Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information for

"Reaction of ketone hydrazones with $TeCl_4$: Isolation and reaction of divinyl telluride"

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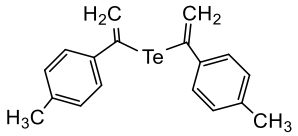
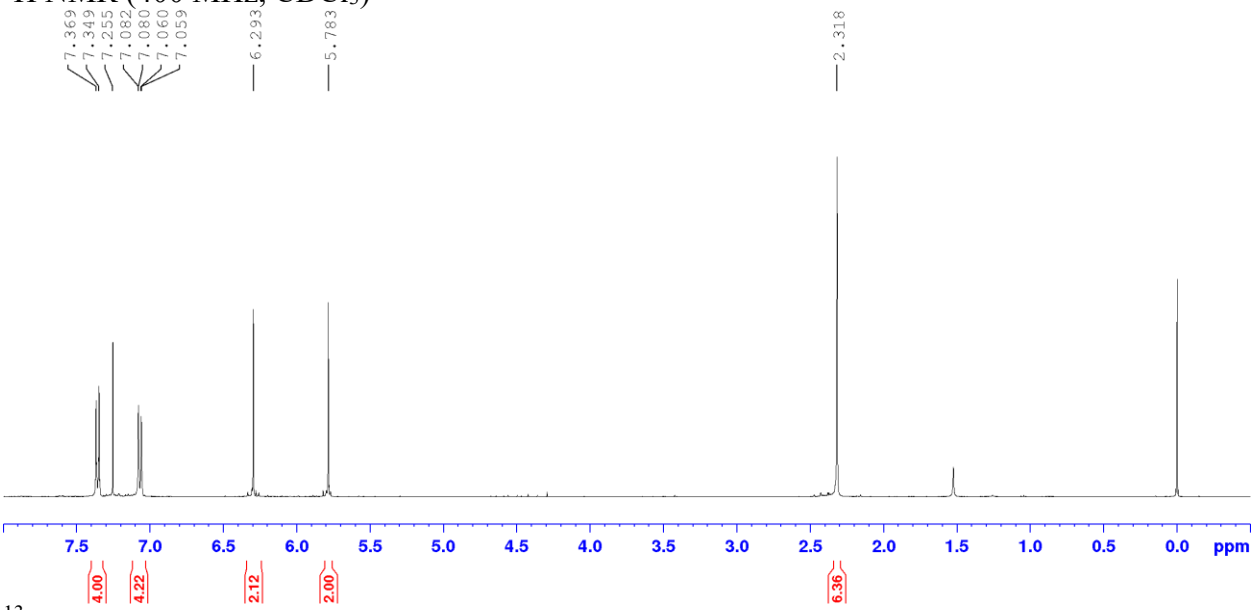
^{1}H- and ^{13}C-NMR Spectra of Products

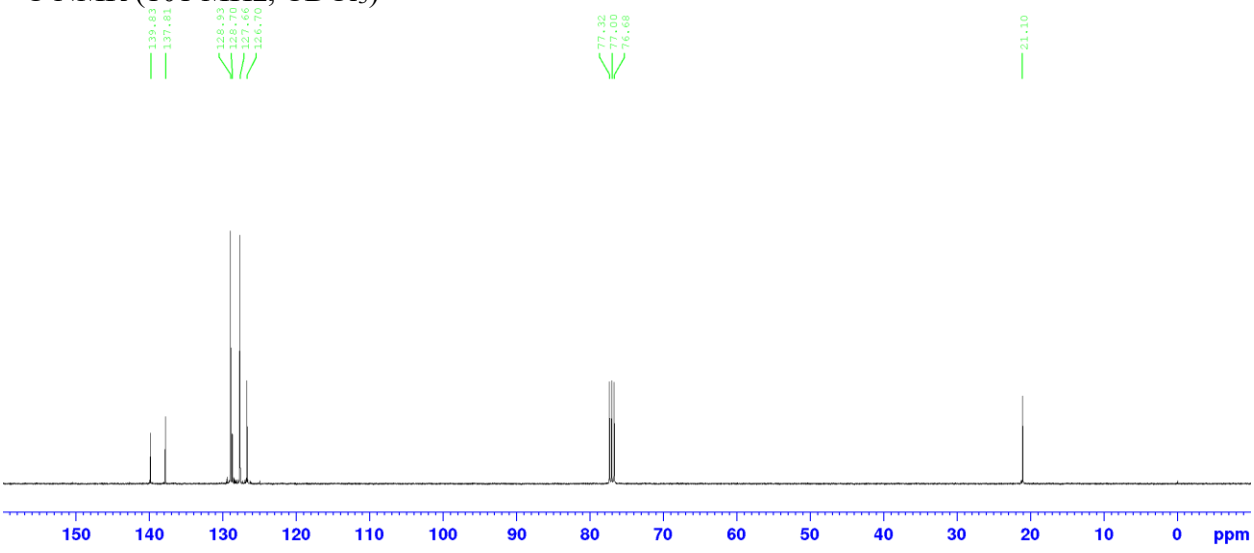
Bis-1-(*p*-tolyl)vinyl telluride **3a**:



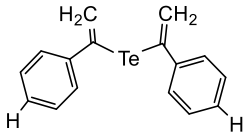
^{1}H NMR (400 MHz, $CDCl_3$)



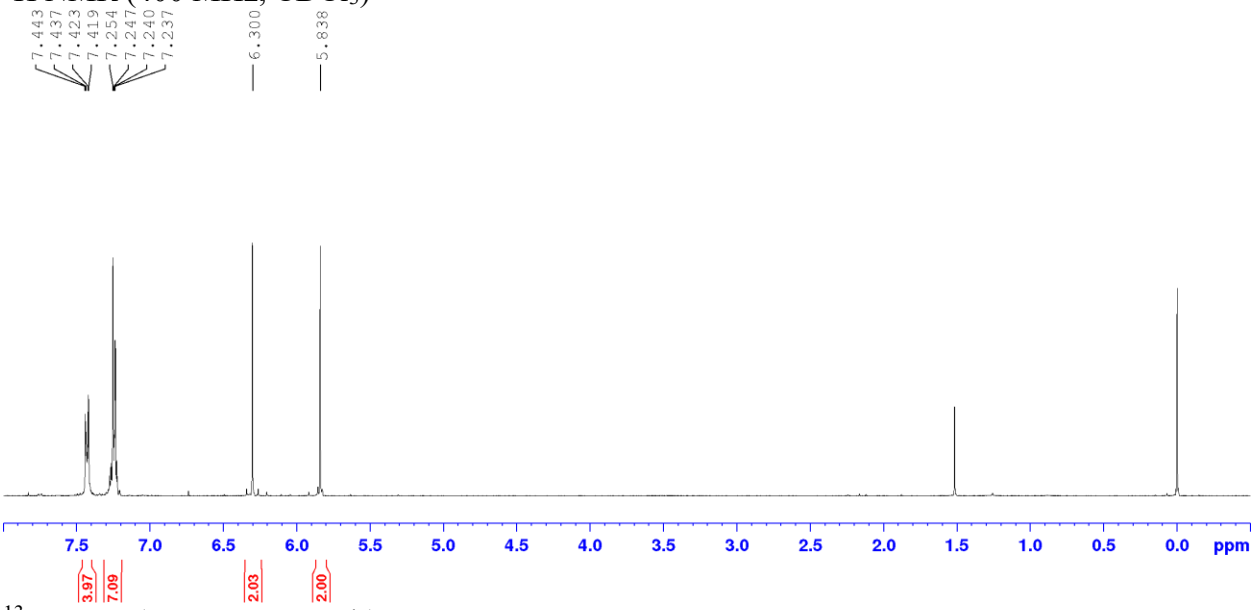
^{13}C NMR (101 MHz, $CDCl_3$)



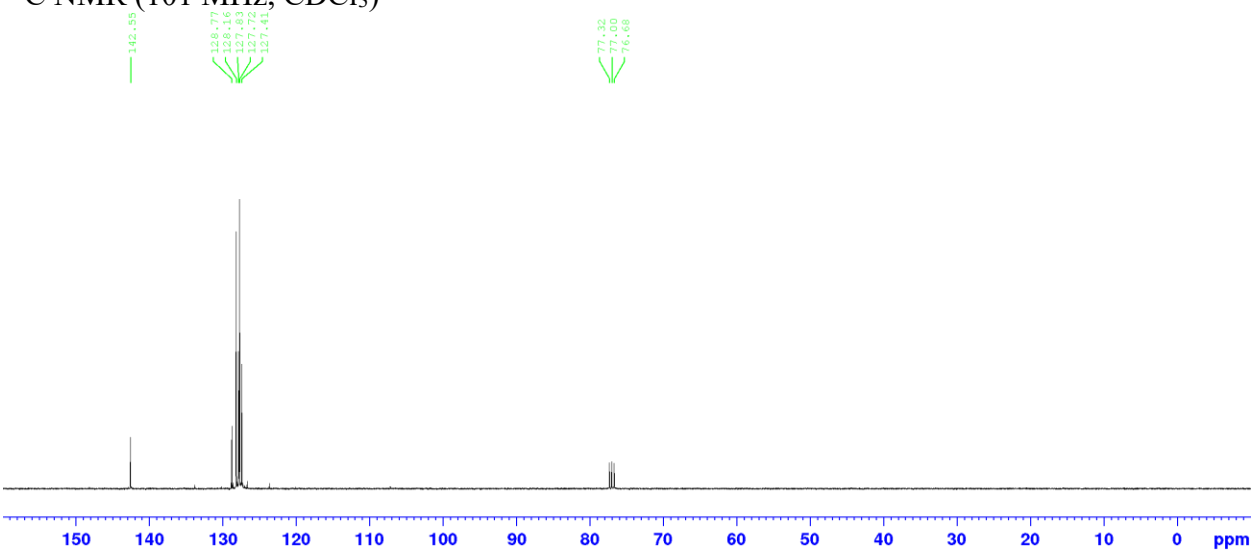
Bis-1-(phenyl)vinyl telluride **3b**:



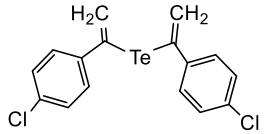
^{1}H NMR (400 MHz, $CDCl_3$)



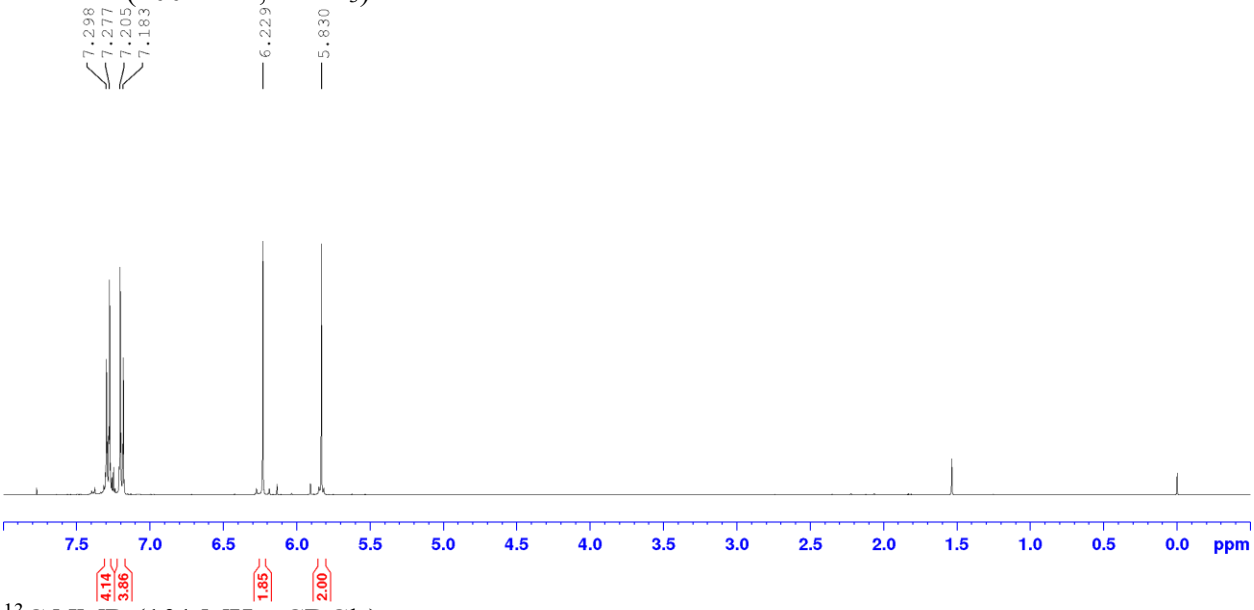
^{13}C NMR (101 MHz, $CDCl_3$)



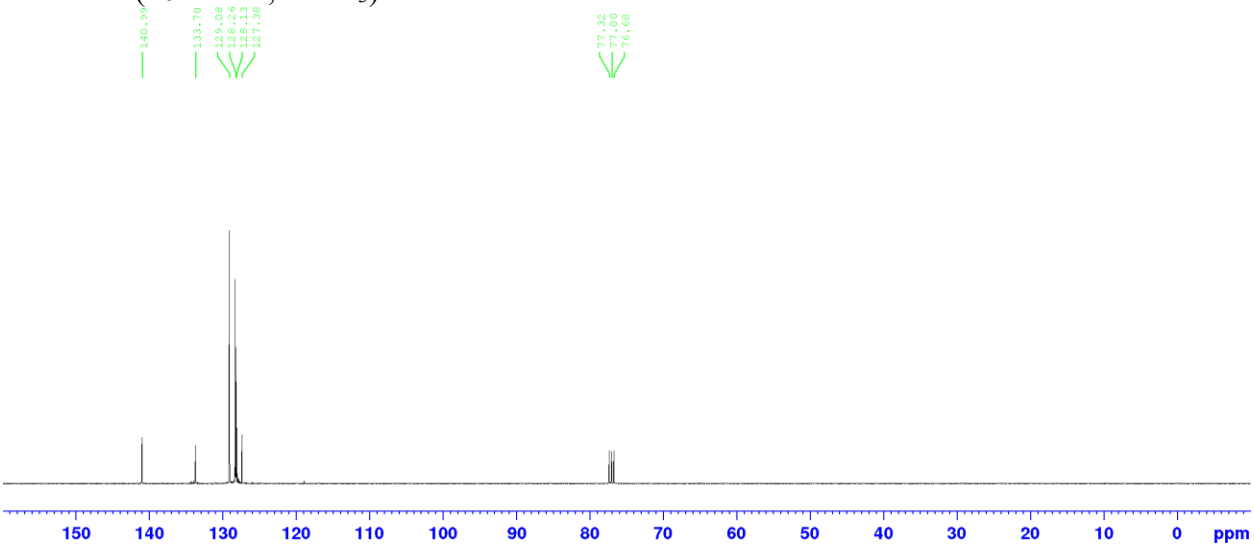
Bis-1-(*p*-chlorophenyl)vinyl telluride **3c**:



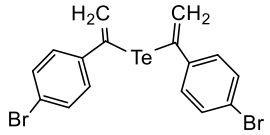
^{1}H NMR (400 MHz, $CDCl_3$)



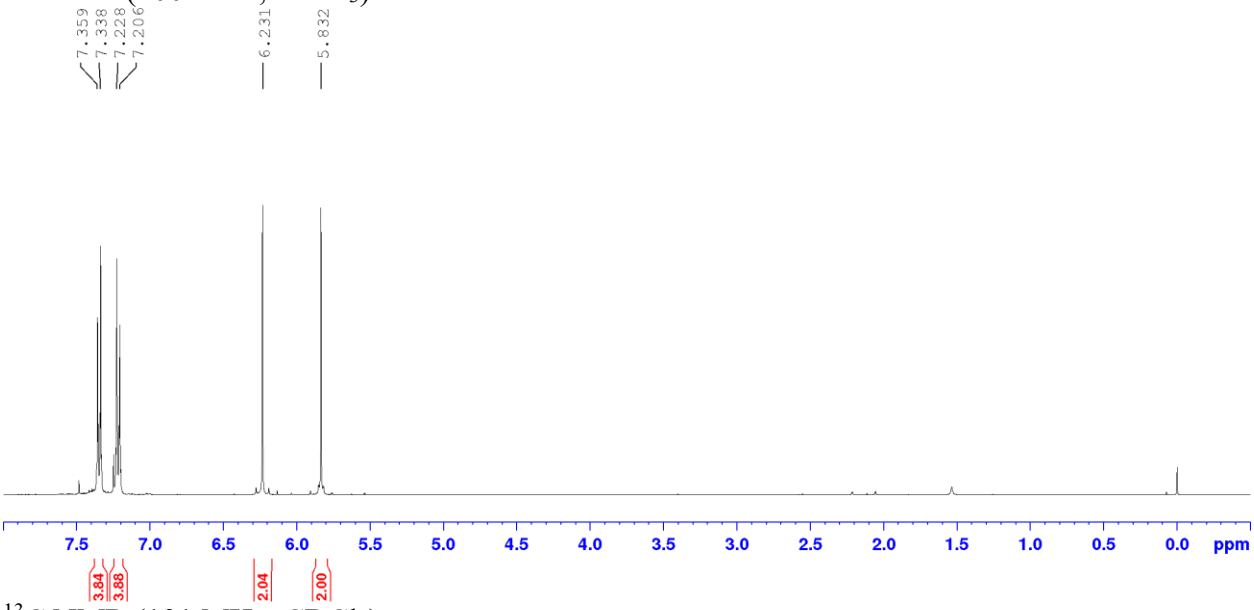
^{13}C NMR (101 MHz, $CDCl_3$)



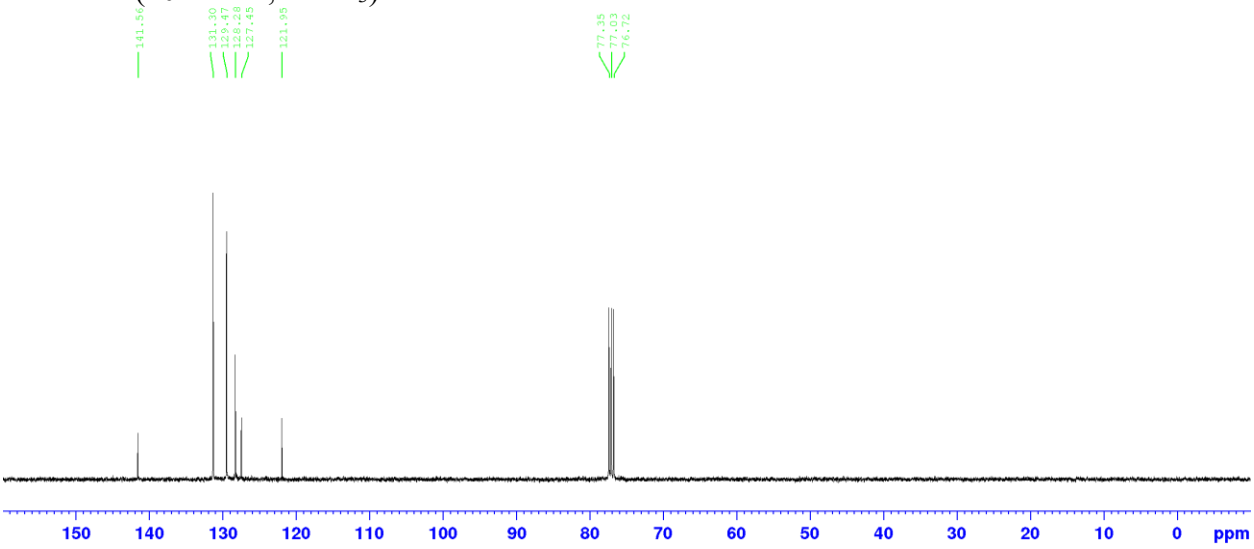
Bis-1-(*p*-bromophenyl)vinyl telluride **3d**:



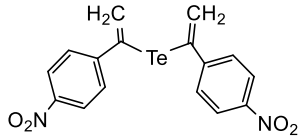
^{1}H NMR (400 MHz, $CDCl_3$)



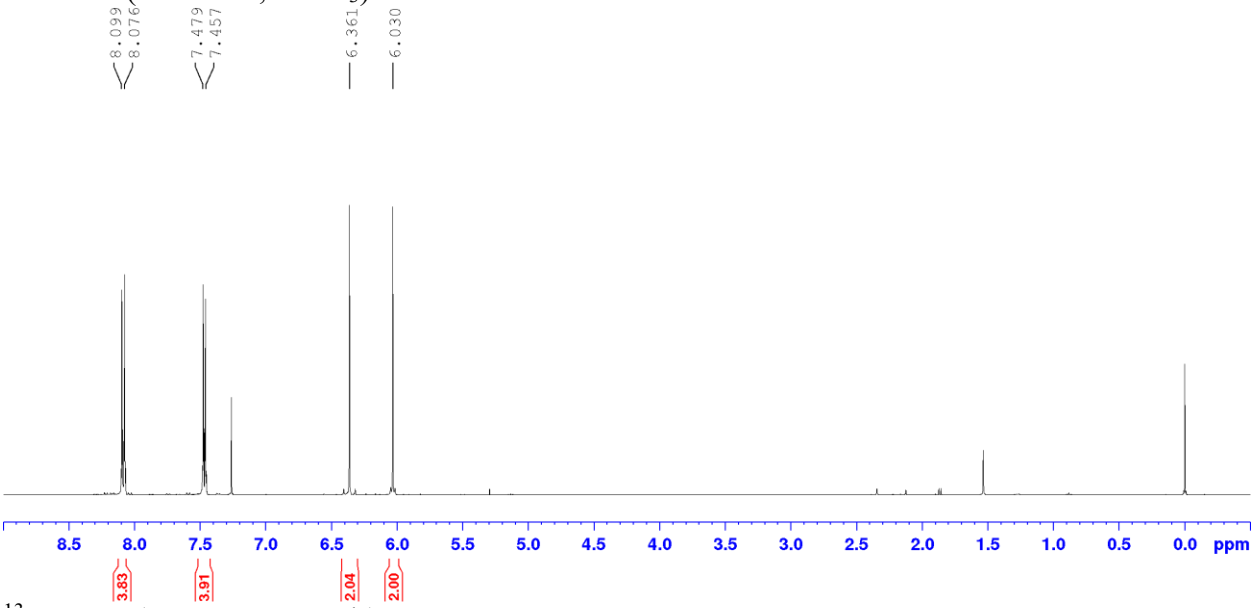
^{13}C NMR (101 MHz, $CDCl_3$)



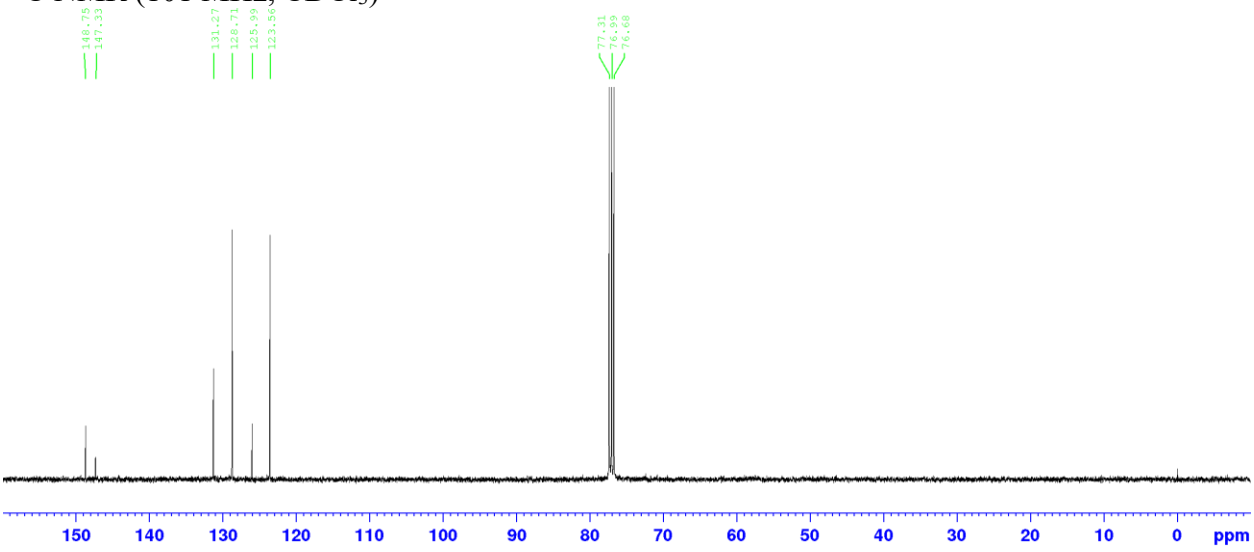
Bis-1-(*p*-nitrophenyl)vinyl telluride **3e**:



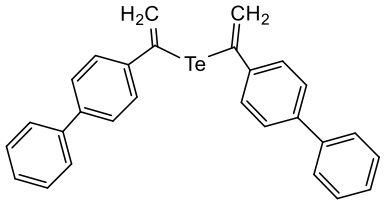
^{1}H NMR (400 MHz, $CDCl_3$)



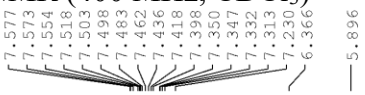
^{13}C NMR (101 MHz, $CDCl_3$)

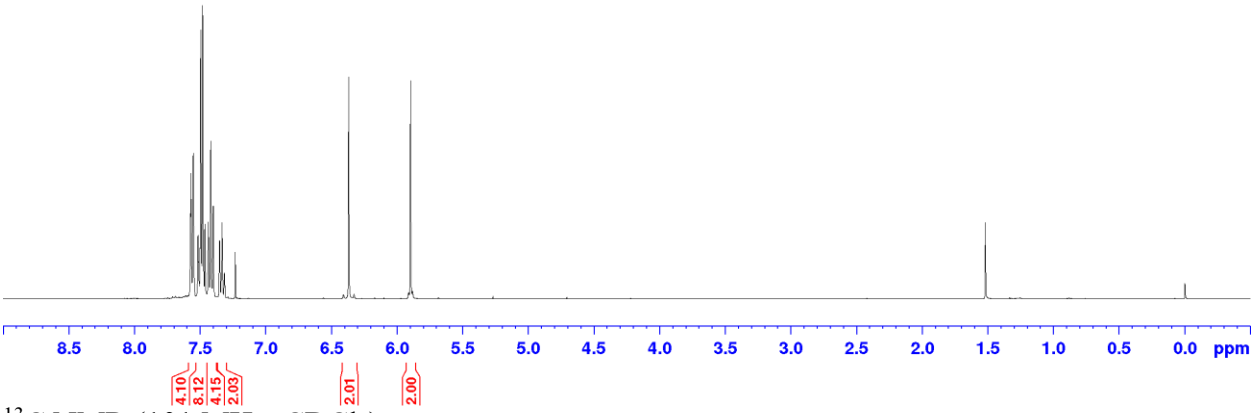


Bis-1-([1,1'-biphenyl]-4-yl)vinyl telluride **3f**:

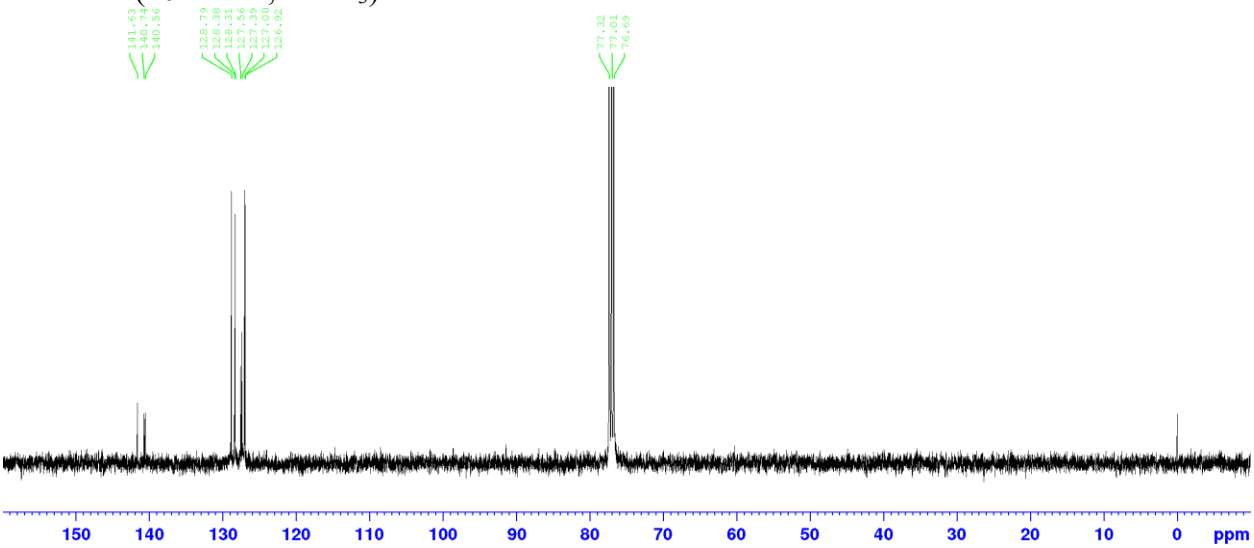


^{1}H NMR (400 MHz, $CDCl_3$)

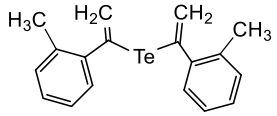




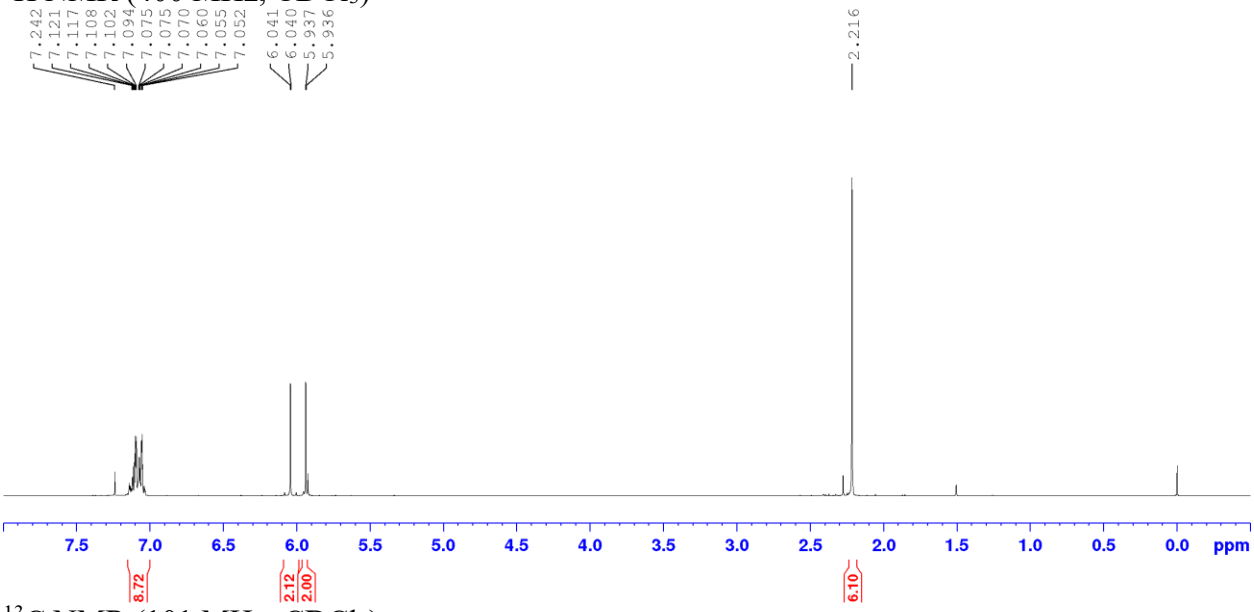
^{13}C NMR (101 MHz, $CDCl_3$)



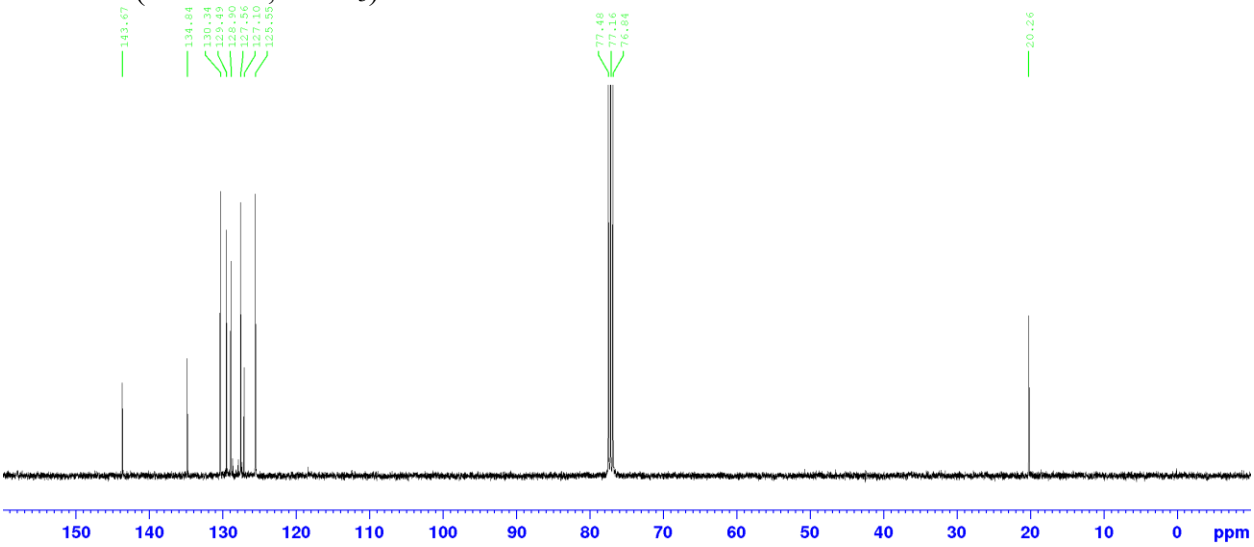
Bis-1-(*o*-tolyl)vinyl telluride **3g**:



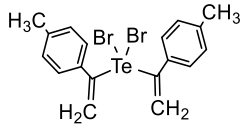
^{1}H NMR (400 MHz, $CDCl_3$)



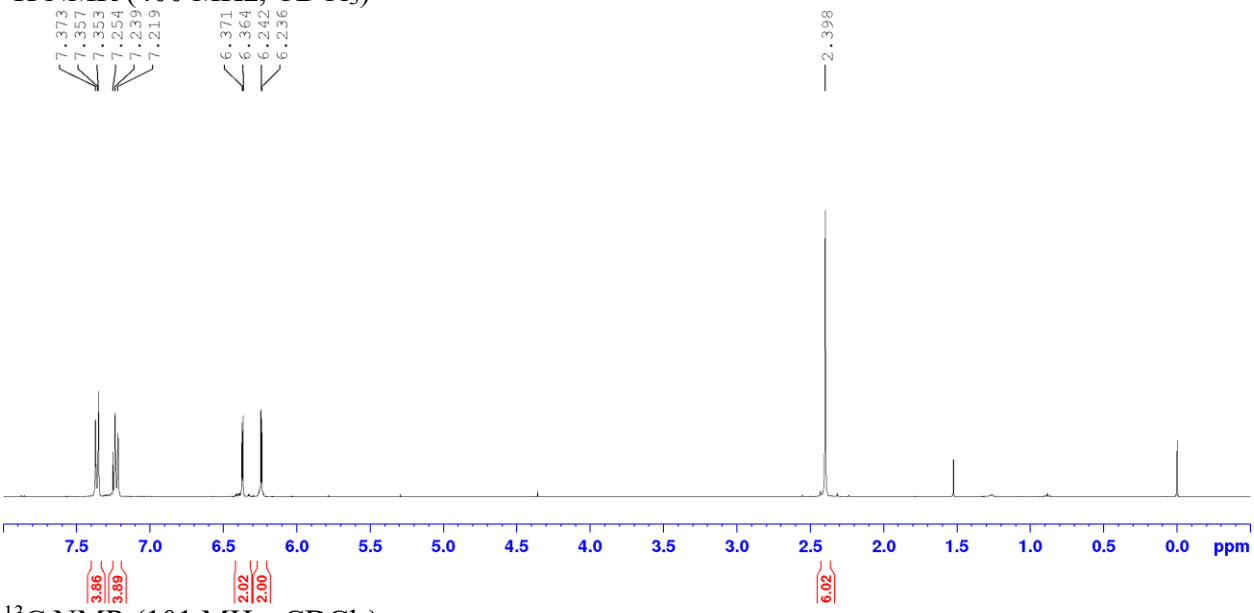
^{13}C NMR (101 MHz, $CDCl_3$)



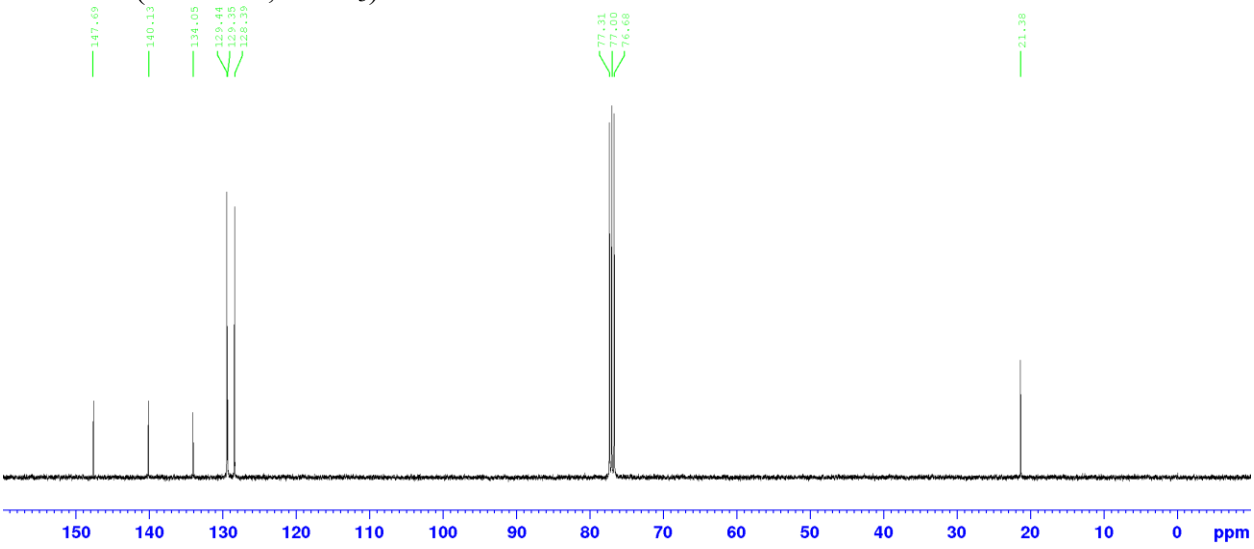
Bis-1-(*p*-methylphenyl)vinyltellurium dibromide **5a**:



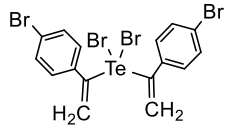
^{1}H NMR (400 MHz, $CDCl_3$)



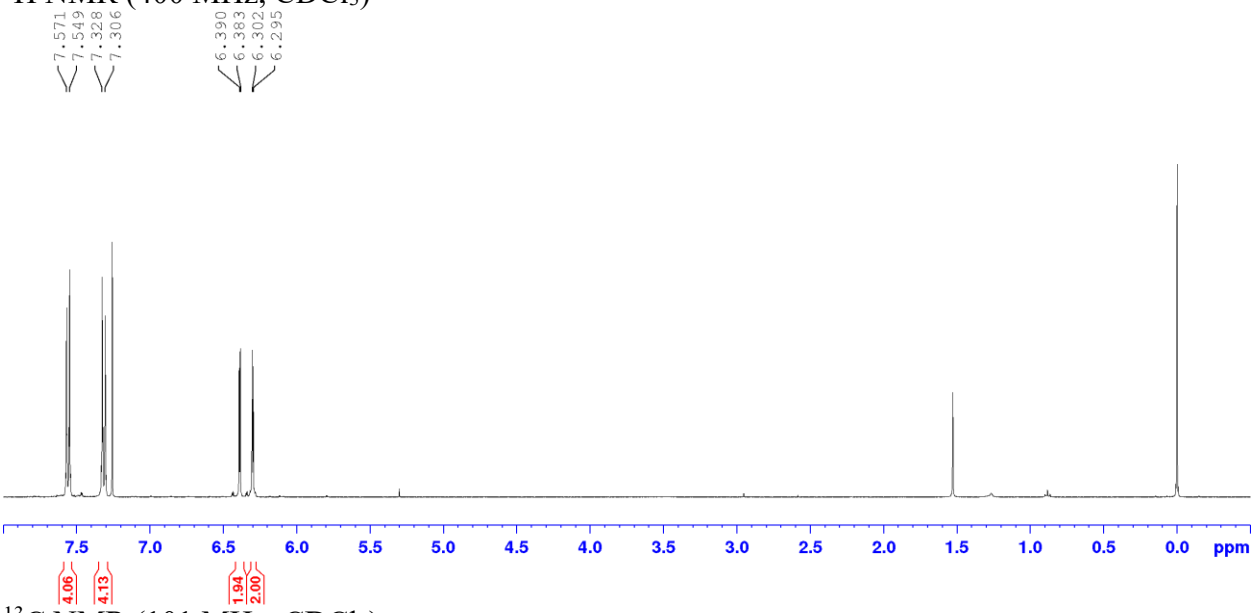
^{13}C NMR (101 MHz, $CDCl_3$)



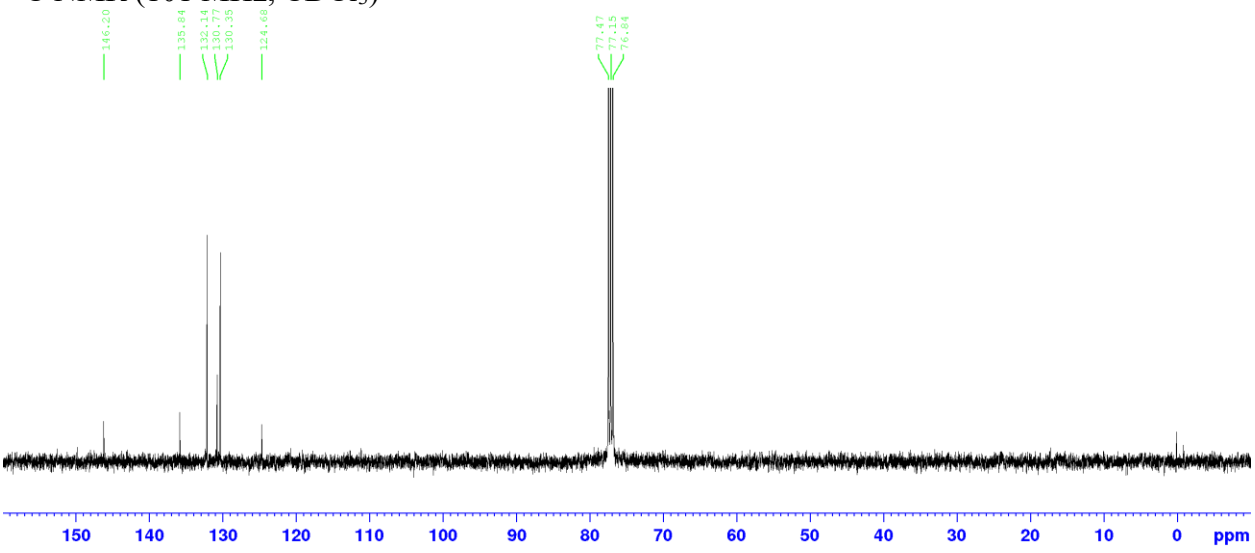
Bis-1-(*p*-bromophenyl)vinyltellurium dibromide **5d**:



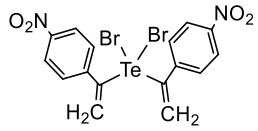
^{1}H NMR (400 MHz, $CDCl_3$)



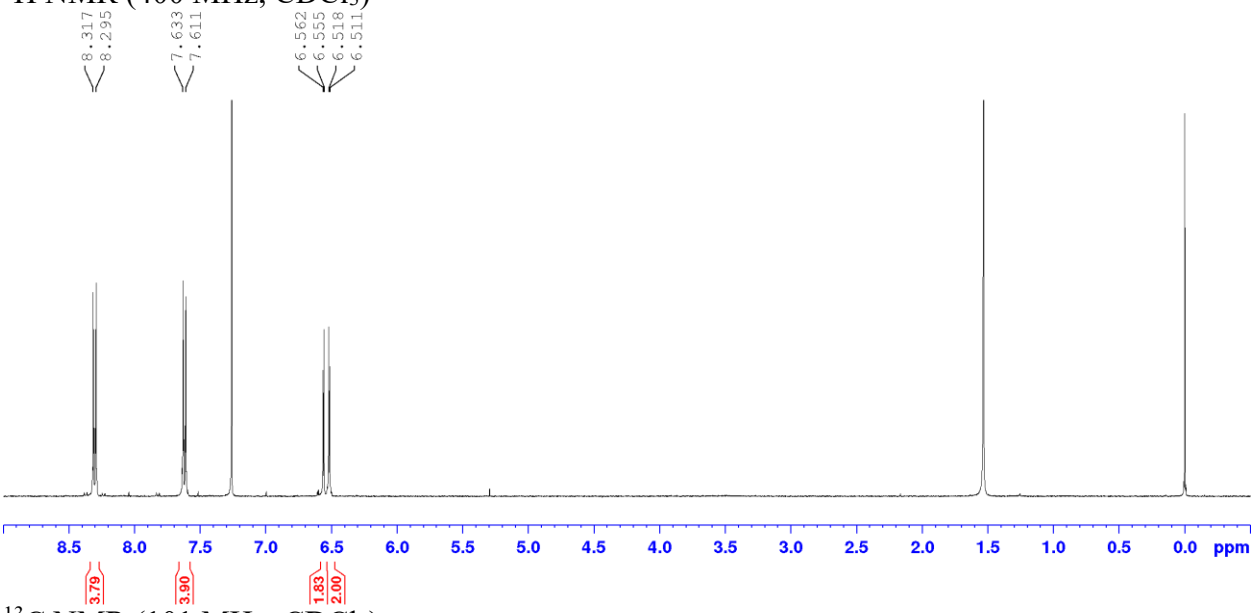
^{13}C NMR (101 MHz, $CDCl_3$)



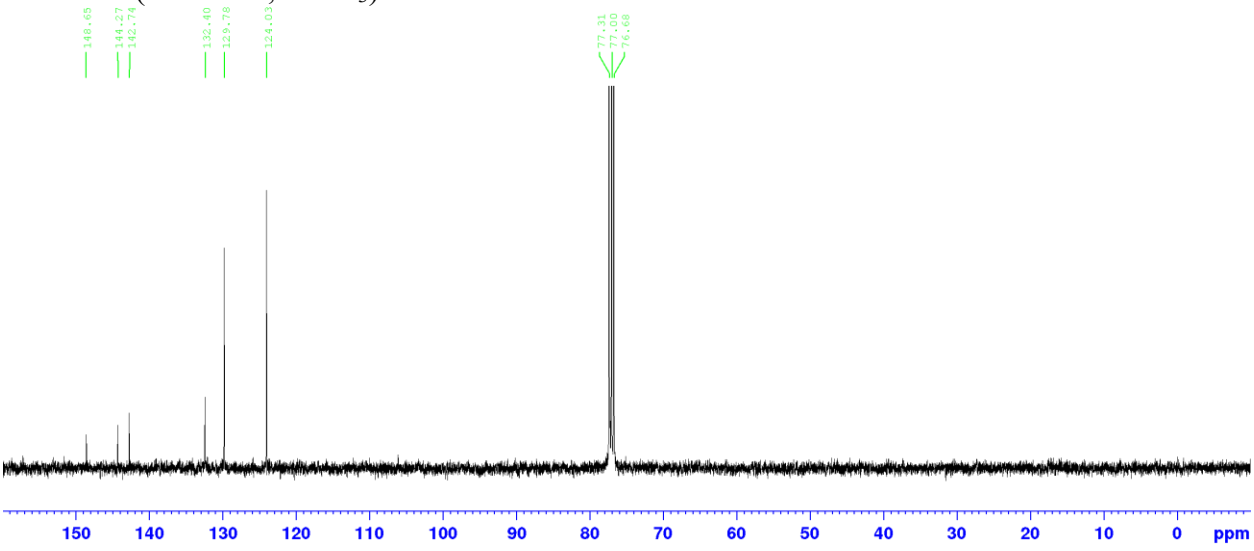
Bis-1-(*p*-nitrophenyl)vinyltellurium dibromide **5e**:



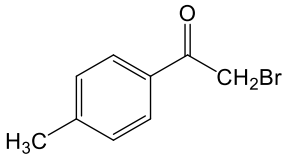
^{1}H NMR (400 MHz, $CDCl_3$)



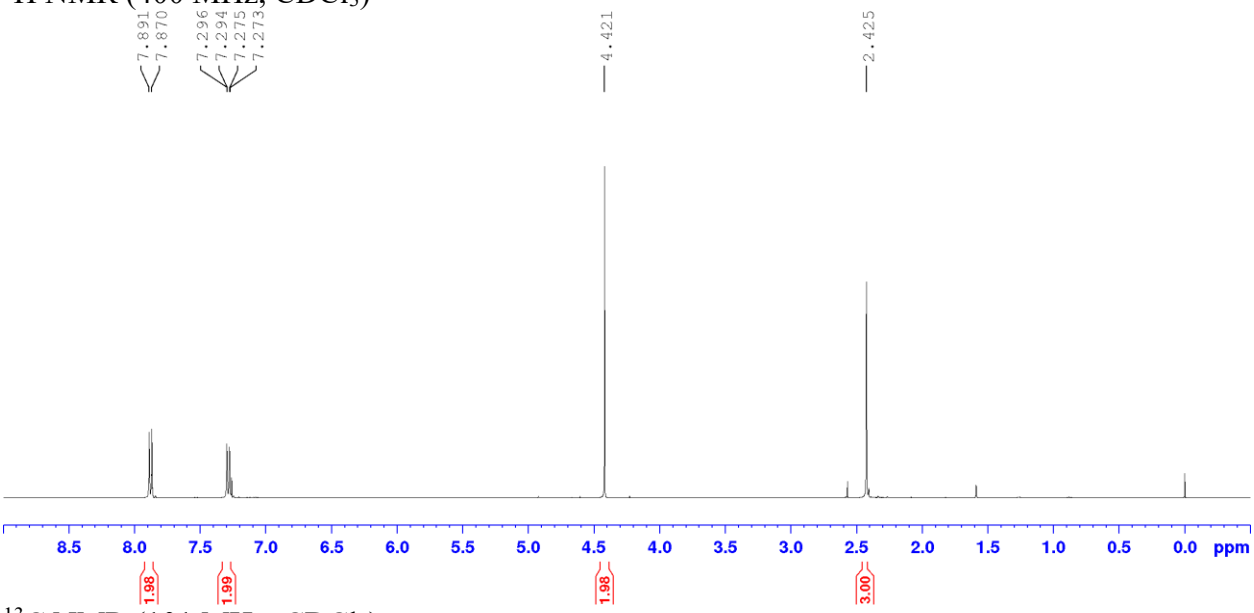
^{13}C NMR (101 MHz, $CDCl_3$)



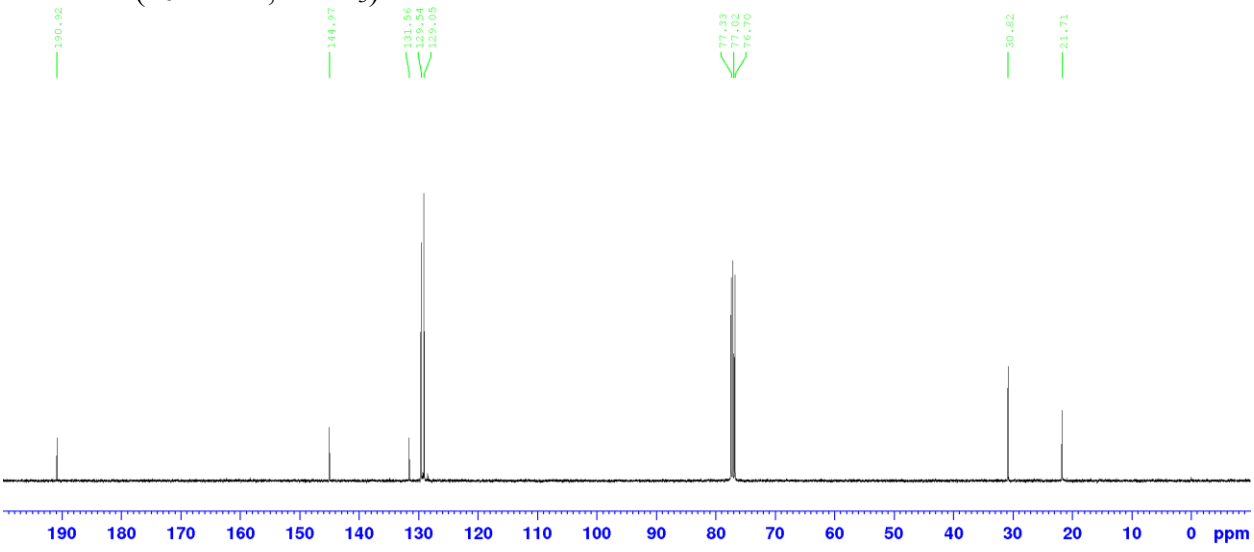
2-bromo-*p*-methylacetophenone **6a**:



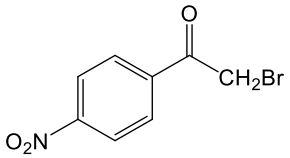
^{1}H NMR (400 MHz, $CDCl_3$)



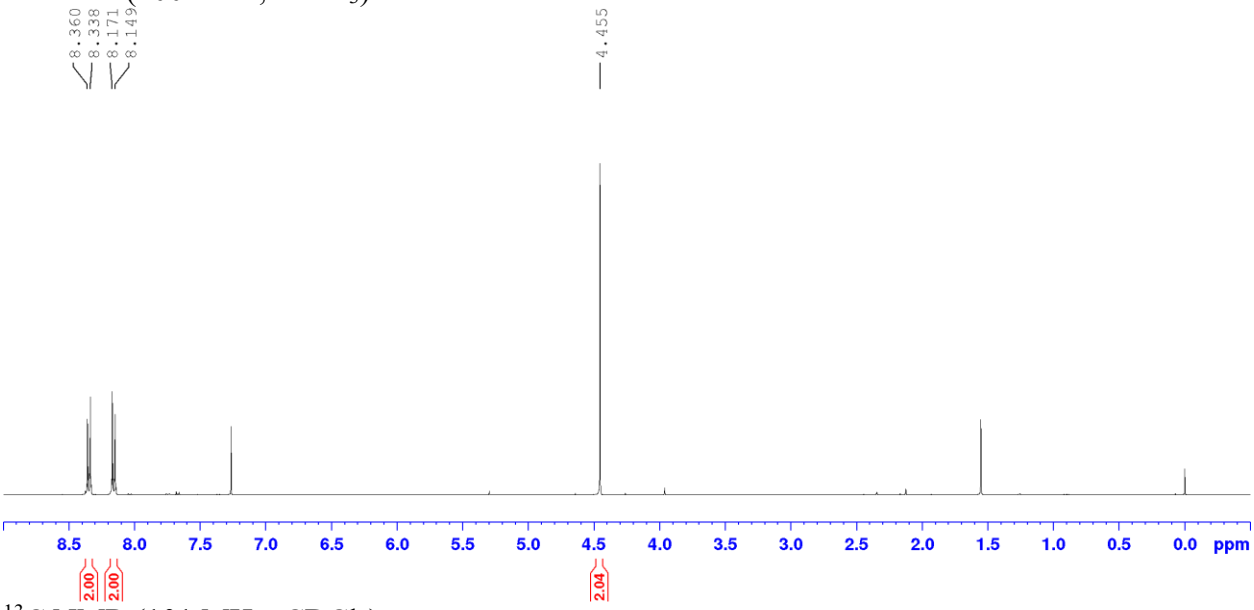
^{13}C NMR (101 MHz, $CDCl_3$)



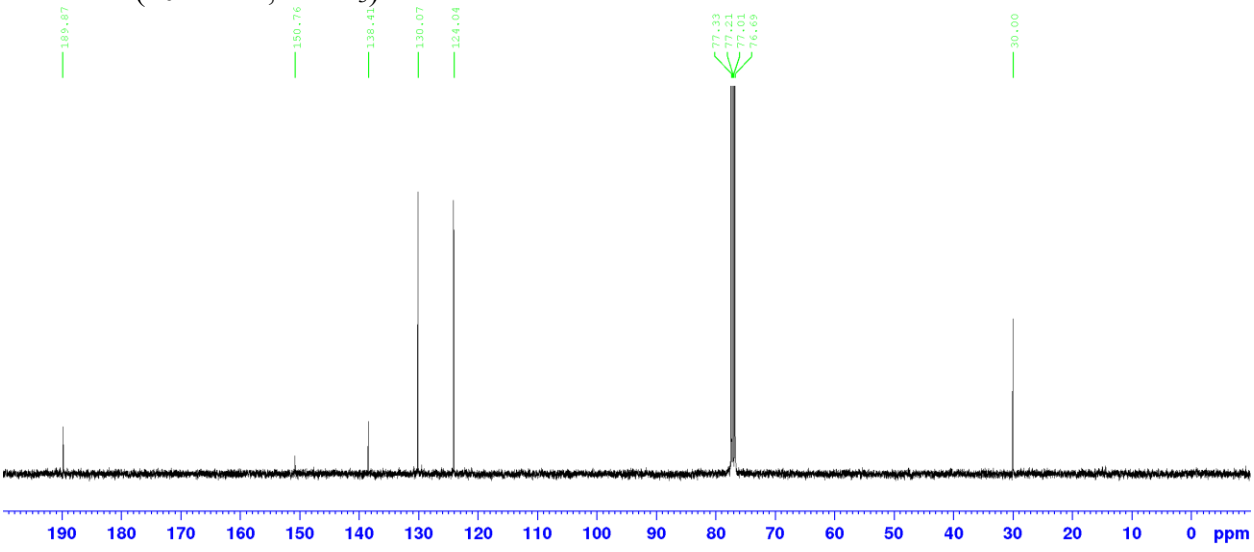
2-bromo-*p*-nitroacetophenone **6b**:



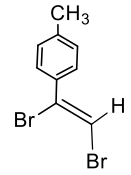
^{1}H NMR (400 MHz, $CDCl_3$)



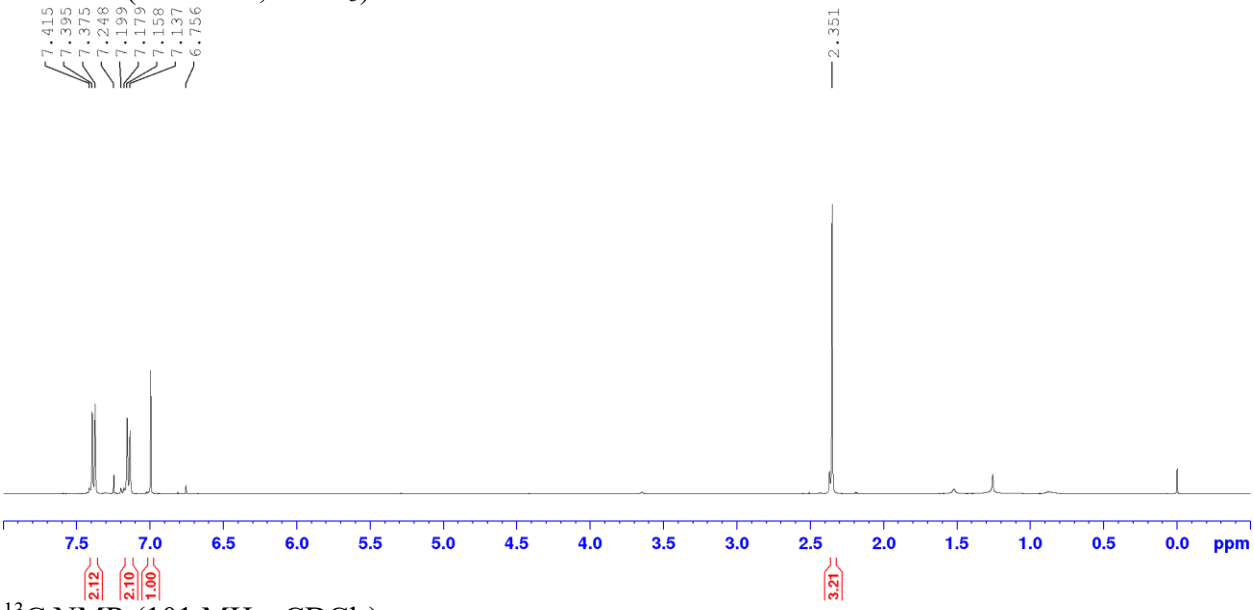
^{13}C NMR (101 MHz, $CDCl_3$)



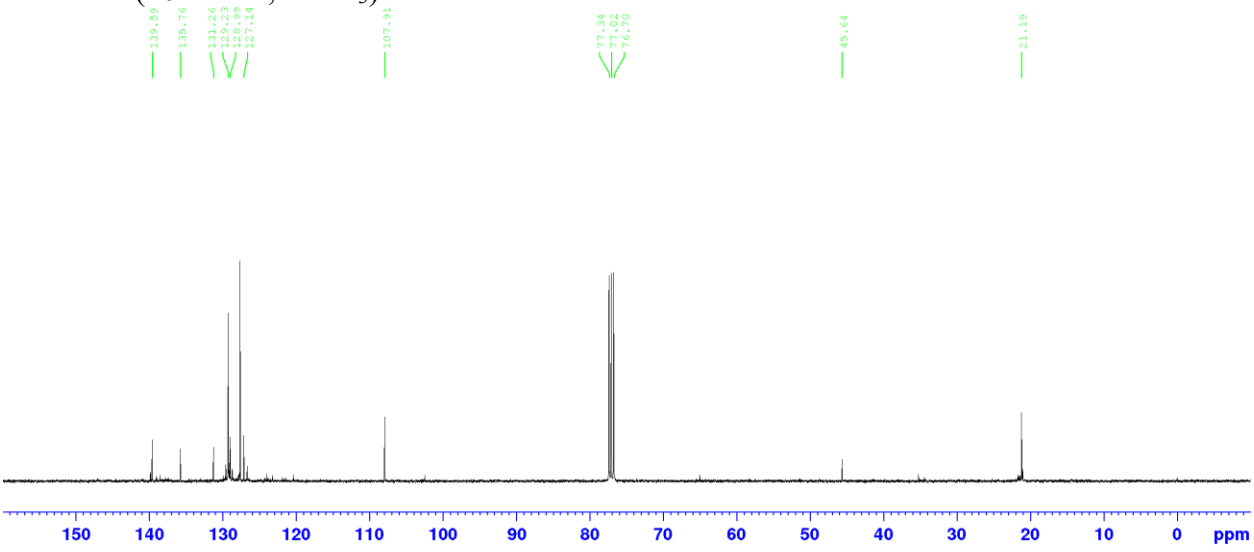
(*Z*)-1,2-dibromo-*p*-methylstyrene **7**:



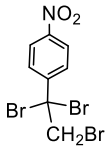
^{1}H NMR (400 MHz, $CDCl_3$)



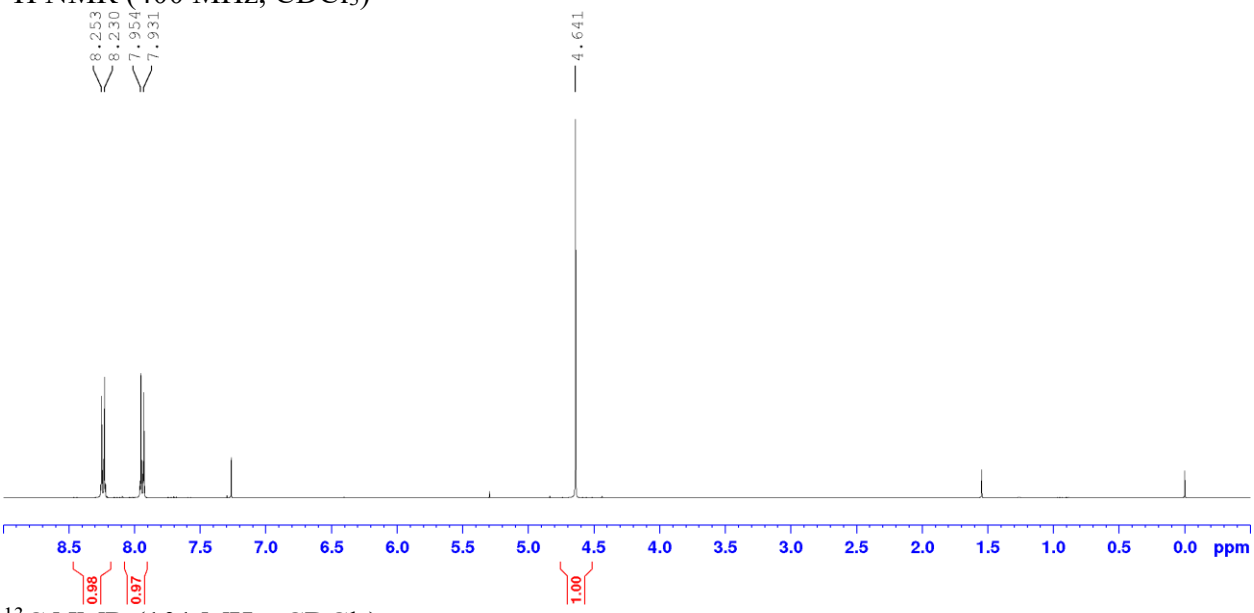
^{13}C NMR (101 MHz, $CDCl_3$)



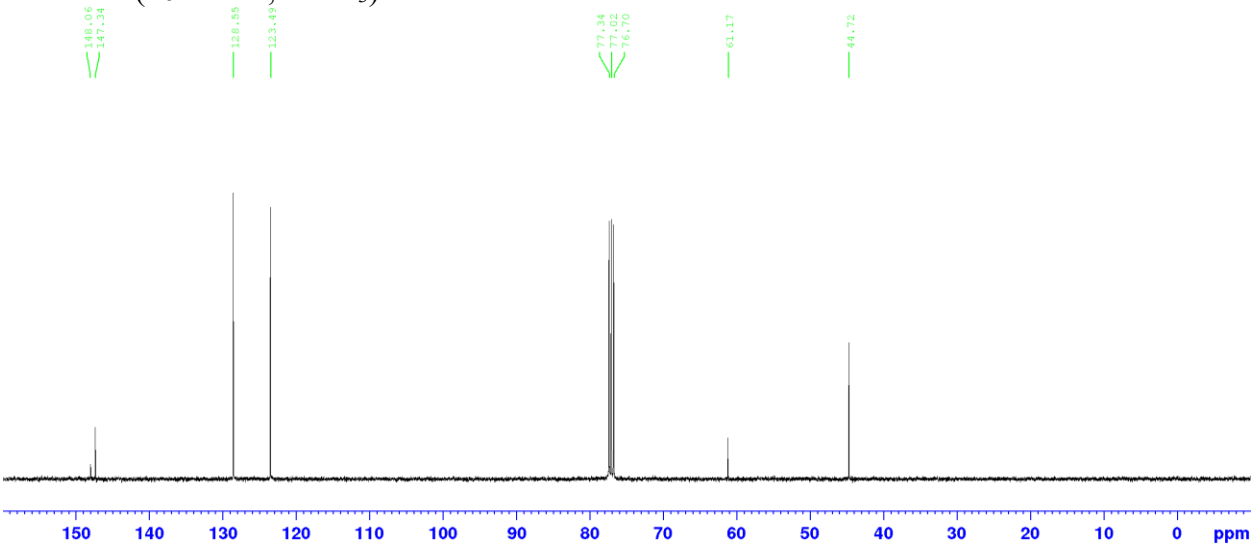
1-nitro-4-(1,1,2-tribromoethyl)benzene **8**:



^{1}H NMR (400 MHz, $CDCl_3$)

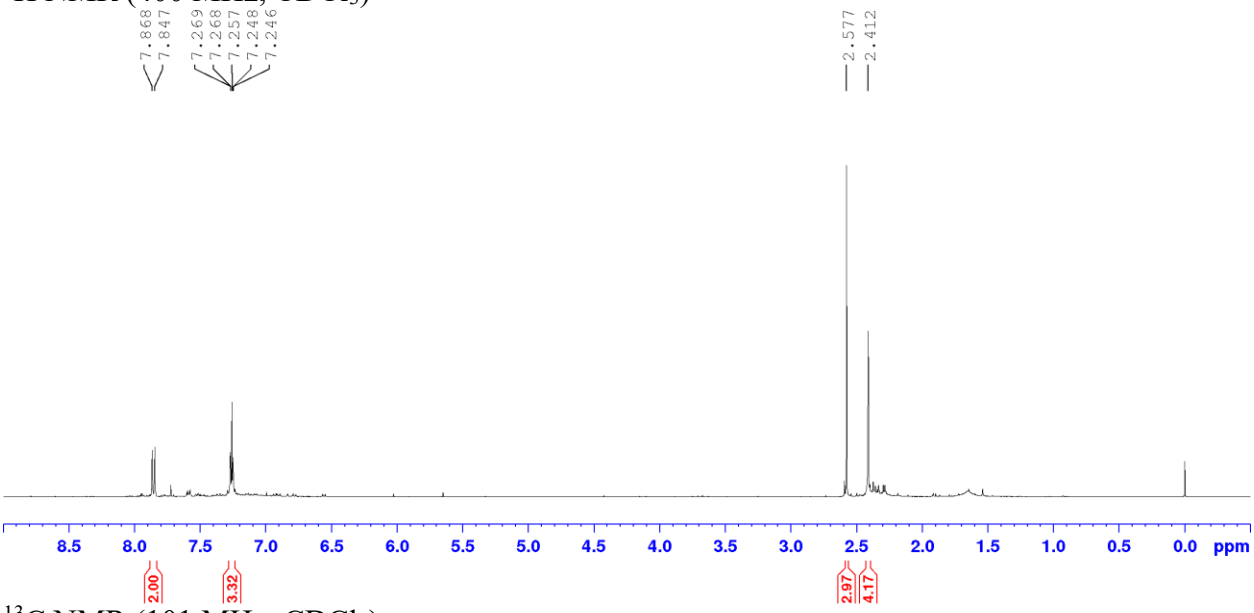


^{13}C NMR (101 MHz, $CDCl_3$)

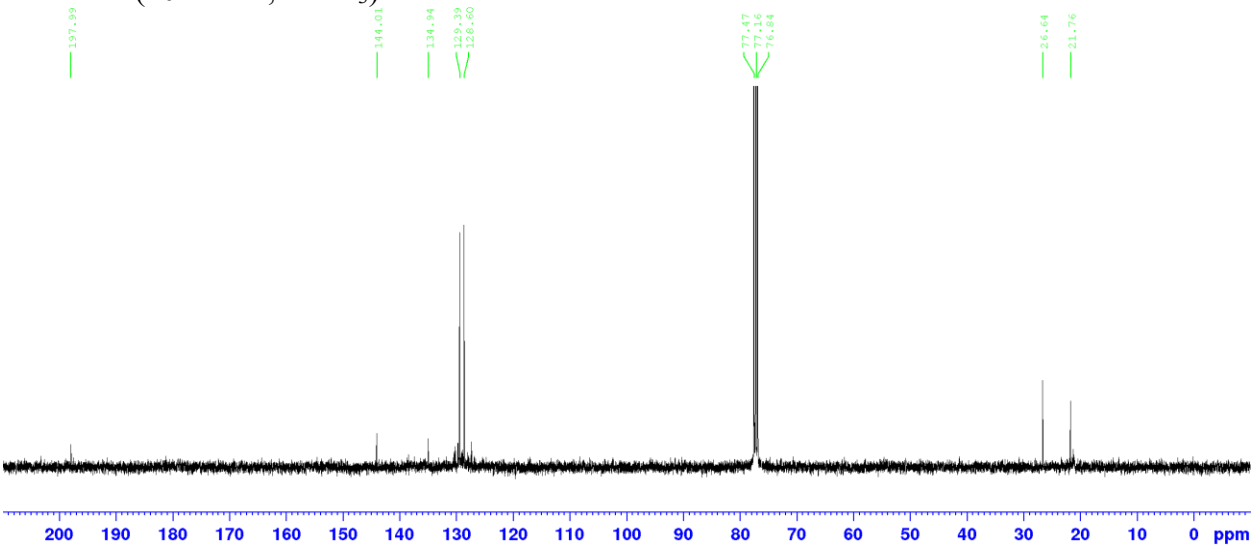


p-methylacetophenone (Oxidation of Dibromide)

^{1}H NMR (400 MHz, $CDCl_3$)

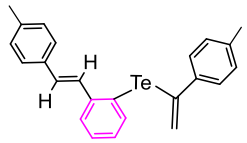


^{13}C NMR (101 MHz, $CDCl_3$)

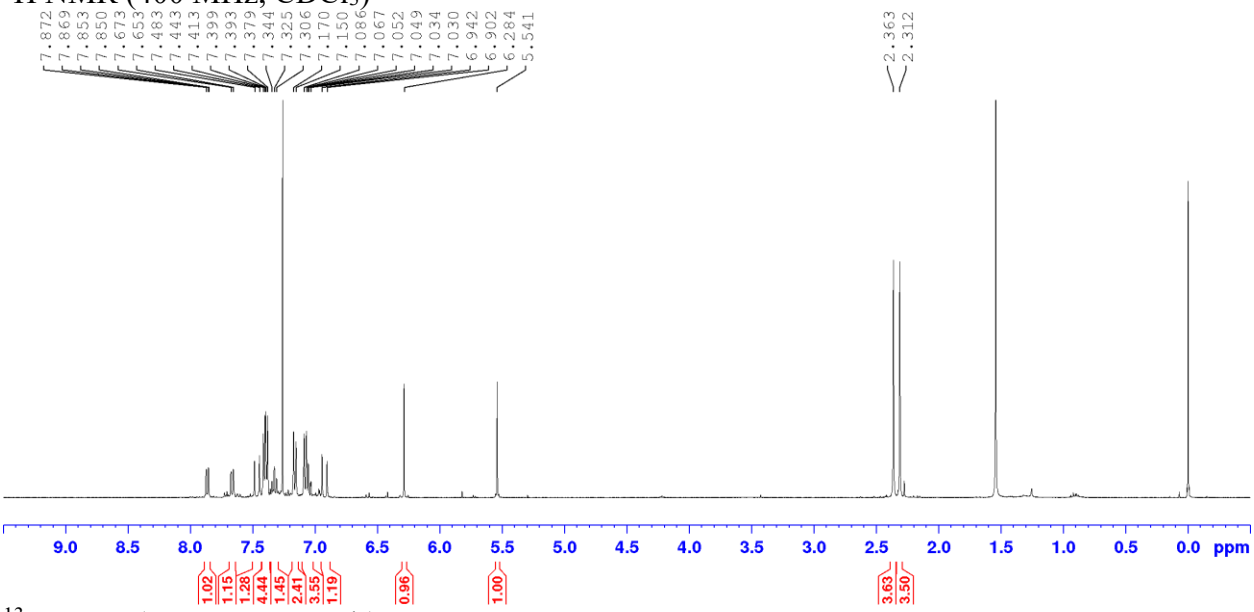


(E)-(2-(4-methylstyryl)phenyl)(1-(*p*-tolyl)vinyl)telluride **10**a:

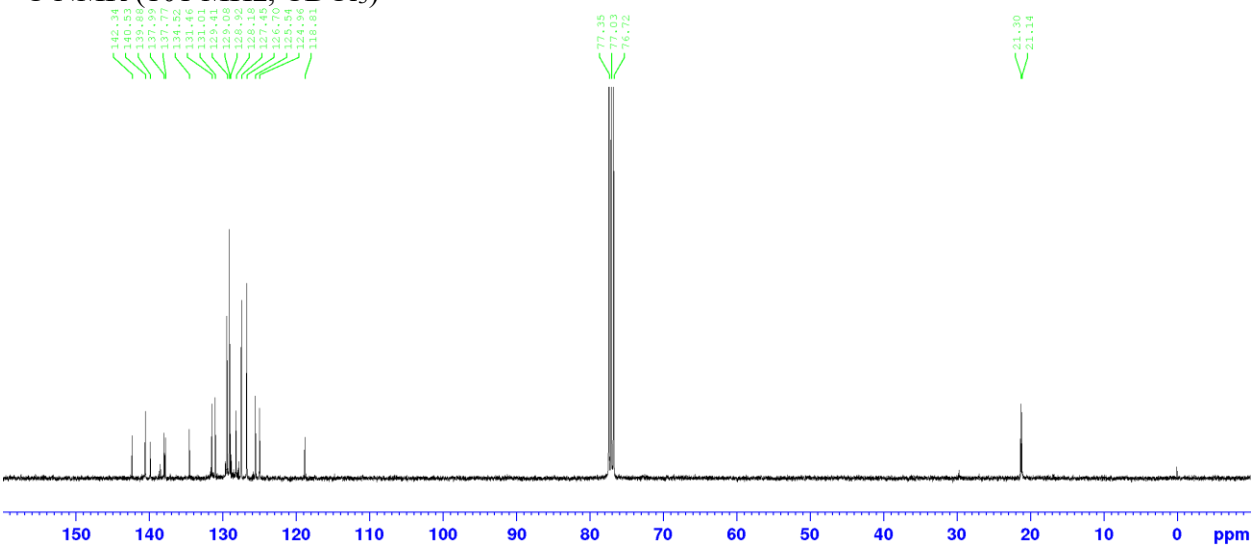
Compound **10** is unstable. Upon standing at rt for 6 h, compound **10a** decomposed to give undefined species.



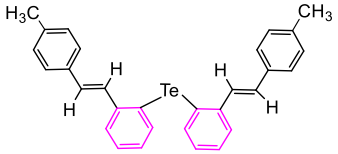
^{1}H NMR (400 MHz, $CDCl_3$)



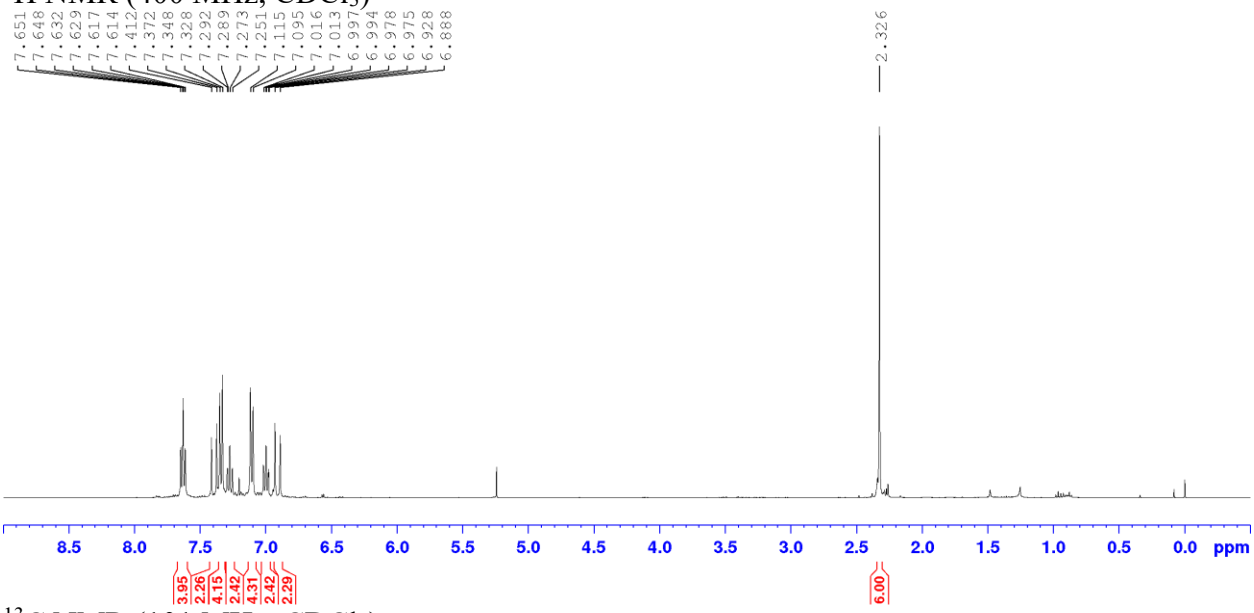
^{13}C NMR (101 MHz, $CDCl_3$)



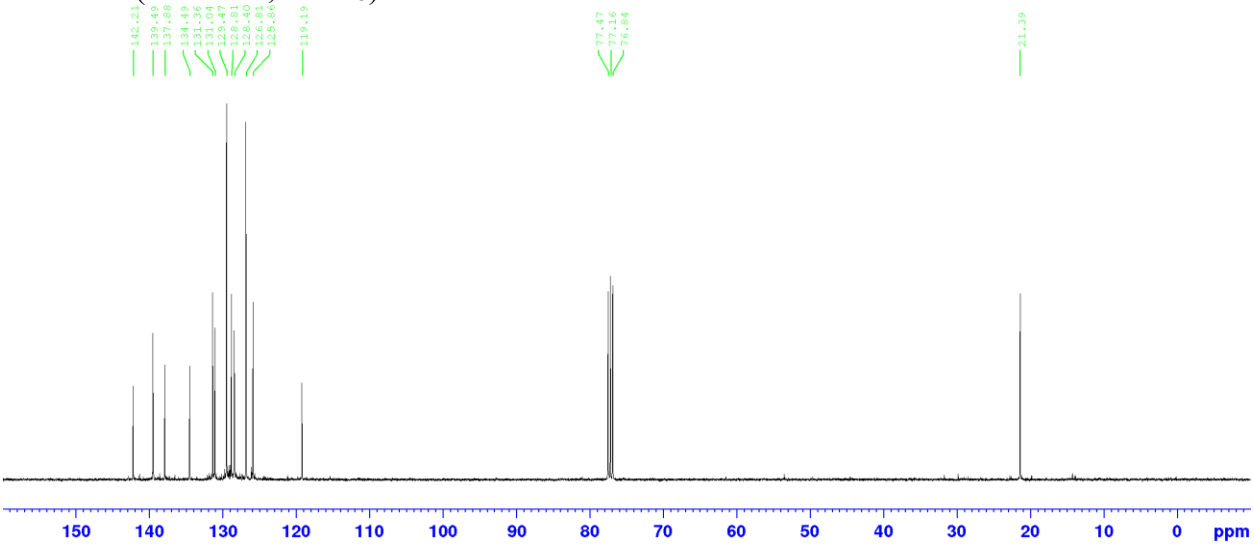
Bis(2-((*E*)-4-methylstyryl)phenyl) telluride **11a**:



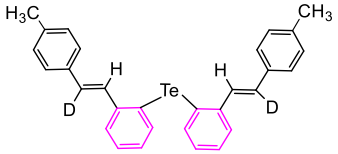
^{1}H NMR (400 MHz, $CDCl_3$)



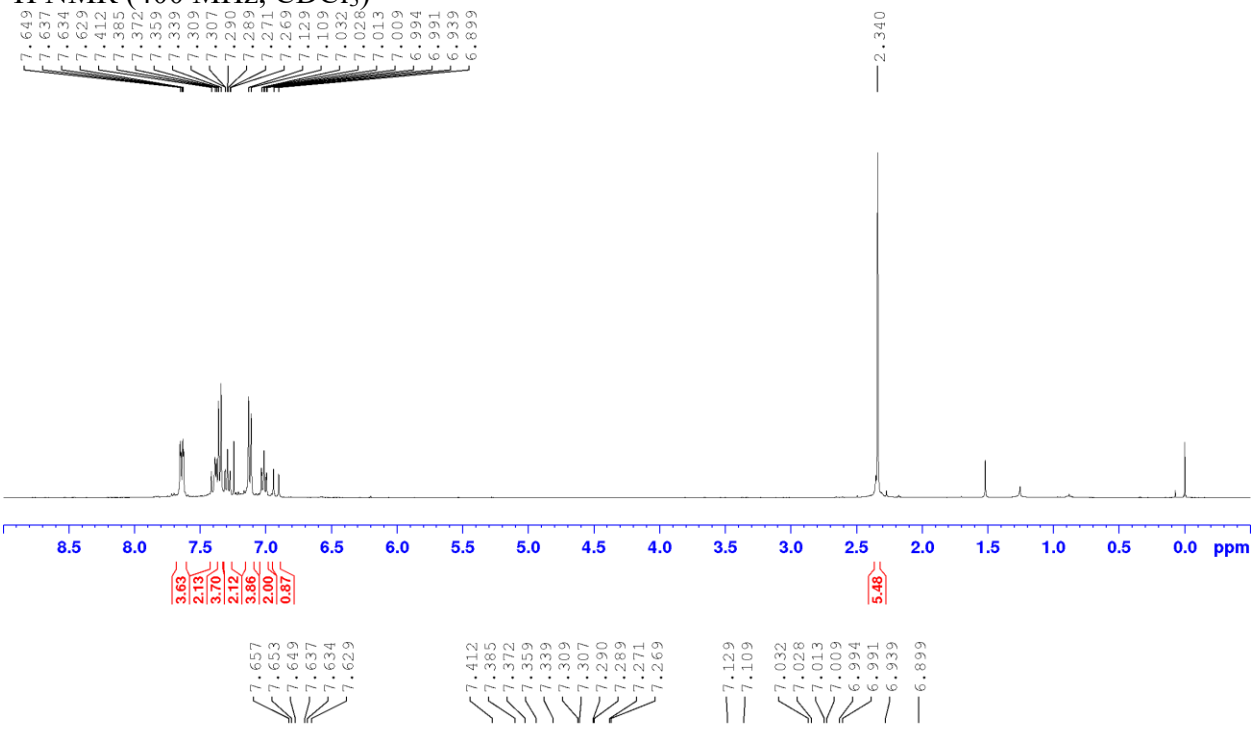
^{13}C NMR (101 MHz, $CDCl_3$)

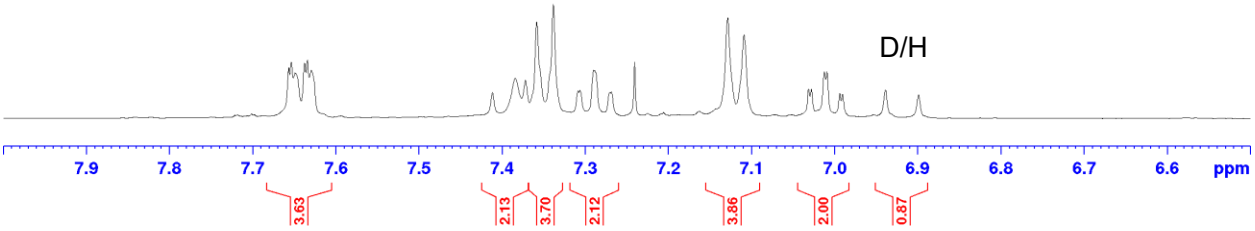


Deuterated Compound **11a-D** (60%D):

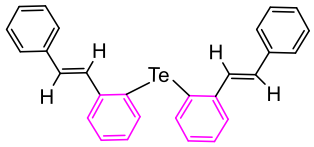


^{1}H NMR (400 MHz, $CDCl_3$)

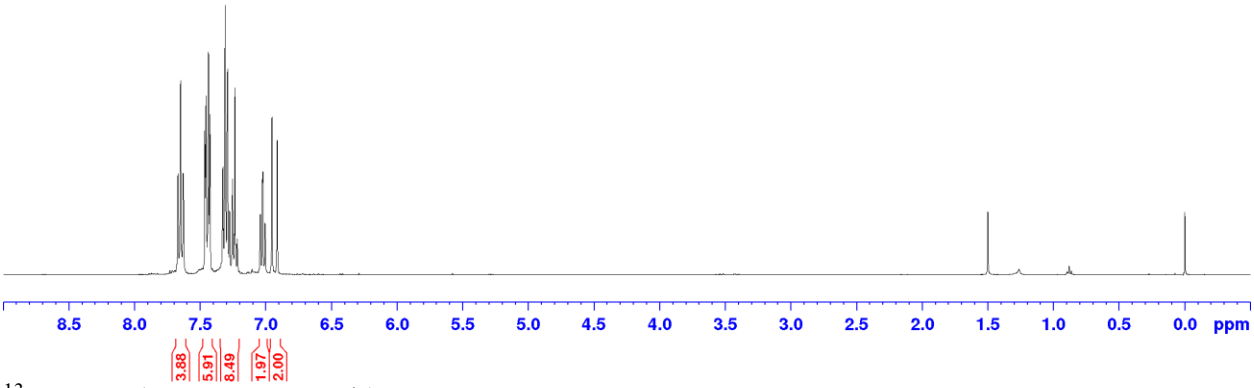




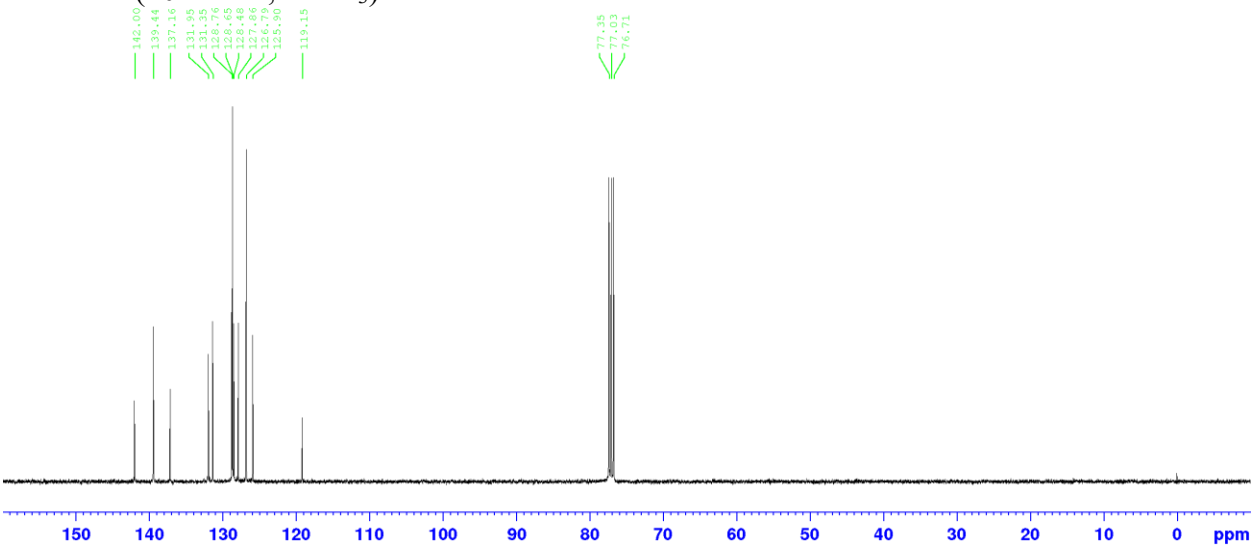
Bis(2-((*E*)-styryl)phenyl) telluride **11b**:



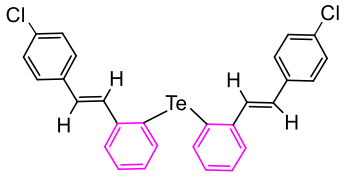
^{1}H NMR (400 MHz, $CDCl_3$)



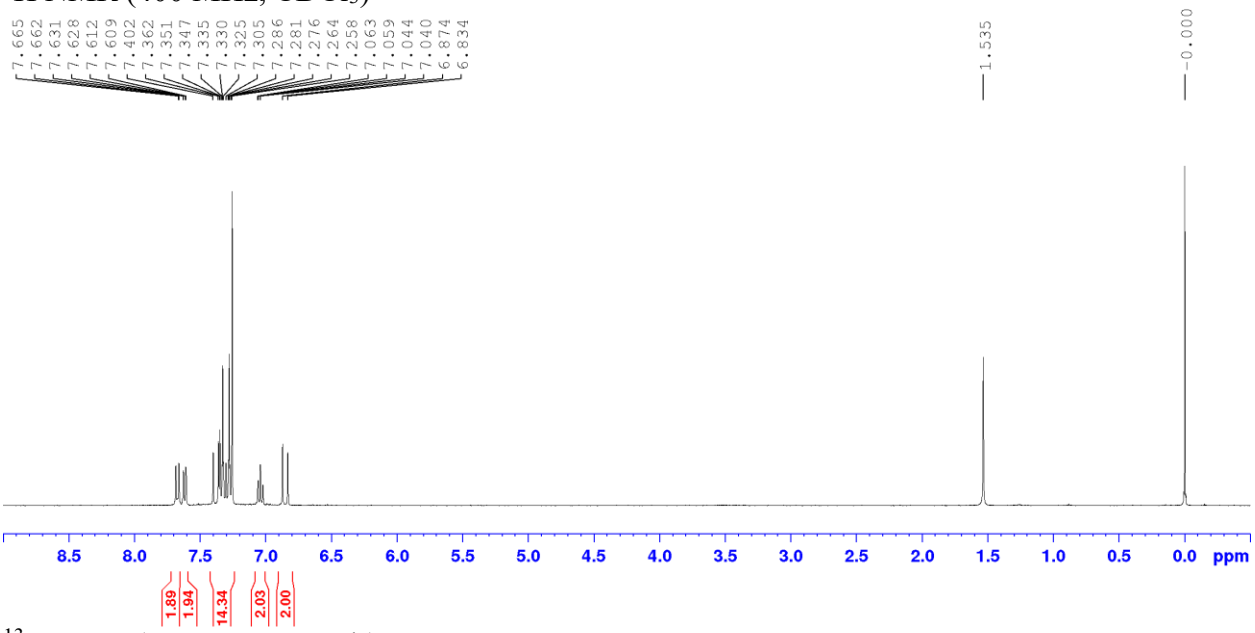
^{13}C NMR (101 MHz, $CDCl_3$)



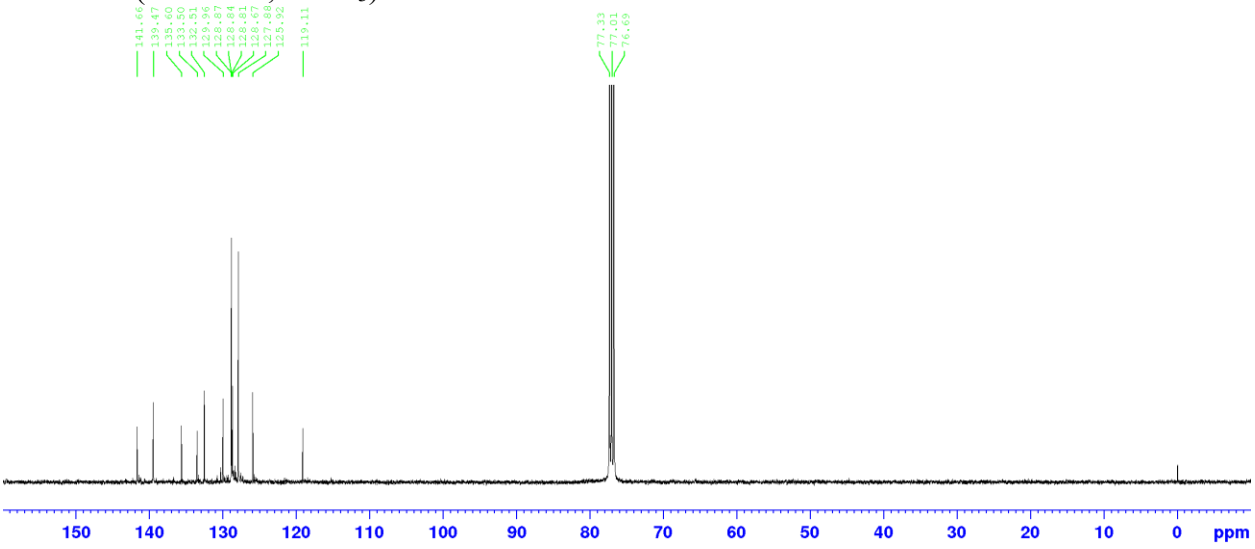
Bis(2-((*E*)-4-chlorostyryl)phenyl) telluride **11c**:



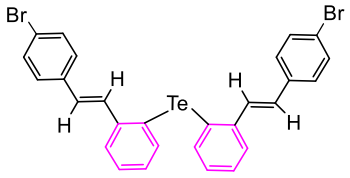
^{1}H NMR (400 MHz, $CDCl_3$)



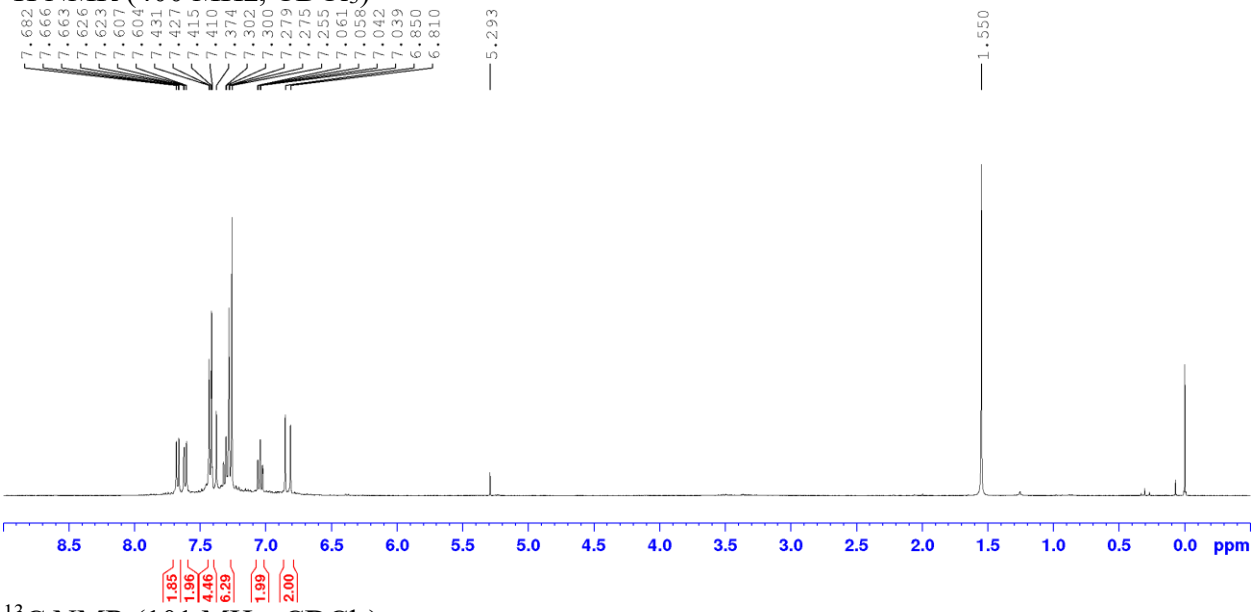
^{13}C NMR (101 MHz, $CDCl_3$)



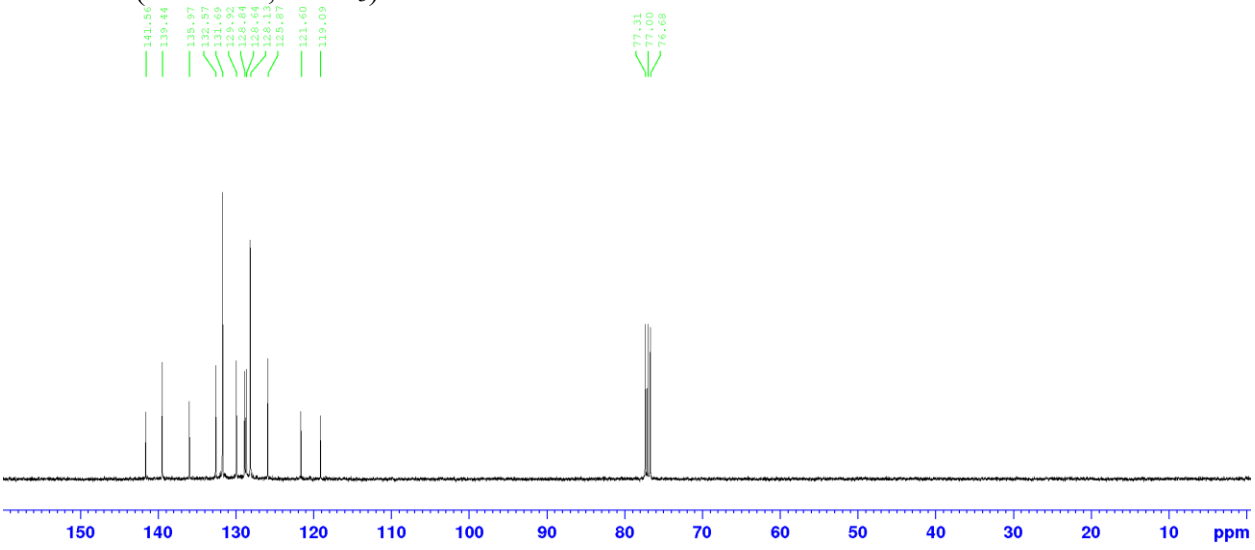
Bis(2-((*E*)-4-bromostyryl)phenyl) telluride **11d**:



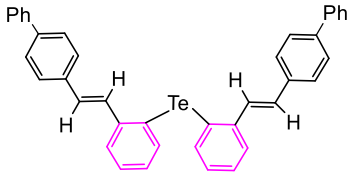
^{1}H NMR (400 MHz, $CDCl_3$)



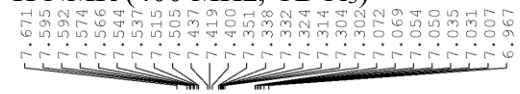
^{13}C NMR (101 MHz, $CDCl_3$)

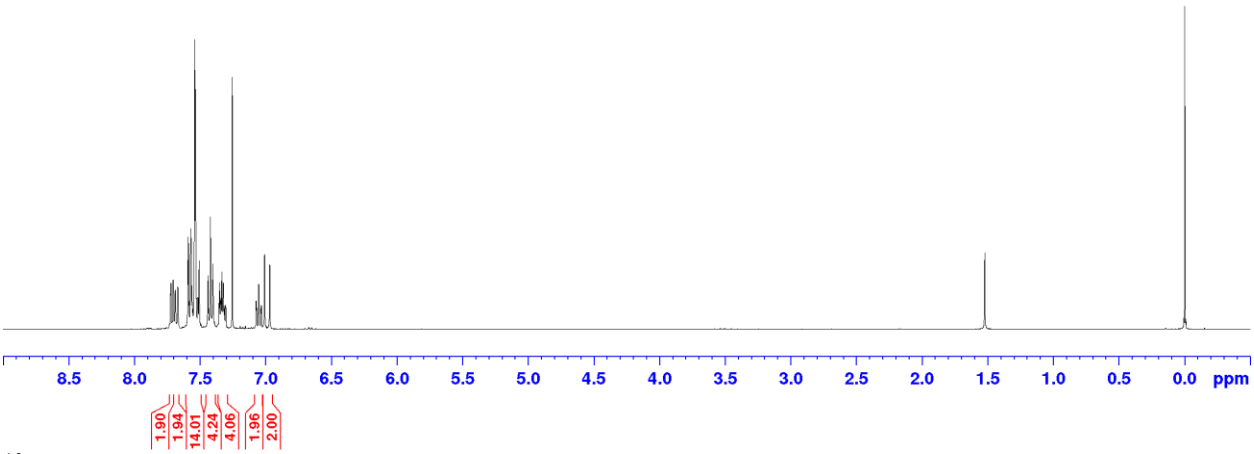


Bis(2-((*E*)-4-phenylstyryl)phenyl) telluride **11f**:

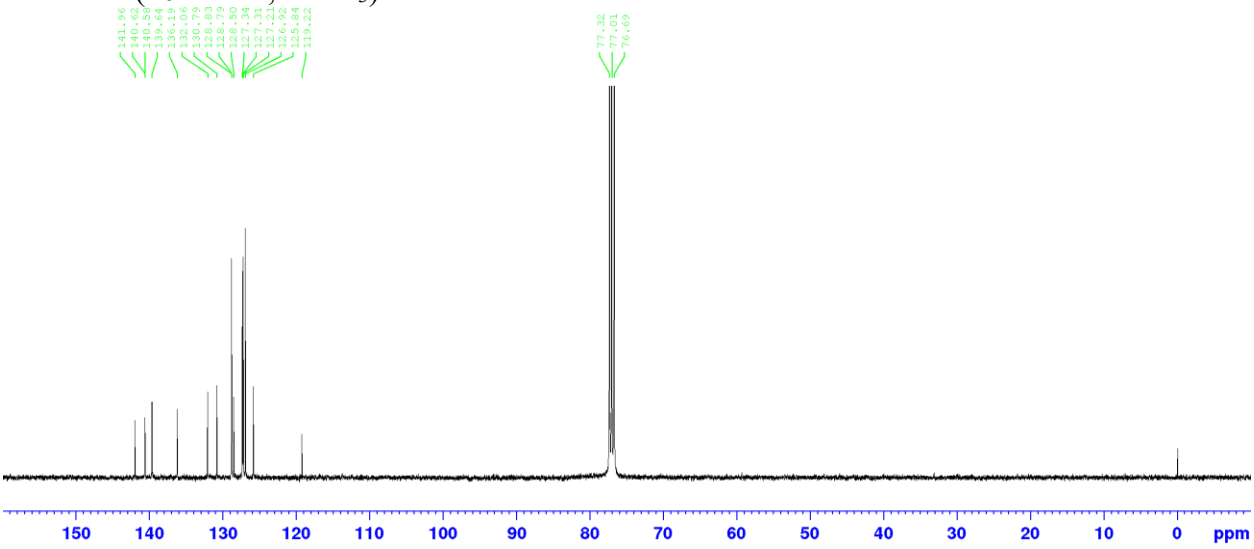


^{1}H NMR (400 MHz, $CDCl_3$)

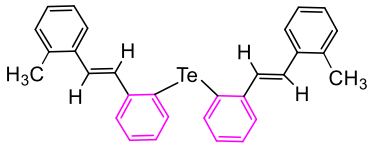




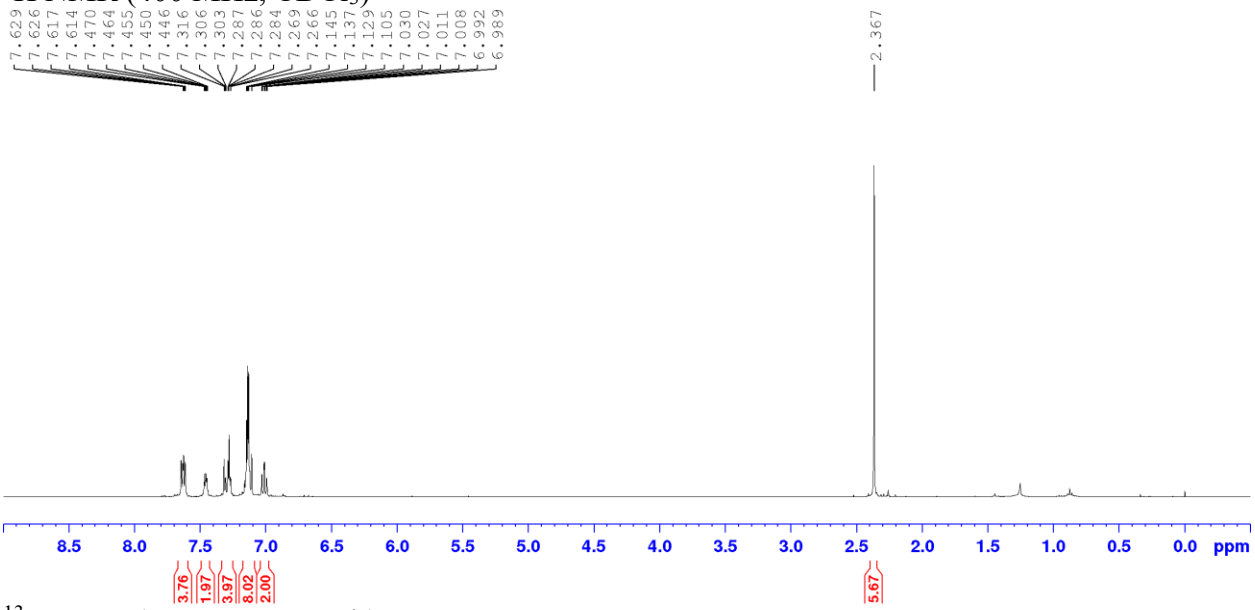
^{13}C NMR (101 MHz, $CDCl_3$)



Bis(2-((*E*)-2-methylstyryl)phenyl) telluride **11g**:



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

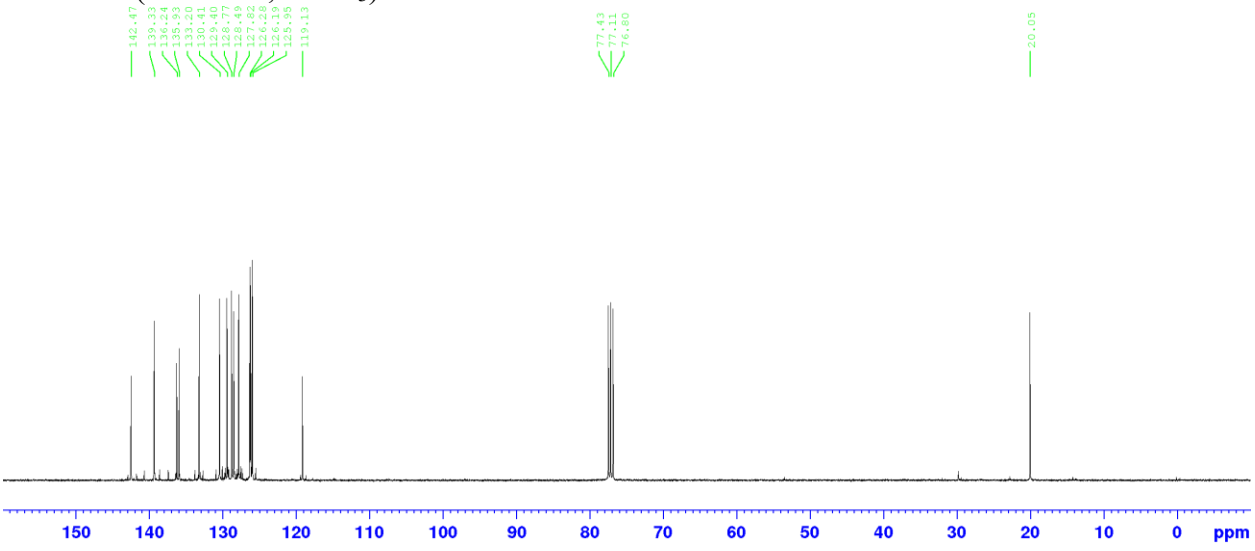


Figure 1. ORTEP Drawing for 1-nitro-4-(112-tribromoethyl)benzene **8**.

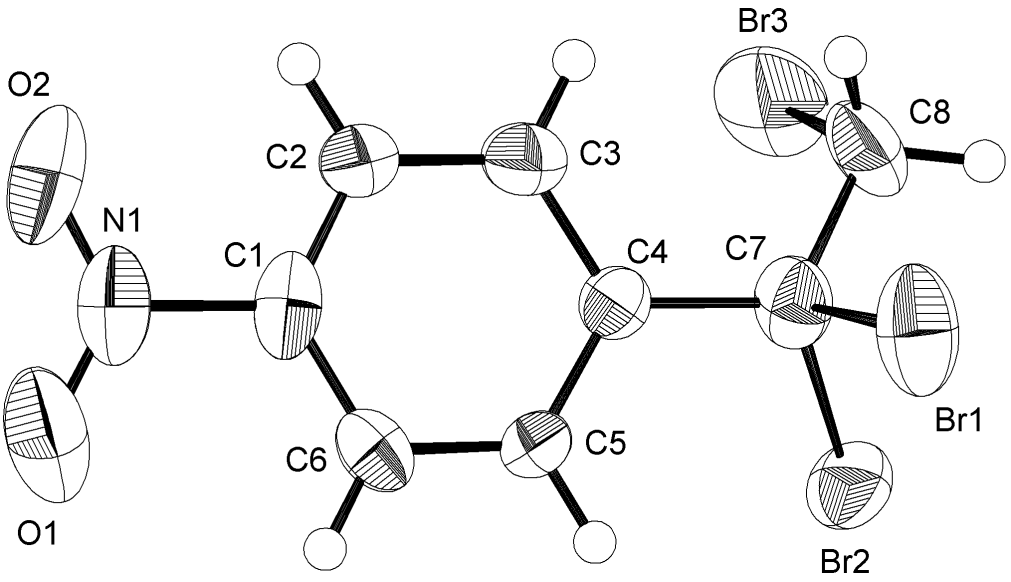


Table 1. Crystal data and structure refinement for 1-nitro-4-(1,1,2-tribromoethyl)benzene **8**.

Identification code	20200111	
Empirical formula	C16 H12 Br6 N2 O4	
Formula weight	775.74	
Temperature	293(2) K	
Wavelength	0.71075 Å	
Crystal system	monoclinic	
Space group	$P2_1/a$	
Unit cell dimensions	a = 7.012(2) Å	α= 90°.
	b = 19.312(7) Å	β= 90.125(7)°.
	c = 16.460(6) Å	γ = 90°.
Volume	2228.9(14) $Å^3$	
Z	4	
Density (calculated)	2.312 Mg/m^3	
Absorption coefficient	10.832 mm^{-1}	
F(000)	1456	
Crystal size	0.35 x 0.20 x 0.10 mm^3	
Theta range for data collection	3.09 to 26.00°.	
Index ranges	-8<=h<=8, -23<=k<=23, -20<=l<=20	

Reflections collected	23139
Independent reflections	4389 [R(int) = 0.1277]
Completeness to theta = 26.00°	99.9 %
Max. and min. transmission	0.4105 and 0.1158
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4389 / 0 / 253
Goodness-of-fit on F^2	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.0881
R indices (all data)	R1 = 0.0951, wR2 = 0.0939
Largest diff. peak and hole	0.992 and -1.285 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 20200111. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7468(10)	2601(5)	7285(5)	49(2)
C(2)	7537(9)	1921(5)	7078(5)	47(2)
C(3)	7345(9)	1422(4)	7685(4)	51(2)
C(4)	7098(9)	1615(4)	8489(4)	39(2)
C(5)	7028(9)	2306(4)	8657(4)	41(2)
C(6)	7211(9)	2807(4)	8079(5)	45(2)
N(1)	7644(10)	3118(5)	6640(5)	64(2)
O(1)	7386(10)	3715(4)	6807(5)	99(3)
O(2)	8053(9)	2920(4)	5967(4)	99(3)
C(7)	6955(9)	1087(5)	9151(4)	50(2)
C(8)	6723(10)	339(4)	8915(5)	63(2)
Br(1)	9428(1)	1081(1)	9745(1)	77(1)
Br(2)	4988(1)	1328(1)	9927(1)	57(1)
Br(3)	4268(1)	199(1)	8367(1)	90(1)
C(9)	12469(9)	-2594(5)	7708(5)	45(2)
C(10)	12540(10)	-1922(5)	7923(4)	50(2)
C(11)	12344(9)	-1416(4)	7325(5)	50(2)
C(12)	12096(9)	-1616(4)	6516(4)	36(2)
C(13)	12051(9)	-2302(4)	6332(4)	40(2)
C(14)	12225(9)	-2797(4)	6917(5)	41(2)
N(2)	12651(10)	-3113(5)	8356(5)	63(2)
O(3)	12414(10)	-3715(4)	8190(4)	95(3)
O(4)	13055(8)	-2929(4)	9031(4)	94(3)
C(15)	11971(9)	-1078(4)	5855(4)	47(2)
C(16)	11720(10)	-337(4)	6100(5)	65(3)
Br(4)	14425(1)	-1081(1)	5255(1)	75(1)
Br(5)	9987(1)	-1328(1)	5074(1)	58(1)
Br(6)	9265(1)	-200(1)	6633(1)	89(1)

Table 3. Bond lengths [Å] and angles [°] for 20200111.

C(1)-C(2)	1.357(10)	C(9)-C(10)	1.347(10)
C(1)-C(6)	1.378(10)	C(9)-C(14)	1.368(9)
C(1)-N(1)	1.463(10)	C(9)-N(2)	1.469(10)
C(2)-C(3)	1.395(9)	C(10)-C(11)	1.394(9)
C(2)-H(1)	0.9300	C(10)-H(7)	0.9300
C(3)-C(4)	1.387(9)	C(11)-C(12)	1.396(9)
C(3)-H(2)	0.9300	C(11)-H(8)	0.9300
C(4)-C(5)	1.363(9)	C(12)-C(13)	1.360(9)
C(4)-C(7)	1.497(9)	C(12)-C(15)	1.507(9)
C(5)-C(6)	1.363(9)	C(13)-C(14)	1.362(9)
C(5)-H(3)	0.9300	C(13)-H(9)	0.9300
C(6)-H(4)	0.9300	C(14)-H(10)	0.9300
N(1)-O(1)	1.199(9)	N(2)-O(4)	1.201(9)
N(1)-O(2)	1.207(9)	N(2)-O(3)	1.206(9)
C(7)-C(8)	1.505(10)	C(15)-C(16)	1.497(10)
C(7)-Br(2)	1.939(7)	C(15)-Br(5)	1.953(7)
C(7)-Br(1)	1.989(7)	C(15)-Br(4)	1.986(7)
C(8)-Br(3)	1.961(7)	C(16)-Br(6)	1.952(7)
C(8)-H(5)	0.9700	C(16)-H(11)	0.9700
C(8)-H(6)	0.9700	C(16)-H(12)	0.9700

C(2)-C(1)-C(6)	121.5(8)	C(3)-C(4)-C(7)	121.4(8)
C(2)-C(1)-N(1)	118.4(9)	C(4)-C(5)-C(6)	123.3(8)
C(6)-C(1)-N(1)	120.2(9)	C(4)-C(5)-H(3)	118.4
C(1)-C(2)-C(3)	119.0(8)	C(6)-C(5)-H(3)	118.4
C(1)-C(2)-H(1)	120.5	C(5)-C(6)-C(1)	118.1(8)
C(3)-C(2)-H(1)	120.5	C(5)-C(6)-H(4)	121.0
C(4)-C(3)-C(2)	120.7(8)	C(1)-C(6)-H(4)	121.0
C(4)-C(3)-H(2)	119.7	O(1)-N(1)-O(2)	123.4(10)
C(2)-C(3)-H(2)	119.7	O(1)-N(1)-C(1)	118.5(10)
C(5)-C(4)-C(3)	117.5(7)	O(2)-N(1)-C(1)	118.0(10)
C(5)-C(4)-C(7)	121.1(7)	C(4)-C(7)-C(8)	118.3(7)

C(4)-C(7)-Br(2)	111.4(6)	C(16)-C(15)-Br(5)	109.2(5)
C(8)-C(7)-Br(2)	108.9(5)	C(12)-C(15)-Br(5)	110.2(5)
C(4)-C(7)-Br(1)	107.5(5)	C(16)-C(15)-Br(4)	103.9(5)
C(8)-C(7)-Br(1)	102.4(5)	C(12)-C(15)-Br(4)	107.9(5)
Br(2)-C(7)-Br(1)	107.4(3)	Br(5)-C(15)-Br(4)	106.8(3)
C(7)-C(8)-Br(3)	110.2(5)	C(15)-C(16)-Br(6)	110.8(5)
C(7)-C(8)-H(5)	109.6	C(15)-C(16)-H(11)	109.5
Br(3)-C(8)-H(5)	109.6	Br(6)-C(16)-H(11)	109.5
C(7)-C(8)-H(6)	109.6	C(15)-C(16)-H(12)	109.5
Br(3)-C(8)-H(6)	109.6	Br(6)-C(16)-H(12)	109.5
H(5)-C(8)-H(6)	108.1	H(11)-C(16)-H(12)	108.1
C(10)-C(9)-C(14)	122.0(8)		
C(10)-C(9)-N(2)	117.6(8)		
C(14)-C(9)-N(2)	120.4(9)		
C(9)-C(10)-C(11)	119.1(8)		
C(9)-C(10)-H(7)	120.4		
C(11)-C(10)-H(7)	120.4		
C(10)-C(11)-C(12)	119.4(8)		
C(10)-C(11)-H(8)	120.3		
C(12)-C(11)-H(8)	120.3		
C(13)-C(12)-C(11)	119.0(7)		
C(13)-C(12)-C(15)	120.7(7)		
C(11)-C(12)-C(15)	120.3(7)		
C(12)-C(13)-C(14)	121.6(7)		
C(12)-C(13)-H(9)	119.2		
C(14)-C(13)-H(9)	119.2		
C(13)-C(14)-C(9)	118.9(8)		
C(13)-C(14)-H(10)	120.6		
C(9)-C(14)-H(10)	120.6		
O(4)-N(2)-O(3)	121.8(9)		
O(4)-N(2)-C(9)	119.4(9)		
O(3)-N(2)-C(9)	118.8(9)		
C(16)-C(15)-C(12)	118.1(7)		

Symmetry transformations used to generate equivalent atoms:

Figure 2. ORTEP drawing for Tellurium dibromide **5e**.

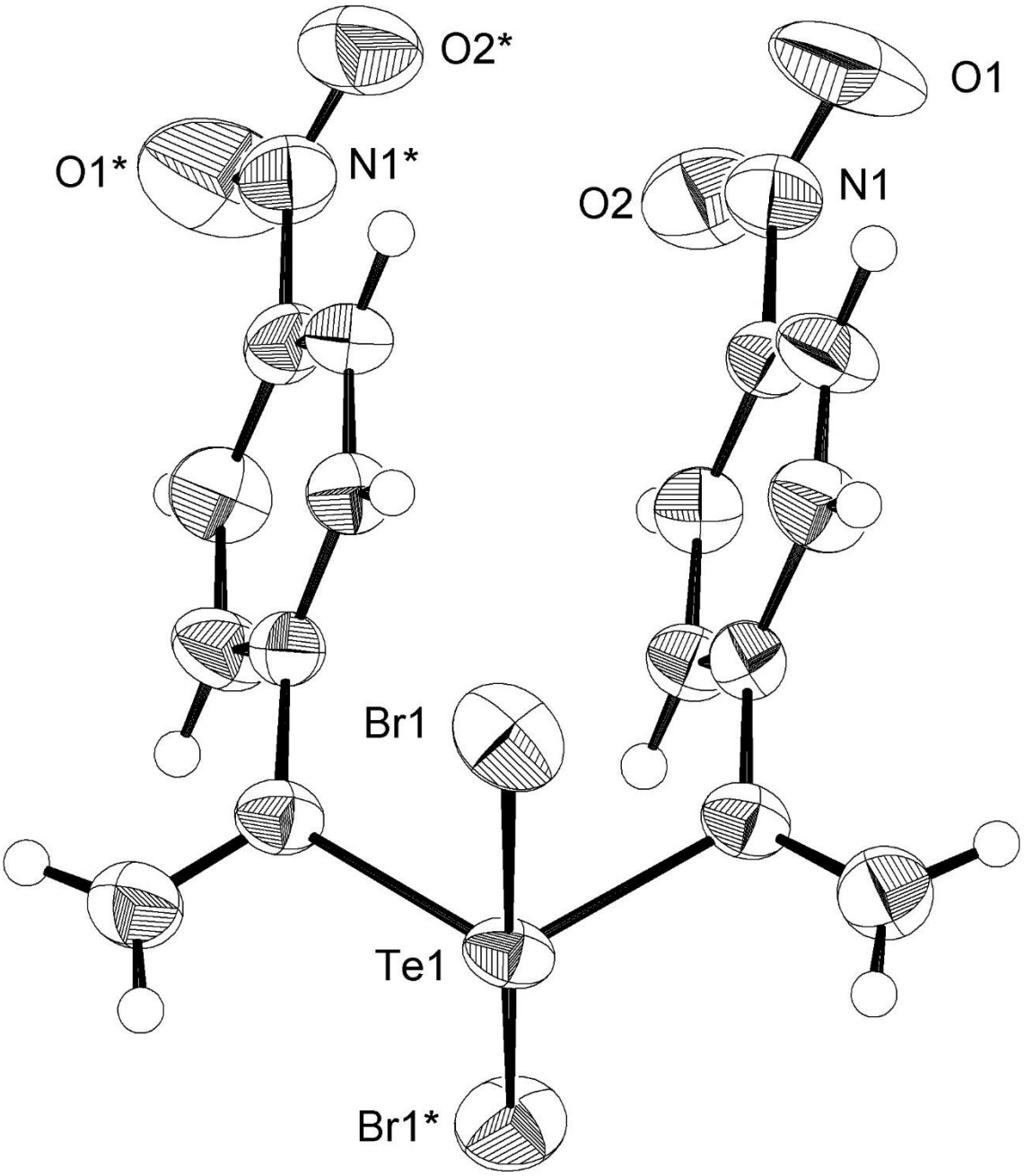


Table 4. Crystal data and structure refinement for tellurium dibromide **5e** (200123).

Identification code	200123	
Empirical formula	C16 H12 Br2 N2 O4 Te	
Formula weight	583.70	
Temperature	293(2) K	
Wavelength	0.71075 Å	
Crystal system	monoclinic	
Space group	*C*2/c	
Unit cell dimensions	a = 15.726(10) Å	α= 90°.
	b = 10.425(5) Å	β= 121.565(8)°.
	c = 13.630(8) Å	γ = 90°.
Volume	1904.0(18) $Å^3$	
Z	4	
Density (calculated)	2.036 Mg/m^3	
Absorption coefficient	5.782 mm^{-1}	
F(000)	1104	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	3.46 to 25.99°.	
Index ranges	-19<=h<=19, -12<=k<=12, -16<=l<=16	
Reflections collected	9702	
Independent reflections	1875 [R(int) = 0.0400]	
Completeness to theta = 25.99°	99.8 %	
Max. and min. transmission	0.5956 and 0.3910	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1875 / 0 / 114	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0720	
R indices (all data)	R1 = 0.0437, wR2 = 0.0764	
Largest diff. peak and hole	1.646 and -0.512 e.$Å^{-3}$	

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 200123. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Te(1)	0	370(1)	7500	39(1)
Br(1)	1837(1)	566(1)	9347(1)	62(1)
C(1)	519(3)	1528(3)	6628(3)	39(1)
C(2)	920(3)	836(4)	6182(4)	54(1)
C(3)	476(3)	2947(3)	6601(3)	36(1)
C(4)	1371(3)	3612(4)	7091(4)	51(1)
C(5)	1375(3)	4938(4)	7064(4)	53(1)
C(6)	479(3)	5562(3)	6541(4)	41(1)
C(7)	-414(3)	4933(4)	6041(3)	42(1)
C(8)	-414(3)	3608(4)	6070(3)	39(1)
N(1)	479(3)	6975(3)	6528(3)	54(1)
O(1)	1247(3)	7534(3)	6865(4)	106(2)
O(2)	-311(3)	7525(3)	6162(3)	75(1)

Table 6. Bond lengths [Å] and angles [°] for 200123.

Te(1)-C(1)#1	2.133(4)	C(4)-H(3)	0.9300
Te(1)-C(1)	2.133(4)	C(5)-C(6)	1.365(6)
Te(1)-Br(1)	2.6669(13)	C(5)-H(4)	0.9300
Te(1)-Br(1)#1	2.6669(13)	C(6)-C(7)	1.366(6)
C(1)-C(2)	1.299(6)	C(6)-N(1)	1.473(5)
C(1)-C(3)	1.481(5)	C(7)-C(8)	1.382(5)
C(2)-H(1)	0.9300	C(7)-H(5)	0.9300
C(2)-H(2)	0.9300	C(8)-H(6)	0.9300
C(3)-C(8)	1.377(5)	N(1)-O(1)	1.195(5)
C(3)-C(4)	1.387(5)	N(1)-O(2)	1.213(5)
C(4)-C(5)	1.383(6)		

C(1)#1-Te(1)-C(1)	111.1(2)	C(6)-C(5)-H(4)	120.9
C(1)#1-Te(1)-Br(1)	88.40(11)	C(4)-C(5)-H(4)	120.9
C(1)-Te(1)-Br(1)	86.63(11)	C(5)-C(6)-C(7)	122.8(4)
C(1)#1-Te(1)-Br(1)#1	86.63(11)	C(5)-C(6)-N(1)	118.5(4)
C(1)-Te(1)-Br(1)#1	88.40(11)	C(7)-C(6)-N(1)	118.7(4)
Br(1)-Te(1)-Br(1)#1	171.20(3)	C(6)-C(7)-C(8)	118.8(4)
C(2)-C(1)-C(3)	124.8(4)	C(6)-C(7)-H(5)	120.6
C(2)-C(1)-Te(1)	111.6(3)	C(8)-C(7)-H(5)	120.6
C(3)-C(1)-Te(1)	123.6(3)	C(3)-C(8)-C(7)	120.0(4)
C(1)-C(2)-H(1)	120.0	C(3)-C(8)-H(6)	120.0
C(1)-C(2)-H(2)	120.0	C(7)-C(8)-H(6)	120.0
H(1)-C(2)-H(2)	120.0	O(1)-N(1)-O(2)	122.5(4)
C(8)-C(3)-C(4)	119.9(4)	O(1)-N(1)-C(6)	119.3(4)
C(8)-C(3)-C(1)	122.3(3)	O(2)-N(1)-C(6)	118.2(4)
C(4)-C(3)-C(1)	117.7(3)		
C(5)-C(4)-C(3)	120.3(4)		
C(5)-C(4)-H(3)	119.9		
C(3)-C(4)-H(3)	119.9		
C(6)-C(5)-C(4)	118.2(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2

Table 7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 200123. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Te(1)	33(1)	28(1)	50(1)	0	18(1)	0
Br(1)	34(1)	74(1)	59(1)	13(1)	13(1)	4(1)
C(1)	32(2)	35(2)	46(2)	2(2)	17(2)	0(2)
C(2)	58(3)	44(2)	64(3)	2(2)	35(3)	5(2)
C(3)	35(2)	35(2)	38(2)	3(2)	20(2)	2(2)
C(4)	36(2)	46(2)	72(3)	4(2)	28(2)	6(2)
C(5)	40(3)	44(2)	74(3)	-4(2)	29(2)	-11(2)
C(6)	51(3)	33(2)	44(3)	0(2)	28(2)	-4(2)
C(7)	41(2)	36(2)	44(2)	6(2)	20(2)	8(2)
C(8)	32(2)	40(2)	42(2)	-1(2)	16(2)	-3(2)
N(1)	68(3)	35(2)	66(3)	0(2)	39(2)	-4(2)
O(1)	84(3)	47(2)	185(5)	-7(2)	69(3)	-21(2)
O(2)	90(3)	42(2)	87(3)	1(2)	43(3)	11(2)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 200123.

	x	y	z	U(eq)
H(1)	1208	1231	5813	65
H(2)	920	-53	6232	65
H(3)	1971	3164	7440	62
H(4)	1971	5392	7393	64
H(5)	-1011	5387	5687	50
H(6)	-1015	3163	5731	47

Table 9. Torsion angles [°] for 200123.

C(1)#1-Te(1)-C(1)-C(2)	174.1(4)
Br(1)-Te(1)-C(1)-C(2)	87.2(3)
Br(1)#1-Te(1)-C(1)-C(2)	-100.1(3)
C(1)#1-Te(1)-C(1)-C(3)	-2.5(3)
Br(1)-Te(1)-C(1)-C(3)	-89.5(3)
Br(1)#1-Te(1)-C(1)-C(3)	83.3(3)
C(2)-C(1)-C(3)-C(8)	118.9(5)
Te(1)-C(1)-C(3)-C(8)	-64.9(5)
C(2)-C(1)-C(3)-C(4)	-58.3(6)
Te(1)-C(1)-C(3)-C(4)	117.9(4)
C(8)-C(3)-C(4)-C(5)	0.9(7)
C(1)-C(3)-C(4)-C(5)	178.3(4)
C(3)-C(4)-C(5)-C(6)	-0.2(7)
C(4)-C(5)-C(6)-C(7)	-0.4(7)
C(4)-C(5)-C(6)-N(1)	178.9(4)
C(5)-C(6)-C(7)-C(8)	0.4(7)
N(1)-C(6)-C(7)-C(8)	-178.9(4)
C(4)-C(3)-C(8)-C(7)	-0.9(6)
C(1)-C(3)-C(8)-C(7)	-178.2(4)
C(6)-C(7)-C(8)-C(3)	0.3(6)
C(5)-C(6)-N(1)-O(1)	7.6(7)
C(7)-C(6)-N(1)-O(1)	-173.1(5)
C(5)-C(6)-N(1)-O(2)	-173.0(4)
C(7)-C(6)-N(1)-O(2)	6.3(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2