Electronic Supplementary Information

For

Oxidation behavior of intramolecularly coordinated unsymmetrical diorganotellurides: Isolation of novel tetraorganoditelluronic acids, [RR´Te(μ-O)(OH)$_2$]$_2$

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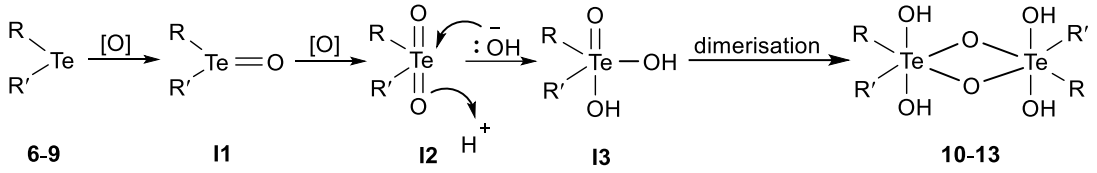
Mechanism for the synthesis of telluronic acids, 10-13

The mechanism for the formation of telluronic acids involves the initial formation of telluroxide, **I1** followed by tellurone **I2** (Scheme S1). In the subsequent step, nucleophilic attack of hydroxyl anion on highly Lewis acidic tellurium centre of tellurone **I2** followed by dimerization leads to the formation of telluronic acids.



Scheme S1. Plausible mechanism for the formation of telluronic acids **10-13**.

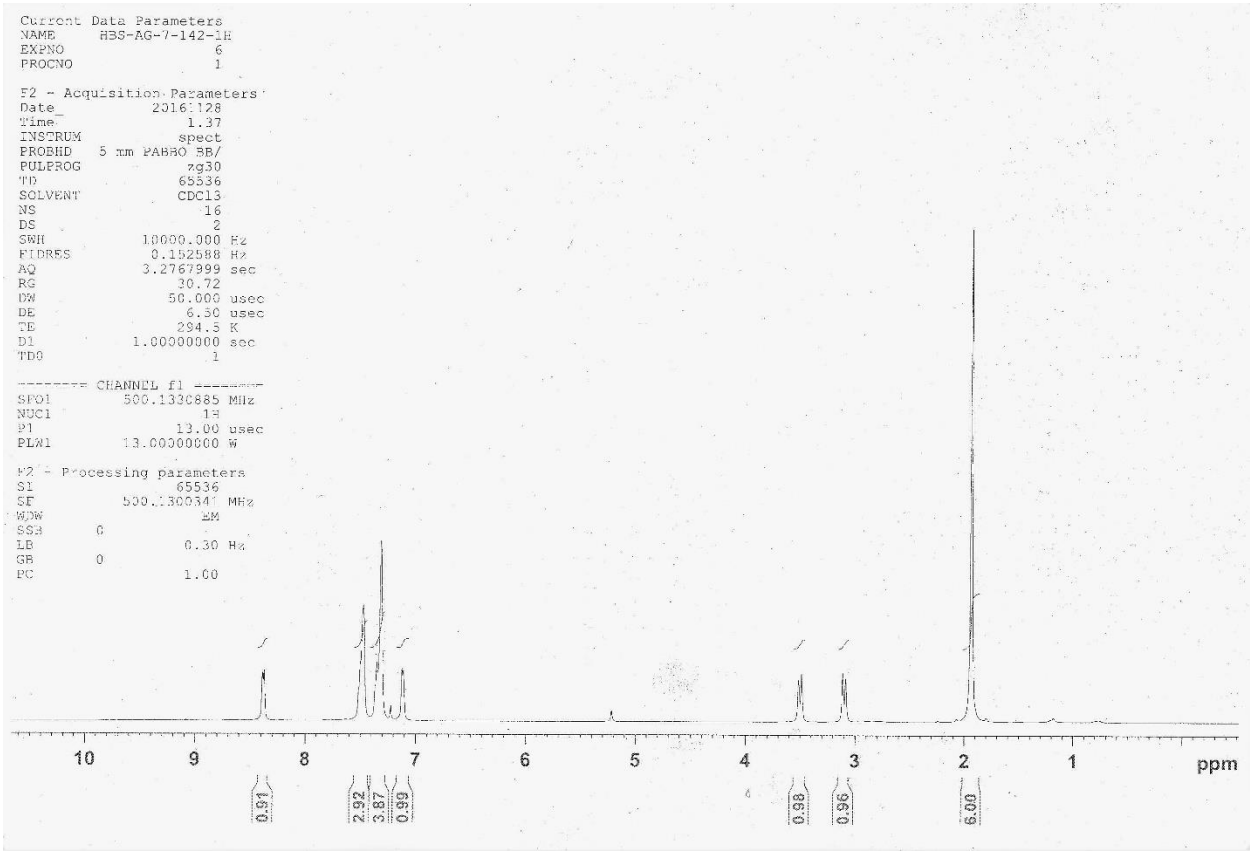


Fig. S1 ^{1}H NMR spectrum of **10**.

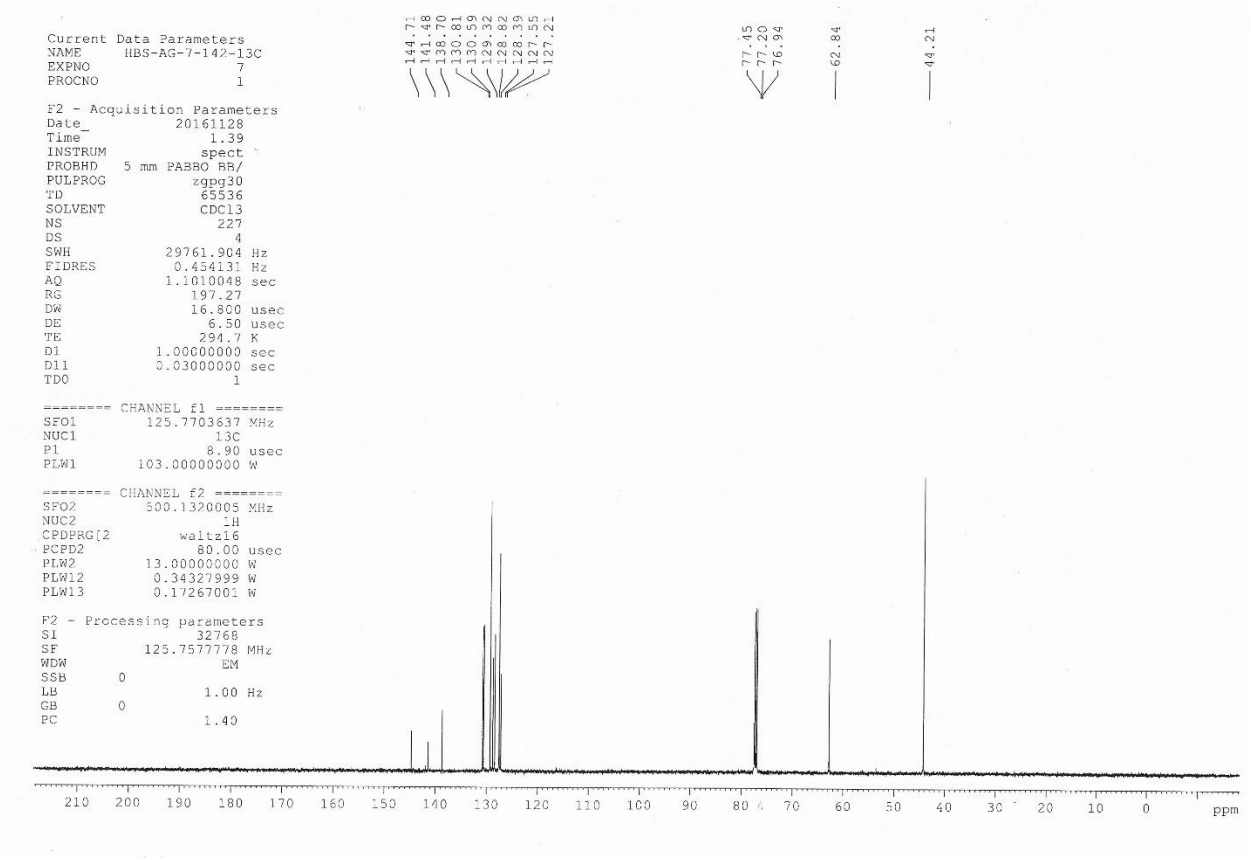


Fig. S2 ^{13}C NMR spectrum of **10**.

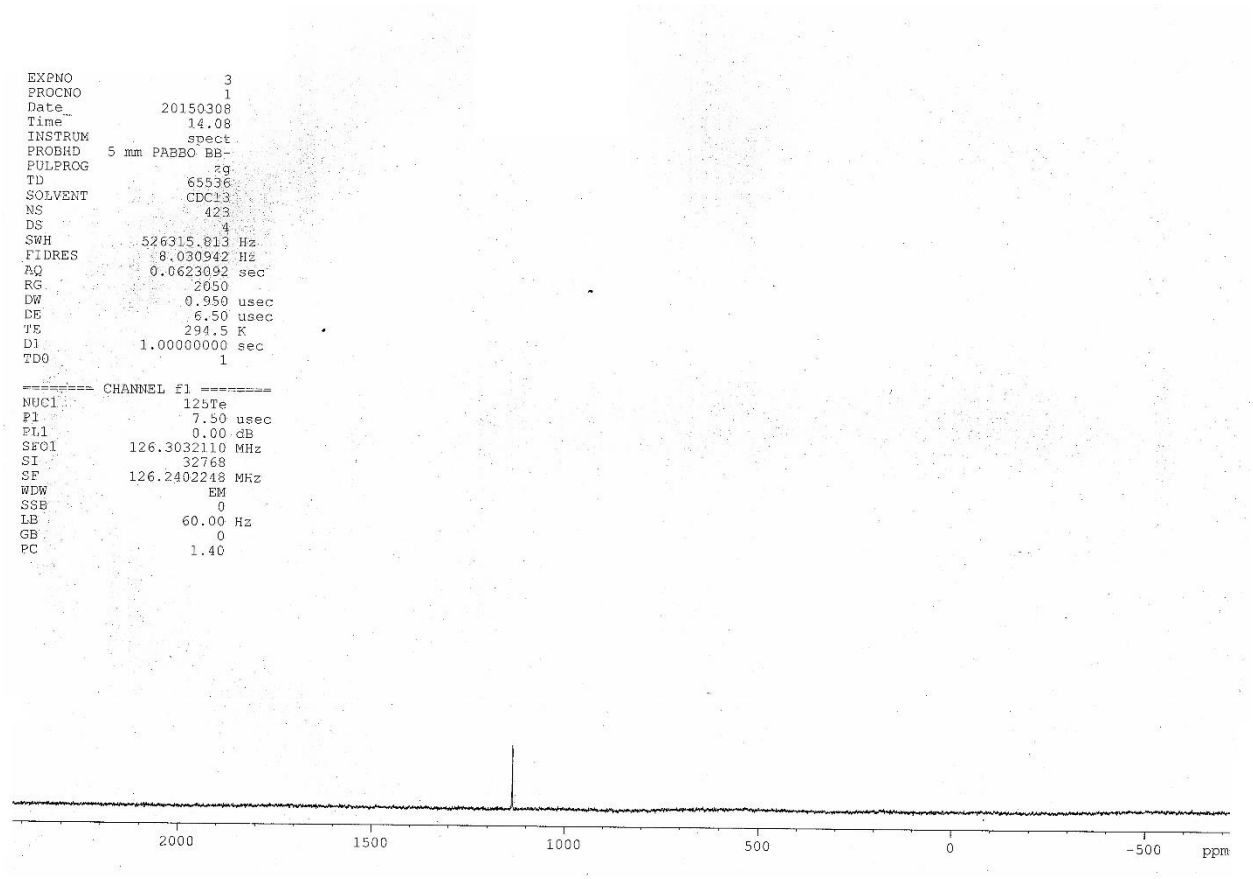


Fig. S3 ^{125}Te NMR spectrum of **10** (δ = 1132 ppm).

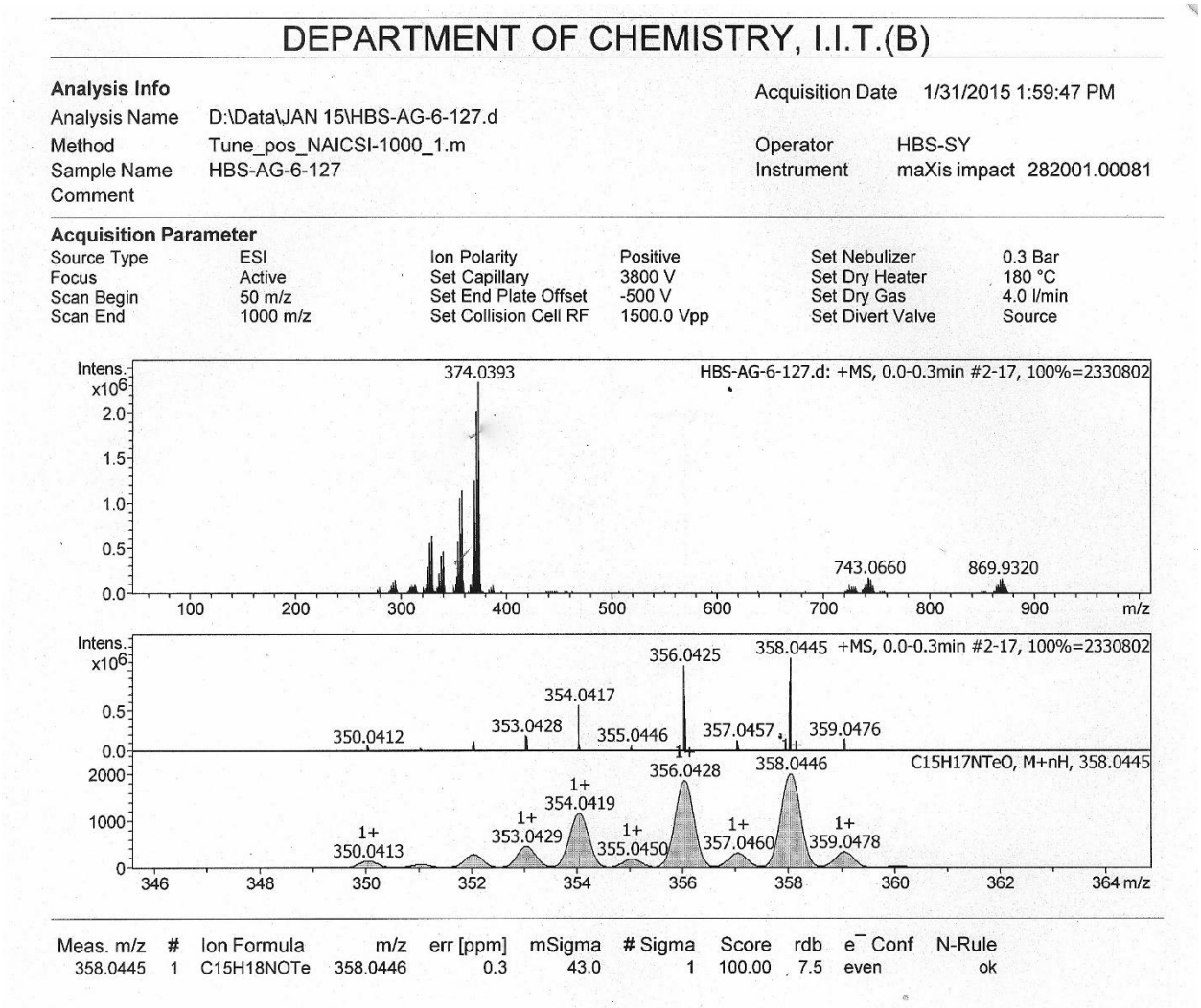


Fig. S4 HRMS of **10**.

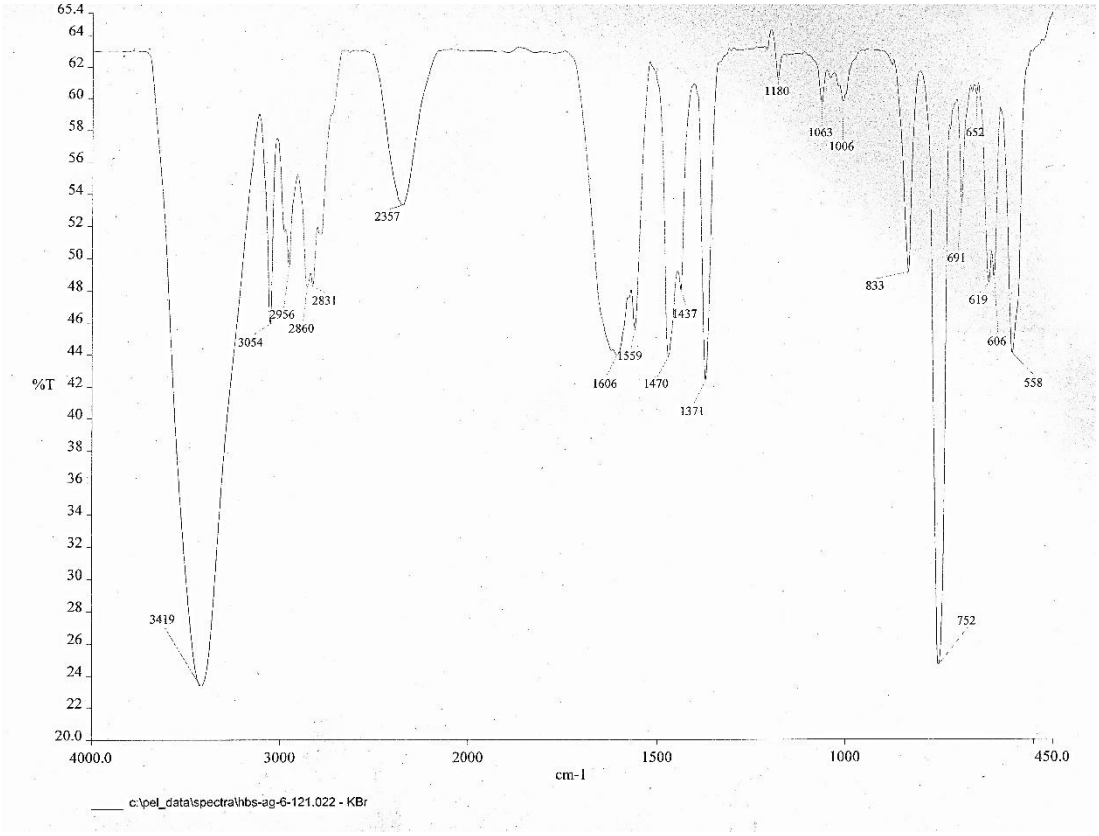


Fig. S5 FT-IR spectrum of **10**.

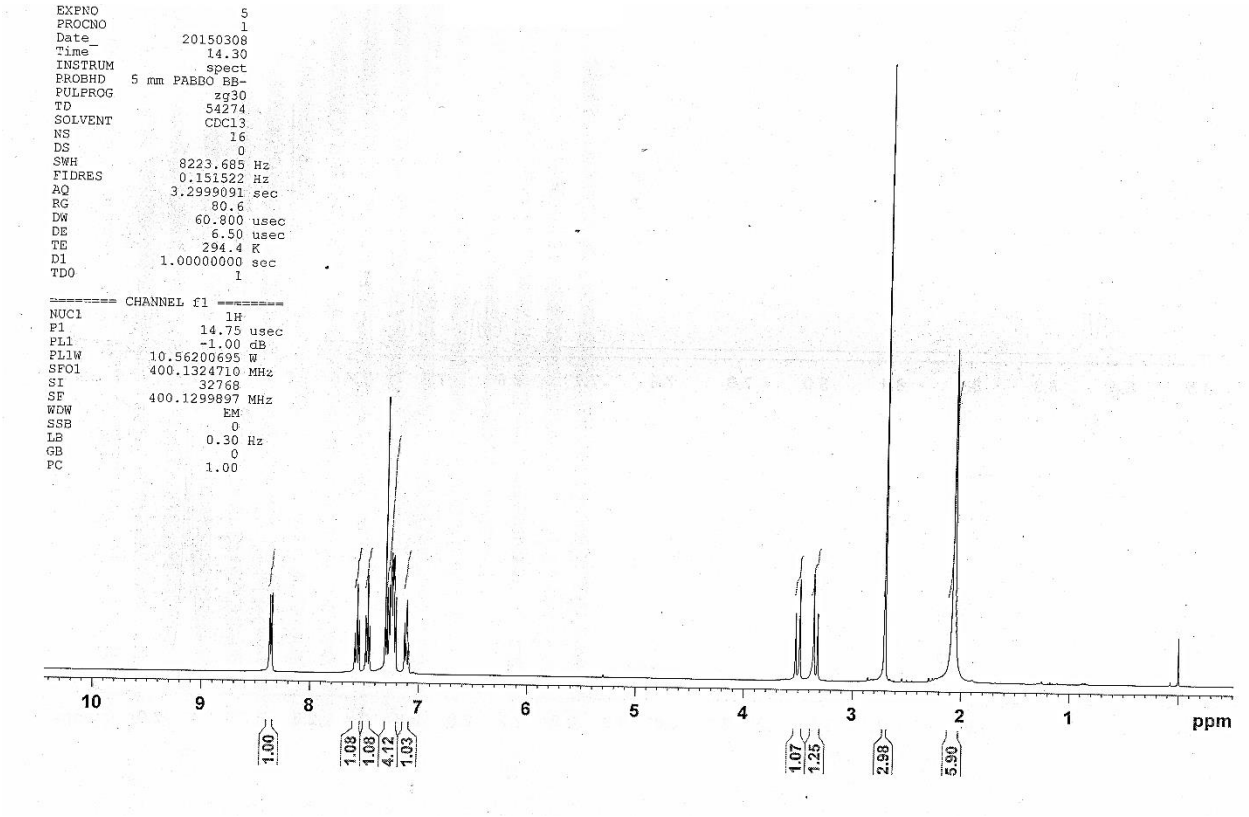


Fig. S6 ^{1}H NMR spectrum of **11**.

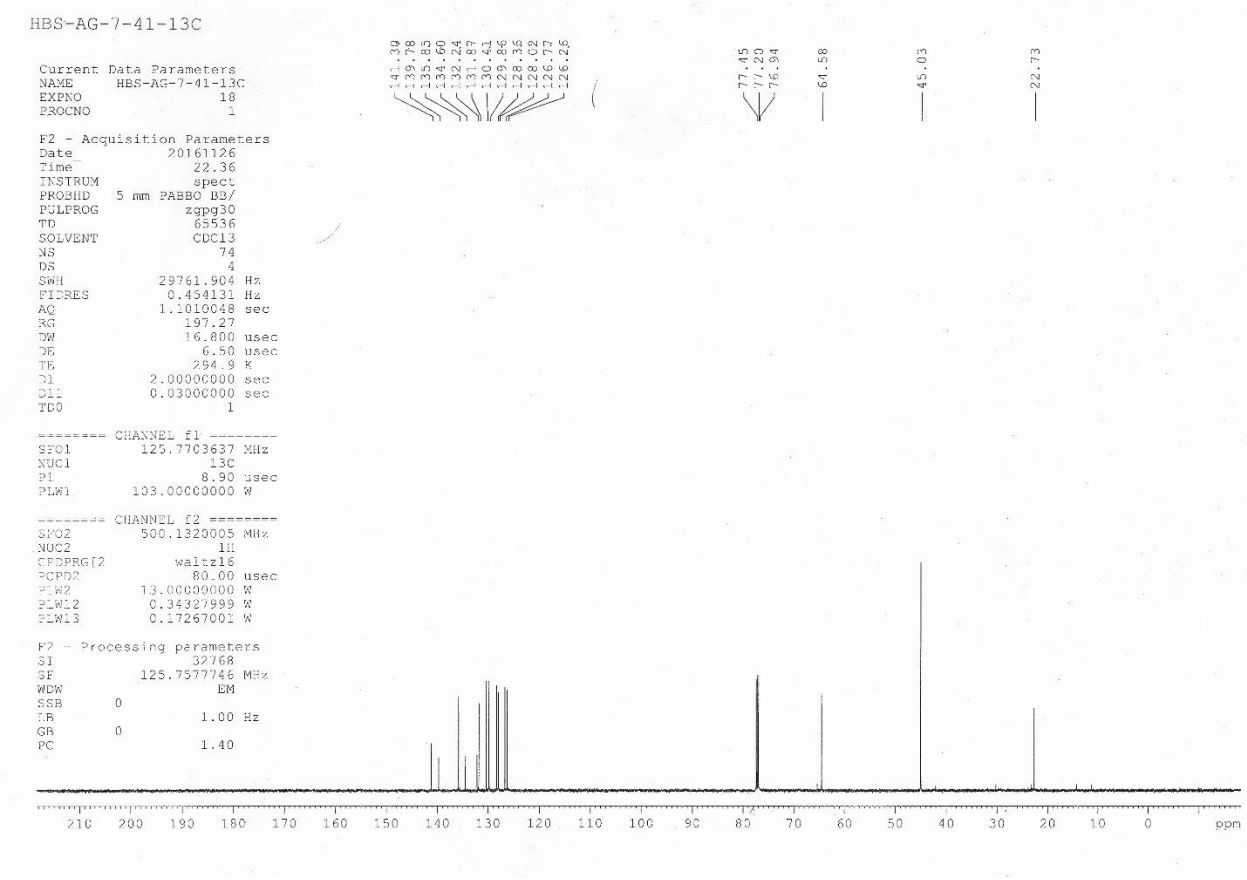


Fig. S7 ^{13}C NMR spectrum of **11**.

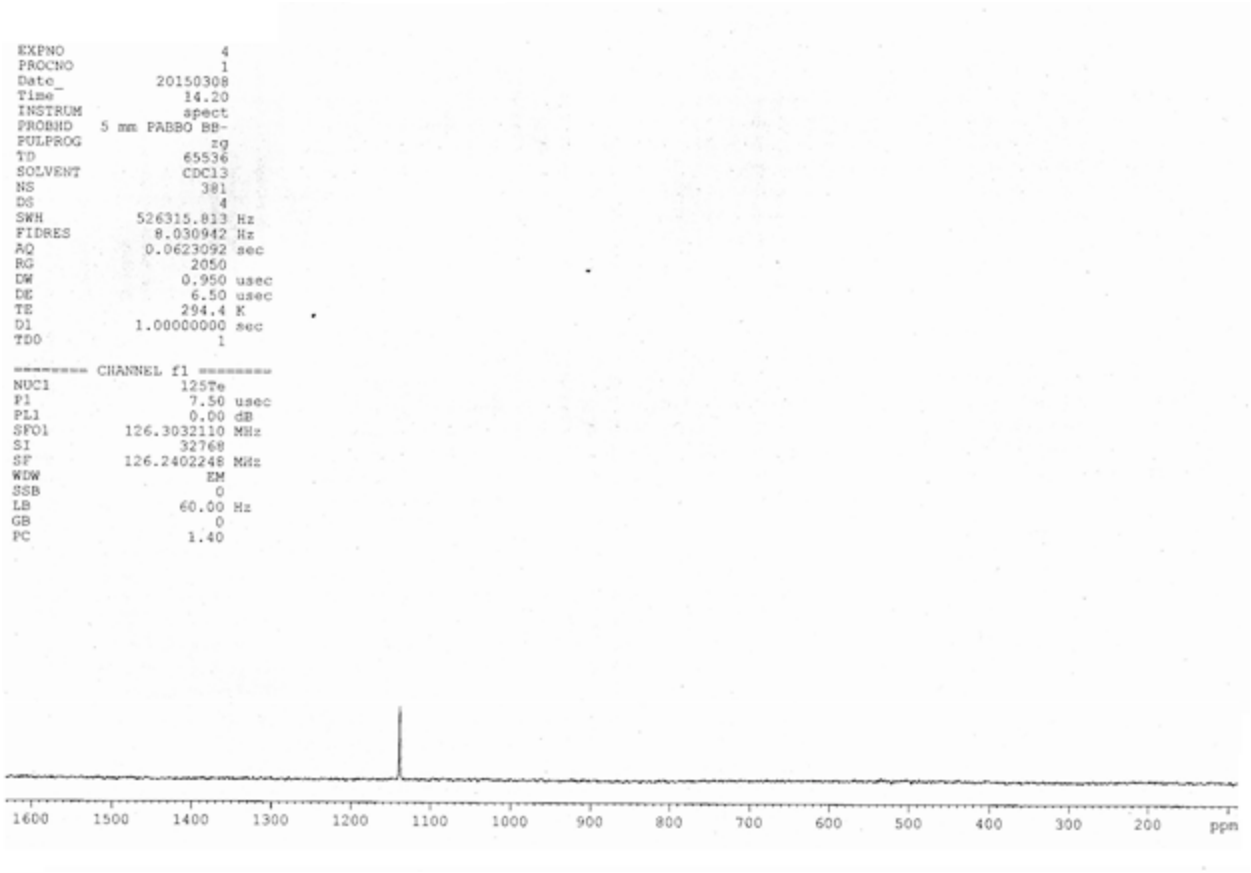


Fig. S8 ^{125}Te NMR spectrum of **11** (δ = 1140 ppm).

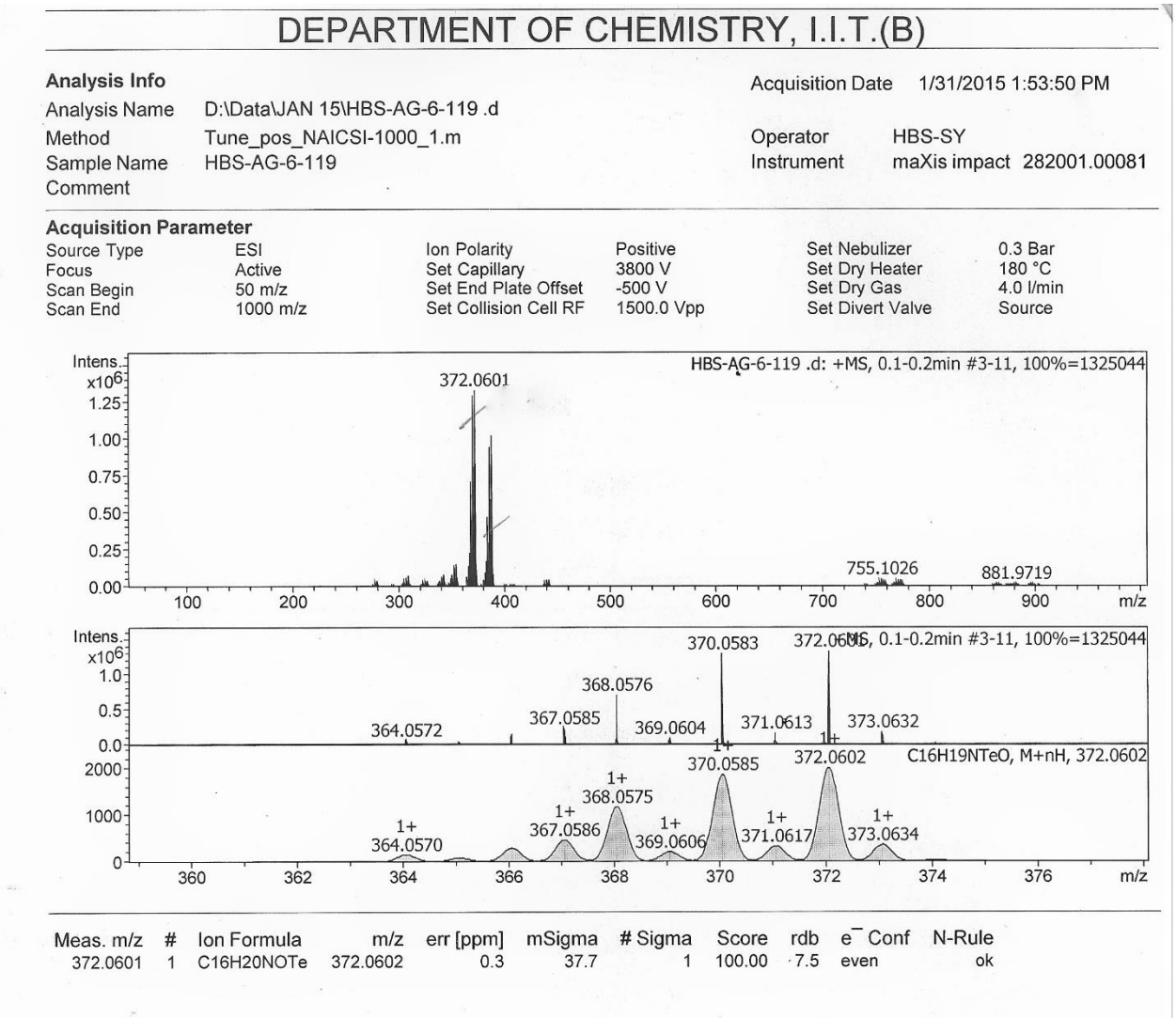


Fig. S9 HRMS of **11**.

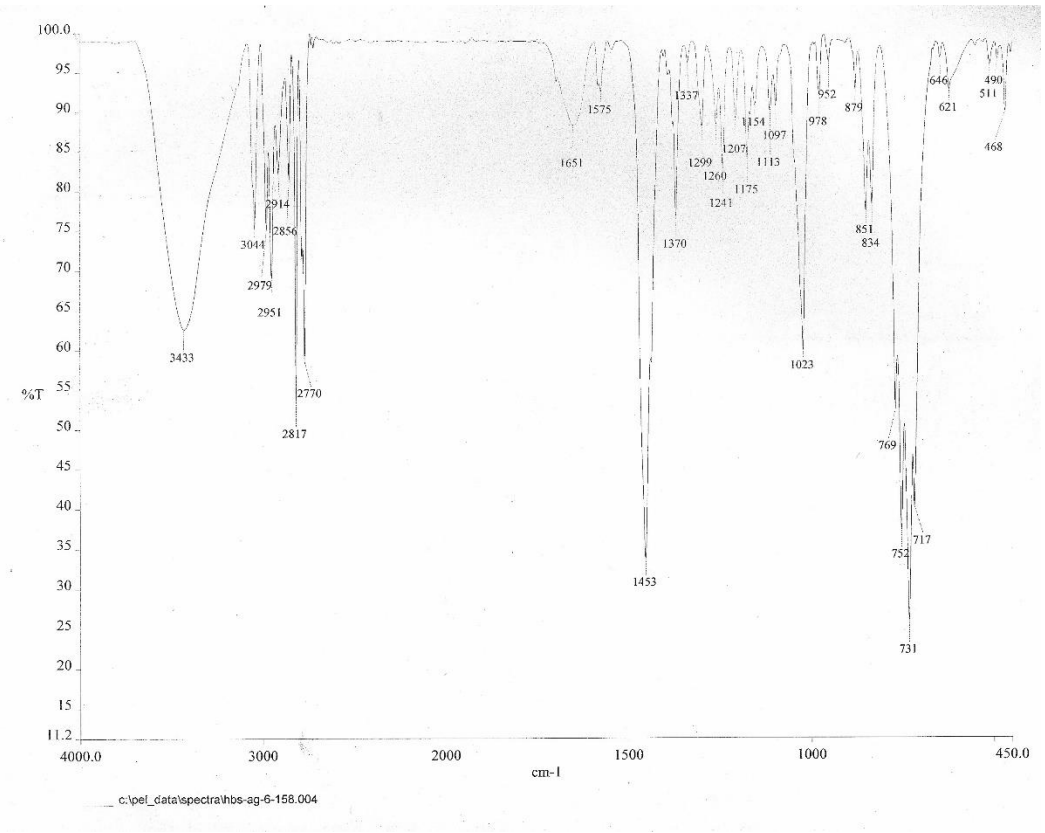


Fig. S10 FT-IR spectrum of **11**.

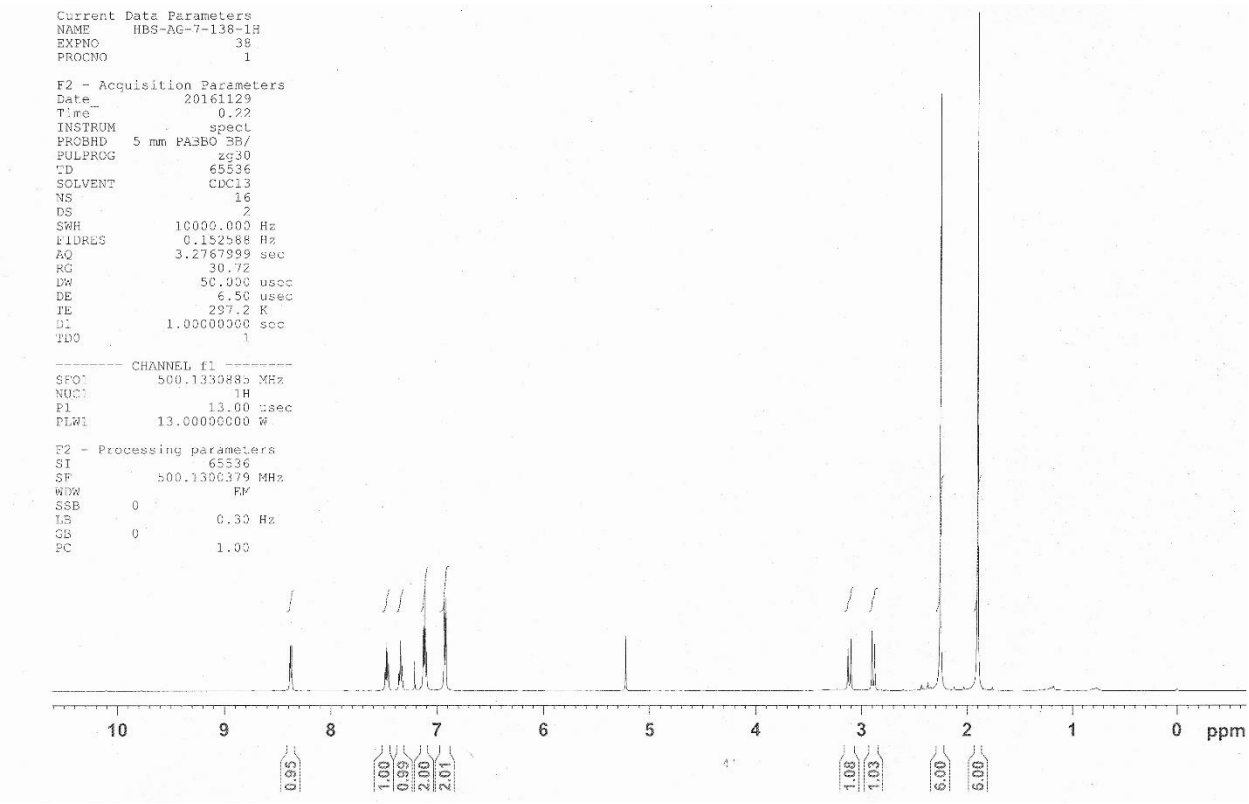


Fig. S11 ^{1}H NMR spectrum of **12**.

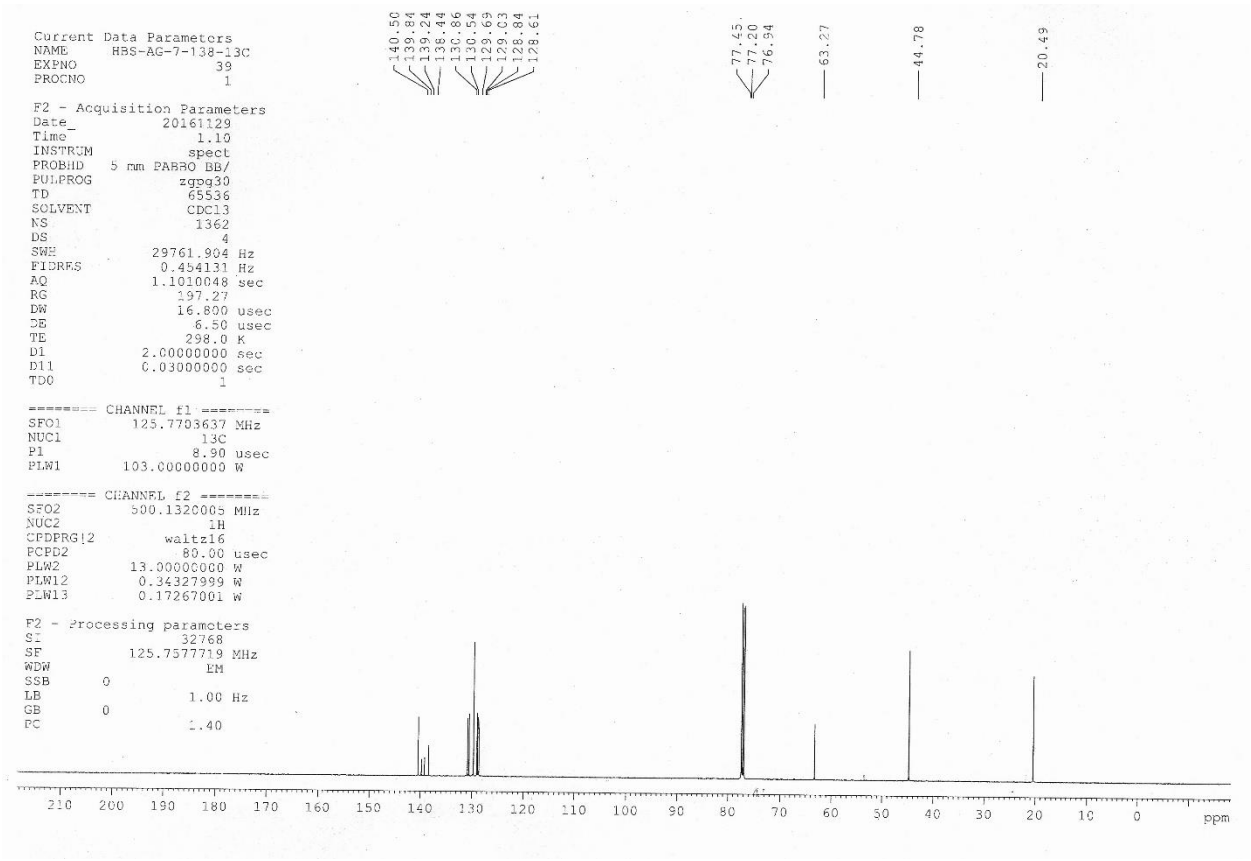


Fig. S12 ^{13}C NMR spectrum of **12**.

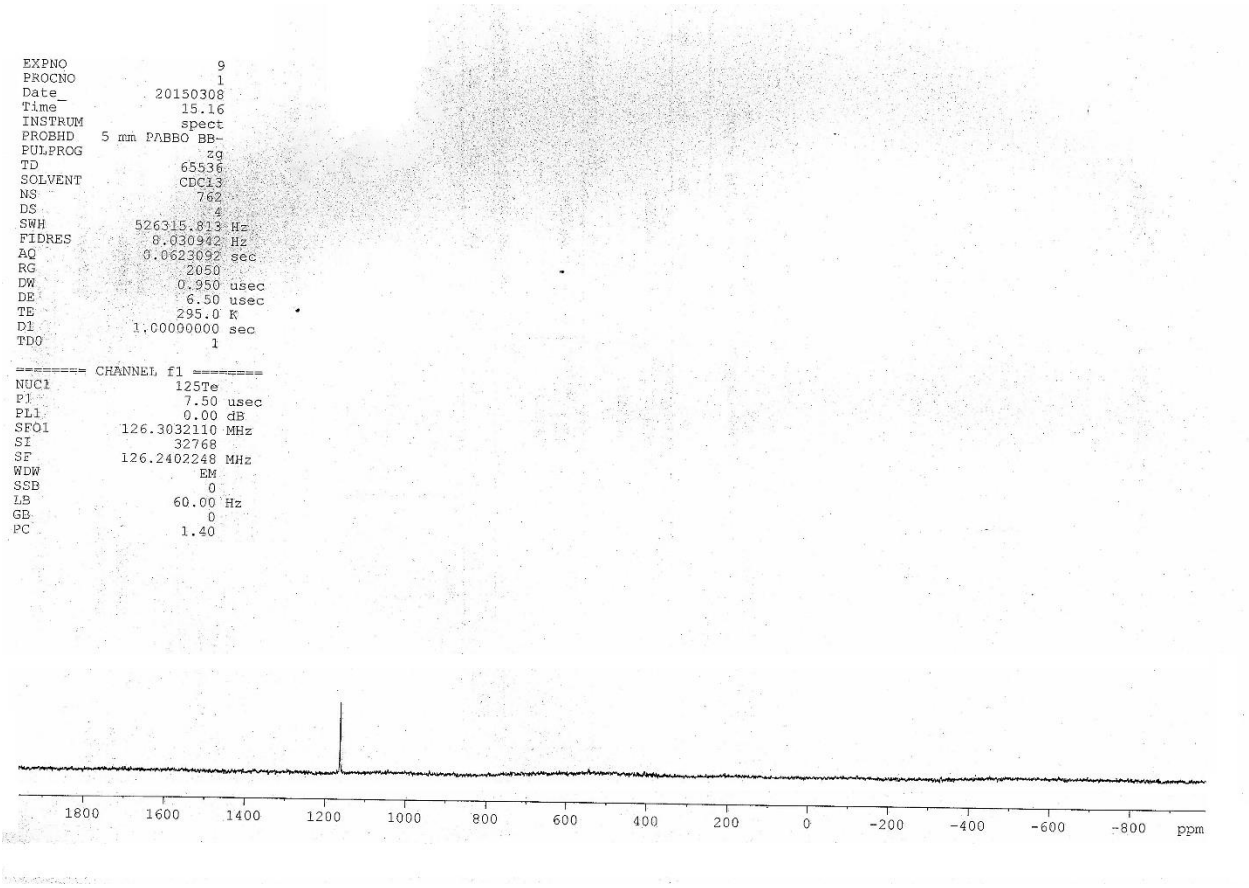


Fig. S13 ^{125}Te NMR spectrum of **12** (δ = 1167 ppm).

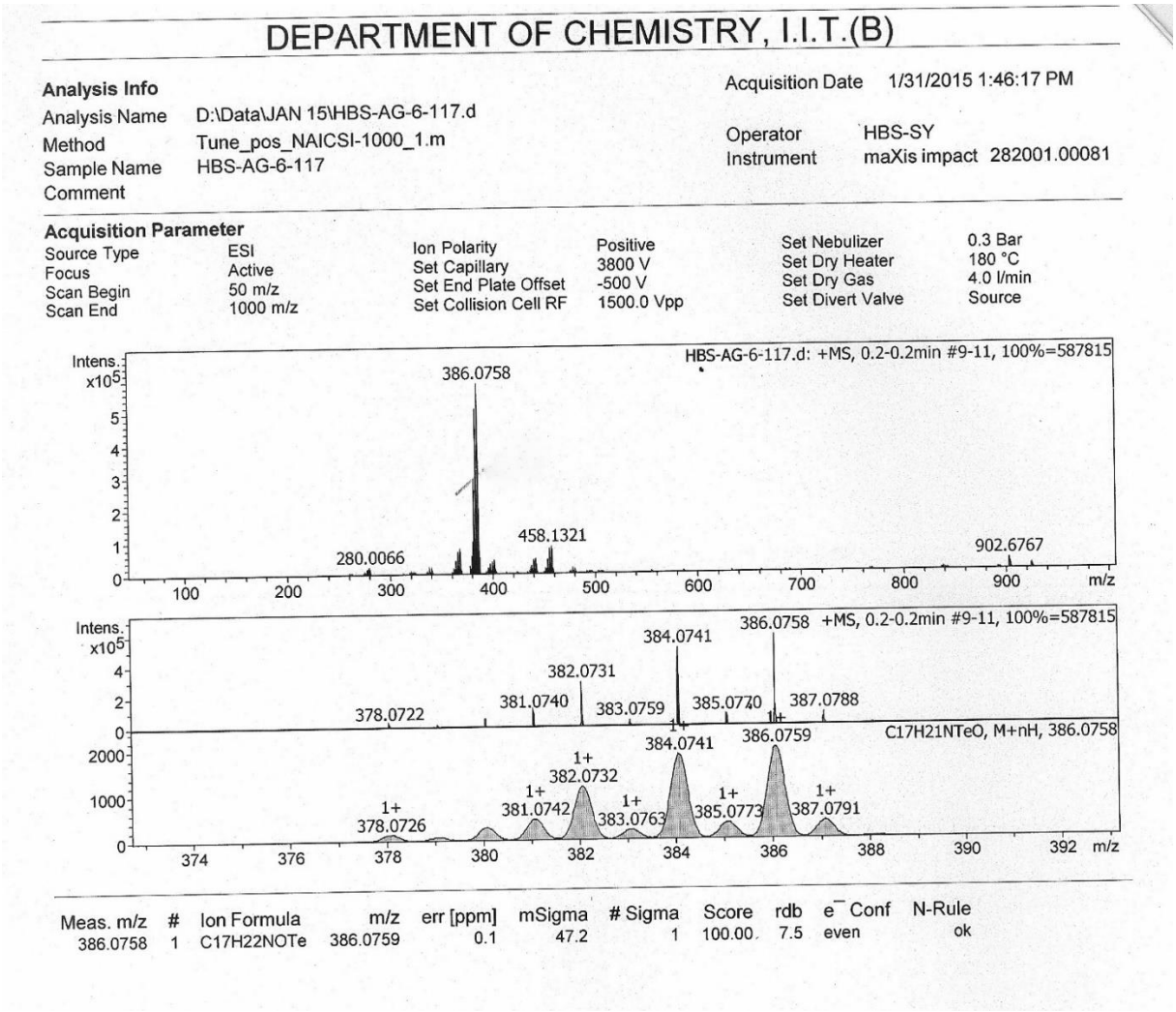


Fig. S14 HRMS of **12**.

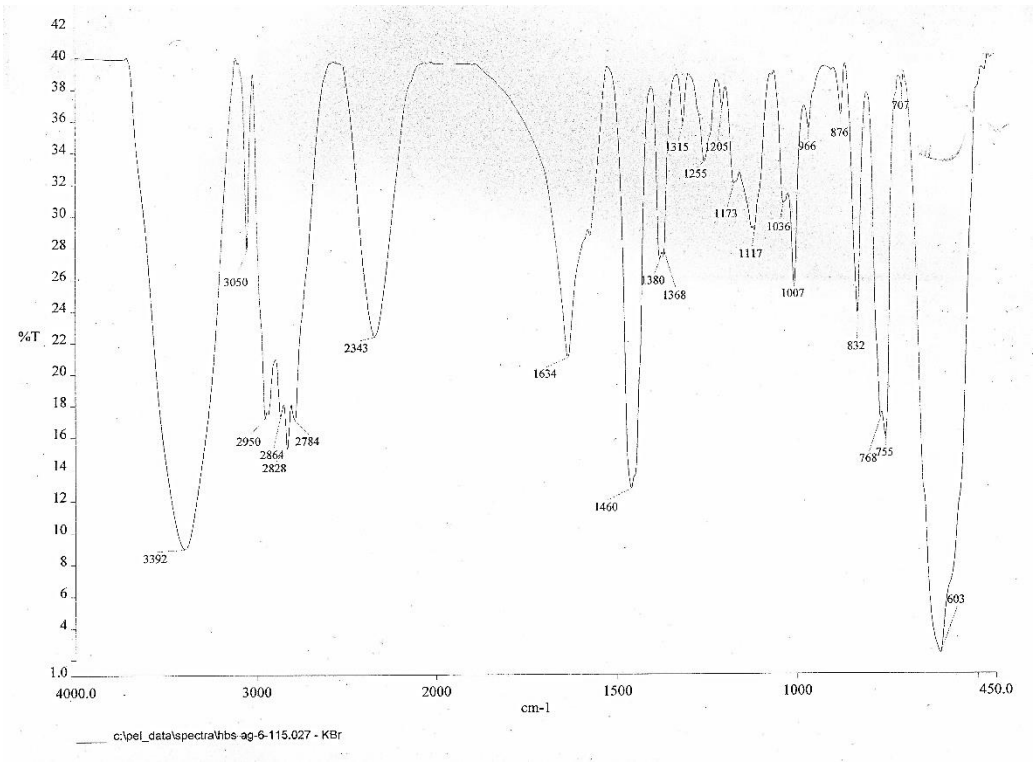


Fig. S15 FT-IR spectrum of **12**

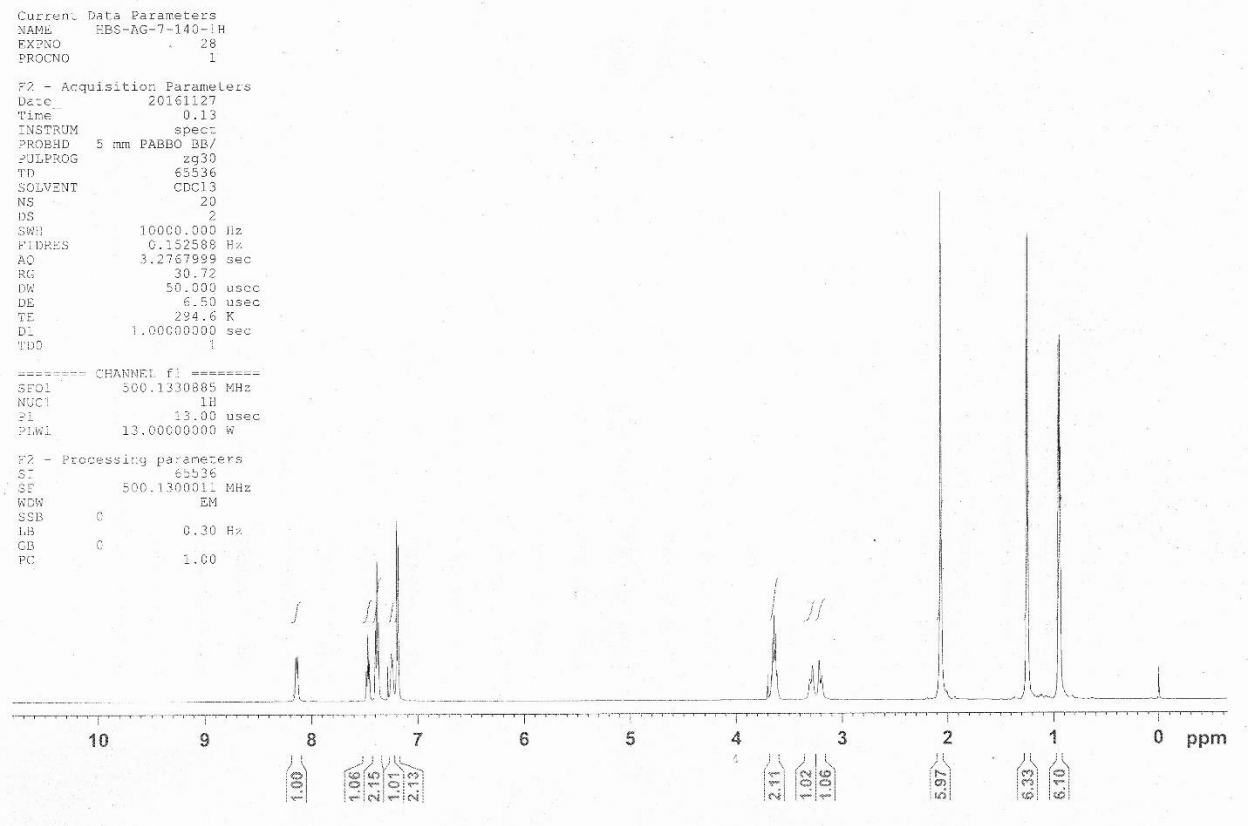


Fig. S16 ^{1}H NMR spectrum of **13**.

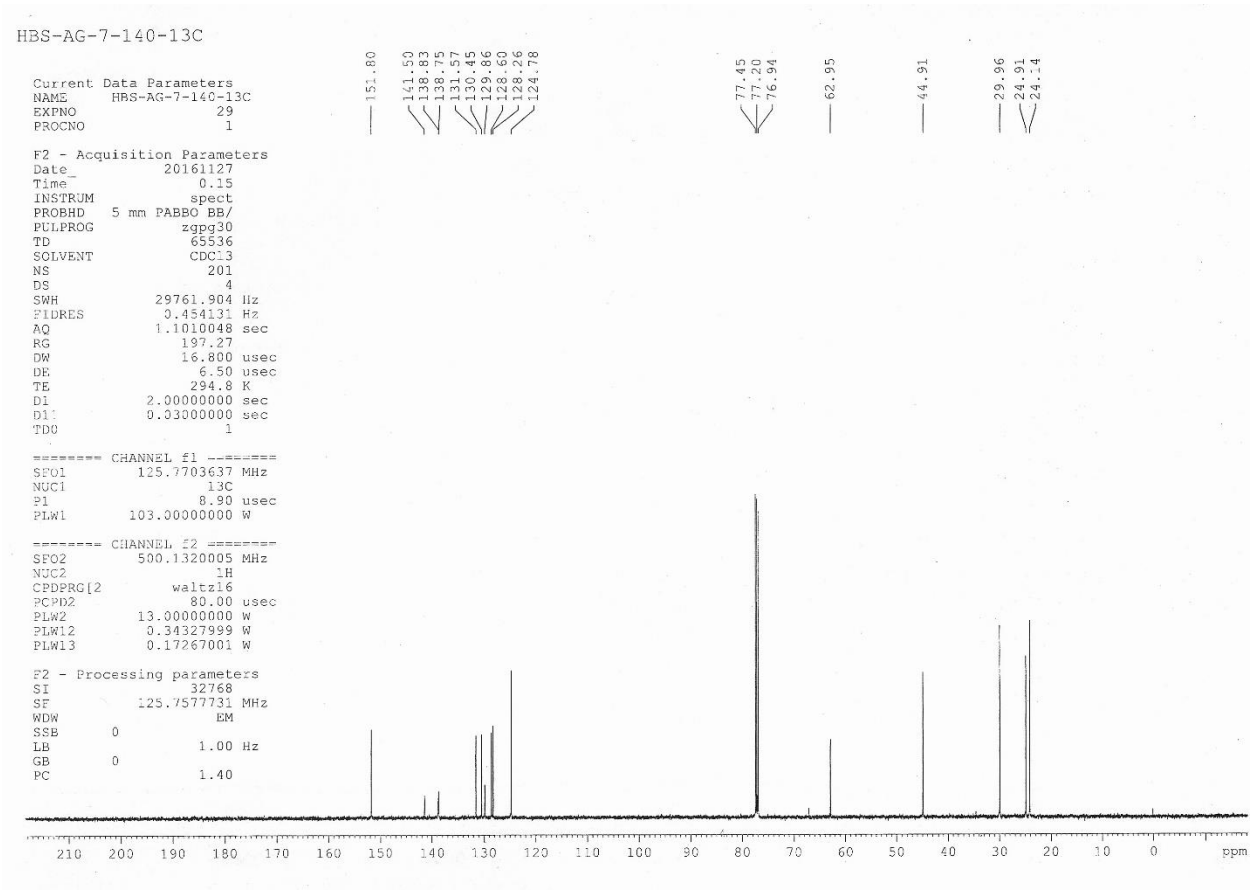


Fig. S17 ^{13}C NMR spectrum of **13**.

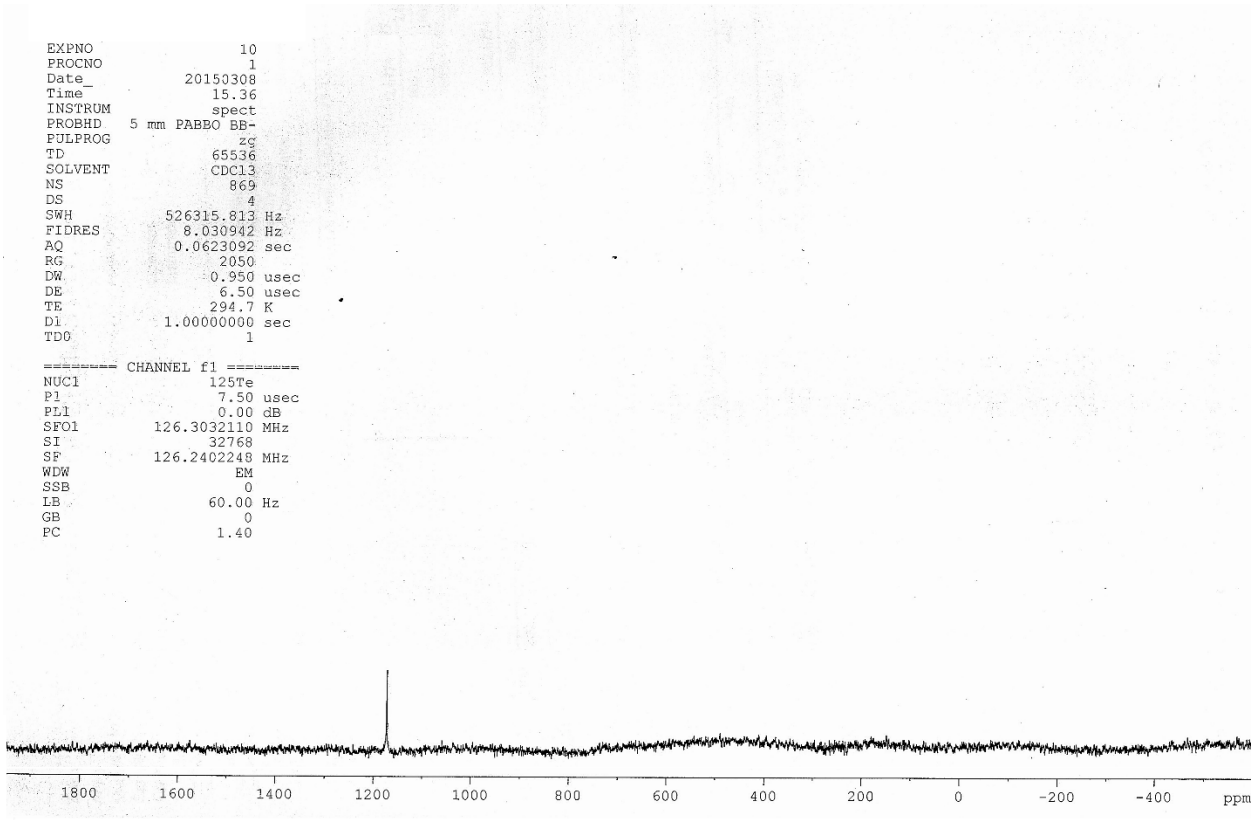


Fig. S18 ^{125}Te NMR spectrum of **13** (δ = 1172 ppm).

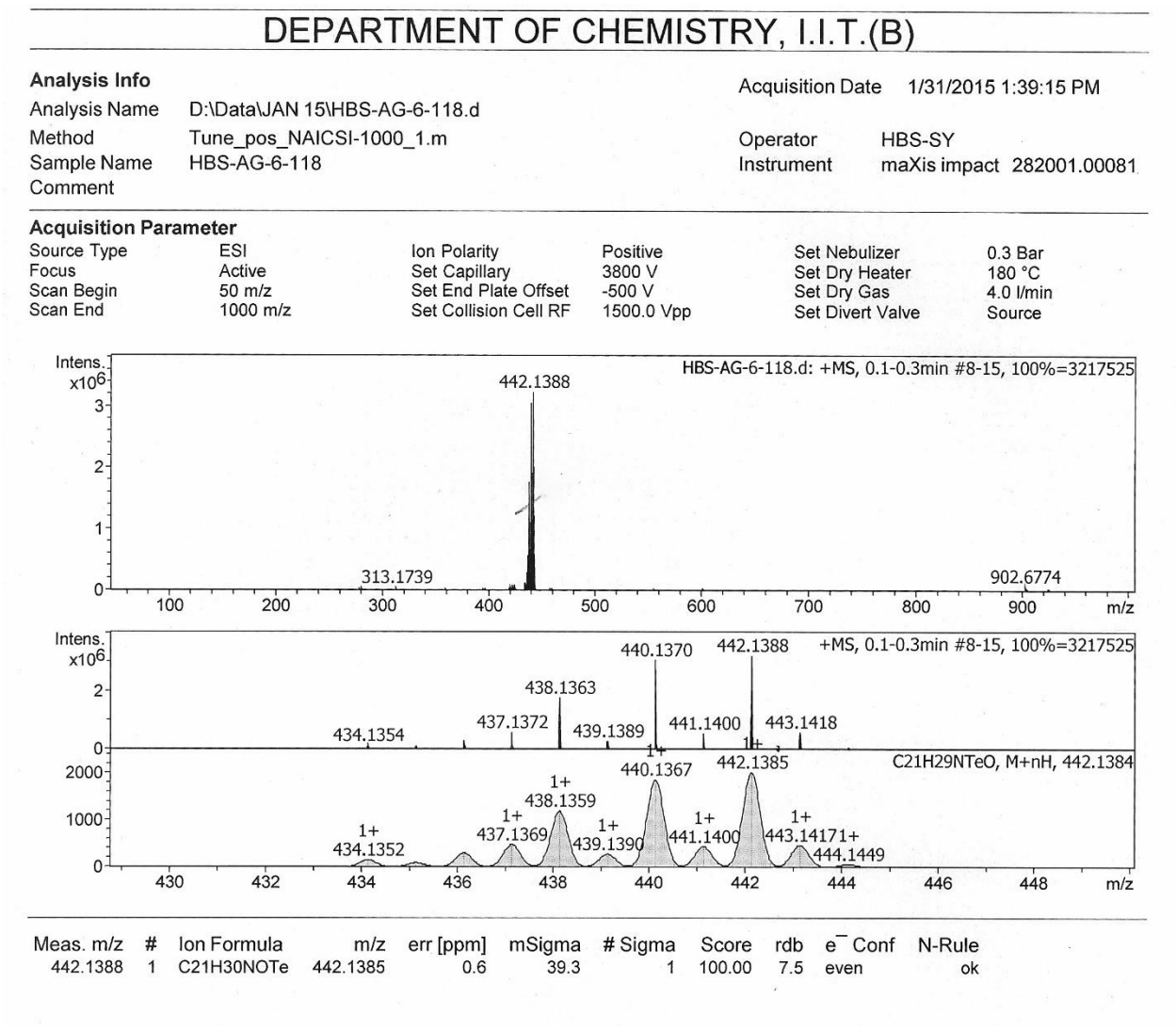


Fig. S19 HRMS of **13**.

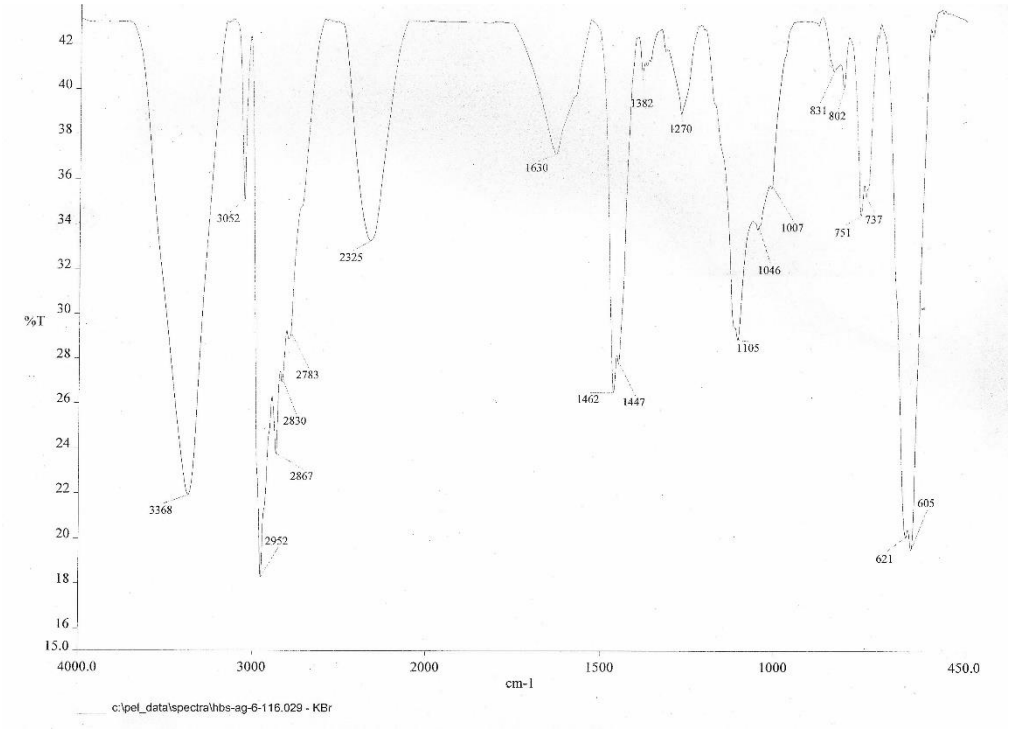


Fig. S20 FT-IR spectrum of **13**.

Table S1 Crystallographic Data and Refinement Details for **10-13**

Compound	**10**	**11**	**12**	**13**
Empirical formula	$C_{30}H_{38}N_2O_6Te_2$	$C_{32}H_{42}N_2O_6Te_2$	$C_{34}H_{46}N_2O_6Te_2$	$C_{46}H_{68}N_4O_6Te_2$
Formula weight	777.82	805.87	833.93	1028.24
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	C2/c	$P2_1/c$	P-1	P-1
a (Å)	28.210(3)	9.7975(6)	9.3292(2)	8.8868(2)
b (Å)	9.1255(3)	9.4758(3)	9.5482(2)	11.3262(4)
c (Å)	18.2830(19)	17.8984(7)	10.8122(2)	13.3415(4)
α (°)	90	90	103.832(2)	67.256(3)
β (°)	140.20(2)	104.004(5)	114.891(2)	72.991(2)
γ (°)	90	90	91.144(2)	77.596(2)
V ($Å^3$)	3012.7(10)	1612.29(13)	840.33(3)	1176.38(7)
Z	4	2	1	1
D(calcd) (Mg/m^3)	1.715	1.660	1.648	1.451
T (K)	100(2) K	100(2) K	100(2) K	100(2) K
Range of □(°)	2.501 to 31.153	2.142 to 31.174	2.430 to 31.193	2.105 to 31.134
Data Compl (25.5°)	98.5 %	99.8 %	99.8 %	99.9 %
Abs coeff (mm^{-1})	1.981	1.854	1.782	1.289
Indep. Ref (R_{int})	4374 (0.0275)	4793 (0.0810)	4956 (0.0394)	6840 (0.0624)
Final R_1	0.0268	0.0815	0.0357	0.0504
Final R_1 [I > 2□(I)]	0.0228	0.0579	0.0305	0.0390
wR_2 (all indices)	0.0537	0.1249	0.0706	0.0814
Data/Restr./Param.	4374 / 2 / 191	4793 / 0 / 197	4956 / 0 / 205	6840 / 21 / 282
Goodness of fit F^2	1.024	1.063	1.060	1.040
Largest diff. peak and hole ($e.Å^{-3}$)	0.554 and -0.903	1.430 and -1.158	1.290 and -0.673	0.937 and -1.085

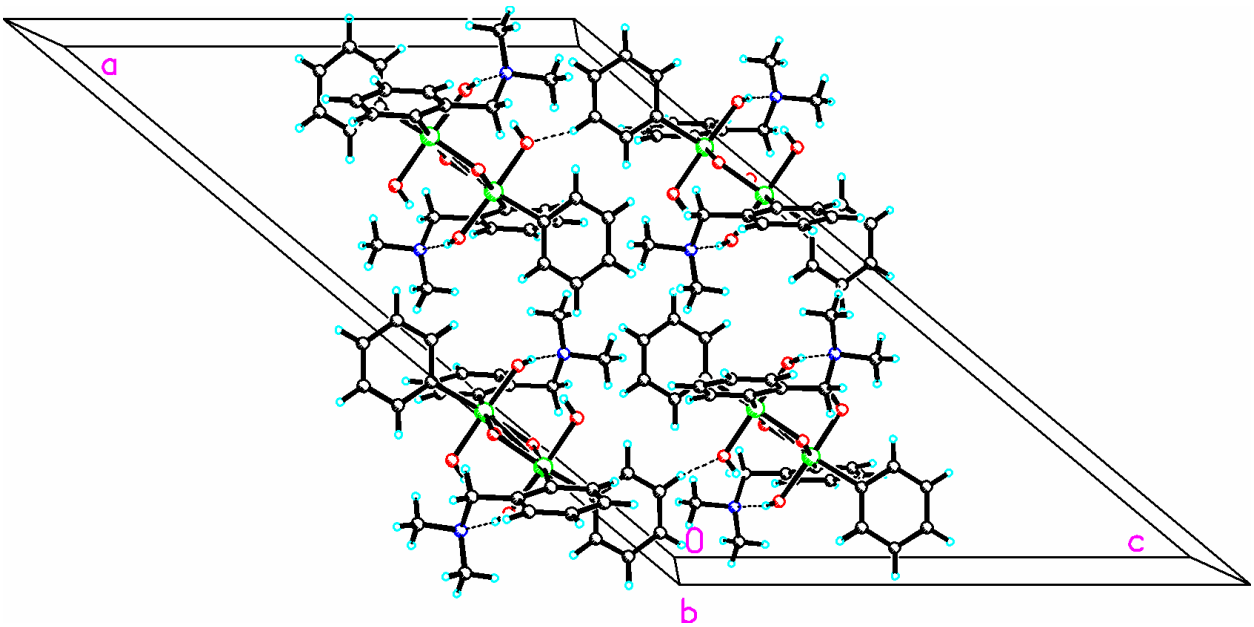


Fig. S21 Packing diagram of **10.**

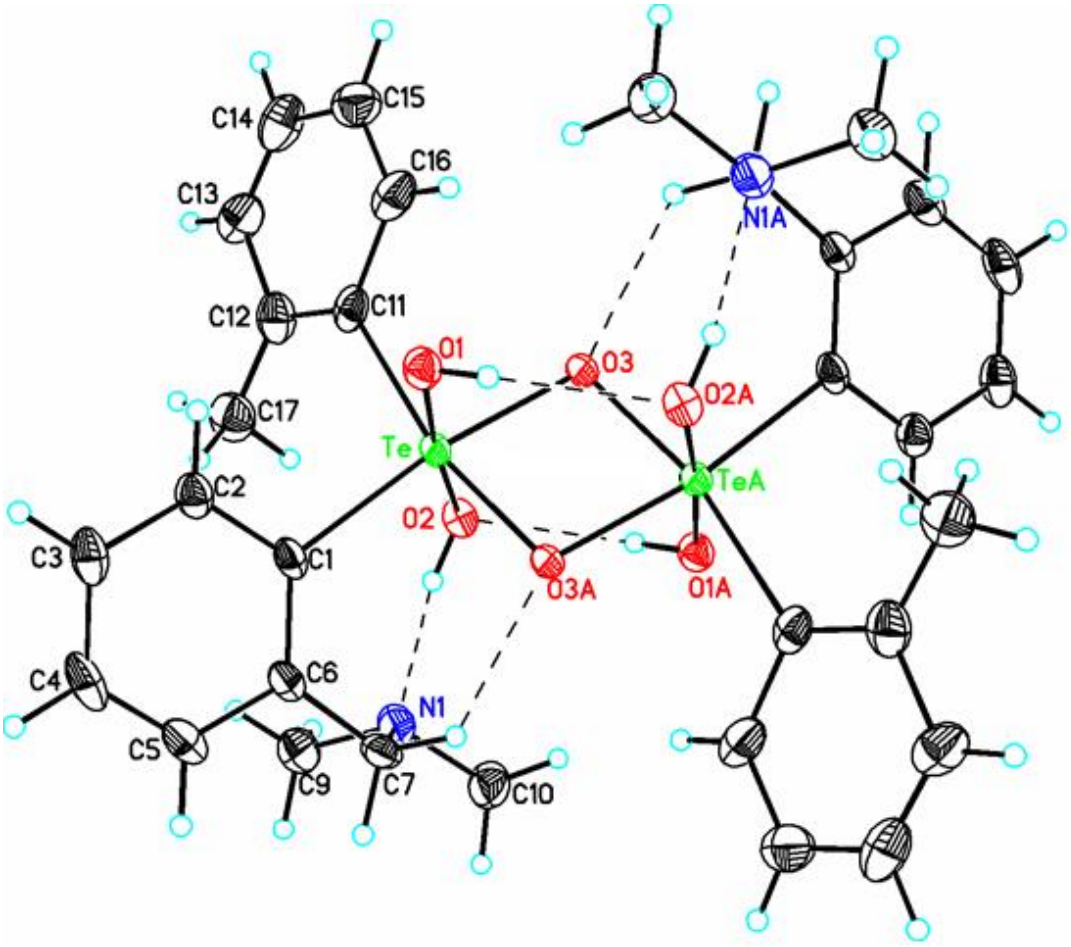


Fig. S22 Molecular structure of **11.**

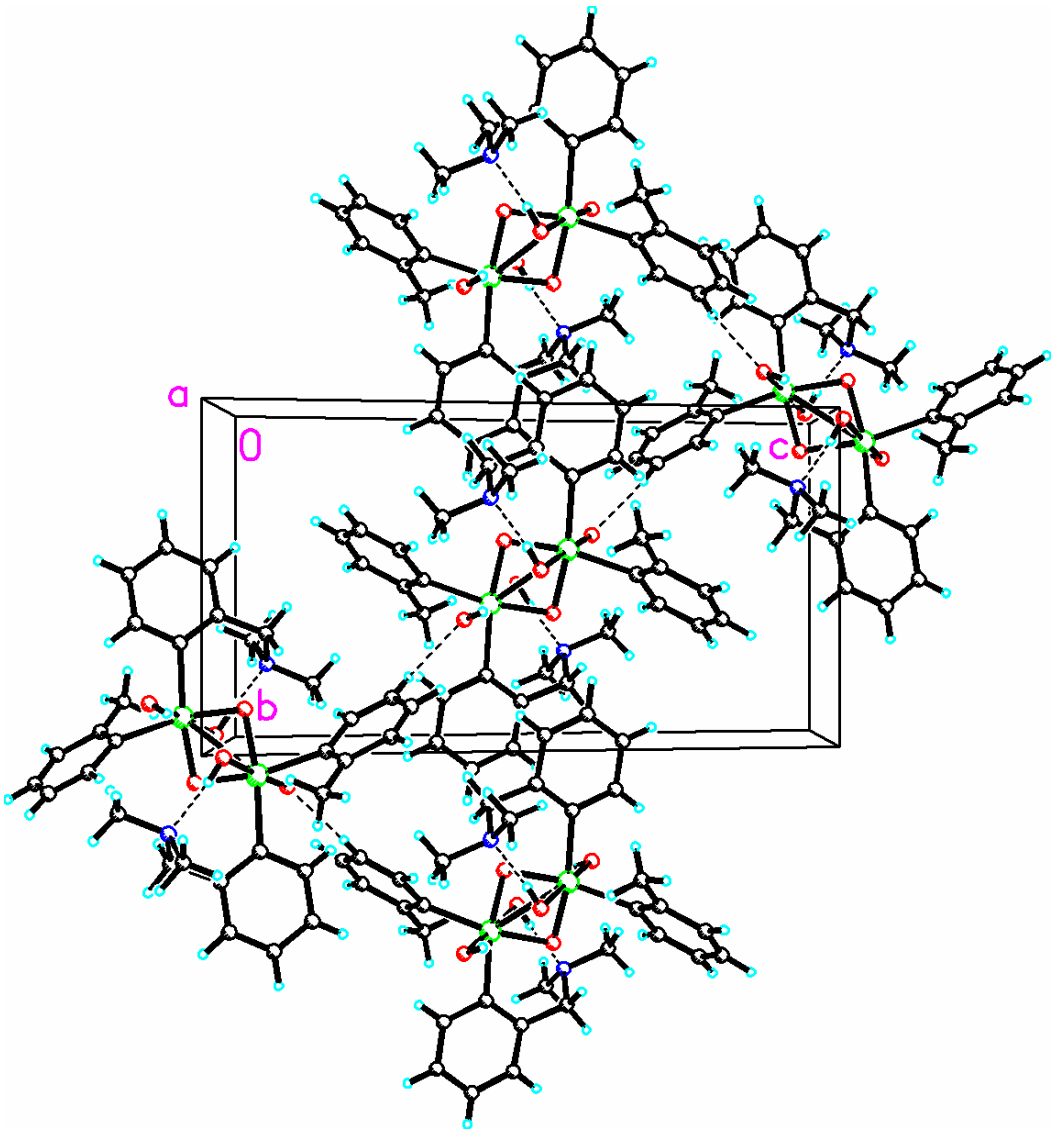


Fig. S23 Packing diagram of **11.**

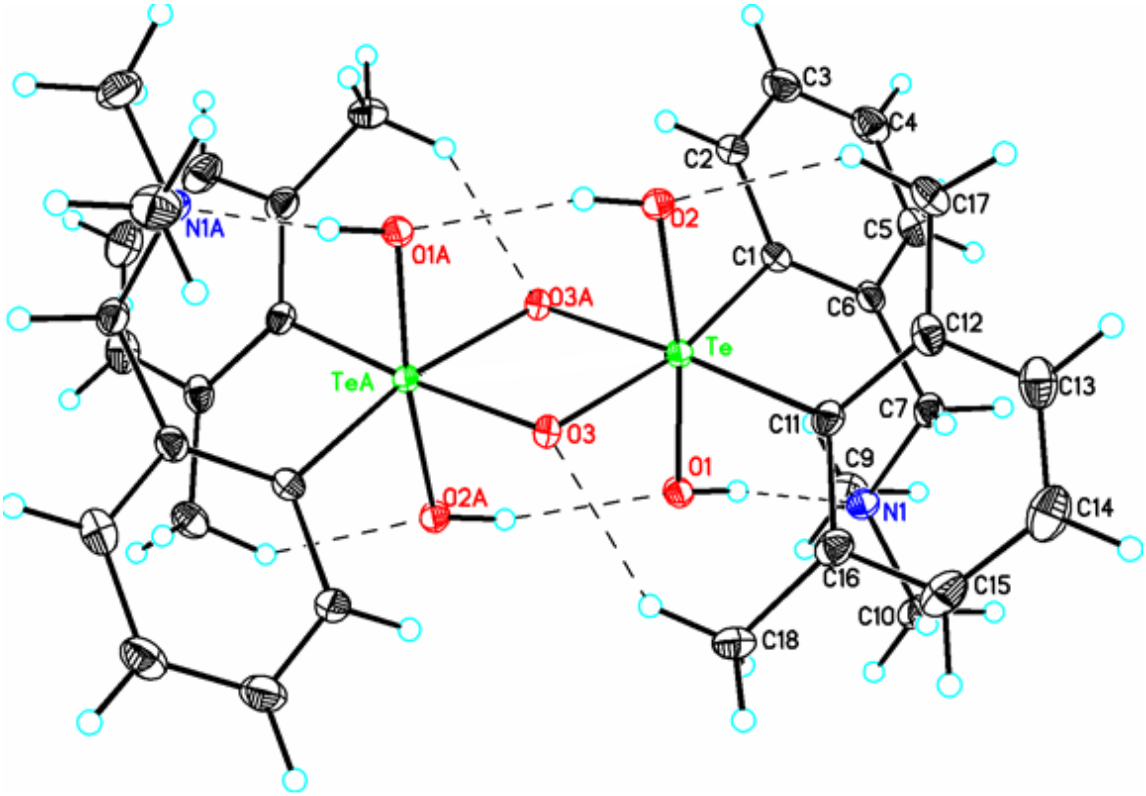


Fig. S24 Molecular structure of **12.**

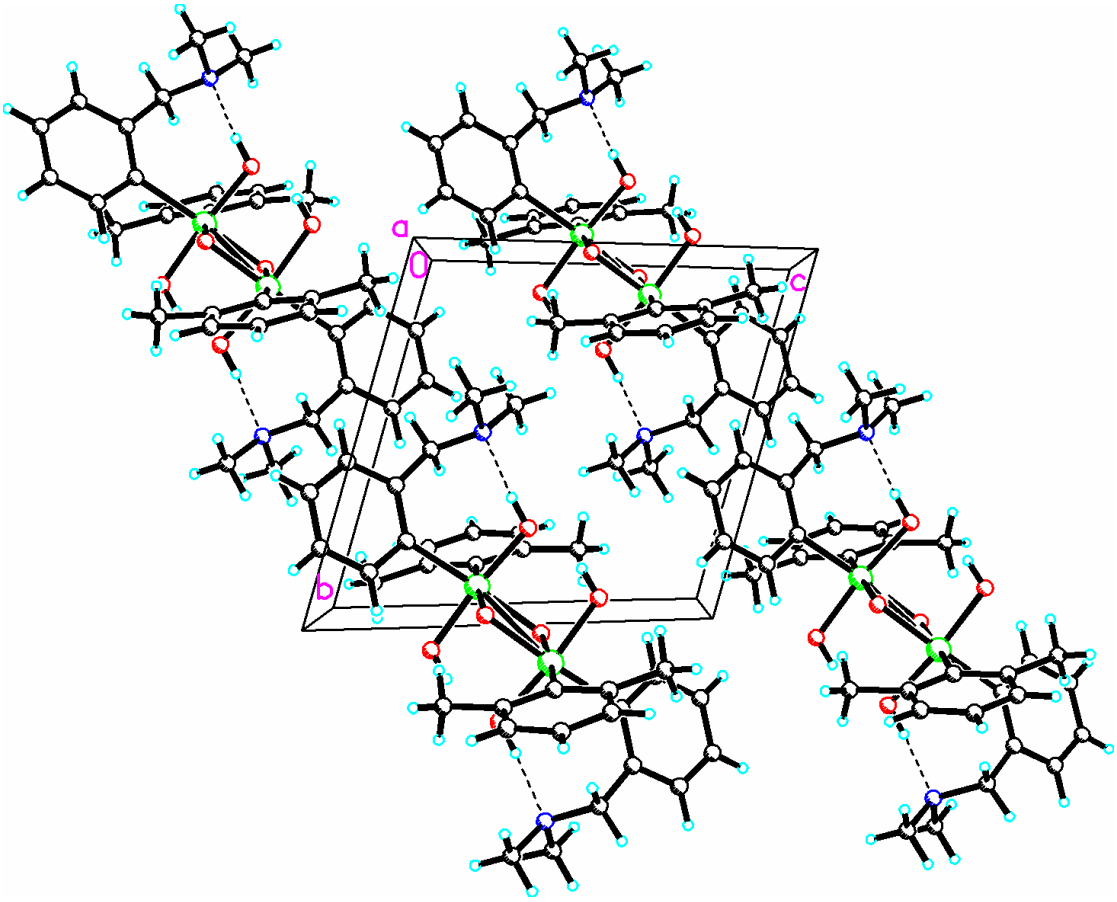


Fig. S25 Packing diagram of **12.**

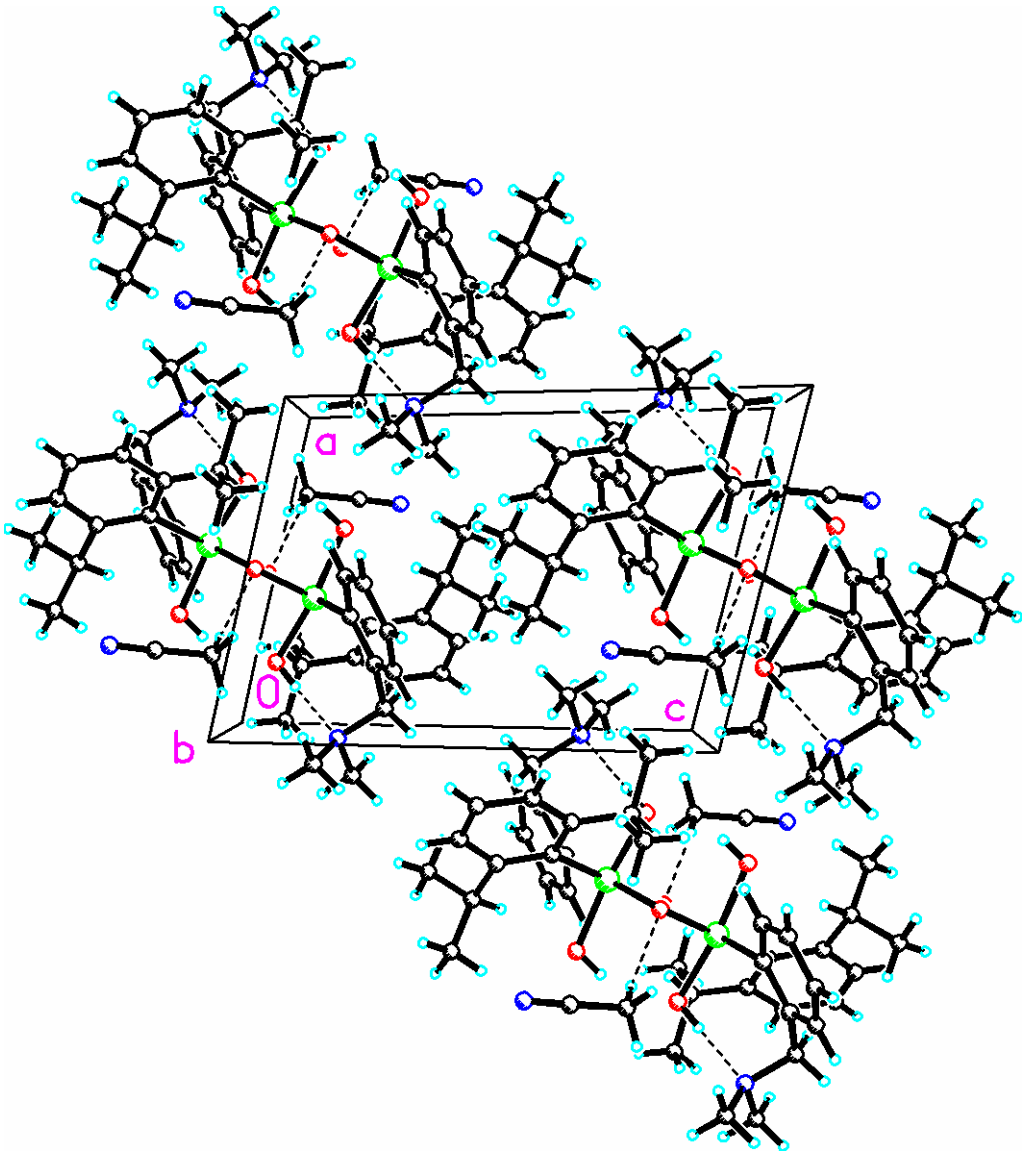


Fig. S26 Packing diagram of **13.**

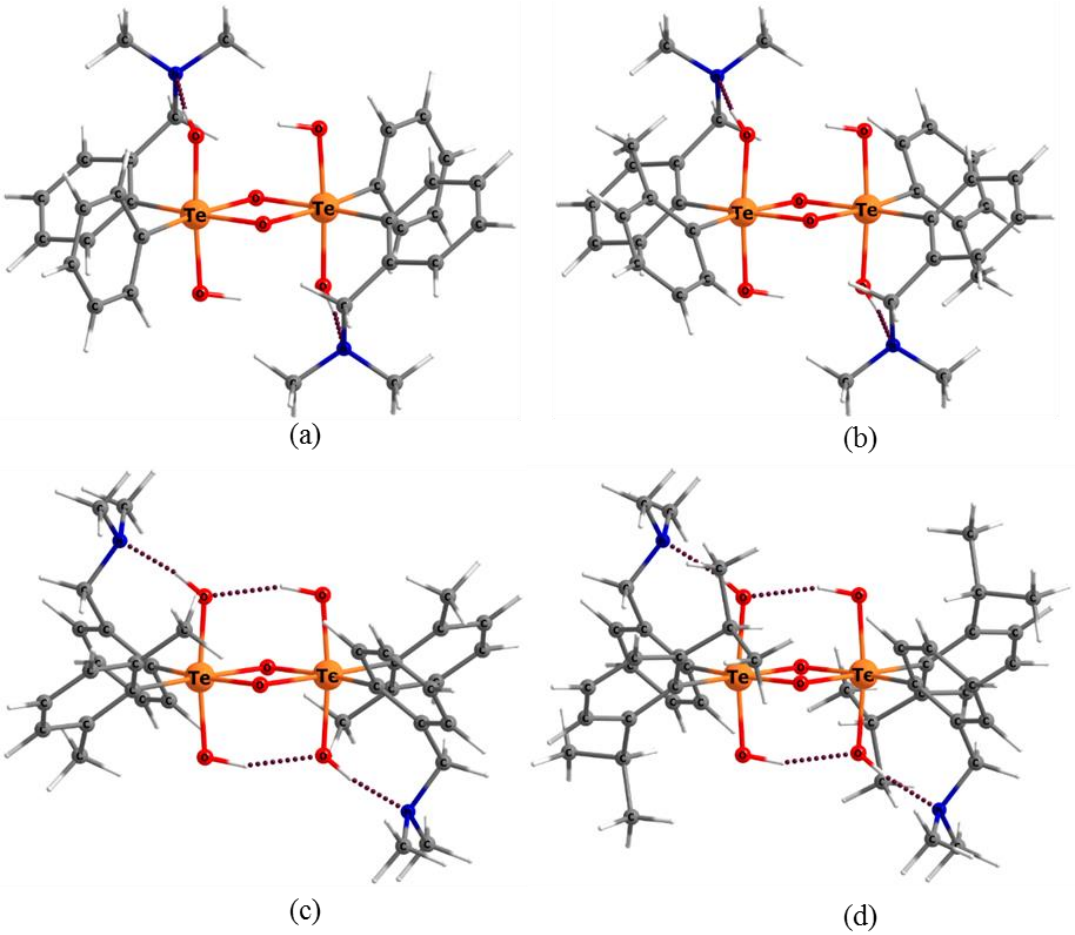


Fig. S27 Optimized geometries of **10-13.**

Table S2: Comparison of the metrical parameters of X-ray structure and optimised structure for **10**.

X-ray Structure		Optimized Structure
Bond length (Å)		
Te1-O1	1.970	1.968
Te1-O2	1.945	1.966
Te1-O3	1.966	1.988
Te1-O31	1.982	1.995
Te1-C1	2.143	2.165
Te1-C11	2.126	2.139
Bond Angle (°)		
O1-Te1-O2	176.68	175.75
O3-Te1-O31	78.49	79.05
C1-Te1-C11	97.82	97.42

Table S3: Comparison of the metrical parameters of X-ray structure and computed Structure for **11**.

X-ray Structure		Optimized Structure
Bond length (Å)		
Te1-O1	1.965	1.968
Te1-O2	1.949	1.968
Te1-O3	1.978	1.996
Te1-O31	1.980	1.991
Te1-C1	2.149	2.162
Te1-C11	2.155	2.155
Bond Angle (°)		
O1-Te1-O2	175.52	174.59
O3-Te1-O31	78.68	79.10
C1-Te1-C11	101.44	98.47

Table S4: Comparison of the metrical parameters of X-ray structure and computed Structure for **12**.

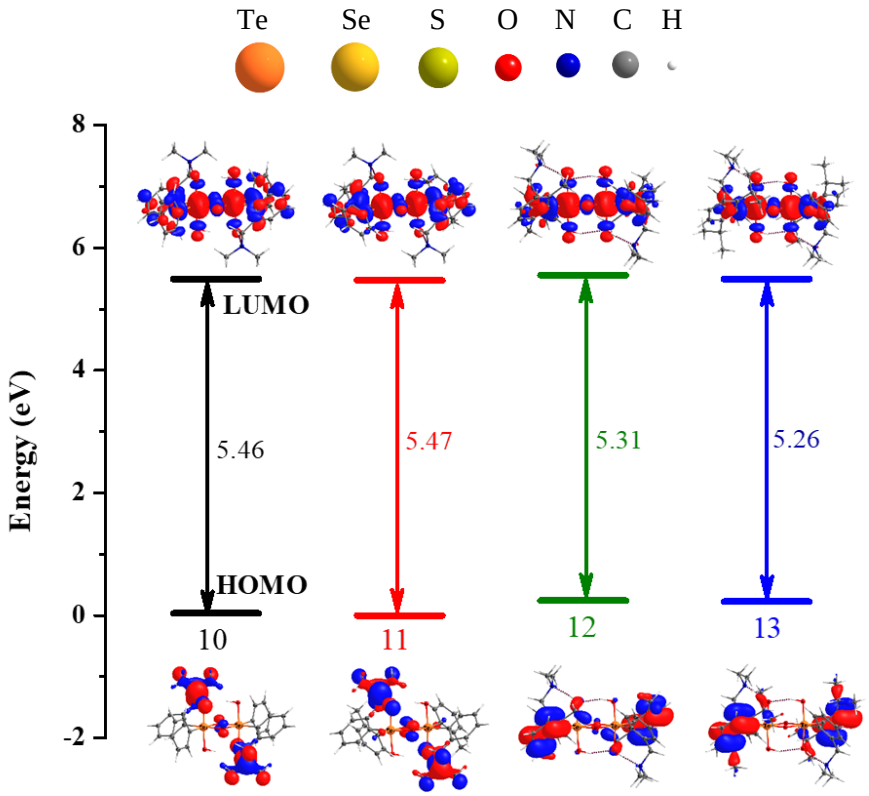
X-ray Structure		Optimized Structure
Bond length (Å)		
Te1-O1	1.963	1.965
Te1-O2	1.950	1.974
Te1-O3	2.000	2.018
Te1-O31	1.962	1.970
Te1-C1	2.163	2.183
Te1-C11	2.170	2.192
Bond Angle (°)		
O1-Te1-O2	175.56	172.87
O3-Te1-O31	77.85	78.54
C1-Te1-C11	101.74	99.97

Table S5: Comparison of the metrical parameters of X-ray structure and computed Structure for **13**

X-ray Structure		Optimized Structure
Bond length (Å)		
Te1-O1	1.954	1.964
Te1-O2	1.947	1.976
Te1-O3	1.992	2.014
Te1-O31	1.951	1.966
Te1-C1	2.158	2.175
Te1-C11	2.159	2.186
Bond Angle (°)		
O1-Te1-O2	173.12	173.06
O3-Te1-O31	78.08	78.79
C1-Te1-C11	100.44	100.68

Discussion on the Frontier molecular orbitals of telluronic acids 10-13

Frontier molecular orbital analysis on the four telluronic acids **10-13**, revealed that the HOMO-LUMO gaps remain almost similar for telluronic acids 1**0** and **11** (5.46 eV and 5.47 eV) and decrease to 5.31 eV (for 1**2**) and 5.26 eV (for **13**) as the substitutions on the aryl ring of R´ group increase from **11** to **13** (Fig. S28a).



(a)

Compounds	**10**	**11**	**12**	**13**
Relative HOMO energy (eV)	0.04	0.00	0.24	0.23
LUMO energy (eV)	5.49	5.47	5.55	5.49

(b)

Fig. S28. (a) Frontier molecular orbitals of telluronic acids **10-13** and their HOMO-LUMO energy gaps; (b) Relative HOMO energies of telluronic acids **10-13** and their corresponding LUMO energies.

Thus, the increase in induction effect of the R´ groups increases the HOMO energies in **12** and **13** and eventually leads to decrease in the HOMO-LUMO gap. The relative HOMO energies

of telluronic acids **10**-**13** are listed in Fig. S28b. The most stable HOMO is observed for telluronic acid **11** and subsequent HOMO-LUMO energies have been plotted by considering the HOMO level of **11** as zero energy. It is further observed that in the cases of telluronic acids **10** and **11**, where R´ = C_6H_5 and 2-MeC_6H_4 respectively, the HOMO, mainly consists of both nitrogen centered sp^3 hybridized orbitals. Interestingly, in telluronic acids **12** and **13**, the HOMO changes to π-bonding orbitals of the R´ aryl rings. It is worth mentioning that the LUMO remains the same in all four telluronic acids and consists of mainly Te-centered s-orbitals.

Cartesian Coordinates for 10-13

Compound 10

78

C30N2H38Te2O6

Te	-1.366306000	-0.701600000	0.002083000
O	-1.197529000	-0.926907000	1.949949000
H	-0.260723000	-0.709652000	2.133619000
O	-1.450950000	-0.358121000	-1.931779000
H	-1.225844000	-1.208420000	-2.424541000
O	0.569827000	-1.119987000	-0.163026000
N	-0.635362000	-2.607377000	-3.159954000
C	-1.929656000	-2.783589000	-0.185550000
C	-2.952869000	-3.164802000	0.684379000
H	-3.385498000	-2.436826000	1.363262000
C	-3.422012000	-4.476890000	0.710484000
H	-4.217049000	-4.752993000	1.397479000
C	-2.858232000	-5.423218000	-0.138236000
H	-3.207569000	-6.451991000	-0.127338000
C	-1.834774000	-5.045083000	-1.002687000
H	-1.387486000	-5.786717000	-1.661092000
C	-1.349545000	-3.730924000	-1.051071000
C	-0.218988000	-3.426619000	-2.009557000
H	0.560993000	-2.870327000	-1.481903000
H	0.216189000	-4.379073000	-2.358915000
C	-1.589010000	-3.296394000	-4.021331000
H	-1.911862000	-2.622118000	-4.819893000
H	-2.467377000	-3.591752000	-3.442687000
H	-1.156197000	-4.200763000	-4.483492000
C	0.531615000	-2.151363000	-3.911526000
H	0.202548000	-1.539933000	-4.756934000
H	1.131142000	-2.990646000	-4.302726000
H	1.157323000	-1.532269000	-3.264323000
C	-3.333718000	0.094178000	0.265411000
C	-3.837087000	0.314783000	1.549717000
H	-3.226684000	0.071053000	2.412557000
C	-5.120822000	0.839768000	1.702935000

H	-5.516429000	1.009340000	2.701071000
C	-5.892517000	1.145920000	0.582828000
H	-6.891404000	1.556076000	0.706163000
C	-5.380418000	0.928219000	-0.695531000
H	-5.977097000	1.172207000	-1.570607000
C	-4.099506000	0.400814000	-0.860573000
H	-3.682235000	0.240730000	-1.848812000
Te	1.366306000	0.701600000	-0.002083000
O	1.197529000	0.926907000	-1.949949000
H	0.260723000	0.709652000	-2.133619000
O	1.450950000	0.358121000	1.931779000
H	1.225844000	1.208420000	2.424541000
O	-0.569827000	1.119987000	0.163026000
N	0.635362000	2.607377000	3.159954000
C	1.929656000	2.783589000	0.185550000
C	2.952869000	3.164802000	-0.684379000
H	3.385498000	2.436826000	-1.363262000
C	3.422012000	4.476890000	-0.710484000
H	4.217049000	4.752993000	-1.397479000
C	2.858232000	5.423218000	0.138236000
H	3.207569000	6.451991000	0.127338000
C	1.834774000	5.045083000	1.002687000
H	1.387486000	5.786717000	1.661092000
C	1.349545000	3.730924000	1.051071000
C	0.218988000	3.426619000	2.009557000
H	-0.560993000	2.870327000	1.481903000
H	-0.216189000	4.379073000	2.358915000
C	1.589010000	3.296394000	4.021331000
H	1.911862000	2.622118000	4.819893000
H	2.467377000	3.591752000	3.442687000
H	1.156197000	4.200763000	4.483492000
C	-0.531615000	2.151363000	3.911526000
H	-0.202548000	1.539933000	4.756934000
H	-1.131142000	2.990646000	4.302726000
H	-1.157323000	1.532269000	3.264323000
C	3.333718000	-0.094178000	-0.265411000
C	3.837087000	-0.314783000	-1.549717000

H	3.226684000	-0.071053000	-2.412557000
C	5.120822000	-0.839768000	-1.702935000
H	5.516429000	-1.009340000	-2.701071000
C	5.892517000	-1.145920000	-0.582828000
H	6.891404000	-1.556076000	-0.706163000
C	5.380418000	-0.928219000	0.695531000
H	5.977097000	-1.172207000	1.570607000
C	4.099506000	-0.400814000	0.860573000
H	3.682235000	-0.240730000	1.848812000

Compound 11

84

C32N2H42Te2O6

Te	-0.673918000	0.759457000	-1.153837000
O	1.119750000	1.155803000	-1.860815000
H	1.719899000	0.945358000	-1.115814000
O	-2.393624000	0.210286000	-0.371100000
H	-2.845070000	1.000347000	0.055498000
O	-0.045208000	-1.069566000	-0.681969000
N	-3.420675000	2.306264000	0.980105000
C	-1.191910000	2.850619000	-1.339674000
C	-0.805949000	3.401628000	-2.563604000
H	-0.299776000	2.780988000	-3.297049000
C	-1.035545000	4.747036000	-2.846323000
H	-0.726717000	5.159426000	-3.802776000
C	-1.645064000	5.553606000	-1.890735000
H	-1.824184000	6.606315000	-2.091316000
C	-2.017262000	5.006597000	-0.665714000
H	-2.481295000	5.641471000	0.086086000
C	-1.805464000	3.654913000	-0.360426000
C	-2.220492000	3.158989000	1.008579000
H	-1.405950000	2.565141000	1.434630000
H	-2.387269000	4.030045000	1.666022000
C	-4.606564000	3.022701000	0.526211000
H	-5.447151000	2.326741000	0.452514000

H	-4.427036000	3.453839000	-0.461147000
H	-4.890329000	3.838404000	1.214134000
C	-3.644313000	1.682480000	2.281986000
H	-4.550763000	1.071689000	2.239616000
H	-3.763781000	2.423809000	3.089999000
H	-2.805267000	1.022963000	2.517730000
C	-1.255821000	0.111830000	-3.124828000
C	-2.530897000	0.292387000	-3.696573000
C	-2.736892000	-0.236299000	-4.979483000
H	-3.714181000	-0.106486000	-5.438907000
C	-1.740398000	-0.916448000	-5.672713000
H	-1.945305000	-1.312301000	-6.663928000
C	-0.487427000	-1.082738000	-5.091811000
H	0.303836000	-1.608224000	-5.619288000
C	-0.252110000	-0.564015000	-3.821225000
H	0.722480000	-0.668947000	-3.361263000
C	-3.673643000	1.010560000	-3.029584000
H	-3.431517000	2.062755000	-2.844660000
H	-3.902746000	0.552713000	-2.065020000
H	-4.563138000	0.979926000	-3.664534000
Te	0.673918000	-0.759457000	1.153837000
O	-1.119750000	-1.155803000	1.860815000
H	-1.719899000	-0.945358000	1.115814000
O	2.393624000	-0.210286000	0.371100000
H	2.845070000	-1.000347000	-0.055498000
O	0.045208000	1.069566000	0.681969000
N	3.420675000	-2.306264000	-0.980105000
C	1.191910000	-2.850619000	1.339674000
C	0.805949000	-3.401628000	2.563604000
H	0.299776000	-2.780988000	3.297049000
C	1.035545000	-4.747036000	2.846323000
H	0.726717000	-5.159426000	3.802776000
C	1.645064000	-5.553606000	1.890735000

H	1.824184000	-6.606315000	2.091316000
C	2.017262000	-5.006597000	0.665714000
H	2.481295000	-5.641471000	-0.086086000
C	1.805464000	-3.654913000	0.360426000
C	2.220492000	-3.158989000	-1.008579000
H	1.405950000	-2.565141000	-1.434630000
H	2.387269000	-4.030045000	-1.666022000
C	4.606564000	-3.022701000	-0.526211000
H	5.447151000	-2.326741000	-0.452514000
H	4.427036000	-3.453839000	0.461147000
H	4.890329000	-3.838404000	-1.214134000
C	3.644313000	-1.682480000	-2.281986000
H	4.550763000	-1.071689000	-2.239616000
H	3.763781000	-2.423809000	-3.089999000
H	2.805267000	-1.022963000	-2.517730000
C	1.255821000	-0.111830000	3.124828000
C	2.530897000	-0.292387000	3.696573000
C	2.736892000	0.236299000	4.979483000
H	3.714181000	0.106486000	5.438907000
C	1.740398000	0.916448000	5.672713000
H	1.945305000	1.312301000	6.663928000
C	0.487427000	1.082738000	5.091811000
H	-0.303836000	1.608224000	5.619288000
C	0.252110000	0.564015000	3.821225000
H	-0.722480000	0.668947000	3.361263000
C	3.673643000	-1.010560000	3.029584000
H	3.431517000	-2.062755000	2.844660000
H	3.902746000	-0.552713000	2.065020000
H	4.563138000	-0.979926000	3.664534000

Compound 12

90

C34N2H46Te2O6

Te	0.894879000	0.556587000	1.119687000

O	0.588035000	2.313272000	0.268410000
H	0.429497000	3.050102000	0.929339000
O	1.047992000	-1.277292000	1.805497000
H	0.580961000	-1.828028000	1.139463000
O	1.033777000	-0.147976000	-0.710156000
N	0.646396000	4.316020000	2.044601000
C	0.188111000	1.226395000	3.064446000
C	-0.628617000	0.287369000	3.697426000
H	-0.813428000	-0.660089000	3.204349000
C	-1.171681000	0.545468000	4.953783000
H	-1.803992000	-0.197770000	5.431653000
C	-0.888723000	1.748857000	5.593403000
H	-1.295158000	1.959660000	6.578773000
C	-0.074507000	2.684498000	4.962566000
H	0.153472000	3.623749000	5.462371000
C	0.470482000	2.453918000	3.690731000
C	1.335001000	3.539104000	3.086523000
H	1.688832000	4.203261000	3.894498000
H	2.225552000	3.099908000	2.623080000
C	-0.527812000	5.025457000	2.538589000
H	-1.234962000	4.319439000	2.978324000
H	-1.020306000	5.530404000	1.702876000
H	-0.268865000	5.783025000	3.298953000
C	1.577822000	5.227356000	1.386775000
H	2.405465000	4.657203000	0.956382000
H	1.990162000	5.979815000	2.080483000
H	1.063336000	5.751311000	0.576250000
C	3.044035000	0.894095000	1.331490000
C	3.684962000	0.552668000	2.546095000
C	5.051364000	0.840222000	2.680413000
H	5.544747000	0.579564000	3.613609000
C	5.775046000	1.432839000	1.657569000

H	6.832954000	1.647000000	1.785263000
C	5.138407000	1.731869000	0.461788000
H	5.703362000	2.171851000	-0.356272000
C	3.775870000	1.467866000	0.262869000
C	3.026365000	-0.103813000	3.736679000
H	3.793561000	-0.571885000	4.359943000
H	2.310924000	-0.870662000	3.439542000
H	2.502052000	0.625103000	4.363173000
C	3.223838000	1.780876000	-1.104904000
H	3.974847000	2.314975000	-1.693613000
H	2.313402000	2.379078000	-1.044546000
H	2.956011000	0.858465000	-1.626162000
Te	-0.894879000	-0.556587000	-1.119687000
O	-0.588035000	-2.313272000	-0.268410000
H	-0.429497000	-3.050102000	-0.929339000
O	-1.047992000	1.277292000	-1.805497000
H	-0.580961000	1.828028000	-1.139463000
O	-1.033777000	0.147976000	0.710156000
N	-0.646396000	-4.316020000	-2.044601000
C	-0.188111000	-1.226395000	-3.064446000
C	0.628617000	-0.287369000	-3.697426000
H	0.813428000	0.660089000	-3.204349000
C	1.171681000	-0.545468000	-4.953783000
H	1.803992000	0.197770000	-5.431653000
C	0.888723000	-1.748857000	-5.593403000
H	1.295158000	-1.959660000	-6.578773000
C	0.074507000	-2.684498000	-4.962566000
H	-0.153472000	-3.623749000	-5.462371000
C	-0.470482000	-2.453918000	-3.690731000
C	-1.335001000	-3.539104000	-3.086523000
H	-1.688832000	-4.203261000	-3.894498000
H	-2.225552000	-3.099908000	-2.623080000

C	0.527812000	-5.025457000	-2.538589000
H	1.234962000	-4.319439000	-2.978324000
H	1.020306000	-5.530404000	-1.702876000
H	0.268865000	-5.783025000	-3.298953000
C	-1.577822000	-5.227356000	-1.386775000
H	-2.405465000	-4.657203000	-0.956382000
H	-1.990162000	-5.979815000	-2.080483000
H	-1.063336000	-5.751311000	-0.576250000
C	-3.044035000	-0.894095000	-1.331490000
C	-3.684962000	-0.552668000	-2.546095000
C	-5.051364000	-0.840222000	-2.680413000
H	-5.544747000	-0.579564000	-3.613609000
C	-5.775046000	-1.432839000	-1.657569000
H	-6.832954000	-1.647000000	-1.785263000
C	-5.138407000	-1.731869000	-0.461788000
H	-5.703362000	-2.171851000	0.356272000
C	-3.775870000	-1.467866000	-0.262869000
C	-3.026365000	0.103813000	-3.736679000
H	-3.793561000	0.571885000	-4.359943000
H	-2.310924000	0.870662000	-3.439542000
H	-2.502052000	-0.625103000	-4.363173000
C	-3.223838000	-1.780876000	1.104904000
H	-3.974847000	-2.314975000	1.693613000
H	-2.313402000	-2.379078000	1.044546000
H	-2.956011000	-0.858465000	1.626162000

Compound 13

114

C42N2H62Te2O6

Te	1.532521000	0.013415000	0.183259000
O	1.609551000	-0.348755000	-1.755944000
H	2.278310000	0.217262000	-2.241981000
O	1.213454000	0.349962000	2.092295000

H	0.235294000	0.318326000	2.185463000
O	0.017254000	-1.244788000	0.207946000
N	3.693180000	0.865349000	-2.947835000
C	2.765228000	1.810466000	0.061032000
C	2.308350000	2.835183000	0.894402000
H	1.447970000	2.648223000	1.526224000
C	2.964786000	4.062125000	0.947947000
H	2.596074000	4.843118000	1.607236000
C	4.095240000	4.274335000	0.164295000
H	4.623907000	5.222797000	0.201405000
C	4.548793000	3.256908000	-0.667794000
H	5.433650000	3.417562000	-1.280031000
C	3.898434000	2.015226000	-0.746653000
C	4.468988000	0.992609000	-1.703385000
H	5.514598000	1.266794000	-1.928375000
H	4.493355000	0.001440000	-1.236719000
C	3.562623000	2.119327000	-3.681525000
H	2.941594000	1.951484000	-4.565882000
H	4.538810000	2.514567000	-4.012701000
H	3.076435000	2.871849000	-3.058033000
C	4.266176000	-0.176268000	-3.793644000
H	4.318001000	-1.115411000	-3.237041000
H	5.281885000	0.079856000	-4.141221000
H	3.629887000	-0.328344000	-4.670103000
C	3.082049000	-1.482399000	0.593453000
C	4.127873000	-1.170217000	1.498150000
C	5.207581000	-2.060222000	1.591347000
H	6.016984000	-1.833027000	2.278833000
C	5.258382000	-3.227002000	0.845407000
H	6.110105000	-3.897037000	0.931152000
C	4.194661000	-3.547789000	0.016766000
H	4.209122000	-4.488188000	-0.527108000

C	3.083587000	-2.704547000	-0.125047000
C	4.146658000	0.006701000	2.469988000
H	3.359880000	0.709255000	2.206955000
C	3.808977000	-0.491906000	3.883392000
H	3.797192000	0.347694000	4.587440000
H	4.545567000	-1.221789000	4.238530000
H	2.820821000	-0.957600000	3.895111000
C	5.467313000	0.786922000	2.457822000
H	5.719337000	1.136592000	1.452324000
H	6.309764000	0.195682000	2.832563000
H	5.379069000	1.666736000	3.103759000
C	1.933139000	-3.257873000	-0.963296000
H	1.166643000	-2.494395000	-1.058857000
C	1.289999000	-4.441434000	-0.223759000
H	0.922672000	-4.128299000	0.757334000
H	1.994332000	-5.268872000	-0.079016000
H	0.436748000	-4.824321000	-0.794379000
C	2.356994000	-3.647974000	-2.382854000
H	2.731640000	-2.777022000	-2.926378000
H	1.493251000	-4.034869000	-2.935010000
H	3.128034000	-4.426339000	-2.401115000
Te	-1.532520000	-0.013436000	-0.183246000
O	-1.609551000	0.348723000	1.755951000
H	-2.278362000	-0.217266000	2.241961000
O	-1.213445000	-0.349978000	-2.092285000
H	-0.235294000	-0.318154000	-2.185484000
O	-0.017252000	1.244764000	-0.207936000
N	-3.693250000	-0.865241000	2.947832000
C	-2.765242000	-1.810474000	-0.061002000
C	-2.308361000	-2.835216000	-0.894338000
H	-1.447972000	-2.648279000	-1.526155000
C	-2.964807000	-4.062154000	-0.947861000

H	-2.596094000	-4.843167000	-1.607125000
C	-4.095274000	-4.274333000	-0.164219000
H	-4.623950000	-5.222791000	-0.201312000
C	-4.548829000	-3.256880000	0.667838000
H	-5.433697000	-3.417510000	1.280065000
C	-3.898458000	-2.015203000	0.746677000
C	-4.469026000	-0.992552000	1.703365000
H	-5.514639000	-1.266734000	1.928347000
H	-4.493391000	-0.001400000	1.236665000
C	-3.562672000	-2.119200000	3.681552000
H	-2.941675000	-1.951319000	4.565924000
H	-4.538855000	-2.514467000	4.012706000
H	-3.076440000	-2.871718000	3.058089000
C	-4.266308000	0.176371000	3.793607000
H	-4.318154000	1.115499000	3.236981000
H	-5.282017000	-0.079784000	4.141161000
H	-3.630048000	0.328489000	4.670079000
C	-3.082042000	1.482376000	-0.593452000
C	-4.127876000	1.170183000	-1.498134000
C	-5.207576000	2.060197000	-1.591338000
H	-6.016985000	1.832998000	-2.278815000
C	-5.258356000	3.226994000	-0.845424000
H	-6.110072000	3.897037000	-0.931178000
C	-4.194621000	3.547792000	-0.016804000
H	-4.209063000	4.488209000	0.527038000
C	-3.083558000	2.704537000	0.125023000
C	-4.146664000	-0.006747000	-2.469956000
H	-3.359889000	-0.709300000	-2.206910000
C	-3.808970000	0.491842000	-3.883365000
H	-3.797191000	-0.347766000	-4.587404000
H	-4.545551000	1.221729000	-4.238512000
H	-2.820808000	0.957524000	-3.895086000

C	-5.467320000	-0.786968000	-2.457788000
H	-5.719352000	-1.136623000	-1.452287000
H	-6.309768000	-0.195737000	-2.832547000
H	-5.379068000	-1.666793000	-3.103709000
C	-1.933069000	3.257874000	0.963210000
H	-1.166602000	2.494369000	1.058797000
C	-1.289905000	4.441362000	0.223575000
H	-0.922629000	4.128151000	-0.757512000
H	-1.994211000	5.268820000	0.078808000
H	-0.436616000	4.824248000	0.794139000
C	-2.356856000	3.648082000	2.382759000
H	-2.731538000	2.777187000	2.926350000
H	-1.493071000	4.034956000	2.934864000
H	-3.127846000	4.426497000	2.401004000