.787518	3.058546	-0.000424
H	6.114641	0.970934	-0.008889
H	5.017753	-1.234860	-0.010320
H	2.326679	3.005740	0.008297
C	2.207701	0.831551	0.004253
C	2.999273	-0.419961	-0.002029
N	0.910418	0.749877	0.007504
N	2.350037	-1.543409	-0.003950
Te	0.372891	-1.166147	0.002114
C	-2.108371	0.780191	-1.220745
C	-4.276992	0.961072	-0.007783
C	-3.452181	1.542168	-1.160004
H	-1.260938	1.457742	-1.317731
H	-2.083808	0.086495	-2.063550
H	-3.281848	2.607324	-0.990735
H	-3.987606	1.440860	-2.104857
C	-2.092568	0.848715	1.185085
H	-1.765332	0.294216	2.066465
H	-1.423621	1.699773	1.061025
C	-3.569151	1.290019	1.309876
H	-4.060511	0.766634	2.132607
H	-3.627361	2.358904	1.519170
H	-5.284814	1.375712	-0.012835
C	-4.325537	-0.561671	-0.165717
H	-5.009252	-1.001340	0.561320
H	-4.693706	-0.818370	-1.160966
C	-2.895666	-1.109012	0.042824
H	-2.795680	-1.602292	1.011895
H	-2.629973	-1.835912	-0.728033
N	-1.907960	-0.016379	0.004629

M062X-CPCM-ACN_donor-Te-diBr.out

C	-0.717744	-2.472831	0.000010
C	0.717732	-2.472835	0.000010
C	1.418795	-1.320333	-0.000016
C	-1.418802	-1.320326	-0.000016
H	-1.230848	-3.424581	0.000000
H	1.230831	-3.424588	0.000000
C	-0.739982	-0.046025	-0.000018
C	0.739983	-0.046029	-0.000018
N	-1.354824	1.103210	-0.000152
N	1.354827	1.103205	-0.000152
Te	0.000006	2.521353	0.000153
Br	-3.303113	-1.337649	-0.000079
Br	3.303107	-1.337660	-0.000079

M062X-CPCM-ACN_donor-Te-nat.out

C	-3.323832	0.720807	0.000001
C	-3.323786	-0.720855	0.000001
C	-2.173956	-1.429238	0.000000
C	-2.174040	1.429223	0.000000
H	-4.275734	1.236144	0.000001
H	-4.275656	-1.236264	0.000001
H	-2.166512	-2.511169	-0.000001
H	-2.166576	2.511165	-0.000000
C	-0.909682	0.737686	0.000000
C	-0.909622	-0.737603	-0.000001
N	0.240222	1.360787	-0.000005
N	0.240241	-1.360827	-0.000004
Te	1.661745	0.000005	0.000001

M062X-CPCM-THF_acceptor-NO3.out

O	0.923281	-0.832505	0.000036
O	0.259569	1.215556	0.000059
O	-1.182823	-0.383080	-0.000008
N	-0.000032	0.000033	-0.000098

M062X-CPCM-THF_acceptor-quin.out

C	-0.785699	0.127767	1.374610
C	1.287048	-0.002332	-0.001939
C	0.755483	0.294914	1.403576
H	-1.280187	0.979704	1.844690
H	-1.090122	-0.768845	1.918454
H	1.030260	1.312069	1.692755
H	1.204452	-0.383393	2.131570
C	-0.787350	1.127623	-0.794728
H	-1.285613	1.110360	-1.765638
H	-1.087560	2.047582	-0.289023
C	0.753193	1.067063	-0.960439
H	1.023669	0.808490	-1.986972
H	1.204439	2.035913	-0.738134
H	2.377582	-0.004393	-0.003530
C	0.749380	-1.366495	-0.446880
H	1.196071	-1.660016	-1.398744
H	1.021102	-2.126708	0.289354
C	-0.791820	-1.250936	-0.576063
H	-1.096547	-1.272058	-1.624473
H	-1.289832	-2.082158	-0.073661
N	-1.287018	0.002549	0.002077

M062X-CPCM-THF_complex-Te-diBr-Br.out

C	2.353229	2.219284	-0.000118
C	3.241620	1.091957	-0.000078
C	2.763714	-0.169467	0.000022
C	1.013790	2.054757	-0.000048
H	2.780753	3.212382	-0.000221
H	4.307167	1.275410	-0.000148
C	0.427153	0.734406	0.000109
C	1.341239	-0.430150	0.000094
N	-0.854341	0.514768	0.000075
N	0.804087	-1.611003	0.000227
Te	-1.181394	-1.431060	0.000197
Br	-4.157034	-0.636263	-0.000217
Br	3.942442	-1.644829	0.000076
Br	-0.132497	3.555270	-0.000199

M062X-CPCM-THF_complex-Te-diBr-Cl.out

C	1.545272	2.460873	0.000404
C	2.613150	1.501546	0.000291
C	2.358301	0.176748	0.000073
C	0.254796	2.067340	0.000304
H	1.796596	3.512687	0.000550
H	3.631564	1.864453	0.000371
C	-0.096831	0.666378	0.000086
C	1.002084	-0.326943	-0.000041
N	-1.321434	0.233271	-0.000092
N	0.670343	-1.579208	-0.000311
Te	-1.328413	-1.741856	-0.000338
Cl	-4.139675	-1.433426	0.000141
Br	-1.136453	3.345626	0.000397
Br	3.779904	-1.068097	-0.000101

M062X-CPCM-THF_complex-Te-diBr-I.out

C	2.832229	2.150552	0.000036
C	3.675195	0.988381	0.000075
C	3.149051	-0.253949	0.000009
C	1.487464	2.039286	-0.000070
H	3.299395	3.125653	0.000014
H	4.747063	1.129722	0.000085
C	0.851096	0.742493	-0.000080
C	1.717806	-0.456676	-0.000021
N	-0.438483	0.573211	-0.000426
N	1.136696	-1.617764	-0.000327
Te	-0.833690	-1.357812	0.000150
I	-4.059974	-0.392754	0.000232
Br	0.397184	3.579860	-0.000306
Br	4.269086	-1.773627	-0.000112

M062X-CPCM-THF_complex-Te-diBr-NO3.out

C	2.576772	2.004700	0.000269
C	3.322095	0.777534	0.000314
C	2.696915	-0.418009	0.000144
C	1.227659	2.001465	0.000050
H	3.122079	2.938429	0.000373
H	4.401926	0.830877	0.000452
C	0.486557	0.760787	-0.000114
C	1.253705	-0.506732	-0.000044
N	-0.811293	0.697648	-0.000482
N	0.577186	-1.613474	-0.000356
Te	-1.369079	-1.194756	-0.000200
O	-3.584929	0.108249	0.000486
O	-5.724306	-0.095521	0.000581
O	-4.483729	-1.852737	-0.000099
N	-4.615969	-0.623670	0.000374
Br	0.261973	3.623758	-0.000096
Br	3.697459	-2.019869	0.000136

M062X-CPCM-THF_complex-Te-diBr-quin.out

C	2.921820	2.254147	0.003916
C	3.847036	1.152654	0.004897
C	3.412848	-0.122497	0.001879
C	1.589933	2.049800	0.000246
H	3.320458	3.259221	0.006039
H	4.905872	1.372277	0.007821
C	1.043081	0.710476	-0.001374
C	1.996190	-0.431625	-0.001277
N	-0.224637	0.452628	-0.002862
N	1.496664	-1.621918	-0.003526
Te	-0.511484	-1.510461	-0.003846
C	-3.205959	0.067488	-1.245539
C	-5.361289	0.009810	0.002655
C	-4.630614	0.662610	-1.174876
H	-2.449377	0.839117	-1.385500
H	-3.114145	-0.648521	-2.064600
H	-4.586958	1.743729	-1.028645
H	-5.163285	0.478219	-2.108588
C	-3.162632	0.227505	1.154674
H	-2.740148	-0.236391	2.047637
H	-2.623052	1.157539	0.978104
C	-4.683505	0.460256	1.301016
H	-5.081785	-0.110331	2.142620
H	-4.885770	1.514347	1.494269
H	-6.414035	0.291280	0.003235
C	-5.212934	-1.510502	-0.119059
H	-5.832721	-2.019008	0.620163
H	-5.544202	-1.837177	-1.106731
C	-3.725753	-1.860808	0.099936
H	-3.560526	-2.291678	1.089530
H	-3.372879	-2.584481	-0.638465
N	-2.885206	-0.653202	0.002287
Br	0.393949	3.511464	-0.002062
Br	4.636412	-1.558397	0.002326

M062X-CPCM-THF_complex-Te-nat-Br.out

C	3.878826	1.687216	0.000033
C	4.431034	0.355691	-0.000030
C	3.636252	-0.736866	-0.000100
C	2.544288	1.899521	0.000035
H	4.559600	2.529079	0.000051
H	5.507789	0.242259	-0.000025
H	4.042889	-1.740172	-0.000145
H	2.124111	2.896980	0.000051
C	1.638108	0.777116	0.000062
C	2.201382	-0.585081	-0.000053
N	0.340637	0.920499	-0.000009
N	1.367075	-1.586451	-0.000078
Te	-0.493229	-0.874266	0.000044
Br	-3.214852	0.737422	-0.000036

M062X-CPCM-THF_complex-Te-nat-Cl.out

C	-3.584411	1.368861	-0.000049
C	-3.964728	-0.021254	-0.000099
C	-3.038085	-1.005150	-0.000015
C	-2.286700	1.745884	0.000068
H	-4.365528	2.118908	-0.000070
H	-5.019008	-0.268553	-0.000192
H	-3.317136	-2.051435	-0.000049
H	-1.994370	2.788317	0.000171
C	-1.245968	0.746372	-0.000007
C	-1.632154	-0.676142	0.000001
N	0.022052	1.053427	0.000178
N	-0.677011	-1.561574	0.000061
Te	1.088054	-0.615925	0.000004
Cl	3.365543	1.179203	-0.000068

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M062X-CPCM-THF_complex-Te-nat-I.out
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C	-4.198781	1.881492	0.000001
C	-4.849293	0.595452	0.000075
C	-4.140432	-0.554742	-0.000016
C	-2.852249	1.992612	-0.000159
H	-4.814238	2.772247	0.000049
H	-5.931485	0.564296	0.000176
H	-4.623040	-1.523682	0.000007
H	-2.356630	2.954774	-0.000248
C	-2.034334	0.804702	-0.000224
C	-2.698186	-0.511156	-0.000150
N	-0.729184	0.848870	-0.000467
N	-1.944187	-1.575685	-0.000330
Te	-0.041680	-1.003370	-0.000211
I	3.080114	0.514060	0.000366

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M062X-CPCM-THF_complex-Te-nat-NO3.out
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C	4.023959	1.508760	0.000165
C	4.464022	0.136223	0.000306
C	3.581544	-0.886862	0.000223
C	2.711672	1.830844	-0.000060
H	4.772337	2.291459	0.000203
H	5.527863	-0.065148	0.000450
H	3.905134	-1.920059	0.000289
H	2.375327	2.859762	-0.000211
C	1.714503	0.787480	-0.000125
C	2.163561	-0.617279	0.000030
N	0.433622	1.036460	-0.000466
N	1.249067	-1.545750	-0.000157
Te	-0.545860	-0.682614	-0.000177
O	-2.463249	1.113587	0.000390
O	-4.598079	1.371177	0.000515
O	-3.759337	-0.609789	-0.000082
N	-3.623573	0.620020	0.000433

==========
M062X-CPCM-THF_complex-Te-nat-quin.out
==========

C	4.251962	2.120459	-0.000340
C	5.030469	0.904405	-0.004990
C	4.441507	-0.309945	-0.005663
C	2.902408	2.097538	0.004159
H	4.776439	3.067713	-0.000643
H	6.110199	0.984086	-0.008132
H	5.019310	-1.225354	-0.009177
H	2.315668	3.007159	0.007397
C	2.203714	0.832996	0.003975
C	2.999363	-0.415996	-0.001736
N	0.906741	0.747514	0.006885
N	2.354811	-1.542006	-0.003430
Te	0.379050	-1.171190	0.001854
C	-2.109664	0.779576	-1.219705
C	-4.278458	0.964545	-0.007152
C	-3.453137	1.542717	-1.160532
H	-1.261142	1.456129	-1.313957
H	-2.083803	0.087345	-2.063734
H	-3.282214	2.608144	-0.993391
H	-3.989082	1.440443	-2.105069
C	-2.094059	0.844892	1.185612
H	-1.770251	0.287332	2.066361
H	-1.419916	1.692193	1.064127
C	-3.568835	1.293123	1.309714
H	-4.062671	0.773949	2.133719
H	-3.622843	2.362708	1.516795
H	-5.285373	1.381586	-0.011822
C	-4.331033	-0.558349	-0.163754
H	-5.014256	-0.995596	0.565316
H	-4.703019	-0.814812	-1.157701
C	-2.901579	-1.108929	0.040903
H	-2.801080	-1.605633	1.008236
H	-2.638514	-1.834257	-0.732383
N	-1.912122	-0.018860	0.004359

==========
M062X-CPCM-THF_donor-Te-diBr.out
==========

C	-0.717849	-2.472117	0.000010
C	0.717837	-2.472121	0.000010
C	1.419723	-1.320221	-0.000015
C	-1.419730	-1.320213	-0.000015
H	-1.231291	-3.423711	0.000001
H	1.231274	-3.423718	0.000001
C	-0.740320	-0.045860	-0.000018
C	0.740321	-0.045863	-0.000018
N	-1.355610	1.102631	-0.000146
N	1.355613	1.102625	-0.000146
Te	0.000006	2.520302	0.000148
Br	-3.303222	-1.336947	-0.000076
Br	3.303216	-1.336958	-0.000076

==========
M062X-CPCM-THF_donor-Te-nat.out
==========

C	-3.322915	0.720875	0.000001
C	-3.322869	-0.720924	0.000001
C	-2.173348	-1.429403	0.000000
C	-2.173432	1.429388	0.000000
H	-4.274826	1.236229	0.000001
H	-4.274748	-1.236350	0.000001
H	-2.165235	-2.511267	-0.000001
H	-2.165303	2.511262	-0.000000
C	-0.908901	0.737896	0.000000
C	-0.908842	-0.737817	-0.000001
N	0.240244	1.361540	-0.000004
N	0.240267	-1.361573	-0.000003
Te	1.661123	0.000005	0.000001

M062X-CPCM-ACN_complex-Te-CN-Br-opp.out

C	-3.372244	1.660247	-0.000109
C	-3.903852	0.316772	-0.000087
C	-3.100654	-0.778696	-0.000062
C	-2.040258	1.874106	-0.000103
H	-4.067125	2.488991	-0.000171
H	-3.506462	-1.781443	-0.000093
H	-1.631422	2.875679	-0.000169
C	-1.126969	0.758907	-0.000031
C	-1.675297	-0.605280	-0.000010
N	0.170412	0.909778	-0.000177
N	-0.833979	-1.603819	-0.000156
Te	1.012770	-0.878168	0.000341
Br	3.707517	0.758940	-0.000301
C	-5.328561	0.146471	-0.000140
N	-6.470019	0.020246	-0.000169

M062X-CPCM-ACN_complex-Te-CN-Cl-opp.out

C	2.985688	1.542528	0.000069
C	3.410577	0.161933	0.000000
C	2.523653	-0.867615	-0.000187
C	1.674215	1.858837	0.000002
H	3.743021	2.314961	0.000189
H	2.852048	-1.898453	-0.000226
H	1.343723	2.889129	0.000062
C	0.676317	0.818191	-0.000057
C	1.115043	-0.585027	-0.000263
N	-0.604212	1.070972	-0.000043
N	0.196109	-1.511513	-0.000379
Te	-1.596764	-0.638884	-0.000048
Cl	-3.935366	1.083328	0.000299
C	4.817993	-0.116807	0.000157
N	5.947138	-0.326956	0.000287

M062X-CPCM-ACN_complex-Te-CN-I-opp.out

C	-3.748358	1.749417	0.000411
C	-4.354447	0.437744	-0.000185
C	-3.614924	-0.701598	-0.000485
C	-2.406678	1.888212	0.000699
H	-4.395174	2.616140	0.000596
H	-4.076374	-1.680000	-0.000945
H	-1.941385	2.864834	0.001110
C	-1.558410	0.723222	0.000480
C	-2.182029	-0.607692	-0.000161
N	-0.254126	0.800188	0.000606
N	-1.400199	-1.654589	-0.000466
Te	0.478378	-1.032291	0.000359
I	3.538940	0.580984	-0.000315
C	-5.786879	0.349488	-0.000498
N	-6.933701	0.290580	-0.000755

M062X-CPCM-ACN_complex-Te-CN-Br-same.out

C	-3.676559	0.662948	0.000007
C	-3.952649	-0.755135	0.000191
C	-2.944317	-1.651240	0.000214
C	-2.410407	1.155660	-0.000143
H	-4.984664	-1.079086	0.000314
H	-3.137506	-2.715799	0.000365
H	-2.214401	2.219359	-0.000275
C	-1.303433	0.241683	-0.000092
C	-1.573633	-1.203859	0.000053
N	-0.061811	0.653307	-0.000214
N	-0.548768	-2.010842	0.000109
Te	1.117162	-0.926819	-0.000092
Br	3.435153	1.233154	0.000110
C	-4.788028	1.570858	-0.000005
N	-5.688283	2.283852	-0.000014

M062X-CPCM-ACN_complex-Te-CN-Cl-same.out

C	3.284432	0.392325	0.000068
C	3.361456	-1.050199	0.000007
C	2.237990	-1.796809	-0.000026
C	2.098009	1.055444	0.000102
H	4.338732	-1.513775	0.000005
H	2.281327	-2.878000	-0.000049
H	2.052250	2.136187	0.000168
C	0.874607	0.304584	0.000059
C	0.941585	-1.164293	-0.000020
N	-0.297344	0.884658	0.000159
N	-0.186168	-1.816686	0.000020
Te	-1.694908	-0.510561	-0.000073
Cl	-3.498294	1.762029	-0.000031
C	4.509331	1.139765	0.000117
N	5.496292	1.727080	0.000158

M062X-CPCM-ACN_complex-Te-CN-I-same.out

C	-4.044757	0.868072	0.000001
C	-4.453359	-0.517682	0.000288
C	-3.535009	-1.505894	0.000344
C	-2.737893	1.237996	-0.000196
H	-5.511400	-0.741887	0.000462
H	-3.829122	-2.547128	0.000552
H	-2.439967	2.277841	-0.000368
C	-1.723217	0.222471	-0.000208
C	-2.128077	-1.190143	0.000109
N	-0.447900	0.513927	-0.000201
N	-1.185523	-2.093185	0.000065
Te	0.570370	-1.171155	-0.000119
I	3.337154	0.910106	0.000091
C	-5.062944	1.879700	-0.000019
N	-5.886061	2.680467	-0.000037

M062X-CPCM-ACN_complex-Te-CN-NO3-opp.out

C	3.464797	1.594458	-0.000019
C	3.916618	0.221983	-0.000002
C	3.050633	-0.824461	0.000007
C	2.147790	1.886171	-0.000028
H	4.207506	2.380921	-0.000023
H	3.397822	-1.848985	0.000022
H	1.798167	2.910033	-0.000039
C	1.169333	0.826673	-0.000019
C	1.637147	-0.568182	-0.000003
N	-0.116290	1.052416	-0.000020
N	0.738303	-1.514460	0.000017
Te	-1.063540	-0.681676	-0.000015
O	-2.984374	1.083227	-0.000089
O	-5.120490	1.325693	0.000081
O	-4.268135	-0.649121	0.000170
N	-4.142056	0.580838	-0.000032
C	5.329116	-0.030437	0.000009
N	6.461753	-0.220288	0.000019

M062X-CPCM-ACN_complex-Te-CN-NO3-same.out

C	3.727662	0.609264	-0.000074
C	3.936226	-0.820348	-0.000129
C	2.886383	-1.666960	-0.000078
C	2.486642	1.162385	0.000027
H	4.951570	-1.192745	-0.000183
H	3.028588	-2.739561	-0.000086
H	2.341961	2.234339	0.000102
C	1.336089	0.302704	0.000058
C	1.538310	-1.154627	0.000000
N	0.115867	0.771201	0.000270
N	0.475682	-1.909680	0.000155
Te	-1.138339	-0.751143	0.000033
O	-2.674002	1.369744	-0.000269
O	-4.718930	2.033547	-0.000173
O	-4.277040	-0.071662	0.000237
N	-3.908131	1.108736	-0.000077
C	4.881054	1.463282	-0.000085
N	5.813306	2.134054	-0.000095

M062X-CPCM-ACN_complex-Te-CN-Quin-opp.out

C	3.889607	1.848495	0.005244
C	4.584929	0.579455	-0.001984
C	3.925420	-0.606467	-0.004033
C	2.542864	1.896593	0.010329
H	4.477557	2.756375	0.006180
H	4.454335	-1.550230	-0.009551
H	2.014131	2.840534	0.015464
C	1.770935	0.676443	0.008170
C	2.485483	-0.615674	0.000628
N	0.470694	0.666583	0.010648
N	1.775558	-1.703770	-0.002350
Te	-0.171742	-1.213123	0.002644
C	-2.540239	0.852559	-1.219571
C	-4.702444	1.113503	-0.009238
C	-3.853128	1.666520	-1.157472
H	-1.666473	1.496670	-1.310465
H	-2.540907	0.162768	-2.065882
H	-3.641272	2.723381	-0.983726
H	-4.390090	1.589811	-2.103651
C	-2.526085	0.909954	1.187570
H	-2.222352	0.339399	2.066967
H	-1.823631	1.734057	1.067544
C	-3.984468	1.408023	1.311252
H	-4.496863	0.900252	2.130837
H	-4.000357	2.477211	1.525804
H	-5.692964	1.567843	-0.014110
C	-4.811015	-0.405860	-0.174727
H	-5.513583	-0.821712	0.548171
H	-5.185908	-0.642775	-1.172299
C	-3.405874	-1.010469	0.035488
H	-3.327872	-1.510290	1.003212
H	-3.168446	-1.745259	-0.737034
N	-2.374438	0.042828	0.003083
C	6.019976	0.591026	-0.007722
N	7.168117	0.614323	-0.012602

M062X-CPCM-ACN_complex-Te-CN-Quin-same.out

C	4.168734	1.074569	-0.000370
C	4.714549	-0.266002	0.008887
C	3.899641	-1.338948	0.009625
C	2.832851	1.314207	-0.008764
H	5.789759	-0.382882	0.015228
H	4.295590	-2.345947	0.016620
H	2.436465	2.320709	-0.015448
C	1.919588	0.203403	-0.006854
C	2.464577	-1.168747	0.002001
N	0.628405	0.367793	-0.011439
N	1.615164	-2.149702	0.003425
Te	-0.254505	-1.408988	-0.002783
C	-2.344700	0.919697	-1.252762
C	-4.398868	1.559346	0.003801
C	-3.504858	1.937896	-1.181871
H	-1.383698	1.409181	-1.407115
H	-2.492335	0.204121	-2.064030
H	-3.118183	2.949746	-1.045115
H	-4.074831	1.926517	-2.111606
C	-2.238752	1.076120	1.146271
H	-1.978645	0.508115	2.041186
H	-1.436314	1.789039	0.961396
C	-3.606756	1.777785	1.297372
H	-4.160666	1.364987	2.143108
H	-3.464015	2.842449	1.485959
H	-5.307807	2.160153	0.004983
C	-4.739461	0.069787	-0.106856
H	-5.485270	-0.212293	0.637110
H	-5.160348	-0.140963	-1.092014
C	-3.438272	-0.733248	0.111550
H	-3.411681	-1.185669	1.104923
H	-3.336624	-1.536361	-0.621786
N	-2.258780	0.145342	0.000625
C	5.082625	2.181149	0.000274
N	5.823416	3.058624	0.001319

M062X-CPCM-ACN_complex-Te-F4-Br.out

C	-3.192754	1.253794	-0.000130
C	-3.640457	-0.112141	-0.000037
C	-2.766384	-1.134316	0.000065
C	-1.883534	1.563651	-0.000148
C	-0.891614	0.521146	-0.000067
C	-1.348582	-0.880167	0.000090
N	0.385051	0.761723	-0.000044
N	-0.446589	-1.811227	0.000114
Te	1.360272	-0.959582	0.000061
Br	3.886216	0.830703	0.000058
F	-4.131828	2.194217	-0.000261
F	-1.490916	2.834078	-0.000281
F	-4.954438	-0.314406	-0.000061
F	-3.198481	-2.391843	0.000125

M062X-CPCM-ACN_complex-Te-F4-Cl.out

C	2.846981	1.070503	0.000074
C	3.151310	-0.334532	0.000022
C	2.176246	-1.261014	-0.000053
C	1.576600	1.512999	0.000043
C	0.482408	0.578816	-0.000021
C	0.790985	-0.863355	-0.000061
N	-0.760834	0.952504	-0.000130
N	-0.204514	-1.691624	-0.000187
Te	-1.922036	-0.653051	-0.000012
Cl	-4.026420	1.260083	0.000122
F	3.878779	1.909101	0.000124
F	1.317677	2.818104	0.000062
F	4.438135	-0.671252	0.000026
F	2.477103	-2.557001	-0.000128

M062X-CPCM-ACN_complex-Te-F4-I.out

C	-3.546382	1.376192	0.000017
C	-4.083074	0.042054	0.000137
C	-3.278051	-1.035233	0.000092
C	-2.219669	1.600254	-0.000160
C	-1.298891	0.494988	-0.000159
C	-1.847641	-0.872737	-0.000037
N	-0.008428	0.650190	-0.000211
N	-1.010347	-1.863570	-0.000013
Te	0.840231	-1.136012	-0.000147
I	3.761034	0.603835	0.000139
F	-4.421421	2.375610	0.000072
F	-1.744857	2.841715	-0.000293
F	-5.406665	-0.073794	0.000302
F	-3.788517	-2.262429	0.000197

M062X-CPCM-ACN_complex-Te-F4-NO3.out

C	3.264719	1.170444	0.000054
C	3.629809	-0.220257	0.000246
C	2.696469	-1.188675	0.000239
C	1.976629	1.557834	-0.000132
C	0.923678	0.576544	-0.000199
C	1.295828	-0.850755	0.000024
N	-0.335113	0.893245	-0.000272
N	0.338537	-1.723979	-0.000001
Te	-1.412913	-0.766294	-0.000391
O	-3.153225	1.109722	-0.000165
O	-5.260809	1.531241	0.000677
O	-4.578809	-0.508525	0.000878
N	-4.351749	0.705775	0.000429
F	4.259230	2.052171	0.000121
F	1.661261	2.849697	-0.000247
F	4.929498	-0.499683	0.000446
F	3.053311	-2.469775	0.000425

M062X-CPCM-ACN_complex-Te-F4-Quin.out

C	-3.662137	1.523233	-0.000091
C	-4.313439	0.238589	0.002996
C	-3.607017	-0.904066	0.002857
C	-2.322369	1.631746	-0.003586
C	-1.497791	0.450759	-0.004291
C	-2.163577	-0.872166	-0.000392
N	-0.205611	0.495680	-0.006337
N	-1.414099	-1.921328	0.000391
Te	0.525012	-1.355722	-0.002929
C	2.776872	0.789791	1.231382
C	4.913766	1.167469	0.007617
C	4.046574	1.668623	1.166127
H	1.873222	1.388136	1.341426
H	2.821452	0.087894	2.066432
H	3.780678	2.714809	1.002595
H	4.593200	1.611335	2.108020
C	2.739704	0.881873	-1.175871
H	2.449517	0.312700	-2.060467
H	2.005267	1.673893	-1.034684
C	4.174395	1.441025	-1.305756
H	4.701073	0.961135	-2.133029
H	4.143058	2.511298	-1.512427
H	5.881815	1.667651	0.011568
C	5.093530	-0.346723	0.157685
H	5.813752	-0.723793	-0.568950
H	5.478418	-0.576274	1.153114
C	3.718564	-1.013547	-0.059652
H	3.659203	-1.496323	-1.037184
H	3.520272	-1.774233	0.698577
N	2.637828	-0.009689	-0.002680
F	-4.448838	2.593695	0.001006
F	-1.741538	2.828290	-0.005983
F	-5.642711	0.241827	0.006124
F	-4.225895	-2.080809	0.005913

M062X-CPCM-ACN_donor-Te-CN.out

C	-2.609954	1.354540	-0.000002
C	-2.836793	-0.072348	-0.000002
C	-1.817022	-0.968832	-0.000003
C	-1.357571	1.854476	-0.000003
H	-3.469460	2.010858	-0.000002
H	-1.994609	-2.035528	-0.000004
H	-1.174869	2.920430	-0.000004
C	-0.225777	0.963782	-0.000003
C	-0.465413	-0.486987	-0.000003
N	1.012016	1.388116	-0.000008
N	0.565731	-1.294769	-0.000007
Te	2.184265	-0.187688	0.000005
C	-4.191976	-0.545557	-0.000002
N	-5.280005	-0.911980	-0.000002

M062X-CPCM-ACN_donor-Te-F4.out

C	-0.000001	-2.538531	0.719018
C	-0.000001	-2.538531	-0.719018
C	-0.000001	-1.390708	-1.421294
C	-0.000001	-1.390708	1.421294
C	-0.000001	-0.126911	0.736581
C	-0.000001	-0.126911	-0.736581
N	-0.000006	1.017790	1.357763
N	-0.000006	1.017790	-1.357763
Te	0.000004	2.437140	0.000000
F	-0.000003	-1.406839	2.748810
F	-0.000001	-3.721301	1.319085
F	-0.000001	-3.721301	-1.319085
F	-0.000003	-1.406839	-2.748810

M062X-CPCM-THF_complex-Te-CN-Br-opp.out

C	-3.375573	1.650001	-0.000078
C	-3.901003	0.304298	-0.000107
C	-3.091082	-0.786947	-0.000098
C	-2.044263	1.869702	-0.000039
H	-4.074668	2.475298	-0.000087
H	-3.492215	-1.791646	-0.000121
H	-1.638908	2.872745	-0.000018
C	-1.125288	0.759249	-0.000029
C	-1.666563	-0.607708	-0.000058
N	0.170630	0.918167	0.000015
N	-0.819025	-1.600539	-0.000048
Te	1.028534	-0.862586	0.000022
Br	3.676983	0.748353	0.000109
C	-5.324767	0.127409	-0.000144
N	-6.466057	-0.001958	-0.000172

M062X-CPCM-THF_complex-Te-CN-Br-same.out

C	-3.677694	0.644443	-0.000037
C	-3.941962	-0.775675	0.000053
C	-2.925887	-1.663294	0.000132
C	-2.414601	1.146449	-0.000046
H	-4.971469	-1.107675	0.000051
H	-3.109766	-2.729596	0.000194
H	-2.226554	2.211647	-0.000118
C	-1.300078	0.241990	0.000032
C	-1.558458	-1.205756	0.000124
N	-0.062420	0.664593	-0.000003
N	-0.526764	-2.002788	0.000189
Te	1.134823	-0.902376	0.000127
Br	3.401740	1.217907	-0.000212
C	-4.797395	1.541850	-0.000127
N	-5.706164	2.244253	-0.000199

M062X-CPCM-THF_complex-Te-CN-Cl-opp.out

C	2.989904	1.535739	0.000174
C	3.411069	0.154255	0.000075
C	2.519813	-0.872349	-0.000121
C	1.678893	1.855148	0.000081
H	3.749514	2.305998	0.000290
H	2.845264	-1.904217	-0.000221
H	1.349959	2.886001	0.000111
C	0.677743	0.817747	-0.000069
C	1.111880	-0.586887	-0.000173
N	-0.601141	1.075964	-0.000239
N	0.189169	-1.508990	-0.000464
Te	-1.605769	-0.627445	-0.000162
Cl	-3.907556	1.064754	0.000638
C	4.817607	-0.128241	0.000160
N	5.946580	-0.340396	0.000223

M062X-CPCM-THF_complex-Te-CN-Cl-same.out

C	3.286144	0.384622	0.000054
C	3.357996	-1.057972	-0.000046
C	2.231519	-1.800576	-0.000068
C	2.100780	1.050689	0.000141
H	4.333862	-1.524681	-0.000081
H	2.270721	-2.882028	-0.000118
H	2.057734	2.131589	0.000242
C	0.874903	0.304400	0.000102
C	0.936490	-1.164888	-0.000016
N	-0.294180	0.889491	0.000265
N	-0.193515	-1.811949	0.000037
Te	-1.701980	-0.495900	-0.000015
Cl	-3.475797	1.735435	-0.000222
C	4.513912	1.126941	0.000093
N	5.504656	1.708209	0.000122

M062X-CPCM-THF_complex-Te-CN-I-opp.out

C	-3.752068	1.736657	0.000241
C	-4.349183	0.421031	-0.000107
C	-3.600275	-0.712729	-0.000291
C	-2.411074	1.884359	0.000409
H	-4.405207	2.598682	0.000353
H	-4.054670	-1.694485	-0.000575
H	-1.951524	2.863742	0.000663
C	-1.554227	0.725643	0.000281
C	-2.168177	-0.609614	-0.000118
N	-0.251078	0.813504	0.000383
N	-1.377628	-1.649493	-0.000322
Te	0.500220	-1.011965	0.000230
I	3.509176	0.571908	-0.000197
C	-5.780732	0.322374	-0.000291
N	-6.927284	0.255527	-0.000452

M062X-CPCM-THF_complex-Te-CN-I-same.out

C	-4.048693	0.842686	0.000013
C	-4.441184	-0.547627	0.000028
C	-3.511167	-1.525223	0.000078
C	-2.745340	1.226249	0.000016
H	-5.496783	-0.783586	-0.000018
H	-3.792704	-2.570036	0.000044
H	-2.458624	2.269298	0.000001
C	-1.719092	0.222676	-0.000021
C	-2.107561	-1.194534	0.000071
N	-0.447802	0.530052	-0.000053
N	-1.154267	-2.085277	0.000037
Te	0.595165	-1.140567	-0.000032
I	3.308192	0.899694	0.000018
C	-5.079460	1.841198	-0.000008
N	-5.915025	2.629151	-0.000036

M062X-CPCM-THF_complex-Te-CN-NO3-opp.out

C	3.468107	1.587080	-0.000039
C	3.915323	0.213312	-0.000032
C	3.044322	-0.829588	-0.000005
C	2.151809	1.883091	-0.000018
H	4.213764	2.370819	-0.000053
H	3.387682	-1.855482	0.000009
H	1.804725	2.907871	-0.000012
C	1.169244	0.827491	0.000005
C	1.631794	-0.569015	0.000009
N	-0.114984	1.059073	0.000057
N	0.728782	-1.511045	0.000069
Te	-1.072479	-0.669418	0.000012
O	-2.965600	1.074138	-0.000103
O	-5.102042	1.312951	-0.000013
O	-4.247211	-0.660873	0.000115
N	-4.124875	0.569311	-0.000048
C	5.326879	-0.043826	-0.000043
N	6.459177	-0.236552	-0.000052

M062X-CPCM-THF_complex-Te-CN-NO3-same.out

C	3.730348	0.599356	-0.000088
C	3.931579	-0.831214	-0.000027
C	2.877420	-1.672817	0.000017
C	2.490783	1.157016	-0.000098
H	4.945414	-1.207926	-0.000036
H	3.014116	-2.746217	0.000042
H	2.350391	2.229596	-0.000164
C	1.336389	0.303122	-0.000039
C	1.531441	-1.155026	0.000021
N	0.118732	0.778051	-0.000111
N	0.465052	-1.904133	-0.000008
Te	-1.145350	-0.735770	0.000102
O	-2.661436	1.360056	0.000547
O	-4.708381	2.017377	0.000200
O	-4.260780	-0.086663	-0.000723
N	-3.897122	1.095240	-0.000081
C	4.887912	1.447424	-0.000169
N	5.824455	2.112455	-0.000236

M062X-CPCM-THF_complex-Te-CN-Quin-opp.out

C	3.885207	1.850501	0.004689
C	4.583403	0.582658	-0.001766
C	3.925886	-0.603973	-0.003507
C	2.538612	1.896864	0.009343
H	4.472192	2.759036	0.005422
H	4.455709	-1.547166	-0.008451
H	2.007839	2.839623	0.013918
C	1.768408	0.675425	0.007502
C	2.485680	-0.615750	0.000704
N	0.468498	0.663704	0.009647
N	1.778728	-1.705233	-0.002091
Te	-0.167768	-1.218677	0.002341
C	-2.541824	0.851280	-1.219565
C	-4.702702	1.119579	-0.008466
C	-3.852558	1.669000	-1.157910
H	-1.665866	1.492316	-1.311076
H	-2.544399	0.161136	-2.065674
H	-3.637950	2.725538	-0.985392
H	-4.390497	1.593268	-2.103674
C	-2.526159	0.909176	1.187055
H	-2.224450	0.337332	2.066361
H	-1.819406	1.729635	1.067373
C	-3.982569	1.413389	1.311124
H	-4.496637	0.909270	2.132002
H	-3.994597	2.482992	1.524012
H	-5.691915	1.576876	-0.012926
C	-4.816097	-0.399736	-0.172454
H	-5.519288	-0.812777	0.551537
H	-5.193489	-0.636230	-1.169247
C	-3.412121	-1.008231	0.036061
H	-3.334570	-1.508880	1.003468
H	-3.177501	-1.743638	-0.736797
N	-2.378242	0.041708	0.002946
C	6.018555	0.598228	-0.007035
N	7.166506	0.625880	-0.011540

M062X-CPCM-THF_complex-Te-CN-Quin-same.out

C	4.164646	1.079836	-0.000374
C	4.712980	-0.259908	0.009155
C	3.900698	-1.334667	0.009931
C	2.828461	1.316416	-0.008995
H	5.788499	-0.374017	0.015670
H	4.297823	-2.341144	0.017130
H	2.429977	2.322044	-0.015873
C	1.917197	0.203764	-0.007037
C	2.465276	-1.167471	0.002097
N	0.625881	0.365504	-0.011771
N	1.618995	-2.150822	0.003585
Te	-0.250365	-1.415048	-0.002868
C	-2.344801	0.919928	-1.251768
C	-4.398259	1.564009	0.003991
C	-3.503131	1.940486	-1.181581
H	-1.382462	1.407353	-1.404300
H	-2.492503	0.205530	-2.064155
H	-3.114614	2.951662	-1.044956
H	-4.073102	1.930574	-2.111397
C	-2.239720	1.073804	1.146719
H	-1.981694	0.504290	2.041329
H	-1.434274	1.783676	0.963150
C	-3.605579	1.779973	1.297712
H	-4.161203	1.369231	2.143408
H	-3.459907	2.844239	1.486467
H	-5.305686	2.167180	0.005299
C	-4.742851	0.075303	-0.107008
H	-5.489242	-0.204916	0.637169
H	-5.165321	-0.133811	-1.091896
C	-3.443220	-0.731095	0.109958
H	-3.417794	-1.185551	1.102514
H	-3.343445	-1.533452	-0.624557
N	-2.262060	0.144296	0.000572
C	5.076784	2.188070	0.000255
N	5.816192	3.066584	0.001303

M062X-CPCM-THF_complex-Te-F4-Br.out

C	-3.197056	1.242017	-0.000066
C	-3.637017	-0.126083	0.000088
C	-2.757100	-1.143321	0.000125
C	-1.889479	1.559387	-0.000172
C	-0.890994	0.522432	-0.000189
C	-1.340112	-0.881841	-0.000026
N	0.383601	0.771286	-0.000201
N	-0.432498	-1.806459	0.000045
Te	1.374362	-0.942097	-0.000292
Br	3.862699	0.821690	0.000445
F	-4.142566	2.177709	-0.000048
F	-1.505838	2.832400	-0.000250
F	-4.951107	-0.335756	0.000228
F	-3.183655	-2.403182	0.000310

M062X-CPCM-THF_complex-Te-F4-Cl.out

C	2.850009	1.064042	0.000062
C	3.150439	-0.341391	-0.000017
C	2.172593	-1.265219	-0.000136
C	1.580586	1.510152	0.000016
C	0.483375	0.579006	-0.000089
C	0.787873	-0.864404	-0.000149
N	-0.758179	0.957032	-0.000251
N	-0.210196	-1.688730	-0.000380
Te	-1.929104	-0.642027	0.000089
Cl	-4.008792	1.244756	0.000139
F	3.885007	1.900634	0.000150
F	1.327213	2.816232	0.000067
F	4.437463	-0.682228	-0.000026
F	2.471677	-2.562046	-0.000269

M062X-CPCM-THF_complex-Te-F4-I.out

C	-3.549526	1.360531	-0.000527
C	-4.075859	0.022769	-0.000605
C	-3.262529	-1.048384	-0.000556
C	-2.224418	1.594769	-0.000342
C	-1.294625	0.496337	-0.000264
C	-1.832809	-0.875821	-0.000435
N	-0.006014	0.662705	-0.000222
N	-0.987268	-1.858905	-0.000390
Te	0.862855	-1.114550	0.000035
I	3.731179	0.598567	0.000717
F	-4.433043	2.354142	-0.000580
F	-1.760621	2.840208	-0.000213
F	-5.399778	-0.103512	-0.000737
F	-3.765374	-2.279199	-0.000596

M062X-CPCM-THF_complex-Te-F4-NO3.out

C	3.268561	1.162135	0.000045
C	3.627841	-0.229774	0.000149
C	2.690480	-1.194567	0.000138
C	1.981864	1.554885	-0.000068
C	0.924657	0.577760	-0.000128
C	1.290857	-0.851304	0.000005
N	-0.332402	0.900300	-0.000159
N	0.329578	-1.719717	-0.000021
Te	-1.420162	-0.752666	-0.000250
O	-3.143054	1.106033	-0.000216
O	-5.252769	1.516452	0.000358
O	-4.560793	-0.520078	0.000738
N	-4.341508	0.695708	0.000266
F	4.267542	2.040251	0.000103
F	1.673257	2.848184	-0.000115
F	4.927349	-0.514806	0.000274
F	3.043647	-2.476906	0.000241

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M062X-CPCM-THF_complex-Te-F4-Quin.out
==========

C	-3.657495	1.527087	-0.000034
C	-4.311706	0.243516	0.002153
C	-3.608085	-0.900959	0.002000
C	-2.317494	1.633394	-0.002727
C	-1.495486	0.450453	-0.003487
C	-2.164334	-0.871527	-0.000309
N	-0.203332	0.492831	-0.005001
N	-1.417762	-1.922534	0.000651
Te	0.520284	-1.361508	-0.002041
C	2.777532	0.789048	1.230464
C	4.913535	1.171585	0.006378
C	4.045859	1.670188	1.165710
H	1.872504	1.385484	1.339377
H	2.822520	0.087752	2.066091
H	3.778159	2.716094	1.003264
H	4.593278	1.613530	2.107255
C	2.739528	0.880064	-1.176015
H	2.450683	0.309778	-2.060397
H	2.002213	1.669485	-1.035285
C	4.172548	1.443797	-1.306460
H	4.700571	0.966398	-2.134419
H	4.138207	2.514135	-1.512474
H	5.880428	1.674110	0.009865
C	5.097151	-0.342291	0.155878
H	5.817749	-0.717476	-0.571465
H	5.484103	-0.571022	1.150768
C	3.723086	-1.012112	-0.059712
H	3.664106	-1.496224	-1.036701
H	3.526890	-1.772777	0.699182
N	2.640659	-0.011186	-0.002865
F	-4.442077	2.598684	0.001030
F	-1.734109	2.828335	-0.004324
F	-5.640684	0.250162	0.004484
F	-4.228792	-2.075859	0.004204

==========
M062X-CPCM-THF_donor-Te-CN.out
==========

C	-2.609125	1.354048	-0.000002
C	-2.836526	-0.073109	-0.000002
C	-1.816912	-0.969256	-0.000003
C	-1.357151	1.854452	-0.000003
H	-3.469004	2.009925	-0.000002
H	-1.994206	-2.035968	-0.000005
H	-1.173898	2.920281	-0.000004
C	-0.224997	0.963841	-0.000003
C	-0.464854	-0.487540	-0.000003
N	1.012077	1.388792	-0.000008
N	0.565477	-1.295506	-0.000008
Te	2.184016	-0.187639	0.000005
C	-4.192203	-0.545316	-0.000002
N	-5.280568	-0.910391	-0.000002

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M062X-CPCM-THF_donor-Te-F4.out
==========

C	-0.000001	-2.537959	0.719294
C	-0.000001	-2.537959	-0.719294
C	-0.000001	-1.390501	-1.422155
C	-0.000001	-1.390501	1.422155
C	-0.000001	-0.126489	0.737044
C	-0.000001	-0.126489	-0.737044
N	-0.000005	1.017548	1.358512
N	-0.000005	1.017548	-1.358512
Te	0.000004	2.436570	0.000000
F	-0.000003	-1.406416	2.749027
F	-0.000001	-3.720690	1.318521
F	-0.000001	-3.720690	-1.318521
F	-0.000003	-1.406416	-2.749027

5.4.3.3 M06-2X-D3 geometries

5.4.3.3.1 Gas phase

==========
M062XD3-null-null_complex-Te-CN-Br-opp.out
==========

C	-3.393607	1.610485	-0.000141
C	-3.897617	0.258043	-0.000126
C	-3.059903	-0.816024	-0.000052
C	-2.064099	1.850866	-0.000078
H	-4.108002	2.423312	-0.000214
H	-3.441378	-1.828776	-0.000036
H	-1.669741	2.858694	-0.000105
C	-1.122824	0.760104	0.000011
C	-1.638563	-0.618271	0.000027
N	0.166174	0.951656	0.000011
N	-0.770028	-1.589623	0.000054
Te	1.088040	-0.800691	0.000214
Br	3.572754	0.703263	-0.000191
C	-5.317896	0.058369	-0.000172
N	-6.458755	-0.083880	-0.000193

==========
M062XD3-null-null_complex-Te-CN-Br-same.out
==========

C	-3.692956	0.588526	-0.000082
C	-3.919036	-0.836780	-0.000032
C	-2.878018	-1.697468	-0.000034
C	-2.436524	1.115366	-0.000121
H	-4.941019	-1.192781	-0.000009
H	-3.030284	-2.769295	-0.000011
H	-2.270723	2.184585	-0.000189
C	-1.298766	0.242931	-0.000095
C	-1.519788	-1.212366	-0.000058
N	-0.075411	0.702116	-0.000203
N	-0.469053	-1.977895	-0.000118
Te	1.186134	-0.818359	-0.000001
Br	3.321277	1.155553	0.000191
C	-4.836223	1.454758	-0.000116
N	-5.768932	2.126927	-0.000139

M062XD3-null-null_complex-Te-CN-Cl-opp.out

C	3.010095	1.511036	0.000122
C	3.419881	0.127518	0.000004
C	2.509493	-0.886329	-0.000018
C	1.699753	1.841267	0.000222
H	3.778263	2.273422	0.000165
H	2.821162	-1.922938	-0.000071
H	1.375307	2.873982	0.000354
C	0.684994	0.818111	0.000176
C	1.104356	-0.592808	0.000031
N	-0.587152	1.097927	0.000424
N	0.170546	-1.500199	0.000113
Te	-1.636668	-0.582637	-0.000018
Cl	-3.830665	0.983443	-0.000331
C	4.823001	-0.168937	-0.000045
N	5.951447	-0.389874	-0.000085

M062XD3-null-null_complex-Te-CN-Cl-same.out

C	3.298387	0.363265	-0.000021
C	3.354022	-1.078804	-0.000016
C	2.217851	-1.809729	0.000103
C	2.112299	1.034013	0.000084
H	4.326578	-1.553490	-0.000061
H	2.242878	-2.892133	0.000161
H	2.074032	2.115344	0.000140
C	0.879504	0.302841	0.000153
C	0.924918	-1.168949	0.000156
N	-0.279393	0.904885	0.000488
N	-0.209604	-1.800863	0.000424
Te	-1.722841	-0.445949	0.000075
Cl	-3.430391	1.635953	-0.000702
C	4.534161	1.091001	-0.000076
N	5.536719	1.654061	-0.000128

M062XD3-null-null_complex-Te-CN-I-opp.out

C	-3.765018	1.686203	-0.000359
C	-4.331152	0.358148	-0.000199
C	-3.545335	-0.753682	-0.000058
C	-2.426113	1.865041	-0.000359
H	-4.440901	2.531134	-0.000483
H	-3.972635	-1.747886	0.000055
H	-1.985381	2.853409	-0.000492
C	-1.537005	0.731279	-0.000176
C	-2.116443	-0.620803	-0.000039
N	-0.240083	0.862186	-0.000220
N	-1.296059	-1.633800	0.000076
Te	0.589717	-0.934831	0.000117
I	3.390655	0.538094	0.000108
C	-5.759303	0.223493	-0.000194
N	-6.905124	0.131253	-0.000226

M062XD3-null-null_complex-Te-CN-I-same.out

C	-4.057002	0.763490	-0.000292
C	-4.399792	-0.638892	-0.000075
C	-3.434489	-1.583853	-0.000001
C	-2.762068	1.183694	-0.000415
H	-5.447872	-0.908918	-0.000010
H	-3.675910	-2.639152	0.000113
H	-2.506231	2.235044	-0.000581
C	-1.701553	0.218617	-0.000324
C	-2.040463	-1.212844	-0.000104
N	-0.444949	0.576249	-0.000524
N	-1.057436	-2.064844	-0.000121
Te	0.682414	-1.043775	-0.000013
I	3.202672	0.867687	0.000341
C	-5.123800	1.722526	-0.000366
N	-5.995056	2.472240	-0.000416

M062XD3-null-null_complex-Te-CN-NO3-opp.out

C	3.486565	1.554044	0.000009
C	3.915346	0.175459	0.000009
C	3.021337	-0.851199	0.000010
C	2.172939	1.867616	0.000009
H	4.244878	2.326126	0.000016
H	3.346989	-1.883279	0.000016
H	1.834496	2.895650	0.000019
C	1.172445	0.829844	0.000006
C	1.612524	-0.574693	0.000004
N	-0.104347	1.088345	0.000038
N	0.692903	-1.498100	0.000030
Te	-1.109521	-0.614246	-0.000047
O	-2.899509	1.038083	-0.000231
O	-5.039955	1.248732	0.000004
O	-4.161181	-0.716193	0.000363
N	-4.065282	0.515797	0.000038
C	5.323299	-0.099825	0.000017
N	6.454889	-0.301780	0.000024

M062XD3-null-null_complex-Te-CN-NO3-same.out

C	3.746972	0.554862	-0.000151
C	3.914984	-0.878932	-0.000184
C	2.840647	-1.696847	-0.000086
C	2.514001	1.132940	-0.000016
H	4.921731	-1.275645	-0.000273
H	2.949205	-2.773937	-0.000090
H	2.392085	2.208020	0.000031
C	1.340856	0.307309	0.000069
C	1.503727	-1.155673	0.000030
N	0.136272	0.812524	0.000278
N	0.422766	-1.878269	0.000188
Te	-1.175113	-0.662852	0.000155
O	-2.616750	1.309660	0.000222
O	-4.673925	1.936144	-0.000125
O	-4.198156	-0.163222	-0.000538
N	-3.861744	1.026387	-0.000242
C	4.923937	1.375255	-0.000244
N	5.880239	2.013034	-0.000325

M062XD3-null-null_complex-Te-CN-Quin-opp.out

C	3.852554	1.864679	0.008268
C	4.570945	0.606870	-0.002653
C	3.926927	-0.585716	-0.005749
C	2.506295	1.896825	0.015358
H	4.430761	2.779046	0.010192
H	4.465167	-1.523783	-0.014070
H	1.960840	2.830948	0.023215
C	1.750613	0.666294	0.011517
C	2.486365	-0.616424	0.001043
N	0.451863	0.640014	0.014848
N	1.799176	-1.717124	-0.003273
Te	-0.142828	-1.256558	0.003689
C	-2.540798	0.848679	-1.216100
C	-4.700259	1.160695	-0.011606
C	-3.839927	1.687591	-1.164465
H	-1.651899	1.473378	-1.298050
H	-2.545248	0.161849	-2.065402
H	-3.610616	2.742608	-1.000624
H	-4.379653	1.615694	-2.109909
C	-2.528946	0.902805	1.185632
H	-2.244065	0.322885	2.065622
H	-1.795781	1.700740	1.070616
C	-3.972691	1.446205	1.306361
H	-4.501266	0.963780	2.131581
H	-3.960391	2.517502	1.511808
H	-5.680152	1.638260	-0.017345
C	-4.845987	-0.357248	-0.169235
H	-5.555810	-0.752952	0.558509
H	-5.235969	-0.588980	-1.162658
C	-3.451311	-0.992270	0.032702
H	-3.381574	-1.501353	0.996815
H	-3.232141	-1.729978	-0.743135
N	-2.400045	0.034625	0.003149
C	6.006103	0.648626	-0.011252
N	7.152658	0.703301	-0.018711

M062XD3-null-null_complex-Te-CN-Quin-same.out

C	4.130583	1.120836	-0.000656
C	4.700092	-0.211200	0.005592
C	3.908962	-1.300656	0.005928
C	2.791254	1.331595	-0.006871
H	5.777844	-0.303264	0.010103
H	4.317945	-2.302107	0.010742
H	2.374890	2.329713	-0.011317
C	1.897750	0.203757	-0.005666
C	2.470847	-1.158783	0.000797
N	0.604817	0.343473	-0.008910
N	1.648575	-2.160751	0.002357
Te	-0.221998	-1.462941	-0.001395
C	-2.335607	0.920768	-1.241758
C	-4.384885	1.605361	0.000929
C	-3.475072	1.964386	-1.179262
H	-1.360738	1.388367	-1.376282
H	-2.484632	0.217399	-2.064109
H	-3.068570	2.968296	-1.040167
H	-4.040841	1.969558	-2.112085
C	-2.246308	1.051588	1.153665
H	-2.010724	0.469065	2.046498
H	-1.415423	1.735383	0.983823
C	-3.592946	1.796806	1.299430
H	-4.166309	1.402652	2.141665
H	-3.421170	2.856717	1.492059
H	-5.277913	2.230150	0.000736
C	-4.765876	0.125472	-0.117091
H	-5.520717	-0.138561	0.625045
H	-5.196462	-0.067523	-1.102090
C	-3.483542	-0.712730	0.093585
H	-3.474401	-1.183583	1.079292
H	-3.398817	-1.508230	-0.650783
N	-2.284753	0.133290	0.001943
C	5.026732	2.242835	0.000659
N	5.753932	3.130945	0.002284

M062XD3-null-null_complex-Te-F4-Br.out

C	-3.214915	1.199465	-0.000074
C	-3.628297	-0.175249	-0.000096
C	-2.727984	-1.176515	0.000014
C	-1.912032	1.542255	0.000061
C	-0.891552	0.524452	0.000150
C	-1.312710	-0.891776	0.000117
N	0.374435	0.804068	0.000403
N	-0.385746	-1.792227	0.000318
Te	1.428653	-0.875577	0.000147
Br	3.783159	0.784879	-0.000349
F	-4.183068	2.121125	-0.000144
F	-1.563535	2.825159	0.000130
F	-4.944828	-0.410479	-0.000188
F	-3.141503	-2.442410	0.000035

M062XD3-null-null_complex-Te-F4-Cl.out

C	2.864518	1.039464	0.000355
C	3.150874	-0.367195	0.000109
C	2.162365	-1.281707	-0.000107
C	1.598040	1.499483	0.000378
C	0.488658	0.580238	0.000149
C	0.778527	-0.869939	-0.000099
N	-0.745781	0.975591	0.000176
N	-0.227970	-1.679082	-0.000283
Te	-1.956951	-0.597266	-0.000202
Cl	-3.959792	1.176102	-0.000125
F	3.913113	1.869518	0.000566
F	1.369512	2.810102	0.000618
F	4.440855	-0.722644	0.000111
F	2.458331	-2.580702	-0.000331

M062XD3-null-null_complex-Te-F4-I.out

C	-3.558766	1.308237	-0.000042
C	-4.052829	-0.040176	0.000054
C	-3.213617	-1.092788	0.000130
C	-2.238200	1.574431	-0.000052
C	-1.279861	0.497843	-0.000033
C	-1.784811	-0.890485	0.000049
N	0.000973	0.701324	0.000207
N	-0.914035	-1.846541	0.000298
Te	0.944333	-1.041897	-0.000286
I	3.628562	0.580437	0.000135
F	-4.470374	2.284718	-0.000016
F	-1.813769	2.833305	-0.000022
F	-5.379958	-0.197727	0.000136
F	-3.698026	-2.332558	0.000297

M062XD3-null-null_complex-Te-F4-NO3.out

C	3.285501	1.125911	0.000028
C	3.620912	-0.270914	-0.000056
C	2.666590	-1.220821	-0.000083
C	2.004445	1.541667	0.000102
C	0.928644	0.582350	0.000108
C	1.270016	-0.856043	-0.000043
N	-0.319638	0.930635	0.000126
N	0.293145	-1.702990	0.000009
Te	-1.454724	-0.692371	0.000037
O	-3.094430	1.079093	-0.000545
O	-5.211089	1.458341	-0.000252
O	-4.490332	-0.570030	0.000548
N	-4.298947	0.650309	-0.000126
F	4.304158	1.989929	0.000053
F	1.727253	2.841493	0.000166
F	4.921165	-0.578795	-0.000122
F	3.006744	-2.507574	-0.000137

M062XD3-null-null_complex-Te-F4-Quin.out

C	-3.618122	1.557561	0.000337
C	-4.295882	0.283906	-0.001819
C	-3.614853	-0.875235	-0.001928
C	-2.276007	1.643530	0.001769
C	-1.476101	0.444684	0.001095
C	-2.169336	-0.868038	0.000061
N	-0.183851	0.465185	0.002094
N	-1.445001	-1.933763	0.000984
Te	0.489163	-1.408055	0.002101
C	2.777301	0.773723	1.229417
C	4.899712	1.212121	-0.001252
C	4.027562	1.682322	1.167074
H	1.858266	1.348816	1.337682
H	2.835312	0.073588	2.065871
H	3.737537	2.724055	1.015651
H	4.582928	1.632642	2.104803
C	2.726284	0.867787	-1.171334
H	2.448289	0.292411	-2.056412
H	1.964327	1.632941	-1.027135
C	4.142667	1.473032	-1.307842
H	4.680509	1.018838	-2.143117
H	4.079593	2.543701	-1.506519
H	5.854102	1.738567	-0.001362
C	5.122549	-0.297736	0.138887
H	5.847221	-0.651638	-0.595676
H	5.526897	-0.520944	1.128521
C	3.760390	-0.998952	-0.065446
H	3.706593	-1.487253	-1.041205
H	3.587402	-1.765097	0.694329
N	2.657578	-0.027575	-0.002108
F	-4.384608	2.639742	0.000826
F	-1.671181	2.825128	0.003832
F	-5.622545	0.317033	-0.003583
F	-4.253169	-2.035336	-0.003916

M062XD3-null-null_complex-Te-diBr-Br.out

C	-2.402635	2.171328	0.000005
C	-3.258612	1.021798	-0.000008
C	-2.740905	-0.225772	-0.000008
C	-1.057433	2.039959	0.000046
H	-2.849882	3.155802	-0.000027
H	-4.330026	1.168201	-0.000009
C	-0.431820	0.738980	0.000088
C	-1.313334	-0.453466	0.000011
N	0.854673	0.562360	0.000172
N	-0.740657	-1.613568	0.000055
Te	1.266933	-1.370757	0.000090
Br	4.064652	-0.628872	-0.000195
Br	-3.886853	-1.731514	-0.000031
Br	0.043051	3.576295	0.000025

M062XD3-null-null_complex-Te-diBr-Cl.out

C	-1.603597	2.430402	0.000031
C	-2.647507	1.448113	0.000037
C	-2.355422	0.129420	0.000024
C	-0.302811	2.063922	0.000005
H	-1.871344	3.478215	0.000035
H	-3.676938	1.779337	0.000058
C	0.086217	0.674447	-0.000024
C	-0.990416	-0.347121	0.000023
N	1.321299	0.276816	-0.000035
N	-0.627115	-1.587086	-0.000012
Te	1.401423	-1.700003	-0.000045
Cl	4.068666	-1.428147	0.000112
Br	1.052693	3.384488	-0.000013
Br	-3.751868	-1.150263	0.000016

M062XD3-null-null_complex-Te-diBr-I.out

C	-2.881602	2.088559	0.000009
C	-3.683167	0.899860	0.000014
C	-3.109991	-0.323202	0.000007
C	-1.532070	2.020327	-0.000005
H	-3.375344	3.050612	0.000013
H	-4.760192	0.996463	0.000021
C	-0.848602	0.748504	-0.000012
C	-1.673458	-0.482979	-0.000003
N	0.444975	0.631893	-0.000039
N	-1.049807	-1.617635	-0.000021
Te	0.937507	-1.281284	-0.000009
I	3.961259	-0.386887	0.000021
Br	-0.498684	3.600883	-0.000019
Br	-4.185728	-1.878640	0.000010

M062XD3-null-null_complex-Te-diBr-NO3.out

C	2.629633	1.942484	0.000106
C	3.335585	0.694612	-0.000081
C	2.670326	-0.480564	-0.000149
C	1.279258	1.978927	0.000218
H	3.197098	2.863064	0.000177
H	4.416778	0.706904	-0.000148
C	0.498439	0.763861	0.000123
C	1.225354	-0.529720	-0.000071
N	-0.799067	0.746689	0.000271
N	0.512766	-1.609960	-0.000095
Te	-1.436544	-1.121526	-0.000081
O	-3.520725	0.130133	-0.000100
O	-5.659604	-0.089058	-0.000155
O	-4.407739	-1.840091	-0.000168
N	-4.558837	-0.613617	-0.000166
Br	0.367842	3.633066	0.000535
Br	3.628596	-2.111290	-0.000346

M062XD3-null-null_complex-Te-diBr-Quin.out

C	2.831760	2.309329	0.002133
C	3.796201	1.241162	0.002546
C	3.413715	-0.050854	0.001009
C	1.507801	2.060481	0.000518
H	3.191189	3.329245	0.002883
H	4.847318	1.495561	0.003795
C	1.014103	0.701117	-0.000010
C	2.007818	-0.406716	-0.000413
N	-0.243045	0.400410	-0.000825
N	1.556402	-1.615558	-0.001946
Te	-0.441576	-1.573138	-0.001454
C	-3.167099	0.049173	-1.230642
C	-5.335203	0.036574	-0.001244
C	-4.578110	0.679447	-1.167669
H	-2.388384	0.803142	-1.342261
H	-3.080460	-0.650345	-2.065084
H	-4.508371	1.758120	-1.012504
H	-5.110244	0.519453	-2.106653
C	-3.138122	0.161616	1.167839
H	-2.740860	-0.333862	2.055920
H	-2.558557	1.071949	1.015482
C	-4.651056	0.450459	1.306074
H	-5.080307	-0.109527	2.140146
H	-4.817881	1.509593	1.506992
H	-6.378927	0.351157	-0.002602
C	-5.236046	-1.486442	-0.139388
H	-5.872835	-1.982306	0.594645
H	-5.582227	-1.791920	-1.129121
C	-3.757391	-1.885341	0.070047
H	-3.605642	-2.347807	1.048117
H	-3.425314	-2.601530	-0.685722
N	-2.882653	-0.706166	0.003051
Br	0.254246	3.469648	-0.001199
Br	4.683134	-1.439035	0.000765

M062XD3-null-null_complex-Te-nat-Br.out

C	-3.922238	1.593115	-0.000054
C	-4.429664	0.246520	-0.000039
C	-3.594212	-0.817779	0.000022
C	-2.592600	1.844489	-0.000008
H	-4.628377	2.415170	-0.000087
H	-5.502823	0.095058	-0.000063
H	-3.964008	-1.835848	0.000053
H	-2.198618	2.852958	-0.000002
C	-1.647695	0.755313	0.000044
C	-2.163761	-0.625181	0.000052
N	-0.358755	0.951100	0.000130
N	-1.295077	-1.593299	0.000160
Te	0.563732	-0.801557	0.000061
Br	3.104503	0.704862	-0.000149

M062XD3-null-null_complex-Te-nat-Cl.out

C	-3.613666	1.313964	-0.000170
C	-3.969166	-0.080393	-0.000140
C	-3.020384	-1.045872	-0.000045
C	-2.319284	1.708874	-0.000113
H	-4.406195	2.053335	-0.000246
H	-5.019361	-0.349362	-0.000187
H	-3.276154	-2.098685	-0.000016
H	-2.038259	2.754839	-0.000135
C	-1.259637	0.730978	-0.000023
C	-1.618744	-0.698505	0.000014
N	-0.001231	1.069453	0.000060
N	-0.647279	-1.562043	0.000091
Te	1.120142	-0.564636	0.000081
Cl	3.284555	1.110283	-0.000109

M062XD3-null-null_complex-Te-nat-I.out

C	-4.250946	1.760377	0.000026
C	-4.842471	0.448120	-0.000007
C	-4.077063	-0.667135	0.000026
C	-2.908488	1.927428	0.000093
H	-4.903843	2.625158	0.000014
H	-5.922973	0.364877	-0.000046
H	-4.509789	-1.659949	0.000021
H	-2.451105	2.908664	0.000135
C	-2.035345	0.780143	0.000119
C	-2.637743	-0.563961	0.000079
N	-0.736026	0.893162	0.000234
N	-1.834000	-1.587668	0.000171
Te	0.062601	-0.917661	0.000115
I	2.962924	0.494931	-0.000207

M062XD3-null-null_complex-Te-nat-NO3.out

C	4.054695	1.437433	-0.000010
C	4.459717	0.056134	0.000024
C	3.547841	-0.943151	0.000024
C	2.748175	1.787464	-0.000042
H	4.820685	2.204089	-0.000022
H	5.518713	-0.174269	0.000040
H	3.841151	-1.985862	0.000039
H	2.429991	2.822503	-0.000078
C	1.724207	0.771465	-0.000036
C	2.135711	-0.643638	-0.000002
N	0.453245	1.060002	-0.000108
N	1.197411	-1.545141	-0.000026
Te	-0.587549	-0.622352	-0.000018
O	-2.390396	1.085470	0.000023
O	-4.528542	1.322655	0.000098
O	-3.672449	-0.652614	0.000073
N	-3.557650	0.579071	0.000084

M062XD3-null-null_complex-Te-nat-Quin.out

C	4.198602	2.168702	0.000446
C	5.002309	0.969416	-0.009956
C	4.439391	-0.256236	-0.012201
C	2.850601	2.118838	0.008868
H	4.703001	3.127007	0.001335
H	6.080215	1.071405	-0.016117
H	5.030661	-1.162422	-0.019822
H	2.242506	3.013934	0.016352
C	2.178276	0.840763	0.006897
C	3.000298	-0.391340	-0.004161
N	0.883724	0.729803	0.012716
N	2.386305	-1.533600	-0.006885
Te	0.416893	-1.203413	0.003901
C	-2.113594	0.770622	-1.214274
C	-4.286084	0.986305	-0.010522
C	-3.453645	1.543824	-1.169486
H	-1.256620	1.438750	-1.292838
H	-2.079278	0.084123	-2.063131
H	-3.277533	2.610706	-1.016297
H	-3.990614	1.435767	-2.113271
C	-2.104624	0.827682	1.186181
H	-1.799642	0.258922	2.066749
H	-1.402858	1.653745	1.074024
C	-3.569483	1.313960	1.303474
H	-4.078322	0.818865	2.133702
H	-3.601195	2.387098	1.497874
H	-5.286910	1.418732	-0.016879
C	-4.363674	-0.537392	-0.156744
H	-5.048604	-0.958674	0.580712
H	-4.752551	-0.793696	-1.144641
C	-2.938557	-1.107381	0.035134
H	-2.840192	-1.617863	0.995976
H	-2.688570	-1.829722	-0.745727
N	-1.937293	-0.034173	0.005201

M062XD3-null-null_donor-Te-CN.out

C	-2.604159	1.350672	-0.000002
C	-2.835391	-0.077882	-0.000002
C	-1.815526	-0.971446	-0.000003
C	-1.354412	1.853729	-0.000003
H	-3.466279	2.003977	-0.000002
H	-1.990616	-2.038351	-0.000004
H	-1.167347	2.918757	-0.000004
C	-0.220120	0.963916	-0.000002
C	-0.461155	-0.490851	-0.000003
N	1.012792	1.392988	-0.000007
N	0.564641	-1.300212	-0.000007
Te	2.182323	-0.187259	0.000004
C	-4.193611	-0.544187	-0.000002
N	-5.284624	-0.900006	-0.000002

M062XD3-null-null_donor-Te-F4-Br.out

C	-0.000001	-2.534553	0.720847
C	-0.000001	-2.534553	-0.720847
C	-0.000001	-1.388848	-1.427393
C	-0.000001	-1.388848	1.427393
C	-0.000001	-0.123638	0.739742
C	-0.000001	-0.123638	-0.739742
N	-0.000005	1.016766	1.363273
N	-0.000005	1.016766	-1.363273
Te	0.000004	2.432883	0.000000
F	-0.000003	-1.404102	2.750212
F	-0.000001	-3.717018	1.315358
F	-0.000001	-3.717018	-1.315358
F	-0.000003	-1.404102	-2.750212

==========
M062XD3-null-null_donor-Te-diBr.out
==========

C	-0.718314	-2.467371	0.000008
C	0.718303	-2.467374	0.000008
C	1.425421	-1.318997	-0.000013
C	-1.425428	-1.318990	-0.000013
H	-1.234325	-3.417771	0.000002
H	1.234309	-3.417778	0.000003
C	-0.742326	-0.044421	-0.000017
C	0.742327	-0.044424	-0.000016
N	-1.360671	1.099825	-0.000116
N	1.360673	1.099820	-0.000116
Te	0.000006	2.514048	0.000116
Br	-3.303878	-1.333181	-0.000060
Br	3.303872	-1.333191	-0.000059

==========
M062XD3-null-null_donor-Te-nat.out
==========

C	-3.317352	0.721163	0.000000
C	-3.317303	-0.721218	0.000000
C	-2.169474	-1.430085	-0.000000
C	-2.169560	1.430067	0.000000
H	-4.269302	1.236702	0.000000
H	-4.269218	-1.236835	0.000000
H	-2.157061	-2.511563	-0.000000
H	-2.157153	2.511553	0.000000
C	-0.903980	0.739058	0.000001
C	-0.903923	-0.739006	-0.000001
N	0.240627	1.366315	-0.000001
N	0.240679	-1.366311	-0.000000
Te	1.657176	0.000005	0.000000

5.4.3.3.2 PCM

==========
M062XD3-PCM-ACN_acceptor-NO3.out
==========

O	-0.231786	-1.220867	-0.000030
O	1.173959	0.409893	-0.000007
O	-0.942277	0.810990	-0.000074
N	0.000118	-0.000019	0.000126

==========
M062XD3-PCM-ACN_acceptor-Quin.out
==========

C	-0.838101	-1.365591	0.021799
C	1.289797	-0.043691	-0.017053
C	0.705451	-1.463044	-0.135765
H	-1.166392	-1.819944	0.971610
H	-1.352439	-1.900127	-0.794935
H	1.131796	-2.113190	0.635040
H	0.970807	-1.891303	-1.108867
C	-0.751885	0.731749	1.209684
H	-1.041575	1.793424	1.144285
H	-1.240104	0.311002	2.104494
C	0.793761	0.583906	1.297967
H	1.266509	1.559432	1.453249
H	1.076171	-0.055675	2.142525
H	2.386493	-0.081341	-0.031897
C	0.768205	0.805524	-1.189914
H	1.093364	1.844367	-1.063071
H	1.184790	0.445274	-2.136075
C	-0.782841	0.711076	-1.202035
H	-1.239523	1.713069	-1.268016
H	-1.133399	0.130980	-2.071167
N	-1.291832	0.043494	0.016390

==========
M062XD3-PCM-ACN_complex-Te-CN-Br-opp.out
==========

C	-3.371100	1.659222	-0.000042
C	-3.902518	0.315539	0.000147
C	-3.098897	-0.779694	0.000230
C	-2.039187	1.873337	-0.000117
H	-4.066256	2.487769	-0.000135
H	-3.504600	-1.782515	0.000385
H	-1.630368	2.874909	-0.000282
C	-1.125547	0.758353	0.000089
C	-1.673527	-0.606106	0.000191
N	0.171632	0.909916	-0.000106
N	-0.831754	-1.604157	0.000374
Te	1.015434	-0.877594	0.000049
Br	3.700823	0.759556	-0.000306
C	-5.327213	0.144981	0.000232
N	-6.468763	0.019448	0.000273

==========
M062XD3-PCM-ACN_complex-Te-CN-Br-same.out
==========

C	-3.678093	0.662062	-0.000052
C	-3.953162	-0.756292	0.000145
C	-2.944211	-1.651679	0.000245
C	-2.412207	1.155625	-0.000144
H	-4.984969	-1.080928	0.000209
H	-3.136555	-2.716397	0.000392
H	-2.216983	2.219455	-0.000293
C	-1.304520	0.242467	-0.000041
C	-1.573813	-1.203345	0.000163
N	-0.063228	0.655049	-0.000116
N	-0.548464	-2.009605	0.000242
Te	1.116869	-0.924335	0.000084
Br	3.437700	1.230019	-0.000140
C	-4.790265	1.568984	-0.000154
N	-5.691250	2.281084	-0.000232

==========
M062XD3-PCM-ACN_complex-Te-CN-Cl-opp.out
==========

C	2.985895	1.542377	-0.000052
C	3.410887	0.161646	-0.000037
C	2.523758	-0.867803	0.000010
C	1.674528	1.858814	-0.000015
H	3.743491	2.314589	-0.000053
H	2.852196	-1.898676	0.000047
H	1.343935	2.889097	0.000025
C	0.676549	0.818197	0.000008
C	1.115135	-0.585180	0.000022
N	-0.603916	1.071080	0.000229
N	0.196070	-1.511460	0.000157
Te	-1.596853	-0.638461	-0.000033
Cl	-3.936007	1.082419	-0.000018
C	4.818335	-0.117264	-0.000031
N	5.947610	-0.326890	-0.000018

M062XD3-PCM-ACN_complex-Te-CN-Cl-same.out

C	3.284053	0.391341	0.000076
C	3.360753	-1.051227	-0.000010
C	2.237175	-1.797749	-0.000040
C	2.097690	1.054570	0.000146
H	4.337956	-1.514997	-0.000033
H	2.280635	-2.878961	-0.000075
H	2.051894	2.135352	0.000233
C	0.874189	0.303834	0.000108
C	0.940675	-1.165160	-0.000013
N	-0.297428	0.884371	0.000251
N	-0.187352	-1.816983	0.000056
Te	-1.696075	-0.509592	-0.000067
Cl	-3.492507	1.762095	-0.000125
C	4.508942	1.138764	0.000116
N	5.495805	1.726264	0.000148

M062XD3-PCM-ACN_complex-Te-CN-I-opp.out

C	-3.747771	1.748954	0.000441
C	-4.353703	0.437195	-0.000197
C	-3.614044	-0.702116	-0.000523
C	-2.406095	1.887808	0.000751
H	-4.394621	2.615665	0.000647
H	-4.075504	-1.680526	-0.001024
H	-1.940685	2.864346	0.001206
C	-1.557708	0.722904	0.000512
C	-2.181090	-0.608193	-0.000186
N	-0.253513	0.800335	0.000680
N	-1.398986	-1.654856	-0.000531
Te	0.479771	-1.031798	0.000395
I	3.536601	0.581035	-0.000344
C	-5.786108	0.348818	-0.000535
N	-6.932931	0.289804	-0.000819

M062XD3-PCM-ACN_complex-Te-CN-I-same.out

C	-4.038751	0.869567	0.000008
C	-4.449080	-0.515805	0.000023
C	-3.532058	-1.504703	-0.000017
C	-2.731557	1.238672	-0.000009
H	-5.507243	-0.738937	0.000045
H	-3.826436	-2.545672	0.000000
H	-2.433411	2.278244	-0.000056
C	-1.717728	0.222250	0.000065
C	-2.125102	-1.190062	-0.000012
N	-0.442030	0.511936	-0.000065
N	-1.183876	-2.094087	0.000051
Te	0.573561	-1.175692	-0.000011
I	3.328399	0.914215	0.000007
C	-5.057169	1.880808	-0.000006
N	-5.881892	2.679946	-0.000001

M062XD3-PCM-ACN_complex-Te-CN-NO3-opp.out

C	3.464452	1.593998	0.000059
C	3.915981	0.221361	0.000102
C	3.049625	-0.824807	0.000044
C	2.147515	1.886142	-0.000044
H	4.207408	2.380239	0.000089
H	3.396470	-1.849492	0.000057
H	1.798142	2.910114	-0.000101
C	1.168613	0.826938	-0.000088
C	1.636167	-0.568162	-0.000044
N	-0.116875	1.053168	-0.000258
N	0.737126	-1.514117	-0.000167
Te	-1.064879	-0.680865	-0.000116
O	-2.979836	1.080963	-0.000111
O	-5.115541	1.326494	0.000316
O	-4.266079	-0.649586	0.000449
N	-4.138427	0.580183	0.000090
C	5.328370	-0.031683	0.000187
N	6.460888	-0.222319	0.000259

M062XD3-PCM-ACN_complex-Te-CN-NO3-same.out

C	3.726475	0.609346	-0.000060
C	3.935529	-0.820197	-0.000068
C	2.885980	-1.667246	-0.000028
C	2.485337	1.162038	-0.000015
H	4.951000	-1.192299	-0.000088
H	3.028646	-2.739780	-0.000012
H	2.339833	2.233855	0.000013
C	1.335082	0.301885	0.000013
C	1.537585	-1.155467	0.000005
N	0.114965	0.770193	0.000135
N	0.475078	-1.910588	0.000110
Te	-1.139345	-0.751888	0.000015
O	-2.670001	1.370908	-0.000071
O	-4.714617	2.035659	0.000034
O	-4.273742	-0.069816	0.000053
N	-3.904260	1.110569	-0.000087
C	4.879502	1.463873	-0.000073
N	5.811415	2.135111	-0.000083

M062XD3-PCM-ACN_complex-Te-CN-Quin-opp.out

C	3.886755	1.849315	0.004534
C	4.583072	0.580587	-0.001717
C	3.924603	-0.605863	-0.003367
C	2.540071	1.896445	0.009117
H	4.474212	2.757515	0.005175
H	4.454208	-1.549260	-0.008157
H	2.010209	2.839770	0.013532
C	1.769053	0.675572	0.007390
C	2.484504	-0.616337	0.000751
N	0.469101	0.664986	0.009450
N	1.775380	-1.704661	-0.001973
Te	-0.172434	-1.215423	0.002260
C	-2.538381	0.851262	-1.220252
C	-4.698926	1.117529	-0.008203
C	-3.849297	1.668298	-1.157382
H	-1.663073	1.493011	-1.312765
H	-2.541509	0.160757	-2.066022
H	-3.634825	2.724714	-0.983986
H	-4.387123	1.592838	-2.103186
C	-2.522164	0.909520	1.187249
H	-2.219498	0.338070	2.066470
H	-1.817092	1.731325	1.067144
C	-3.979171	1.411493	1.311532
H	-4.492281	0.906041	2.132114
H	-3.992206	2.480959	1.524956
H	-5.688530	1.573884	-0.012496
C	-4.810863	-0.401808	-0.172798
H	-5.513755	-0.815821	0.550866
H	-5.187326	-0.638380	-1.169891
C	-3.406765	-1.009368	0.036358
H	-3.328807	-1.509145	1.004145
H	-3.171435	-1.744873	-0.736156
N	-2.373335	0.041907	0.002768
C	6.018115	0.593438	-0.006877
N	7.166248	0.617783	-0.011284

M062XD3-PCM-ACN_complex-Te-CN-Quin-same.out

C	4.165908	1.075817	-0.000376
C	4.712810	-0.264394	0.009010
C	3.898884	-1.338104	0.009754
C	2.829827	1.314258	-0.008889
H	5.788127	-0.380372	0.015445
H	4.295717	-2.344758	0.016847
H	2.432245	2.320309	-0.015674
C	1.917621	0.202600	-0.006951
C	2.463621	-1.169232	0.002027
N	0.626460	0.366059	-0.011576
N	1.614978	-2.150785	0.003475
Te	-0.255289	-1.411399	-0.002808
C	-2.341509	0.919208	-1.252769
C	-4.394349	1.563249	0.003846
C	-3.499361	1.940009	-1.181753
H	-1.379400	1.406523	-1.407006
H	-2.490593	0.204020	-2.064154
H	-3.110311	2.950932	-1.044759
H	-4.069224	1.930308	-2.111587
C	-2.235339	1.075169	1.146405
H	-1.976330	0.506508	2.041257
H	-1.431159	1.786125	0.961634
C	-3.601793	1.779834	1.297524
H	-4.156689	1.368322	2.143262
H	-3.456659	2.844164	1.486252
H	-5.302008	2.165998	0.005040
C	-4.738217	0.074361	-0.106892
H	-5.484663	-0.206103	0.637072
H	-5.159788	-0.135407	-1.091987
C	-3.438742	-0.731596	0.111323
H	-3.413070	-1.184391	1.104581
H	-3.338776	-1.534821	-0.622175
N	-2.257413	0.144513	0.000597
C	5.078788	2.183226	0.000276
N	5.818651	3.061493	0.001327

M062XD3-PCM-ACN_complex-Te-F4-Br.out

C	-3.192520	1.253029	-0.000019
C	-3.639780	-0.113070	-0.000130
C	-2.765381	-1.134987	0.000092
C	-1.883373	1.563453	0.000274
C	-0.891028	0.521105	0.000391
C	-1.347595	-0.880508	0.000390
N	0.385514	0.762016	0.000550
N	-0.445390	-1.811284	0.000423
Te	1.361698	-0.958700	0.000370
Br	3.882872	0.830687	-0.000812
F	-4.132085	2.193038	-0.000279
F	-1.491556	2.834091	0.000351
F	-4.953746	-0.315816	-0.000441
F	-3.197241	-2.392520	-0.000034

M062XD3-PCM-ACN_complex-Te-F4-Cl.out

C	2.847147	1.070627	-0.000001
C	3.151445	-0.334522	-0.000055
C	2.176449	-1.261199	-0.000058
C	1.576688	1.513039	0.000045
C	0.482689	0.578631	0.000028
C	0.791070	-0.863692	-0.000016
N	-0.760385	0.952551	0.000069
N	-0.204555	-1.691750	-0.000027
Te	-1.922080	-0.652552	0.000038
Cl	-4.027050	1.258873	-0.000059
F	3.878960	1.909151	0.000011
F	1.317218	2.817826	0.000110
F	4.438254	-0.671163	-0.000109
F	2.477750	-2.557043	-0.000113

M062XD3-PCM-ACN_complex-Te-F4-I.out

C	-3.549184	1.374098	-0.000166
C	-4.084161	0.039240	0.000009
C	-3.277740	-1.037028	-0.000176
C	-2.222758	1.599915	-0.000643
C	-1.300365	0.495877	-0.000740
C	-1.847422	-0.872694	-0.000422
N	-0.010186	0.653073	-0.000759
N	-1.008876	-1.862362	-0.000549
Te	0.841070	-1.132116	-0.000553
I	3.762525	0.601854	0.001071
F	-4.425562	2.372404	0.000022
F	-1.749691	2.841862	-0.000934
F	-5.407640	-0.078275	0.000353
F	-3.786691	-2.264842	-0.000108

M062XD3-PCM-ACN_complex-Te-F4-NO3.out

C	3.265499	1.169263	-0.000018
C	3.629678	-0.221741	0.000120
C	2.695733	-1.189639	0.000158
C	1.977659	1.557600	-0.000104
C	0.924014	0.576942	-0.000125
C	1.295256	-0.850724	0.000051
N	-0.334512	0.894528	-0.000077
N	0.337357	-1.723204	0.000055
Te	-1.413534	-0.764170	-0.000211
O	-3.153719	1.111150	0.000217
O	-5.262520	1.526853	0.000422
O	-4.574934	-0.510993	0.000153
N	-4.351216	0.704025	0.000175
F	4.260684	2.050297	-0.000001
F	1.663273	2.849618	-0.000163
F	4.929224	-0.501953	0.000222
F	3.051789	-2.470951	0.000281

M062XD3-PCM-ACN_complex-Te-F4-Quin.out

C	-3.660022	1.524099	-0.000094
C	-4.312126	0.239709	0.002735
C	-3.606482	-0.903484	0.002623
C	-2.320174	1.631938	-0.003324
C	-1.496403	0.450328	-0.004029
C	-2.162959	-0.872366	-0.000395
N	-0.204331	0.494490	-0.005913
N	-1.414116	-1.921856	0.000383
Te	0.525348	-1.357422	-0.002678
C	2.774460	0.789976	1.231289
C	4.910815	1.169744	0.006977
C	4.043421	1.669918	1.165826
H	1.870215	1.387539	1.340568
H	2.819266	0.088551	2.066761
H	3.776453	2.715884	1.002589
H	4.590381	1.613090	2.107576
C	2.736859	0.880913	-1.176099
H	2.447489	0.310823	-2.060404
H	2.001002	1.671664	-1.035317
C	4.170644	1.442371	-1.306192
H	4.697969	0.963662	-2.133756
H	4.137511	2.512651	-1.512633
H	5.878249	1.671139	0.010563
C	5.092644	-0.344264	0.157074
H	5.812856	-0.720543	-0.570016
H	5.478675	-0.573238	1.152217
C	3.718312	-1.012901	-0.059104
H	3.658959	-1.496628	-1.036206
H	3.521123	-1.773230	0.699813
N	2.636447	-0.010318	-0.002437
F	-4.446193	2.594928	0.000969
F	-1.738493	2.827998	-0.005476
F	-5.641416	0.243908	0.005641
F	-4.225914	-2.079894	0.005486

M062XD3-PCM-ACN_complex-Te-diBr-Br.out

C	2.352764	2.222263	-0.000092
C	3.243541	1.096339	-0.000132
C	2.768608	-0.165879	-0.000029
C	1.013761	2.056153	0.000083
H	2.779754	3.215607	-0.000238
H	4.308579	1.282694	-0.000290
C	0.429341	0.734616	0.000292
C	1.346373	-0.427889	0.000145
N	-0.852009	0.511330	0.000359
N	0.813099	-1.610978	0.000224
Te	-1.168083	-1.436740	0.000291
Br	-4.184683	-0.634650	-0.000391
Br	3.948189	-1.639570	-0.000141
Br	-0.134992	3.554680	-0.000048

M062XD3-PCM-ACN_complex-Te-diBr-Cl.out

C	1.538670	2.464503	0.000062
C	2.609744	1.508067	0.000046
C	2.359990	0.182534	-0.000016
C	0.249453	2.067973	0.000015
H	1.788195	3.516765	0.000118
H	3.626616	1.875246	0.000064
C	-0.097528	0.665633	0.000073
C	1.004716	-0.324024	-0.000025
N	-1.320765	0.227580	0.000022
N	0.677960	-1.578180	-0.000024
Te	-1.314841	-1.747194	-0.000067
Cl	-4.168076	-1.433226	0.000151
Br	-1.146186	3.341093	-0.000034
Br	3.784002	-1.058436	0.000028

M062XD3-PCM-ACN_complex-Te-diBr-I.out

C	2.820807	2.164956	-0.000010
C	3.674019	1.009831	0.000030
C	3.159385	-0.237033	0.000103
C	1.477240	2.042901	0.000019
H	3.280541	3.143597	-0.000039
H	4.744464	1.161531	0.000026
C	0.852147	0.740499	0.000080
C	1.729705	-0.450979	0.000110
N	-0.436016	0.558569	0.000183
N	1.159881	-1.618143	0.000278
Te	-0.808347	-1.376540	0.000037
I	-4.086655	-0.393511	-0.000292
Br	0.373866	3.574287	0.000032
Br	4.290559	-1.747801	0.000207

M062XD3-PCM-ACN_complex-Te-diBr-NO3.out

C	2.563978	2.018405	0.000154
C	3.318549	0.796230	0.000106
C	2.702604	-0.403781	0.000010
C	1.215251	2.006084	0.000110
H	3.103708	2.955379	0.000253
H	4.397889	0.858772	0.000175
C	0.482986	0.759883	-0.000000
C	1.259833	-0.502066	-0.000064
N	-0.814375	0.686404	0.000021
N	0.592081	-1.614271	-0.000076
Te	-1.354849	-1.211401	-0.000301
O	-3.593960	0.100000	-0.000165
O	-5.734340	-0.092526	0.000180
O	-4.502638	-1.855848	0.000453
N	-4.626817	-0.625908	0.000120
Br	0.238262	3.621831	0.000221
Br	3.712670	-1.999157	0.000039

M062XD3-PCM-ACN_complex-Te-diBr-Quin.out

C	2.928440	2.249733	0.001858
C	3.850428	1.145533	0.001670
C	3.411906	-0.128131	0.000091
C	1.596037	2.048588	0.000263
H	3.330373	3.253476	0.003141
H	4.909813	1.362486	0.002631
C	1.045032	0.710886	-0.000258
C	1.994556	-0.434068	-0.000353
N	-0.223436	0.456674	-0.000531
N	1.490628	-1.622578	-0.000484
Te	-0.519625	-1.505151	0.000779
C	-3.203206	0.069512	-1.247822
C	-5.359925	0.008003	-0.002745
C	-4.628190	0.663440	-1.178195
H	-2.447432	0.841730	-1.388861
H	-3.110722	-0.647871	-2.065653
H	-4.585382	1.744344	-1.030078
H	-5.158875	0.479933	-2.113139
C	-3.164244	0.232231	1.153260
H	-2.741087	-0.229153	2.047172
H	-2.628466	1.164310	0.975924
C	-4.685990	0.459282	1.297341
H	-5.083220	-0.113830	2.137633
H	-4.891819	1.512500	1.491489
H	-6.413281	0.286920	-0.004207
C	-5.207474	-1.511904	-0.125391
H	-5.828524	-2.022785	0.611036
H	-5.533961	-1.838304	-1.114708
C	-3.720674	-1.858975	0.099216
H	-3.557642	-2.287289	1.090238
H	-3.363232	-2.583040	-0.636610
N	-2.882334	-0.648961	0.001786
Br	0.404171	3.514016	-0.000351
Br	4.632680	-1.567624	-0.000950

M062XD3-PCM-ACN_complex-Te-nat-Br.out

C	3.868721	1.710659	-0.000016
C	4.432454	0.383474	0.000278
C	3.647808	-0.716009	0.000392
C	2.532819	1.912402	-0.000204
H	4.542642	2.557887	-0.000019
H	5.510071	0.279797	0.000459
H	4.063301	-1.715605	0.000644
H	2.105311	2.906679	-0.000337
C	1.636418	0.782162	-0.000292
C	2.211819	-0.575515	0.000057
N	0.337264	0.912984	-0.000265
N	1.386981	-1.585152	0.000099
Te	-0.475723	-0.891243	-0.000124
Br	-3.243819	0.743943	0.000160

M062XD3-PCM-ACN_complex-Te-nat-Cl.out

C	-3.579440	1.382849	-0.000020
C	-3.965991	-0.005962	0.000008
C	-3.044478	-0.994120	0.000088
C	-2.280683	1.755314	0.000013
H	-4.357783	2.135644	-0.000036
H	-5.021313	-0.248092	-0.000030
H	-3.328393	-2.039016	0.000090
H	-1.985286	2.796852	0.000058
C	-1.244292	0.751030	-0.000115
C	-1.637500	-0.670118	0.000014
N	0.025869	1.050834	0.000023
N	-0.687138	-1.561246	0.000019
Te	1.078240	-0.627179	-0.000017
Cl	3.398087	1.189815	0.000035

M062XD3-PCM-ACN_complex-Te-nat-I.out

C	-4.190628	1.904683	0.000122
C	-4.852481	0.624038	0.000066
C	-4.154568	-0.532474	0.000040
C	-2.843514	2.004945	0.000115
H	-4.798871	2.800264	0.000133
H	-5.934791	0.602917	0.000060
H	-4.646415	-1.496669	-0.000000
H	-2.340528	2.963253	0.000131
C	-2.036124	0.809723	0.000062
C	-2.711940	-0.500853	0.000089
N	-0.730454	0.841057	0.000082
N	-1.968168	-1.572844	-0.000011
Te	-0.063190	-1.018789	0.000053
I	3.106271	0.516404	-0.000124

M062XD3-PCM-ACN_complex-Te-nat-NO3.out

C	4.017484	1.524816	0.000154
C	4.465541	0.154500	0.000239
C	3.589803	-0.874019	0.000175
C	2.703778	1.840060	0.000005
H	4.761612	2.311421	0.000201
H	5.530482	-0.040257	0.000356
H	3.920184	-1.904985	0.000237
H	2.362503	2.867329	-0.000074
C	1.713007	0.790538	-0.000054
C	2.170398	-0.612007	0.000045
N	0.430314	1.030879	-0.000187
N	1.261465	-1.546340	-0.000026
Te	-0.536388	-0.695232	-0.000215
O	-2.482592	1.123089	-0.000019
O	-4.617868	1.377202	0.000514
O	-3.775170	-0.601943	0.000357
N	-3.640013	0.628093	0.000247

M062XD3-PCM-ACN_complex-Te-nat-Quin.out

C	4.256087	2.115392	-0.000267
C	5.032158	0.897678	-0.005347
C	4.440825	-0.315670	-0.006160
C	2.906427	2.094861	0.004532
H	4.782539	3.061519	-0.000523
H	6.112036	0.975365	-0.008716
H	5.017804	-1.231717	-0.010014
H	2.321505	3.005722	0.008083
C	2.205412	0.831489	0.004200
C	2.998321	-0.419263	-0.001937
N	0.908340	0.748444	0.007369
N	2.350346	-1.543397	-0.003845
Te	0.372817	-1.168168	0.002047
C	-2.105829	0.780408	-1.220407
C	-4.274460	0.963510	-0.007596
C	-3.448925	1.543730	-1.159812
H	-1.257599	1.457075	-1.316403
H	-2.081329	0.087335	-2.063749
H	-3.277471	2.608734	-0.990619
H	-3.984400	1.443073	-2.104728
C	-2.090283	0.847260	1.185618
H	-1.764386	0.291378	2.066648
H	-1.419365	1.696908	1.062677
C	-3.566098	1.291370	1.310123
H	-4.058582	0.769209	2.132977
H	-3.622327	2.360418	1.519210
H	-5.281740	1.379507	-0.012514
C	-4.325176	-0.559236	-0.165801
H	-5.009243	-0.998084	0.561434
H	-4.694326	-0.815242	-1.160889
C	-2.895919	-1.108640	0.041832
H	-2.796229	-1.603156	1.010335
H	-2.631281	-1.835119	-0.729822
N	-1.906873	-0.017264	0.004516

M062XD3-PCM-ACN_donor-Te-CN.out

C	-2.609915	1.354557	-0.000002
C	-2.836815	-0.072374	-0.000002
C	-1.817042	-0.968874	-0.000003
C	-1.357545	1.854522	-0.000003
H	-3.469398	2.010919	-0.000002
H	-1.994600	-2.035591	-0.000004
H	-1.174820	2.920475	-0.000004
C	-0.225708	0.963806	-0.000003
C	-0.465364	-0.487048	-0.000003
N	1.012036	1.388173	-0.000008
N	0.565720	-1.294857	-0.000008
Te	2.184261	-0.187689	0.000005
C	-4.192032	-0.545537	-0.000002
N	-5.280077	-0.911929	-0.000002

M062XD3-PCM-ACN_donor-Te-F4.out

C	-0.000001	-2.538524	0.719056
C	-0.000001	-2.538524	-0.719056
C	-0.000001	-1.390712	-1.421423
C	-0.000001	-1.390712	1.421423
C	-0.000001	-0.126863	0.736640
C	-0.000001	-0.126863	-0.736640
N	-0.000006	1.017802	1.357822
N	-0.000006	1.017802	-1.357822
Te	0.000004	2.437147	0.000000
F	-0.000003	-1.406889	2.748869
F	-0.000001	-3.721315	1.319014
F	-0.000001	-3.721315	-1.319014
F	-0.000003	-1.406889	-2.748869

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M062XD3-PCM-ACN_donor-Te-diBr.out
==========

C	-0.717764	-2.472752	0.000010
C	0.717752	-2.472756	0.000010
C	1.418906	-1.320291	-0.000016
C	-1.418913	-1.320283	-0.000016
H	-1.230975	-3.424448	0.000000
H	1.230957	-3.424455	0.000000
C	-0.740045	-0.045925	-0.000018
C	0.740046	-0.045929	-0.000018
N	-1.354939	1.103247	-0.000152
N	1.354941	1.103242	-0.000152
Te	0.000006	2.521354	0.000154
Br	-3.303196	-1.337699	-0.000080
Br	3.303190	-1.337710	-0.000079

==========
M062XD3-PCM-ACN_donor-Te-nat.out
==========

C	-3.323787	0.720825	0.000001
C	-3.323741	-0.720873	0.000001
C	-2.173956	-1.429298	0.000000
C	-2.174039	1.429283	0.000000
H	-4.275680	1.236183	0.000001
H	-4.275603	-1.236303	0.000001
H	-2.166483	-2.511240	-0.000001
H	-2.166547	2.511236	-0.000000
C	-0.909621	0.737736	0.000000
C	-0.909561	-0.737654	-0.000001
N	0.240216	1.360873	-0.000005
N	0.240235	-1.360912	-0.000004
Te	1.661719	0.000005	0.000001

==========
M062XD3-PCM-THF_acceptor-NO3.out
==========

O	1.183156	0.381876	0.000030
O	-0.922391	0.833472	0.000053
O	-0.260779	-1.215468	-0.000014
N	0.000017	0.000138	-0.000080

==========
M062XD3-PCM-THF_acceptor-Quin.out
==========

C	-0.749212	-0.447155	1.326306
C	1.286931	0.019965	-0.031028
C	0.792004	-0.277154	1.387378
H	-1.238775	0.132367	2.110346
H	-1.030373	-1.492699	1.467869
H	1.065479	0.547418	2.050285
H	1.265623	-1.180489	1.777542
C	-0.816880	1.338183	-0.259263
H	-1.340089	1.701663	-1.146112
H	-1.111358	1.975247	0.577858
C	0.719904	1.373695	-0.468643
H	0.964060	1.552767	-1.518428
H	1.171084	2.180849	0.111662
H	2.376911	0.037881	-0.058690
C	0.745890	-1.062400	-0.970755
H	1.170591	-0.947325	-1.969573
H	1.039061	-2.047962	-0.602431
C	-0.797776	-0.927420	-1.011858
H	-1.127469	-0.528257	-1.972966
H	-1.278262	-1.898419	-0.880034
N	-1.287379	-0.019905	0.031408

==========
M062XD3-PCM-THF_complex-Te-CN-Br-opp.out
==========

C	-3.371137	1.648569	0.000028
C	-3.897084	0.302946	-0.000041
C	-3.087507	-0.788672	-0.000140
C	-2.039803	1.867410	0.000030
H	-4.069999	2.474140	0.000082
H	-3.489284	-1.793143	-0.000181
H	-1.632949	2.869776	0.000075
C	-1.121252	0.756533	0.000070
C	-1.662632	-0.610640	-0.000117
N	0.174145	0.916211	0.000038
N	-0.814914	-1.603005	-0.000070
Te	1.034496	-0.863752	0.000055
Br	3.660671	0.752818	-0.000048
C	-5.320943	0.127486	-0.000002
N	-6.462500	0.000207	0.000018

==========
M062XD3-PCM-THF_complex-Te-CN-Br-same.out
==========

C	-3.685061	0.641436	-0.000024
C	-3.945451	-0.779407	0.000058
C	-2.926836	-1.664011	0.000124
C	-2.423212	1.146893	-0.000042
H	-4.974103	-1.114104	0.000061
H	-3.106901	-2.730930	0.000183
H	-2.238377	2.212525	-0.000113
C	-1.305835	0.245898	0.000026
C	-1.560736	-1.202630	0.000114
N	-0.069352	0.672133	-0.000027
N	-0.527262	-1.997047	0.000174
Te	1.131762	-0.892093	0.000099
Br	3.417410	1.203437	-0.000176
C	-4.807671	1.535142	-0.000099
N	-5.719494	2.233644	-0.000158

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M062XD3-PCM-THF_complex-Te-CN-Cl-opp.out
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C	2.991074	1.535108	0.000317
C	3.412226	0.153530	0.000493
C	2.520416	-0.872870	0.000299
C	1.680204	1.854798	-0.000001
H	3.751087	2.305075	0.000441
H	2.845965	-1.904836	0.000407
H	1.350926	2.885606	-0.000165
C	0.678992	0.817465	-0.000090
C	1.112609	-0.587286	0.000009
N	-0.599713	1.076411	-0.000265
N	0.189120	-1.508867	-0.000110
Te	-1.605619	-0.625605	-0.000370
Cl	-3.912001	1.060449	0.000082
C	4.818901	-0.128937	0.000886
N	5.947977	-0.340810	0.001189

M062XD3-PCM-THF_complex-Te-CN-Cl-same.out

C	3.284913	0.382236	-0.000066
C	3.356099	-1.060425	0.000007
C	2.229486	-1.802958	0.000031
C	2.099642	1.048401	-0.000088
H	4.331920	-1.527359	0.000080
H	2.269025	-2.884460	0.000163
H	2.056376	2.129398	-0.000075
C	0.873540	0.302348	-0.000020
C	0.934072	-1.167321	-0.000060
N	-0.294611	0.888570	0.000208
N	-0.196404	-1.813089	0.000206
Te	-1.704900	-0.493577	-0.000052
Cl	-3.460522	1.736094	0.000043
C	4.512650	1.124521	-0.000020
N	5.503008	1.706519	0.000025

M062XD3-PCM-THF_complex-Te-CN-I-opp.out

C	-3.751928	1.733047	0.000047
C	-4.346747	0.416343	-0.000033
C	-3.595543	-0.715938	-0.000077
C	-2.411189	1.882911	0.000092
H	-4.406663	2.593927	0.000057
H	-4.048366	-1.698417	-0.000134
H	-1.952758	2.862671	0.000147
C	-1.551921	0.726019	0.000067
C	-2.163491	-0.610617	-0.000027
N	-0.249172	0.817498	0.000104
N	-1.370847	-1.648527	-0.000054
Te	0.506967	-1.006024	0.000049
I	3.499077	0.569337	-0.000044
C	-5.778108	0.314780	-0.000064
N	-6.924552	0.245449	-0.000092

M062XD3-PCM-THF_complex-Te-CN-I-same.out

C	-4.046466	0.840157	-0.000045
C	-4.437867	-0.550485	-0.000187
C	-3.507276	-1.527584	-0.000210
C	-2.743263	1.224464	0.000080
H	-5.493375	-0.787121	-0.000276
H	-3.788219	-2.572613	-0.000298
H	-2.456883	2.267701	0.000285
C	-1.716317	0.221423	0.000060
C	-2.103712	-1.196230	-0.000194
N	-0.445458	0.530174	0.000122
N	-1.149654	-2.086027	-0.000098
Te	0.599766	-1.138603	0.000113
I	3.300268	0.900331	-0.000069
C	-5.077974	1.837872	0.000051
N	-5.914358	2.625018	0.000081

M062XD3-PCM-THF_complex-Te-CN-NO3-opp.out

C	3.468821	1.585250	0.000111
C	3.914633	0.210920	0.000153
C	3.042107	-0.830725	0.000057
C	2.152898	1.883126	-0.000026
H	4.215617	2.367959	0.000171
H	3.383883	-1.857279	0.000068
H	1.806980	2.908359	-0.000082
C	1.168533	0.828881	-0.000107
C	1.629848	-0.568442	-0.000066
N	-0.115237	1.062428	-0.000306
N	0.726038	-1.509309	-0.000228
Te	-1.075166	-0.665678	-0.000189
O	-2.958168	1.068052	-0.000206
O	-5.093985	1.310766	0.000358
O	-4.242929	-0.664738	0.000701
N	-4.118818	0.565245	0.000217
C	5.325752	-0.048543	0.000278
N	6.457627	-0.243969	0.000383

M062XD3-PCM-THF_complex-Te-CN-NO3-same.out

C	3.724876	0.601102	-0.004218
C	3.928586	-0.829008	0.021079
C	2.875967	-1.672592	0.026787
C	2.484191	1.155869	-0.022941
H	4.943221	-1.203517	0.035550
H	3.014390	-2.745554	0.045857
H	2.340967	2.227808	-0.040954
C	1.331336	0.300006	-0.015120
C	1.528782	-1.157830	0.009136
N	0.113480	0.773495	-0.024860
N	0.463668	-1.908305	0.015793
Te	-1.149216	-0.741193	-0.001588
O	-2.641736	1.351355	0.035134
O	-4.678909	2.036858	0.056822
O	-4.260947	-0.068949	-0.079792
N	-3.881149	1.104905	0.003784
C	4.880776	1.451377	-0.007384
N	5.816334	2.117852	-0.008888

M062XD3-PCM-THF_complex-Te-CN-Quin-opp.out

C	3.880399	1.851826	0.004165
C	4.580296	0.584792	-0.001593
C	3.924341	-0.602731	-0.003047
C	2.533792	1.896540	0.008494
H	4.466398	2.761027	0.004666
H	4.455341	-1.545289	-0.007472
H	2.001257	2.838303	0.012583
C	1.765227	0.674030	0.006978
C	2.484106	-0.616502	0.000779
N	0.465563	0.660914	0.008907
N	1.778743	-1.706872	-0.001929
Te	-0.168085	-1.222399	0.002067
C	-2.538383	0.849269	-1.220250
C	-4.697775	1.125400	-0.008028
C	-3.847299	1.670056	-1.159545
H	-1.660774	1.487962	-1.312068
H	-2.541987	0.158355	-2.065794
H	-3.630122	2.726534	-0.989803
H	-4.386259	1.593668	-2.104697
C	-2.520987	0.909390	1.186459
H	-2.221495	0.336774	2.066069
H	-1.809969	1.726049	1.066421
C	-3.975263	1.420032	1.310153
H	-4.490912	0.920866	2.133070
H	-3.982880	2.490318	1.519858
H	-5.685639	1.585627	-0.012318
C	-4.816141	-0.393998	-0.168817
H	-5.519331	-0.803541	0.557190
H	-5.196606	-0.631247	-1.164303
C	-3.413501	-1.006441	0.037875
H	-3.335739	-1.507254	1.005285
H	-3.182020	-1.742857	-0.735050
N	-2.376839	0.040425	0.003010
C	6.015423	0.602404	-0.006439
N	7.163355	0.631971	-0.010593

M062XD3-PCM-THF_complex-Te-CN-Quin-same.out

C	4.160374	1.082176	-0.000335
C	4.710471	-0.256945	0.010411
C	3.899804	-1.332908	0.011329
C	2.823869	1.316744	-0.009946
H	5.786186	-0.369469	0.017712
H	4.298022	-2.338920	0.019434
H	2.423450	2.321613	-0.017720
C	1.914219	0.202791	-0.007735
C	2.464080	-1.167912	0.002501
N	0.622952	0.363105	-0.013031
N	1.619381	-2.152452	0.004111
Te	-0.250613	-1.418855	-0.003312
C	-2.340844	0.919570	-1.251382
C	-4.392225	1.569876	0.004726
C	-3.495601	1.944108	-1.180520
H	-1.376703	1.403556	-1.403241
H	-2.490672	0.206308	-2.064456
H	-3.103477	2.953787	-1.043052
H	-4.065392	1.937452	-2.110485
C	-2.235499	1.071145	1.147308
H	-1.979446	0.499982	2.041484
H	-1.426929	1.777632	0.964587
C	-3.598776	1.782243	1.298636
H	-4.156066	1.373422	2.144205
H	-3.449284	2.845867	1.488075
H	-5.297605	2.176110	0.006400
C	-4.742043	0.082349	-0.107107
H	-5.489394	-0.195684	0.636946
H	-5.165858	-0.124662	-1.091884
C	-3.445084	-0.728796	0.108888
H	-3.421108	-1.184593	1.100939
H	-3.348174	-1.530901	-0.626397
N	-2.261091	0.142613	0.000362
C	5.070957	2.191689	0.000176
N	5.809062	3.071334	0.001129

M062XD3-PCM-THF_complex-Te-F4-Br.out

C	-3.206661	1.233649	-0.000078
C	-3.639745	-0.136413	-0.000021
C	-2.754047	-1.148617	0.000054
C	-1.900634	1.558624	-0.000025
C	-0.895581	0.527388	0.000057
C	-1.338543	-0.879271	0.000068
N	0.378125	0.782582	0.000050
N	-0.427281	-1.800006	0.000106
Te	1.376425	-0.927550	0.000248
Br	3.870773	0.808865	-0.000374
F	-4.157382	2.164283	-0.000145
F	-1.526830	2.834240	-0.000045
F	-4.952811	-0.353298	-0.000068
F	-3.173622	-2.410545	0.000120

M062XD3-PCM-THF_complex-Te-F4-Cl.out

C	2.850772	1.063334	0.000103
C	3.150649	-0.342320	-0.000027
C	2.172536	-1.266106	-0.000034
C	1.581340	1.509804	0.000199
C	0.484012	0.578738	0.000292
C	0.787753	-0.864954	0.000164
N	-0.756922	0.958439	0.000050
N	-0.210926	-1.688415	0.000028
Te	-1.929743	-0.639270	0.000131
Cl	-4.008766	1.239146	-0.000398
F	3.886330	1.899507	-0.000054
F	1.327203	2.815218	0.000087
F	4.437789	-0.683518	-0.000264
F	2.471815	-2.562828	-0.000298

M062XD3-PCM-THF_complex-Te-F4-I.out

C	-3.563534	1.350571	0.000127
C	-4.081383	0.009482	0.001194
C	-3.261267	-1.056590	0.000815
C	-2.239876	1.593632	-0.001295
C	-1.302738	0.501114	-0.001338
C	-1.832520	-0.874759	-0.000448
N	-0.015317	0.676088	-0.002118
N	-0.981031	-1.852468	-0.000346
Te	0.865320	-1.095761	-0.001272
I	3.740777	0.588501	0.001228
F	-4.453904	2.338148	0.000625
F	-1.784690	2.841777	-0.002350
F	-5.404556	-0.124789	0.002577
F	-3.756348	-2.290358	0.001808

M062XD3-PCM-THF_complex-Te-F4-NO3.out

C	3.270131	1.159653	0.001837
C	3.627661	-0.232844	0.007424
C	2.689054	-1.196154	0.006812
C	1.983995	1.554826	-0.004344
C	0.925208	0.579361	-0.005288
C	1.290128	-0.850305	0.000666
N	-0.331525	0.903217	-0.010695
N	0.327888	-1.717263	0.000188
Te	-1.420453	-0.748810	-0.008612
O	-3.147722	1.114117	-0.015441
O	-5.261168	1.503129	0.038922
O	-4.549072	-0.526181	0.006066
N	-4.341704	0.692253	0.010319
F	4.270022	2.036787	0.003124
F	1.677858	2.848407	-0.009376
F	4.926699	-0.520075	0.013201
F	3.039597	-2.479017	0.011951

M062XD3-PCM-THF_complex-Te-F4-Quin.out

C	-3.655060	1.527828	-0.000021
C	-4.310103	0.244436	0.001399
C	-3.607143	-0.900593	0.001264
C	-2.314909	1.633916	-0.001951
C	-1.493474	0.450429	-0.002707
C	-2.163283	-0.871393	-0.000310
N	-0.201436	0.491938	-0.003762
N	-1.417686	-1.922839	0.000601
Te	0.520278	-1.363258	-0.001231
C	2.775578	0.789280	1.230532
C	4.910377	1.173778	0.004554
C	4.043803	1.670655	1.165499
H	1.870288	1.385458	1.338497
H	2.820230	0.088493	2.066690
H	3.775634	2.716691	1.004789
H	4.592381	1.613226	2.106355
C	2.735612	0.878814	-1.176091
H	2.448108	0.306928	-2.059932
H	1.995697	1.665897	-1.036144
C	4.167233	1.446166	-1.307091
H	4.695725	0.971716	-2.136466
H	4.130253	2.516750	-1.511387
H	5.876678	1.677469	0.007016
C	5.096390	-0.339990	0.152834
H	5.815766	-0.713928	-0.576407
H	5.486498	-0.568759	1.146515
C	3.722524	-1.011496	-0.059400
H	3.662250	-1.497451	-1.035485
H	3.528161	-1.771240	0.700981
N	2.639238	-0.011863	-0.002298
F	-4.439317	2.599736	0.001013
F	-1.731404	2.828546	-0.002781
F	-5.639115	0.252178	0.003025
F	-4.227739	-2.075289	0.002759

M062XD3-PCM-THF_complex-Te-diBr-Br.out

C	2.381410	2.199556	0.000015
C	3.256090	1.061475	0.000092
C	2.761716	-0.193579	0.000091
C	1.039651	2.052290	-0.000073
H	2.821196	3.187331	0.000049
H	4.323961	1.230855	0.000158
C	0.435602	0.739566	-0.000067
C	1.336318	-0.435578	-0.000013
N	-0.848911	0.535976	-0.000120
N	0.786421	-1.610078	0.000036
Te	-1.196937	-1.407709	-0.000045
Br	-4.166925	-0.630993	-0.000016
Br	3.918853	-1.685858	0.000237
Br	-0.087120	3.567109	-0.000151

M062XD3-PCM-THF_complex-Te-diBr-Cl.out

C	1.558581	2.455385	0.000499
C	2.621805	1.490665	0.000365
C	2.359881	0.167172	0.000108
C	0.265799	2.069002	0.000390
H	1.814826	3.506038	0.000657
H	3.642133	1.848333	0.000450
C	-0.093463	0.669973	0.000139
C	1.000754	-0.328709	0.000022
N	-1.320481	0.243825	0.000145
N	0.662696	-1.578952	-0.000337
Te	-1.337031	-1.731786	-0.000274
Cl	-4.148092	-1.436894	-0.000239
Br	-1.118644	3.354292	0.000419
Br	3.773232	-1.087701	-0.000151

M062XD3-PCM-THF_complex-Te-diBr-I.out

C	2.834181	2.147031	0.000070
C	3.675007	0.983338	0.000058
C	3.146156	-0.257863	0.000023
C	1.489022	2.038830	0.000022
H	3.302959	3.121395	0.000141
H	4.747256	1.122185	0.000104
C	0.849692	0.743178	-0.000110
C	1.714520	-0.457705	-0.000002
N	-0.440201	0.576759	0.000038
N	1.131723	-1.617660	-0.000116
Te	-0.839370	-1.353565	-0.000247
I	-4.052228	-0.392652	0.000122
Br	0.402941	3.582119	0.000144
Br	4.262002	-1.780468	0.000037

M062XD3-PCM-THF_complex-Te-diBr-NO3.out

C	2.576895	2.002665	0.000281
C	3.321302	0.774986	0.000363
C	2.695172	-0.420064	0.000208
C	1.227675	2.001129	0.000033
H	3.122843	2.936064	0.000357
H	4.401219	0.827160	0.000509
C	0.485006	0.760976	-0.000125
C	1.251716	-0.507444	0.000008
N	-0.812849	0.699237	-0.000587
N	0.574571	-1.613476	-0.000325
Te	-1.371992	-1.193029	-0.000218
O	-3.577049	0.107057	0.000739
O	-5.716588	-0.093598	0.000686
O	-4.478627	-1.852902	-0.000351
N	-4.609312	-0.623369	0.000509
Br	0.265105	3.625153	-0.000217
Br	3.694443	-2.022879	0.000219

M062XD3-PCM-THF_complex-Te-diBr-Quin.out

C	2.928219	2.249855	0.002300
C	3.850299	1.145722	0.002372
C	3.411884	-0.127972	0.000520
C	1.595837	2.048618	0.000193
H	3.330089	3.253624	0.003828
H	4.909665	1.362772	0.003741
C	1.044916	0.710879	-0.000622
C	1.994549	-0.434024	-0.000534
N	-0.223502	0.456550	-0.001342
N	1.490721	-1.622554	-0.001048
Te	-0.519574	-1.505322	-0.000255
C	-3.203816	0.069423	-1.247760
C	-5.359803	0.007937	-0.001362
C	-4.628792	0.663268	-1.177313
H	-2.448143	0.841646	-1.389269
H	-3.111814	-0.648048	-2.065563
H	-4.585959	1.744191	-1.029336
H	-5.160024	0.479625	-2.111923
C	-3.163403	0.232441	1.153254
H	-2.739605	-0.228717	2.046981
H	-2.627873	1.164577	0.975417
C	-4.685085	0.459342	1.298278
H	-5.081713	-0.113809	2.138828
H	-4.890866	1.512546	1.492548
H	-6.413172	0.286816	-0.002236
C	-5.207359	-1.511974	-0.123855
H	-5.827881	-2.022701	0.613125
H	-5.534493	-1.838614	-1.112875
C	-3.720368	-1.858945	0.099794
H	-3.556663	-2.287250	1.090713
H	-3.363357	-2.582981	-0.636276
N	-2.882144	-0.648919	0.001752
Br	0.403860	3.513954	-0.000695
Br	4.632760	-1.567380	-0.000207

M062XD3-PCM-THF_complex-Te-nat-Br.out

C	3.874238	1.683977	-0.000039
C	4.425818	0.352181	-0.000299
C	3.630570	-0.740071	-0.000284
C	2.539823	1.896312	0.000255
H	4.555041	2.525879	-0.000120
H	5.502588	0.238305	-0.000559
H	4.036895	-1.743483	-0.000506
H	2.118954	2.893356	0.000381
C	1.633116	0.774322	0.000402
C	2.195473	-0.588423	0.000008
N	0.336176	0.919688	0.000094
N	1.360309	-1.588757	-0.000073
Te	-0.501456	-0.873681	0.000098
Br	-3.194497	0.740887	-0.000134

M062XD3-PCM-THF_complex-Te-nat-Cl.out

C	-3.588318	1.362572	0.000012
C	-3.965263	-0.028466	-0.000118
C	-3.036149	-1.009866	-0.000169
C	-2.291631	1.742943	0.000086
H	-4.371503	2.110519	0.000111
H	-5.018954	-0.278499	-0.000129
H	-3.312127	-2.057020	-0.000207
H	-2.001995	2.786184	0.000286
C	-1.247925	0.746099	-0.000028
C	-1.630912	-0.677544	-0.000189
N	0.019145	1.056524	0.000288
N	-0.673846	-1.560457	-0.000157
Te	1.089825	-0.610057	0.000105
Cl	3.363398	1.169111	-0.000236

M062XD3-PCM-THF_complex-Te-nat-I.out

C	-4.217799	1.868805	0.000132
C	-4.860694	0.578896	-0.000083
C	-4.145100	-0.567017	-0.000182
C	-2.871985	1.987773	0.000211
H	-4.838500	2.755951	0.000185
H	-5.942734	0.541258	-0.000161
H	-4.621972	-1.538772	-0.000349
H	-2.381450	2.952468	0.000331
C	-2.046944	0.804808	0.000175
C	-2.703096	-0.515061	0.000013
N	-0.742171	0.857422	0.000192
N	-1.942842	-1.575000	-0.000122
Te	-0.043918	-0.990448	-0.000024
I	3.093155	0.506910	-0.000015

M062XD3-PCM-THF_complex-Te-nat-NO3.out

C	4.025514	1.506408	0.000203
C	4.464294	0.133382	0.000078
C	3.581324	-0.889271	0.000067
C	2.713595	1.829441	0.000325
H	4.774566	2.288521	0.000142
H	5.528064	-0.068652	-0.000046
H	3.904399	-1.922675	-0.000062
H	2.377234	2.858416	0.000352
C	1.715805	0.786454	0.000252
C	2.163246	-0.618909	0.000165
N	0.435514	1.036740	0.000051
N	1.247564	-1.546115	-0.000036
Te	-0.546577	-0.679695	-0.000174
O	-2.466769	1.119778	-0.001170
O	-4.603446	1.361496	0.000028
O	-3.750241	-0.613287	0.001213
N	-3.623263	0.617889	0.000209

M062XD3-PCM-THF_complex-Te-nat-Quin.out

C	4.246237	2.124363	-0.000465
C	5.026960	0.909689	-0.004268
C	4.440375	-0.305748	-0.004692
C	2.896822	2.098995	0.003483
H	4.769006	3.072586	-0.000937
H	6.106579	0.991328	-0.006962
H	5.019637	-1.220234	-0.007557
H	2.307966	3.007237	0.006153
C	2.200532	0.833129	0.003532
C	2.998401	-0.414615	-0.001358
N	0.903897	0.745602	0.005994
N	2.356209	-1.541882	-0.002982
Te	0.380297	-1.174097	0.001526
C	-2.106990	0.781028	-1.218332
C	-4.276184	0.967729	-0.006425
C	-3.449735	1.545639	-1.159199
H	-1.257359	1.456480	-1.309879
H	-2.080426	0.090851	-2.064053
H	-3.277654	2.610806	-0.991472
H	-3.985608	1.444911	-2.103981
C	-2.092366	0.840870	1.187230
H	-1.771205	0.279946	2.066836
H	-1.414703	1.685810	1.069199
C	-3.565936	1.293669	1.310833
H	-4.061874	0.776136	2.134639
H	-3.616926	2.363366	1.518218
H	-5.282329	1.386687	-0.010612
C	-4.331873	-0.555004	-0.164768
H	-5.015577	-0.991727	0.564216
H	-4.705575	-0.809561	-1.158606
C	-2.903186	-1.108660	0.037780
H	-2.803132	-1.608619	1.003557
H	-2.641655	-1.832335	-0.737634
N	-1.911957	-0.020452	0.004048

M062XD3-PCM-THF_donor-Te-CN.out

C	-2.608844	1.353993	-0.000002
C	-2.836439	-0.073239	-0.000002
C	-1.816831	-0.969381	-0.000004
C	-1.356945	1.854475	-0.000003
H	-3.468720	2.009922	-0.000002
H	-1.993934	-2.036138	-0.000005
H	-1.173443	2.920241	-0.000004
C	-0.224702	0.963856	-0.000003
C	-0.464626	-0.487734	-0.000004
N	1.012171	1.389010	-0.000009
N	0.565446	-1.295853	-0.000008
Te	2.183877	-0.187627	0.000005
C	-4.192247	-0.545201	-0.000002
N	-5.280717	-0.910016	-0.000002

M062XD3-PCM-THF_donor-Te-F4.out

C	-0.000001	-2.537806	0.719388
C	-0.000001	-2.537806	-0.719388
C	-0.000001	-1.390398	-1.422524
C	-0.000001	-1.390398	1.422524
C	-0.000001	-0.126298	0.737196
C	-0.000001	-0.126298	-0.737196
N	-0.000006	1.017582	1.358766
N	-0.000006	1.017582	-1.358766
Te	0.000004	2.436407	-0.000000
F	-0.000003	-1.406359	2.749101
F	-0.000001	-3.720600	1.318256
F	-0.000001	-3.720600	-1.318256
F	-0.000003	-1.406359	-2.749101

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M062XD3-PCM-THF_donor-Te-diBr.out
==========

C	-0.717878	-2.471884	0.000009
C	0.717866	-2.471888	0.000009
C	1.419994	-1.320118	-0.000015
C	-1.420001	-1.320110	-0.000015
H	-1.231745	-3.423262	0.000001
H	1.231726	-3.423270	0.000001
C	-0.740463	-0.045667	-0.000018
C	0.740464	-0.045671	-0.000018
N	-1.356009	1.102556	-0.000146
N	1.356012	1.102550	-0.000146
Te	0.000007	2.519964	0.000147
Br	-3.303237	-1.336784	-0.000076
Br	3.303231	-1.336796	-0.000076

==========
M062XD3-PCM-THF_donor-Te-nat.out
==========

C	-3.322564	0.720904	0.000001
C	-3.322518	-0.720953	0.000001
C	-2.173172	-1.429534	0.000000
C	-2.173255	1.429519	0.000000
H	-4.274456	1.236318	0.000001
H	-4.274378	-1.236439	0.000001
H	-2.164761	-2.511394	-0.000000
H	-2.164830	2.511389	-0.000000
C	-0.908617	0.738021	0.000000
C	-0.908559	-0.737945	-0.000001
N	0.240245	1.361872	-0.000004
N	0.240269	-1.361902	-0.000003
Te	1.660902	0.000005	0.000001

5.4.3.3.3 CPCM

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M062XD3-CPCM-ACN_acceptor-NO3.out
==========

O	-0.247249	-1.217809	-0.000061
O	1.178924	0.394932	-0.000038
O	-0.931788	0.822823	-0.000106
N	0.000129	0.000062	0.000235

==========
M062XD3-CPCM-ACN_acceptor-Quin.out
==========

C	-0.786031	-1.123648	-0.802052
C	1.286792	-0.001153	0.004208
C	0.753866	-1.260670	-0.685852
H	-1.285579	-2.033894	-0.465481
H	-1.083882	-0.949737	-1.838138
H	1.021516	-2.142360	-0.098731
H	1.207147	-1.375708	-1.672232
C	-0.792704	-0.129841	1.370544
H	-1.292112	0.617918	1.989160
H	-1.095261	-1.113153	1.736479
C	0.747661	0.033488	1.437732
H	1.016819	0.981868	1.908896
H	1.195367	-0.765021	2.032429
H	2.377288	-0.002032	0.007889
C	0.756073	1.225668	-0.744605
H	1.205318	2.138045	-0.347863
H	1.029616	1.159025	-1.800304
C	-0.784946	1.255220	-0.576204
H	-1.087349	2.064875	0.091235
H	-1.279545	1.419301	-1.535250
N	-1.287658	0.000927	-0.004388

==========
M062XD3-CPCM-ACN_complex-Te-CN-Br-opp.out
==========

C	-3.372056	1.660403	-0.000112
C	-3.903777	0.316928	-0.000057
C	-3.100688	-0.778653	-0.000041
C	-2.040043	1.874146	-0.000154
H	-4.066837	2.489226	-0.000153
H	-3.506621	-1.781365	-0.000036
H	-1.631111	2.875694	-0.000235
C	-1.126870	0.758823	-0.000112
C	-1.675287	-0.605368	-0.000049
N	0.170520	0.909577	-0.000277
N	-0.834021	-1.603954	-0.000173
Te	1.012829	-0.878435	0.000125
Br	3.707251	0.759265	0.000024
C	-5.328406	0.146712	-0.000054
N	-6.469867	0.020498	-0.000044

==========
M062XD3-CPCM-ACN_complex-Te-CN-Br-same.out
==========

C	-3.676302	0.662972	0.000007
C	-3.952491	-0.755133	0.000192
C	-2.944236	-1.651351	0.000215
C	-2.410093	1.155582	-0.000144
H	-4.984519	-1.079043	0.000316
H	-3.137601	-2.715892	0.000367
H	-2.213938	2.219271	-0.000277
C	-1.303194	0.241481	-0.000093
C	-1.573478	-1.204086	0.000053
N	-0.061559	0.653030	-0.000217
N	-0.548632	-2.011087	0.000109
Te	1.117444	-0.927111	-0.000092
Br	3.434272	1.233704	0.000111
C	-4.787666	1.571012	-0.000005
N	-5.687776	2.284190	-0.000013

==========
M062XD3-CPCM-ACN_complex-Te-CN-Cl-opp.out
==========

C	2.985616	1.542622	0.000069
C	3.410583	0.162010	-0.000000
C	2.523713	-0.867616	-0.000188
C	1.674119	1.858868	0.000003
H	3.742883	2.315120	0.000190
H	2.852201	-1.898441	-0.000226
H	1.343562	2.889152	0.000064
C	0.676283	0.818130	-0.000056
C	1.115053	-0.585118	-0.000264
N	-0.604248	1.070853	-0.000040
N	0.196127	-1.511614	-0.000378
Te	-1.596855	-0.639015	-0.000047
Cl	-3.935040	1.083719	0.000295
C	4.818011	-0.116694	0.000157
N	5.947150	-0.326882	0.000286

M062XD3-CPCM-ACN_complex-Te-CN-Cl-same.out

C	3.284410	0.392290	0.000069
C	3.361448	-1.050272	0.000008
C	2.237999	-1.796937	-0.000026
C	2.097957	1.055388	0.000103
H	4.338715	-1.513868	0.000006
H	2.281448	-2.878138	-0.000049
H	2.052116	2.136143	0.000169
C	0.874566	0.304469	0.000059
C	0.941543	-1.164450	-0.000021
N	-0.297378	0.884536	0.000159
N	-0.186228	-1.816808	0.000018
Te	-1.695046	-0.510628	-0.000074
Cl	-3.497699	1.762467	-0.000031
C	4.509270	1.139800	0.000119
N	5.496152	1.727251	0.000160

M062XD3-CPCM-ACN_complex-Te-CN-I-opp.out

C	-3.748015	1.749584	0.000409
C	-4.354268	0.437943	-0.000184
C	-3.614883	-0.701516	-0.000482
C	-2.406312	1.888227	0.000695
H	-4.394702	2.616403	0.000593
H	-4.076485	-1.679864	-0.000940
H	-1.940890	2.864804	0.001104
C	-1.558190	0.723098	0.000478
C	-2.181945	-0.607798	-0.000160
N	-0.253906	0.799919	0.000604
N	-1.400192	-1.654752	-0.000462
Te	0.478529	-1.032636	0.000357
I	3.538565	0.581261	-0.000313
C	-5.786714	0.349816	-0.000496
N	-6.933538	0.290944	-0.000752

M062XD3-CPCM-ACN_complex-Te-CN-I-same.out

C	-4.044291	0.868291	0.000000
C	-4.453126	-0.517436	0.000279
C	-3.534958	-1.505837	0.000335
C	-2.737348	1.237990	-0.000191
H	-5.511197	-0.741497	0.000449
H	-3.829341	-2.547008	0.000537
H	-2.439180	2.277783	-0.000358
C	-1.722850	0.222253	-0.000203
C	-2.127936	-1.190339	0.000106
N	-0.447497	0.513507	-0.000195
N	-1.185491	-2.093491	0.000064
Te	0.570635	-1.171700	-0.000116
I	3.336419	0.910577	0.000089
C	-5.062264	1.880136	-0.000018
N	-5.885140	2.681152	-0.000036

M062XD3-CPCM-ACN_complex-Te-CN-NO3-opp.out

C	3.464480	1.594564	-0.000018
C	3.916402	0.222078	0.000001
C	3.050485	-0.824455	0.000008
C	2.147442	1.886188	-0.000029
H	4.207109	2.381102	-0.000021
H	3.397786	-1.848958	0.000023
H	1.797733	2.910035	-0.000041
C	1.169070	0.826584	-0.000021
C	1.636944	-0.568295	-0.000004
N	-0.116541	1.052248	-0.000027
N	0.738117	-1.514584	0.000012
Te	-1.063830	-0.681889	-0.000017
O	-2.983373	1.083527	-0.000087
O	-5.119461	1.326097	0.000087
O	-4.267185	-0.648764	0.000173
N	-4.141089	0.581192	-0.000029
C	5.328915	-0.030284	0.000013
N	6.461550	-0.220155	0.000024

M062XD3-CPCM-ACN_complex-Te-CN-NO3-same.out

C	3.727411	0.609232	-0.000073
C	3.936007	-0.820419	-0.000129
C	2.886195	-1.667098	-0.000078
C	2.486351	1.162308	0.000027
H	4.951350	-1.192820	-0.000184
H	3.028528	-2.739696	-0.000086
H	2.341569	2.234265	0.000103
C	1.335833	0.302553	0.000058
C	1.538065	-1.154818	0.000000
N	0.115626	0.771023	0.000271
N	0.475418	-1.909836	0.000155
Te	-1.138673	-0.751301	0.000033
O	-2.672858	1.370025	-0.000272
O	-4.717687	2.034087	-0.000175
O	-4.276047	-0.071185	0.000241
N	-3.907026	1.109178	-0.000077
C	4.880754	1.463321	-0.000085
N	5.812923	2.134210	-0.000094

M062XD3-CPCM-ACN_complex-Te-CN-quin-opp.out

C	3.887295	1.849163	0.004563
C	4.583403	0.580337	-0.001723
C	3.924757	-0.606020	-0.003401
C	2.540607	1.896464	0.009144
H	4.474835	2.757301	0.005229
H	4.454251	-1.549476	-0.008216
H	2.010981	2.839929	0.013578
C	1.769426	0.675709	0.007392
C	2.484663	-0.616262	0.000729
N	0.469433	0.665251	0.009456
N	1.775286	-1.704458	-0.001970
Te	-0.172562	-1.215014	0.002274
C	-2.538742	0.851501	-1.220272
C	-4.699325	1.116899	-0.008143
C	-3.849725	1.668383	-1.157012
H	-1.663563	1.493410	-1.312992
H	-2.542099	0.161037	-2.066066
H	-3.635366	2.724729	-0.983047
H	-4.387482	1.593269	-2.102880
C	-2.522505	0.909641	1.187216
H	-2.219235	0.338469	2.066406
H	-1.818251	1.732126	1.066847
C	-3.979835	1.410519	1.311817
H	-4.492573	0.904078	2.132026
H	-3.993537	2.479833	1.525965
H	-5.689079	1.572929	-0.012384
C	-4.810668	-0.402408	-0.173336
H	-5.513660	-0.816930	0.549937
H	-5.186547	-0.638769	-1.170690
C	-3.406467	-1.009527	0.036224
H	-3.328629	-1.509067	1.004118
H	-3.170743	-1.745059	-0.736127
N	-2.373315	0.042110	0.002694
C	6.018450	0.592917	-0.006887
N	7.166583	0.616957	-0.011297

M062XD3-CPCM-ACN_complex-Te-CN-quin-same.out

C	4.166415	1.075419	-0.000397
C	4.713071	-0.264883	0.008611
C	3.898915	-1.338434	0.009314
C	2.830377	1.314145	-0.008608
H	5.788354	-0.381104	0.014799
H	4.295676	-2.345131	0.016126
H	2.433068	2.320306	-0.015116
C	1.917973	0.202652	-0.006748
C	2.463693	-1.169249	0.001900
N	0.626799	0.366282	-0.011201
N	1.614754	-2.150588	0.003330
Te	-0.255501	-1.410906	-0.002662
C	-2.341848	0.919088	-1.252994
C	-4.394864	1.562527	0.003639
C	-3.500207	1.939336	-1.182193
H	-1.380026	1.406900	-1.407516
H	-2.490688	0.203565	-2.064112
H	-3.111650	2.950504	-1.045599
H	-4.070196	1.928897	-2.111943
C	-2.235500	1.075910	1.146134
H	-1.976112	0.507684	2.041147
H	-1.431825	1.787346	0.960963
C	-3.602304	1.779894	1.297184
H	-4.156867	1.368250	2.143068
H	-3.457673	2.844354	1.485583
H	-5.302806	2.164856	0.004737
C	-4.738024	0.073446	-0.106632
H	-5.484244	-0.207151	0.637510
H	-5.159479	-0.136828	-1.091665
C	-3.438166	-0.731808	0.111759
H	-3.412176	-1.184225	1.105165
H	-3.337814	-1.535168	-0.621512
N	-2.257229	0.144858	0.000636
C	5.079478	2.182676	0.000304
N	5.819455	3.060838	0.001397

M062XD3-CPCM-ACN_complex-Te-F4-Br.out

C	-3.192504	1.253968	-0.000131
C	-3.640366	-0.111957	-0.000037
C	-2.766431	-1.134273	0.000066
C	-1.883241	1.563686	-0.000150
C	-0.891444	0.521018	-0.000069
C	-1.348555	-0.880308	0.000089
N	0.385230	0.761451	-0.000046
N	-0.446628	-1.811417	0.000114
Te	1.360416	-0.959915	0.000061
Br	3.885685	0.831076	0.000059
F	-4.131478	2.194488	-0.000262
F	-1.490464	2.834075	-0.000284
F	-4.954371	-0.314059	-0.000059
F	-3.198754	-2.391736	0.000128

M062XD3-CPCM-ACN_complex-Te-F4-Cl.out

C	2.846940	1.070586	0.000073
C	3.151331	-0.334476	0.000021
C	2.176324	-1.261044	-0.000054
C	1.576532	1.513037	0.000044
C	0.482378	0.578758	-0.000020
C	0.791000	-0.863464	-0.000061
N	-0.760864	0.952389	-0.000130
N	-0.204494	-1.691724	-0.000188
Te	-1.922135	-0.653162	-0.000010
Cl	-4.026128	1.260380	0.000118
F	3.878707	1.909217	0.000123
F	1.317537	2.818137	0.000062
F	4.438172	-0.671125	0.000023
F	2.477324	-2.557011	-0.000130

M062XD3-CPCM-ACN_complex-Te-F4-I.out

C	-3.546102	1.376392	0.000017
C	-4.082965	0.042280	0.000138
C	-3.278097	-1.035144	0.000093
C	-2.219355	1.600302	-0.000160
C	-1.298715	0.494873	-0.000160
C	-1.847627	-0.872847	-0.000037
N	-0.008249	0.649913	-0.000214
N	-1.010416	-1.863737	-0.000014
Te	0.840334	-1.136371	-0.000148
I	3.760706	0.604060	0.000140
F	-4.421025	2.375909	0.000071
F	-1.744385	2.841714	-0.000294
F	-5.406571	-0.073389	0.000304
F	-3.788792	-2.262258	0.000200

M062XD3-CPCM-ACN_complex-Te-F4-NO3.out

C	3.264471	1.170570	0.000055
C	3.629660	-0.220147	0.000244
C	2.696410	-1.188679	0.000238
C	1.976341	1.557868	-0.000131
C	0.923474	0.576449	-0.000198
C	1.295698	-0.850887	0.000024
N	-0.335308	0.893062	-0.000271
N	0.338430	-1.724120	-0.000003
Te	-1.413132	-0.766522	-0.000389
O	-3.152393	1.110065	-0.000171
O	-5.259971	1.531542	0.000670
O	-4.577906	-0.508216	0.000884
N	-4.350909	0.706098	0.000427
F	4.258927	2.052357	0.000121
F	1.660834	2.849708	-0.000244
F	4.929373	-0.499466	0.000444
F	3.053443	-2.469742	0.000422

M062XD3-CPCM-ACN_complex-Te-F4-Quin.out

C	-3.659122	1.524687	-0.000070
C	-4.311652	0.240566	0.002365
C	-3.606505	-0.902913	0.002224
C	-2.319258	1.631778	-0.002944
C	-1.496067	0.449822	-0.003666
C	-2.162975	-0.872628	-0.000347
N	-0.203988	0.493571	-0.005272
N	-1.414342	-1.922345	0.000533
Te	0.525507	-1.358387	-0.002269
C	2.774613	0.787887	1.232135
C	4.909574	1.171086	0.006564
C	4.042465	1.669372	1.166461
H	1.869776	1.384199	1.343363
H	2.821217	0.085276	2.066496
H	3.774170	2.715171	1.004266
H	4.590144	1.612354	2.107778
C	2.734893	0.882464	-1.175042
H	2.444493	0.313826	-2.059941
H	1.999279	1.673055	-1.032018
C	4.168377	1.444355	-1.305908
H	4.695175	0.966224	-2.134142
H	4.134729	2.514751	-1.511678
H	5.876604	1.673255	0.010070
C	5.092595	-0.342930	0.155035
H	5.812988	-0.717918	-0.572540
H	5.478797	-0.572676	1.149930
C	3.718757	-1.012354	-0.061786
H	3.659357	-1.494199	-1.039791
H	3.522599	-1.774281	0.695775
N	2.636056	-0.010716	-0.002656
F	-4.444812	2.595848	0.000987
F	-1.736765	2.827533	-0.004739
F	-5.640939	0.245153	0.004892
F	-4.226811	-2.078936	0.004643

M062XD3-CPCM-ACN_complex-Te-diBr-Br.out

C	2.341618	2.229818	-0.000093
C	3.237753	1.108180	-0.000085
C	2.769179	-0.156428	0.000002
C	1.003540	2.057052	-0.000002
H	2.763718	3.225235	-0.000202
H	4.301839	1.299945	-0.000176
C	0.425865	0.732642	0.000156
C	1.348204	-0.425603	0.000108
N	-0.854249	0.502988	0.000132
N	0.820159	-1.611184	0.000201
Te	-1.161795	-1.445932	0.000218
Br	-4.180496	-0.636501	-0.000240
Br	3.956641	-1.623765	-0.000010
Br	-0.152446	3.550171	-0.000145

M062XD3-CPCM-ACN_complex-Te-diBr-Cl.out

C	1.536081	2.465440	0.000325
C	2.608050	1.510033	0.000284
C	2.359722	0.184285	0.000156
C	0.247380	2.067507	0.000248
H	1.784744	3.517901	0.000387
H	3.624515	1.878294	0.000349
C	-0.098140	0.664787	0.000135
C	1.005014	-0.323881	0.000093
N	-1.320847	0.225421	-0.000007
N	0.679408	-1.578348	-0.000033
Te	-1.313206	-1.749305	-0.000312
Cl	-4.167130	-1.431725	-0.000102
Br	-1.149547	3.339263	0.000200
Br	3.785549	-1.054450	0.000086

M062XD3-CPCM-ACN_complex-Te-diBr-I.out

C	2.819240	2.166461	0.000043
C	3.673465	1.012086	0.000043
C	3.160034	-0.235265	-0.000006
C	1.475838	2.043037	-0.000015
H	3.278119	3.145490	-0.000032
H	4.743748	1.164818	-0.000032
C	0.852041	0.740105	0.000024
C	1.730545	-0.450595	0.000060
N	-0.435958	0.556865	-0.000425
N	1.161541	-1.618250	-0.000371
Te	-0.806669	-1.378532	0.000485
I	-4.087899	-0.393525	-0.000004
Br	0.370884	3.573325	-0.000326
Br	4.293045	-1.744614	-0.000254

M062XD3-CPCM-ACN_complex-Te-diBr-NO3.out

C	2.564369	2.018738	0.000299
C	3.318976	0.796657	0.000341
C	2.703124	-0.403475	0.000154
C	1.215611	2.006078	0.000069
H	3.103916	2.955807	0.000409
H	4.398304	0.859252	0.000485
C	0.483809	0.759801	-0.000104
C	1.260465	-0.501857	-0.000047
N	-0.813678	0.686109	-0.000488
N	0.592680	-1.614288	-0.000385
Te	-1.354038	-1.211577	-0.000216
O	-3.597180	0.100602	0.000554
O	-5.737477	-0.093235	0.000600
O	-4.504371	-1.855648	-0.000140
N	-4.629510	-0.625874	0.000392
Br	0.237865	3.621376	-0.000094
Br	3.713433	-1.998635	0.000132

M062XD3-CPCM-ACN_complex-Te-diBr-Quin.out

C	2.927488	2.250385	0.003548
C	3.849989	1.146645	0.004334
C	3.412047	-0.127231	0.001544
C	1.595175	2.048569	0.000212
H	3.328979	3.254300	0.005561
H	4.909251	1.364171	0.006967
C	1.044839	0.710611	-0.001257
C	1.994871	-0.433851	-0.001191
N	-0.223508	0.455557	-0.002511
N	1.491372	-1.622602	-0.003068
Te	-0.519002	-1.506336	-0.003113
C	-3.204988	0.068477	-1.247029
C	-5.359796	0.009310	0.001704
C	-4.629735	0.662761	-1.175880
H	-2.449119	0.840470	-1.388850
H	-3.113365	-0.648969	-2.064766
H	-4.586542	1.743892	-1.029529
H	-5.162042	0.477785	-2.109622
C	-3.161869	0.231875	1.153810
H	-2.738057	-0.229722	2.047304
H	-2.625483	1.163377	0.975369
C	-4.683110	0.461150	1.300122
H	-5.079692	-0.110555	2.141672
H	-4.887117	1.514887	1.493389
H	-6.412884	0.289286	0.001815
C	-5.209122	-1.510820	-0.119284
H	-5.828572	-2.019857	0.619777
H	-5.538629	-1.838458	-1.107168
C	-3.721988	-1.859233	0.101595
H	-3.556841	-2.287784	1.092135
H	-3.367733	-2.583553	-0.635423
N	-2.882624	-0.649997	0.002223
Br	0.402777	3.513729	-0.001736
Br	4.633694	-1.566083	0.001833

M062XD3-CPCM-ACN_complex-Te-nat-Br.out

C	3.867899	1.712498	0.000025
C	4.432509	0.385619	-0.000101
C	3.648635	-0.714373	-0.000176
C	2.531882	1.913462	0.000070
H	4.541384	2.560056	0.000061
H	5.510189	0.282760	-0.000125
H	4.064793	-1.713709	-0.000256
H	2.103854	2.907566	0.000143
C	1.636230	0.782560	0.000103
C	2.212533	-0.574767	-0.000072
N	0.337039	0.912255	0.000102
N	1.388436	-1.584937	-0.000037
Te	-0.474606	-0.892738	0.000057
Br	-3.245633	0.744699	-0.000066

M062XD3-CPCM-ACN_complex-Te-nat-Cl.out

C	-3.577923	1.385239	0.000006
C	-3.965708	-0.003217	-0.000036
C	-3.045155	-0.992326	-0.000063
C	-2.278793	1.756435	0.000022
H	-4.355481	2.138826	0.000027
H	-5.021236	-0.244369	-0.000048
H	-3.330359	-2.036847	-0.000088
H	-1.982463	2.797694	0.000048
C	-1.243550	0.751119	0.000068
C	-1.637889	-0.669615	-0.000031
N	0.027004	1.049561	0.000018
N	-0.688282	-1.561715	-0.000017
Te	1.077625	-0.629407	0.000022
Cl	3.398594	1.193713	-0.000052

M062XD3-CPCM-ACN_complex-Te-nat-I.out

C	-4.184835	1.908284	0.000059
C	-4.848873	0.628808	0.000080
C	-4.152896	-0.528919	0.000076
C	-2.837532	2.006237	0.000034
H	-4.791493	2.804930	0.000065
H	-5.931201	0.609500	0.000097
H	-4.646384	-1.492279	0.000087
H	-2.333059	2.963772	0.000028
C	-2.032189	0.809637	0.000022
C	-2.710231	-0.499768	0.000042
N	-0.726437	0.838643	-0.000001
N	-1.968310	-1.573077	0.000058
Te	-0.062267	-1.022547	-0.000068
I	3.101935	0.518526	0.000018

M062XD3-CPCM-ACN_complex-Te-nat-NO3.out

C	4.016741	1.525305	0.000056
C	4.465112	0.155100	0.000113
C	3.589465	-0.873493	0.000111
C	2.702946	1.840362	-0.000001
H	4.760740	2.312021	0.000069
H	5.530067	-0.039514	0.000169
H	3.919941	-1.904428	0.000167
H	2.361764	2.867655	-0.000031
C	1.712246	0.790798	-0.000021
C	2.170078	-0.611641	0.000043
N	0.429420	1.030863	-0.000012
N	1.261468	-1.546267	0.000069
Te	-0.536690	-0.696092	-0.000140
O	-2.479722	1.120641	-0.000040
O	-4.614252	1.380967	0.000271
O	-3.777228	-0.600617	0.000236
N	-3.638679	0.628906	0.000139

M062XD3-CPCM-ACN_complex-Te-nat-Quin.out

C	4.256728	2.114840	-0.000239
C	5.032500	0.896929	-0.005614
C	4.440845	-0.316285	-0.006496
C	2.907041	2.094624	0.004773
H	4.783412	3.060830	-0.000459
H	6.112386	0.974364	-0.009157
H	5.017688	-1.232423	-0.010581
H	2.322415	3.005685	0.008520
C	2.205725	0.831419	0.004371
C	2.998316	-0.419500	-0.002050
N	0.908606	0.748612	0.007699
N	2.349946	-1.543425	-0.003993
Te	0.372330	-1.167858	0.002161
C	-2.106138	0.779247	-1.221184
C	-4.274336	0.963264	-0.007813
C	-3.449124	1.542727	-1.160646
H	-1.257973	1.455838	-1.318475
H	-2.082261	0.085152	-2.063704
H	-3.277514	2.607812	-0.992116
H	-3.984838	1.441467	-2.105354
C	-2.089798	0.848854	1.184759
H	-1.763094	0.294274	2.066312
H	-1.419572	1.698821	1.060213
C	-3.565764	1.292252	1.309516
H	-4.057662	0.770209	2.132789
H	-3.622405	2.361390	1.518025
H	-5.281686	1.379081	-0.012868
C	-4.324763	-0.559608	-0.164794
H	-5.008738	-0.998027	0.562777
H	-4.693711	-0.816484	-1.159725
C	-2.895449	-1.108569	0.043432
H	-2.795602	-1.601730	1.012594
H	-2.630774	-1.835994	-0.727306
N	-1.906542	-0.017019	0.004589

M062XD3-CPCM-ACN_donor-Te-CN.out

C	-2.610003	1.354589	-0.000002
C	-2.836859	-0.072331	-0.000002
C	-1.817079	-0.968836	-0.000003
C	-1.357609	1.854535	-0.000003
H	-3.469479	2.010947	-0.000002
H	-1.994691	-2.035545	-0.000004
H	-1.174967	2.920513	-0.000004
C	-0.225789	0.963814	-0.000003
C	-0.465430	-0.486994	-0.000003
N	1.012013	1.388116	-0.000008
N	0.565726	-1.294761	-0.000007
Te	2.184310	-0.187696	0.000005
C	-4.192038	-0.545570	-0.000002
N	-5.280045	-0.912063	-0.000002

M062XD3-CPCM-ACN_donor-Te-F4.out

C	-0.000001	-2.538575	0.719035
C	-0.000001	-2.538575	-0.719035
C	-0.000001	-1.390749	-1.421335
C	-0.000001	-1.390749	1.421335
C	-0.000001	-0.126911	0.736607
C	-0.000001	-0.126911	-0.736607
N	-0.000006	1.017798	1.357756
N	-0.000006	1.017798	-1.357756
Te	0.000004	2.437206	-0.000000
F	-0.000003	-1.406936	2.748861
F	-0.000001	-3.721345	1.319096
F	-0.000001	-3.721345	-1.319096
F	-0.000003	-1.406936	-2.748861

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M062XD3-CPCM-ACN_donor-Te-diBr.out
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C	-0.717760	-2.472801	0.000010
C	0.717748	-2.472805	0.000010
C	1.418854	-1.320310	-0.000016
C	-1.418861	-1.320302	-0.000016
H	-1.230845	-3.424562	0.000000
H	1.230828	-3.424569	0.000000
C	-0.740017	-0.045957	-0.000018
C	0.740018	-0.045960	-0.000018
N	-1.354836	1.103291	-0.000153
N	1.354838	1.103286	-0.000152
Te	0.000006	2.521478	0.000154
Br	-3.303227	-1.337780	-0.000080
Br	3.303220	-1.337791	-0.000080

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M062XD3-CPCM-ACN_donor-Te-nat.out
==========

C	-3.323898	0.720821	0.000001
C	-3.323851	-0.720868	0.000001
C	-2.174017	-1.429269	0.000000
C	-2.174100	1.429254	0.000000
H	-4.275796	1.236162	0.000001
H	-4.275718	-1.236282	0.000001
H	-2.166637	-2.511215	-0.000001
H	-2.166701	2.511211	-0.000000
C	-0.909700	0.737707	0.000000
C	-0.909640	-0.737624	-0.000001
N	0.240215	1.360787	-0.000005
N	0.240234	-1.360826	-0.000004
Te	1.661787	0.000005	0.000001

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M062XD3-CPCM-THF_acceptor-NO3.out
==========

O	0.923266	-0.832523	0.000036
O	0.259592	1.215552	0.000059
O	-1.182830	-0.383058	-0.000008
N	-0.000032	0.000033	-0.000098

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M062XD3-CPCM-THF_acceptor-Quin.out
==========

C	-0.781831	1.361720	-0.247799
C	1.286970	-0.007522	-0.001996
C	0.761626	1.375845	-0.399615
H	-1.266181	1.747717	-1.146615
H	-1.096904	1.989294	0.588457
H	1.047649	1.595008	-1.430937
H	1.205577	2.147296	0.232535
C	-0.796952	-0.890118	-1.048702
H	-1.286681	-1.857987	-0.926490
H	-1.117196	-0.480312	-2.008727
C	0.746152	-1.039346	-0.997426
H	1.028499	-2.044440	-0.675558
H	1.183537	-0.878115	-1.984601
H	2.377603	-0.014181	-0.003697
C	0.754342	-0.349369	1.393307
H	1.188102	-1.287420	1.745069
H	1.047129	0.430441	2.100233
C	-0.790427	-0.458094	1.300558
H	-1.115326	-1.493014	1.425607
H	-1.270768	0.132062	2.083019
N	-1.286332	0.007851	0.001677

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M062XD3-CPCM-THF_complex-Te-CN-Br-opp.out
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C	-3.375376	1.650130	-0.000078
C	-3.900928	0.304432	-0.000108
C	-3.091102	-0.786913	-0.000099
C	-2.044040	1.869722	-0.000039
H	-4.074373	2.475511	-0.000087
H	-3.492359	-1.791581	-0.000122
H	-1.638584	2.872740	-0.000018
C	-1.125170	0.759151	-0.000030
C	-1.666534	-0.607815	-0.000060
N	0.170750	0.917972	0.000015
N	-0.819038	-1.600680	-0.000049
Te	1.028657	-0.862825	0.000022
Br	3.676638	0.748671	0.000111
C	-5.324709	0.127623	-0.000144
N	-6.465998	-0.001751	-0.000173

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M062XD3-CPCM-THF_complex-Te-CN-Br-same.out
==========

C	-3.677502	0.644488	-0.000038
C	-3.941868	-0.775653	0.000054
C	-2.925869	-1.663384	0.000133
C	-2.414355	1.146395	-0.000046
H	-4.971388	-1.107613	0.000051
H	-3.109923	-2.729670	0.000196
H	-2.226158	2.211584	-0.000118
C	-1.299904	0.241813	0.000033
C	-1.558366	-1.205960	0.000125
N	-0.062233	0.664341	-0.000002
N	-0.526690	-2.003011	0.000192
Te	1.135045	-0.902642	0.000129
Br	3.401075	1.218379	-0.000216
C	-4.797105	1.542021	-0.000129
N	-5.705742	2.244597	-0.000201

==========
M062XD3-CPCM-THF_complex-Te-CN-Cl-opp.out
==========

C	2.989837	1.535830	0.000174
C	3.411077	0.154327	0.000076
C	2.519876	-0.872354	-0.000123
C	1.678802	1.855176	0.000078
H	3.749380	2.306154	0.000291
H	2.845421	-1.904209	-0.000223
H	1.349802	2.886022	0.000106
C	0.677714	0.817683	-0.000073
C	1.111891	-0.586982	-0.000177
N	-0.601172	1.075846	-0.000251
N	0.189188	-1.509093	-0.000474
Te	-1.605863	-0.627568	-0.000164
Cl	-3.907233	1.065133	0.000654
C	4.817628	-0.128129	0.000163
N	5.946595	-0.340323	0.000229

M062XD3-CPCM-THF_complex-Te-CN-Cl-same.out

C	3.286128	0.384593	0.000056
C	3.357996	-1.058040	-0.000045
C	2.231539	-1.800702	-0.000068
C	2.100734	1.050636	0.000143
H	4.333855	-1.524765	-0.000081
H	2.270855	-2.882163	-0.000118
H	2.057602	2.131550	0.000244
C	0.874868	0.304285	0.000102
C	0.936457	-1.165044	-0.000016
N	-0.294209	0.889368	0.000265
N	-0.193566	-1.812073	0.000036
Te	-1.702111	-0.495965	-0.000016
Cl	-3.475249	1.735854	-0.000223
C	4.513855	1.126985	0.000095
N	5.504522	1.708388	0.000125

M062XD3-CPCM-THF_complex-Te-CN-I-opp.out

C	-3.751758	1.736817	0.000241
C	-4.349026	0.421217	-0.000108
C	-3.600248	-0.712656	-0.000291
C	-2.410740	1.884376	0.000409
H	-4.404773	2.598936	0.000354
H	-4.054791	-1.694362	-0.000576
H	-1.951067	2.863717	0.000664
C	-1.554030	0.725525	0.000282
C	-2.168106	-0.609721	-0.000118
N	-0.250881	0.813251	0.000384
N	-1.377629	-1.649651	-0.000321
Te	0.500366	-1.012287	0.000230
I	3.508834	0.572169	-0.000197
C	-5.780589	0.322681	-0.000291
N	-6.927144	0.255864	-0.000452

M062XD3-CPCM-THF_complex-Te-CN-I-same.out

C	-4.048349	0.842853	0.000013
C	-4.441022	-0.547450	0.000027
C	-3.511147	-1.525202	0.000077
C	-2.744931	1.226242	0.000016
H	-5.496643	-0.783308	-0.000019
H	-3.792915	-2.569966	0.000044
H	-2.458009	2.269252	0.000002
C	-1.718819	0.222494	-0.000021
C	-2.107461	-1.194712	0.000071
N	-0.447503	0.529715	-0.000053
N	-1.154244	-2.085533	0.000036
Te	0.595391	-1.140993	-0.000031
I	3.307617	0.900071	0.000017
C	-5.078947	1.841544	-0.000008
N	-5.914314	2.629709	-0.000035

M062XD3-CPCM-THF_complex-Te-CN-NO3-opp.out

C	3.467827	1.587197	-0.000038
C	3.915146	0.213419	-0.000030
C	3.044213	-0.829572	-0.000005
C	2.151498	1.883118	-0.000019
H	4.213404	2.371012	-0.000051
H	3.387685	-1.855446	0.000009
H	1.804328	2.907883	-0.000014
C	1.169019	0.827413	0.000004
C	1.631632	-0.569117	0.000008
N	-0.115201	1.058913	0.000053
N	0.728642	-1.511165	0.000066
Te	-1.072716	-0.669629	0.000011
O	-2.964793	1.074461	-0.000102
O	-5.101218	1.313289	-0.000010
O	-4.246383	-0.660546	0.000117
N	-4.124075	0.569642	-0.000045
C	5.326716	-0.043663	-0.000040
N	6.459012	-0.236414	-0.000048

M062XD3-CPCM-THF_complex-Te-CN-NO3-same.out

C	3.730117	0.599345	-0.000087
C	3.931391	-0.831260	-0.000025
C	2.877269	-1.672939	0.000018
C	2.490511	1.156954	-0.000097
H	4.945227	-1.207971	-0.000033
H	3.014101	-2.746335	0.000043
H	2.350008	2.229537	-0.000164
C	1.336157	0.302979	-0.000039
C	1.531230	-1.155208	0.000021
N	0.118512	0.777872	-0.000113
N	0.464829	-1.904292	-0.000009
Te	-1.145648	-0.735940	0.000100
O	-2.660419	1.360371	0.000542
O	-4.707291	2.017873	0.000202
O	-4.259859	-0.086215	-0.000712
N	-3.896129	1.095669	-0.000079
C	4.887628	1.447491	-0.000166
N	5.824086	2.112644	-0.000232

M062XD3-CPCM-THF_complex-Te-CN-Quin-opp.out

C	3.882414	1.851245	0.004552
C	4.581502	0.583820	-0.001706
C	3.924891	-0.603352	-0.003360
C	2.535794	1.896621	0.009113
H	4.468745	2.760198	0.005215
H	4.455490	-1.546125	-0.008159
H	2.004140	2.838905	0.013538
C	1.766606	0.674550	0.007365
C	2.484668	-0.616242	0.000748
N	0.466799	0.661937	0.009419
N	1.778342	-1.706115	-0.002007
Te	-0.168620	-1.220827	0.002258
C	-2.539256	0.850547	-1.220057
C	-4.699228	1.122981	-0.008182
C	-3.848605	1.670497	-1.158262
H	-1.662234	1.490059	-1.312055
H	-2.543143	0.160033	-2.065883
H	-3.632083	2.726752	-0.986295
H	-4.387013	1.595330	-2.103817
C	-2.522576	0.909499	1.186654
H	-2.221353	0.337540	2.066080
H	-1.814348	1.728578	1.066265
C	-3.978067	1.416260	1.311048
H	-4.492665	0.913504	2.132445
H	-3.988118	2.486006	1.523392
H	-5.687684	1.581936	-0.012466
C	-4.815276	-0.396304	-0.171444
H	-5.518917	-0.807883	0.552967
H	-5.193481	-0.632610	-1.167992
C	-3.412232	-1.007084	0.036784
H	-3.335027	-1.507475	1.004368
H	-3.179052	-1.743227	-0.735832
N	-2.376673	0.041215	0.002818
C	6.016645	0.600393	-0.006872
N	7.164580	0.628802	-0.011296

M062XD3-CPCM-THF_complex-Te-CN-Quin-same.out

C	4.162303	1.080677	-0.000401
C	4.711476	-0.258798	0.008852
C	3.899945	-1.334158	0.009590
C	2.825966	1.316346	-0.008819
H	5.787066	-0.372249	0.015198
H	4.297880	-2.340332	0.016587
H	2.426565	2.321634	-0.015502
C	1.915560	0.203009	-0.006918
C	2.464368	-1.167976	0.001987
N	0.624254	0.363988	-0.011506
N	1.618558	-2.151707	0.003479
Te	-0.251385	-1.416968	-0.002737
C	-2.341875	0.919346	-1.251979
C	-4.394198	1.567201	0.003810
C	-3.498394	1.941958	-1.181889
H	-1.378711	1.405092	-1.404643
H	-2.490766	0.205021	-2.064236
H	-3.107991	2.952442	-1.045389
H	-4.068352	1.933013	-2.111736
C	-2.236455	1.073570	1.146608
H	-1.979174	0.503821	2.041312
H	-1.429767	1.781952	0.962774
C	-3.601106	1.782060	1.297530
H	-4.157405	1.372459	2.143350
H	-3.453542	2.846110	1.486124
H	-5.300621	2.171897	0.005025
C	-4.741364	0.078984	-0.106846
H	-5.488186	-0.199762	0.637481
H	-5.164373	-0.129625	-1.091626
C	-3.443082	-0.729644	0.110125
H	-3.418292	-1.184113	1.102706
H	-3.344588	-1.532230	-0.624339
N	-2.260475	0.143817	0.000589
C	5.073611	2.189587	0.000288
N	5.812195	3.068794	0.001385

M062XD3-CPCM-THF_complex-Te-F4-Br.out

C	-3.196881	1.242165	-0.000067
C	-3.636970	-0.125937	0.000089
C	-2.757166	-1.143296	0.000125
C	-1.889268	1.559426	-0.000175
C	-0.890878	0.522331	-0.000193
C	-1.340110	-0.881968	-0.000028
N	0.383722	0.771066	-0.000209
N	-0.432543	-1.806616	0.000040
Te	1.374486	-0.942360	-0.000296
Br	3.862326	0.821983	0.000455
F	-4.142312	2.177931	-0.000048
F	-1.505499	2.832410	-0.000255
F	-4.951080	-0.335477	0.000231
F	-3.183921	-2.403103	0.000311

M062XD3-CPCM-THF_complex-Te-F4-Cl.out

C	2.849972	1.064124	0.000062
C	3.150463	-0.341338	-0.000018
C	2.172673	-1.265250	-0.000137
C	1.580524	1.510190	0.000017
C	0.483349	0.578949	-0.000088
C	0.787890	-0.864512	-0.000149
N	-0.758205	0.956920	-0.000249
N	-0.210173	-1.688828	-0.000381
Te	-1.929203	-0.642132	0.000090
Cl	-4.008520	1.245036	0.000137
F	3.884941	1.900747	0.000150
F	1.327082	2.816265	0.000070
F	4.437504	-0.682104	-0.000029
F	2.471899	-2.562058	-0.000272

M062XD3-CPCM-THF_complex-Te-F4-I.out

C	-3.546782	1.361960	0.000016
C	-4.074202	0.024886	0.000282
C	-3.262310	-1.047419	0.000219
C	-2.221478	1.594352	-0.000270
C	-1.293173	0.494762	-0.000301
C	-1.832175	-0.876884	-0.000102
N	-0.004568	0.660133	-0.000622
N	-0.987771	-1.860940	-0.000174
Te	0.863355	-1.116728	-0.000270
I	3.728149	0.600002	0.000278
F	-4.429283	2.356337	0.000113
F	-1.755820	2.839064	-0.000480
F	-5.398171	-0.099824	0.000557
F	-3.767753	-2.277195	0.000458

M062XD3-CPCM-THF_complex-Te-F4-NO3.out

C	3.268321	1.162275	0.000045
C	3.627710	-0.229648	0.000149
C	2.690444	-1.194561	0.000137
C	1.981582	1.554925	-0.000067
C	0.924465	0.577665	-0.000128
C	1.290748	-0.851433	0.000005
N	-0.332587	0.900110	-0.000158
N	0.329498	-1.719864	-0.000021
Te	-1.420356	-0.752909	-0.000249
O	-3.142299	1.106360	-0.000219
O	-5.252002	1.516767	0.000353
O	-4.559991	-0.519765	0.000743
N	-4.340748	0.696033	0.000264
F	4.267242	2.040458	0.000103
F	1.672831	2.848200	-0.000113
F	4.927243	-0.514566	0.000272
F	3.043809	-2.476862	0.000239

M062XD3-CPCM-THF_complex-Te-F4-Quin.out

C	-3.653994	1.528756	-0.000072
C	-4.309628	0.245814	0.002147
C	-3.607461	-0.899595	0.002049
C	-2.313887	1.633418	-0.002691
C	-1.493462	0.449400	-0.003414
C	-2.163627	-0.872004	-0.000278
N	-0.201407	0.490316	-0.004969
N	-1.418060	-1.923681	0.000660
Te	0.520787	-1.364607	-0.002051
C	2.774245	0.786983	1.231282
C	4.908680	1.175809	0.006325
C	4.040420	1.671229	1.166675
H	1.867781	1.381097	1.340963
H	2.821116	0.085000	2.066248
H	3.770015	2.716639	1.005437
H	4.588520	1.615037	2.107866
C	2.734698	0.880503	-1.175107
H	2.446195	0.310677	-2.059924
H	1.995821	1.668161	-1.032752
C	4.166346	1.447472	-1.305945
H	4.694987	0.972004	-2.134641
H	4.129433	2.517907	-1.511109
H	5.874363	1.680665	0.009819
C	5.096049	-0.337818	0.154311
H	5.817261	-0.710639	-0.573668
H	5.483984	-0.566597	1.148826
C	3.723444	-1.010742	-0.061351
H	3.665008	-1.493939	-1.038841
H	3.529321	-1.772734	0.696769
N	2.638702	-0.012413	-0.002831
F	-4.437394	2.601189	0.000981
F	-1.728671	2.827492	-0.004274
F	-5.638606	0.254012	0.004406
F	-4.229808	-2.073652	0.004225

M062XD3-CPCM-THF_complex-Te-diBr-Br.out

C	2.353735	2.218888	-0.000117
C	3.241898	1.091340	-0.000077
C	2.763734	-0.170002	0.000024
C	1.014235	2.054724	-0.000050
H	2.781508	3.211879	-0.000220
H	4.307482	1.274576	-0.000145
C	0.427273	0.734455	0.000107
C	1.341159	-0.430360	0.000094
N	-0.854268	0.515046	0.000072
N	0.803747	-1.611091	0.000226
Te	-1.181757	-1.430774	0.000196
Br	-4.157477	-0.636061	-0.000214
Br	3.942246	-1.645606	0.000079
Br	-0.131518	3.555719	-0.000202

M062XD3-CPCM-THF_complex-Te-diBr-Cl.out

C	1.545647	2.460643	0.000401
C	2.613399	1.501124	0.000287
C	2.358363	0.176349	0.000070
C	0.255072	2.067379	0.000304
H	1.797169	3.512409	0.000547
H	3.631862	1.863892	0.000365
C	-0.096806	0.666425	0.000086
C	1.002016	-0.327123	-0.000043
N	-1.321465	0.233469	-0.000082
N	0.670073	-1.579327	-0.000304
Te	-1.328766	-1.741726	-0.000338
Cl	-4.140118	-1.433324	0.000128
Br	-1.135797	3.346186	0.000404
Br	3.779866	-1.068696	-0.000103

M062XD3-CPCM-THF_complex-Te-diBr-I.out

C	2.833062	2.149929	0.000037
C	3.675657	0.987453	0.000076
C	3.149116	-0.254725	0.000010
C	1.488239	2.039180	-0.000069
H	3.300585	3.124859	0.000015
H	4.747569	1.128452	0.000085
C	0.851398	0.742556	-0.000079
C	1.717764	-0.456963	-0.000020
N	-0.438240	0.573647	-0.000430
N	1.136276	-1.617862	-0.000329
Te	-0.834077	-1.357311	0.000153
I	-4.060668	-0.392538	0.000232
Br	0.398716	3.580355	-0.000308
Br	4.268759	-1.774746	-0.000113

M062XD3-CPCM-THF_complex-Te-diBr-NO3.out

C	2.575984	2.005367	0.000264
C	3.321715	0.778395	0.000307
C	2.696951	-0.417391	0.000140
C	1.226859	2.001721	0.000050
H	3.121014	2.939258	0.000366
H	4.401528	0.832110	0.000441
C	0.486180	0.760752	-0.000111
C	1.253728	-0.506595	-0.000043
N	-0.811623	0.697205	-0.000470
N	0.577517	-1.613521	-0.000348
Te	-1.368927	-1.195388	-0.000197
O	-3.584104	0.108072	0.000476
O	-5.723409	-0.096243	0.000568
O	-4.482345	-1.853136	-0.000097
N	-4.614951	-0.624104	0.000366
Br	0.260620	3.623753	-0.000092
Br	3.698107	-2.018933	0.000131

M062XD3-CPCM-THF_complex-Te-diBr-Quin.out

C	2.928732	2.249567	-0.001968
C	3.850605	1.145273	-0.001848
C	3.411946	-0.128345	-0.000215
C	1.596306	2.048559	-0.000249
H	3.330769	3.253269	-0.003320
H	4.910012	1.362115	-0.002883
C	1.045165	0.710926	0.000345
C	1.994566	-0.434137	0.000387
N	-0.223328	0.456850	0.000756
N	1.490523	-1.622597	0.000611
Te	-0.519729	-1.504957	-0.000560
C	-3.164505	0.232049	-1.153533
C	-5.360177	0.007866	0.002494
C	-4.686284	0.458748	-1.297757
H	-2.628997	1.164306	-0.976249
H	-2.741156	-0.229364	-2.047340
H	-4.892280	1.511841	-1.492405
H	-5.083366	-0.114836	-2.137797
C	-3.203424	0.070220	1.247501
H	-3.110601	-0.646690	2.065699
H	-2.447675	0.842578	1.387712
C	-4.628548	0.663752	1.177749
H	-5.159184	0.480292	2.112735
H	-4.586051	1.744639	1.029428
H	-6.413569	0.286657	0.003869
C	-5.207542	-1.511988	0.125568
H	-5.534073	-1.838208	1.114924
H	-5.828447	-2.023078	-0.610835
C	-3.720644	-1.858946	-0.098773
H	-3.363162	-2.582579	0.637467
H	-3.557479	-2.287765	-1.089561
N	-2.882495	-0.648820	-0.001835
Br	0.404598	3.514114	0.000423
Br	4.632575	-1.567964	0.000799

M062XD3-CPCM-THF_complex-Te-nat-Br.out

C	3.878595	1.687436	0.000033
C	4.430938	0.355933	-0.000033
C	3.636281	-0.736735	-0.000103
C	2.544027	1.899612	0.000037
H	4.559284	2.529366	0.000052
H	5.507703	0.242605	-0.000028
H	4.043098	-1.739984	-0.000150
H	2.123732	2.897037	0.000054
C	1.637962	0.777077	0.000064
C	2.201356	-0.585117	-0.000055
N	0.340487	0.920342	-0.000007
N	1.367107	-1.586531	-0.000080
Te	-0.493343	-0.874486	0.000045
Br	-3.214517	0.737666	-0.000038

M062XD3-CPCM-THF_complex-Te-nat-Cl.out

C	-3.584327	1.368997	-0.000048
C	-3.964729	-0.021126	-0.000094
C	-3.038161	-1.005114	-0.000011
C	-2.286585	1.745946	0.000066
H	-4.365398	2.119092	-0.000070
H	-5.019023	-0.268361	-0.000186
H	-3.317366	-2.051373	-0.000042
H	-1.994172	2.788370	0.000166
C	-1.245912	0.746329	-0.000010
C	-1.632165	-0.676215	0.000002
N	0.022115	1.053313	0.000170
N	-0.677041	-1.561664	0.000060
Te	1.088151	-0.616058	0.000003
Cl	3.365167	1.179580	-0.000063

M062XD3-CPCM-THF_complex-Te-nat-I.out

C	-4.198134	1.881985	0.000001
C	-4.848940	0.596060	0.000074
C	-4.140363	-0.554328	-0.000016
C	-2.851570	1.992804	-0.000156
H	-4.813392	2.772876	0.000049
H	-5.931140	0.565150	0.000174
H	-4.623277	-1.523130	0.000007
H	-2.355708	2.954857	-0.000245
C	-2.033928	0.804666	-0.000221
C	-2.698068	-0.511099	-0.000148
N	-0.728780	0.848551	-0.000461
N	-1.944263	-1.575763	-0.000326
Te	-0.041550	-1.003831	-0.000209
I	3.079650	0.514328	0.000362

M062XD3-CPCM-THF_complex-Te-nat-NO3.out

C	4.023603	1.508925	0.000165
C	4.463775	0.136389	0.000305
C	3.581393	-0.886800	0.000222
C	2.711279	1.830905	-0.000058
H	4.771918	2.291683	0.000203
H	5.527632	-0.064898	0.000449
H	3.905154	-1.919959	0.000288
H	2.374831	2.859805	-0.000208
C	1.714196	0.787424	-0.000124
C	2.163343	-0.617357	0.000029
N	0.433324	1.036308	-0.000463
N	1.248878	-1.545846	-0.000157
Te	-0.546171	-0.682825	-0.000177
O	-2.462239	1.113848	0.000385
O	-4.597037	1.371566	0.000516
O	-3.758397	-0.609455	-0.000077
N	-3.622601	0.620350	0.000429

M062XD3-CPCM-THF_complex-Te-nat-Quin.out

C	4.248703	2.122258	-0.000368
C	5.028285	0.906826	-0.005094
C	4.440473	-0.308109	-0.005745
C	2.899178	2.098105	0.004241
H	4.772355	3.069966	-0.000707
H	6.107942	0.987484	-0.008319
H	5.019222	-1.222938	-0.009316
H	2.311435	3.007102	0.007530
C	2.201743	0.832867	0.004063
C	2.998399	-0.415533	-0.001740
N	0.904937	0.746256	0.007018
N	2.354707	-1.542012	-0.003442
Te	0.378491	-1.172883	0.001878
C	-2.107515	0.778595	-1.220190
C	-4.275821	0.966683	-0.007132
C	-3.450137	1.543278	-1.161121
H	-1.258265	1.454170	-1.314896
H	-2.082451	0.085908	-2.063892
H	-3.277895	2.608613	-0.994647
H	-3.986408	1.441137	-2.105501
C	-2.091253	0.845124	1.185226
H	-1.767826	0.287594	2.066160
H	-1.415958	1.691408	1.063129
C	-3.565443	1.295281	1.309399
H	-4.059716	0.777334	2.133926
H	-3.617982	2.365088	1.515780
H	-5.282275	1.384866	-0.011774
C	-4.330216	-0.556332	-0.162825
H	-5.013723	-0.992384	0.566719
H	-4.702901	-0.812950	-1.156488
C	-2.901316	-1.108474	0.041603
H	-2.800966	-1.604947	1.009087
H	-2.639240	-1.834409	-0.731475
N	-1.910691	-0.019463	0.004301

M062XD3-CPCM-THF_donor-Te-CN.out

C	-2.609173	1.354097	-0.000002
C	-2.836591	-0.073092	-0.000002
C	-1.816969	-0.969261	-0.000003
C	-1.357189	1.854510	-0.000003
H	-3.469022	2.010014	-0.000002
H	-1.994287	-2.035985	-0.000005
H	-1.173995	2.920364	-0.000004
C	-0.225009	0.963873	-0.000003
C	-0.464870	-0.487546	-0.000003
N	1.012075	1.388793	-0.000008
N	0.565473	-1.295499	-0.000008
Te	2.184060	-0.187647	0.000005
C	-4.192264	-0.545329	-0.000002
N	-5.280608	-0.910473	-0.000002

M062XD3-CPCM-THF_donor-Te-F4.out

C	-0.000001	-2.538003	0.719312
C	-0.000001	-2.538003	-0.719312
C	-0.000001	-1.390541	-1.422195
C	-0.000001	-1.390541	1.422195
C	-0.000001	-0.126488	0.737070
C	-0.000001	-0.126488	-0.737070
N	-0.000005	1.017556	1.358506
N	-0.000005	1.017556	-1.358506
Te	0.000004	2.436636	0.000000
F	-0.000003	-1.406512	2.749078
F	-0.000001	-3.720735	1.318532
F	-0.000001	-3.720735	-1.318532
F	-0.000003	-1.406512	-2.749078

==========
M062XD3-CPCM-THF_donor-Te-diBr.out
==========

C	-0.717866	-2.472087	0.000010
C	0.717854	-2.472091	0.000010
C	1.419782	-1.320198	-0.000015
C	-1.419789	-1.320190	-0.000015
H	-1.231288	-3.423692	0.000001
H	1.231271	-3.423699	0.000001
C	-0.740355	-0.045791	-0.000018
C	0.740356	-0.045795	-0.000018
N	-1.355621	1.102711	-0.000147
N	1.355624	1.102706	-0.000147
Te	0.000006	2.520428	0.000148
Br	-3.303335	-1.337078	-0.000077
Br	3.303329	-1.337089	-0.000077

==========
M062XD3-CPCM-THF_donor-Te-nat.out
==========

C	-3.322980	0.720888	0.000001
C	-3.322934	-0.720937	0.000001
C	-2.173409	-1.429434	0.000000
C	-2.173492	1.429419	0.000000
H	-4.274888	1.236247	0.000001
H	-4.274810	-1.236368	0.000001
H	-2.165360	-2.511313	-0.000001
H	-2.165427	2.511308	-0.000000
C	-0.908918	0.737917	0.000000
C	-0.908859	-0.737839	-0.000001
N	0.240237	1.361539	-0.000004
N	0.240260	-1.361572	-0.000003
Te	1.661165	0.000005	0.000001

5.4.4 TD-DFT geometries

5.4.4.1 B97D3

==========
B97D3_complex.out
==========

C	-1.707004	2.394054	-0.000385
C	-2.710599	1.383078	-0.000419
C	-2.363905	0.058428	-0.000177
C	-0.377525	2.062797	-0.000111
H	-2.007683	3.437091	-0.000490
H	-3.755837	1.676075	-0.000563
C	0.062843	0.696247	0.000082
C	-0.992058	-0.375447	0.000013
N	1.332660	0.348871	0.000703
N	-0.589567	-1.621496	0.000445
Te	1.475706	-1.668389	0.000185
Cl	4.180605	-1.391213	-0.000684
Br	0.932351	3.468160	0.000104
Br	-3.752798	-1.271384	-0.000074

==========
B97D3_donor.out
==========

C	-3.345430	0.716150	0.000004
C	-3.345380	-0.716169	0.000005
C	-2.179751	-1.431632	-0.000000
C	-2.179836	1.431622	0.000000
H	-4.298512	1.239289	0.000005
H	-4.298429	-1.239384	0.000006
H	-2.171487	-2.517456	-0.000003
H	-2.171488	2.517461	-0.000003
C	-0.922047	0.742012	0.000001
C	-0.922003	-0.741942	-0.000002
N	0.235694	1.394252	-0.000015
N	0.235685	-1.394340	-0.000014
Te	1.673210	0.000009	0.000003

5.4.4.2 B2PLYP

==========
B2PLYP_complex.out
==========

C	-3.629785	1.300654	0.000073
C	-3.977497	-0.082148	0.000360
C	-3.012921	-1.049709	0.000129
C	-2.322991	1.699203	-0.000409
H	-4.419707	2.042222	0.000260
H	-5.024374	-0.361424	0.000819
H	-3.265893	-2.102500	0.000382
H	-2.048299	2.746189	-0.000586
C	-1.273833	0.729158	-0.000563
C	-1.627912	-0.693903	-0.000448
N	0.002644	1.082843	-0.000575
N	-0.639675	-1.570638	-0.000747
Te	1.122781	-0.571385	-0.000658
Cl	3.252891	1.109868	0.001737

==========
B2PLYP_donor.out
==========

C	-3.627445	1.298440	0.000048
C	-3.964907	-0.089827	0.000016
C	-3.003985	-1.054995	-0.000699
C	-2.330757	1.713716	-0.000649
H	-4.424819	2.029688	0.000908
H	-5.009102	-0.372600	0.000836
H	-3.250033	-2.107475	-0.000416
H	-2.064180	2.761242	-0.000323
C	-1.280365	0.745440	-0.000813
C	-1.625672	-0.678485	-0.000810
N	0.000292	1.101378	0.000042
N	-0.649431	-1.581652	0.000074
Te	1.050446	-0.572957	0.001836

5.4.5 2-$H_2PO_4^-$ and 2-HSO_4^- complex geometries

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B97D3-null-null_complex-Te-nat-H2PO4.out
==========

C	-3.695672	2.186535	0.043708
C	-4.515182	1.035155	-0.171855
C	-3.966674	-0.219658	-0.245543
C	-2.335552	2.077385	0.185081
H	-4.166075	3.166981	0.094732
H	-5.590757	1.166279	-0.278497
H	-4.581903	-1.101429	-0.410199
H	-1.708375	2.950643	0.347180
C	-1.705692	0.791548	0.118383
C	-2.549798	-0.409074	-0.105226
N	-0.400486	0.633080	0.247367
N	-1.953340	-1.585300	-0.162054
Te	0.066959	-1.332927	0.076936
F	2.972740	0.697540	0.028399
O	2.257023	-0.615098	0.398026
O	2.893126	0.724568	-1.625351
H	3.626049	1.278774	-1.924886
O	2.022550	1.919950	0.483367
H	1.075434	1.615084	0.426157
O	4.372406	0.928953	0.465757

==========
B97D3-null-null_complex-Te-nat-HSO4.out
==========

C	-3.686927	2.154108	-0.049243
C	-4.491404	0.995383	0.185139
C	-3.929803	-0.252819	0.263599
C	-2.328035	2.059322	-0.205768
H	-4.168699	3.128752	-0.100926
H	-5.566746	1.116190	0.303617
H	-4.533180	-1.139390	0.443909
H	-1.711724	2.937668	-0.379851
C	-1.684782	0.780313	-0.136372
C	-2.512804	-0.425634	0.109755
N	-0.379234	0.634356	-0.283088
N	-1.905112	-1.597651	0.174912
Te	0.096973	-1.321468	-0.088002
O	2.341666	-0.515122	-0.540729
O	4.283679	0.964182	-0.284995
O	2.059478	1.938762	-0.478950
H	1.108463	1.642541	-0.418129
O	2.670555	0.682314	1.577912
S	2.923700	0.709282	0.143510

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