

Supplementary Information

Isolation and Structural Characterization of Some Aryltellurium Halides and their Hydrolysed Products Stabilized by Intramolecular Te $\cdots$ N Interaction

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General experimental Procedures:

X-ray Crystallography: The diffraction measurements for compounds **10**, **11**, **12**, **13**, **14**, **17**, **20-21**, **23** and **23A** were performed on a Oxford Gemini system and Bruker Apex 2 on graphite-monochromated Mo-K α radiation ($\lambda = 0.7107 \text{ \AA}$). The crystal data for **6**, **22** was collected on a Oxford diffraction X-Calibur diffractometer using Cu radiation ($\lambda = 1.5418 \text{ \AA}$). X-ray diffraction data were obtained on an Oxford XCalibur system using Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$). The structure solutions were achieved by using direct methods as implemented in SHELXS-97.¹ The structures were refined by full least-squares methods using SHELXL-97.²

Computational Details: All geometries were optimized using analytical gradient techniques implemented in the Gaussian03 suite of quantum chemical program.³ Geometry optimization for **11**, **13**, **14** and **15** were performed by B3LYP method with 6-311G(d,p) basis set for H, C, N, O and Lanl2dz(d,p) basis set with corresponding pseudo-potential for Te. Optimized structure of all compounds was confirmed as minima by performing frequency analysis. NBO analyses⁴ on all optimized geometries were performed at B3LYP/Lanl2dz(d,p) (Te), 6-311G(d,p) (H, C, N, O) level. AIM analysis on the optimized geometries of all the compounds were performed by B3LYP method with 6-311G(d,p) basis set for H, C, N, O and WTBS basis set for Te with AIM2000⁵ package.

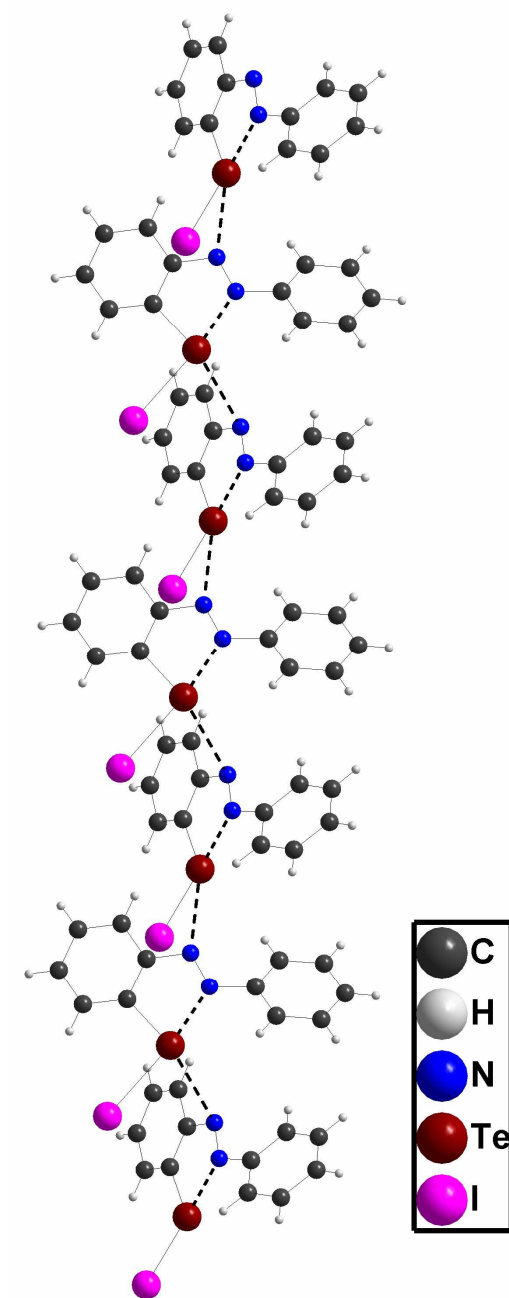


Figure S1. Extended diagram of **12** showing intermolecular C-Te...N interaction

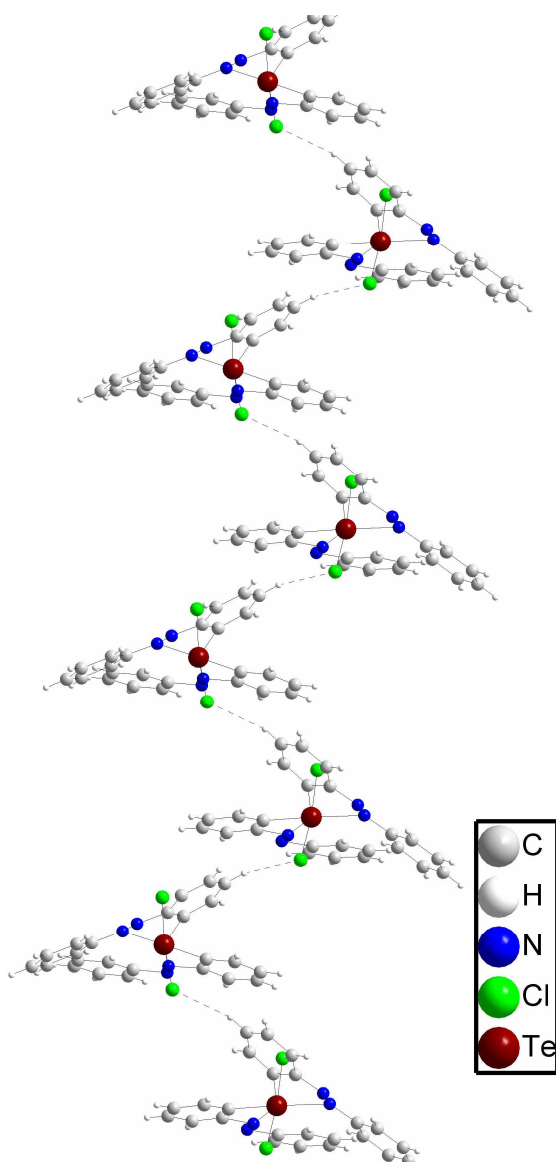


Figure S2. Extended diagram of **13** showing intermolecular C–H⋯Cl hydrogen bonding

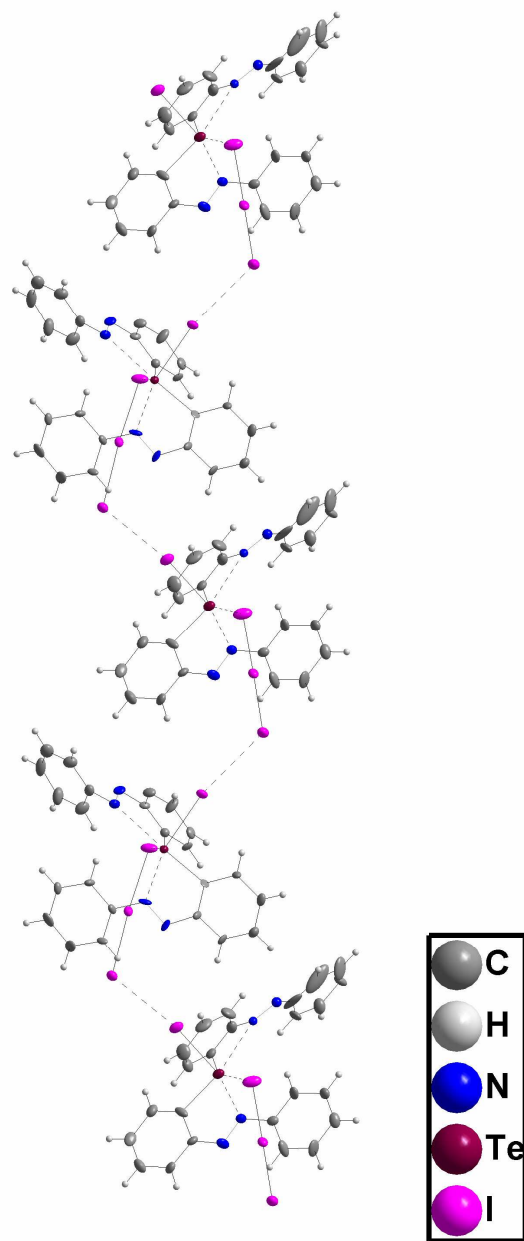


Figure S3. Extended diagram of **14** showing intermolecular I₃⁻ and iodine interaction

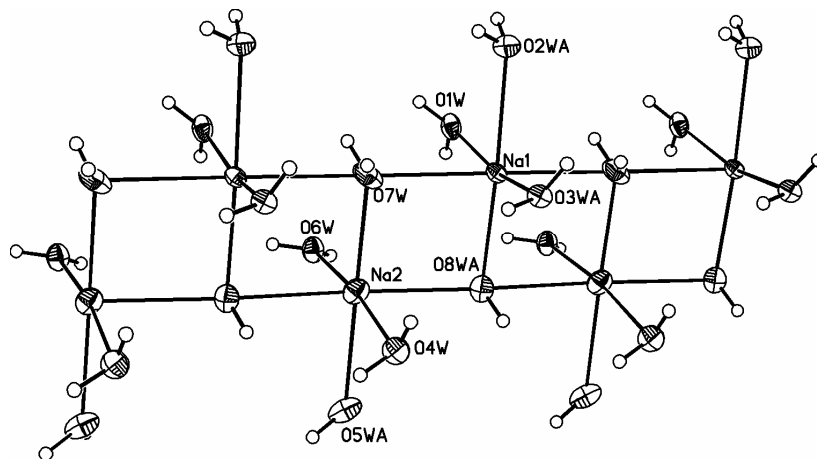


Figure S4. Packing arrangement of Na and H₂O in tellurinc acid salt (**21**)

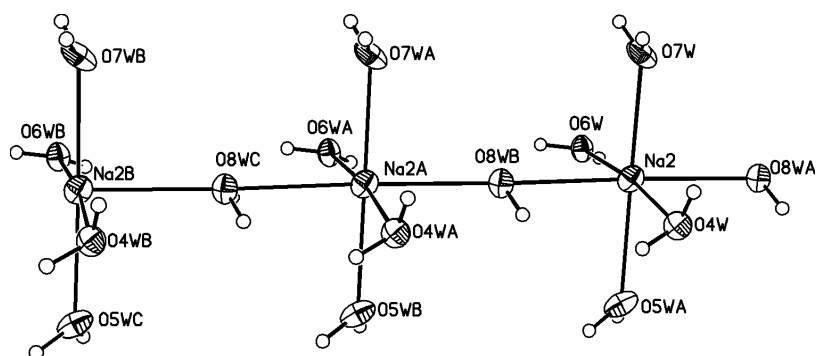


Figure S5. Packing arrangement of Na and H₂O in tellurinc acid (**20**) and its salt (**21**)

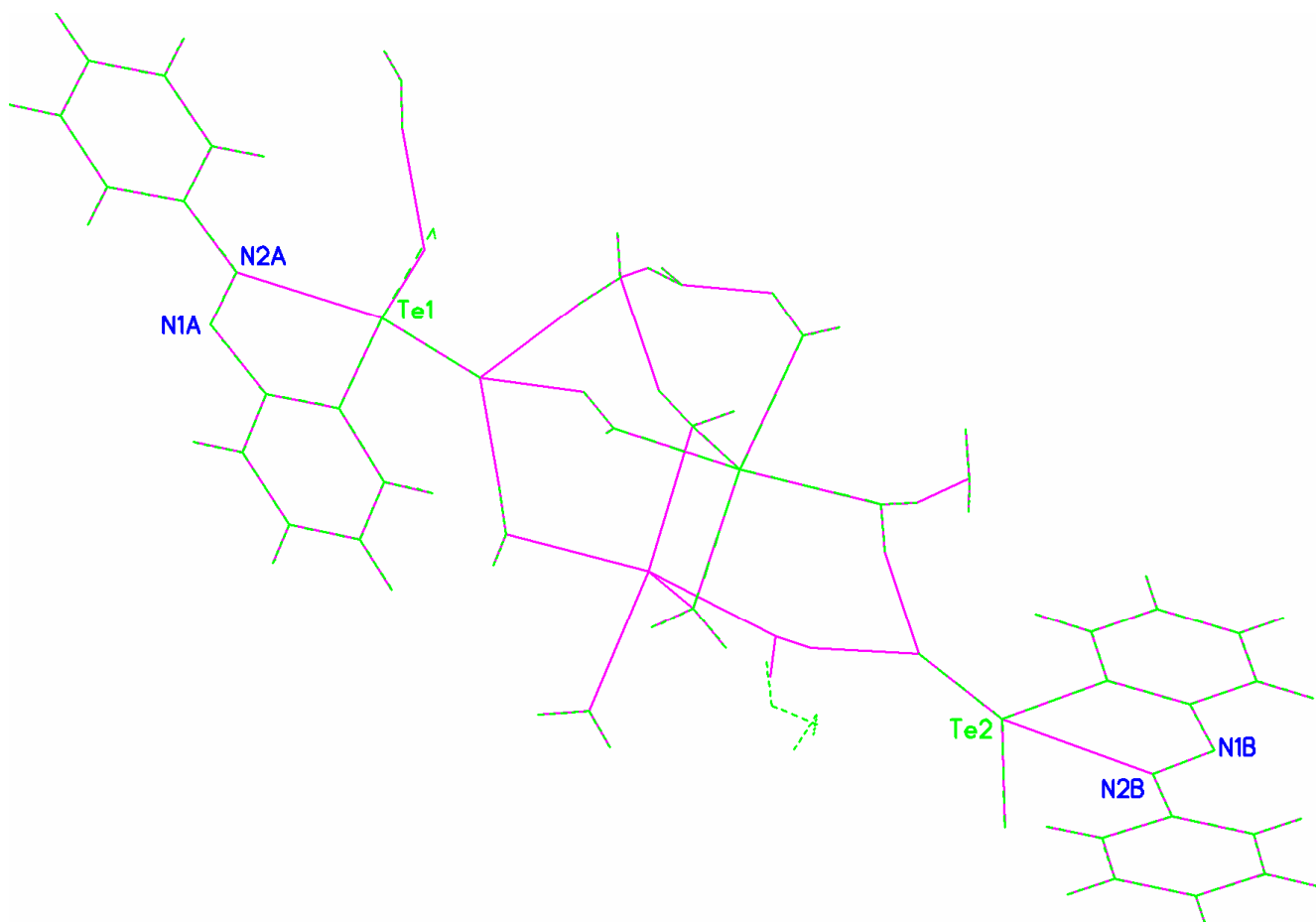


Figure S6. Superimposition of the crystallization arrangement of **20–21**.

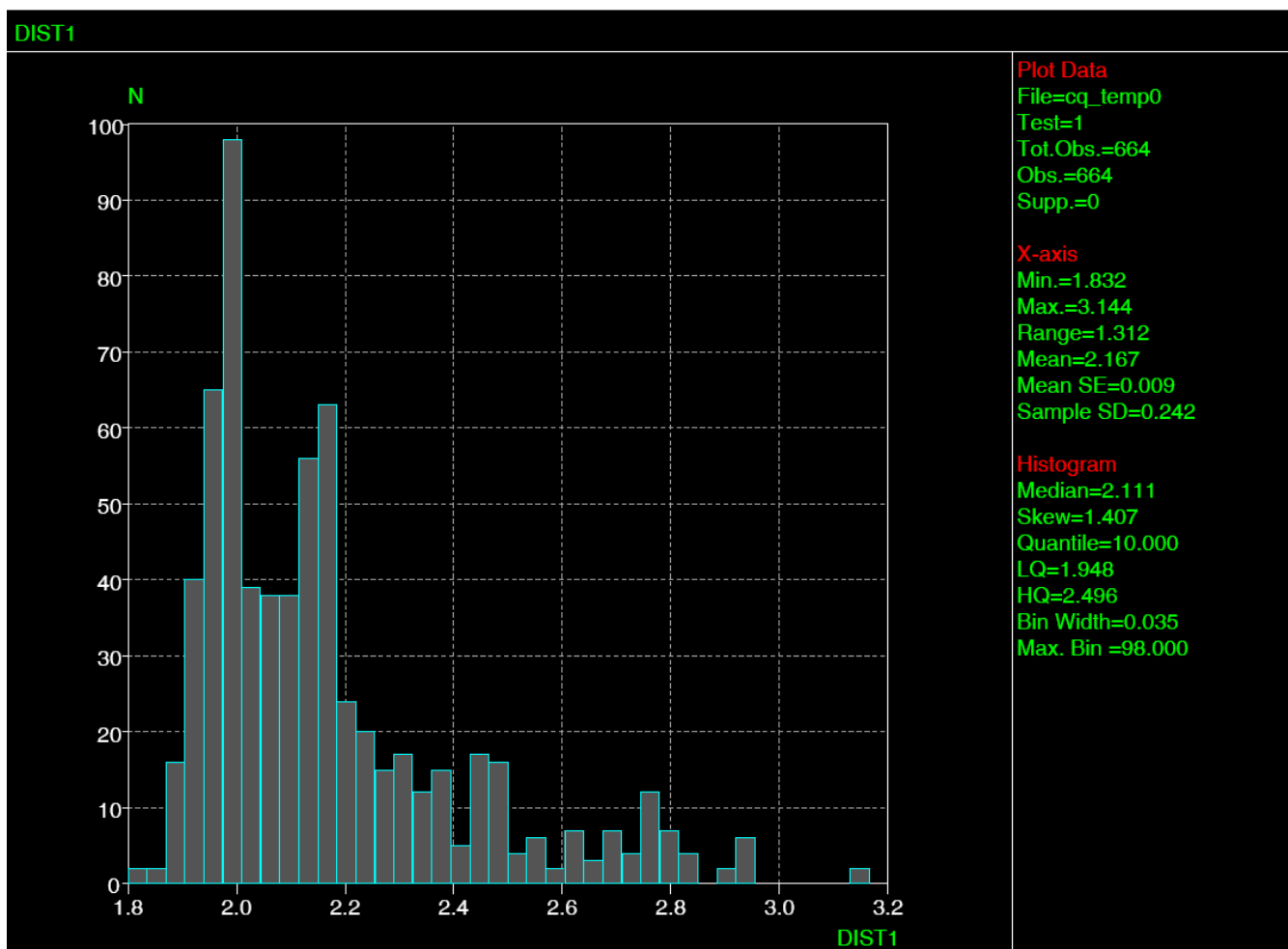


Figure S7. CSD plot for Te–O distance of 20–21.

Entry	Anionic-multitellur-oxane ^a	Oligotellur-oxane ^b	Polymeric Ditetellur-oxane ^c	Macrocyclic Multi-Telluranes ^d	Tellurinic Acid ^e	5 ^f	20 and 21
Te–O (short bonds)	1.908- 1.941 (sixteen bonds)	1.890(8) 1.896(8) 1.916(8)			1.897(5)	1.863- 1.891 1.911- 1.913	1.842(14)- 1.876(2) 1.870(14)- 1.885(14)
Te–O (intermediate bonds)		1.964(7)	2.025(2)	1.99(2)- 2.03(2)		1.987- 2.023	
Te–O (long bonds)	2.091- 2.157 (sixteen bonds)	2.089(8) 2.116(8)	2.100(2)	2.23(2)- 2.29(2)	2.143(5) and 2.232(4)	2.063- 2.106 2.174- 2.249	

Table S1: Comparison of Te-O Bond Lengths of **20** and **21** with related Telluroxanes

^a H. Citeau, K. Kirschbaum, O. Conrad, D. M. Giolando, *Chem. Commun.* **2001**, 2006.

^b K. Kobayashi, N. Deguchi, O. Takahashi, K. Tanaka, E. Horn, O. Kikuchi, N. Furukawa, *Angew. Chem. Int. Ed.* **1999**, 38, 1638.

^c J. Beckmann, D. Dakternieks, A. Duthie, F. Ribot, M. Schürmann, N. A. Lewcenko, *Organometallics* **2003**, 22, 3257.

^d K. Kobayashi, H. Izawa, K. Yamaguchi, E. Horn, N. Furukawa, *Chem. Commun.* **2001**, 1428.

^e J. Beckmann, P. Finke, M. Hesse, B. Wettig, *Angew. Chem. Int. Ed.* **2008**, 47, 9982.

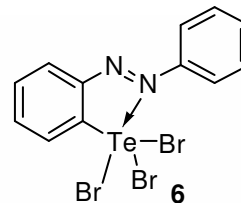
^f K. Srivastava, S. Sharma, H. B. Singh, U. P. Singh, R. J. Butcher, *Chem. Commun.* **2010**, 46, 1130.

Eager 300 Report

Page: 1 Sample: KR-AZOTEBR3 (KR-AZOTEBR3)

Method Name : sp200608
Method File : D:\CHNS2008\SP200608.mth
Chromatogram : KR-AZOTEBR3_
Operator ID : MANOJA
Analysed : 06/20/2008 14:06
Sample ID : KR-AZOTEBR3 (# 19)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 6/20/2008 16:15
Instrument N. : Instrument #1
Sample weight : 1.433



Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	5.3437	43	83098	RS	12.475580	.108519E+07
Carbon	26.9309	67	1036696	RS	1.000000	.265871E+07
Hydrogen	1.4208	175	132499	RS	7.824180	.601503E+07
Totals	33.6954		1252293			

Figure S8.Elemental analysis (C, H, N) of 6

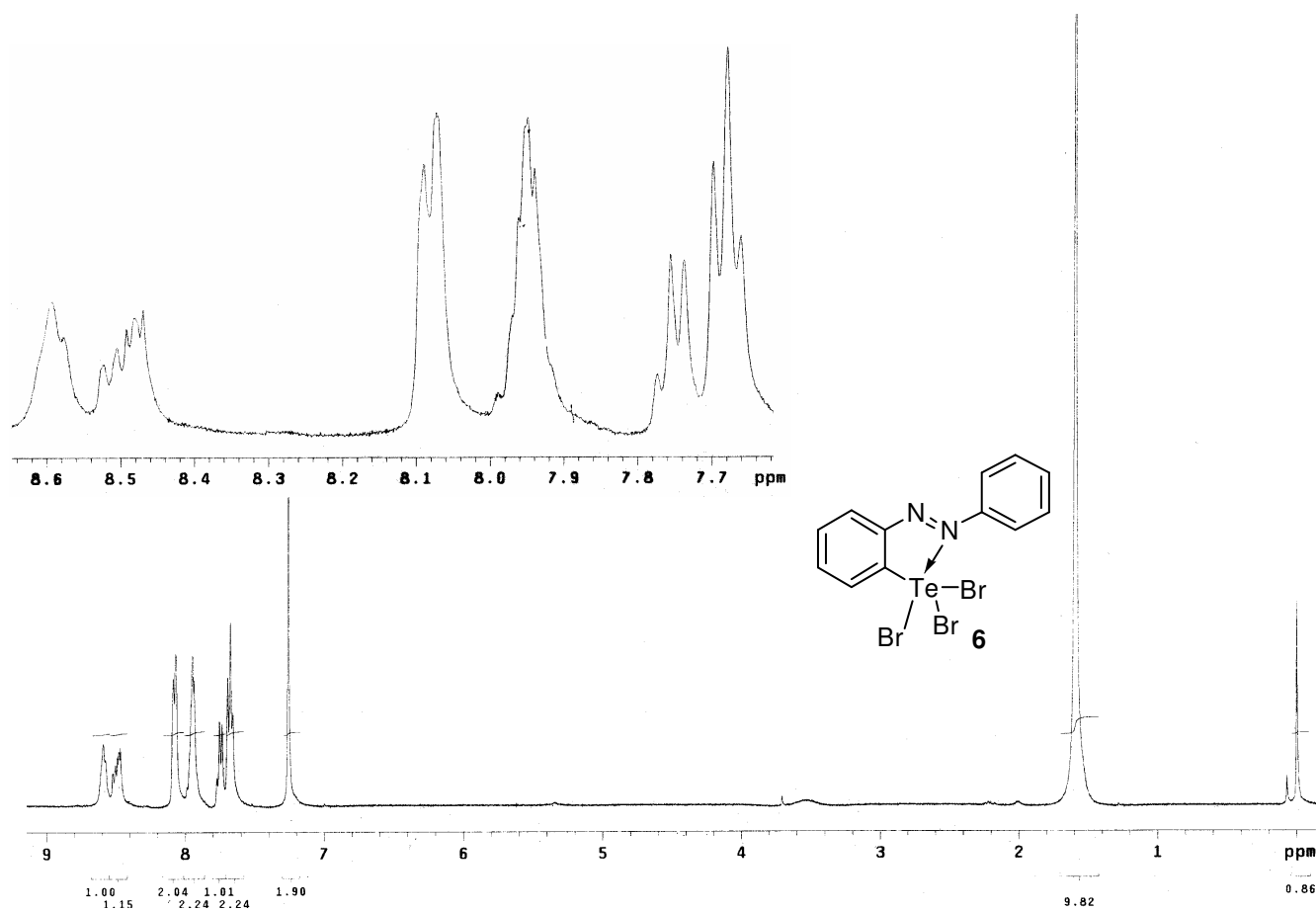


Figure S9. ^1H -NMR spectrum of **6**

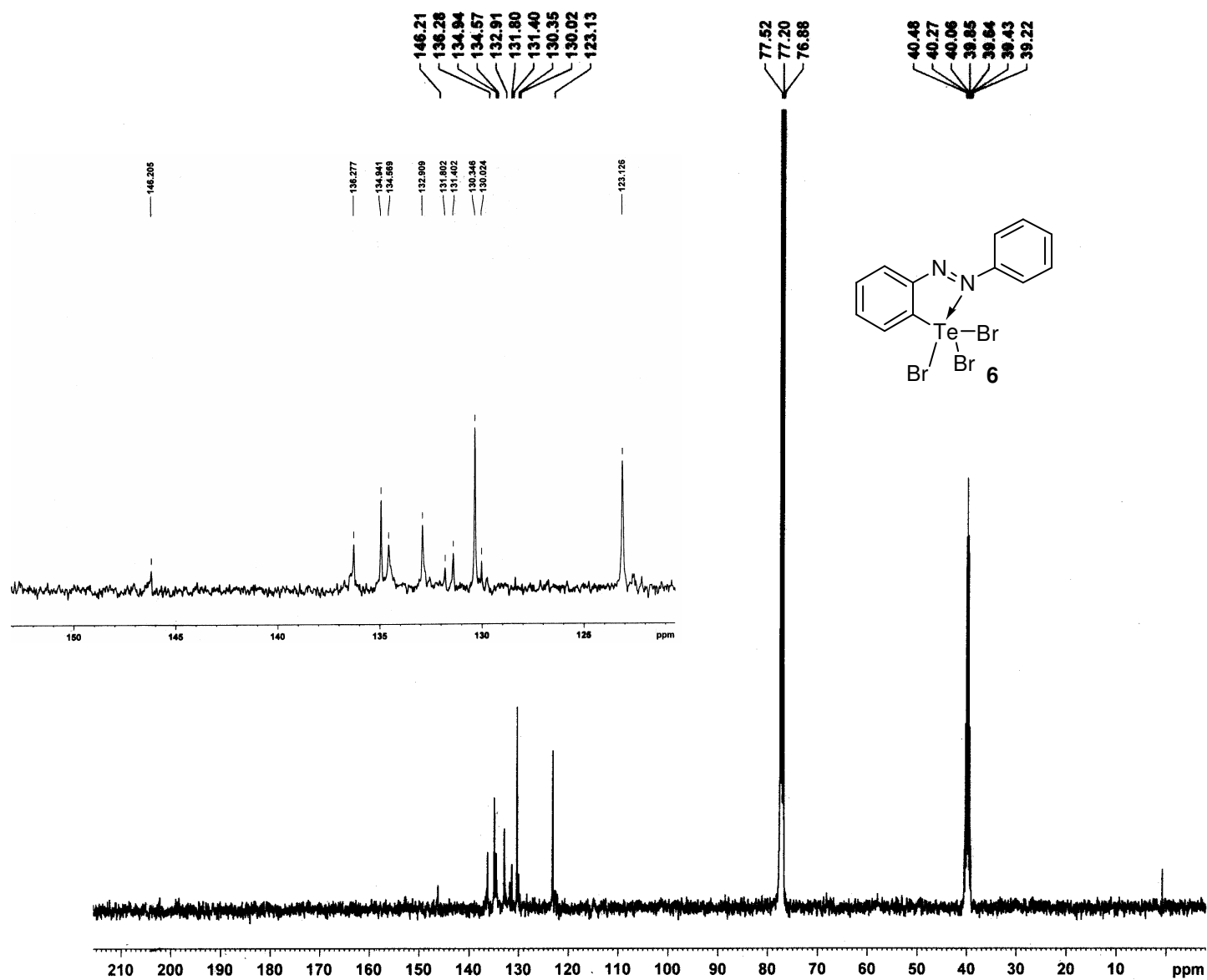


Figure S10. ¹³C-NMR spectrum of **6** in CDCl₃ + 2drops of DMSO-*d*₆

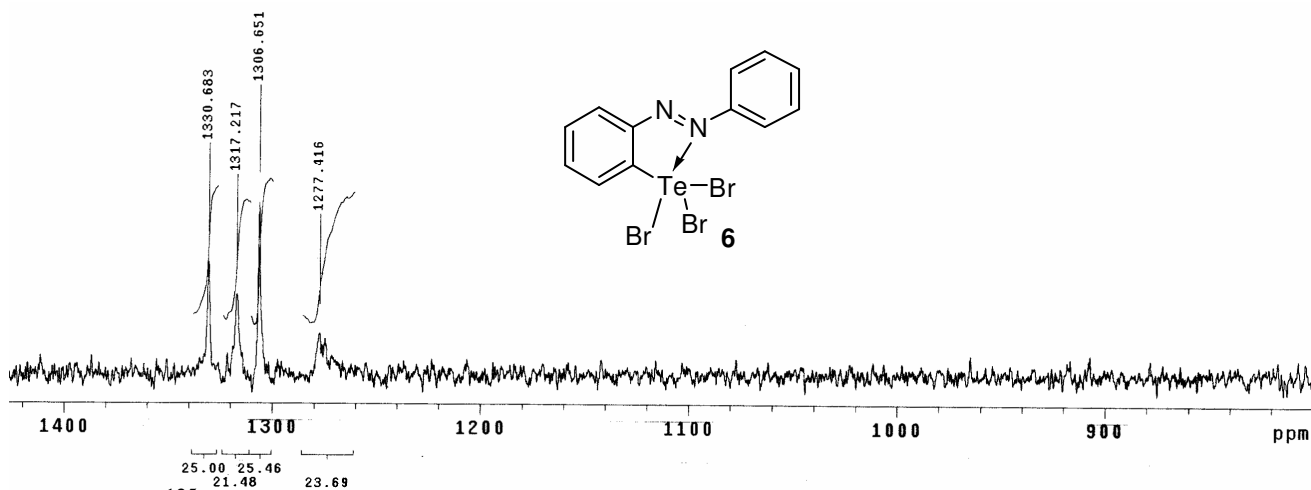


Figure S11. ¹²⁵Te-NMR spectrum of **6**

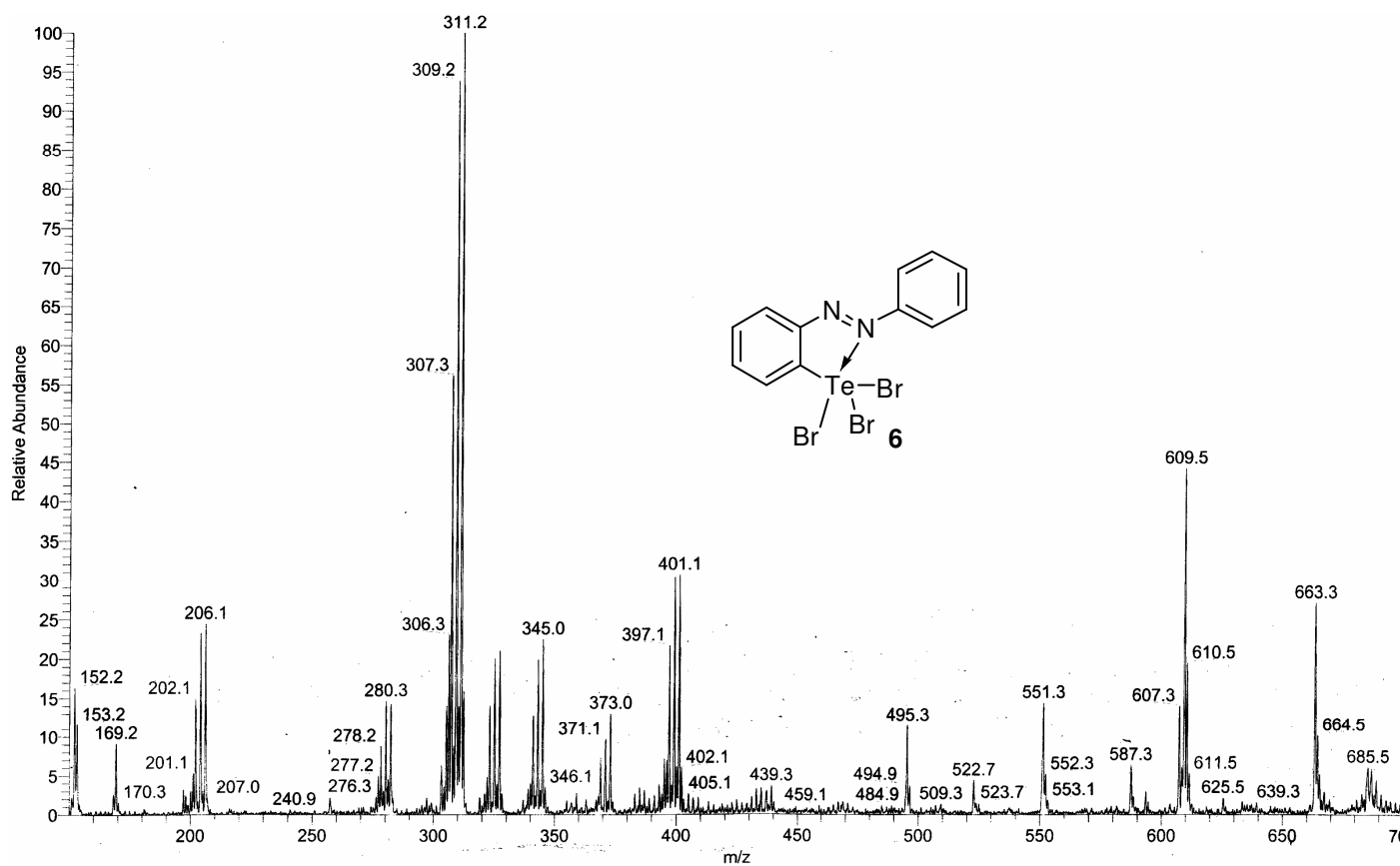


Figure S12.ESI-MS of **6**

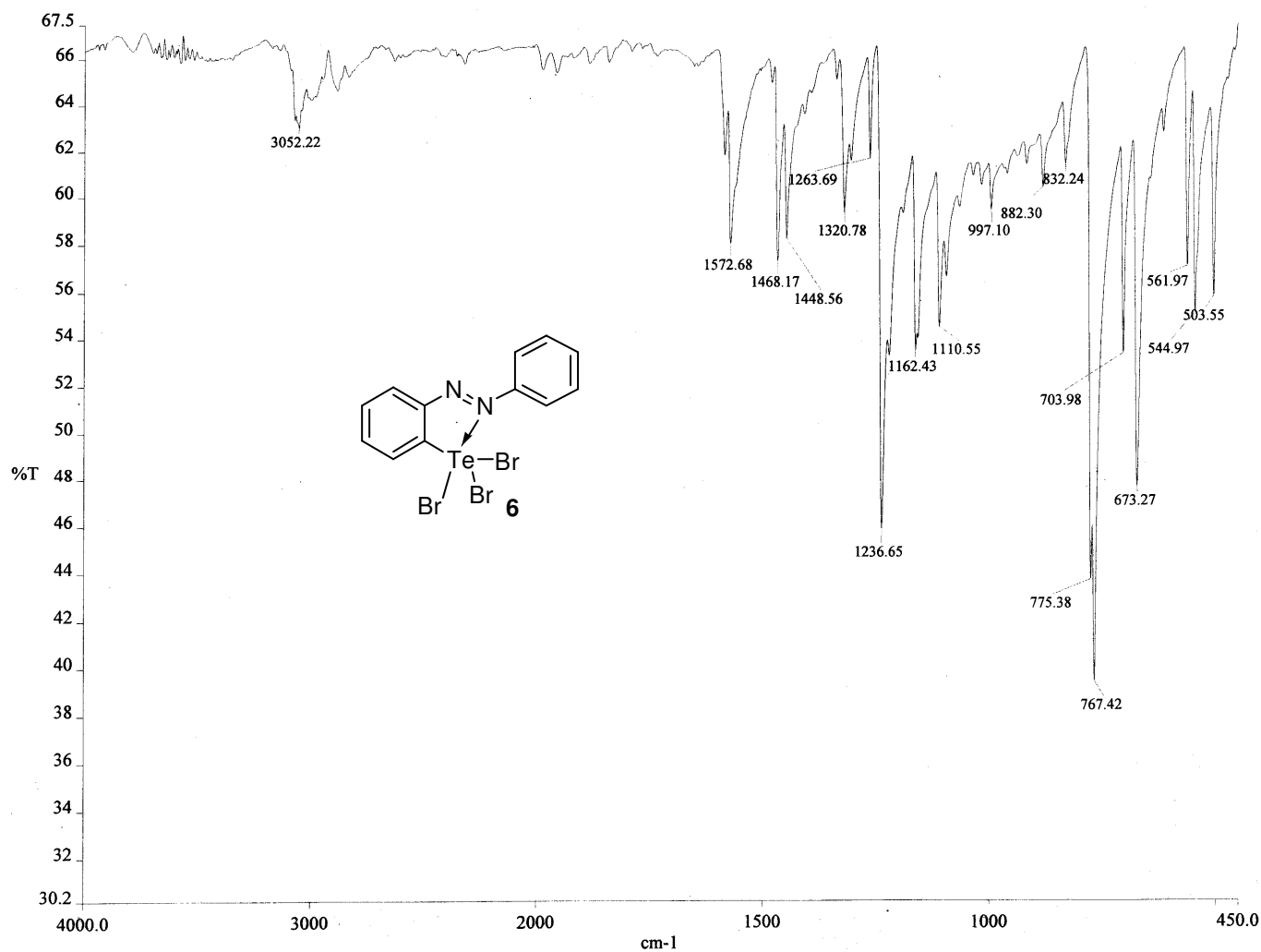


Figure S13.FT-IR spectrum of **6**

MonoTelluride

Eager 300 Report

Page: 1 Sample: HBS-KR (HBS-KR)

Method Name : sp280208

Method File : G:\eager300\Eager 300 EA1112\sp280208.mth

Chromatogram : HBS-KR

Operator ID : MANOJA

Analysed : 02/28/2008 14:55

Sample ID : HBS-KR (# 24)

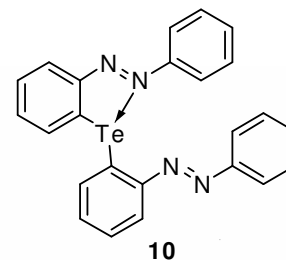
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments

Printed : 2/28/2008 17:32

Instrument N. : Instrument #1

Sample weight : 1.272



Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	10.2907	43	185121	FU	10.843060	.141424E+07
Carbon	58.1897	65	2007280	FU	1.000000	.269258E+07
Hydrogen	3.3366	166	324445	RS	6.186810	.629924E+07
Totals	71.8170		2516846			

Figure S14. Elemental analysis (C, H, N) of 10

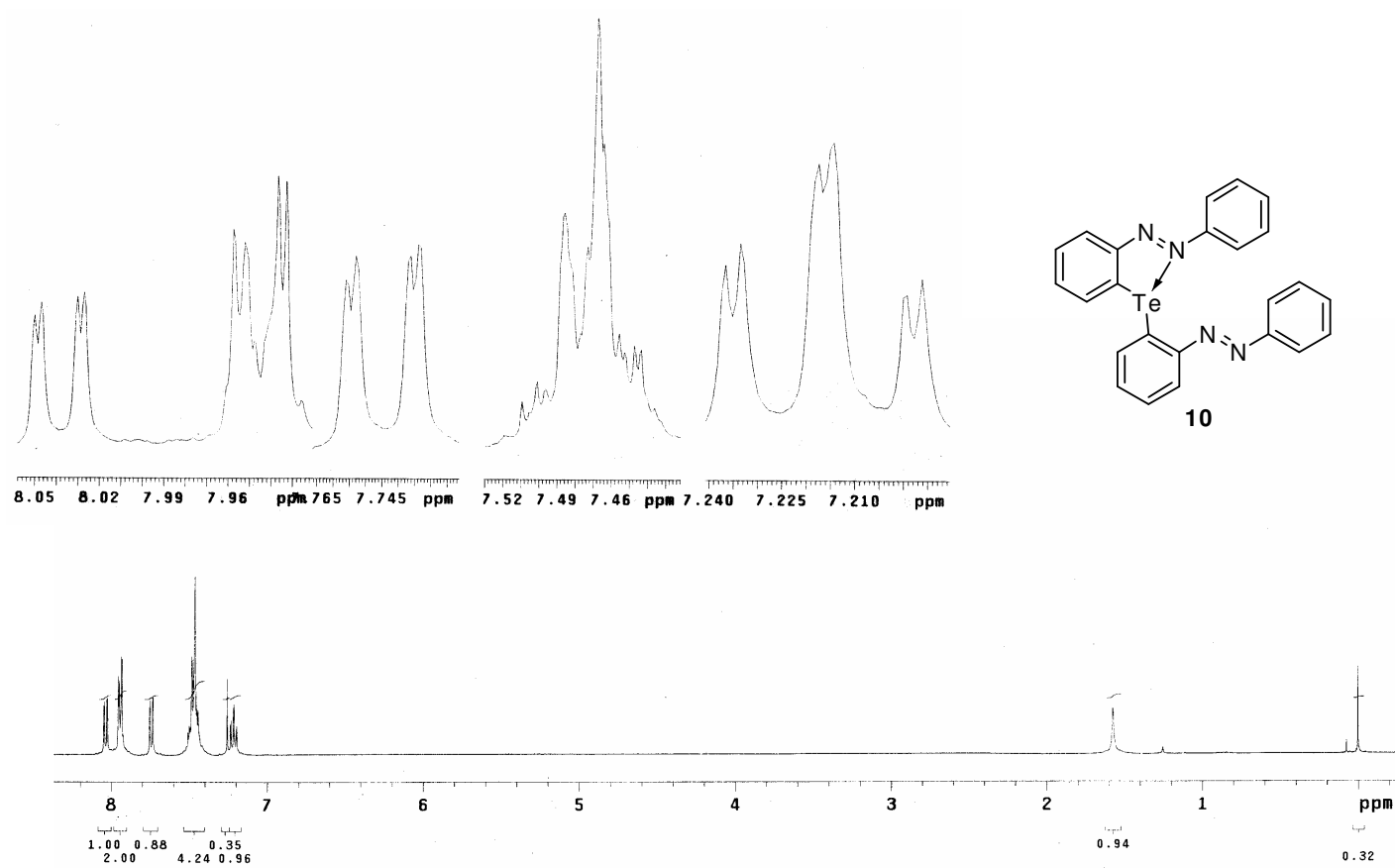


Figure S15. ^1H -NMR spectrum of **10**

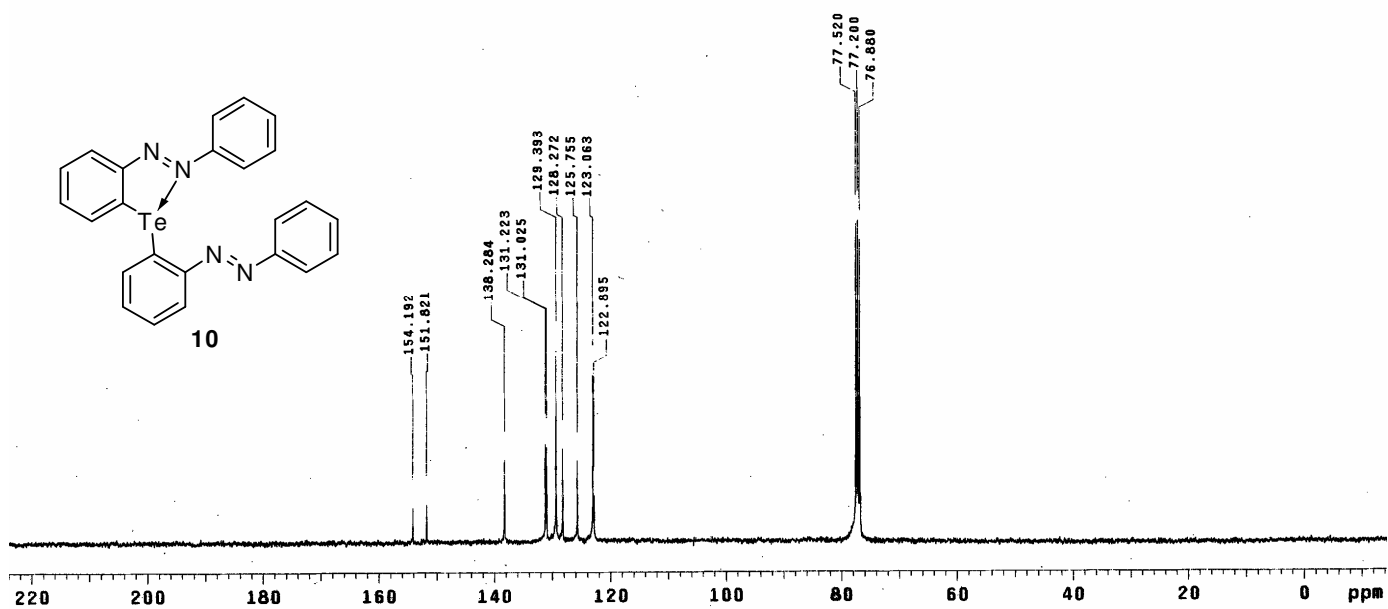


Figure S16. ¹³C-NMR spectrum of **10**

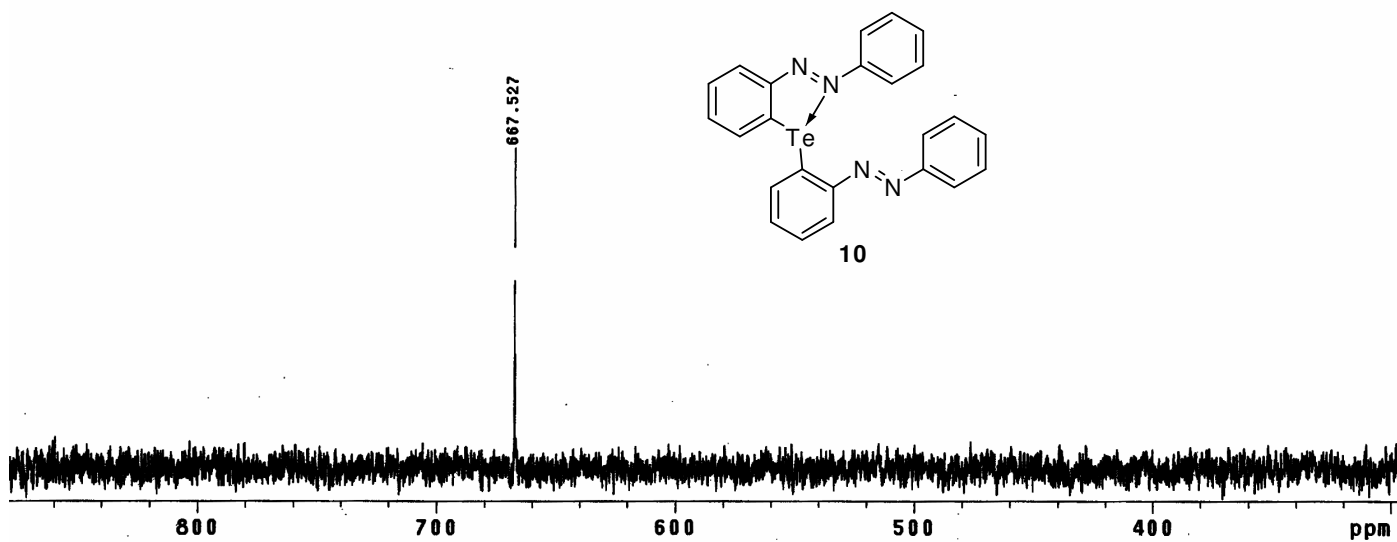


Figure S17. ¹²⁵Te-NMR spectrum of **10**

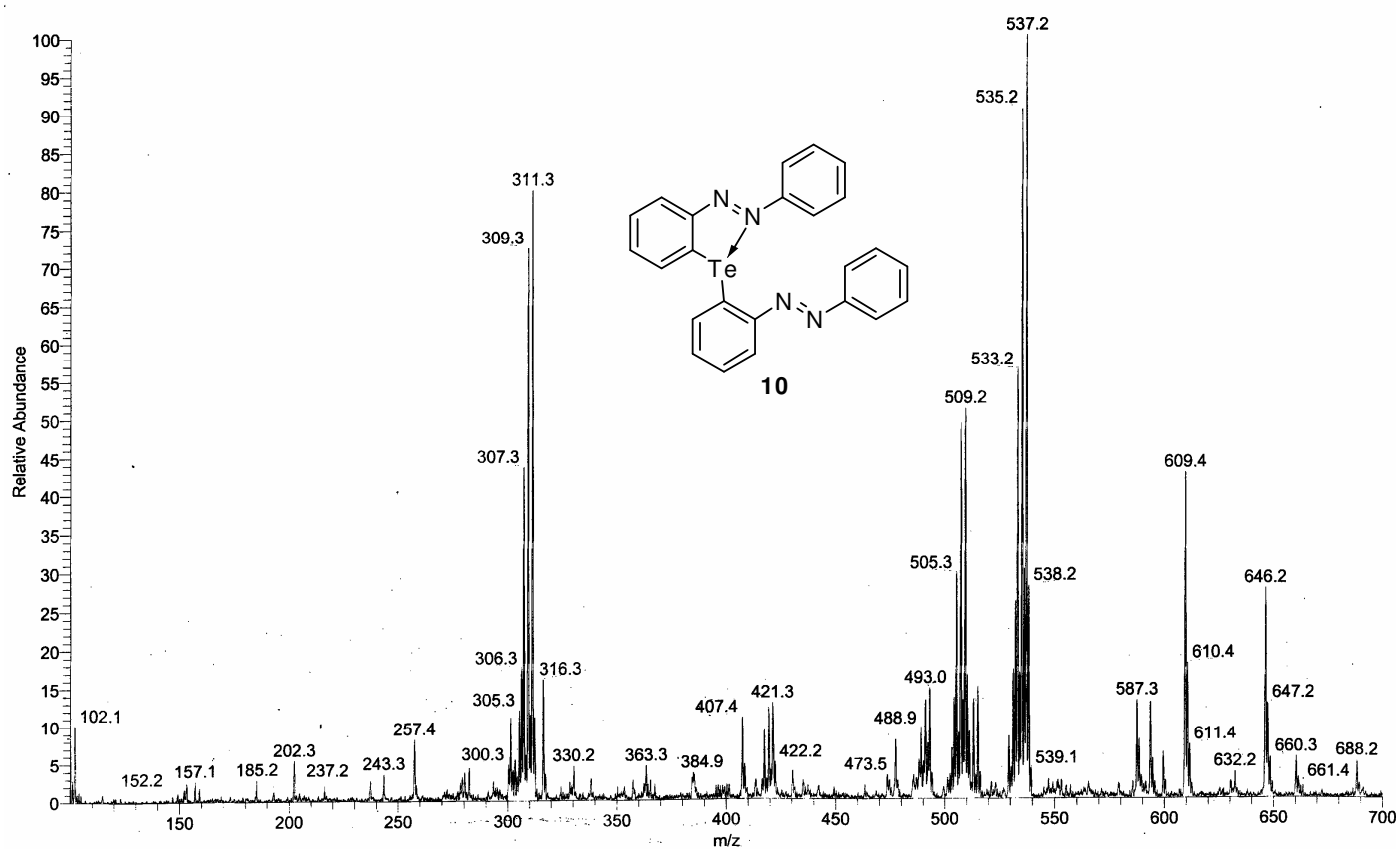


Figure S18. ESI-MS of **10**

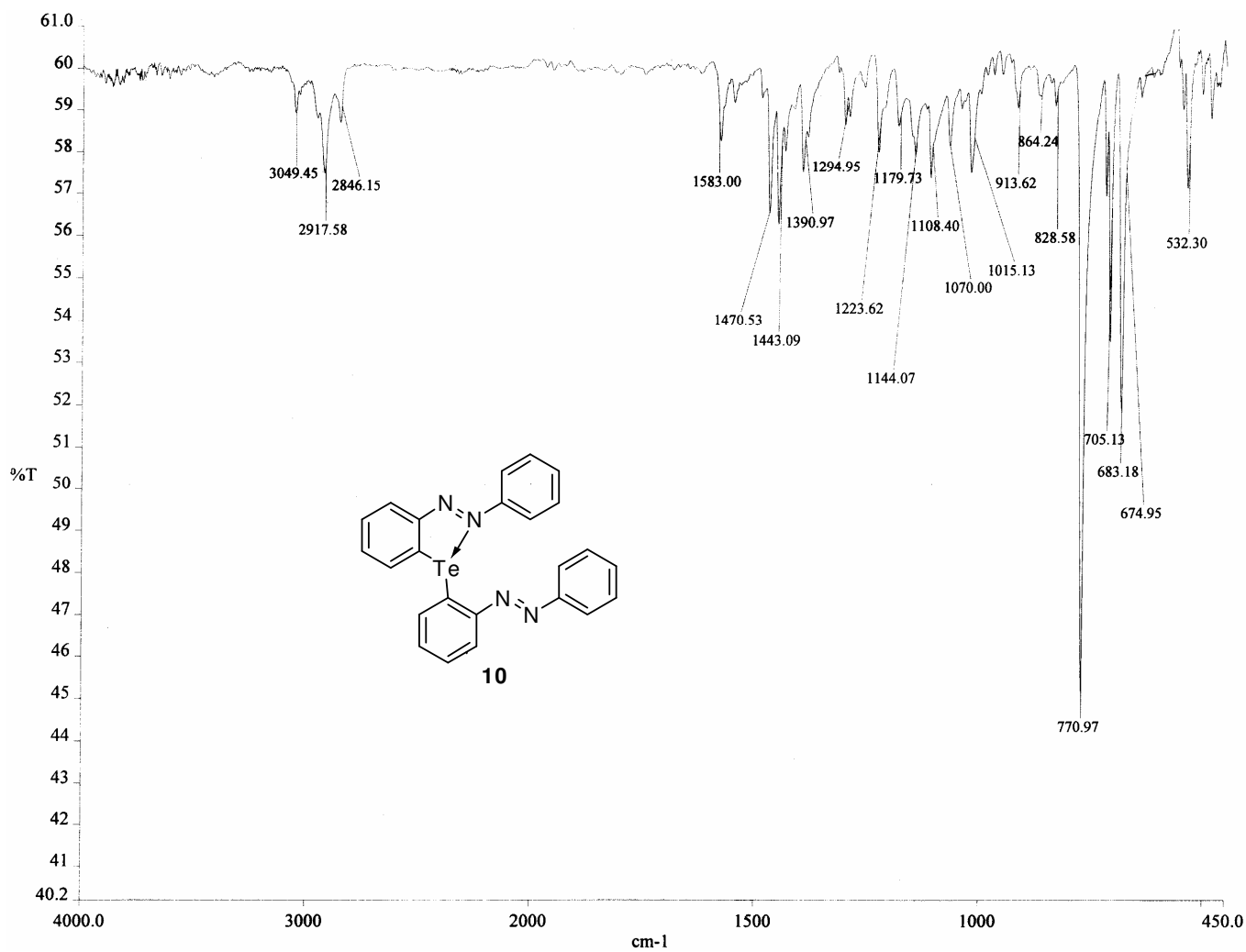


Figure S19. FT-IR spectrum of **10**

Eager 300 Report

Page: 1 Sample: KRTECL2r (KRTECL2r)

Method Name : sp140508
 Method File : G:\eager300\Eager 300 EA1112\sp140508.mth
 Chromatogram : KRTECL2r
 Operator ID : SP
 Analysed : 05/14/2008 16:27
 Sample ID : KRTECL2r (# 30)
 Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
 Printed : 5/14/2008 17:05
 Instrument N. : Instrument #1
 Sample weight : 1.718

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.9556	43	197723	RS	11.820470	.128511E+07
Carbon	51.6610	65	2337174	RS	1.000000	.262987E+07
Hydrogen	3.0495	169	353432	RS	6.612795	.657154E+07
Totals	63.6661		2888328			

Figure S20. Elemental analysis (C, H, N) of 13

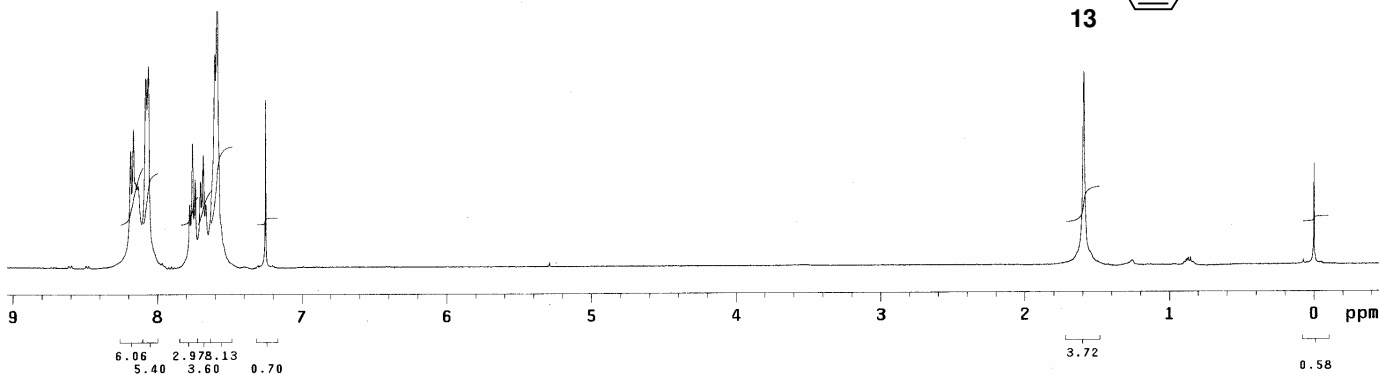
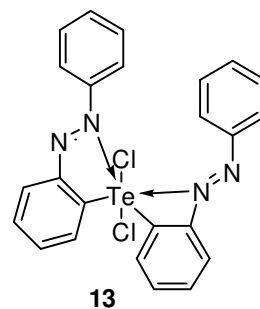
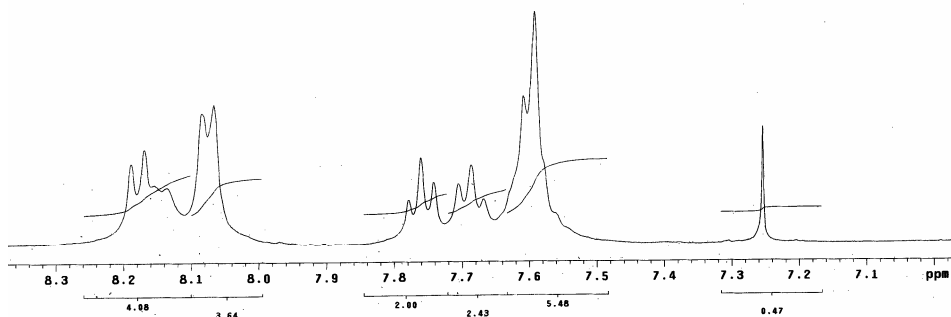


Figure S21. ¹H-NMR spectrum of 13

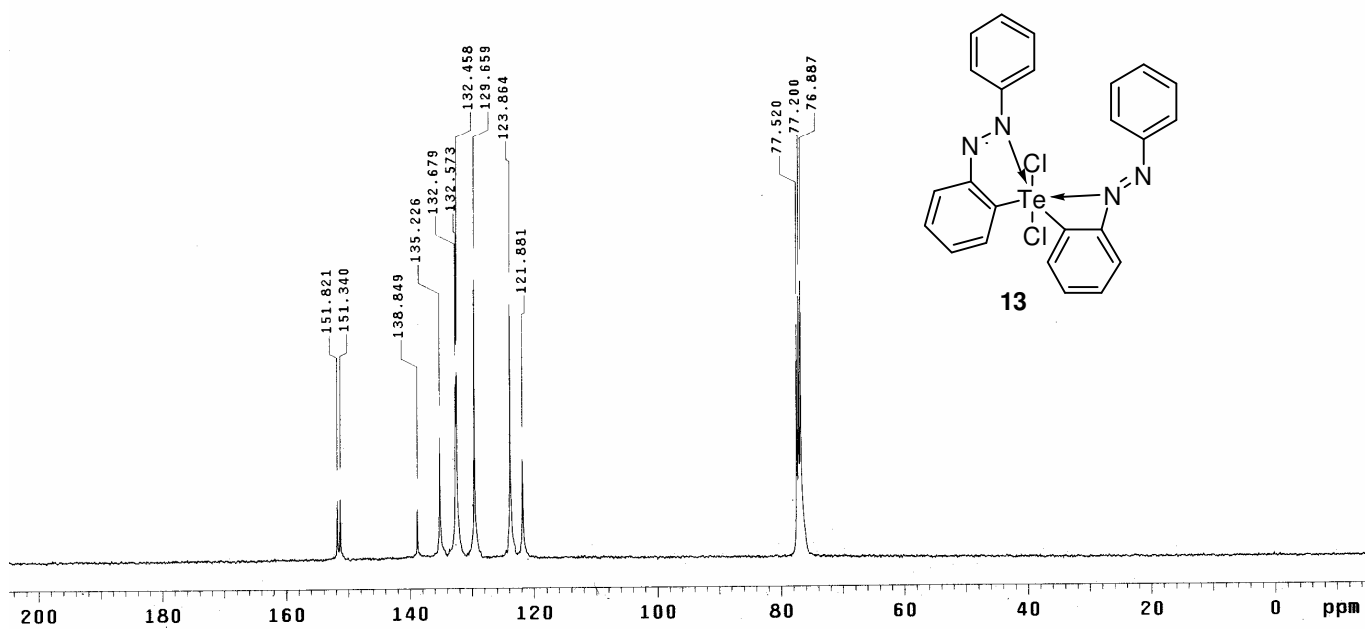


Figure S22. ^{13}C -NMR spectrum of **13**

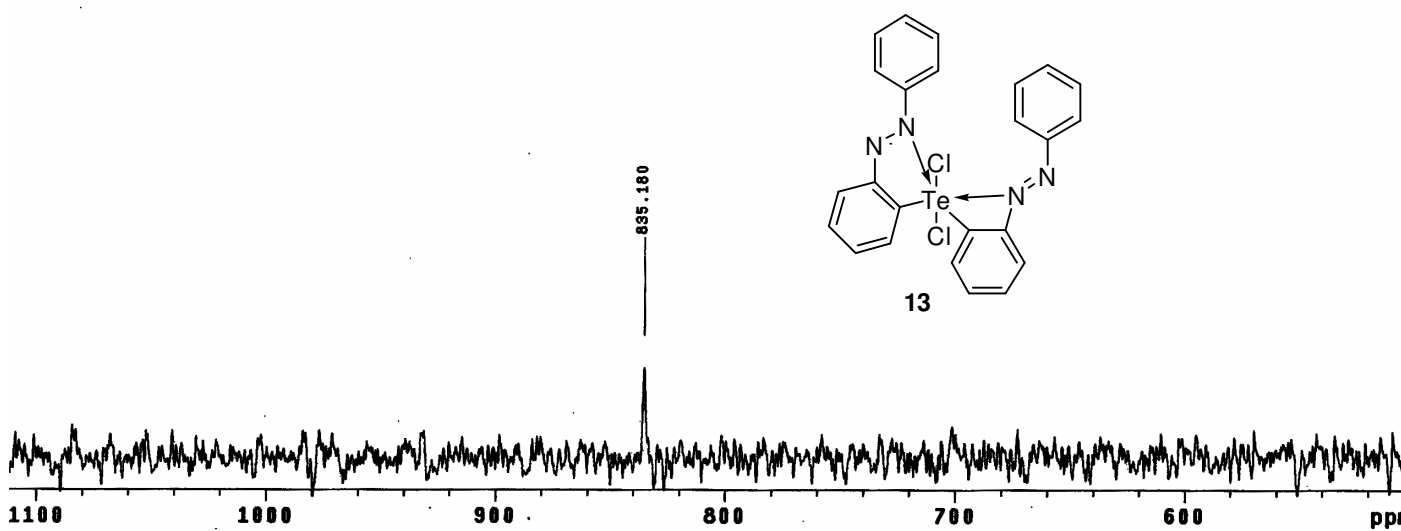


Figure S23. ^{125}Te -NMR spectrum of **13**

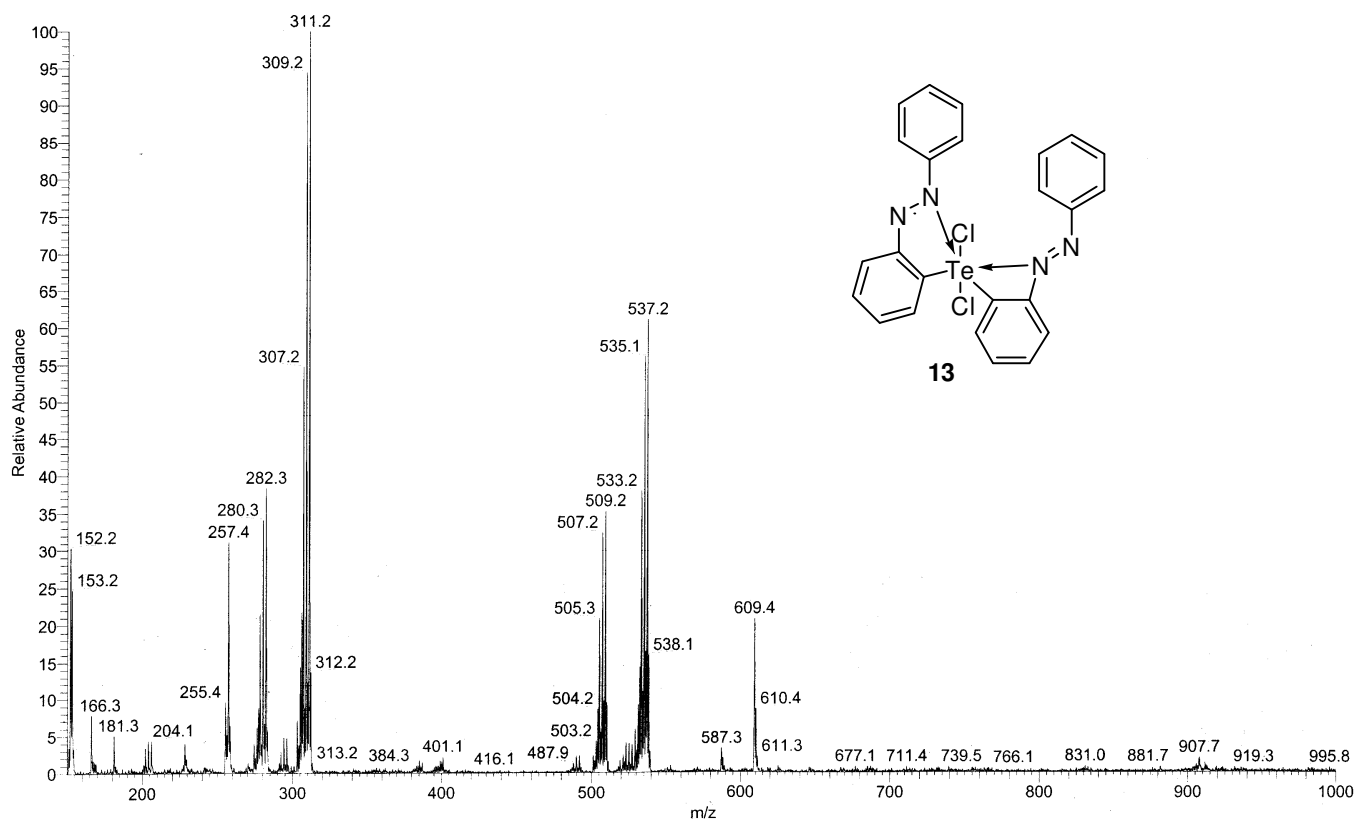


Figure S24. ESI-MS of **13**

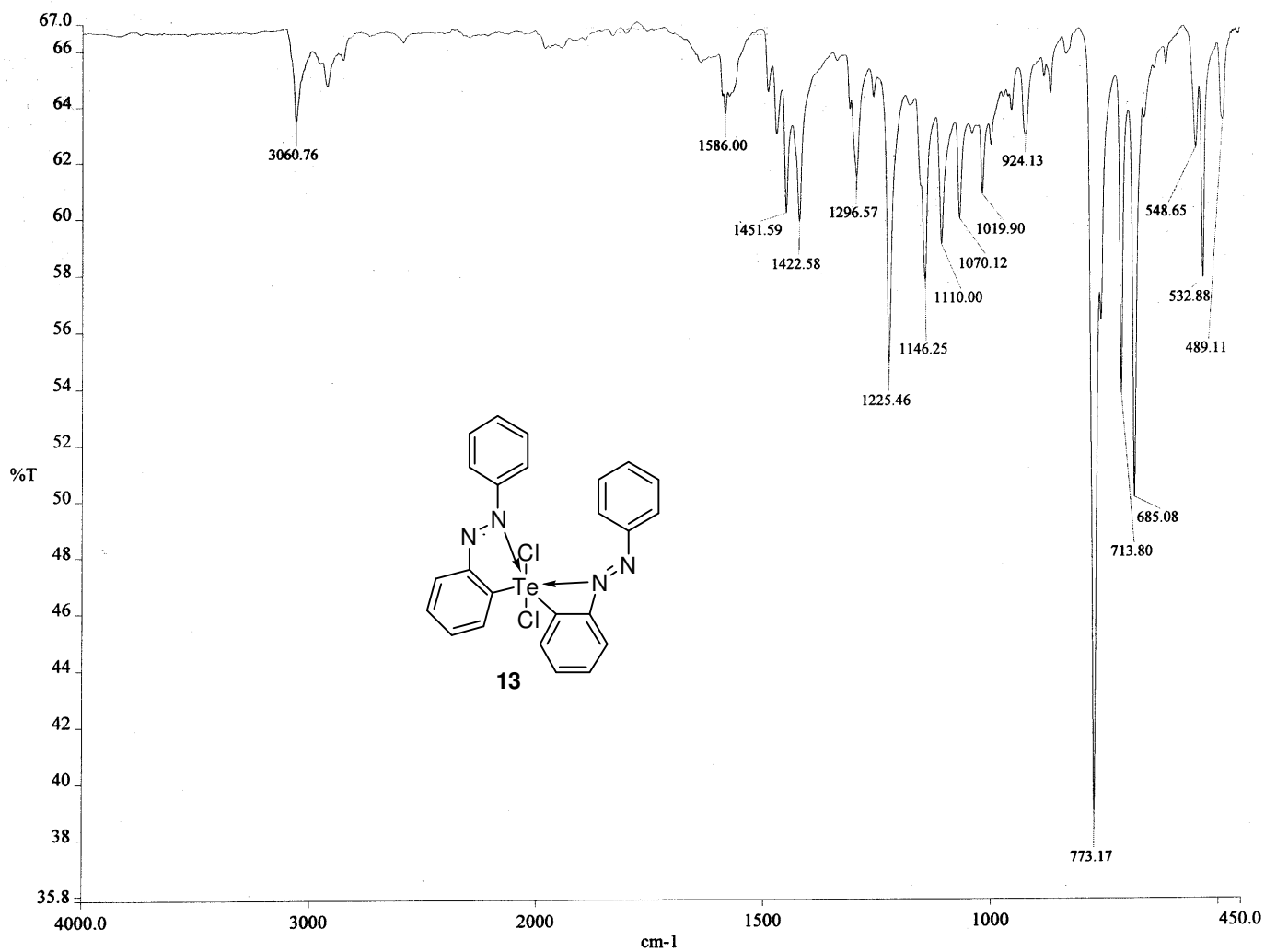


Figure S25.FT-IR spectrum of **13**

Eager 300 Report

Page: 1 Sample: HBSKRTE1 (HBSKRTE1)

Method Name : sp040707

Method File : G:\eager300\Eager 300 EA1112\sp040707.mth

Chromatogram : HBSKRTE1

Operator ID : sp

Analysed : 07/04/2007 15:01

Sample ID : HBSKRTE1 (# 11)

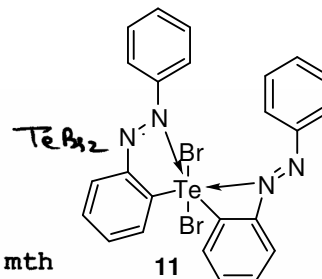
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments

Printed : 7/4/2007 16:36

Instrument N. : Instrument #1

Sample weight : 1.764



Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.5935	45	174415	FU	11.343110	.115058E+07
Carbon	44.3618	67	1978403	FU	1.000000	.252462E+07
Hydrogen	1.7206	187	144379	RS	13.702840	.475693E+07
Totals	54.6758		2297197			

Figure S26.Elemental analysis (C, H, N) of 11

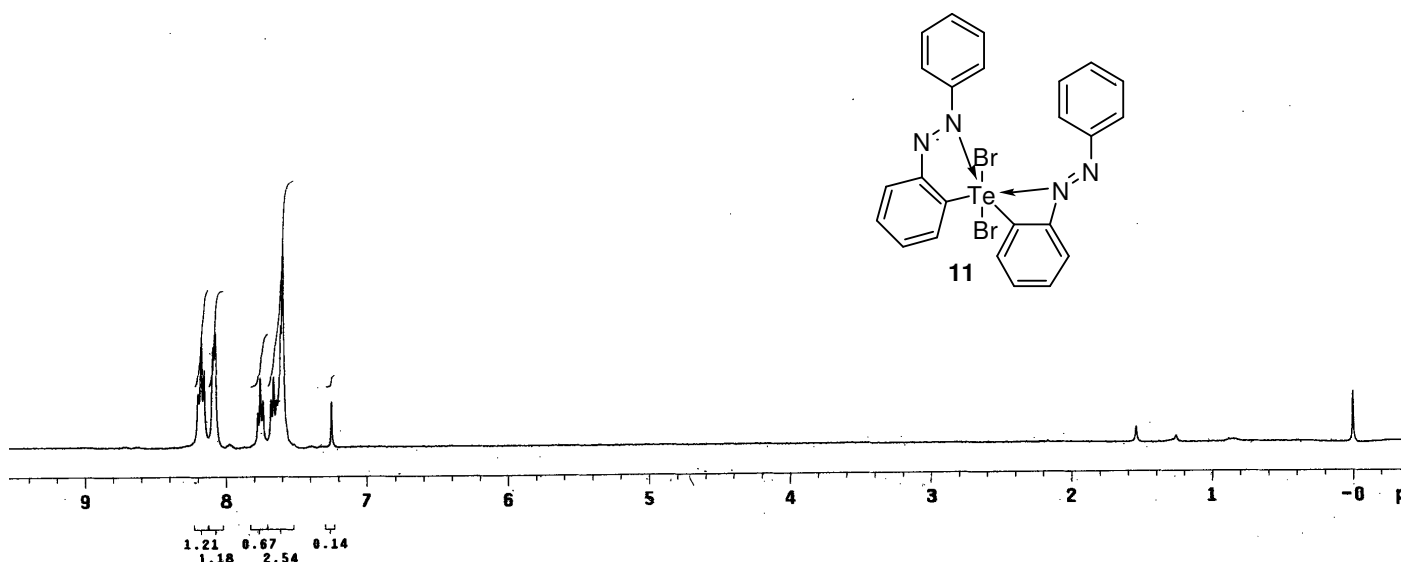
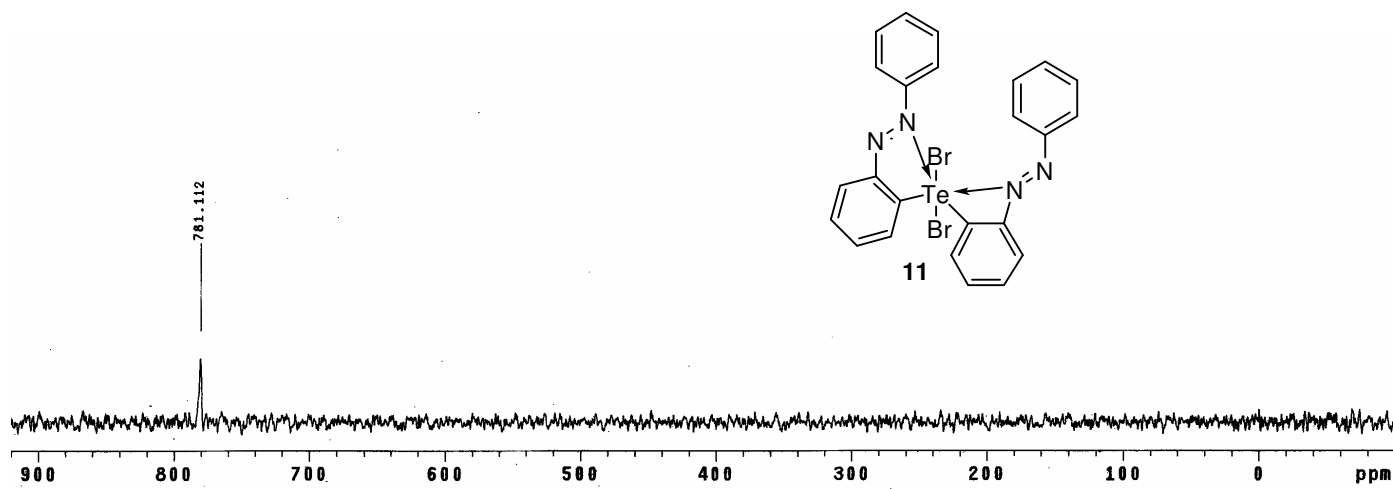
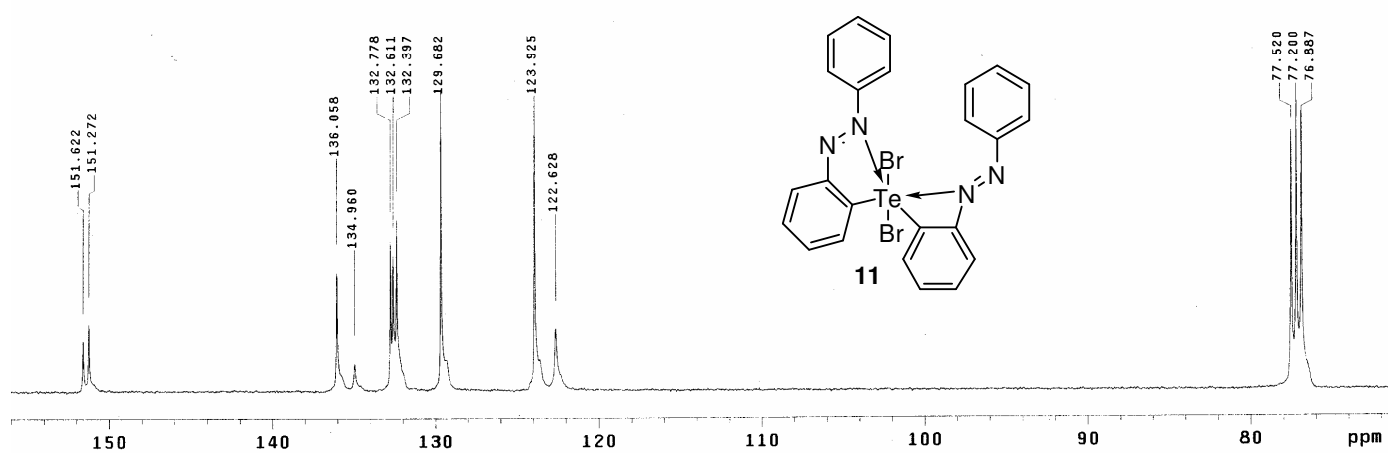


Figure S27. ¹H-NMR spectrum of 11



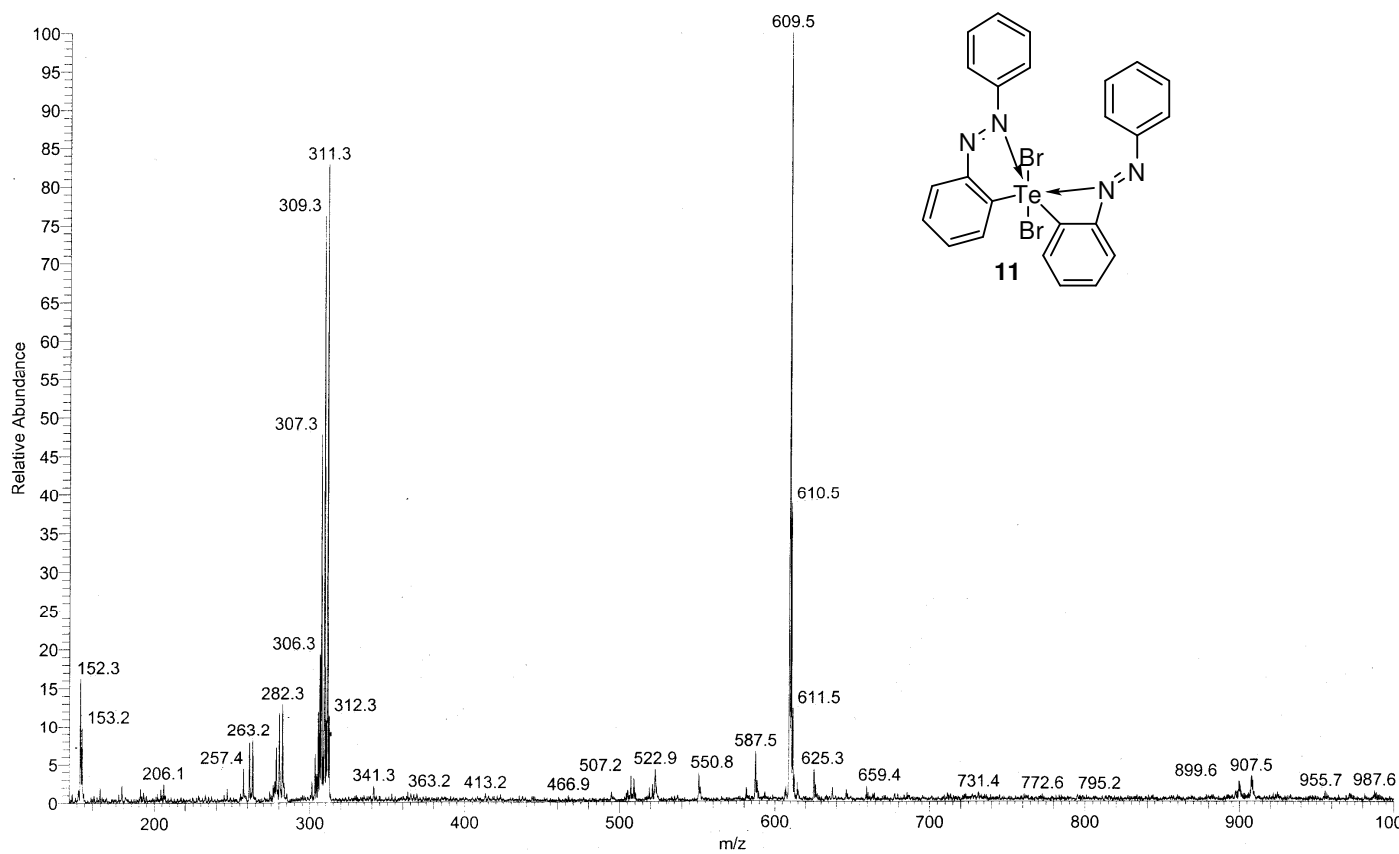


Figure S30. ESI-MS of **11**

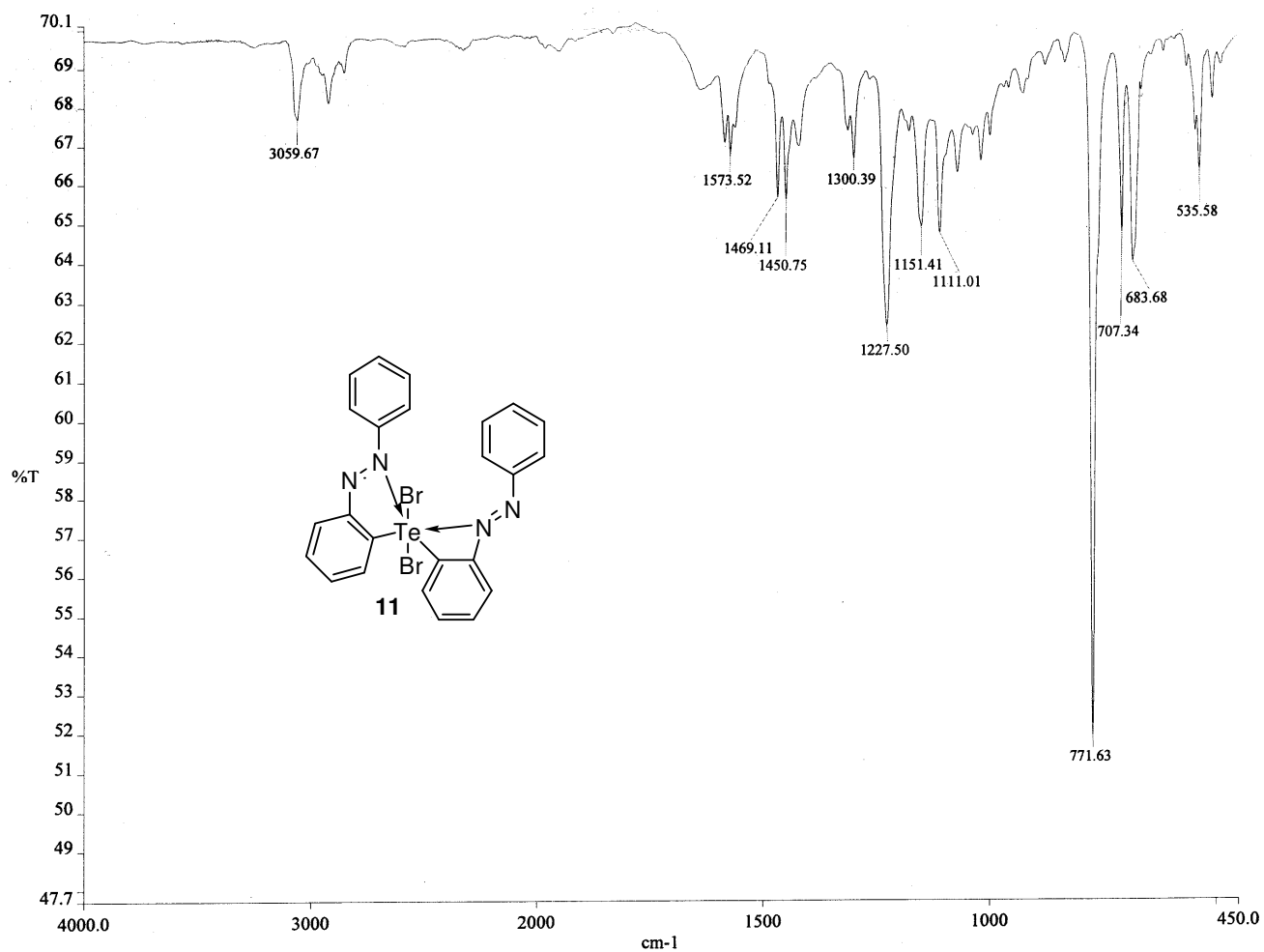


Figure S31. FT-IR spectrum of **11**

Eager 300 Report

Page: 1 Sample: KRTEI2 (KRTEI2)

Method Name : sp300508
 Method File : D:\CHNS2008\SP300508.mth
 Chromatogram : KRTEI2
 Operator ID : SP
 Analysed : 05/30/2008 14:51
 Sample ID : KRTEI2 (# 24)
 Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
 Printed : 5/30/2008 15:17
 Instrument N. : Instrument #1
 Sample weight : 1.788

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	5.7144	43	112533	RS	12.379320	.110140E+07
Carbon	28.8226	66	1393083	RS	1.000000	.269794E+07
Hydrogen	1.5832	172	194008	RS	7.180542	.656808E+07
Totals	36.1201		1699624			

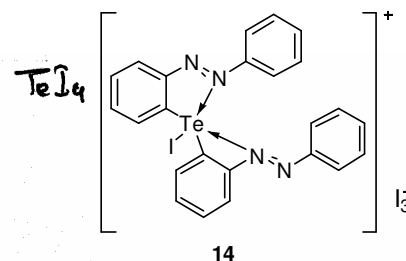


Figure S32.Elemental analysis (C, H, N) of 14

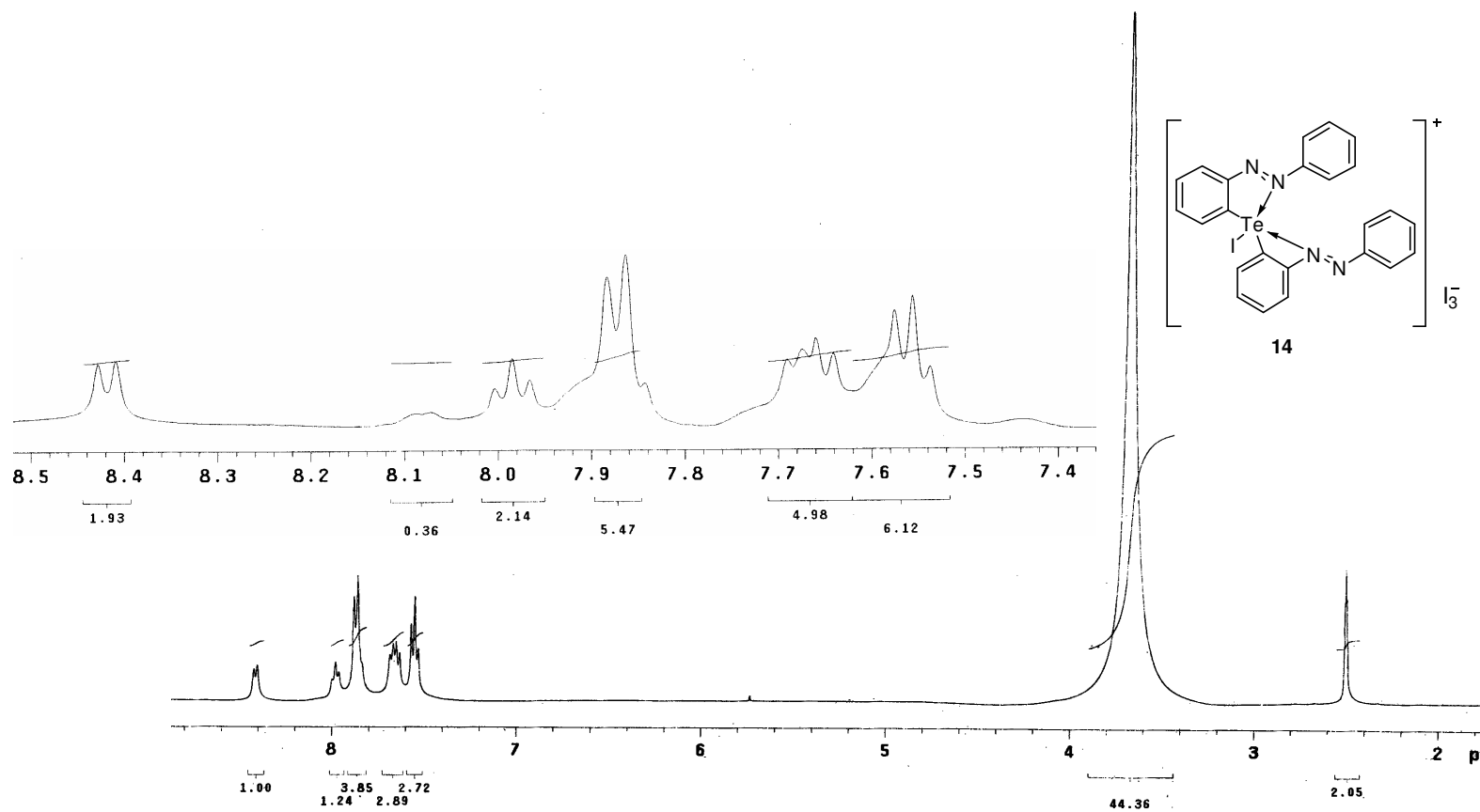
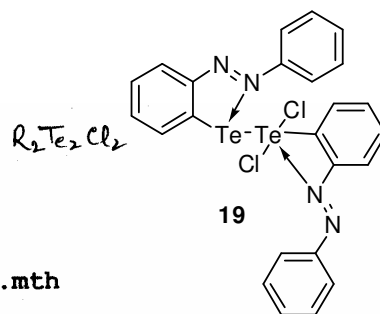


Figure S33. ^1H -NMR spectrum of **14**

Eager 300 Report

Page: 1 Sample: DITECL2(DITECL2)

Method Name : sp090508 Method File : G:\eager300\Eager 300 EA1112\sp090508.mth Chromatogram : DITECL2 Operator ID : SP Analysed : 05/09/2008 13:57 Sample ID : DITECL2# 21) Analysis Type : UnkNown (Area)	Company Name : C.E. Instruments Printed : 5/9/2008 15:31 Instrument N. : Instrument #1 Sample weight : 1.71
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Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.0118	43	207854	RS	8.868044	.110383E+07
Carbon	40.8242	65	1843254	RS	1.000000	.264041E+07
Hydrogen	3.0073	169	354578	RS	5.198444	.678613E+07
Totals	54.8433		2405686			

Figure S34.Elemental analysis of 19

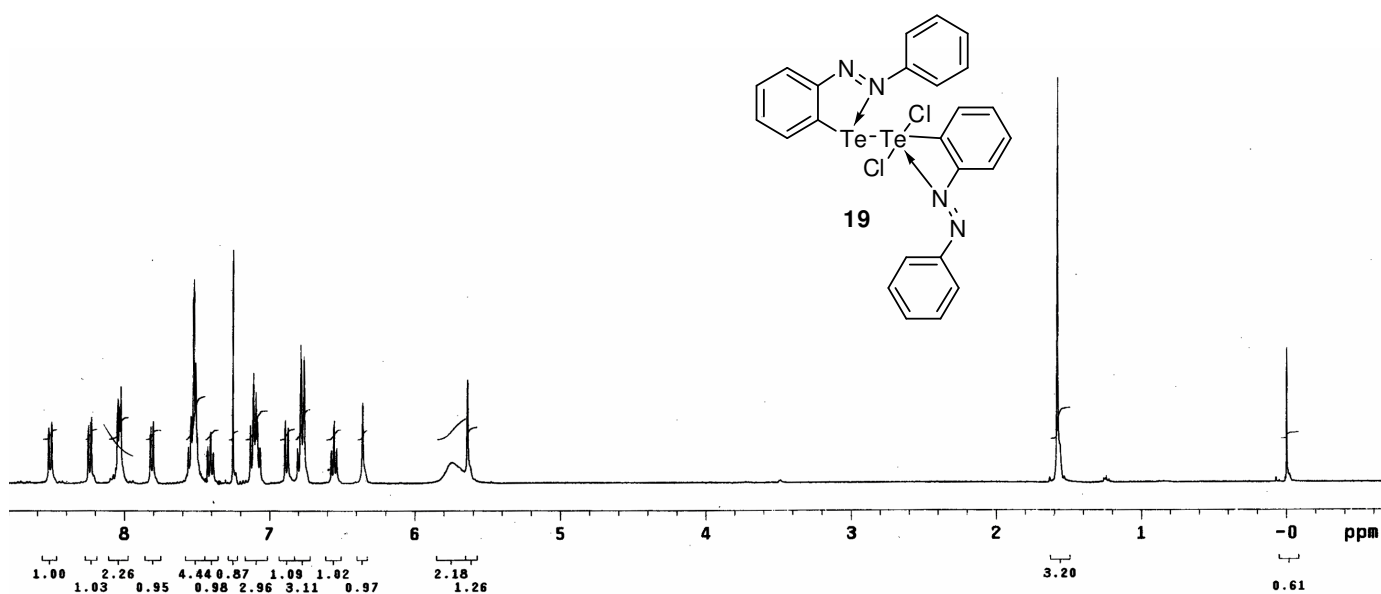


Figure S35. ^1H -NMR spectrum of **19**

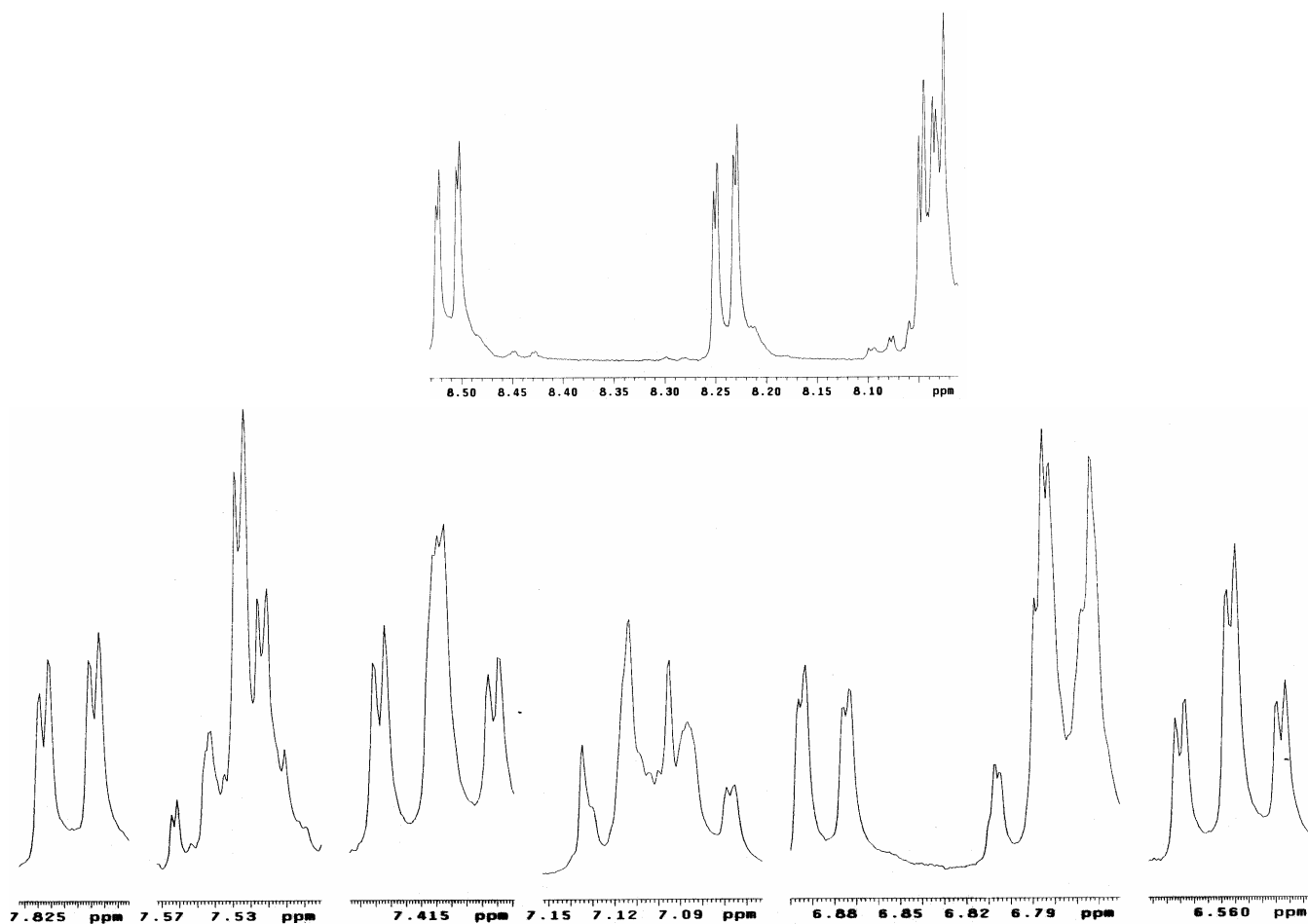


Figure S36. Expansion of ^1H -NMR spectrum of **19**

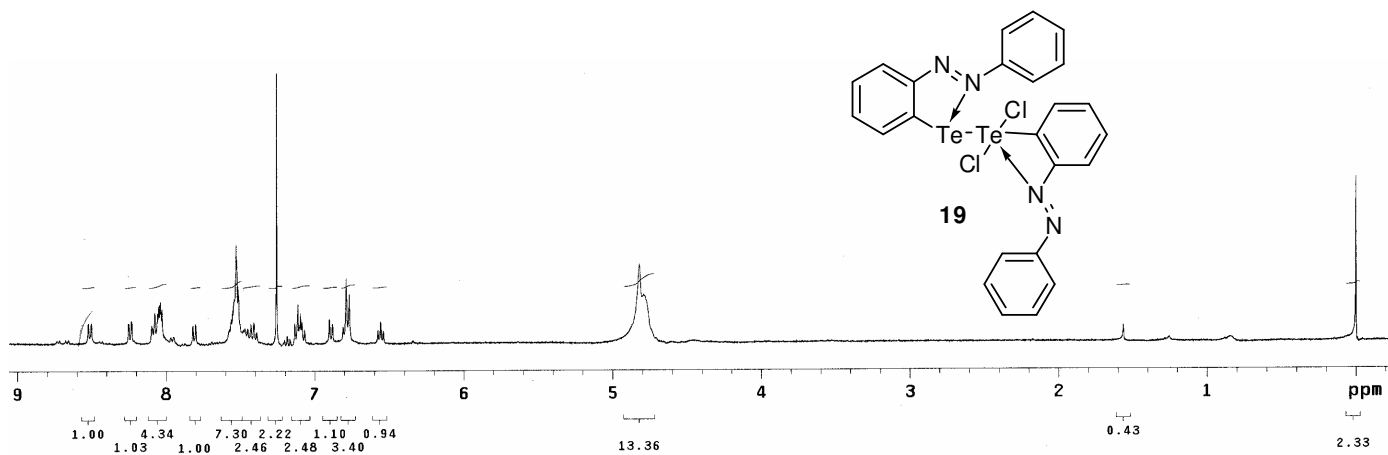


Figure S37. ¹H-NMR spectrum of **19** after D₂O exchange

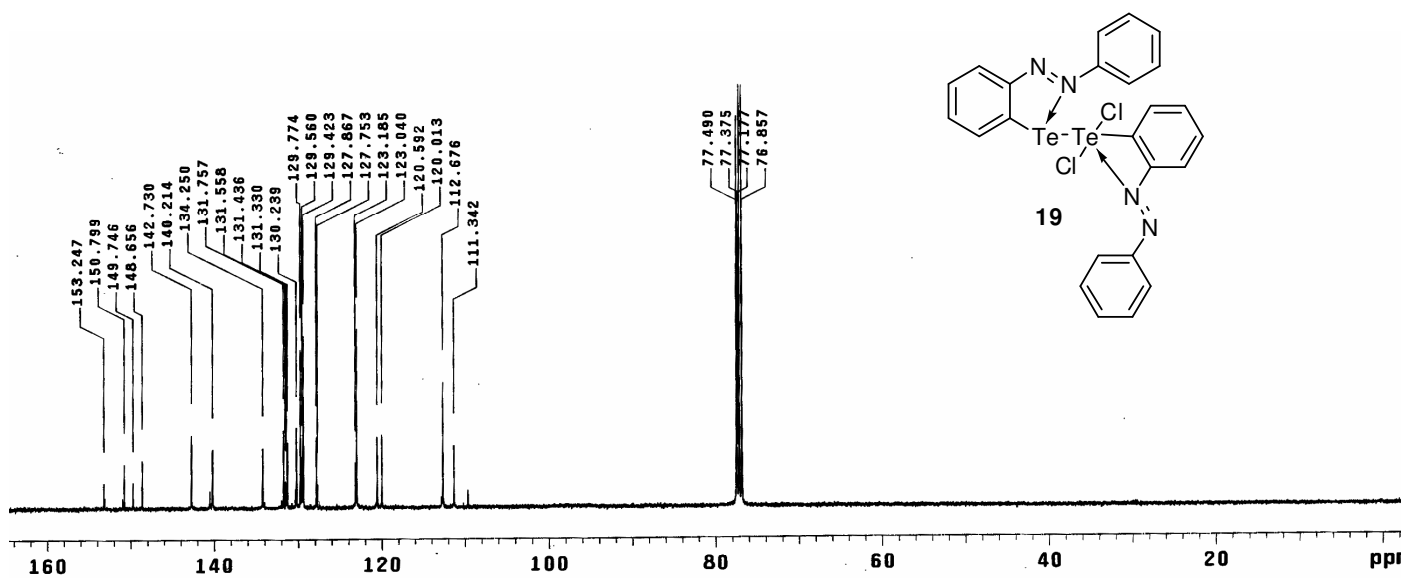


Figure S38. ¹³C-NMR spectrum of **19**

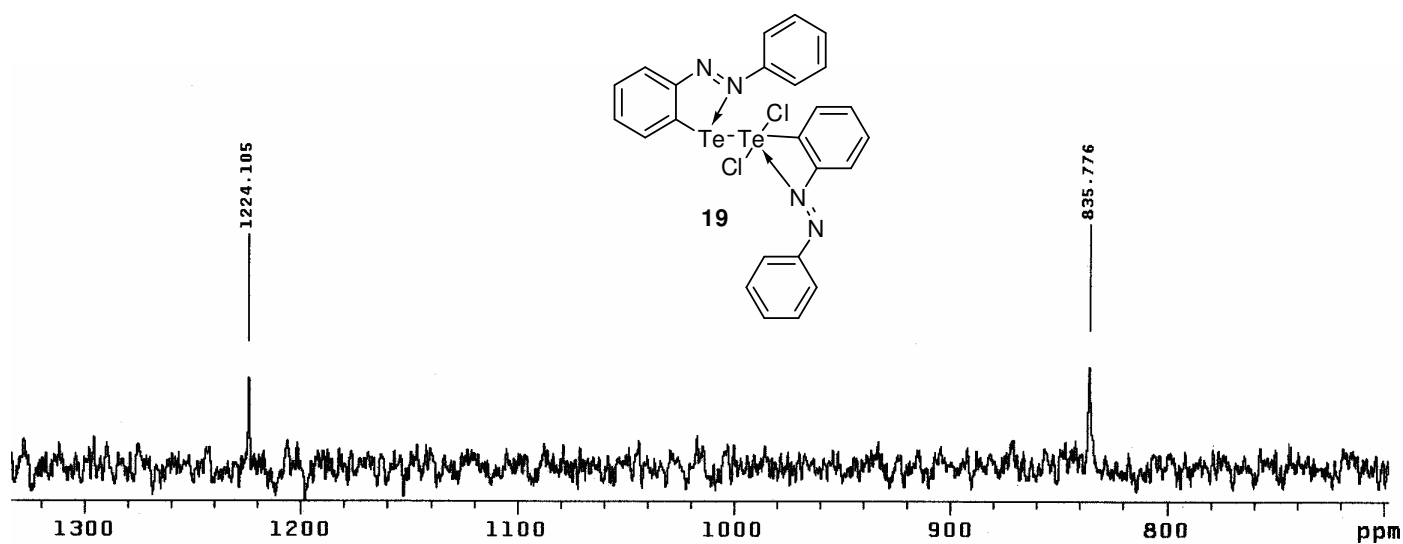


Figure S39. ^{125}Te -NMR spectrum of **19**

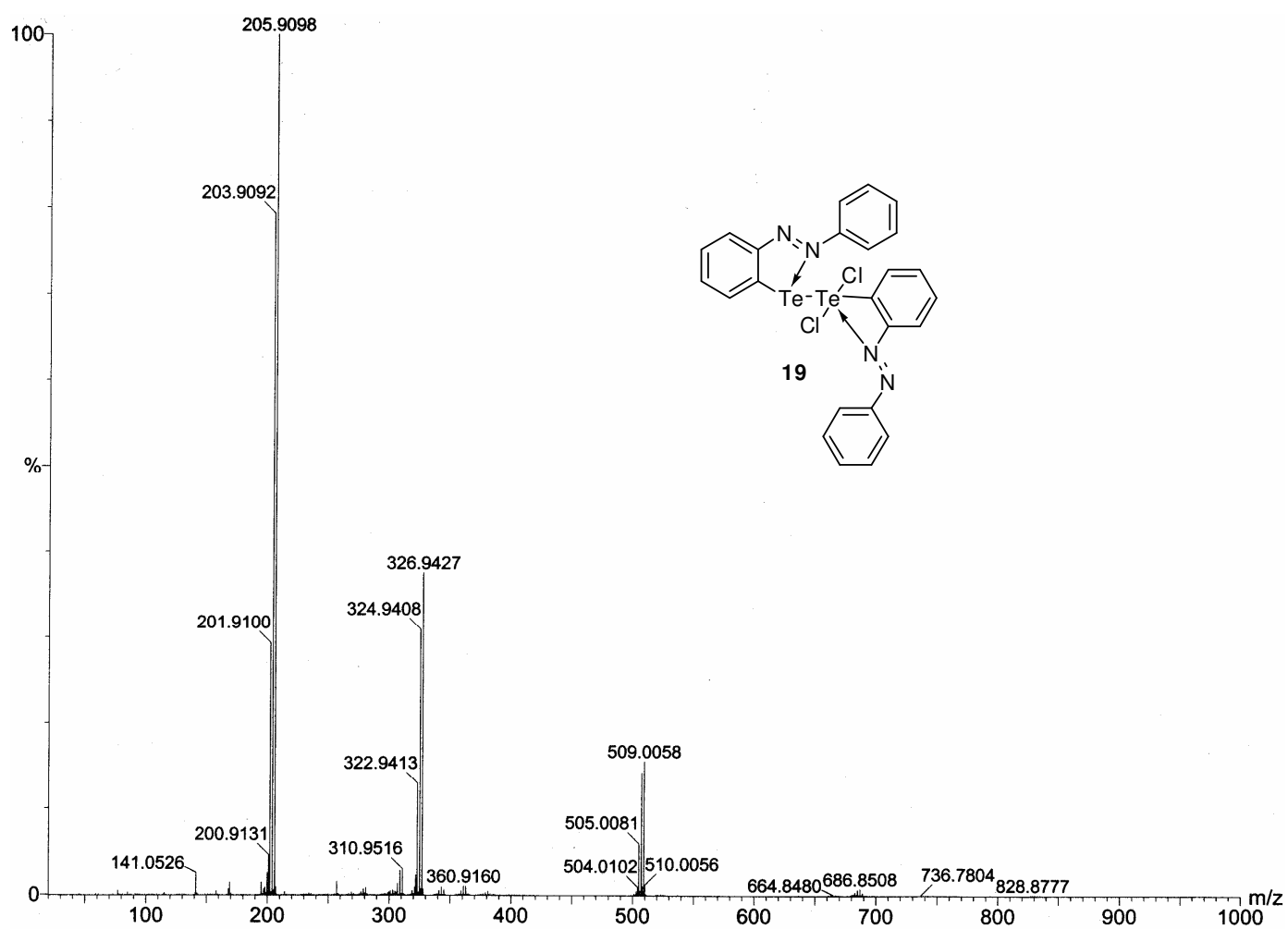


Figure S40. ES-MS of **19**

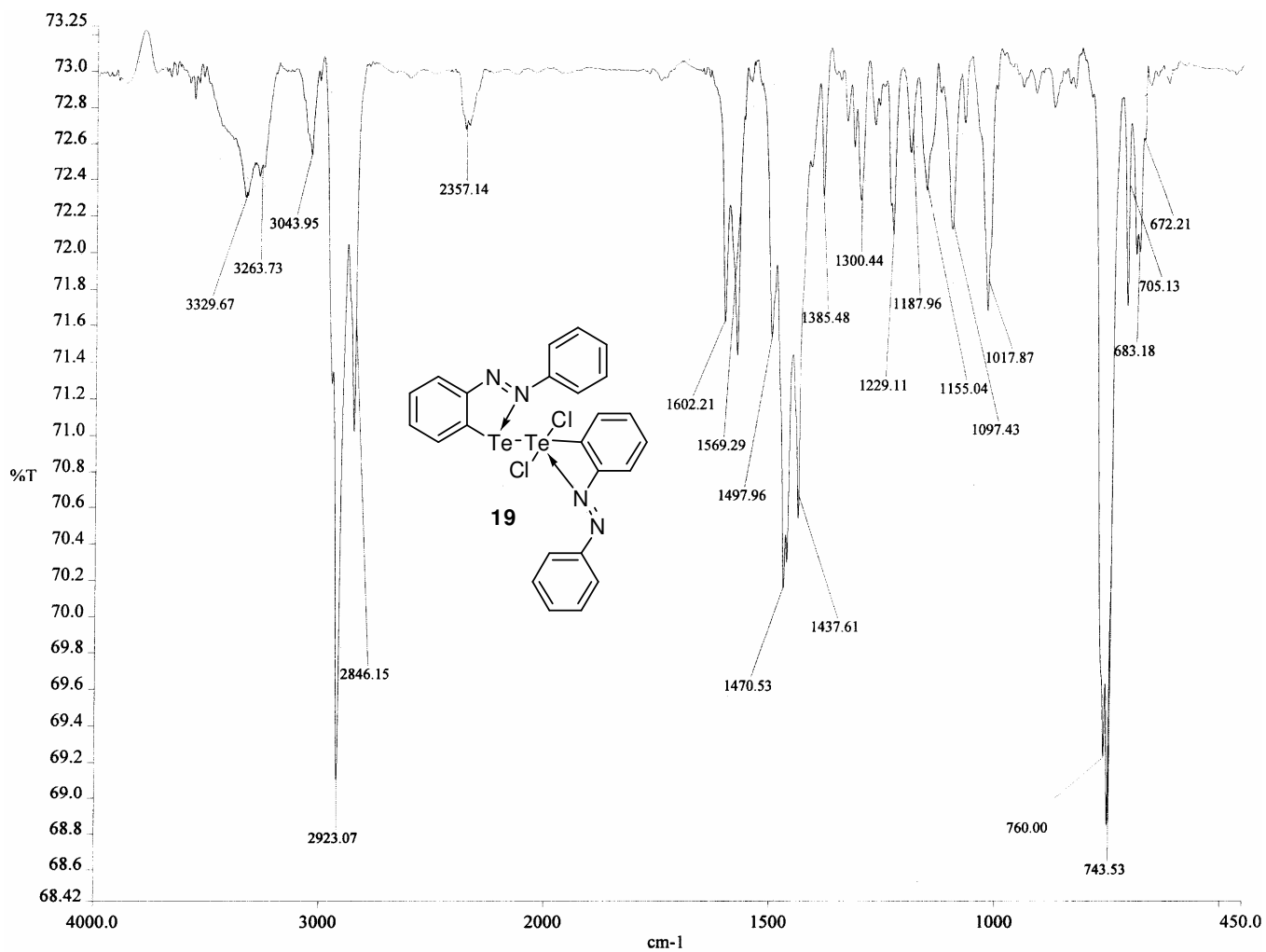


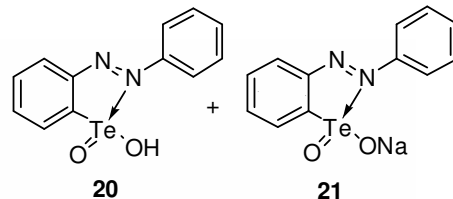
Figure S41.FT-IR spectrum of **19**

Eager 300 Report

Page: 1 Sample: HBS-KR-TEOONAW (HBS-KR-TEOONAW)

Method Name : SP260210
 Method File : D:\CHNS2008\SP260210.mth
 Chromatogram : HBS-KR-TEOONAW
 Operator ID : SP
 Analysed : 02/26/2010 13:50
 Sample ID : HBS-KR-TEOONAW (# 22)
 Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
 Printed : 2/26/2010 15:24
 Instrument N. : Instrument #1
 Sample weight : .989



Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.0310	43	68416	RS	11.456430	.114702E+07
Carbon	29.8224	66	783803	RS	1.000000	.264963E+07
Hydrogen	4.0189	169	315758	RS	2.482290	.676466E+07
Totals	39.8723		1167977			

Figure S42. Elemental analysis (C, H, N) of 20-21

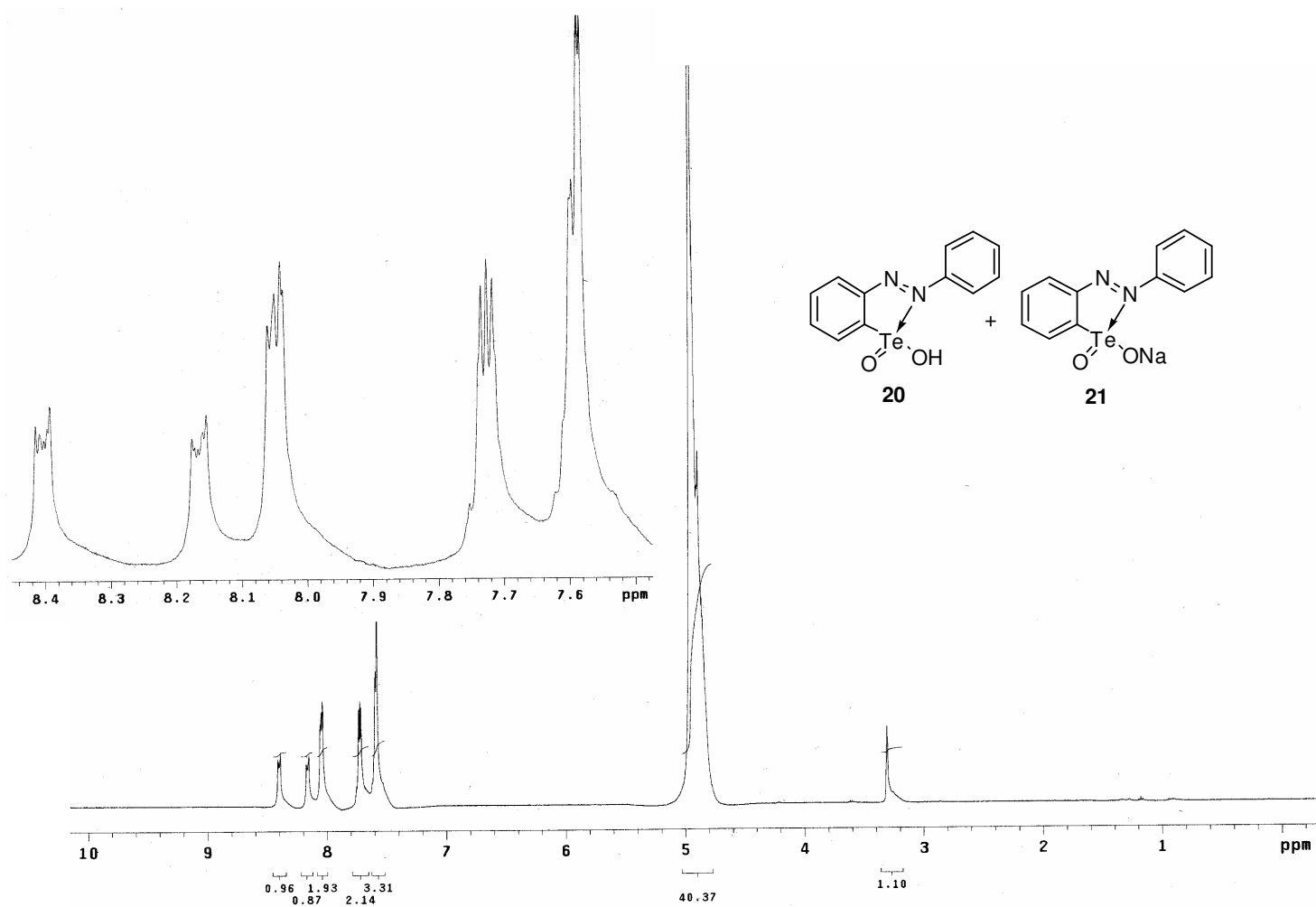


Figure S43. ^1H -NMR spectrum of **20-21**

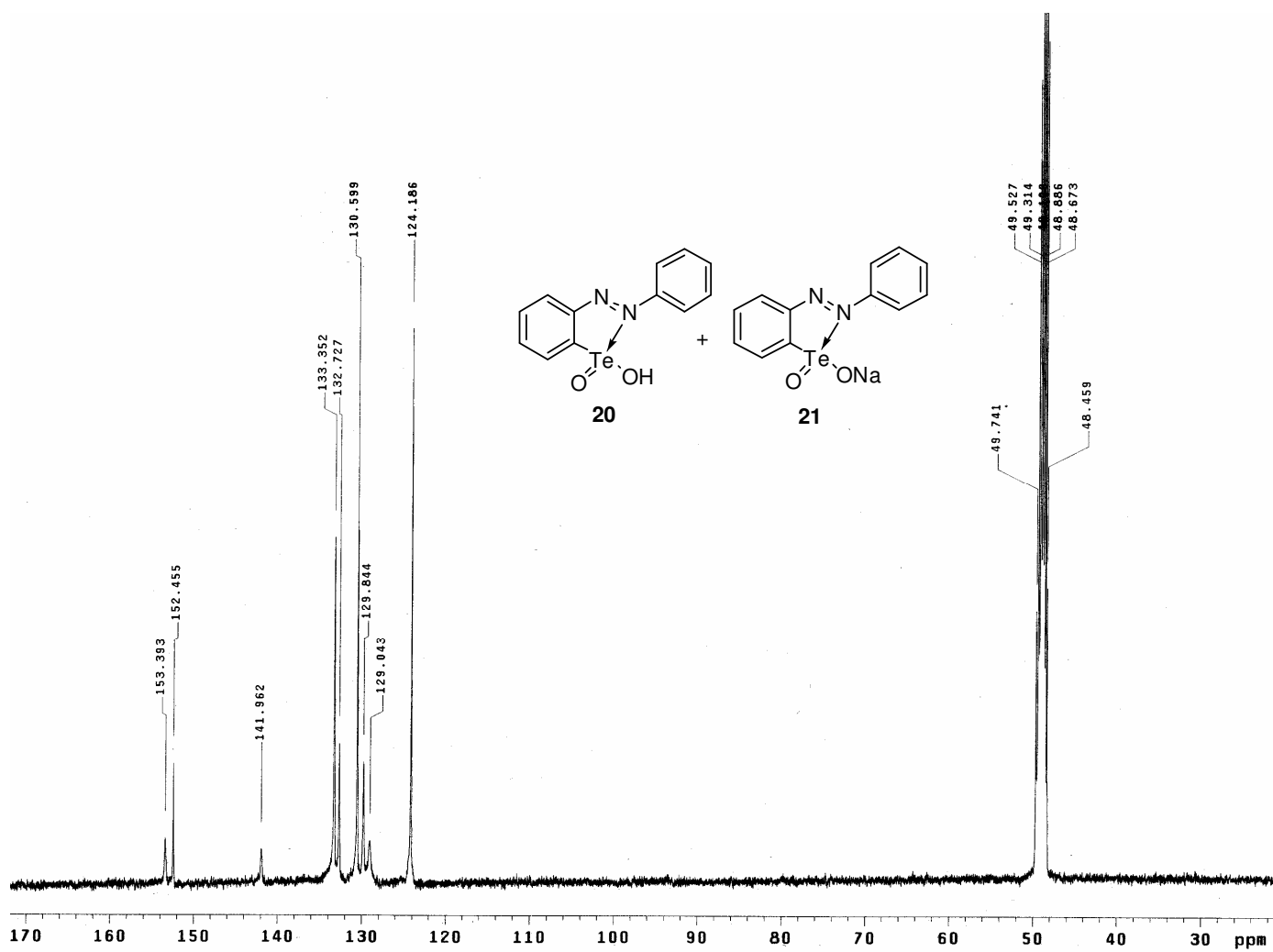


Figure S44. ^{13}C -NMR spectrum of 20-21

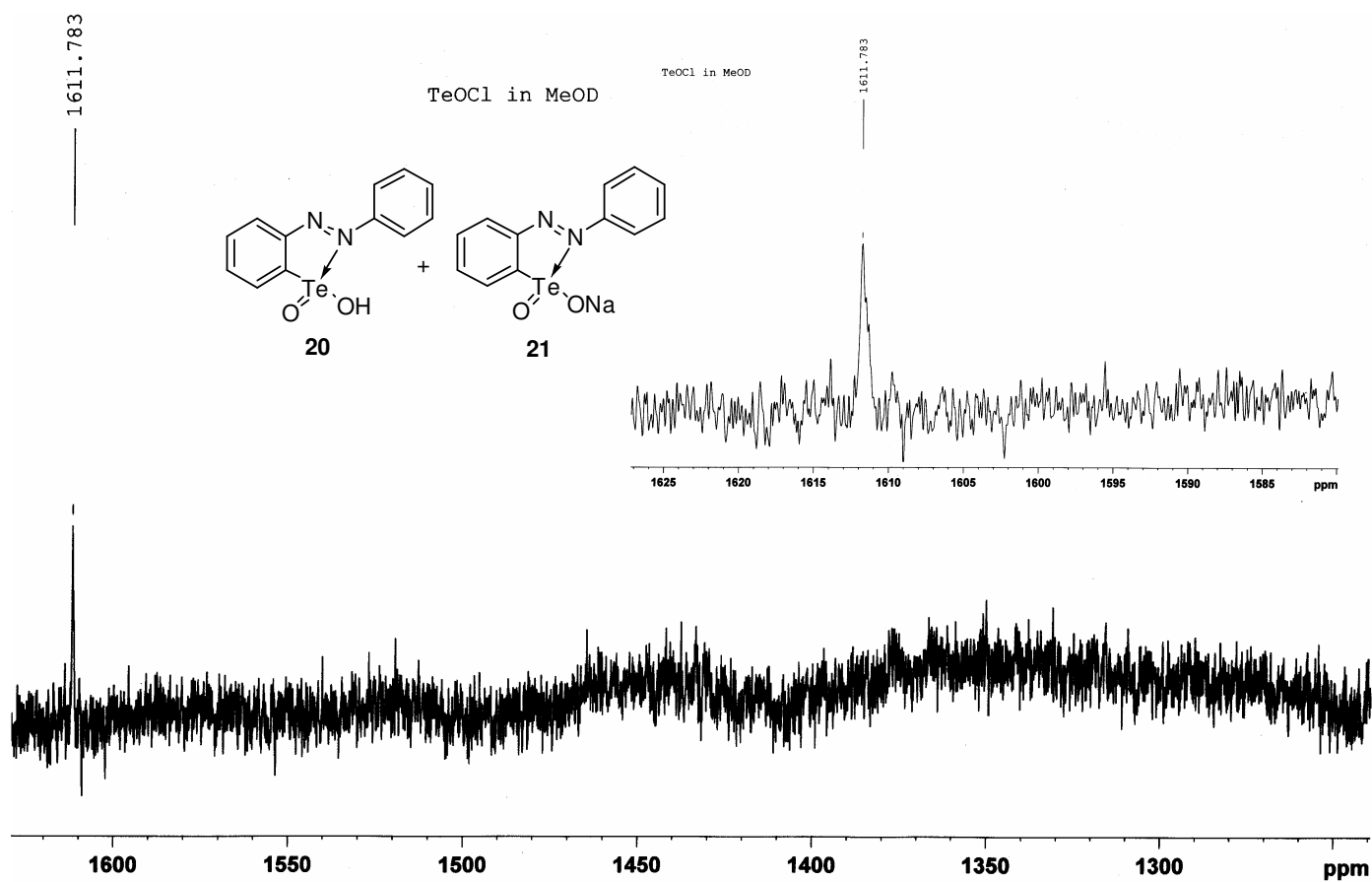


Figure S45. ^{125}Te -NMR spectrum of 20-21

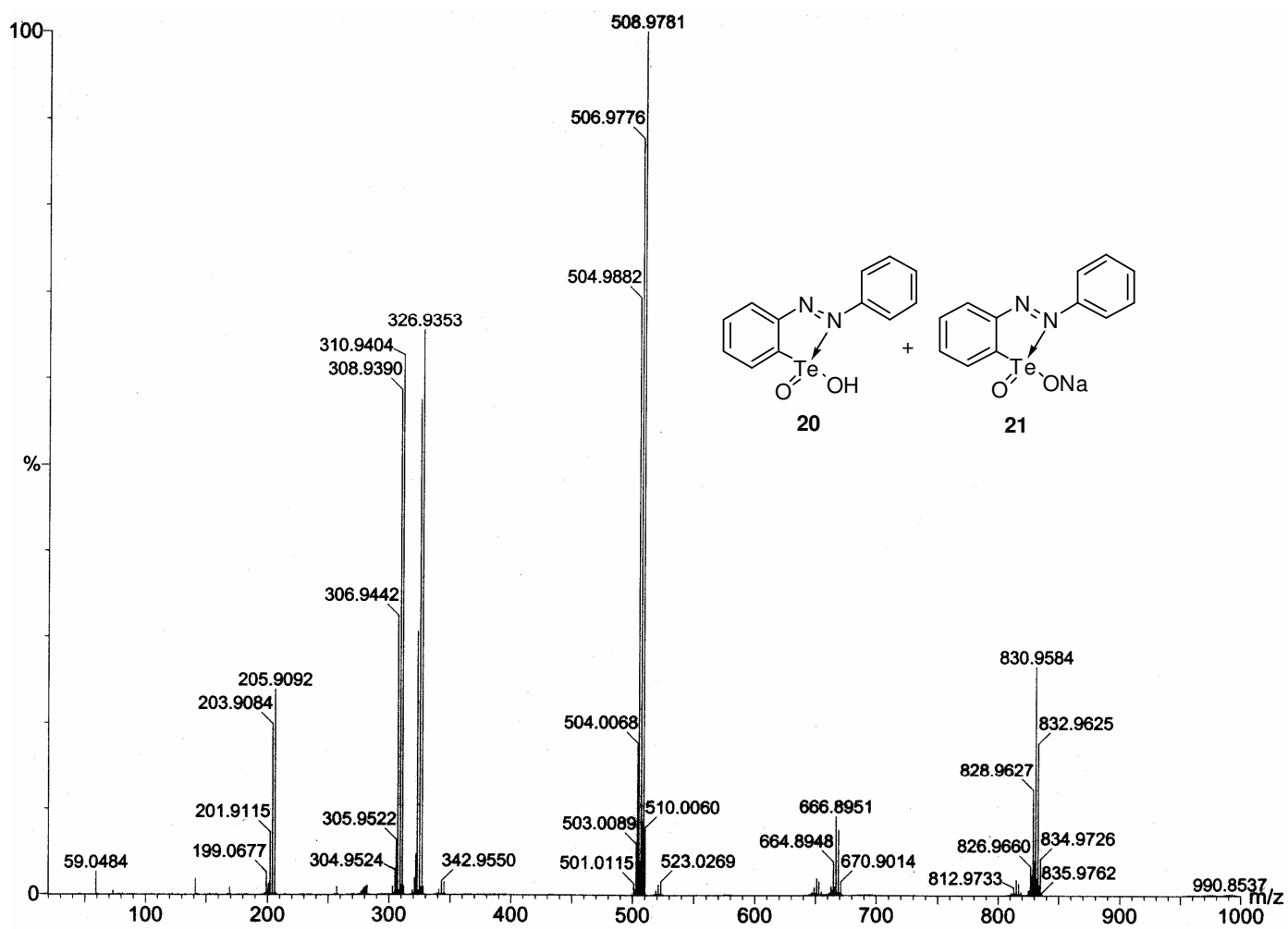


Figure S46. ES-MS of 20-21

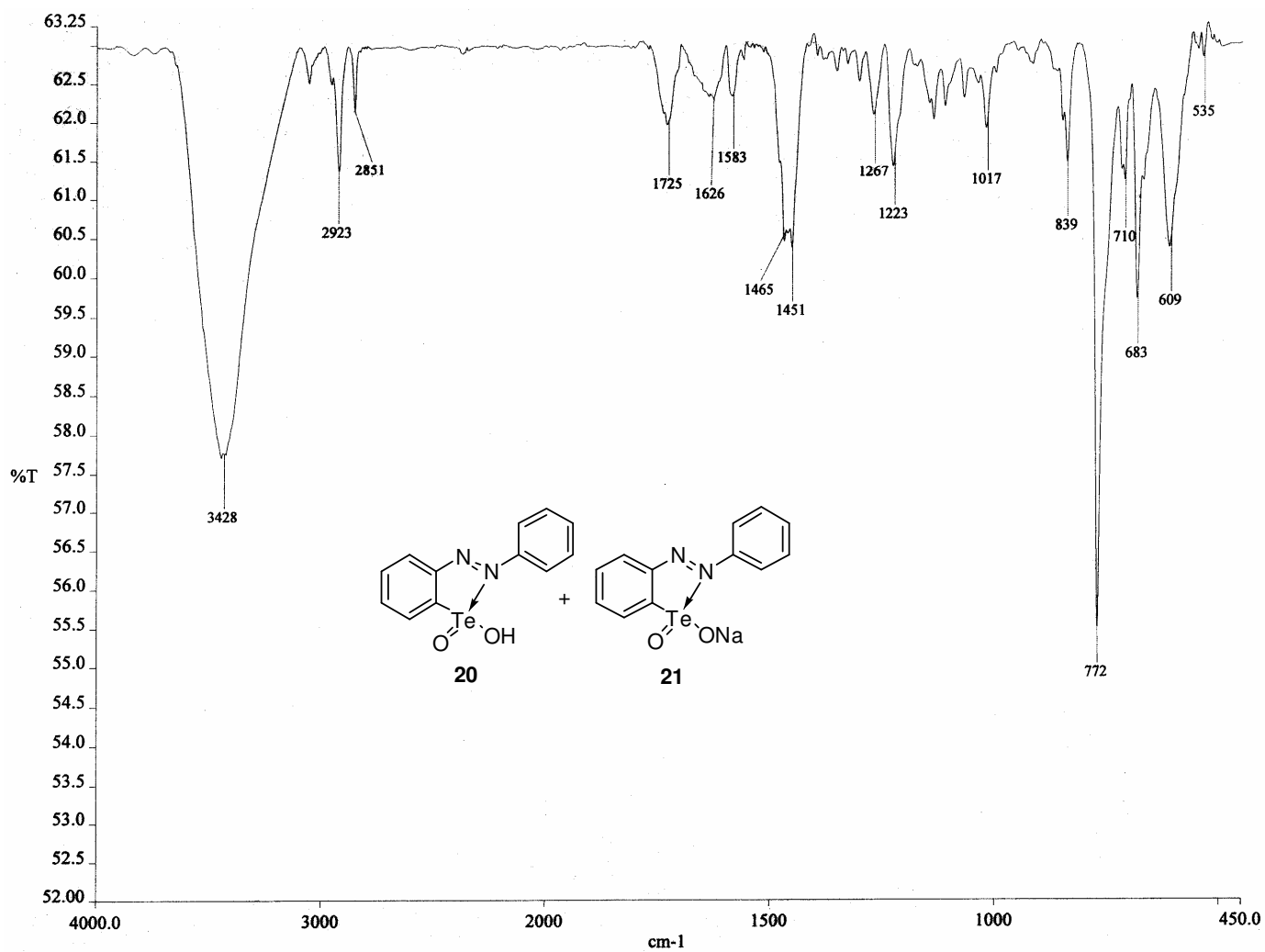


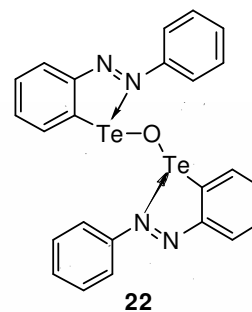
Figure S47. FT-IR spectrum of 20-21

Eager 300 Report

Page: 1 Sample: AZOTEOTA-2 (AZOTEOTA-2)

Method Name : sp190908
Method File : D:\CHNS2008\SP190908.mth
Chromatogram : AZOTEOTA-2
Operator ID : SP
Analysed : 09/19/2008 14:44
Sample ID : AZOTEOTA-2 (# 24)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 9/19/2008 15:48
Instrument N. : Instrument #1
Sample weight : 1.675



Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.8899	44	155841	RS	12.966180	.104658E+07
Carbon	45.3717	66	2020662	RS	1.000000	.265466E+07
Hydrogen	2.6270	169	306059	RS	6.602198	.658512E+07
Totals	56.8887		2482562			

Figure S48.Elemental analysis (C, H, N) of 22

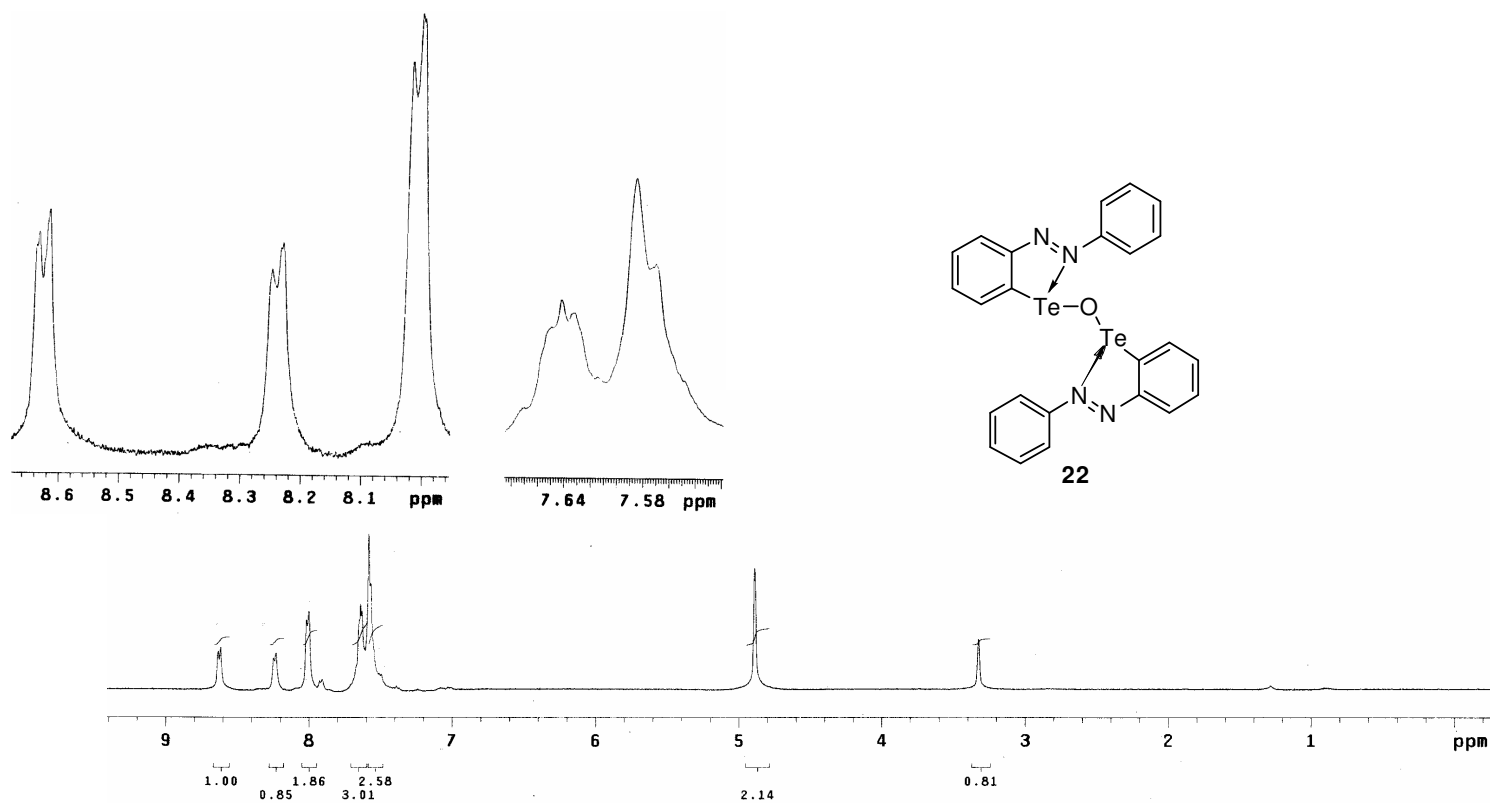


Figure S49. ^1H -NMR spectrum of **22**

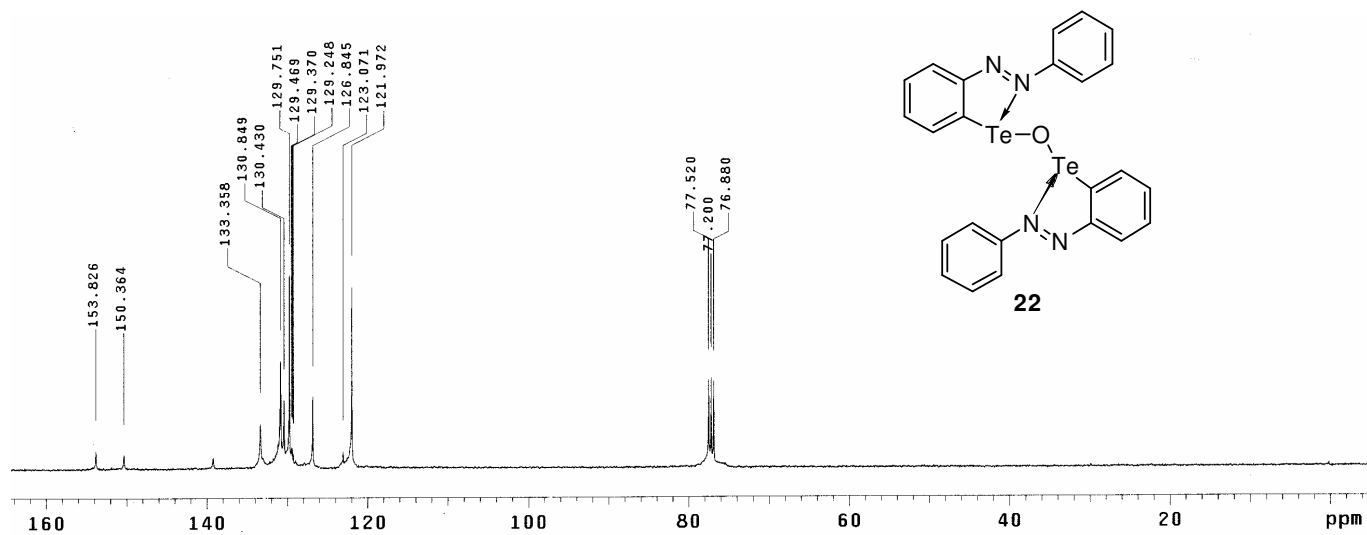


Figure S50. ^{13}C -NMR spectrum of **22**

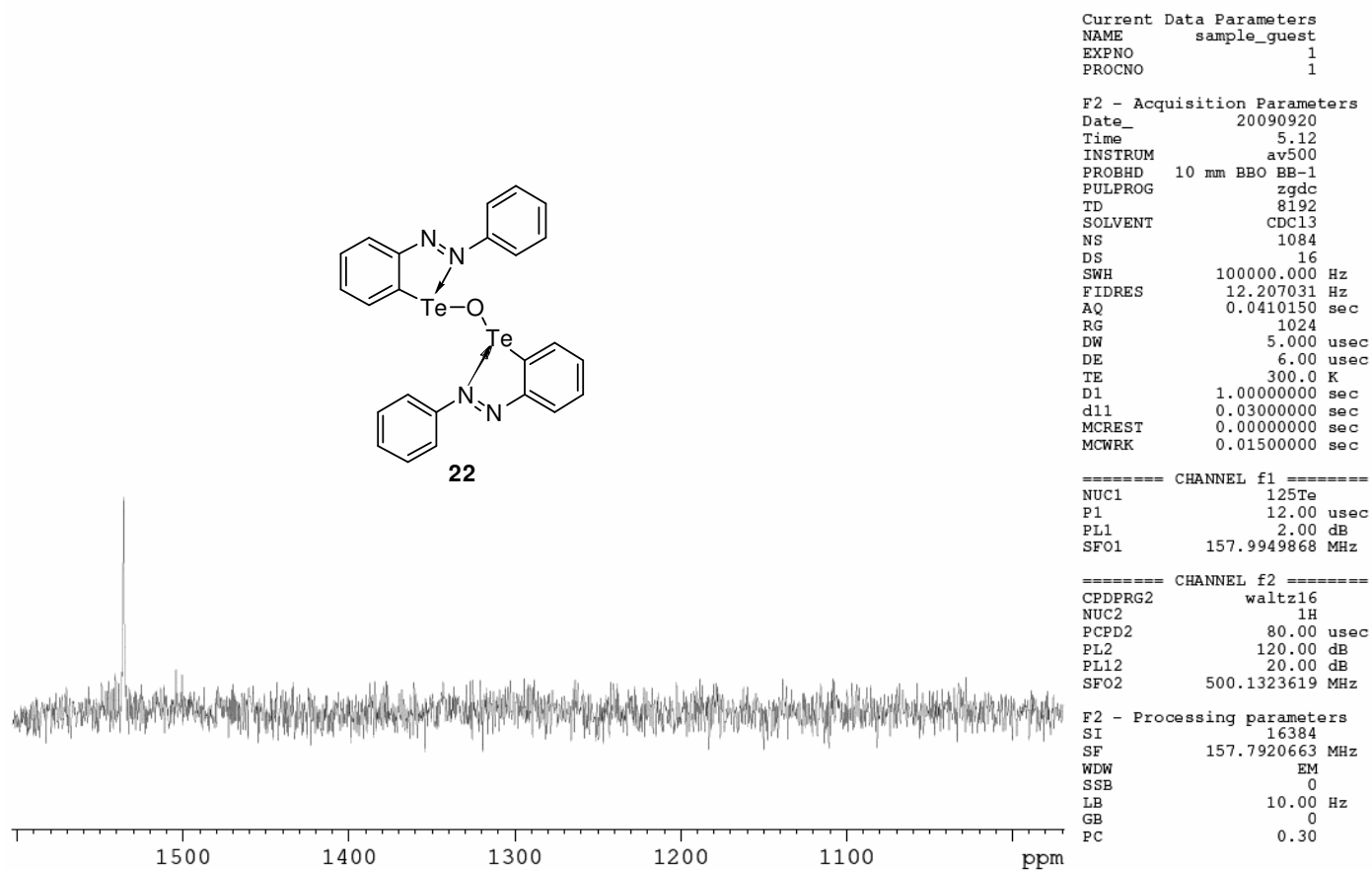


Figure S51. ^{125}Te -NMR spectrum of **22**

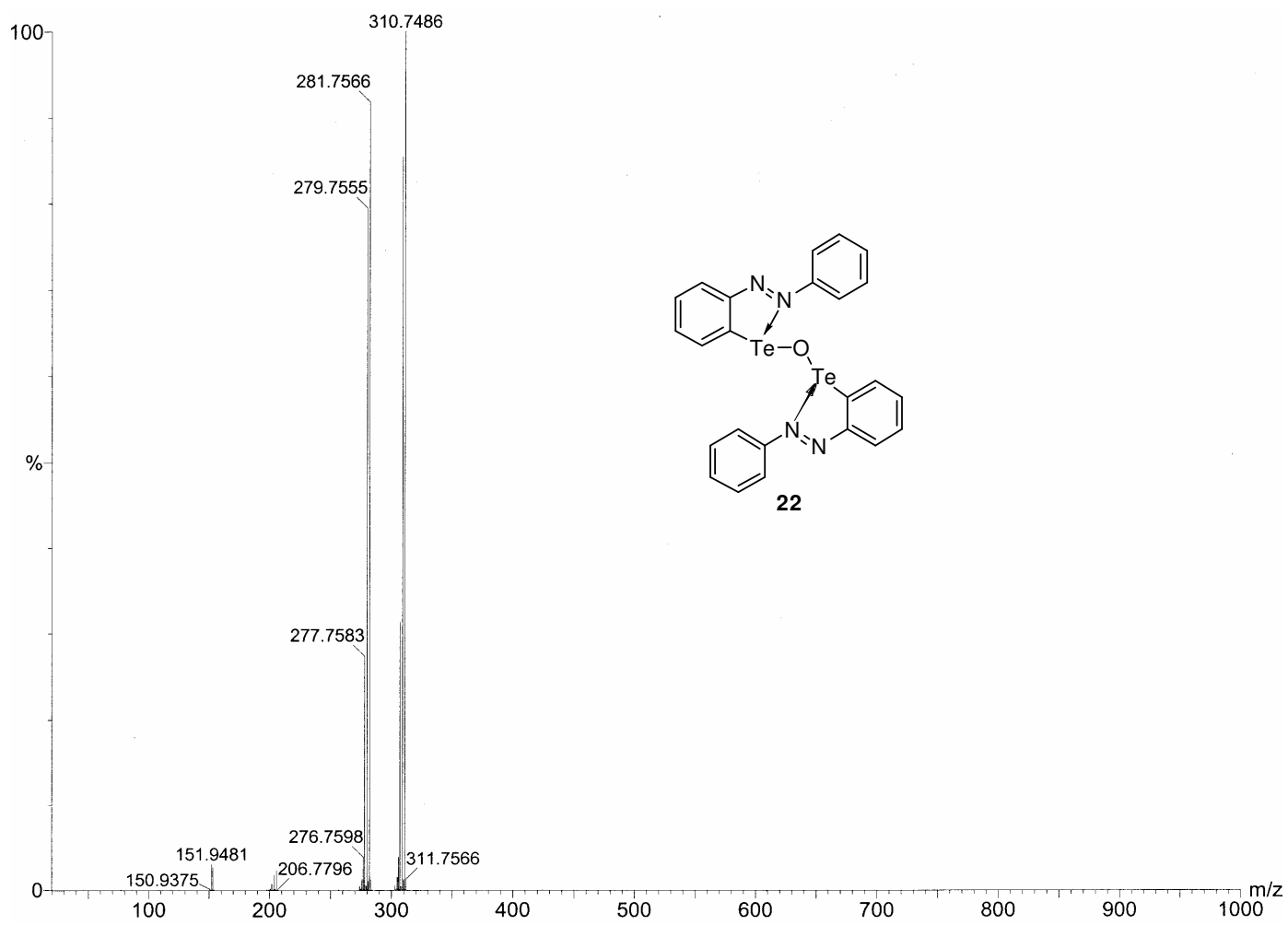


Figure S52. ES-MS of **22**

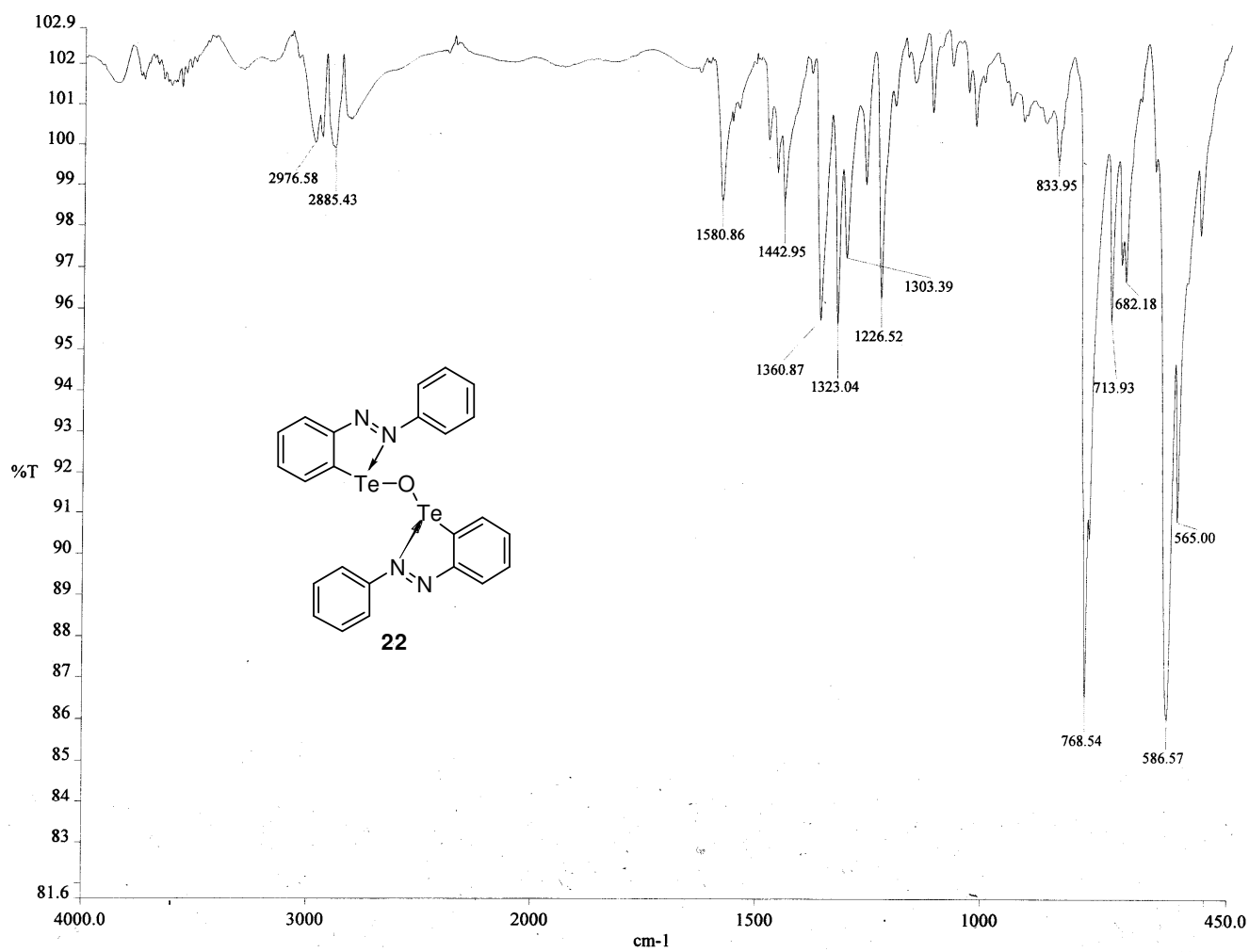


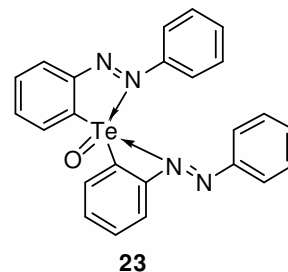
Figure S53. FT-IR spectrum of **22**

Eager 300 Report

Page: 1 Sample: KRTEO (KRTEO)

Method Name : sp300508
Method File : D:\CHNS2008\SP300508.mth
Chromatogram : KRTEO
Operator ID : SP
Analysed : 05/30/2008 14:43
Sample ID : KRTEO (# 23)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 5/30/2008 15:17
Instrument N. : Instrument #1
Sample weight : 1.716



Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	10.2250	43	193252	RS	13.420400	.110140E+07
Carbon	55.9612	64	2593519	RS	1.000000	.269794E+07
Hydrogen	3.9146	169	449300	RS	5.772355	.656808E+07
Totals	70.1008		3236071			

Figure S54.Elemental analysis (C, H, N) of 23

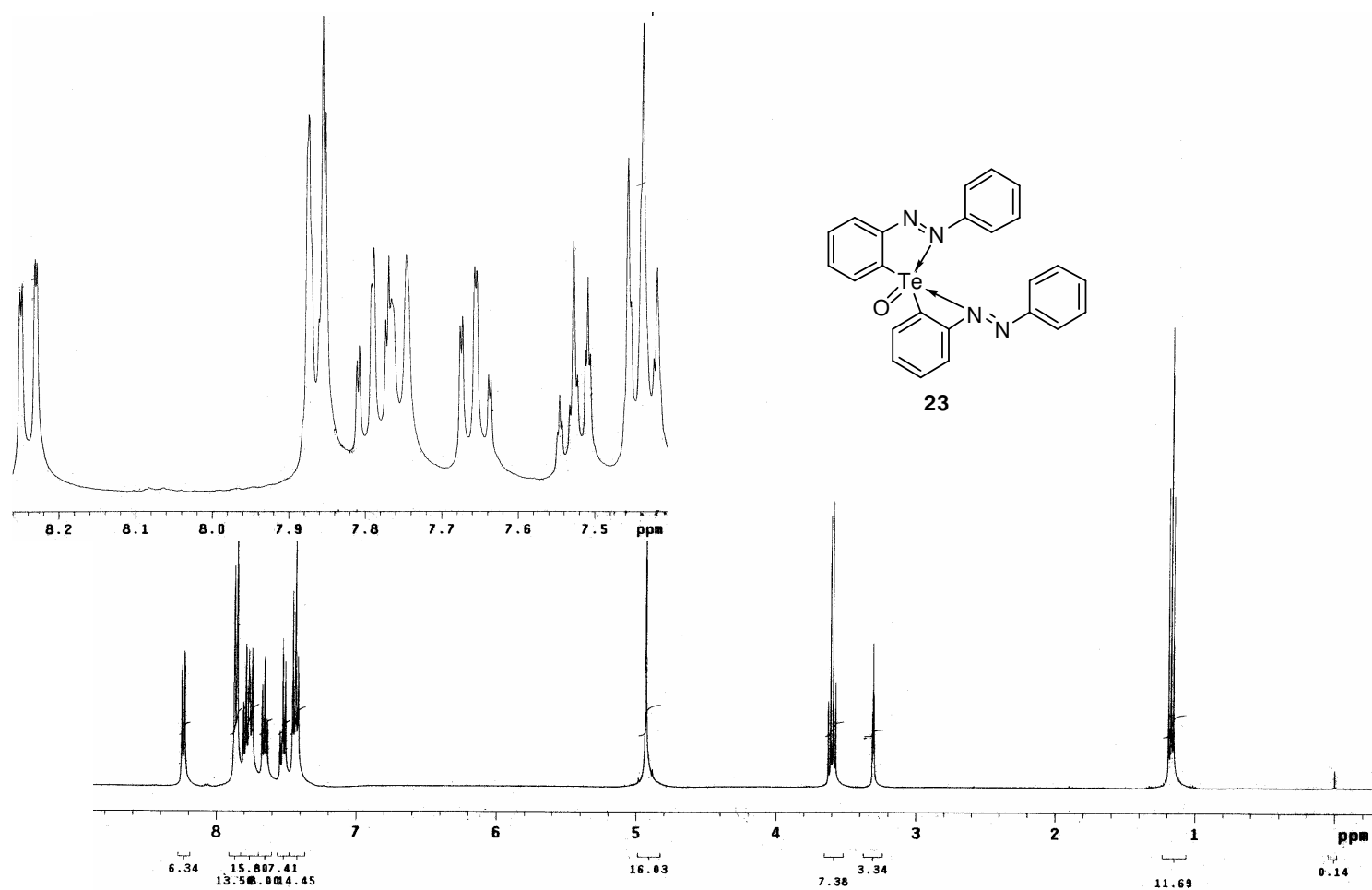


Figure S55. ^1H -NMR spectrum of **23**

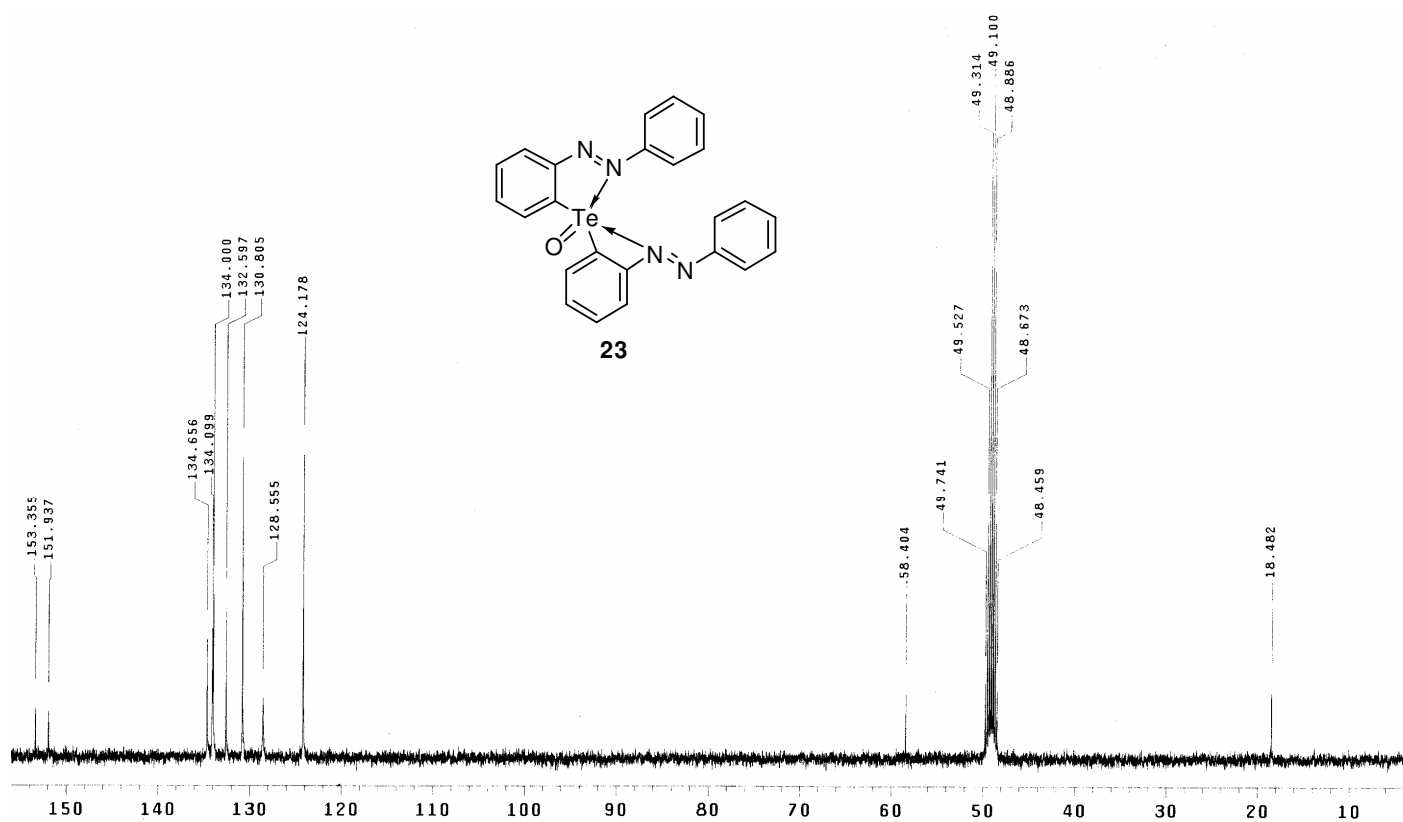


Figure S56. ^{13}C -NMR spectrum of **23**

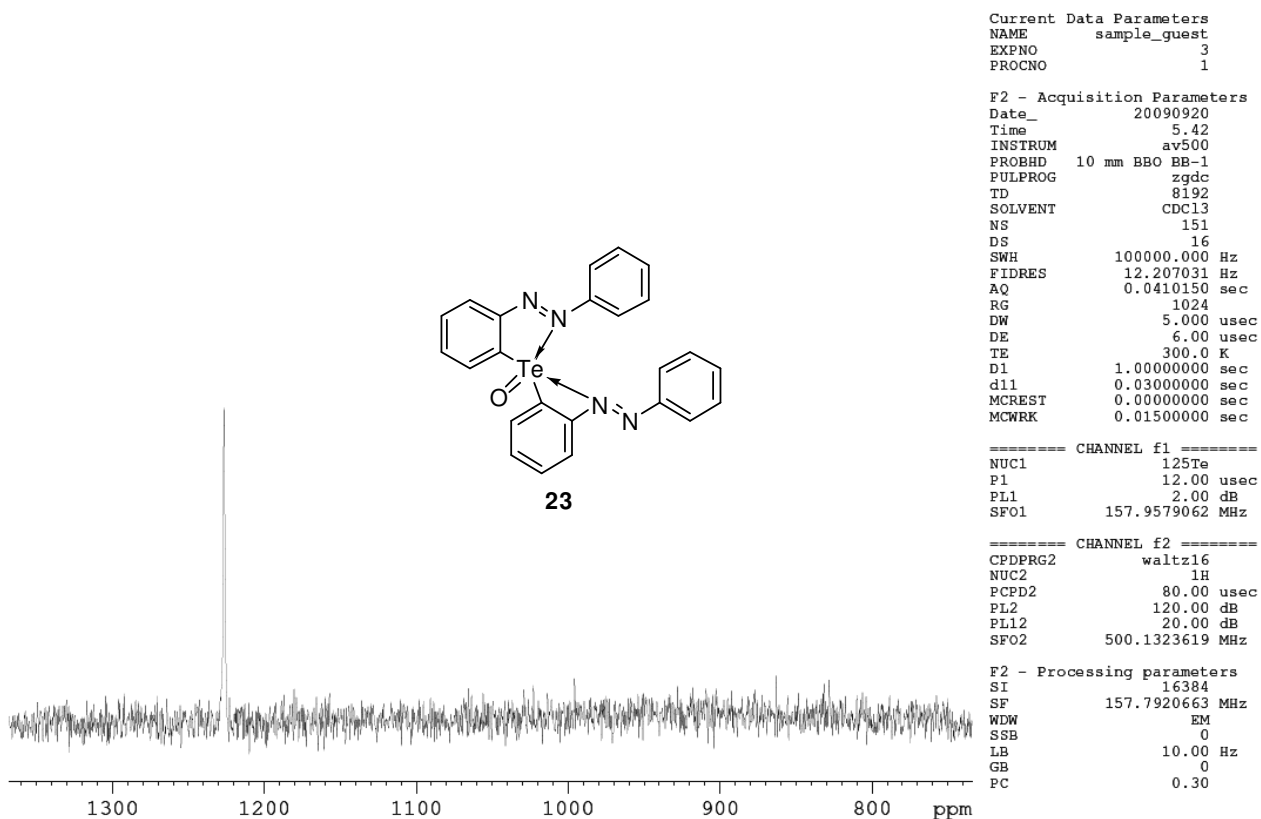


Figure S57. ^{125}Te -NMR spectrum of **23**

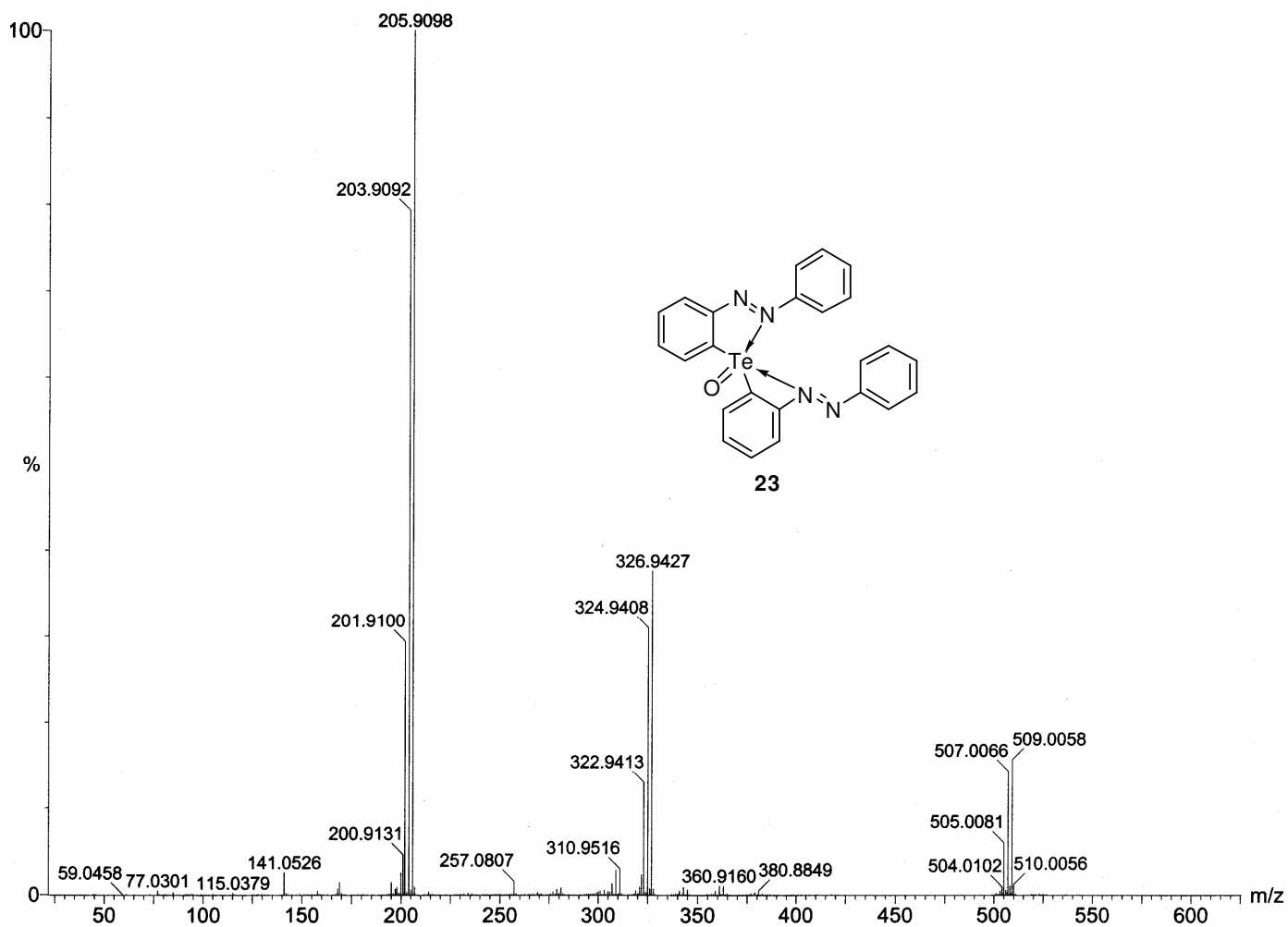


Figure S58. ESI-MS of **23**

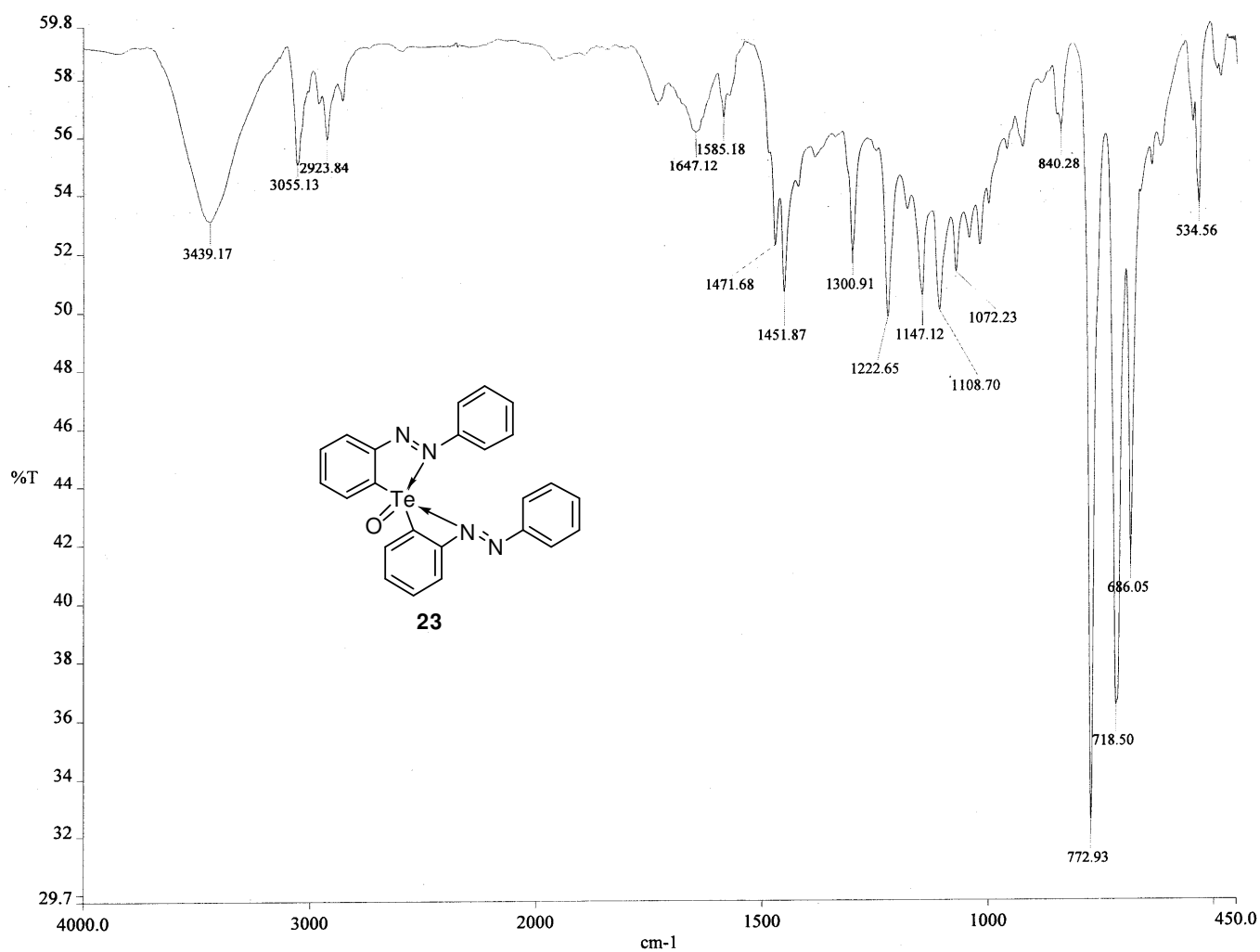
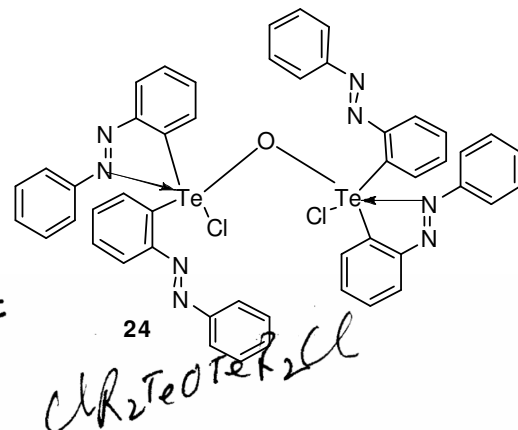


Figure S59.FT-IR spectrum of **23**



Eager 300 Report

Page: 1 Sample: HBS-KR-TECO3 (HBS-KR-TECO3)

Method Name	: sp250908	Company Name	: C.E. Instruments
Method File	: D:\CHNS2008\SP250908.mth	Printed	: 9/25/2008 16:35
Chromatogram	: HBS-KR-TECO3	Instrument N.	: Instrument #1
Operator ID	: MANOJA	Sample weight	: 1.405
Analysed	: 09/25/2008 16:21		
Sample ID	: HBS-KR-TECO3 (# 30)		
Analysis Type	: UnkNown (Area)		

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	10.9517	43	167484	RS	11.649020	.108847E+07
Carbon	51.6936	66	1951025	RS	1.000000	.265878E+07
Hydrogen	3.2553	169	333180	RS	5.855769	.679697E+07
Totals	65.9006		2451689			

Figure S60.Elemental analysis (C, H, N) of 24

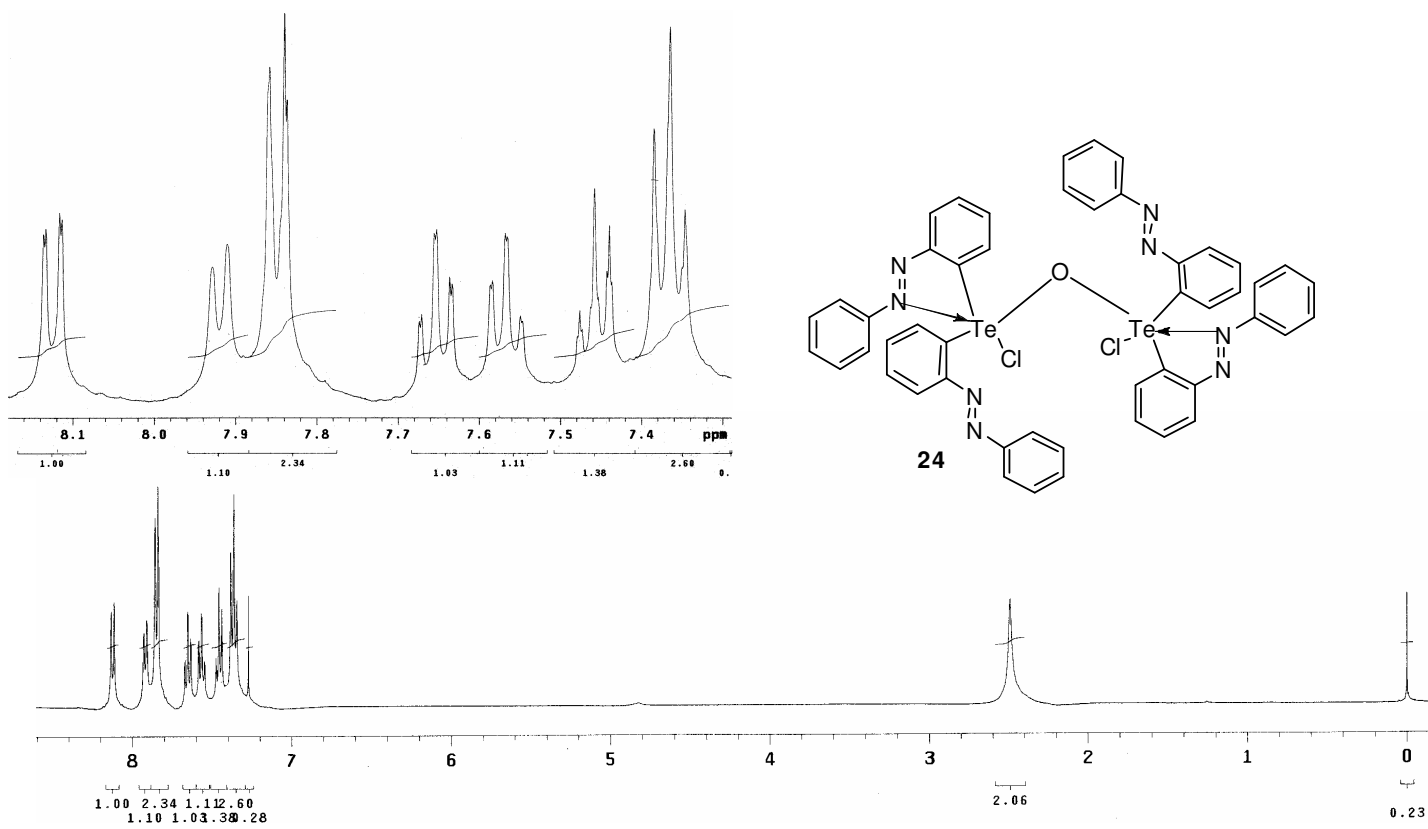


Figure S61. ^1H -NMR spectrum of **24**

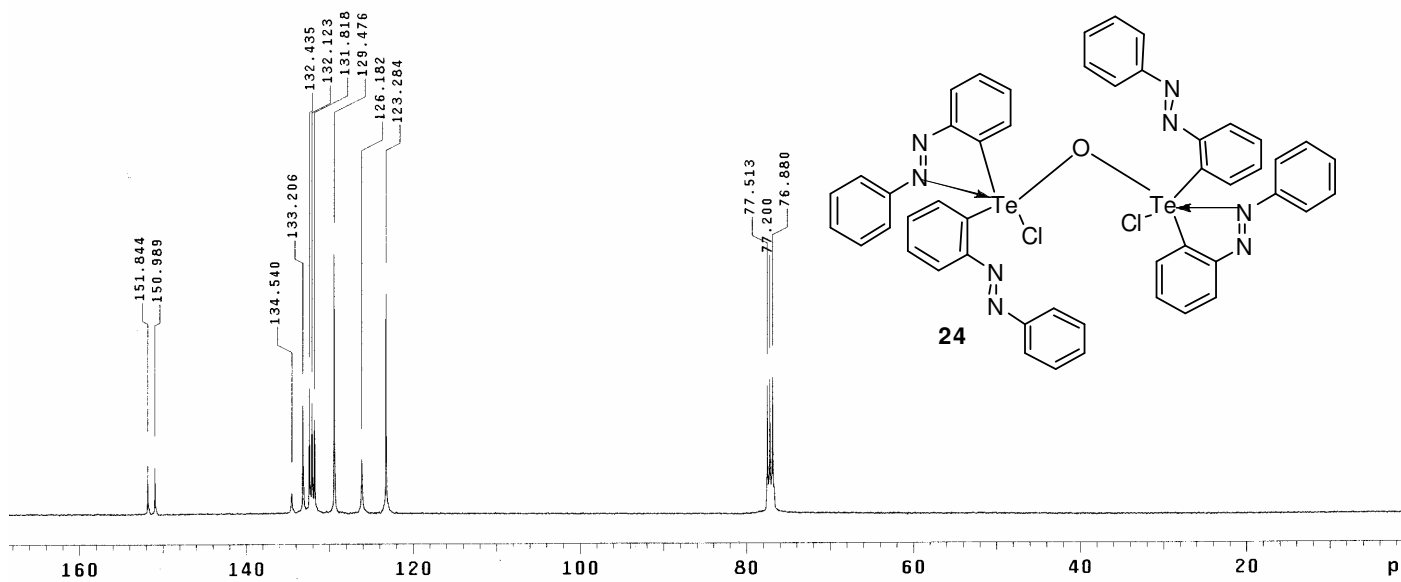


Figure S62. ¹³C-NMR spectrum of **24**

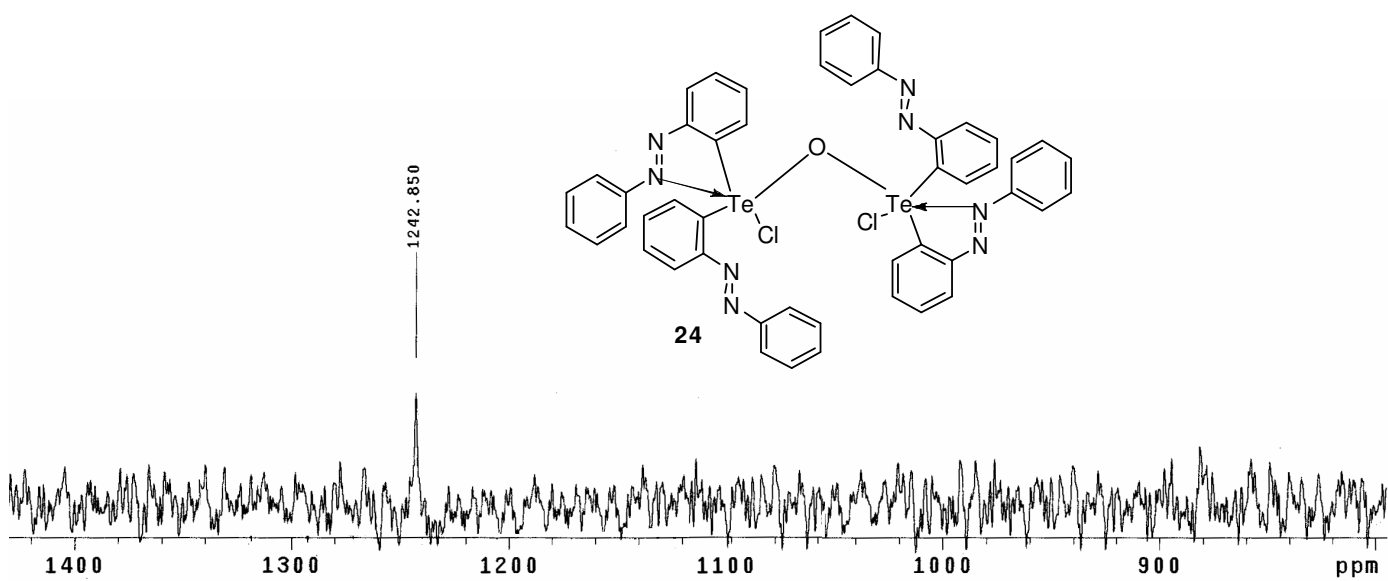


Figure S63. ¹²⁵Te-NMR spectrum of **24**

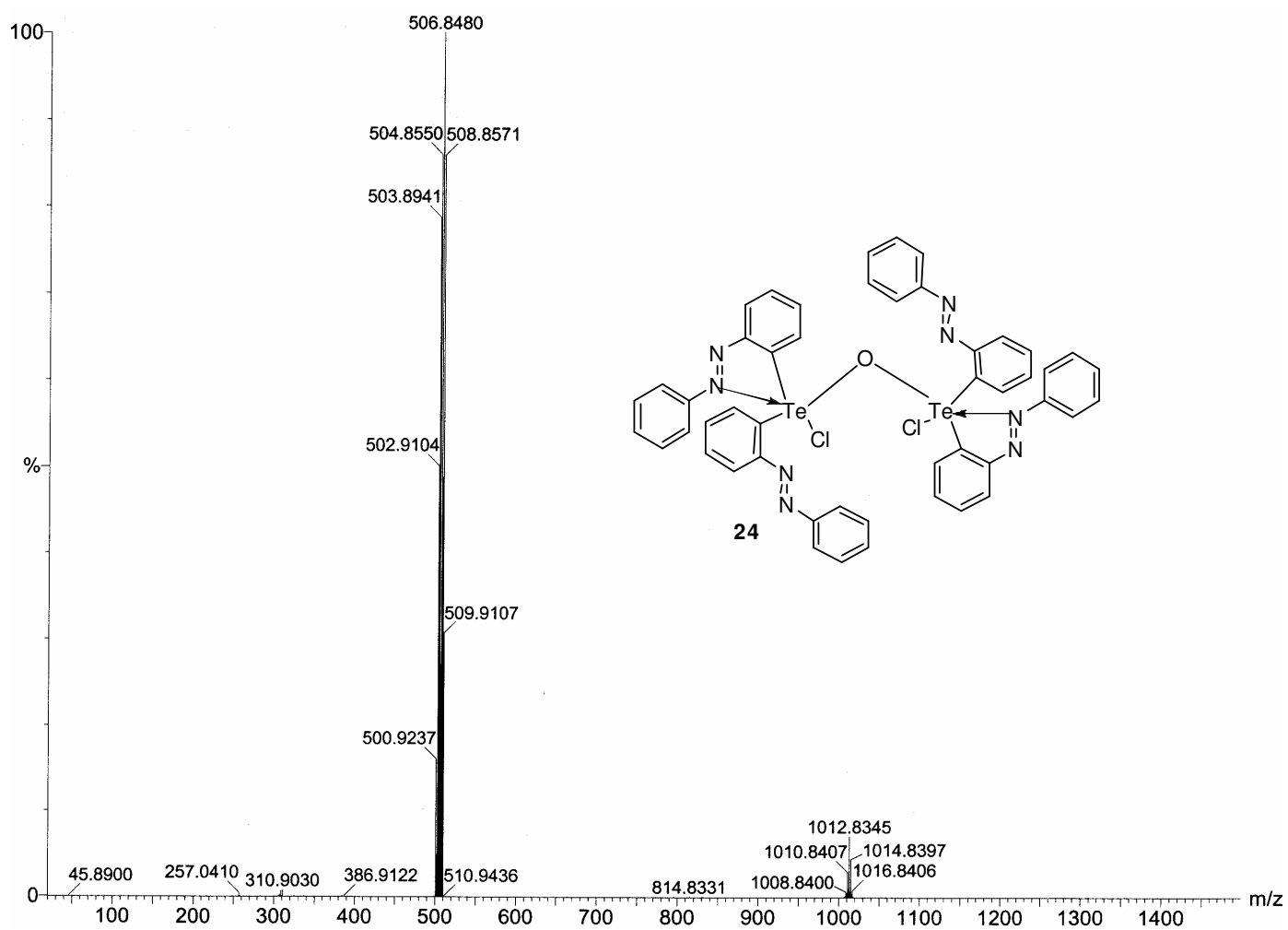


Figure S64.ESI-MS of **24**

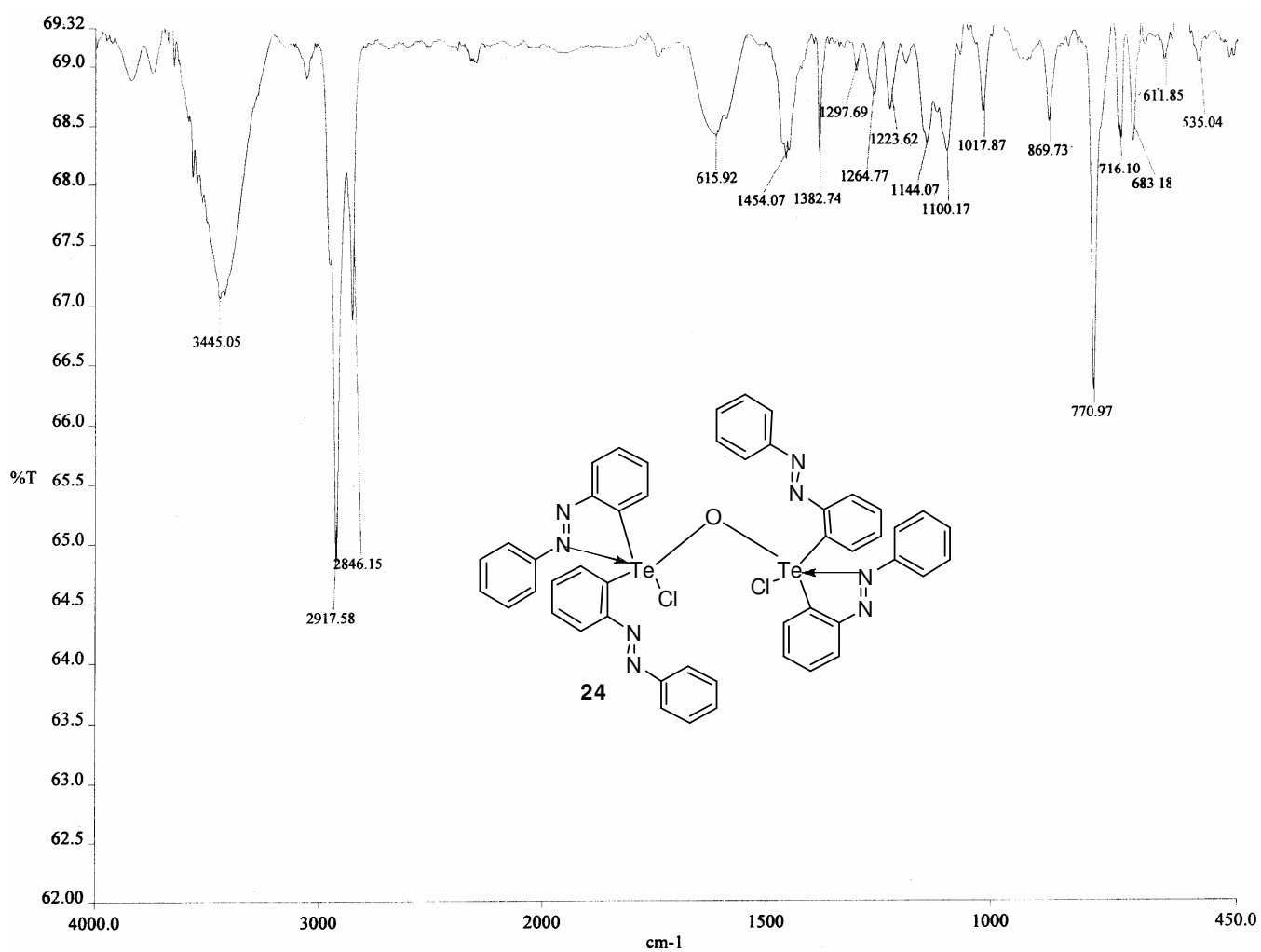


Figure S65.FT-IR spectrum of **22**

Table S2. Optimized coordinates and Energy of **13**: (B3LYP/6-311G(d,p);Lanl2dz(dp) level)

52	-0.247013000	-0.387943000	-0.031454000
17	-1.278569000	-0.491047000	-2.364395000
17	0.633665000	-0.548644000	2.382080000
7	2.726047000	-0.484620000	-0.252871000
7	3.943680000	-0.206465000	-0.329829000
7	-3.578054000	0.312528000	0.331023000
7	-2.618751000	1.096957000	0.162952000
6	0.981214000	-2.044899000	-0.667446000
6	0.496621000	-3.256490000	-1.154467000
1	-0.567708000	-3.443397000	-1.208352000
6	1.392685000	-4.224284000	-1.601271000
1	1.015656000	-5.168589000	-1.977052000
6	2.768613000	-3.978831000	-1.578581000
1	3.458499000	-4.738719000	-1.927386000
6	3.254166000	-2.760596000	-1.130326000
1	4.312109000	-2.534070000	-1.124712000
6	2.356903000	-1.781448000	-0.683719000
6	4.309745000	1.070464000	0.151960000
6	5.550815000	1.552330000	-0.279387000
1	6.138031000	0.938404000	-0.951640000
6	5.998017000	2.798334000	0.144851000
1	6.952853000	3.177331000	-0.200453000
6	5.222065000	3.551123000	1.025027000
1	5.576307000	4.516361000	1.368939000
6	3.997760000	3.055342000	1.481366000
1	3.410360000	3.630984000	2.187639000
6	3.533361000	1.821059000	1.048329000
1	2.603564000	1.408940000	1.418677000
6	-1.911064000	-1.535302000	0.699783000
6	-1.701004000	-2.807061000	1.222022000
1	-0.699524000	-3.210797000	1.286834000
6	-2.771662000	-3.572357000	1.688542000
1	-2.582666000	-4.562436000	2.086833000
6	-4.067022000	-3.066444000	1.644130000
1	-4.900893000	-3.660086000	1.999187000
6	-4.282032000	-1.783883000	1.158729000
1	-5.270703000	-1.342198000	1.136063000
6	-3.214415000	-0.999246000	0.706607000
6	-2.941335000	2.417532000	-0.227931000
6	-4.222817000	2.812238000	-0.638969000
1	-5.015081000	2.076525000	-0.665906000
6	-4.444271000	4.129993000	-1.008469000
1	-5.431507000	4.438658000	-1.332684000

6	-3.400438000	5.059510000	-0.972573000
1	-3.581889000	6.087116000	-1.266139000
6	-2.127127000	4.665475000	-0.568186000
1	-1.316158000	5.383626000	-0.543104000
6	-1.894201000	3.344405000	-0.201224000
1	-0.911123000	3.019543000	0.116496000

Energy (**E**) of **13**: -2073.1201465 a.u

Table S3. Optimized coordinates and Energy of **11**: (B3LYP/6-311G(d,p);Lanl2dz(dp) level)

52	-0.226428000	-0.363846000	-0.020241000
35	0.717543000	-0.522459000	2.554698000
35	-1.326085000	-0.391738000	-2.512883000
7	2.719446000	-0.518434000	-0.337822000
7	3.933286000	-0.249347000	-0.481358000
6	0.943655000	-2.064973000	-0.661977000
6	0.431541000	-3.278937000	-1.114268000
1	-0.635670000	-3.453311000	-1.140392000
6	1.302485000	-4.266580000	-1.567531000
1	0.902574000	-5.212148000	-1.915536000
6	2.681551000	-4.039818000	-1.587705000
1	3.351586000	-4.815454000	-1.940439000
6	3.194261000	-2.819015000	-1.178632000
1	4.254388000	-2.605021000	-1.209019000
6	2.321996000	-1.820308000	-0.726131000
6	4.330849000	1.037214000	-0.053554000
6	5.562481000	1.487138000	-0.543004000
1	6.118449000	0.842083000	-1.212638000
6	6.039821000	2.740812000	-0.178238000
1	6.987229000	3.093945000	-0.568459000
6	5.303434000	3.534981000	0.699420000
1	5.681000000	4.506885000	0.996528000
6	4.088501000	3.072747000	1.212753000
1	3.532094000	3.681483000	1.916411000
6	3.594514000	1.830548000	0.839746000
1	2.671988000	1.445916000	1.254804000
7	-3.498634000	0.510509000	0.451090000
7	-2.499205000	1.238820000	0.262820000
6	-1.934586000	-1.441047000	0.723360000
6	-1.787928000	-2.735094000	1.212208000
1	-0.810530000	-3.196824000	1.246436000
6	-2.889560000	-3.447873000	1.689170000

1	-2.748642000	-4.456149000	2.060926000
6	-4.153904000	-2.866907000	1.690714000
1	-5.012023000	-3.419503000	2.054068000
6	-4.304186000	-1.561838000	1.243115000
1	-5.264742000	-1.061711000	1.259218000
6	-3.203933000	-0.829649000	0.780509000
6	-2.752387000	2.587861000	-0.078896000
6	-4.023629000	3.077407000	-0.412206000
1	-4.863980000	2.396657000	-0.415120000
6	-4.174237000	4.416731000	-0.737244000
1	-5.153638000	4.798989000	-1.001182000
6	-3.069561000	5.273797000	-0.733620000
1	-3.196025000	6.318947000	-0.991993000
6	-1.806756000	4.785485000	-0.406372000
1	-0.949062000	5.447604000	-0.406564000
6	-1.645143000	3.442335000	-0.084048000
1	-0.671677000	3.043562000	0.173453000

Energy (E) of **11**: -6300.9719068 a.u

Table S4. Optimized coordinates and Energy of **14**: (B3LYP/6-311G(d,p);Lanl2dz(dp) level)

52	0.676356000	-0.329734000	-0.516148000
53	0.547190000	-3.153191000	-0.473265000
7	2.516144000	2.318886000	-0.516680000
7	1.282243000	2.118173000	-0.438664000
6	2.803382000	-0.143539000	-0.512386000
6	3.676882000	-1.219730000	-0.559899000
1	3.299787000	-2.234795000	-0.557689000
6	5.058544000	-0.997266000	-0.607423000
1	5.729143000	-1.847508000	-0.640334000
6	5.568489000	0.297449000	-0.618184000
1	6.638089000	0.461954000	-0.657819000
6	4.700125000	1.382761000	-0.584799000
1	5.063245000	2.402826000	-0.601112000
6	3.318174000	1.172962000	-0.532507000
6	0.417318000	3.236978000	-0.466846000
6	0.904776000	4.552326000	-0.550335000
1	1.971521000	4.722669000	-0.591918000
6	0.007028000	5.606269000	-0.579540000
1	0.376182000	6.622568000	-0.644600000
6	-1.369890000	5.365132000	-0.528301000
1	-2.064135000	6.196522000	-0.553961000

6	-1.850616000	4.060073000	-0.445731000
1	-2.916455000	3.872601000	-0.406846000
6	-0.960777000	2.993385000	-0.413466000
1	-1.334699000	1.979451000	-0.344350000
6	0.383217000	-0.127855000	1.580800000
6	1.402859000	-0.034913000	2.519713000
1	2.443791000	-0.043341000	2.222810000
6	1.056941000	0.059717000	3.866803000
1	1.837335000	0.131824000	4.614675000
6	-0.286554000	0.054332000	4.253773000
1	-0.541681000	0.124221000	5.304391000
6	-1.298236000	-0.044398000	3.308494000
1	-2.343023000	-0.055759000	3.589567000
6	-0.965137000	-0.136654000	1.952380000
6	-4.035503000	-0.410248000	0.164090000
6	-5.372835000	-0.360979000	0.584016000
1	-5.576396000	-0.236957000	1.640422000
6	-6.399731000	-0.470324000	-0.345659000
1	-7.432092000	-0.431220000	-0.020577000
6	-6.095158000	-0.637322000	-1.694895000
1	-6.893475000	-0.729192000	-2.421932000
6	-4.761558000	-0.696420000	-2.117549000
1	-4.535330000	-0.838235000	-3.167641000
6	-3.731826000	-0.583621000	-1.198602000
1	-2.700673000	-0.644324000	-1.518398000
7	-1.879394000	-0.249598000	0.878471000
7	-3.092166000	-0.286993000	1.196067000

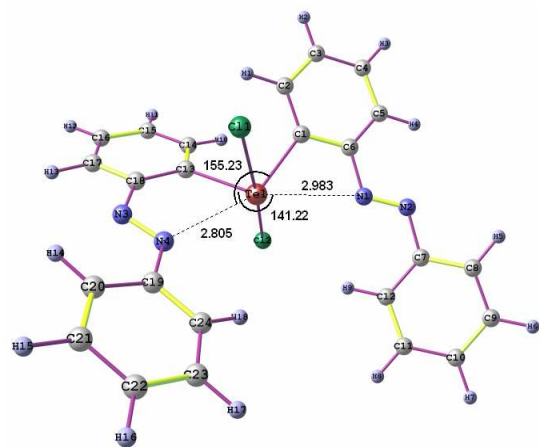
Energy (**E**) of **14**: -8071.97262143 a.u

Table S5. Optimized coordinates and Energy of **15**: (B3LYP/6-311G(d,p);Lanl2dz(dp) level)

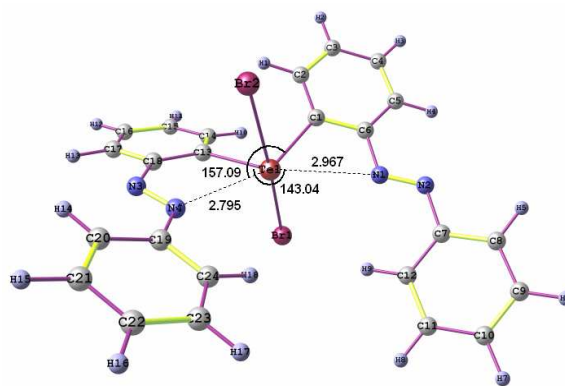
52	-0.216833000	-0.357827000	-0.011534000
7	2.689668000	-0.574611000	-0.493340000
7	3.884620000	-0.311623000	-0.758375000
7	-3.383663000	0.697178000	0.685688000
7	-2.354578000	1.358963000	0.423139000
6	0.875027000	-2.099208000	-0.695044000
6	0.323177000	-3.309836000	-1.109093000
1	-0.745988000	-3.470036000	-1.081057000
6	1.154132000	-4.314316000	-1.599139000
1	0.721880000	-5.256467000	-1.916284000
6	2.533031000	-4.108712000	-1.695814000

1	3.172035000	-4.897651000	-2.075434000
6	3.083695000	-2.890945000	-1.329256000
1	4.143243000	-2.692069000	-1.420693000
6	2.251540000	-1.875398000	-0.840834000
6	4.331498000	0.975313000	-0.386262000
6	5.513882000	1.405933000	-0.999586000
1	5.996974000	0.745173000	-1.709221000
6	6.034140000	2.660695000	-0.704195000
1	6.941911000	2.998490000	-1.190323000
6	5.392059000	3.475966000	0.226560000
1	5.803873000	4.449061000	0.469197000
6	4.228752000	3.033609000	0.862454000
1	3.747531000	3.658723000	1.606019000
6	3.691213000	1.790276000	0.560071000
1	2.810422000	1.422311000	1.070172000
6	-1.943106000	-1.362256000	0.791715000
6	-1.856956000	-2.679102000	1.232682000
1	-0.914004000	-3.206658000	1.195322000
6	-2.973131000	-3.332237000	1.757980000
1	-2.878081000	-4.359030000	2.091563000
6	-4.191968000	-2.668667000	1.859302000
1	-5.061349000	-3.174599000	2.261597000
6	-4.278786000	-1.341750000	1.463170000
1	-5.198843000	-0.778398000	1.558320000
6	-3.162168000	-0.669379000	0.950958000
6	-2.536146000	2.736259000	0.154357000
6	-3.795234000	3.337208000	0.010152000
1	-4.682603000	2.726219000	0.103666000
6	-3.875640000	4.695675000	-0.254317000
1	-4.846282000	5.163870000	-0.371191000
6	-2.712893000	5.462357000	-0.377391000
1	-2.785176000	6.523357000	-0.587428000
6	-1.463032000	4.864109000	-0.236229000
1	-0.560708000	5.455922000	-0.333698000
6	-1.372275000	3.501454000	0.026253000
1	-0.408782000	3.020793000	0.142106000
53	-1.491730000	-0.272430000	-2.712736000
53	0.900449000	-0.513110000	2.783989000

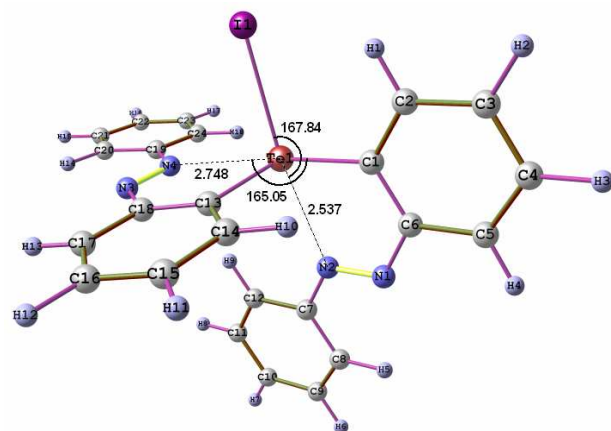
Energy (E) of **15**: -14991.7379425 a.u



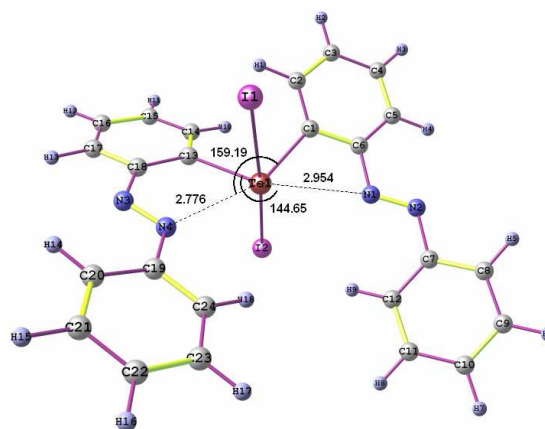
13



11

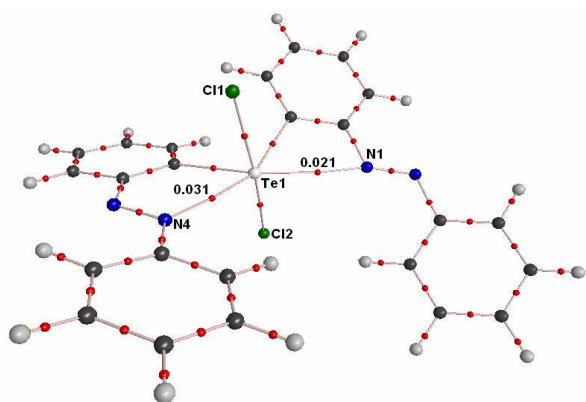


14

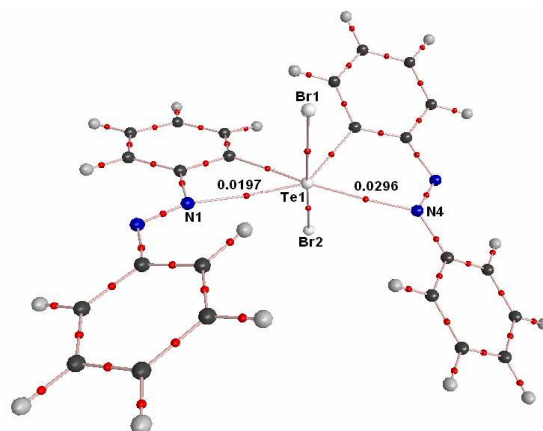


15

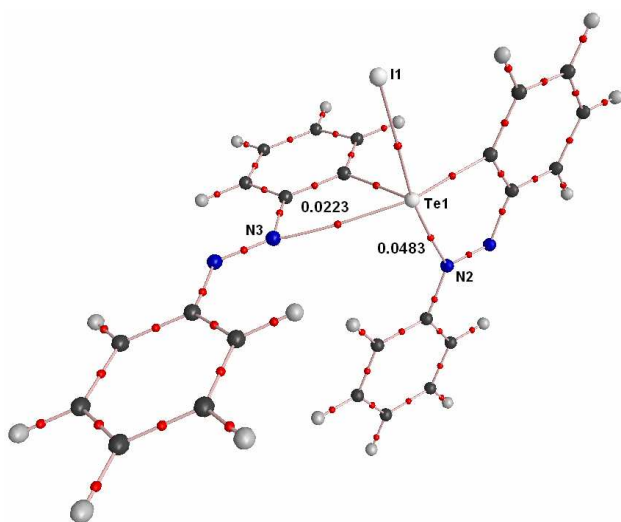
Figure S66. Optimized geometries for compounds **13**, **11**, **14** and **15** at B3LYP/6-311G(d,p);Lanl2dz(d,p)



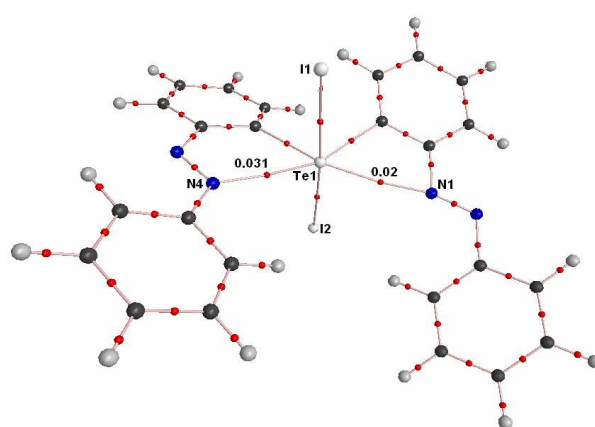
13



11



14



15

Figure S67. Molecular graph of 13, 11, 14 and 15 obtained from AIM analysis

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