Electronic Supplementary Material (ESI) for Dalton Transactions
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Supporting Information

Isolation and molecular structures of novel organotellurium(IV) halides, oxyhalide and mixed halide

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[b] *Department of Chemistry, Howard University, Washington, DC* 20059, *USA*

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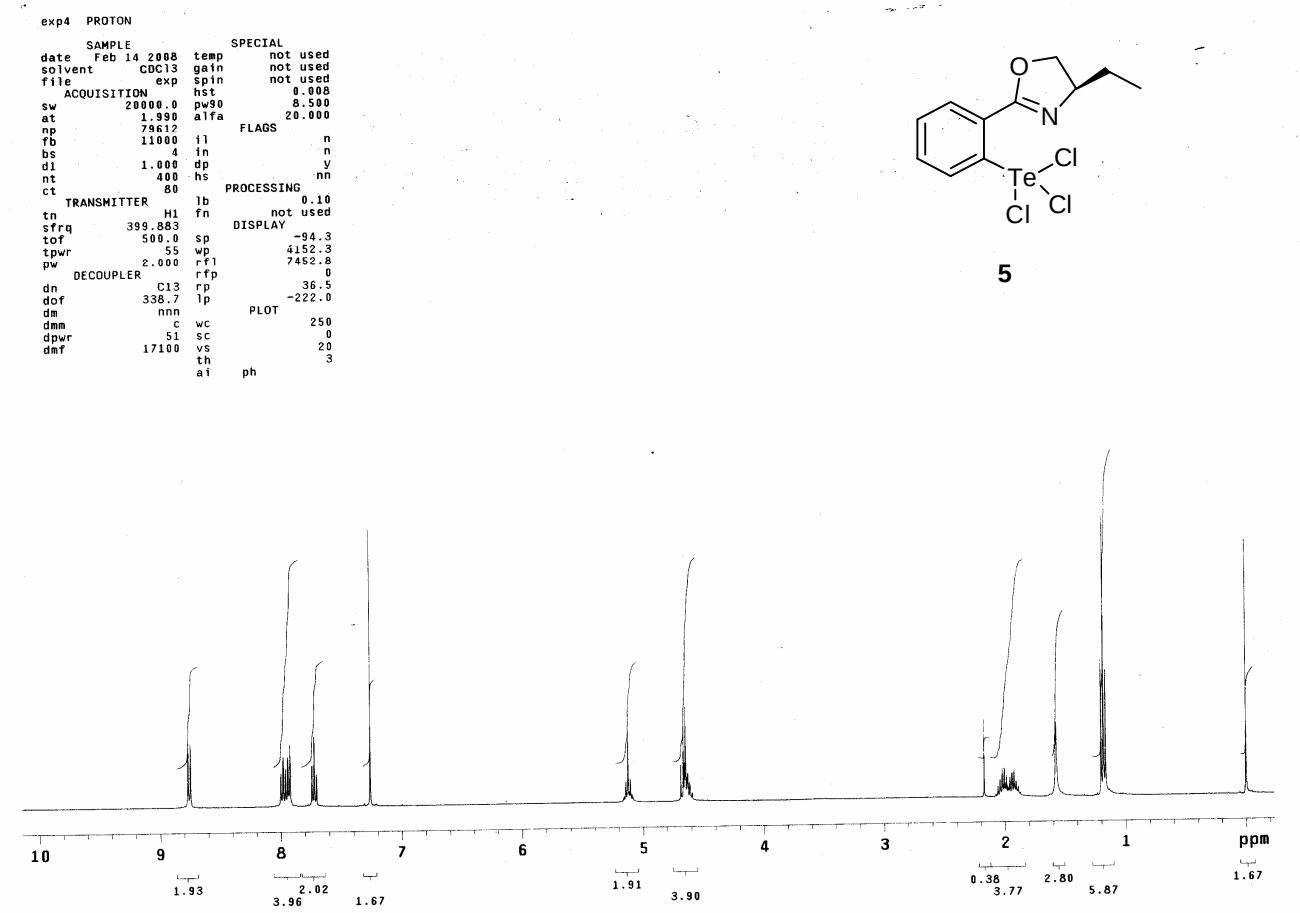

Figure S1. ^{1}H NMR spectrum of compound **5**.

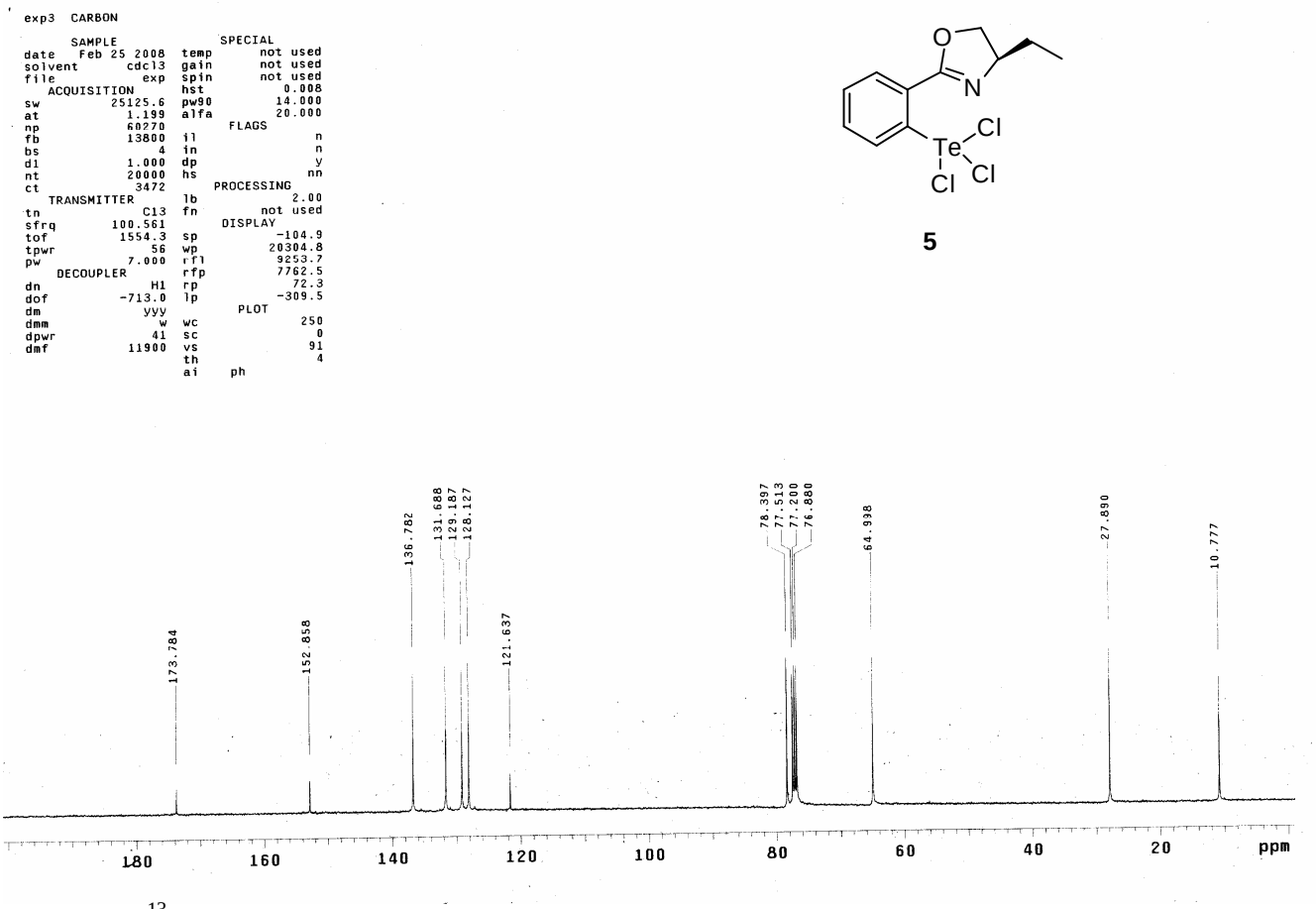

Figure S2. ^{13}C NMR spectrum of compound **5**.

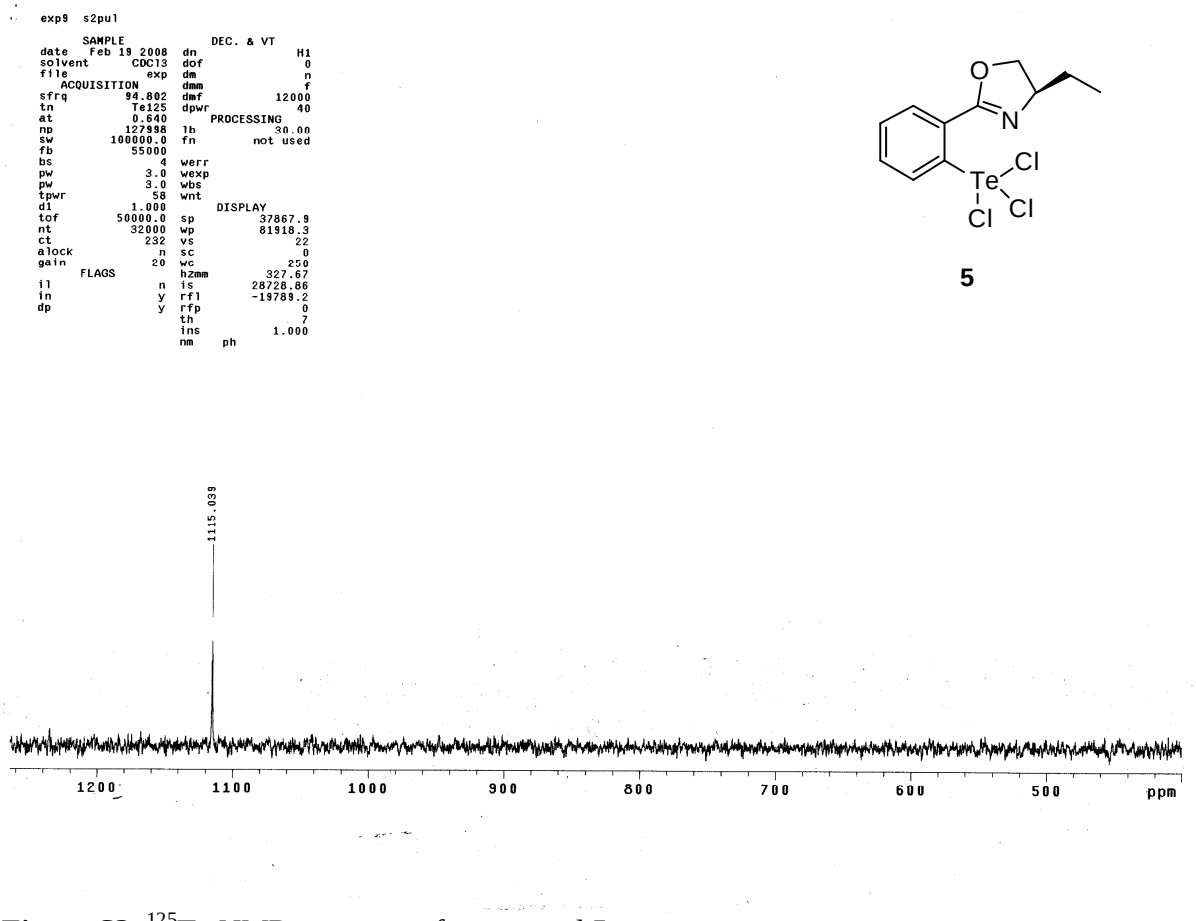

Figure S3. ^{125}Te NMR spectrum of compound **5**.

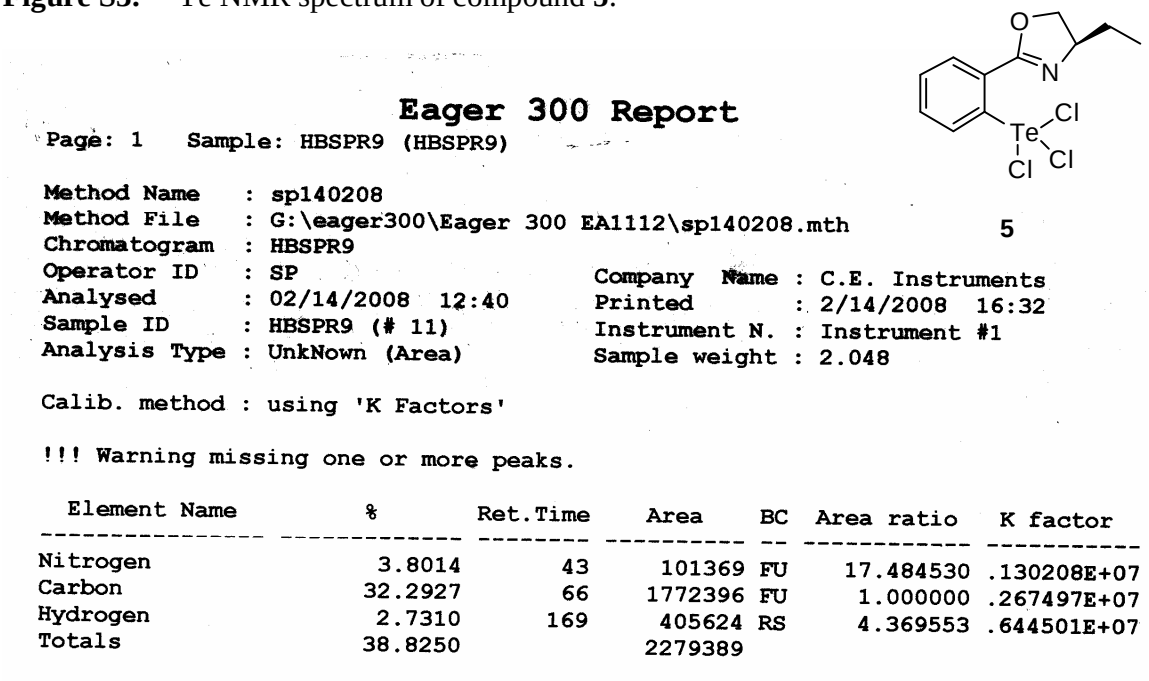

Figure S4. CHN analysis of compound **5**.

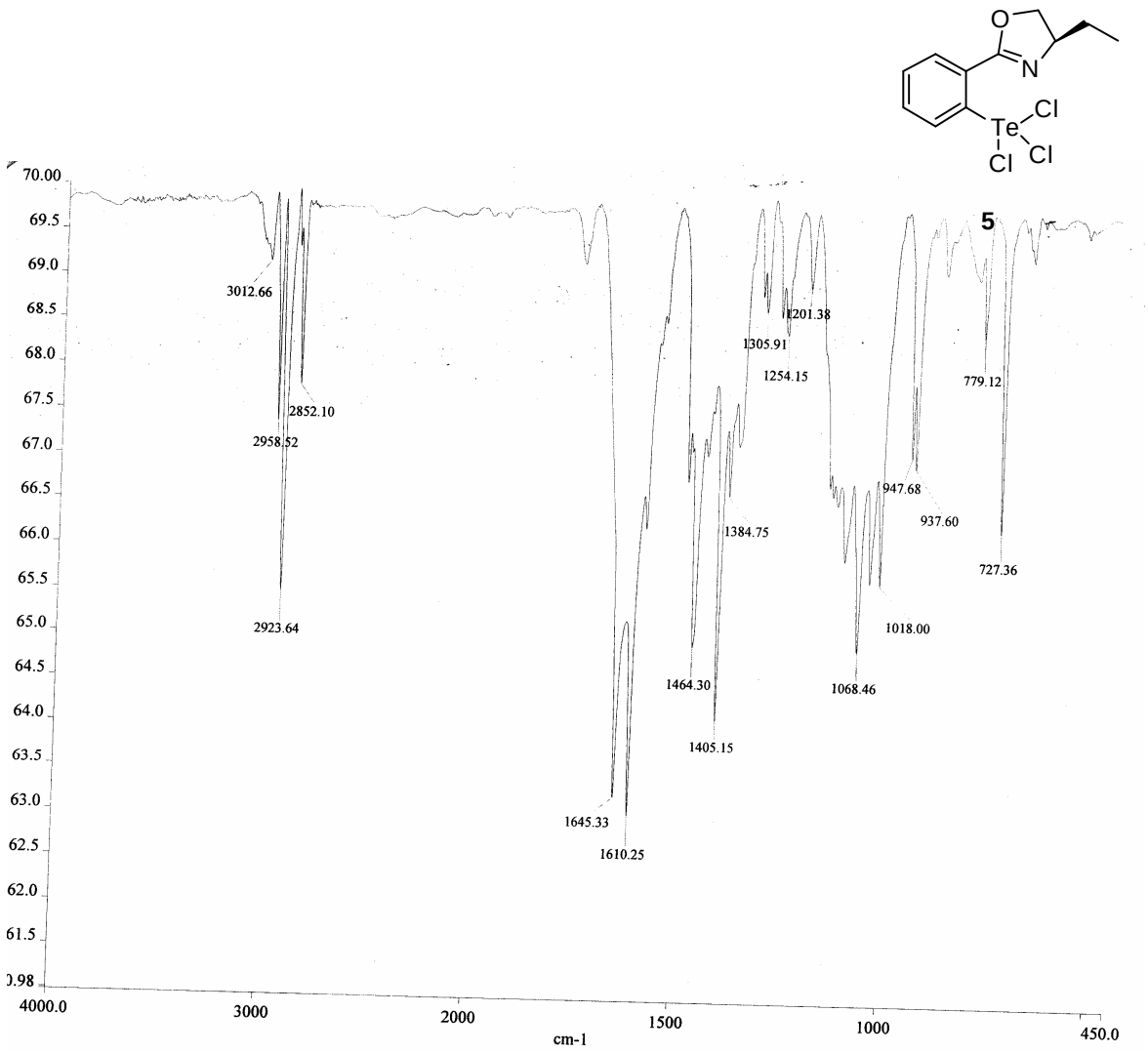

Figure S5. FT-IR spectrum of compound **5**.

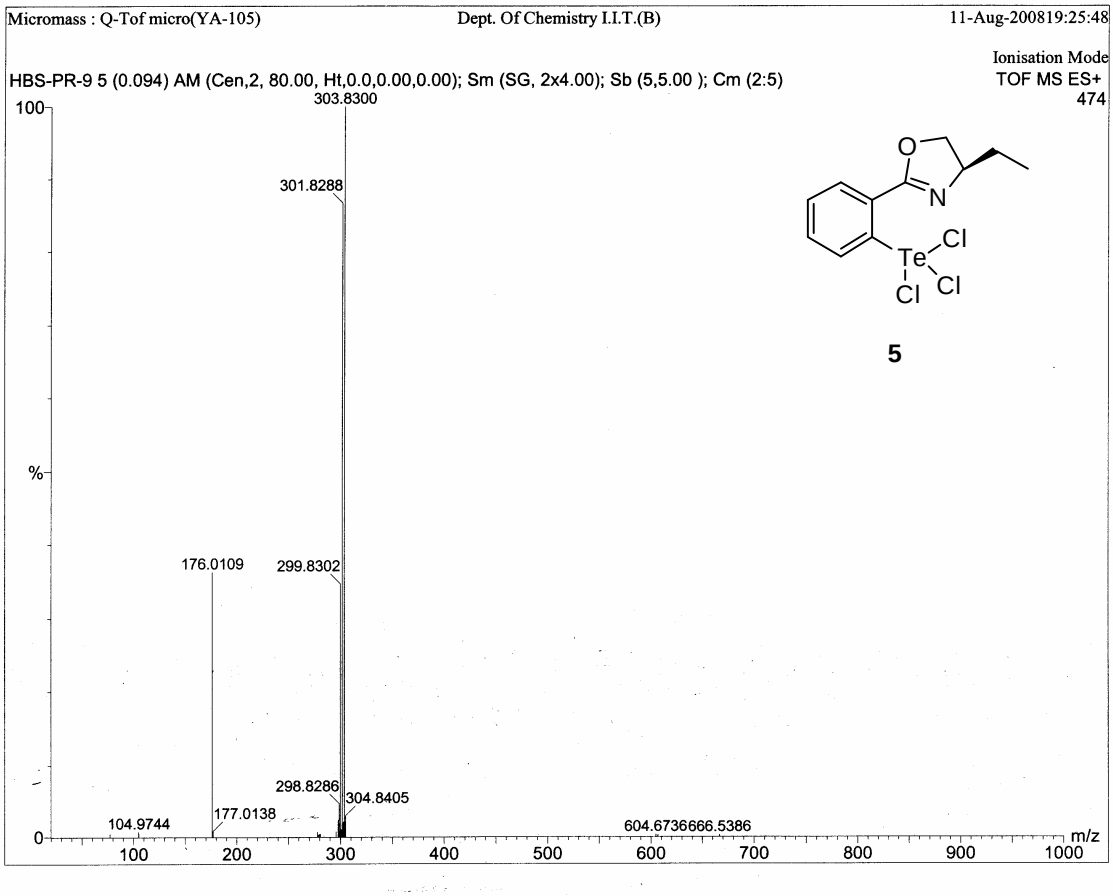

Figure S6. ESI Mass spectrum of compound **5**.

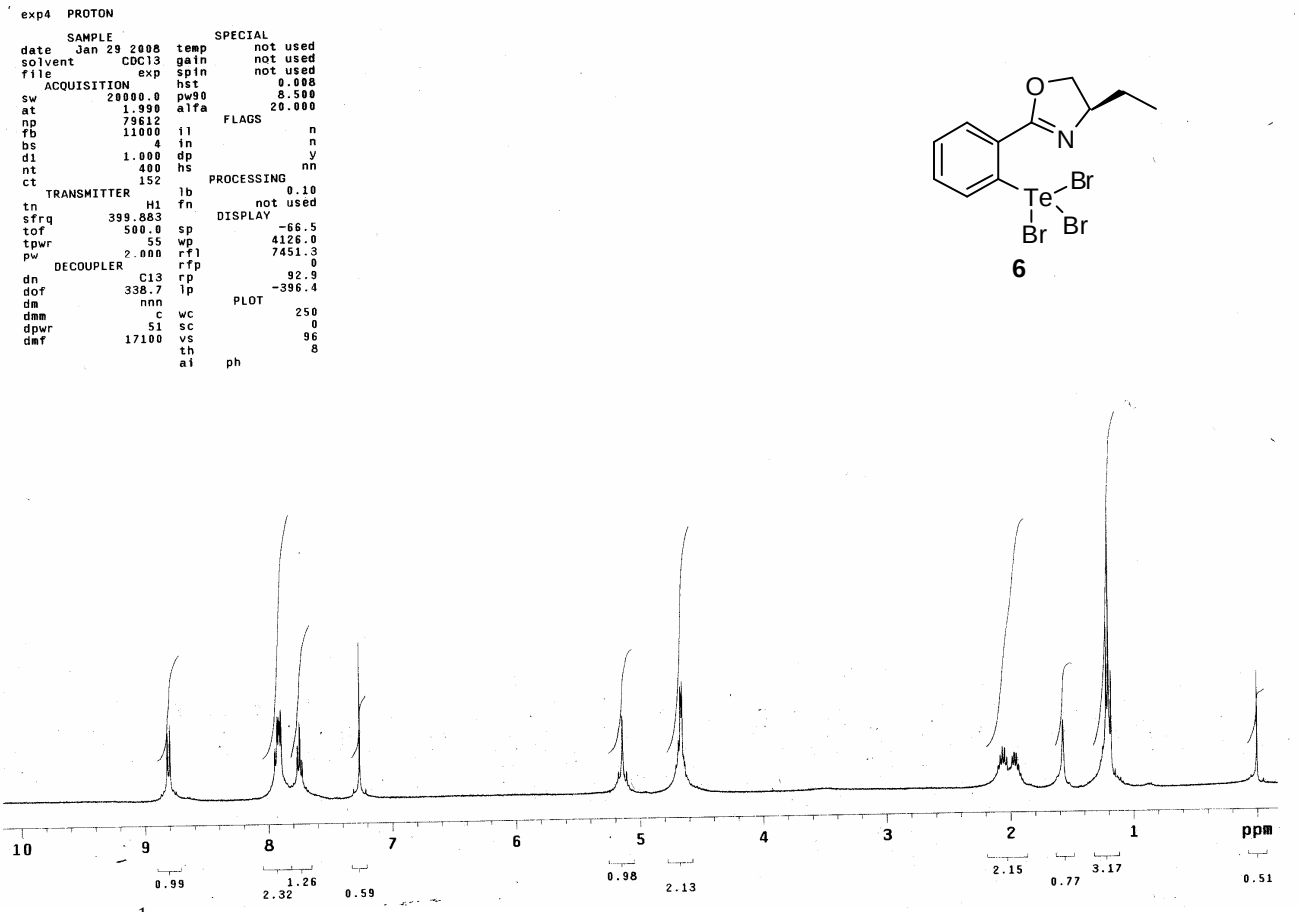

Figure S7. ^{1}H NMR spectrum of compound **6**.

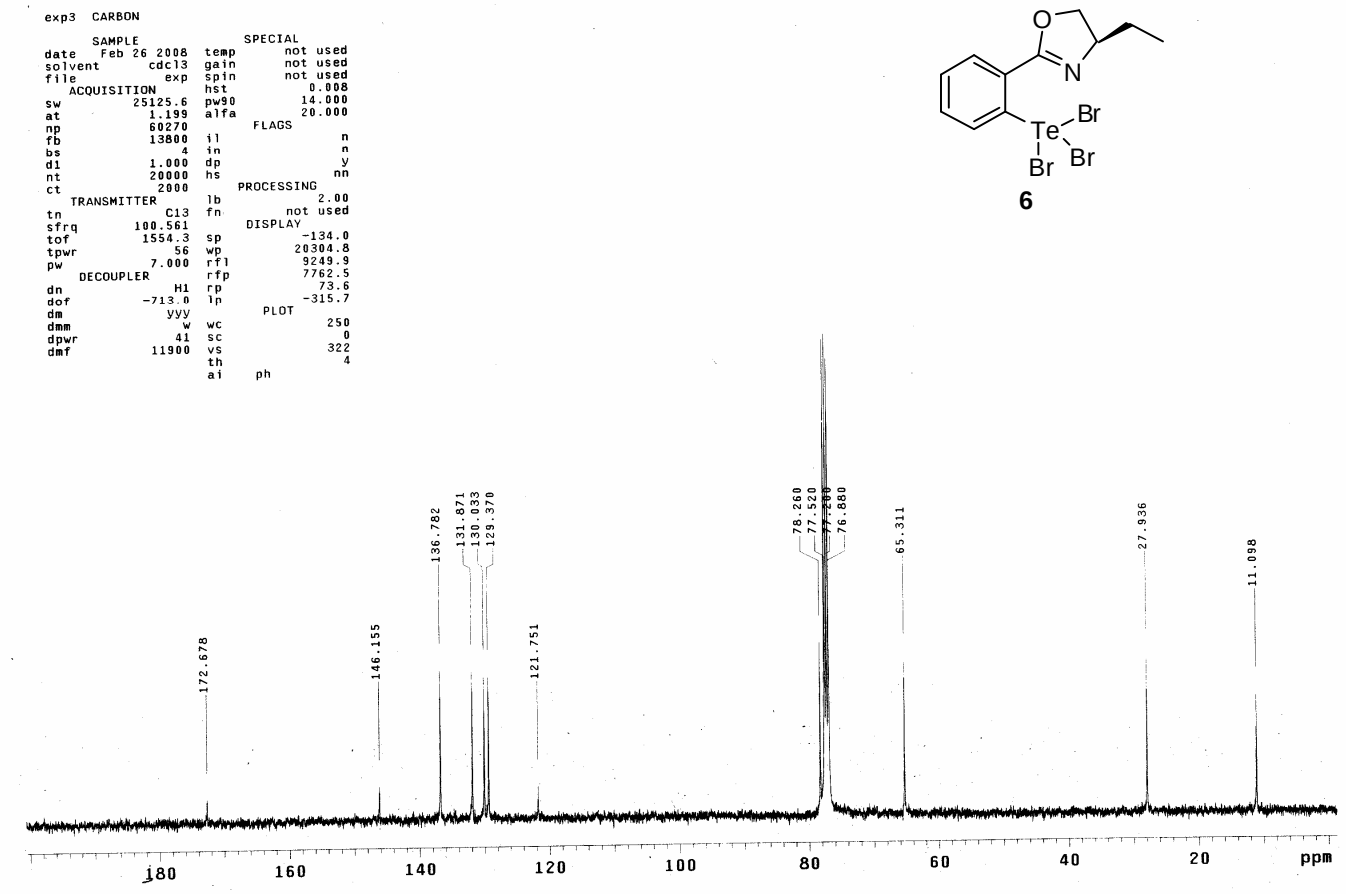

Figure S8. ^{13}C NMR spectrum of compound **6**.

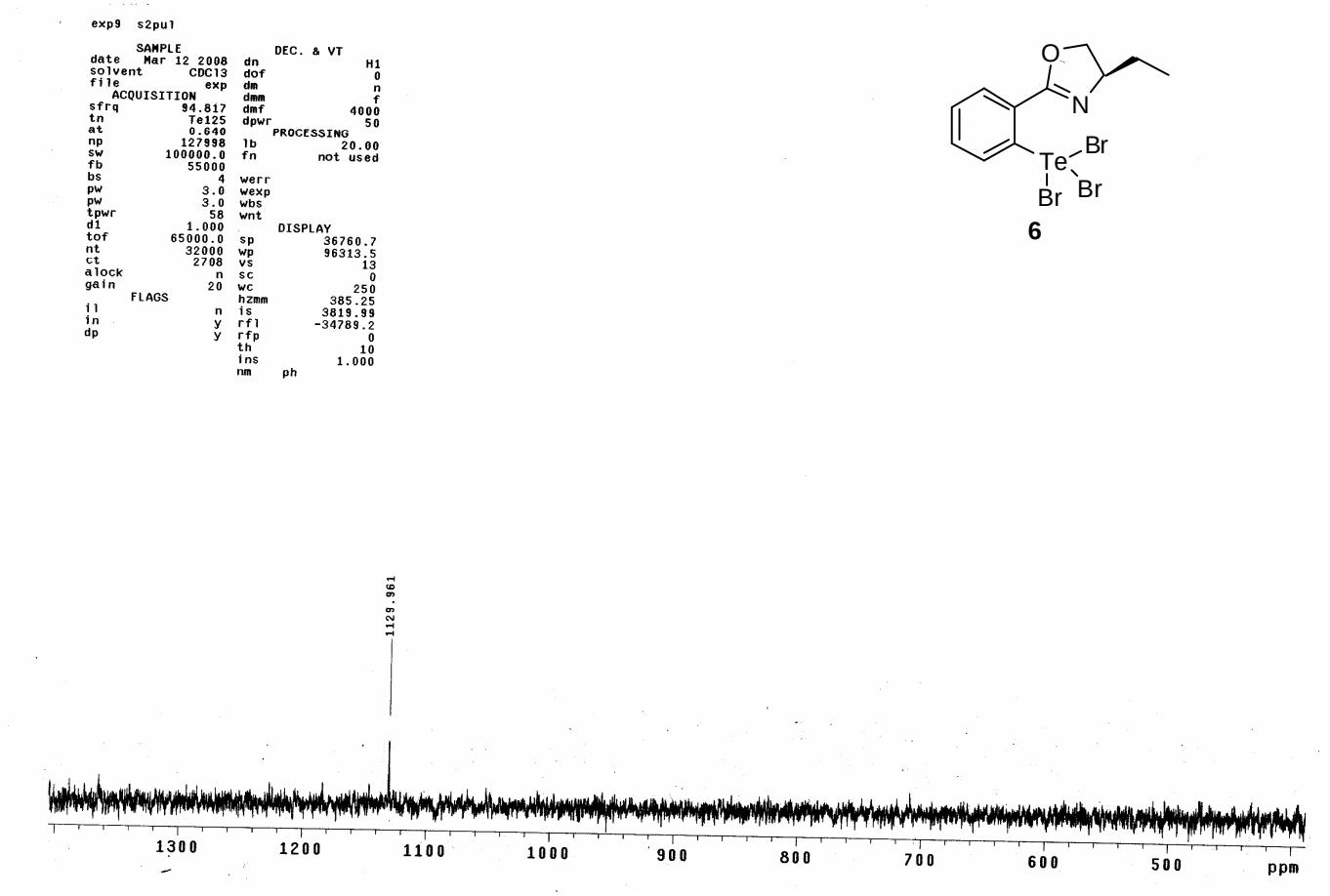

Figure S9. ^{125}Te NMR spectrum of compound **6**.

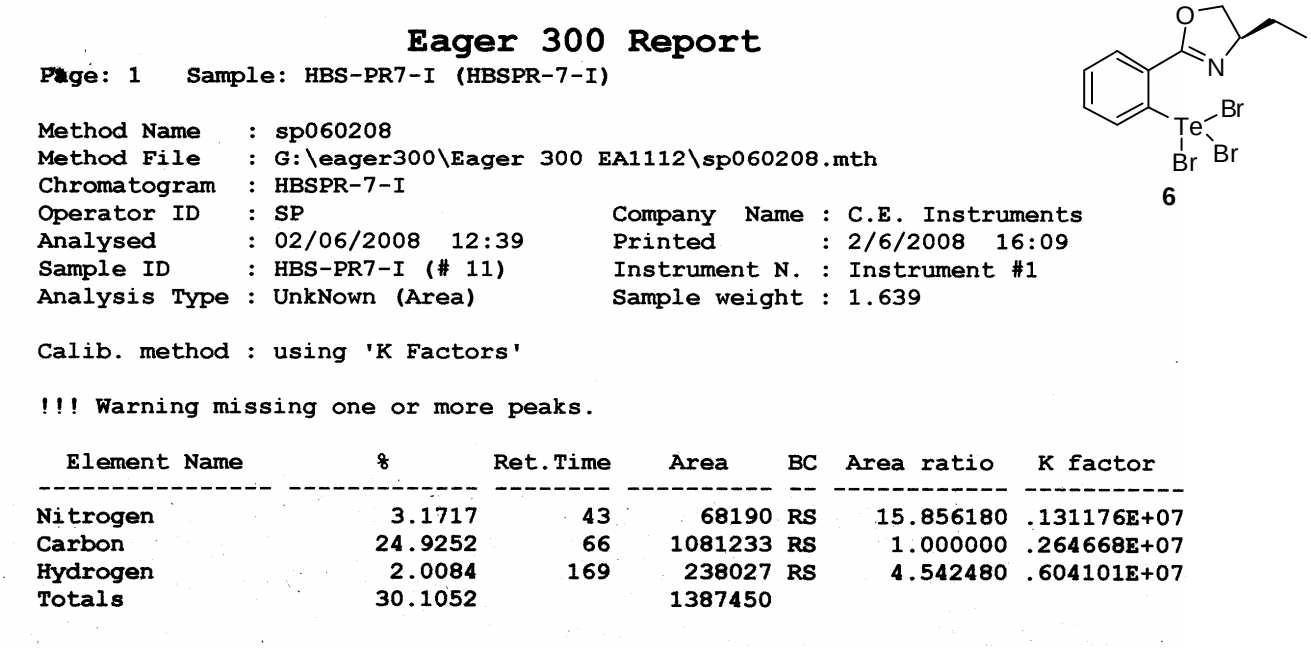

Figure S10. CHN analysis of compound **6**.

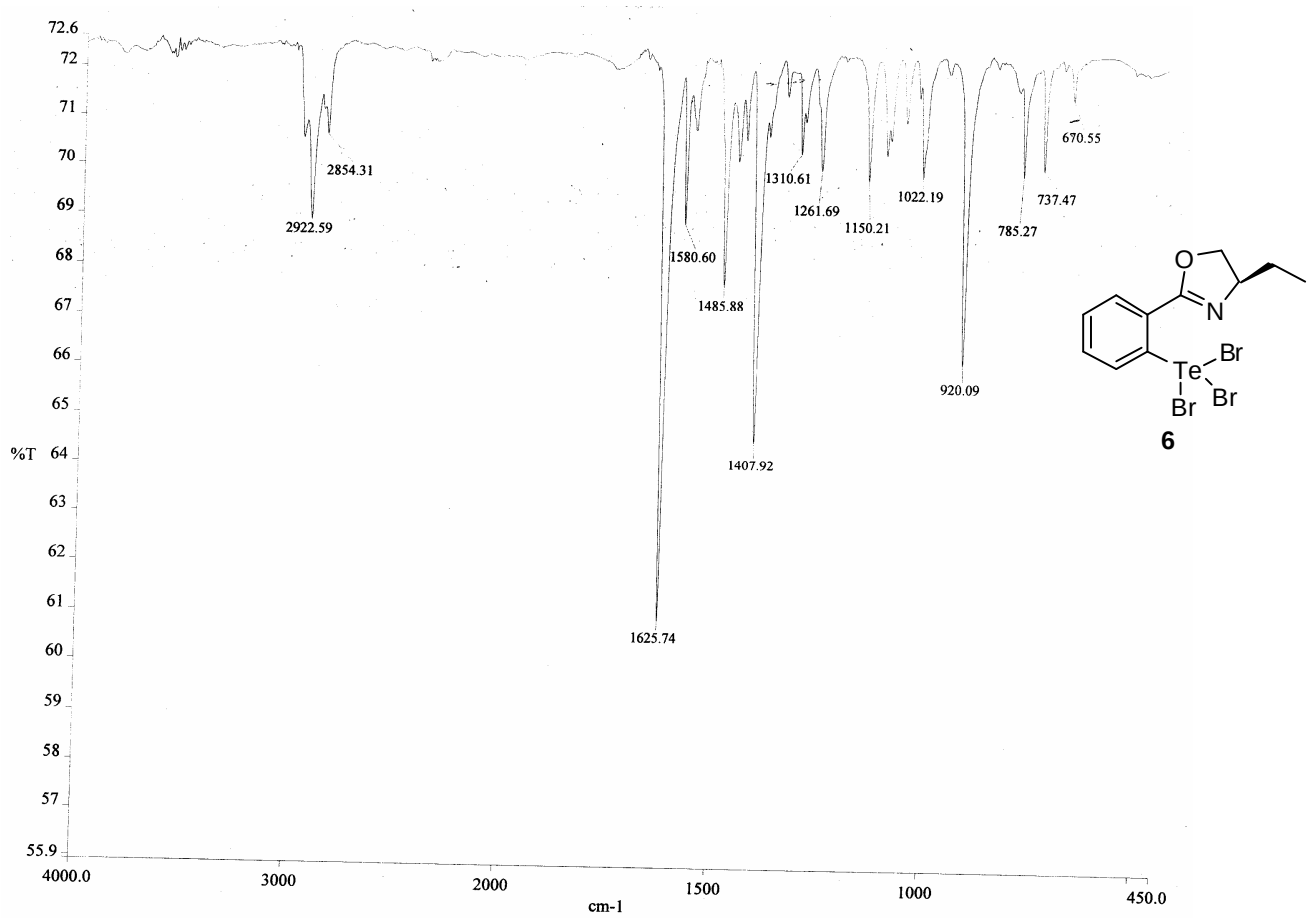

Figure S11. FT-IR spectrum of compound **6**.

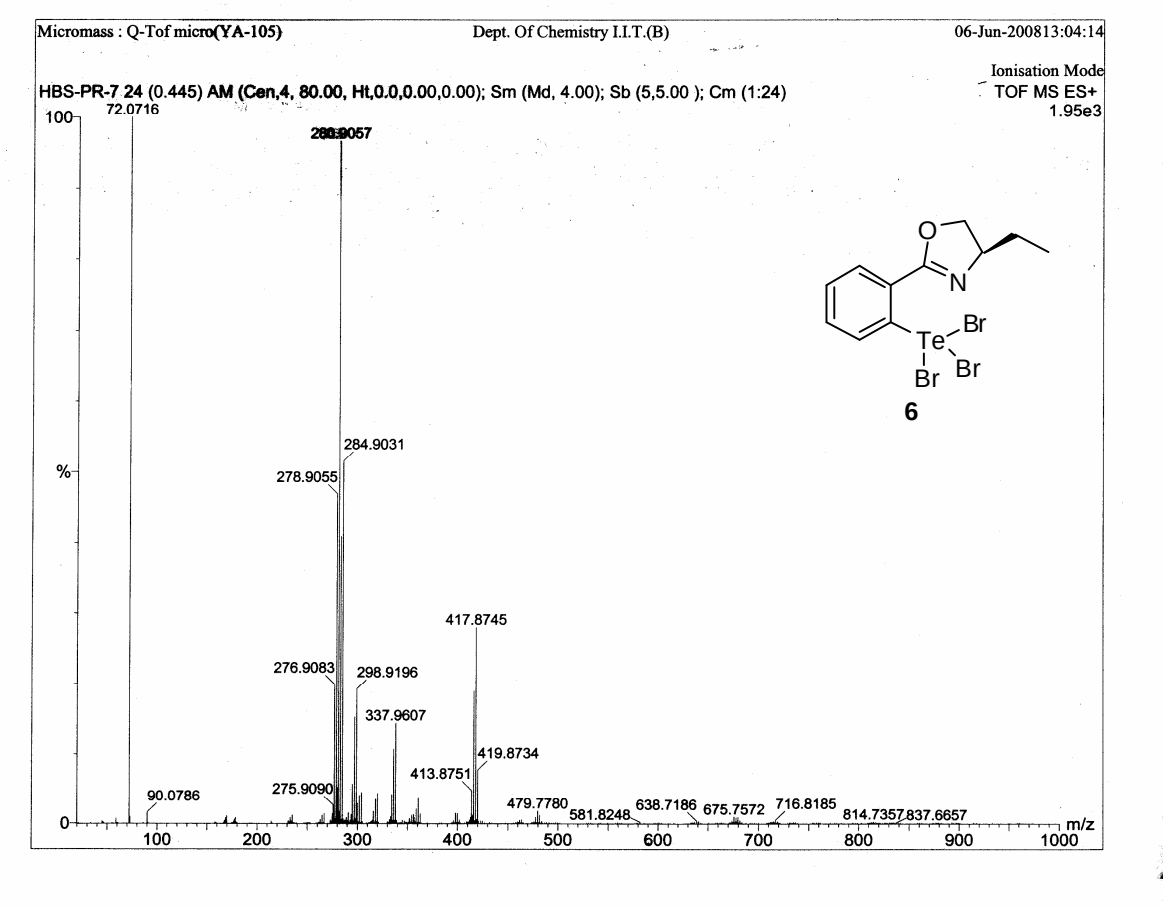

Figure S12. ESI Mass spectrum of compound **6**.

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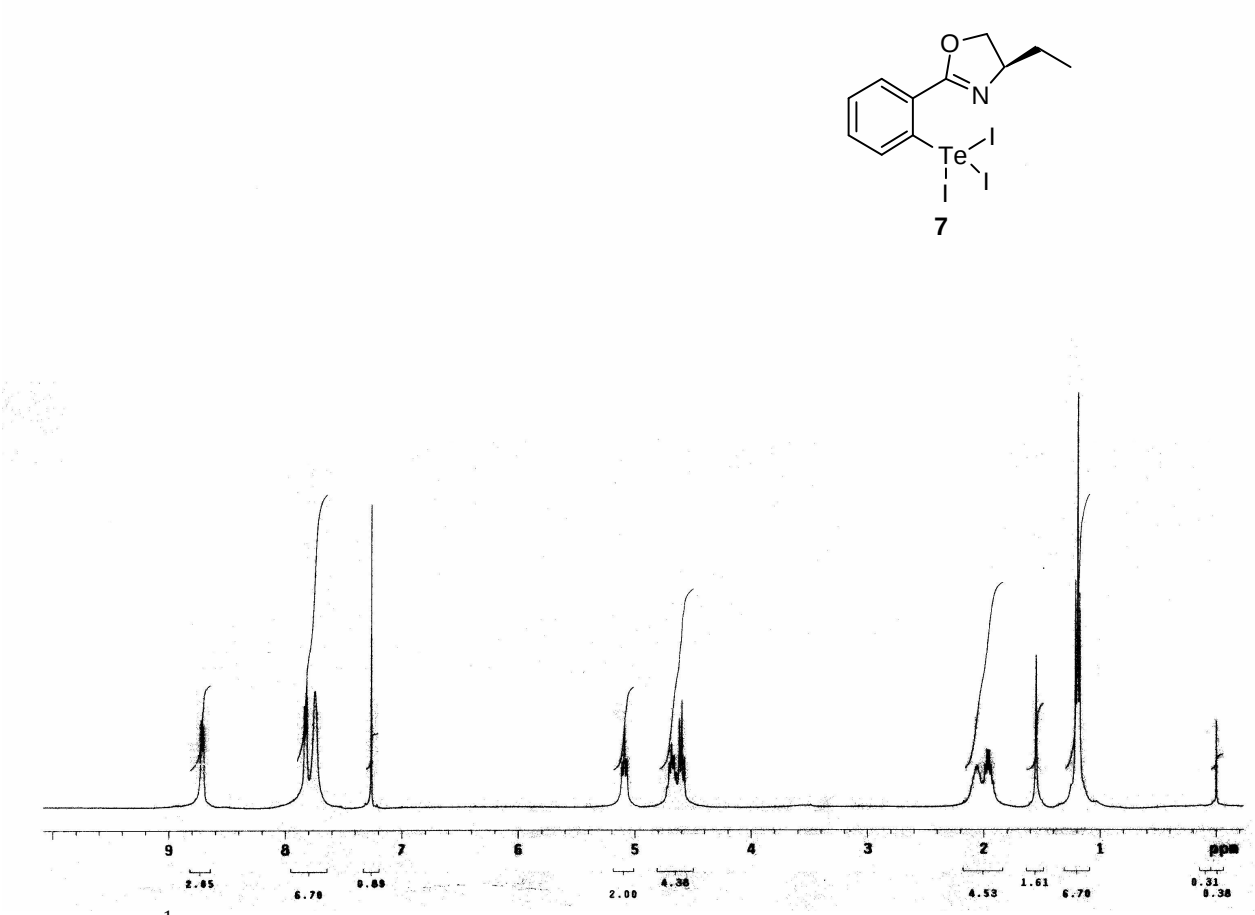


Figure S13. ^{1}H NMR spectrum of compound **7**.

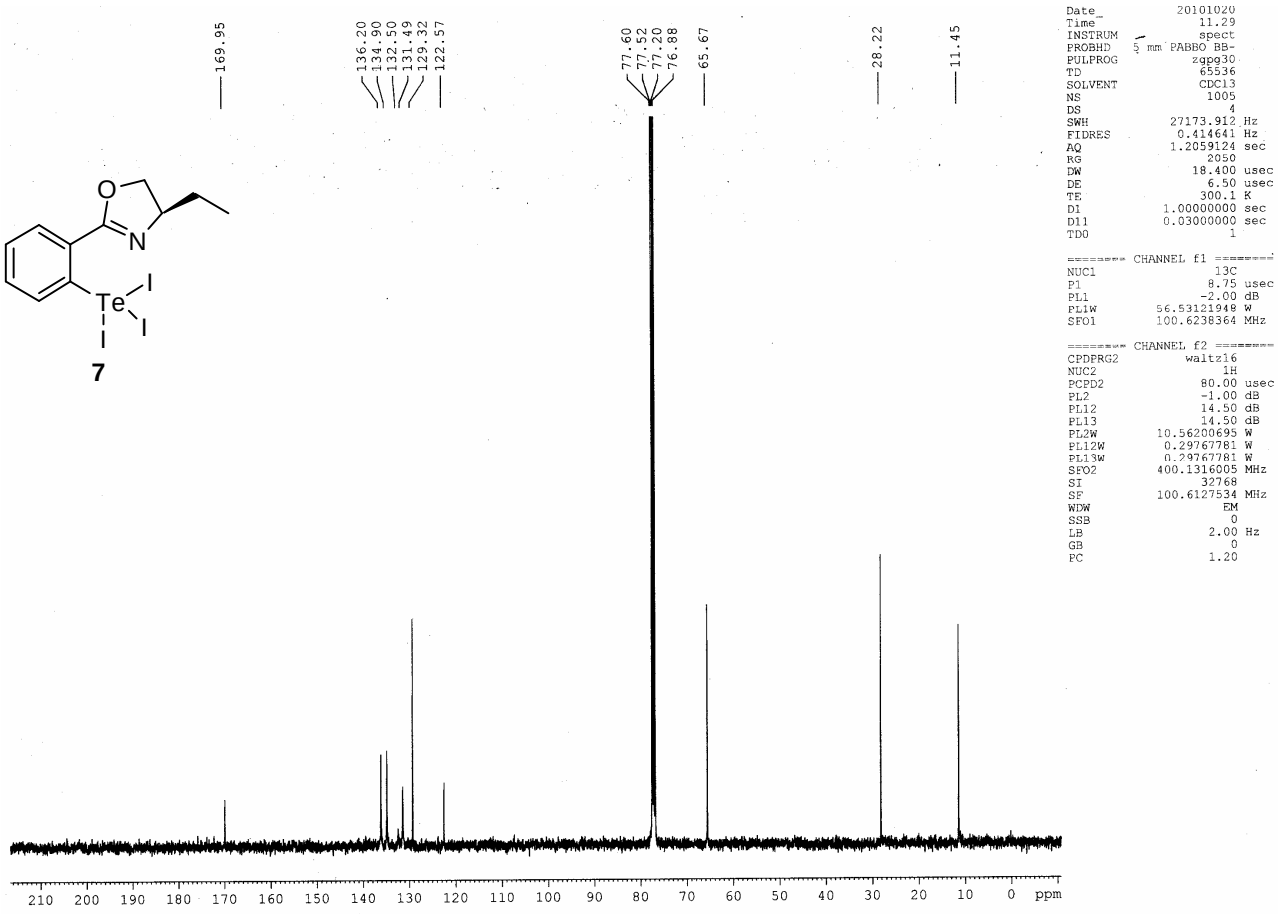
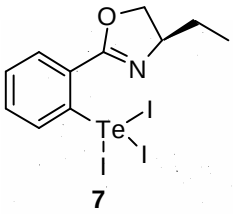


Figure S14. ^{13}C NMR spectrum of compound **7**.



7

1096.66

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RG	32
DW	1.000 usec
DE	6.50 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
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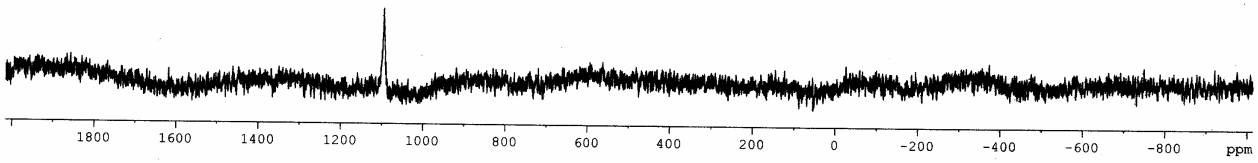
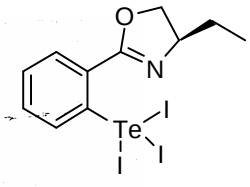


Figure S15. ^{125}Te NMR spectrum of compound **7**.



7

Eager 300 Report

Page: 1 Sample: PR8 (PR8)

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Method File : D:\CHNS2008\SP290708.mth
Chromatogram : PR8
Operator ID : SP **Company Name : C.E. Instruments**
Analysed : 07/29/2008 11:47 **Printed : 7/29/2008 15:29**
Sample ID : PR8 (# 6) **Instrument N. : Instrument #1**
Analysis Type : UnkNown (Area) **Sample weight : 1.474**

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	2.0339	2.05 43	28987	RS	24.846210	966894.1000
Carbon	19.8849	19.36 67	720217	RS	1.000000	.244629E+07
Hydrogen	1.6081	1.77 172	164111	RS	4.388597	.631820E+07
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Figure S16. CHN analysis of compound **7**.

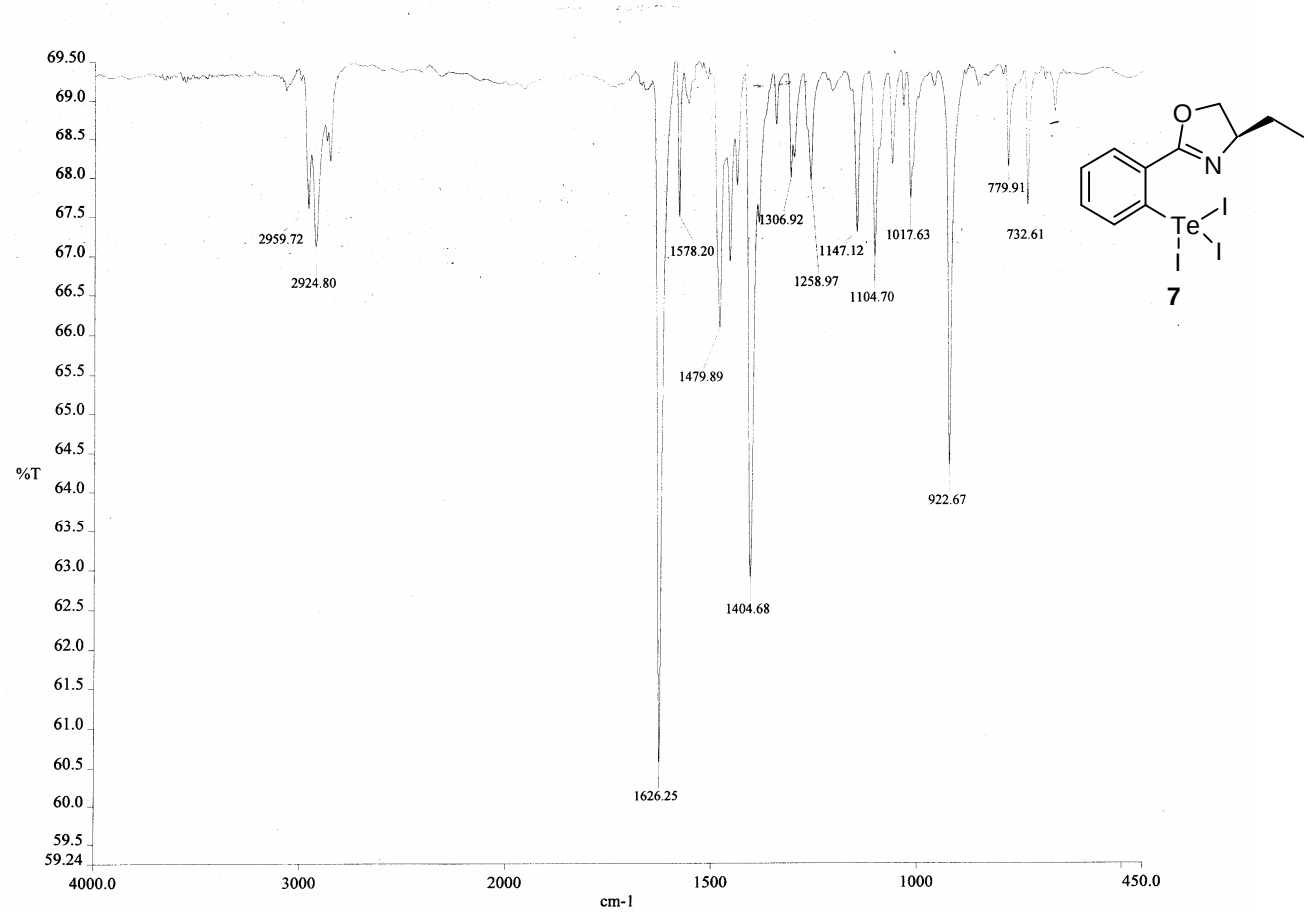


Figure S17. FT-IR spectrum of compound **7**.

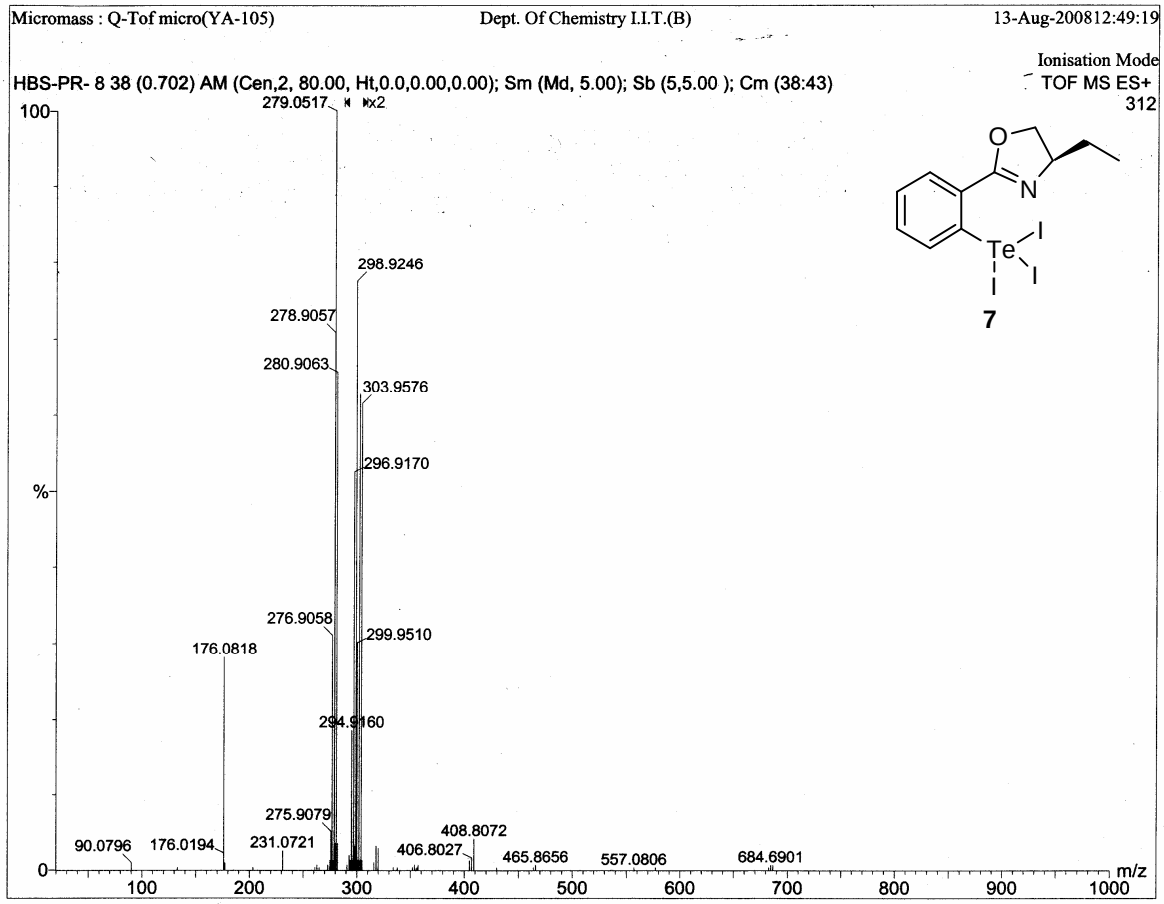


Figure S18. ESI Mass spectrum of compound **7**.

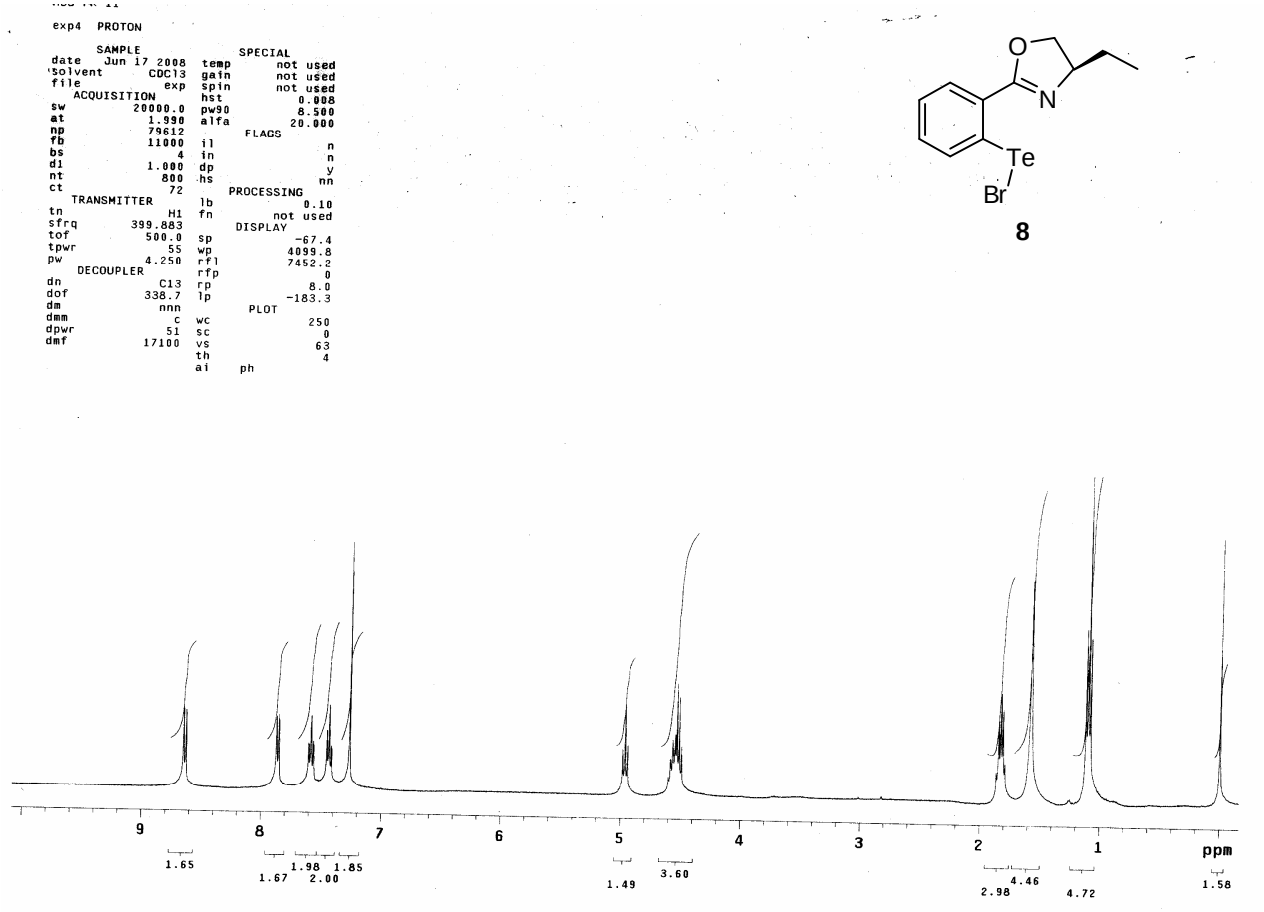


Figure S19. ^{1}H NMR spectrum of compound **8**.

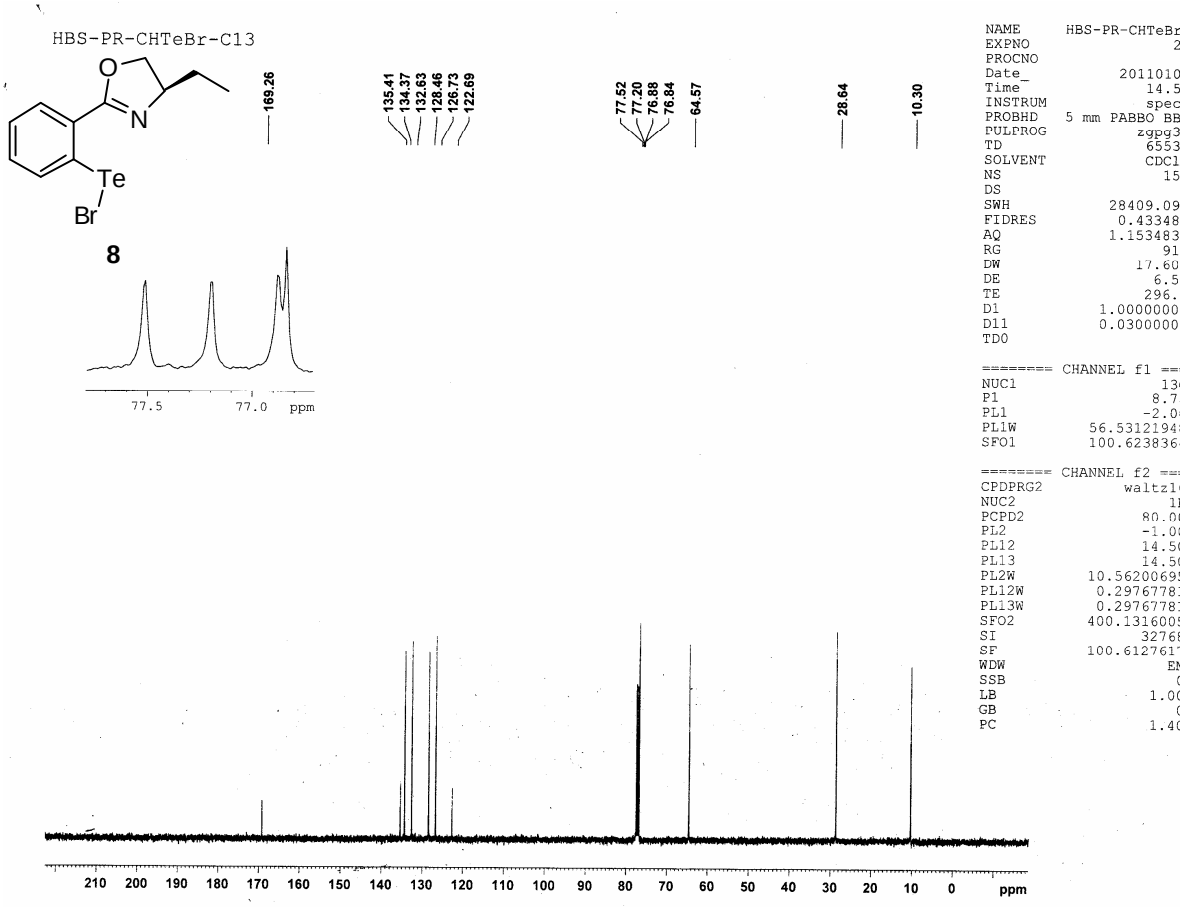


Figure S20. ^{13}C NMR spectrum of compound **8**.

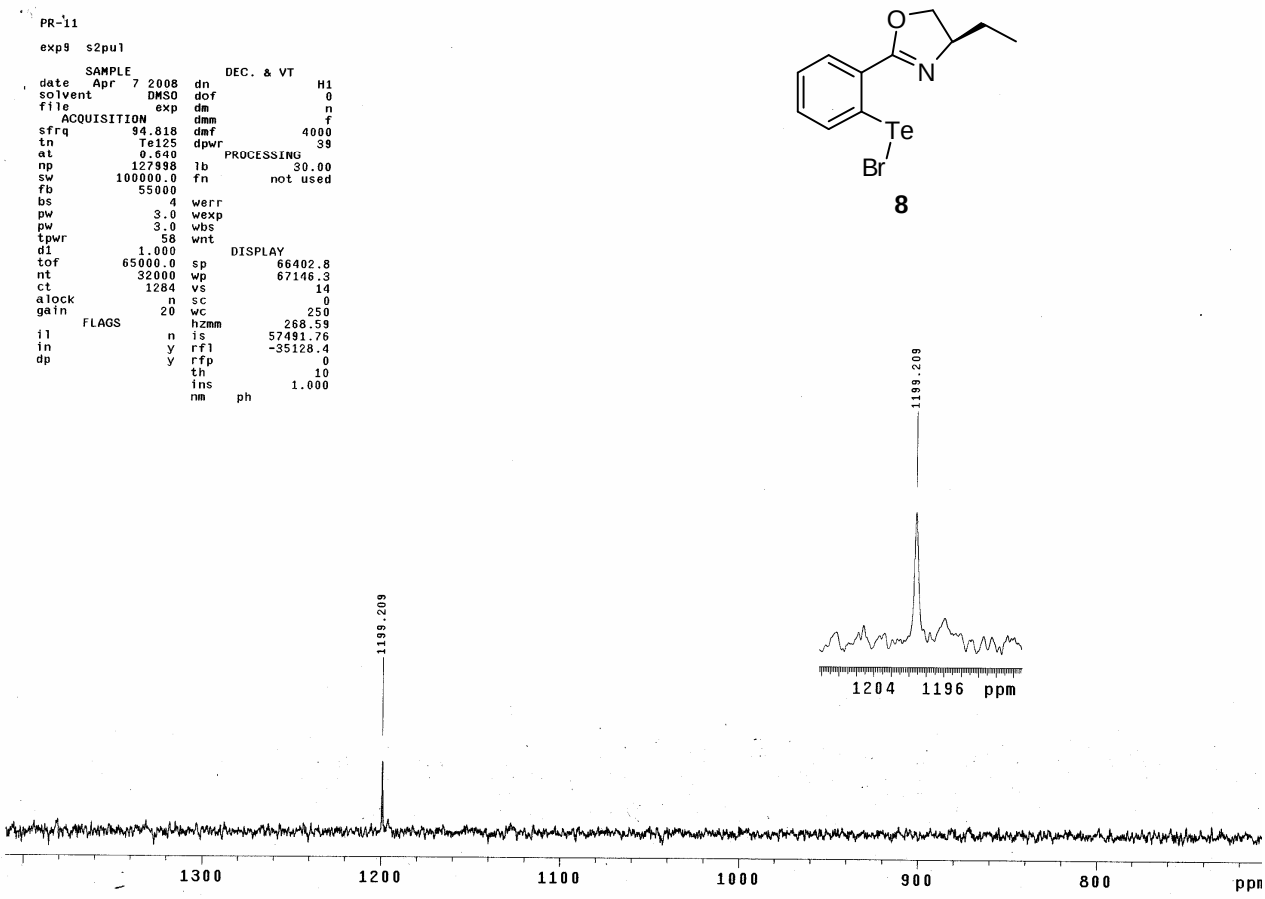


Figure S21. ^{125}Te NMR spectrum of compound **8**.

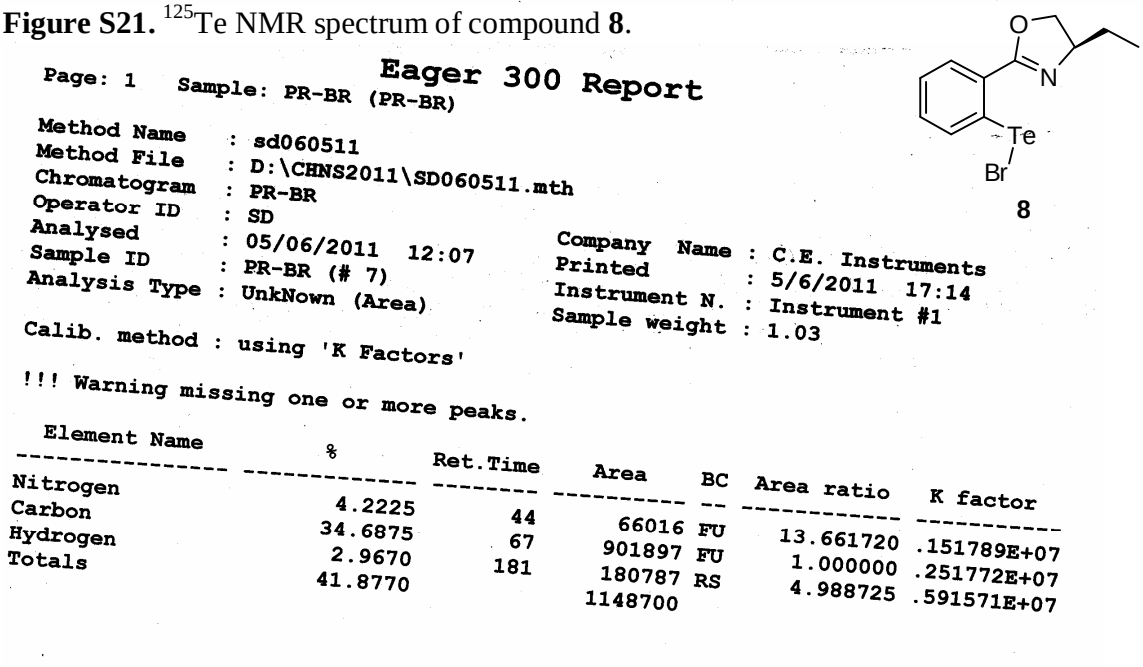


Figure S22. CHN analysis of compound **8**.

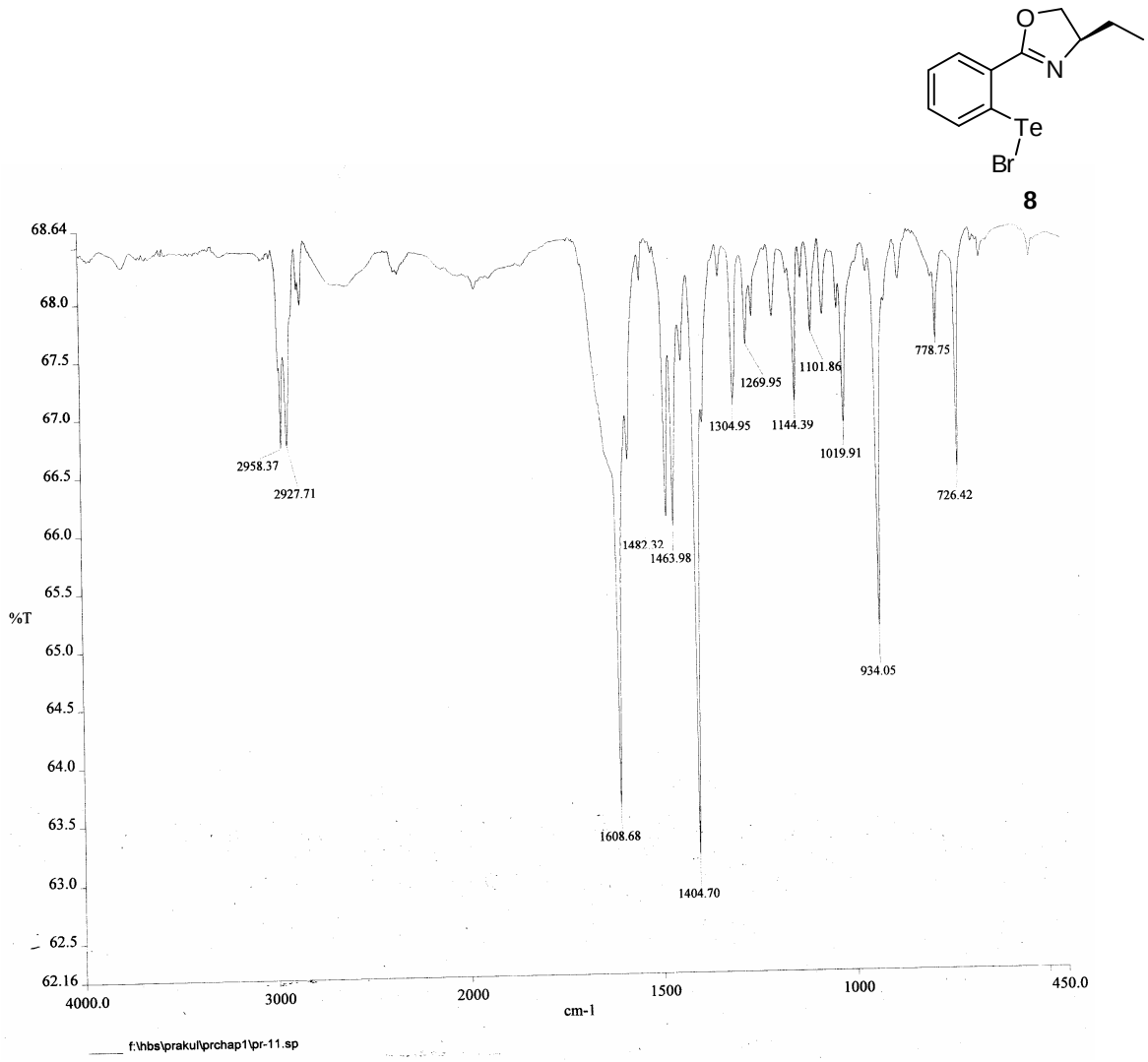


Figure S23. FT-IR spectrum of compound **8**.

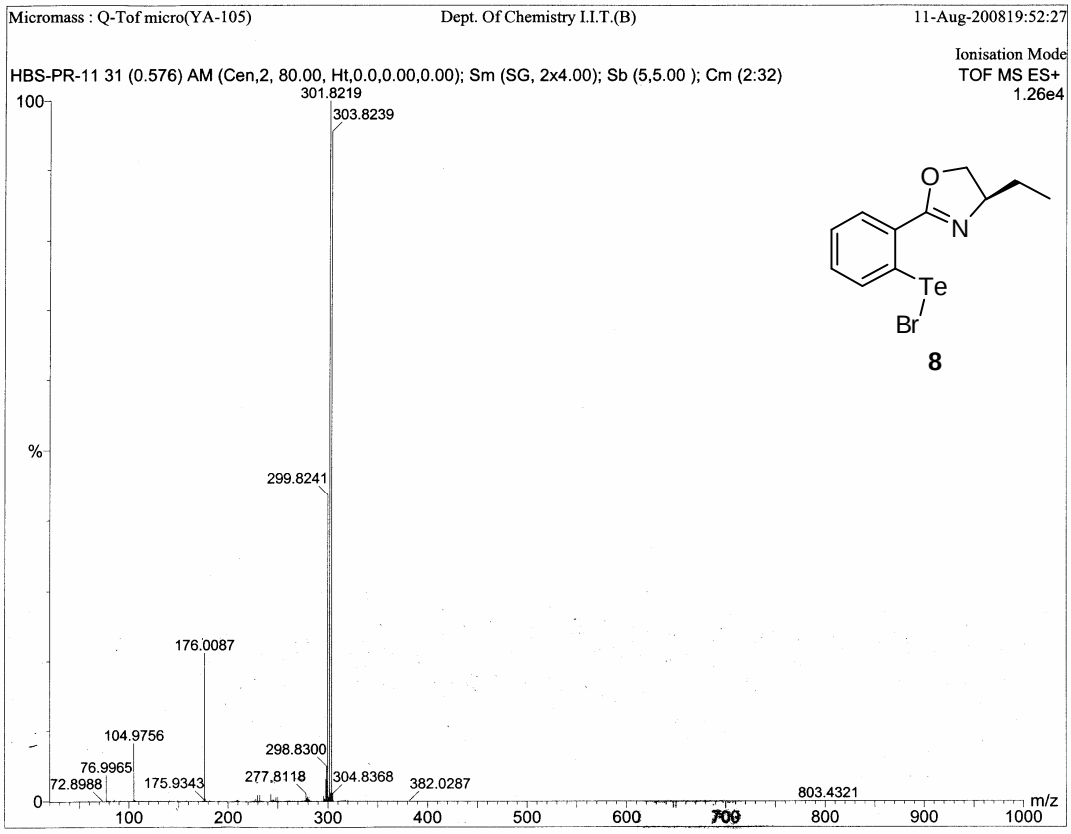
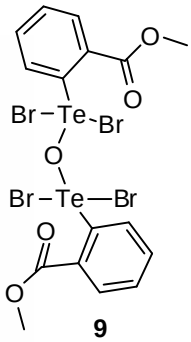


Figure S24. ESI Mass spectrum of compound **8**.



Eager 300 Report

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Operator ID : SP
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Sample ID : PR10 (# 9)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 2/21/2008 14:59
Instrument N. : Instrument #1
Sample weight : 1.884

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

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Figure S25. CHN analysis of compound **9.**

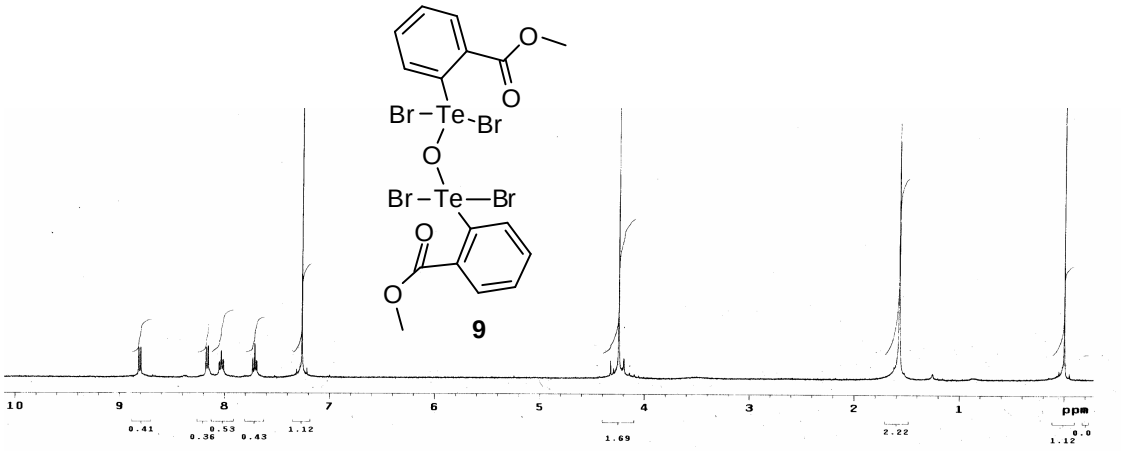

Figure S26. ^{1}H NMR spectrum of compound **9.**

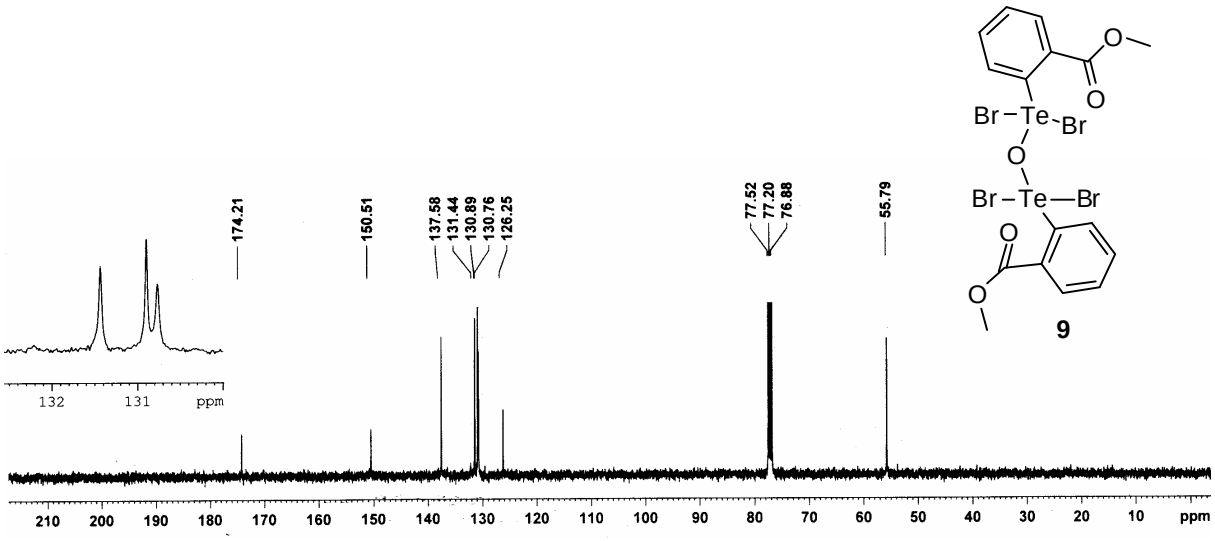

Figure S27. ^{13}C NMR spectrum of compound **9.**

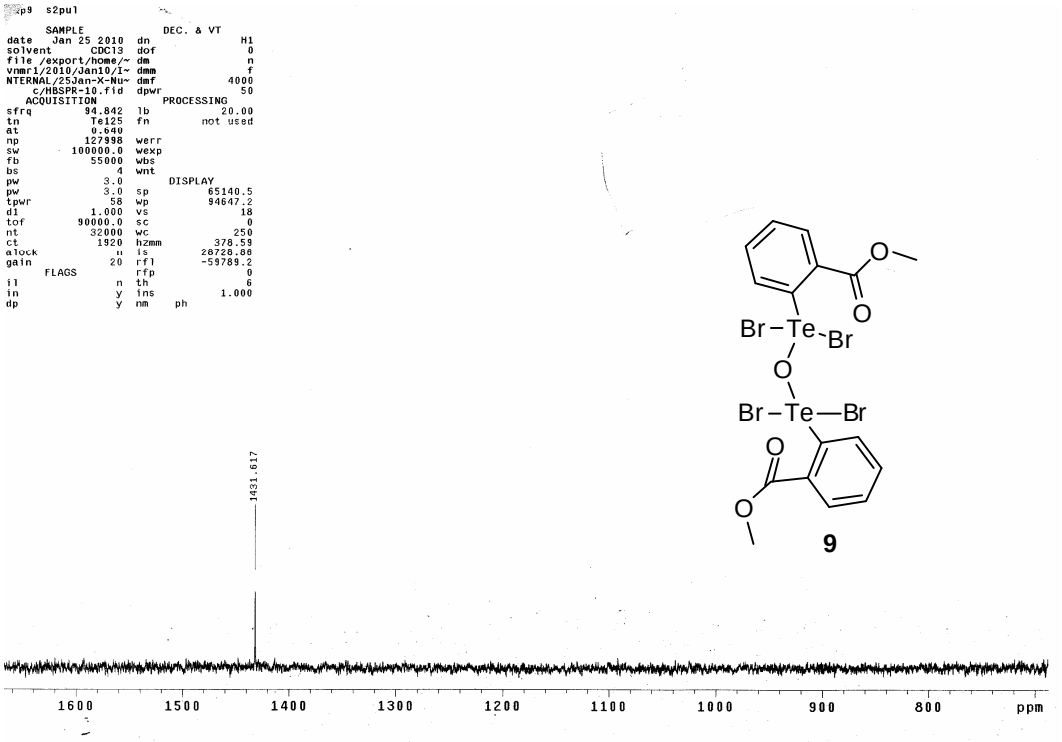

Figure S28. ^{125}Te NMR spectrum of compound **9.**

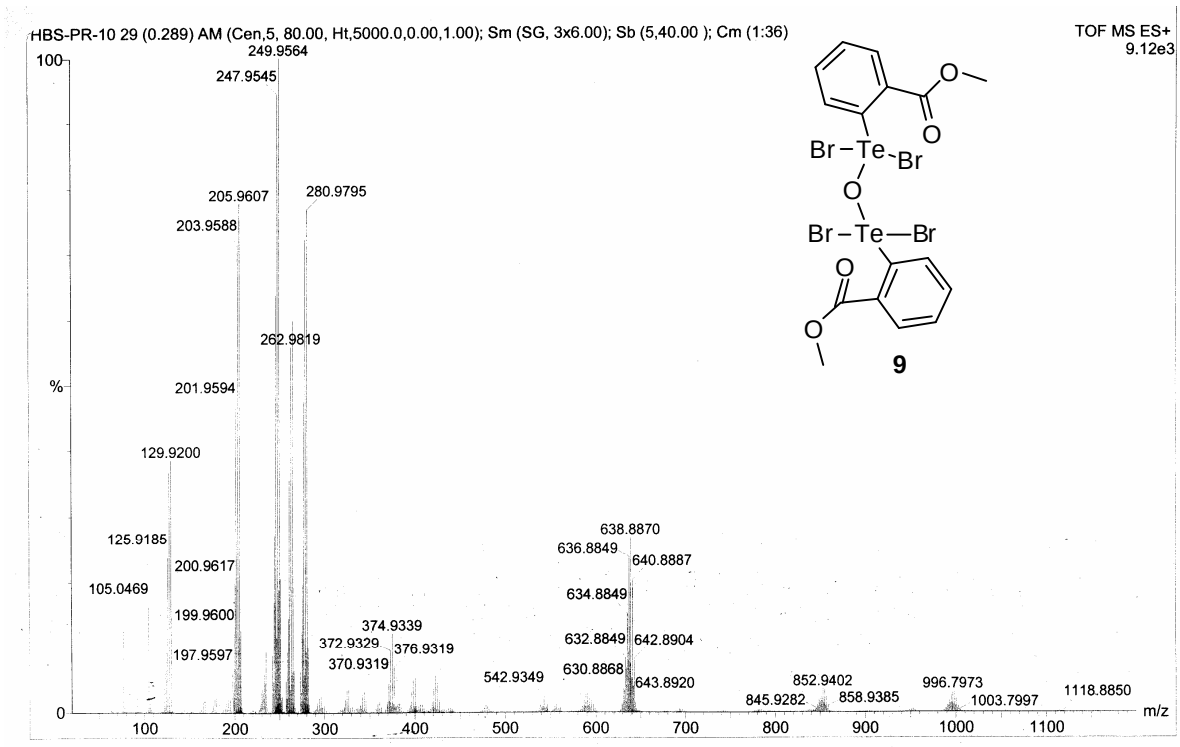

Figure S29. ESI Mass spectrum of compound **9.**

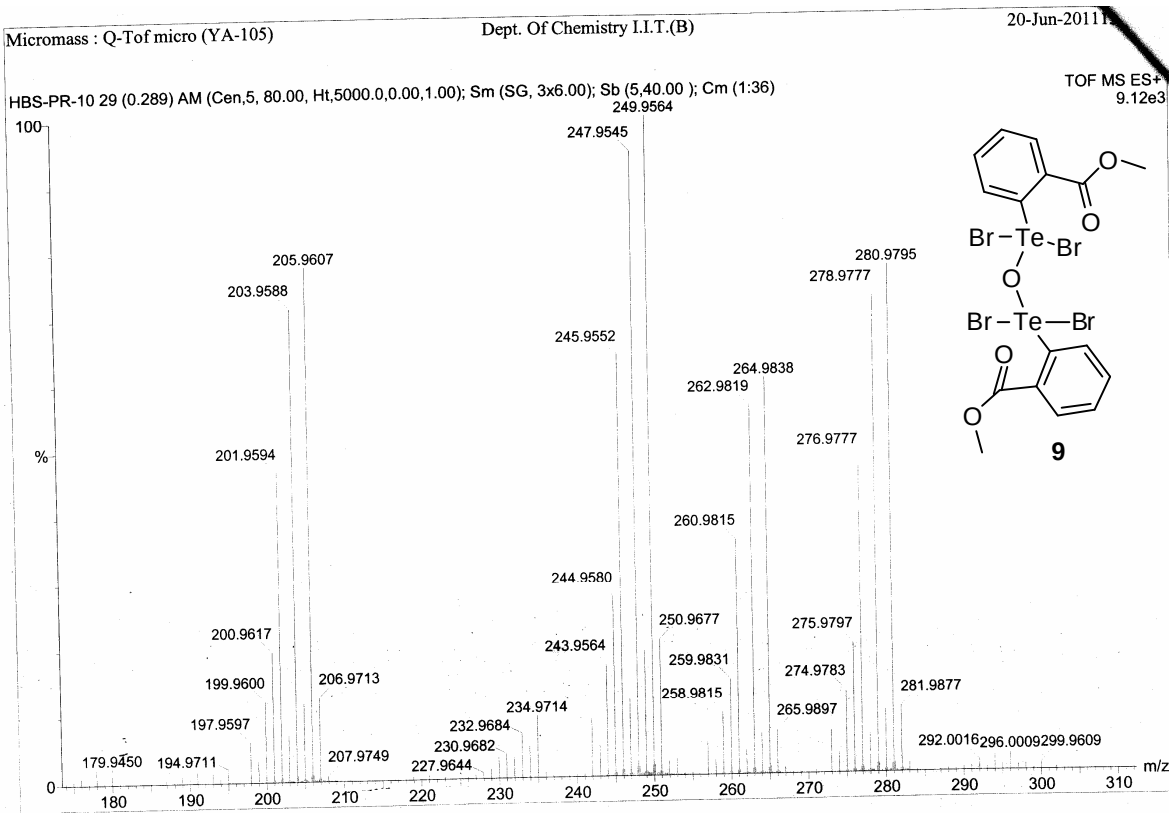

Figure S30. Expansion of ESI Mass spectrum of compound **9.**

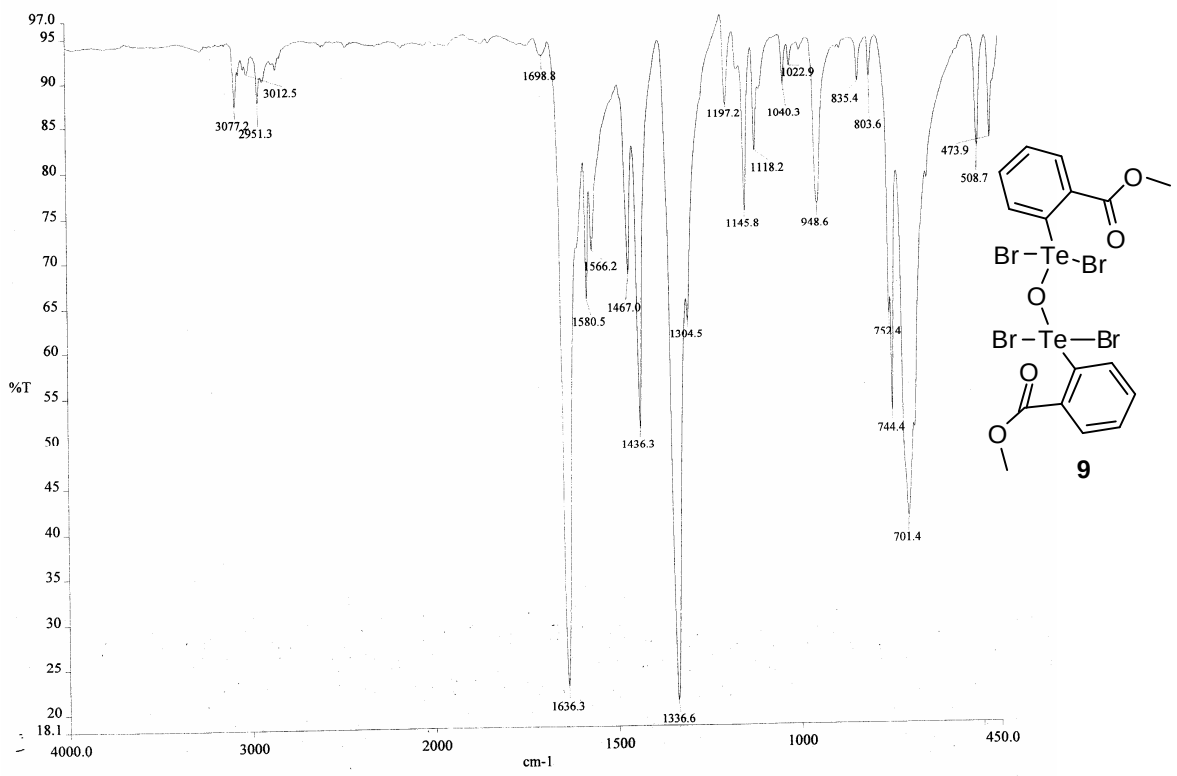

Figure S31. FT-IR spectrum of compound **9.**

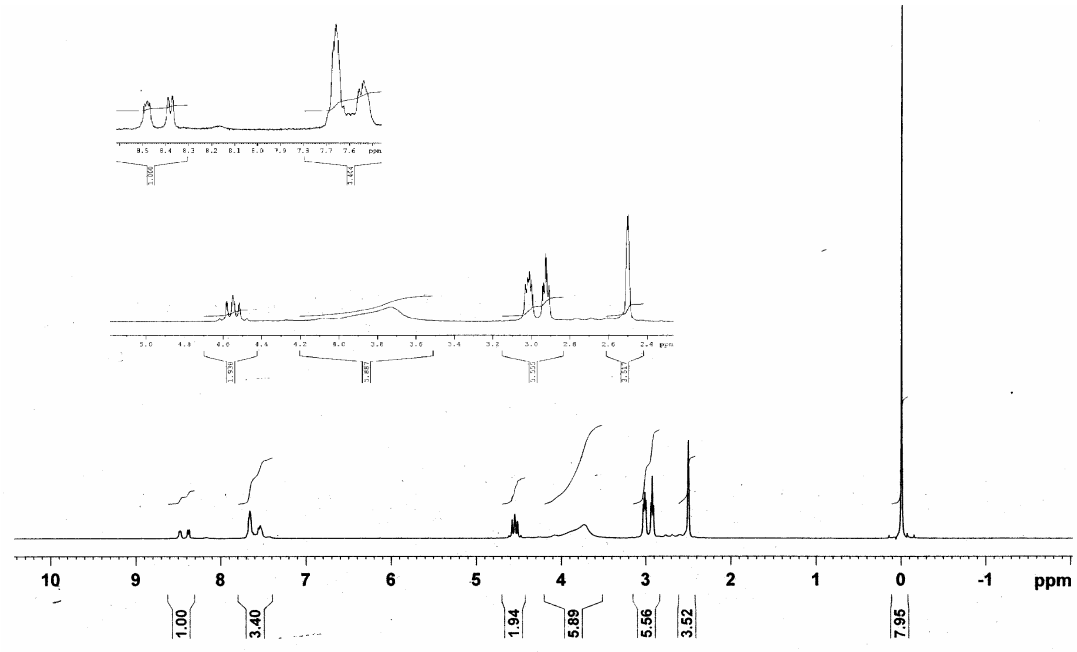

Figure S32. ^{1}H NMR spectrum of compound **12** at 400 MHz (room temperature)**.**

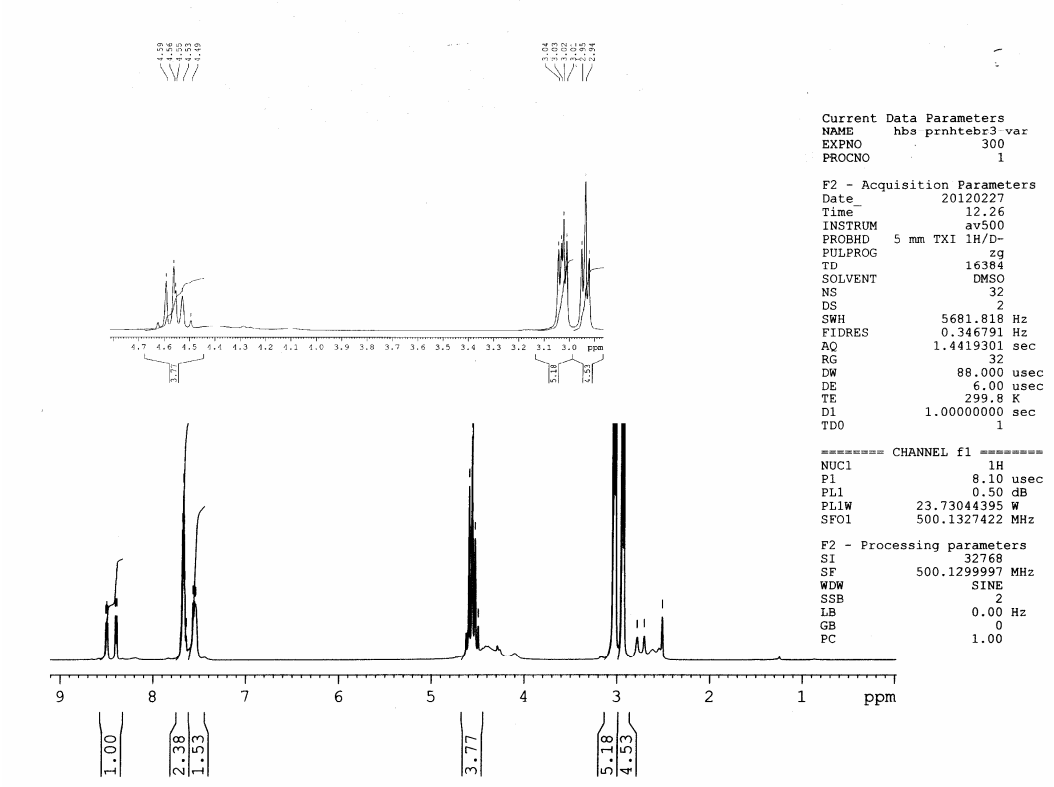

Figure S33. ^{1}H NMR spectrum of compound **12** at 500 MHz (room temperature)**.**

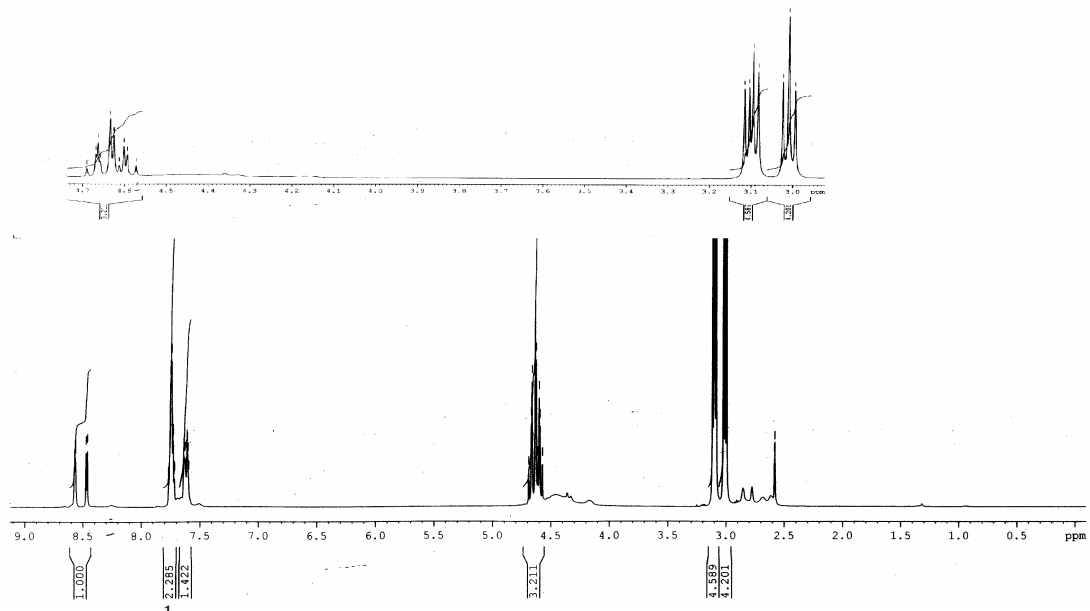

Figure S34. ^{1}H NMR spectrum of compound **12** at 700 MHz (room temperature)**.**

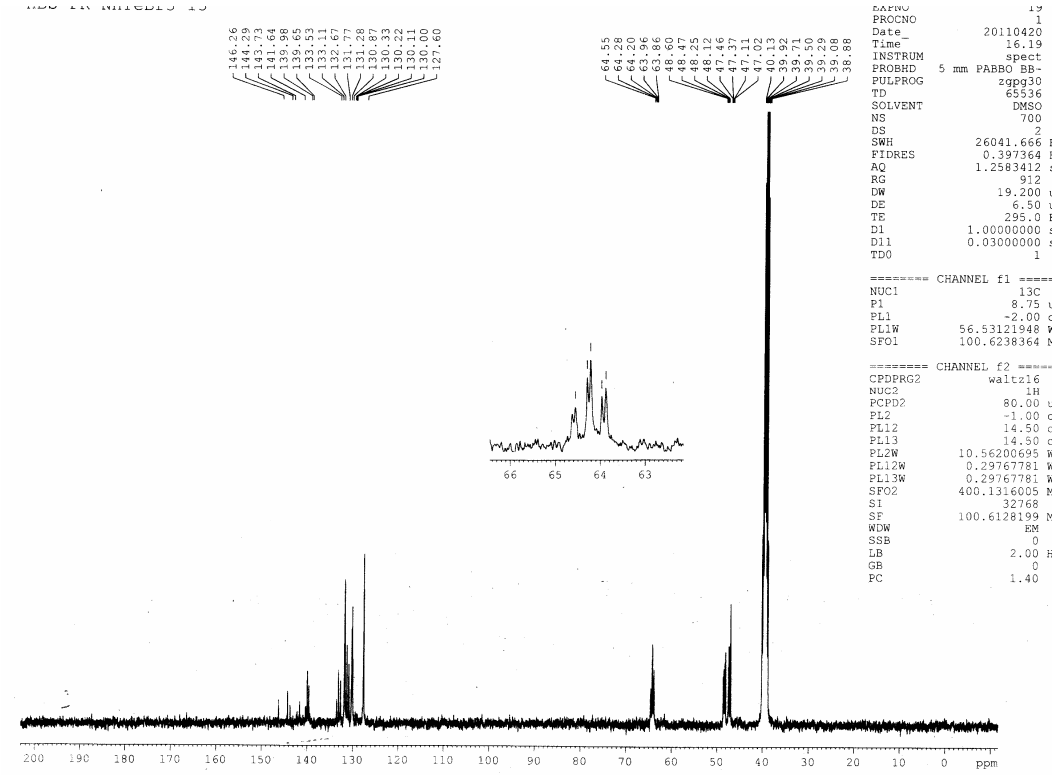

Figure S35. ^{13}C NMR spectrum of compound **12** at 400 MHz (room temperature)

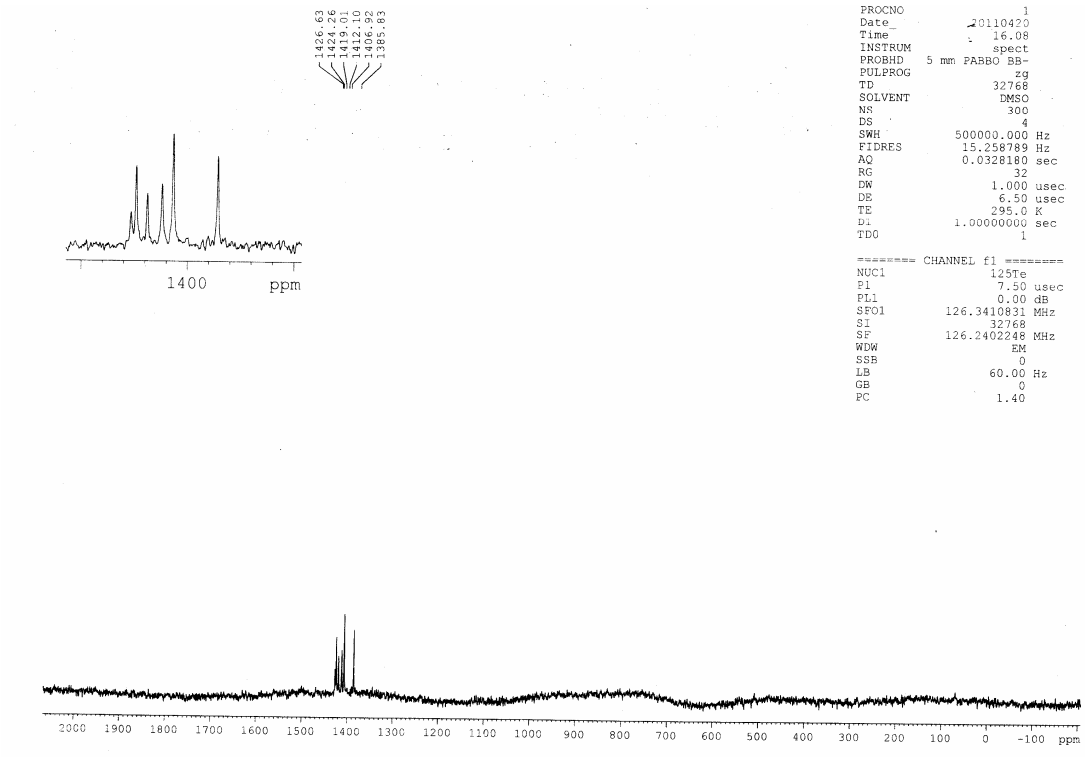

Figure S36. ^{125}Te NMR spectrum of compound **12** at 400 MHz (room temperature)

Eager 300 Report

Page: 1 Sample: TE-BRN (TE-BRN)

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Method File : D:\CHNS2008\SP260210.mth
Chromatogram : TE-BRN
Operator ID : SP
Analysed : 02/26/2010 13:24
Sample ID : TE-BRN (# 19)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 2/26/2010 15:24
Instrument N. : Instrument #1
Sample weight : .819

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

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Nitrogen	3.4733	43	32629	RS	16.060970	.114702E+07
Carbon	24.0429	67	524054	RS	1.000000	.264963E+07
Hydrogen	2.5778	172	189699	RS	2.762553	.676466E+07
Totals	30.0940		756875			

Figure S37. CHN analysis of compound **12**

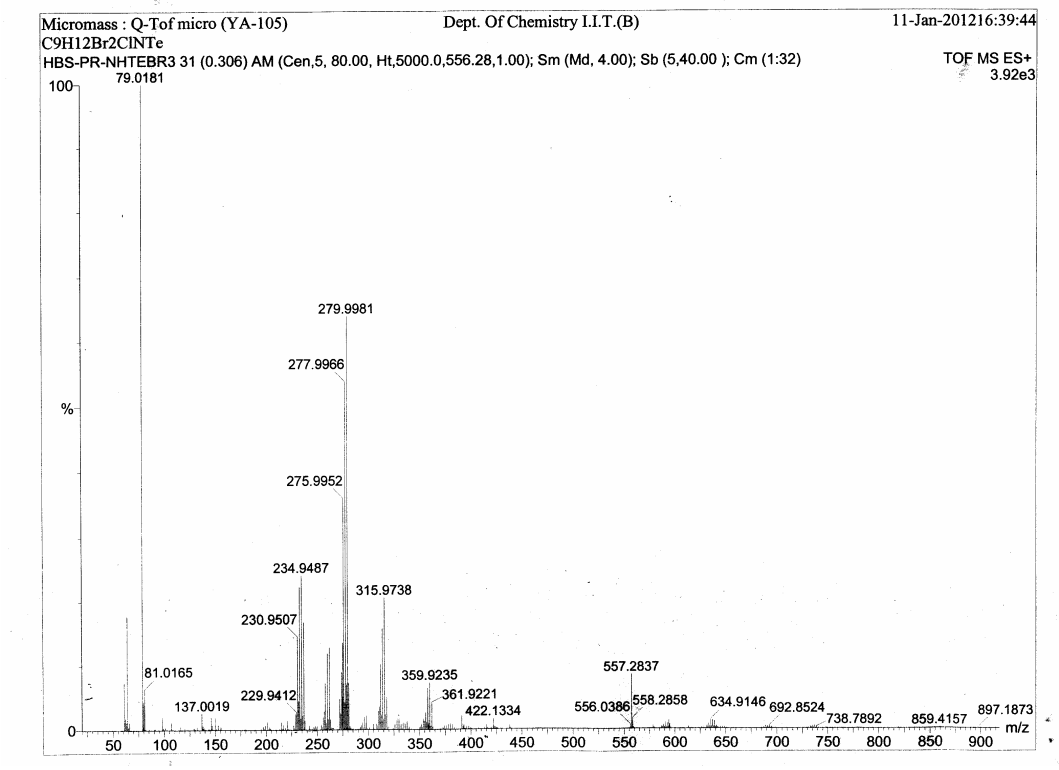
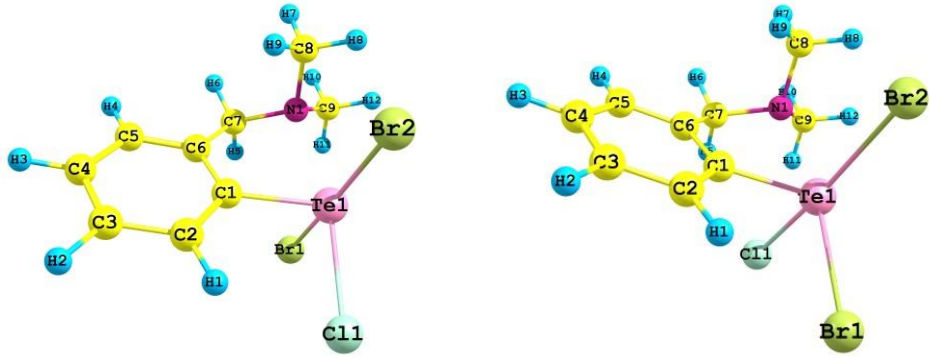


Figure S38. ESI Mass spectrum of compound **12**



12a **12b**

Figure S39. Optimized geometries of **12a** and **12b**.

Table S1. Comparison of the experimentally obtained structural parameters (Å and °) with those computed at b3pw91/ lanl2dz level for 12a and 12b

Bond lengths (Å) / Bond Angle (°)	**12a**		**12b**	
	Optimizd geometry	Crystal structure	Optimized geometry	Crystal structure
Te1···N1	2.4681	2.4315(11)	2.4694	2.421(5)
Te1-Cl1	2.5608	2.440(1)	2.6498	2.601(1)
Te1-Br1	2.8527	2.730(2)	2.7545	2.640(2)
Te1- Br2	2.8259	2.647(2)	2.8214	2.600(2)
Br2-Te-Br1	176.57	174.4(3)	91.38	89.4(3)
Cl1-Te1-N1	167.43	171.6(2)	83.24	92.6(2)
N1-Te1-Br2	85.05	89.1(13)	168.83	170.9.1(13)

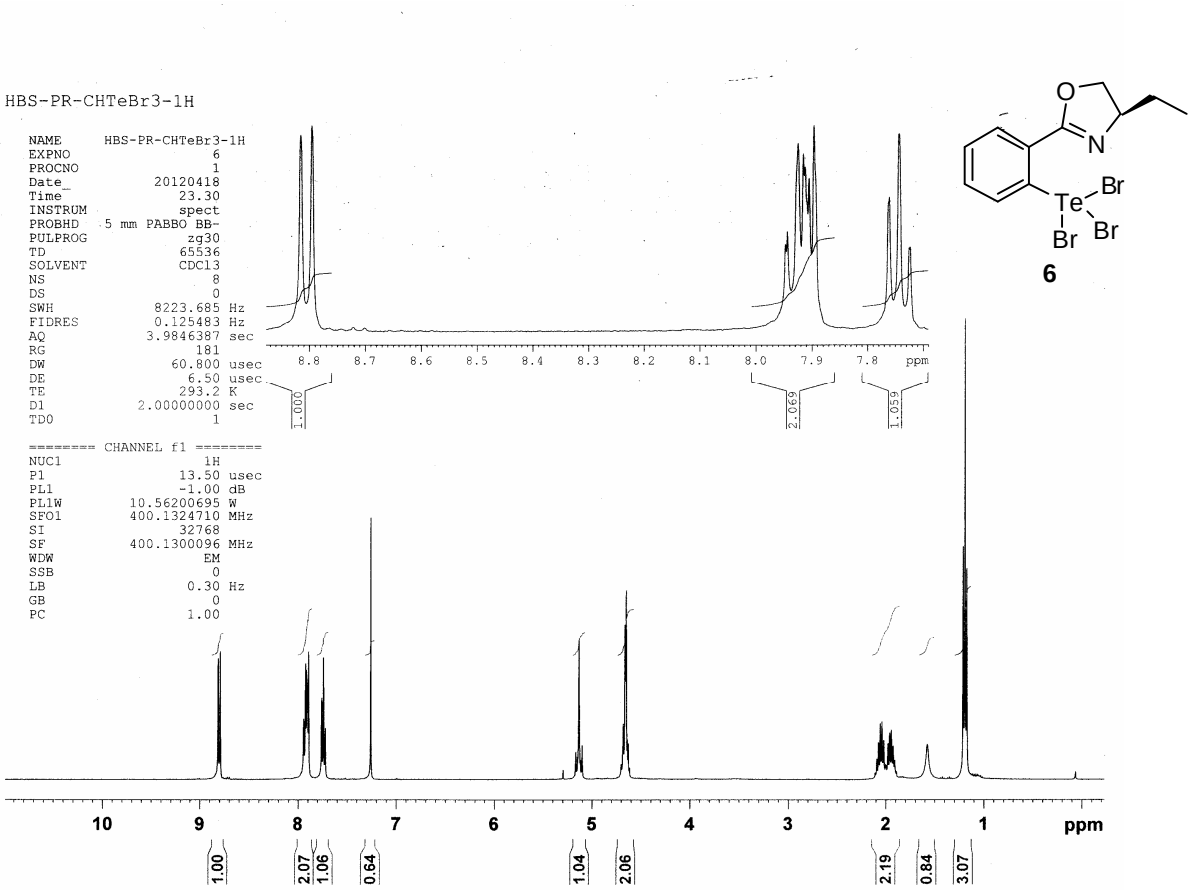


Figure S40. ^{1}H NMR spectrum of compound **6**.

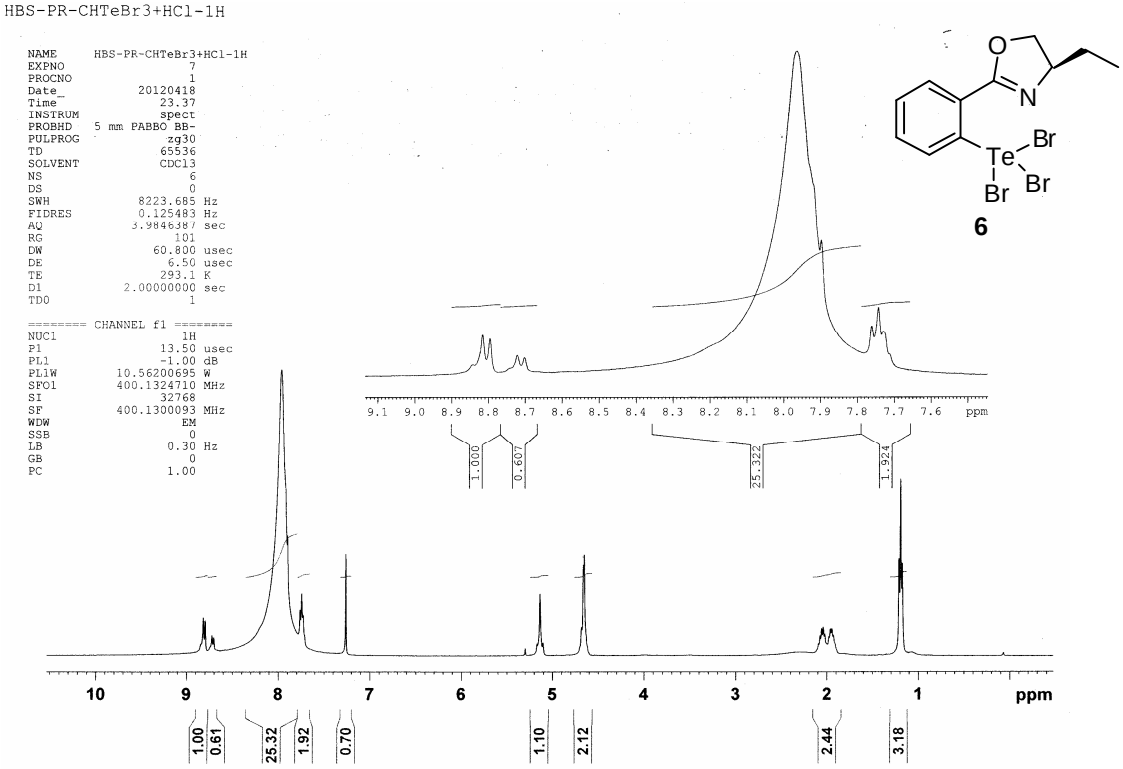


Figure S41. ^{1}H NMR spectrum of compound **6** after the addition of dil. HCl.

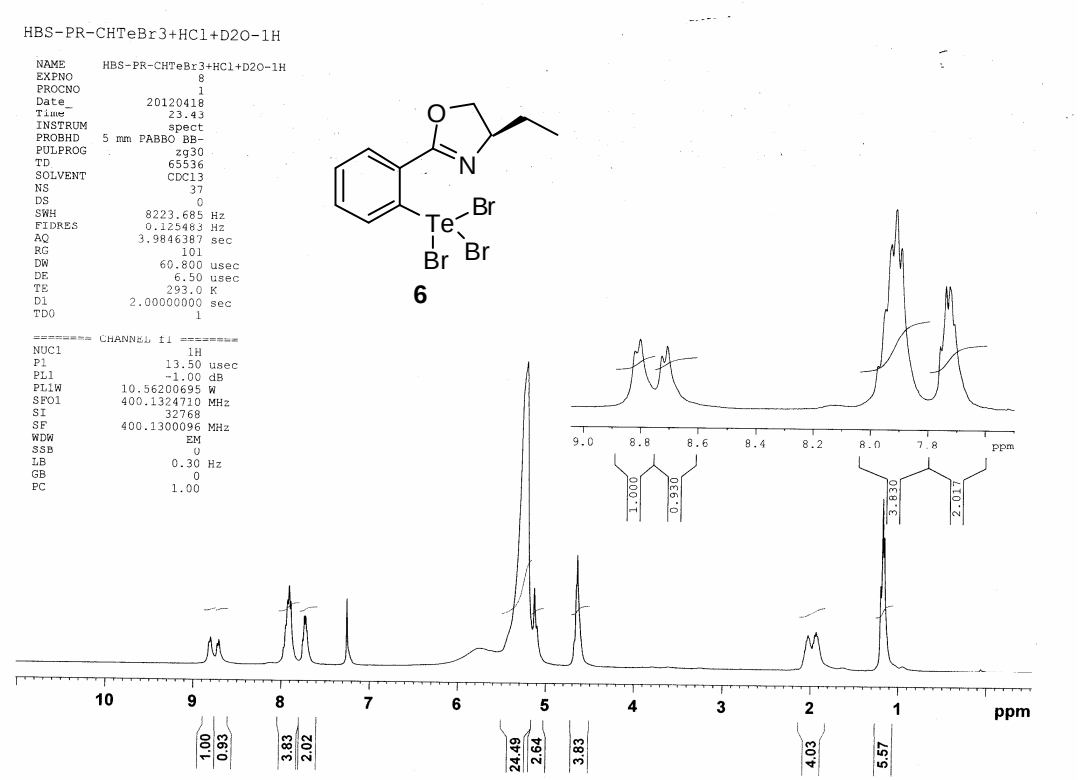


Figure S42. ^{1}H NMR spectrum of compound **6** after the addition of D_2O.

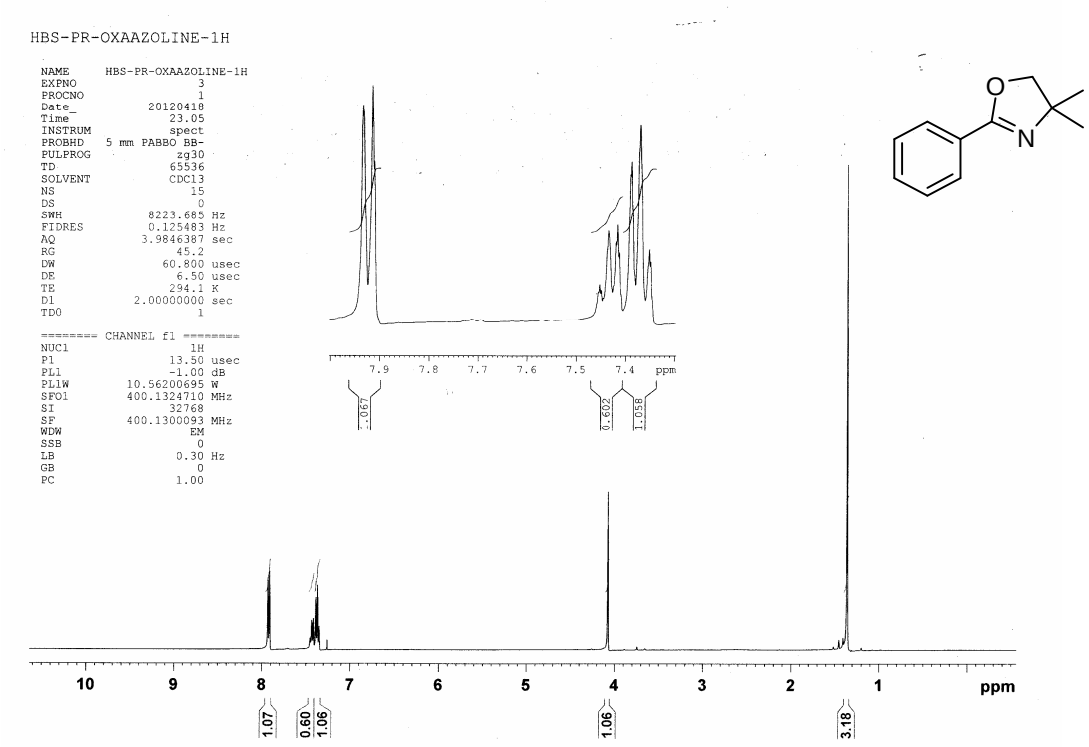


Figure S43. ^{1}H NMR spectrum of 4,4-dimethyl-2-phenyl-2-oxazoline.

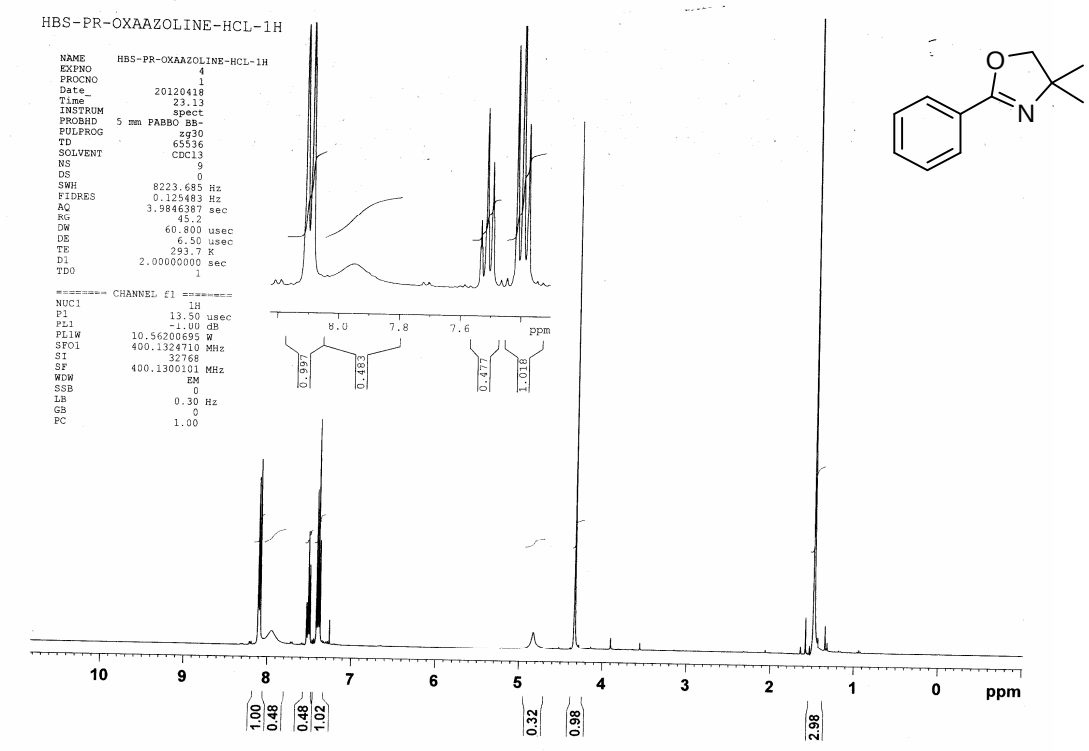


Figure S44. ^{1}H NMR spectrum of 4,4-dimethyl-2-phenyl-2-oxazoline after the addition of dil. HCl.

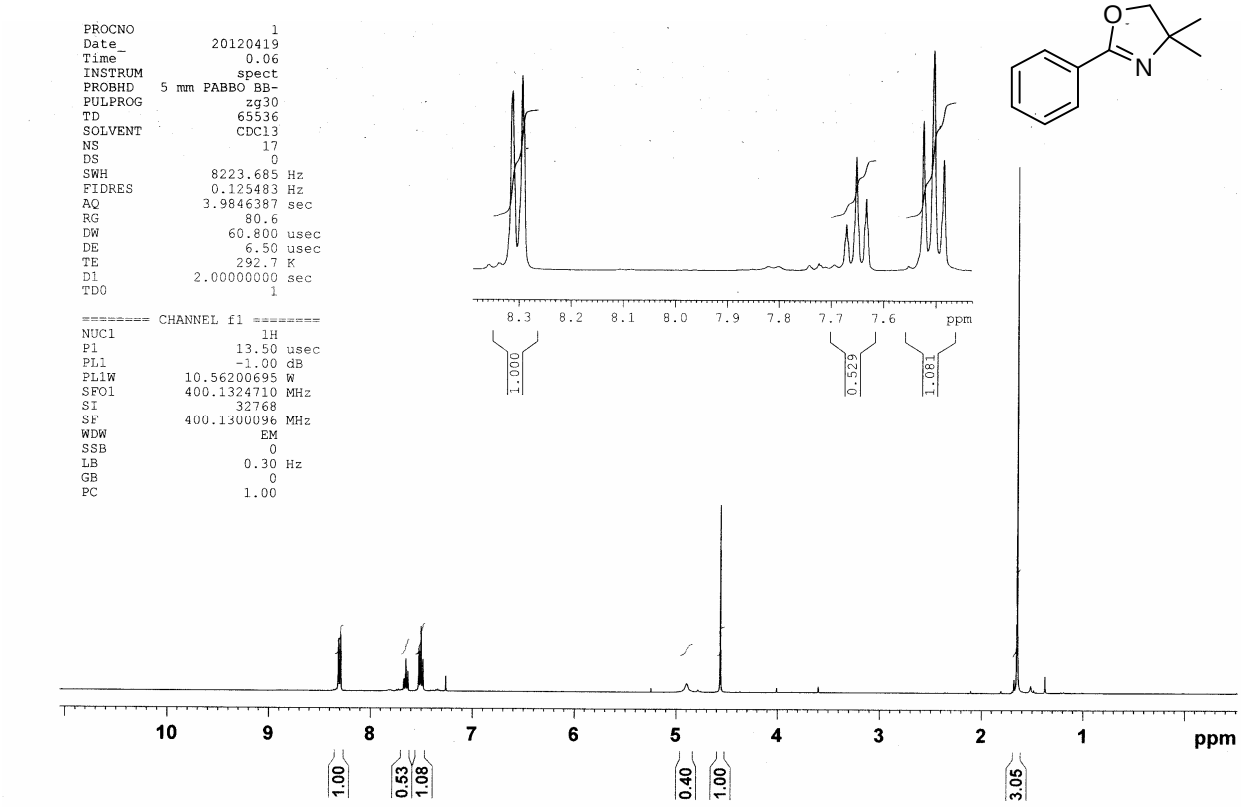


Figure S45. ^{1}H NMR spectrum of 4,4-dimethyl-2-phenyl-2-oxazoline after the addition of D_2O.