**Electronic Supporting Information**

# Isolation of the novel example of a monomeric organotellurinic acid

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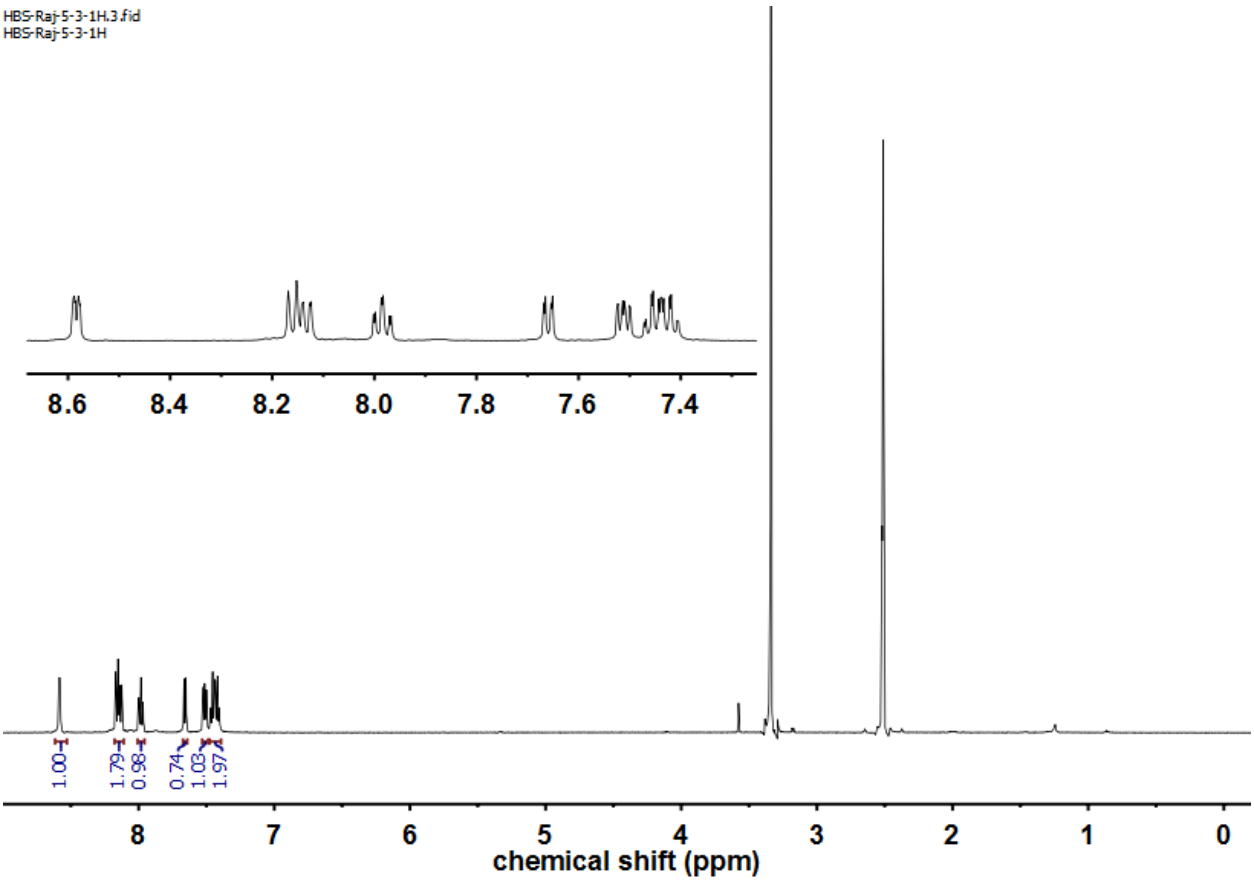



**Fig S1**. $^{1}$H NMR Spectrum of **5**. Inset showing expanded aromatic region.

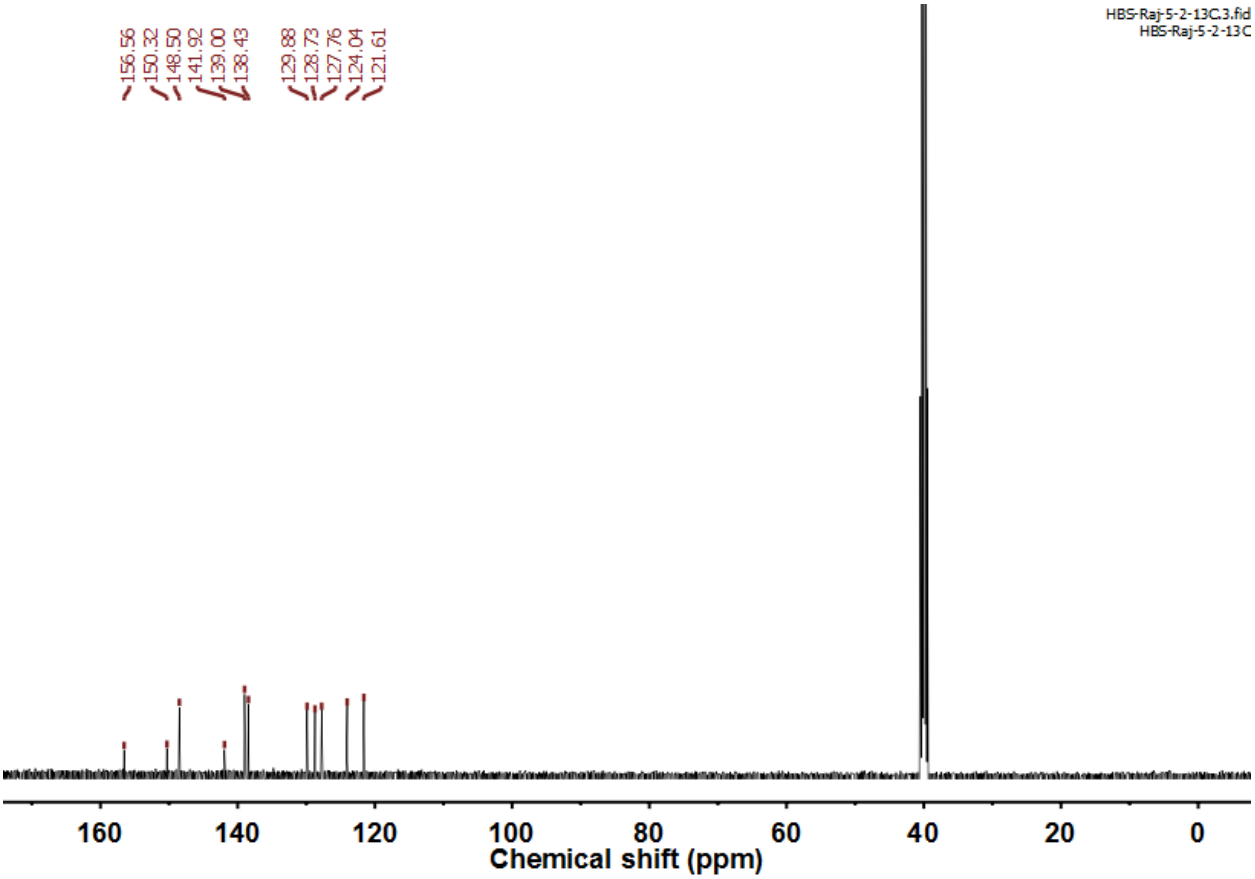



**Fig S2**. $^{13}$C NMR Spectrum of **5**.

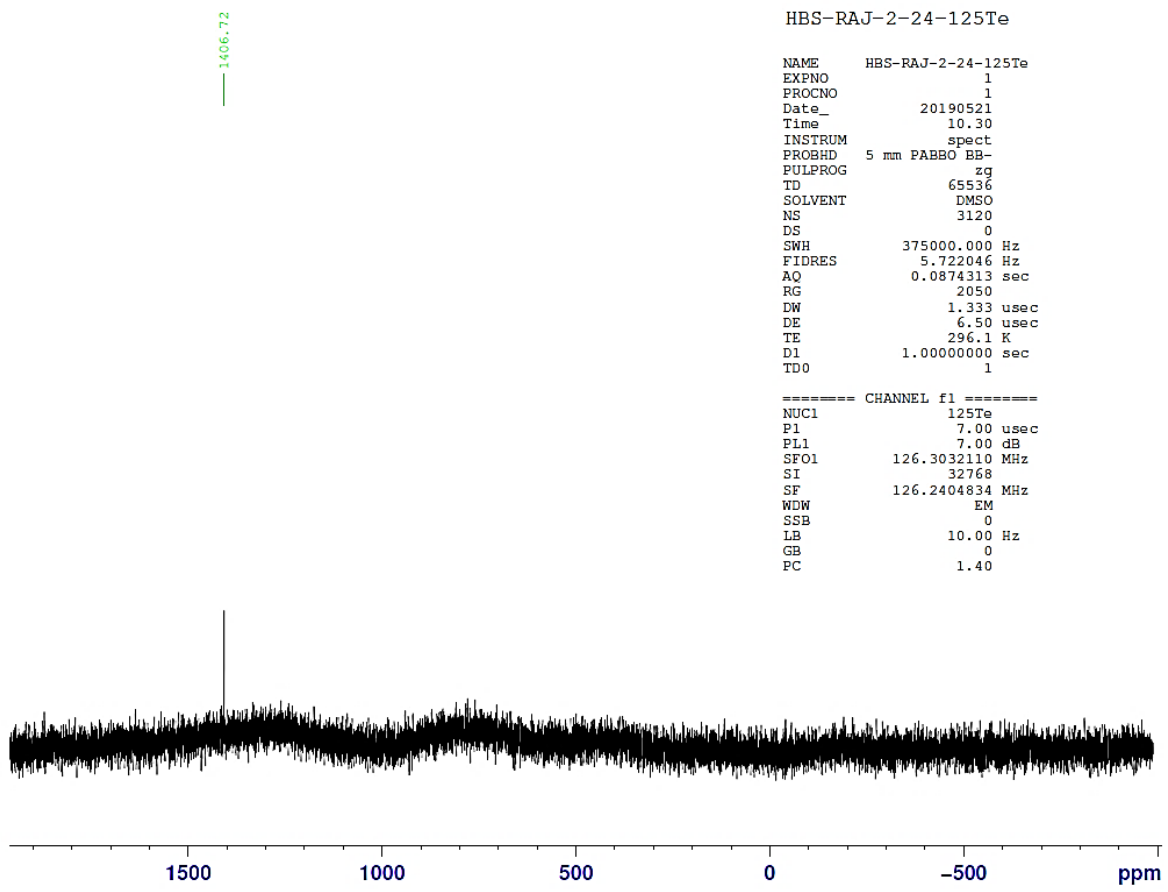



**Fig. S3** $^{125}$Te NMR spectrum of **5**.

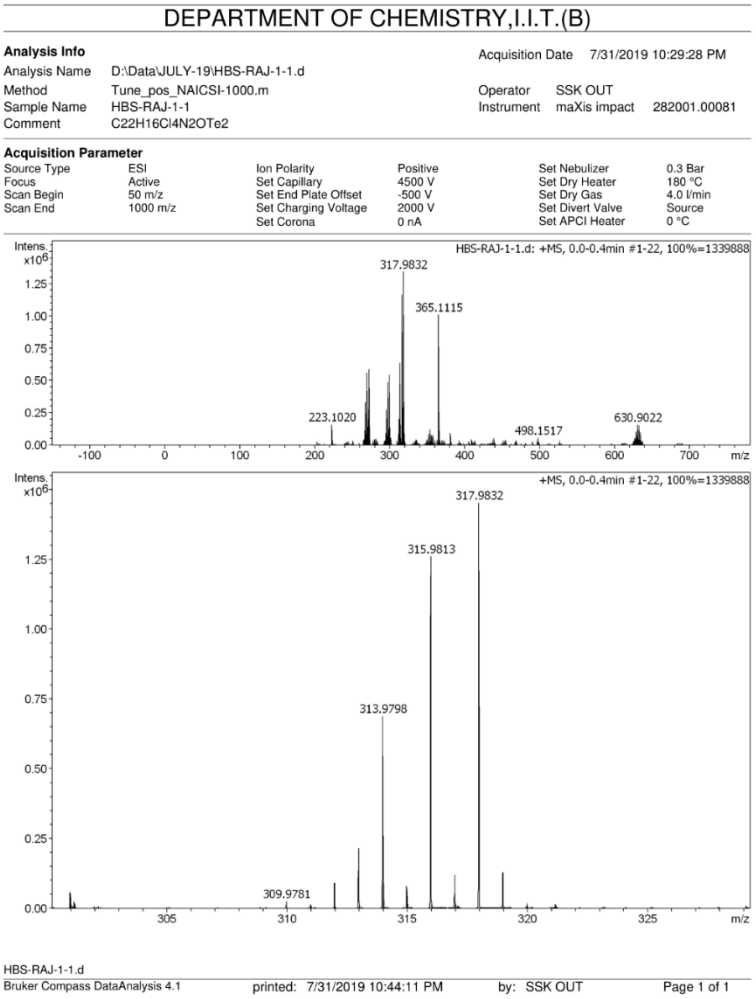



**Fig S4**. ESI-mass spectrum (positive mode) of **5**.

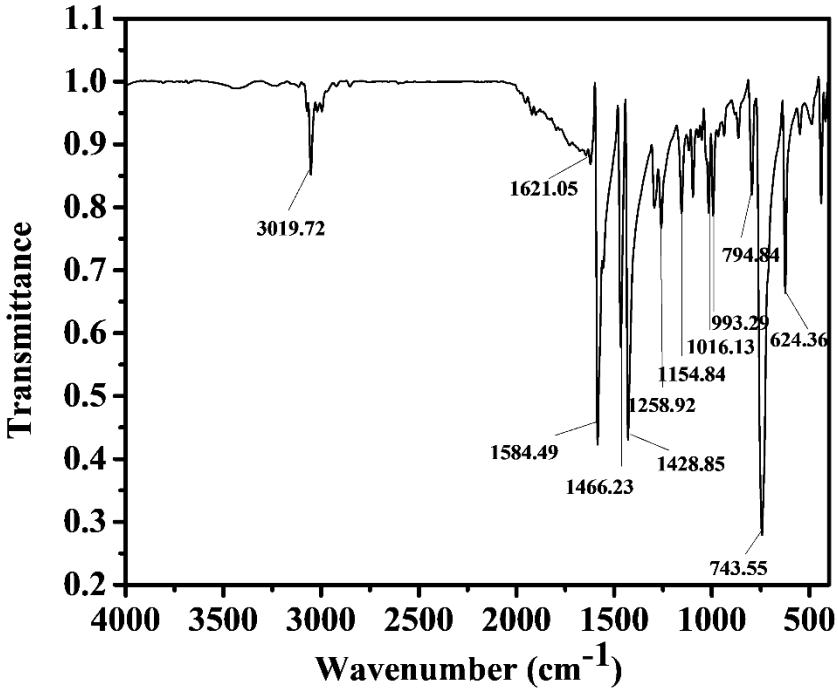



**Fig S5**. FT-IR spectrum (KBr pellet) of **5**.

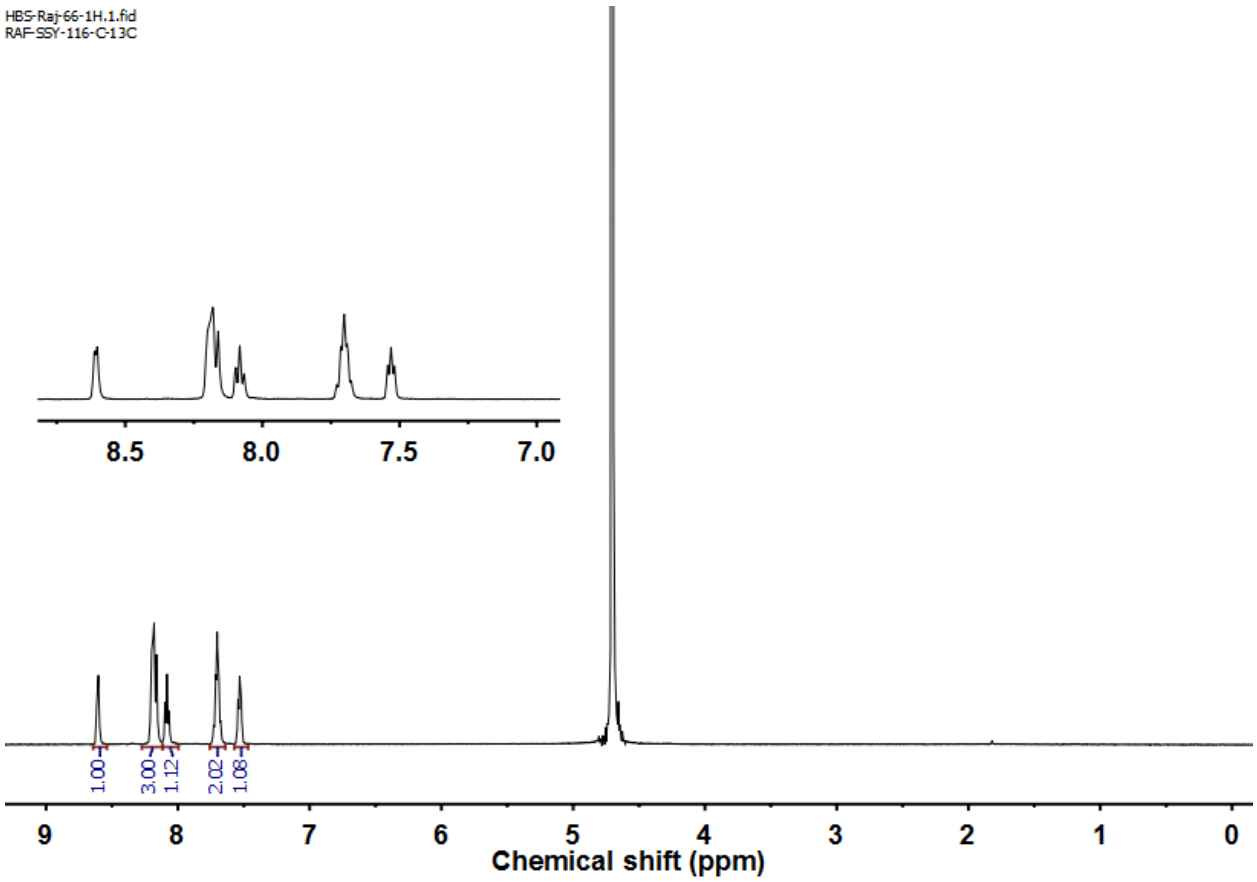



**Fig S6**. $^{1}$H NMR Spectrum of **6**. Inset showing expanded aromatic region.

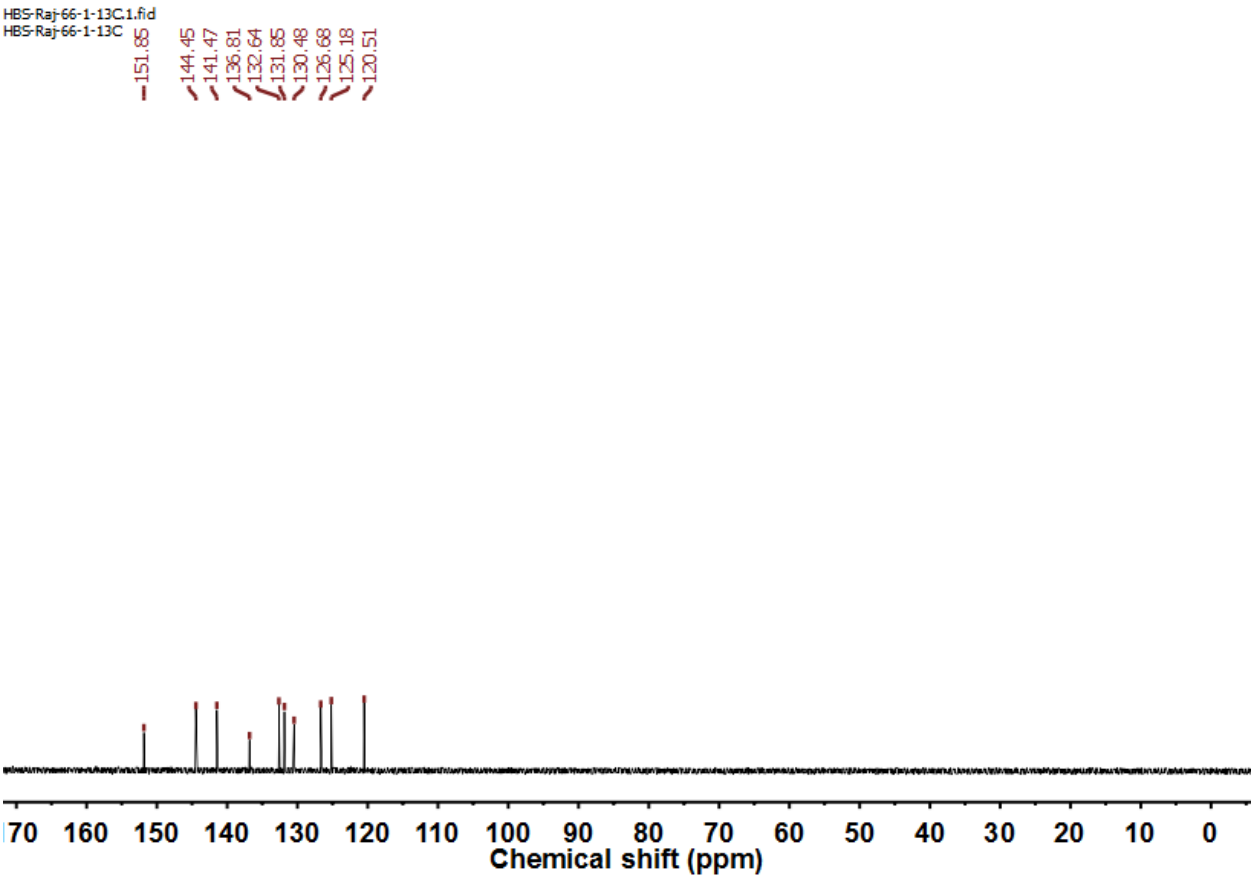



**Fig S7**. $^{13}$C NMR Spectrum of **6**.

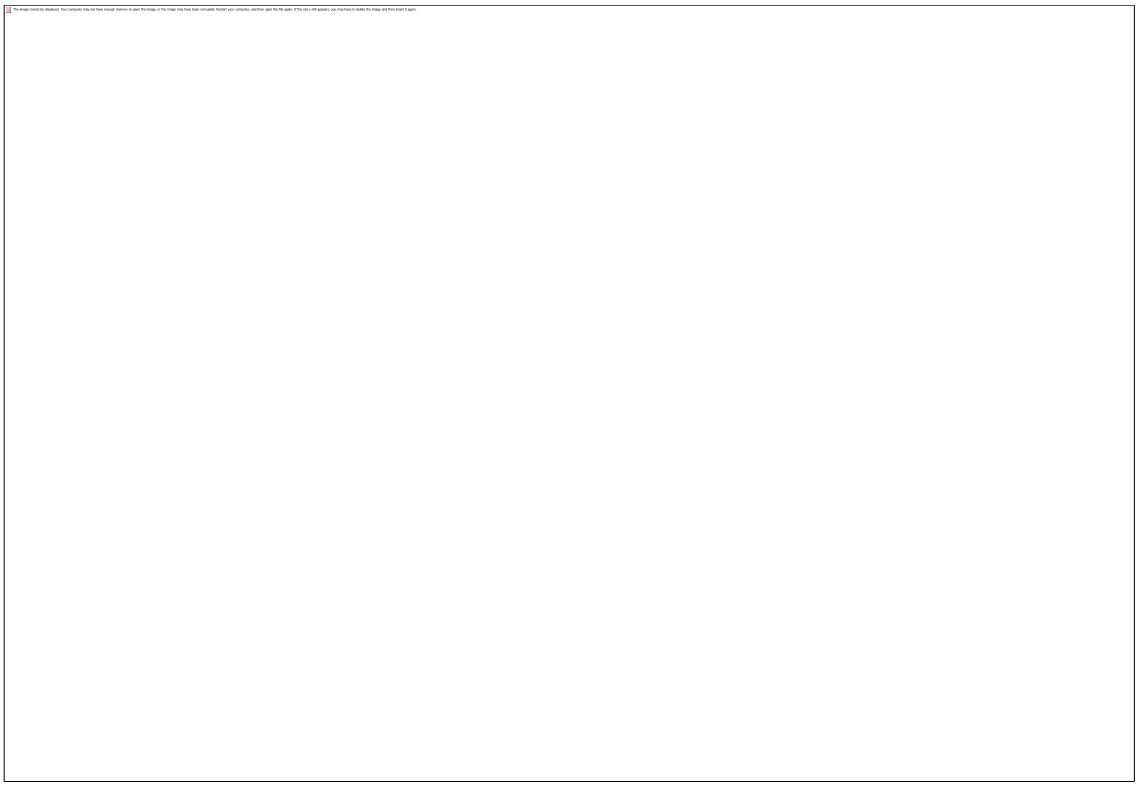


**Fig S8**. $^{125}$Te NMR Spectrum of **6**.

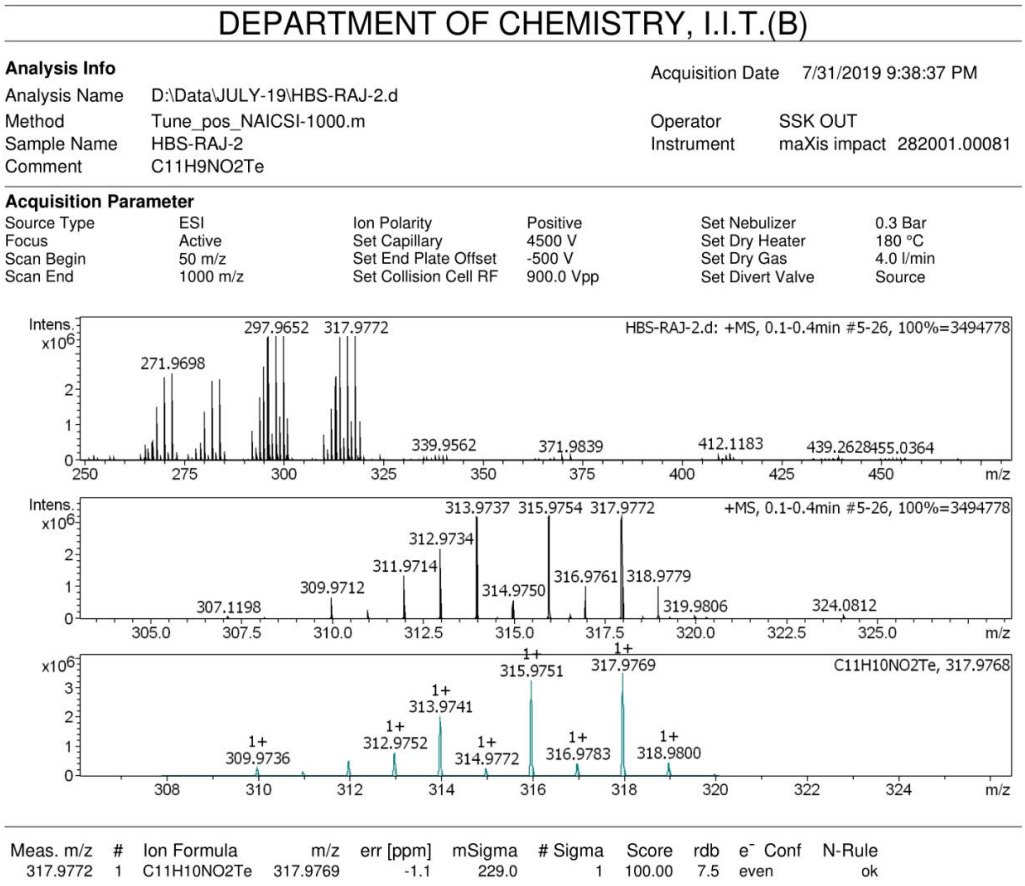



**Fig S9**. High Resolution ESI-mass spectra (positive mode) of **6**. (experimental spectra is depicted in black, simulated pattern is depicted in blue)

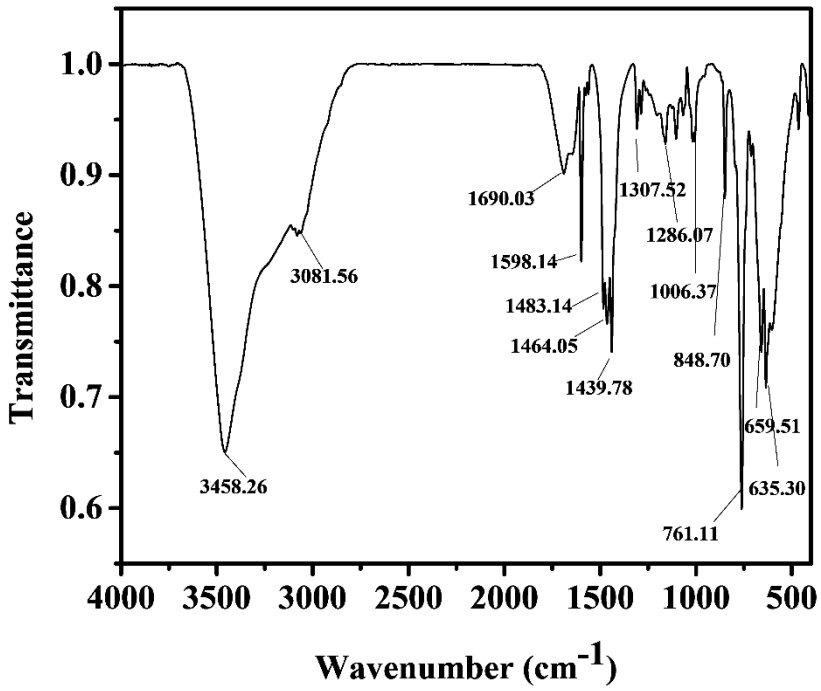



**Fig S10**. FT-IR spectrum (KBr pellet) of **6**.

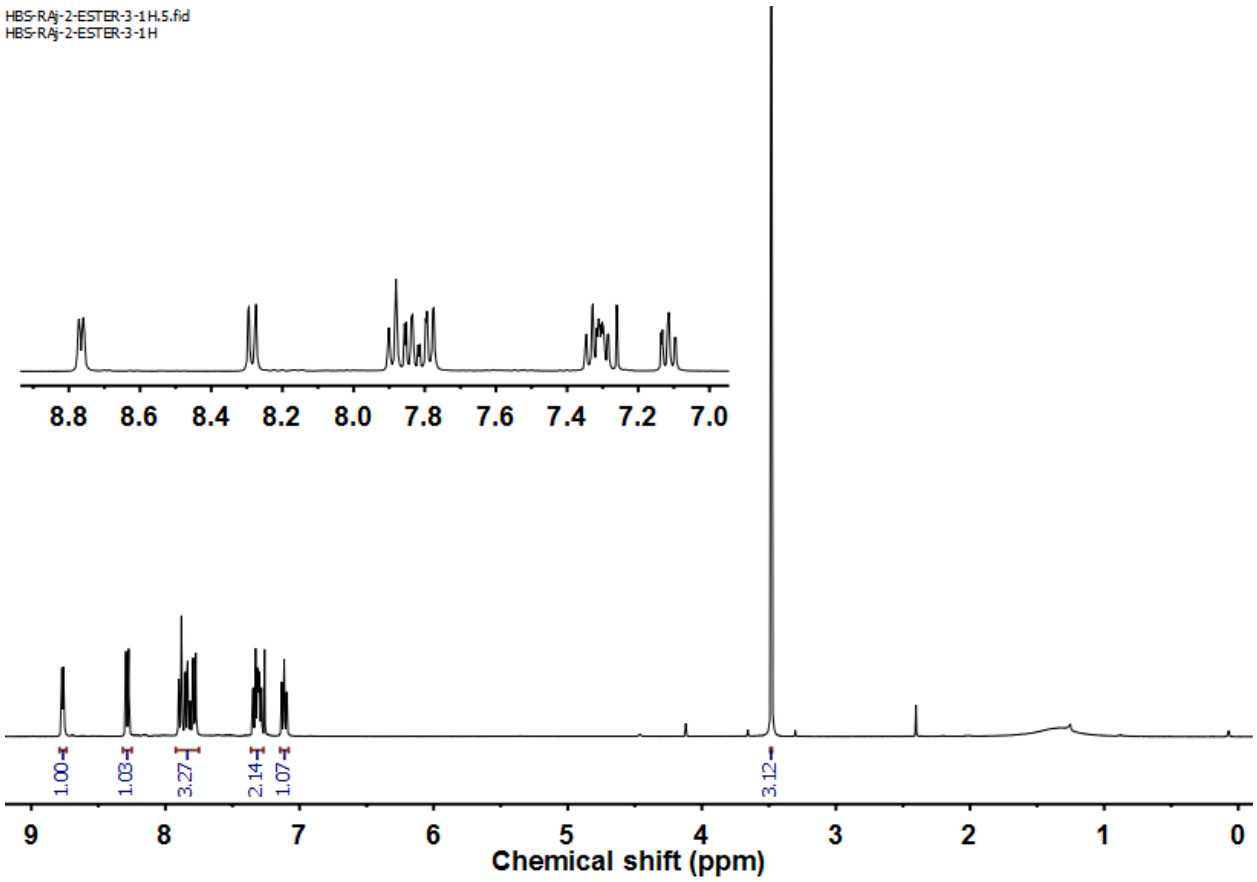



**Fig S11**. $^{1}$H NMR Spectrum of **8**. Inset showing expanded aromatic region.

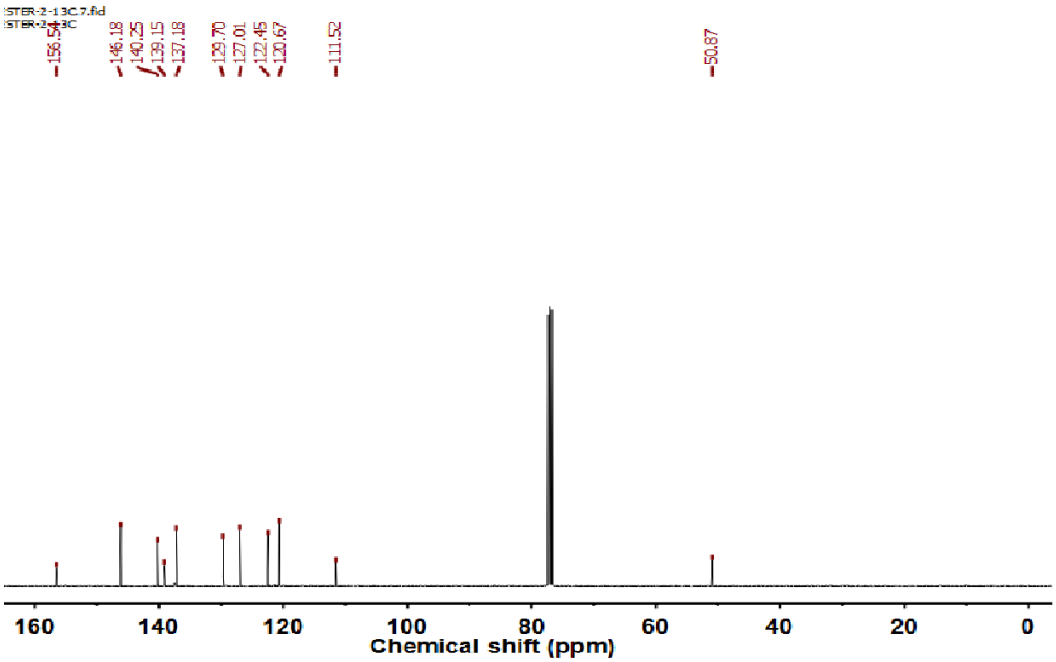



**Fig S12**. $^{13}$C NMR Spectrum of **8**.

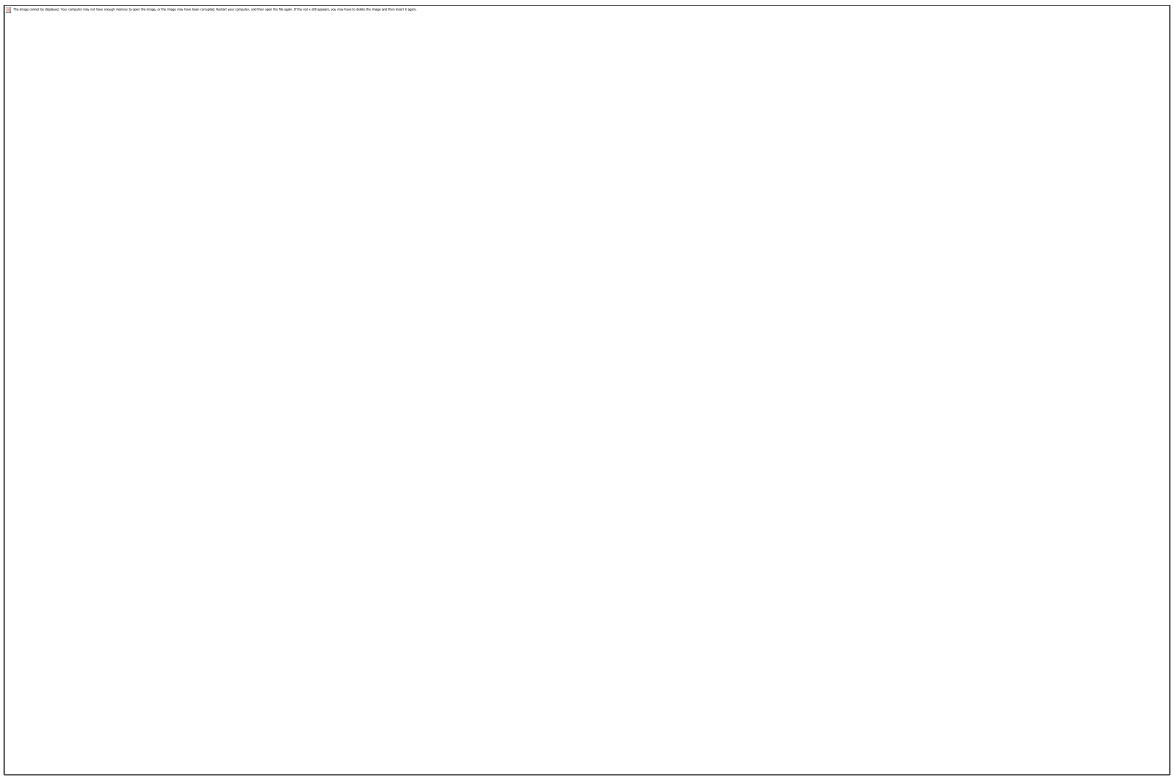


**Fig S13**. $^{125}$Te NMR Spectrum of **8**.

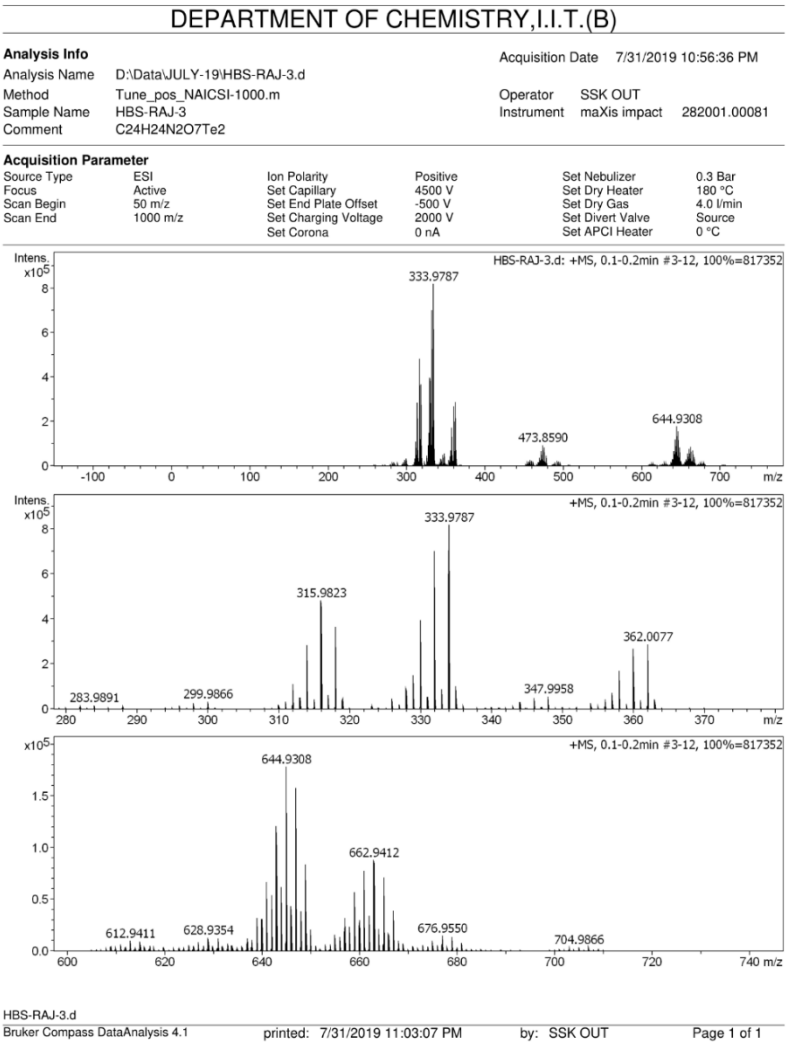



**Fig S14**. High Resolution ESI-mass spectra (positive mode) of **8**.

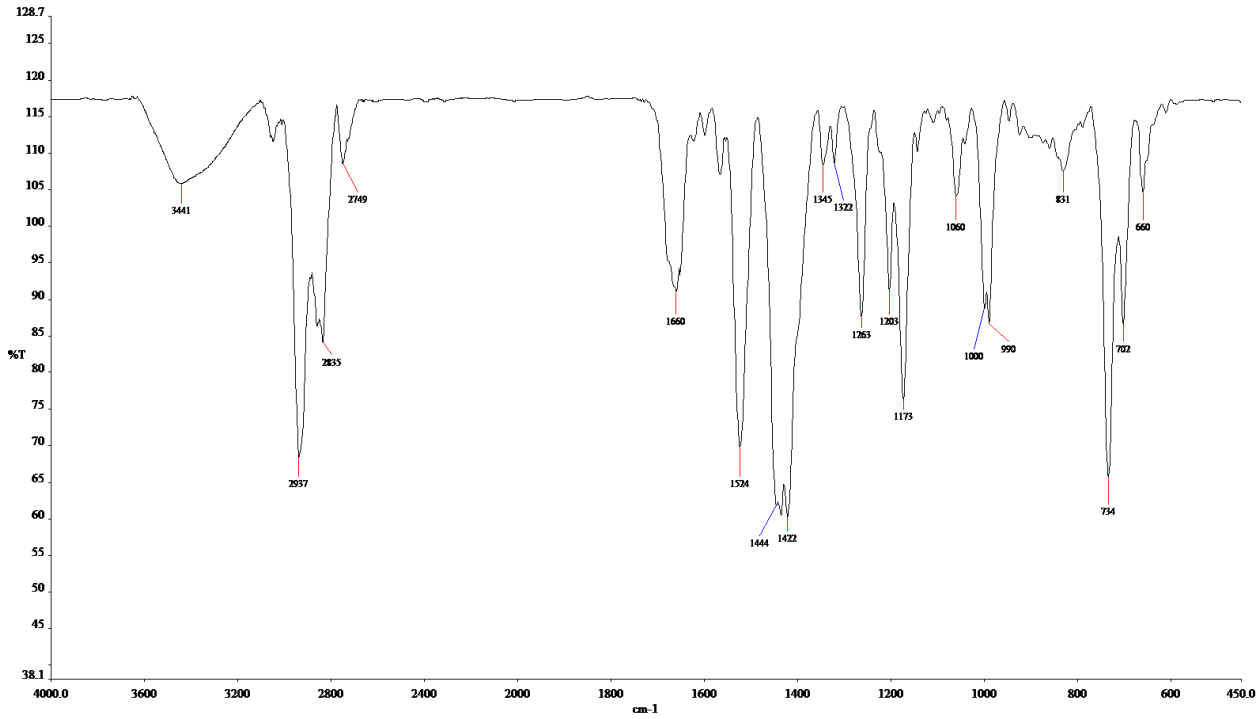



**Fig S15**. FT-IR spectrum (KBr pellet) of **8**.

**Table S1.** Refinement details for the X-ray structures of **4-6, 8**

| **Compound** | **4a** | **4b** | **5** | **6** | **8** |
|---|---|---|---|---|---|
| Formula | $C_{11}H_8Cl_3NTe$ | $C_{11}H_8Cl_3NTe$ | $C_{23}H_{20}Cl_4N_2O_2Te_2$ | $C_{11}H_{13}NO_4Te$ | $C_{24}H_{24}N_2O_7Te_2$ |
| Crystal System | Monoclinic | Orthorhombic | Monoclinic | Triclinic | Monoclinic |
| Space group | *P21/n* | $P2_12_12_1$ | *I2/a* | *P-1* | *P2/c* |
| T/K | 100(2) | 100(2) | 100(2) | 100(2) | 100(2) |
| a [Å] | 6.8410(3) | 6.8250(2) | 17.756(4) | 7.4274(5) | 11.5515(4) |
| b [Å] | 12.7707(6) | 8.4104(3) | 8.602(3) | 8.7073(4) | 10.5679(3) |
| c [Å] | 14.5049(7) | 22.4903(8) | 35.078(5) | 9.5745(6) | 21.3676(6) |
| α [°] | 90 | 90 | 90 | 89.309(4) | 90 |
| β [°] | 97.292(4) | 90 | 99.697(19) | 74.711(5) | 104.168(3) |
| γ [°] | 90 | 90 | 90 | 83.026(4) | 90 |
| V [$A^3$] | 1256.98(10) | 1290.98(9) | 5281(2) | 592.74(6) | 2529.11(14) |
| Z | 4 | 4 | 8 | 2 | 4 |
| $\rho_{cal}g/cm^3$ | 2.051 | 1.997 | 1.895 | 1.966 | 1.858 |
| $\mu/mm^{-1}$ | 2.974 | 2.896 | 2.638 | 2.512 | 2.353 |
| GOF | 1.063 | 1.027 | 1.168 | 1.060 | 1.023 |
| $2\theta$ range (deg) | 5.662- 49.996 | 5.172-49.988 | 4.712- 49.998 | 4.412-62.238 | 3.932-62.15 |
| Refs collected | 11664 | 8593 | 56157 | 3377 | 20319 |
| Unique/observed | 2200 | 2259 | 4644 | 3377 | 7298 |
| Parameters | 145 | 145 | 311 | 189 | 318 |

| | | | | | |
|---|---|---|---|---|---|
| $R_{int}$ | 0.0535 | 0.0645 | 0.0608 | 0.0510 | 0.0600 |
| $R_1$, $wR2[I>2\sigma(I)]$ | 0.0329, 0.0592 | 0.0354, 0.0653 | 0.0345, 0.0712 | 0.0311, 0.0707 | 0.0490, 0.1139 |
| $R_1$, $wR2[I>2\sigma(I)]$ | 0.0438, 0.0652 | 0.0403, 0.0683 | 0.0362, 0.0723 | 0.0380, 0.0732 | 0.0699, 0.1265 |

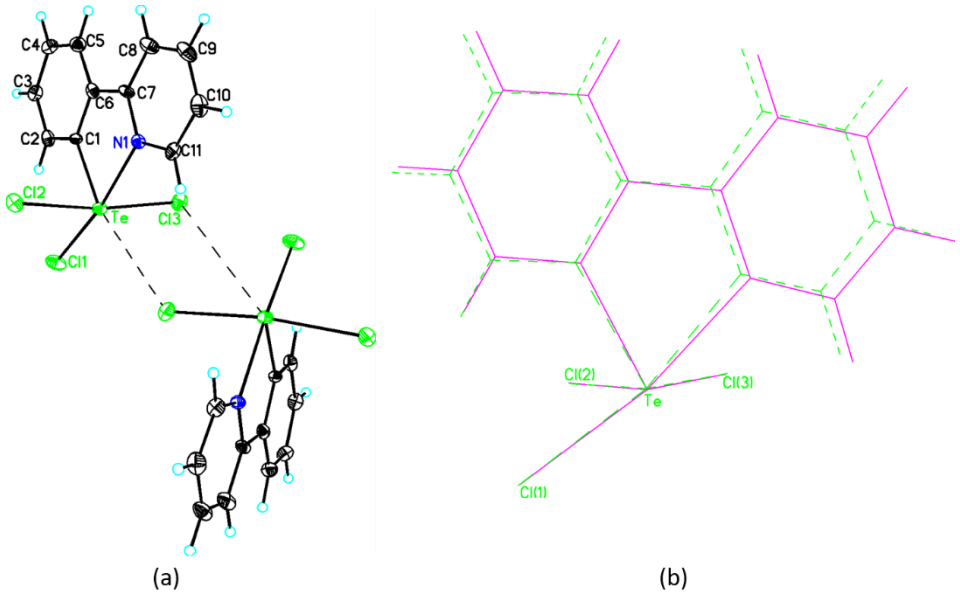



**Fig. S16**. Molecular structures of (a) **4b**, thermal ellipsoids are set at the 50% probability level. Selected bond distances and bond angles [Å, °]: C1-Te 2.105 (7), N1-Te 2.286 (6), Cl1-Te 2.455 (2), Cl2-Te 2.504 (2), Cl3-Te 2.515 (2), N1-Te-C1 76.0 (3), N1-Te-Cl1 169.1 (2), N1-Te-Cl2 89.1 (2), N1-Te-Cl3 85.7 (2); (b) Superimposition of the crystallization arrangement of **4a** and **4b**.

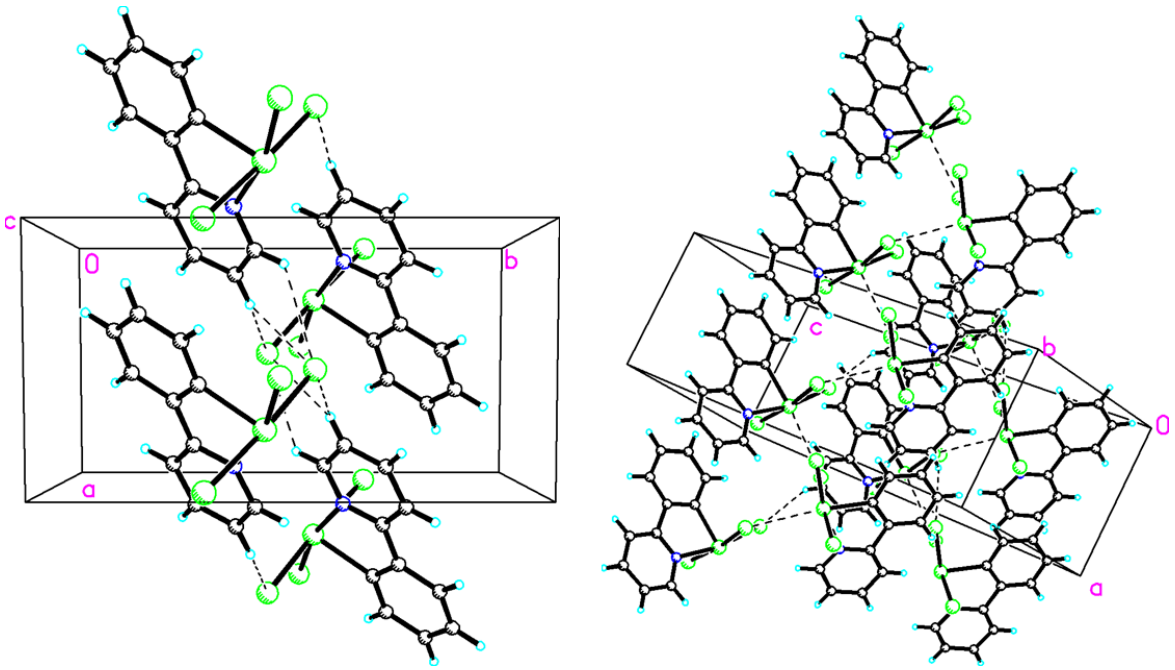


**Fig S17.** Packing diagrams of **4a** (left) and **4b** (right).

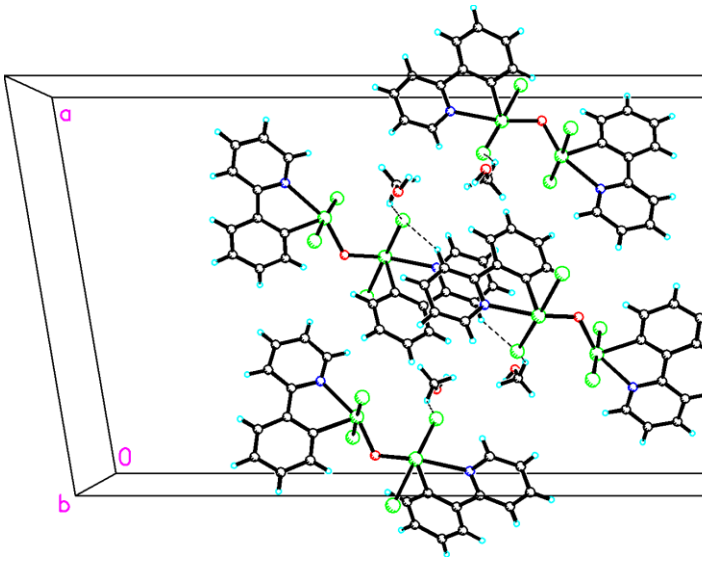
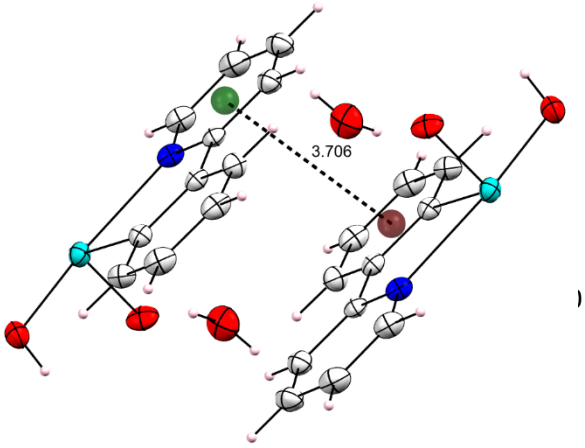



**Fig S18.** Packing diagram of **5**.



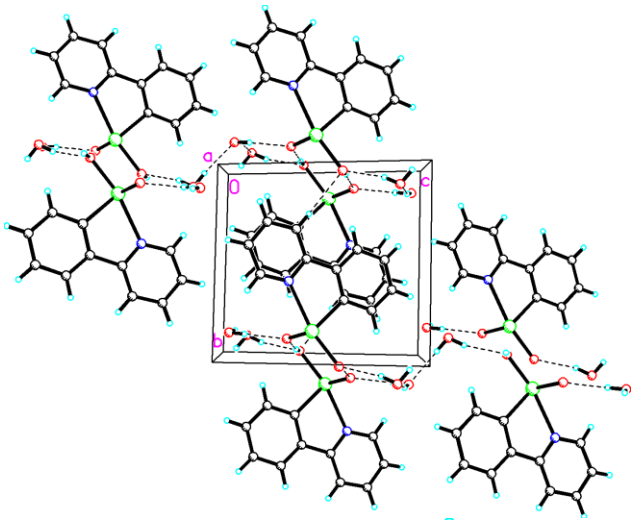


**Fig S19.** Packing diagram of **6**.

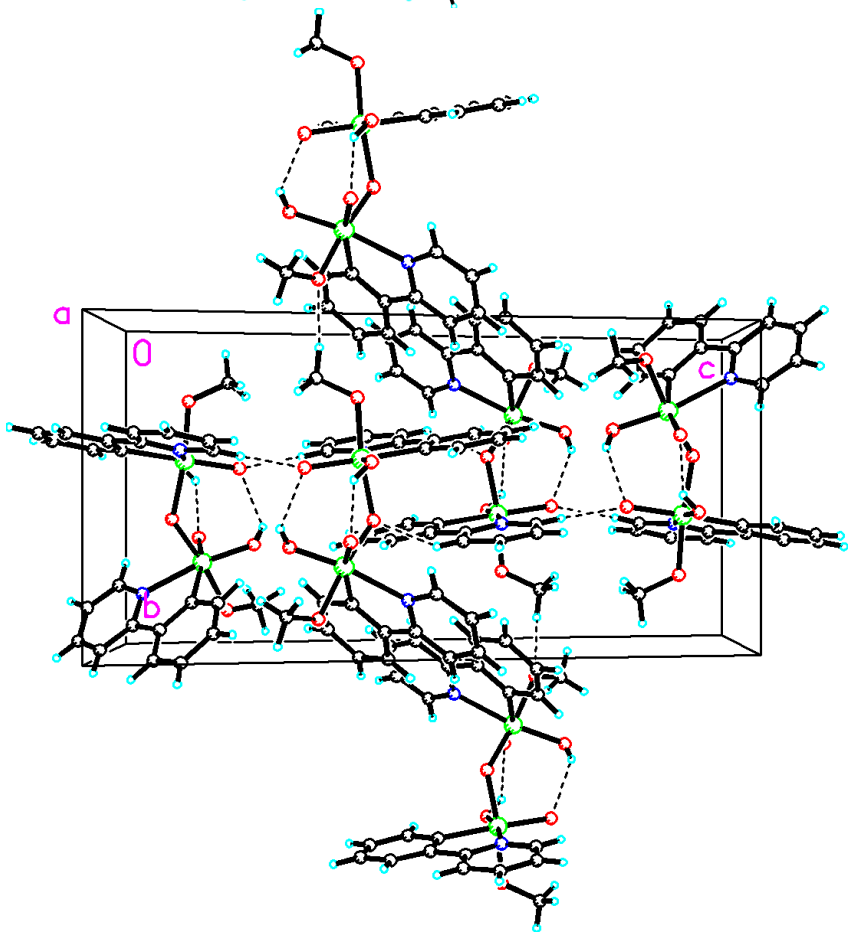


**Fig S20.** Packing diagram of **8**.

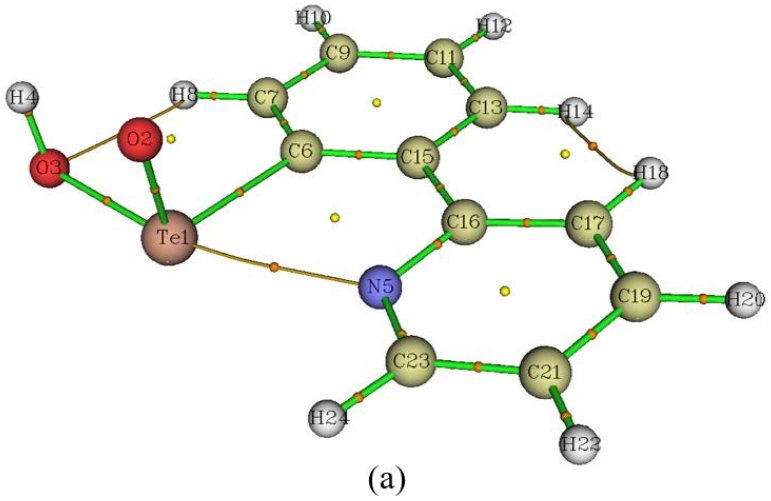
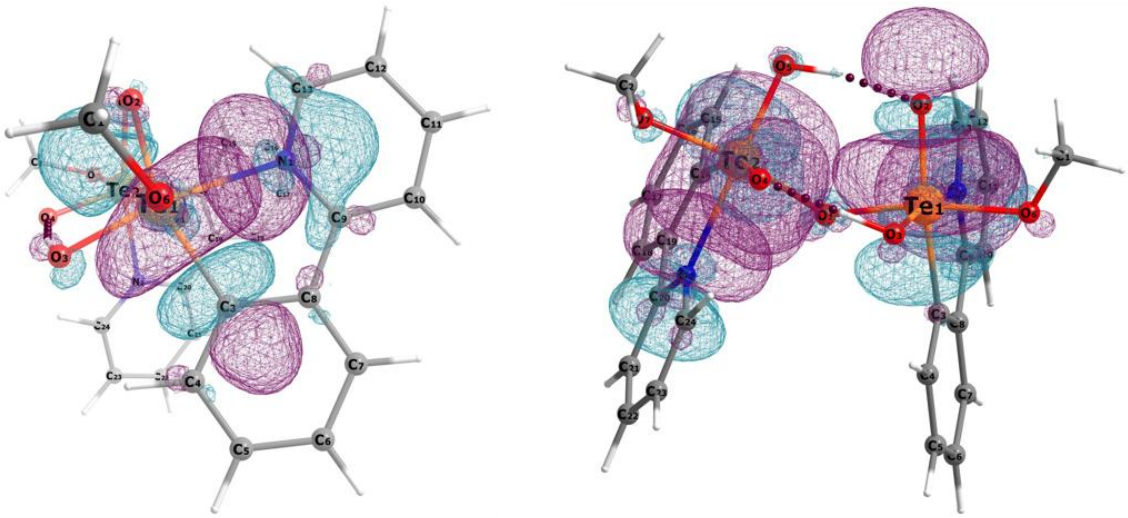



**Fig S21.** Atoms in molecule (AIM) bond topology of **6**.

**Table S2**. Topological parameters for N-Te bcp of compound **6**.

| $\rho(r)$ | $\nabla^2\rho(r)$ | V(r) | G(r) | H(r) | H/$\rho$(r) | \|V(r)/G(r)\| |
|---|---|---|---|---|---|---|
| 0.0460 | 0.0897 | -0.0302 | 0.0227 | -0.0075 | -0.1630 | 1.3303 |



(a) (b)

**Fig S22**. Natural bond orbital (NBO) plot showing (a) *lp*(N) → $\sigma^*$(Te-C), stabilization energy, ΔE = 21.59 kcal/mol; (b) *lp*(N) → $\sigma^*$(Te=O), stabilization energy, ΔE = 20.39 kcal/mol.

**Cartesian Coordinates for 6**

$C_{11}NH_9TeO_2$

Electronic energy: -637.655864671 Eh

Sum of electronic and zero-point Energies = -637.478819 hartree

Sum of electronic and thermal Energies = -637.465568 hartree

Sum of electronic and thermal Enthalpies = -637.464624 hartree

| | | | |
|---|---|---|---|
| Te | -1.089460000 | -1.140076000 | -0.202511000 |
| O | -0.811993000 | -1.781458000 | 1.457220000 |
| O | -3.041602000 | -0.869461000 | -0.027357000 |
| H | -3.209147000 | -0.981721000 | 0.921108000 |
| N | 1.400905000 | -0.719805000 | -0.254398000 |
| C | -0.734399000 | 0.981756000 | -0.062828000 |
| C | -1.827265000 | 1.845891000 | -0.036355000 |
| H | -2.828731000 | 1.425888000 | -0.068992000 |
| C | -1.635249000 | 3.225913000 | 0.033393000 |
| H | -2.493033000 | 3.892395000 | 0.059030000 |
| C | -0.342935000 | 3.746022000 | 0.064084000 |
| H | -0.185670000 | 4.819887000 | 0.108580000 |
| C | 0.753451000 | 2.890193000 | 0.032763000 |

| | | | |
|---|---|---|---|
| H | 1.751704000 | 3.317019000 | 0.044847000 |
| C | 0.575441000 | 1.501190000 | -0.026164000 |
| C | 1.720407000 | 0.568174000 | -0.045165000 |
| C | 3.057143000 | 0.937749000 | 0.157398000 |
| H | 3.323336000 | 1.971815000 | 0.341769000 |
| C | 4.042212000 | -0.041620000 | 0.141554000 |
| H | 5.081235000 | 0.231564000 | 0.301597000 |
| C | 3.686342000 | -1.373938000 | -0.065267000 |
| H | 4.426536000 | -2.166533000 | -0.071002000 |
| C | 2.340734000 | -1.664159000 | -0.253942000 |
| H | 1.992830000 | -2.683399000 | -0.401313000 |

**Cartesian Coordinates for Model Compound of 6**

$C_{11}NH_9TeO_2$

Electronic energy: -637.615053836 hartree

Sum of electronic and zero-point Energies = -637.438576 hartree

Sum of electronic and thermal Energies = -637.425085 hartree

Sum of electronic and thermal Enthalpies = -637.424140 hartree

Sum of electronic and thermal Free Energies = -637.480446 hartree

| | | | |
|---|---|---|---|
| Te | -1.253676000 | -1.050298000 | -0.291581000 |
| O | -1.297940000 | -1.818818000 | 1.337282000 |
| O | -3.145602000 | -0.603257000 | -0.483337000 |
| H | -3.529344000 | -0.814085000 | 0.383508000 |
| N | 2.868829000 | 0.714232000 | -0.675628000 |
| C | -0.663798000 | 0.979007000 | 0.077948000 |
| C | -1.668180000 | 1.948002000 | 0.129668000 |

| | | | |
|---|---|---|---|
| H | -2.707666000 | 1.641495000 | 0.058075000 |
| C | -1.336809000 | 3.297235000 | 0.234525000 |
| H | -2.123450000 | 4.045111000 | 0.283232000 |
| C | 0.003256000 | 3.681673000 | 0.253101000 |
| H | 0.268173000 | 4.733367000 | 0.317671000 |
| C | 1.006064000 | 2.720782000 | 0.184132000 |
| H | 2.052877000 | 3.007978000 | 0.184663000 |
| C | 0.692269000 | 1.356320000 | 0.116180000 |
| C | 1.807356000 | 0.374738000 | 0.076919000 |
| C | 1.763588000 | -0.818253000 | 0.816376000 |
| H | 0.929300000 | -1.036905000 | 1.478286000 |
| C | 2.833606000 | -1.707178000 | 0.716359000 |
| H | 2.820159000 | -2.637677000 | 1.276889000 |
| C | 3.916840000 | -1.372019000 | -0.087265000 |
| H | 4.772314000 | -2.031862000 | -0.192629000 |
| C | 3.886970000 | -0.141315000 | -0.745705000 |
| H | 4.728357000 | 0.171118000 | -1.363079000 |

**Cartesian Coordinates for 8**

$C_{24}N_2H_{24}Te_2O_7$

Electronic energy: -1580.68291448 hartree

Sum of electronic and zero-point Energies= -1580.236333 hartree

Sum of electronic and thermal Energies = -1580.202557 hartree

Sum of electronic and thermal Enthalpies = -1580.201612 hartree

Sum of electronic and thermal Free Energies = -1580.303713 hartree

| | | | |
|---|---|---|---|
| Te | 1.692352000 | -1.077162000 | -0.311234000 |

| | | | |
|---|---|---|---|
| Te | -1.692315000 | -1.077008000 | 0.311752000 |
| O | 0.000020000 | -0.133517000 | 0.000048000 |
| O | 1.443734000 | -2.243271000 | 1.066121000 |
| O | 1.052871000 | -2.018150000 | -1.832565000 |
| H | 0.079076000 | -2.197978000 | -1.625477000 |
| O | -1.443680000 | -2.243774000 | -1.065045000 |
| O | -1.052837000 | -2.017245000 | 1.833566000 |
| H | -0.079053000 | -2.197196000 | 1.626581000 |
| O | 3.547852000 | -1.558434000 | -0.638219000 |
| O | -3.547795000 | -1.558157000 | 0.638995000 |
| N | 2.439842000 | 0.404413000 | 1.298287000 |
| N | -2.439917000 | 0.403695000 | -1.298475000 |
| C | 3.988872000 | -2.865848000 | -0.299135000 |
| H | 5.057831000 | -2.908543000 | -0.536832000 |
| H | 3.465297000 | -3.632810000 | -0.883434000 |
| H | 3.840678000 | -3.085070000 | 0.763687000 |
| C | -3.988760000 | -2.865796000 | 0.300671000 |
| H | -5.057800000 | -2.908290000 | 0.538034000 |
| H | -3.465397000 | -3.632344000 | 0.885698000 |
| H | -3.840206000 | -3.085751000 | -0.761943000 |
| C | 2.211082000 | 0.687483000 | -1.362040000 |
| C | 2.051565000 | 0.761191000 | -2.738507000 |
| H | 1.680332000 | -0.105303000 | -3.276628000 |
| C | 2.369800000 | 1.950337000 | -3.395909000 |
| H | 2.253750000 | 2.020082000 | -4.474007000 |
| C | 2.838930000 | 3.047565000 | -2.672287000 |
| H | 3.088621000 | 3.971552000 | -3.185752000 |
| C | 2.990002000 | 2.966149000 | -1.291320000 |

| | | | |
|---|---|---|---|
| H | 3.355061000 | 3.830651000 | -0.744956000 |
| C | 2.673841000 | 1.778304000 | -0.620251000 |
| C | 2.783613000 | 1.618015000 | 0.842611000 |
| C | 3.184765000 | 2.603980000 | 1.748915000 |
| H | 3.466386000 | 3.590816000 | 1.401103000 |
| C | 3.210943000 | 2.302397000 | 3.106157000 |
| H | 3.519303000 | 3.059979000 | 3.820948000 |
| C | 2.836560000 | 1.032456000 | 3.545347000 |
| H | 2.841977000 | 0.771390000 | 4.597686000 |
| C | 2.449120000 | 0.096883000 | 2.594811000 |
| H | 2.129084000 | -0.917328000 | 2.817643000 |
| C | -2.211015000 | 0.688168000 | 1.361695000 |
| C | -2.051388000 | 0.762613000 | 2.738110000 |
| H | -1.680092000 | -0.103586000 | 3.276659000 |
| C | -2.369595000 | 1.952102000 | 3.394903000 |
| H | -2.253454000 | 2.022426000 | 4.472953000 |
| C | -2.838811000 | 3.048934000 | 2.670736000 |
| H | -3.088477000 | 3.973188000 | 3.183733000 |
| C | -2.989995000 | 2.966782000 | 1.289825000 |
| H | -3.355118000 | 3.830988000 | 0.743037000 |
| C | -2.673858000 | 1.778586000 | 0.619364000 |
| C | -2.783725000 | 1.617520000 | -0.843403000 |
| C | -3.184999000 | 2.602990000 | -1.750189000 |
| H | -3.466658000 | 3.589982000 | -1.402855000 |
| C | -3.211258000 | 2.300714000 | -3.107274000 |
| H | -3.519710000 | 3.057912000 | -3.822432000 |
| C | -2.836841000 | 1.030566000 | -3.545833000 |
| H | -2.842313000 | 0.768942000 | -4.598033000 |

| | | | |
|---|---|---|---|
| C | -2.449284000 | 0.095505000 | -2.594844000 |
| H | -2.129230000 | -0.918804000 | -2.817185000 |