Supplementary Information

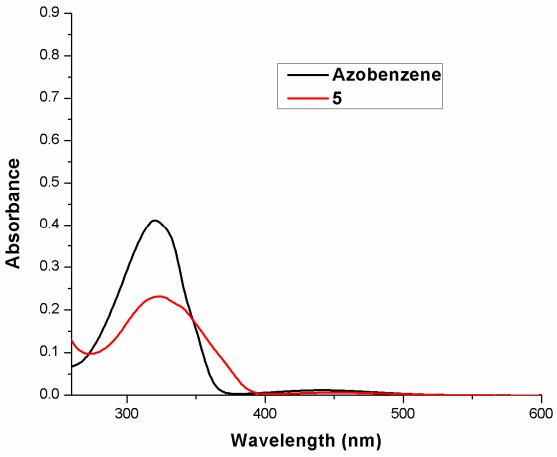
Intramolecularly coordinated azobenzene selenium derivatives: Effect of strength of the Se···N intramolecular interaction on luminescence†

Kriti Srivastava,[a] Tapash Chakraborty,[a] Harkesh B. Singh,*[a] and Ray J. Butcher[b]

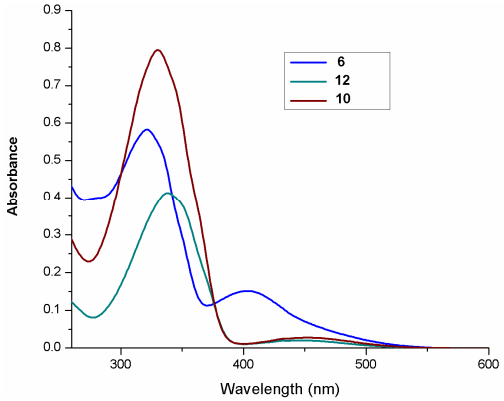
[a]*Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai-400076, India. Fax:+91 22 2572 3480; Tel: +91 22 2576 7190; E-mail: chhbsia@chem.iitb.ac.in*

[b]*Department of Chemistry, Howard University, Washington, D.C 20059, USA.*

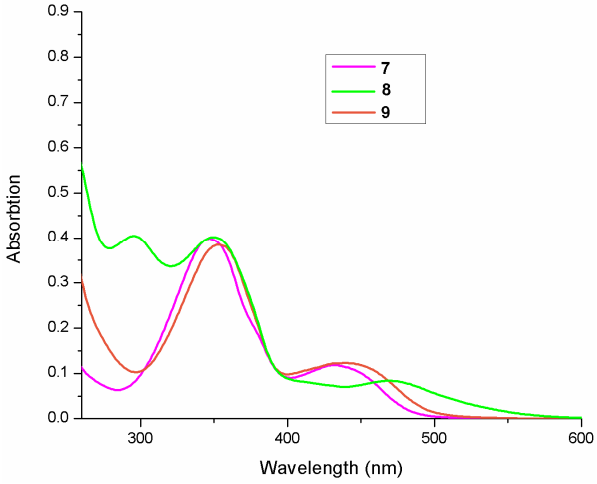
CONTENTS **Page No**



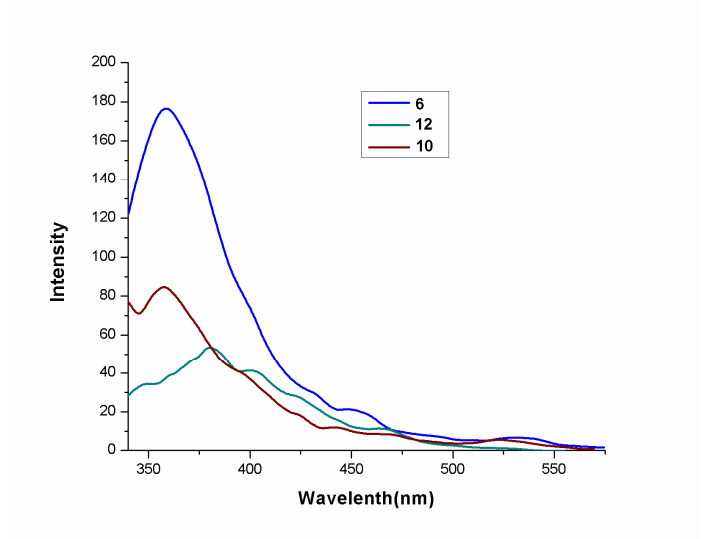
FigureS1 Graphical representation of UV-vis spectra for azobenzene and **5** in $CHCl_3$ at 10^{-5} concentration



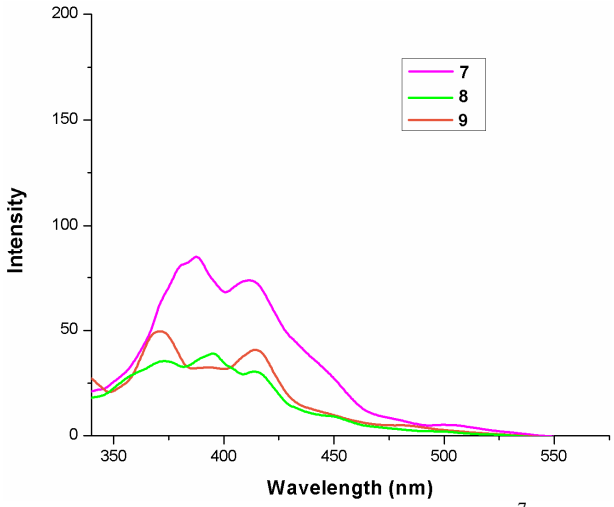
FigureS2 Graphical representation of UV-vis spectra for **6**, **10** and **12** in $CHCl_3$ at 10^{-5} concentration



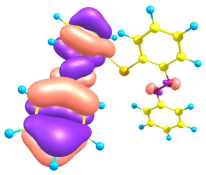
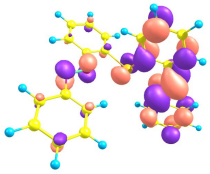
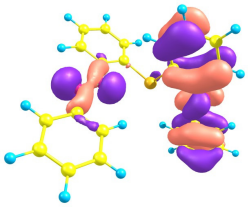
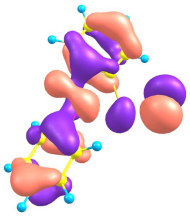
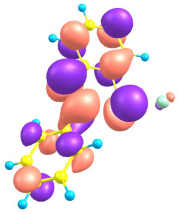
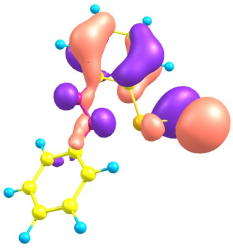
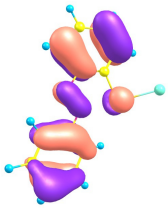
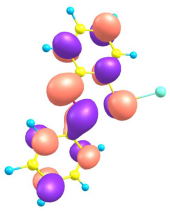
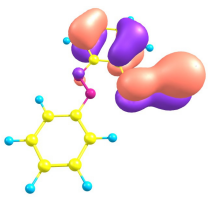
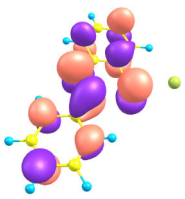
FigureS3 Graphical representation of UV-vis spectra for **7**-**9** in $CHCl_3$ at 10^{-5} concentration

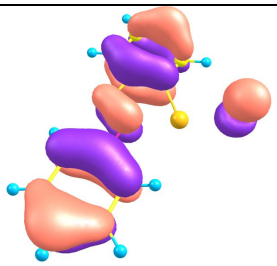
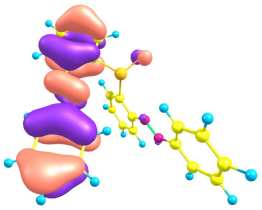
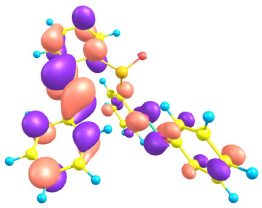
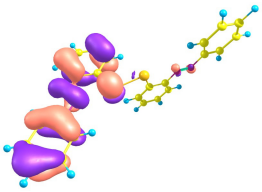
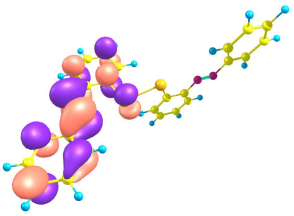


FigureS4 Emission spectra of compound **6**, **12** and **10** at 2 x 10^{-7} M in $CHCl_3$



FigureS5 Emission spectra of compound **7-9** at 2 x 10^{-7} M in $CHCl_3$

Compound	MO	LUMO/LUMO+1
6	 HOMO-2	 LUMO+1
	 HOMO-3	
7	 HOMO-2	 LUMO
	 HOMO-3	
8	 HOMO-4	 LUMO
9	 HOMO-4	 LUMO

	 HOMO-2	
10	 HOMO-2	 LUMO
12	 HOMO-4	 LUMO

TableS1 Pictorial representation of molecular orbitals involved in U.V-visible transition (B3LYP/6-31+G(d))

Entry	MO		LUMO	Excitation Wavelength		Oscillatory Strength (*f*)
				λ_{max}(exp)	λ_{max}(cal)	
6	HOMO	(27%)	LUMO	404	451	0.1005
		(66%)	LUMO+1		439	0.0651
7	HOMO	(46%)	LUMO	432	423	0.0633
	HOMO-1	(39%)			413	0.0304
8	HOMO-2	(66%)	LUMO		481	0.0008
9	HOMO	(85%)	LUMO	439	466	0.0816
10	HOMO-4	(27%)	LUMO	450	439	0.0096
	HOMO	(29%)	LUMO+1		433	0.0061
12	HOMO	(56%)	LUMO+1	445	470	0.1240

TableS2 Comparison of the experimental and computed absorption wavelength for n-π* transition along with their respective oscillatory strength and percentage contribution of molecular orbital at B3LYP/6-31+G(d)

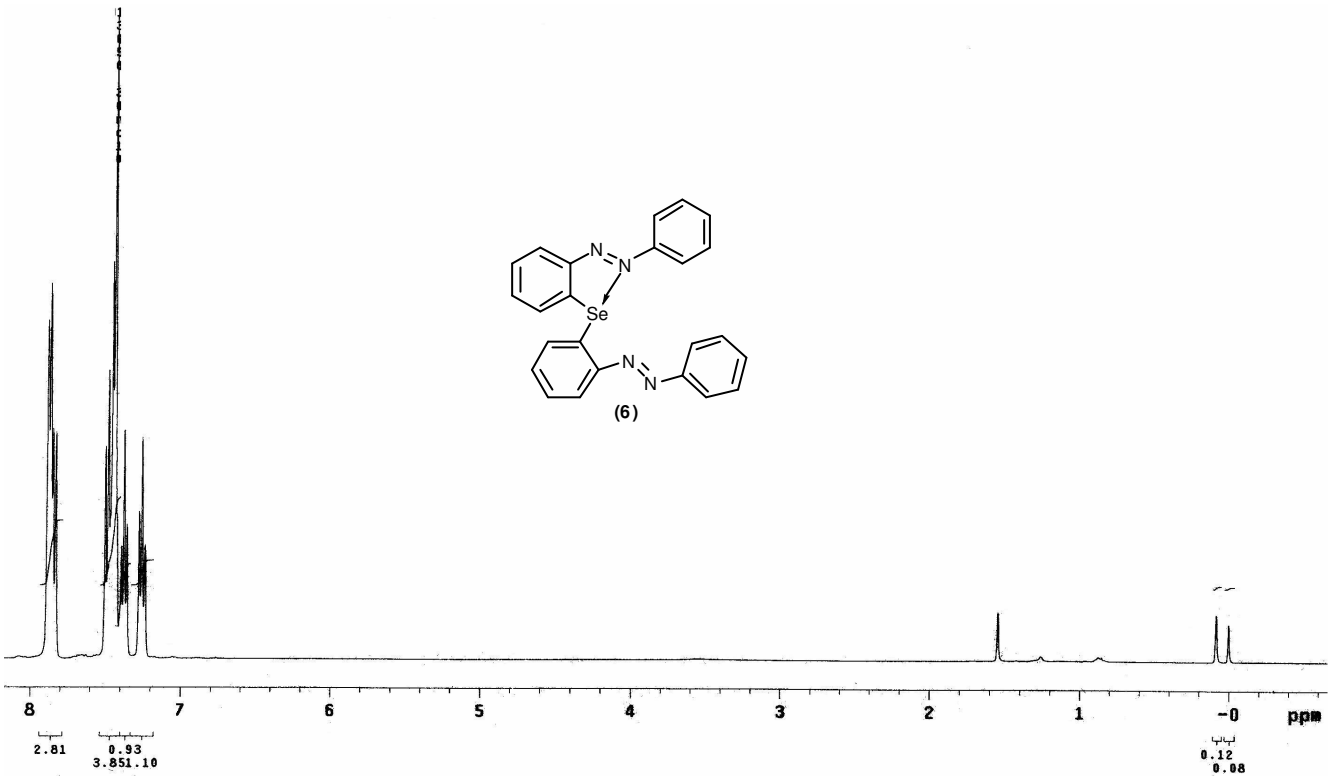


Figure S6: ^{1}H NMR spectrum of **6**

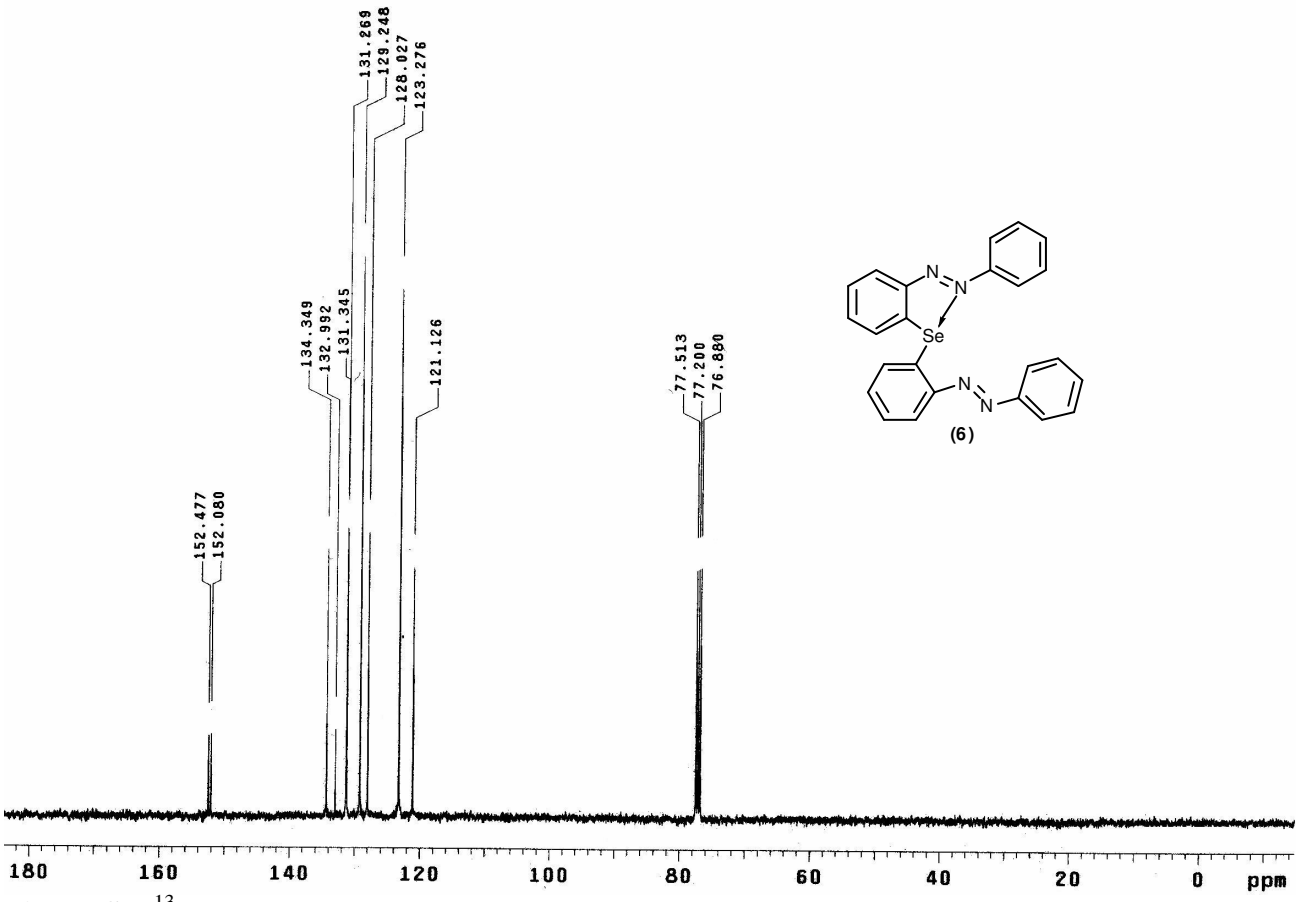


Figure S7: ^{13}C NMR spectrum of **6**

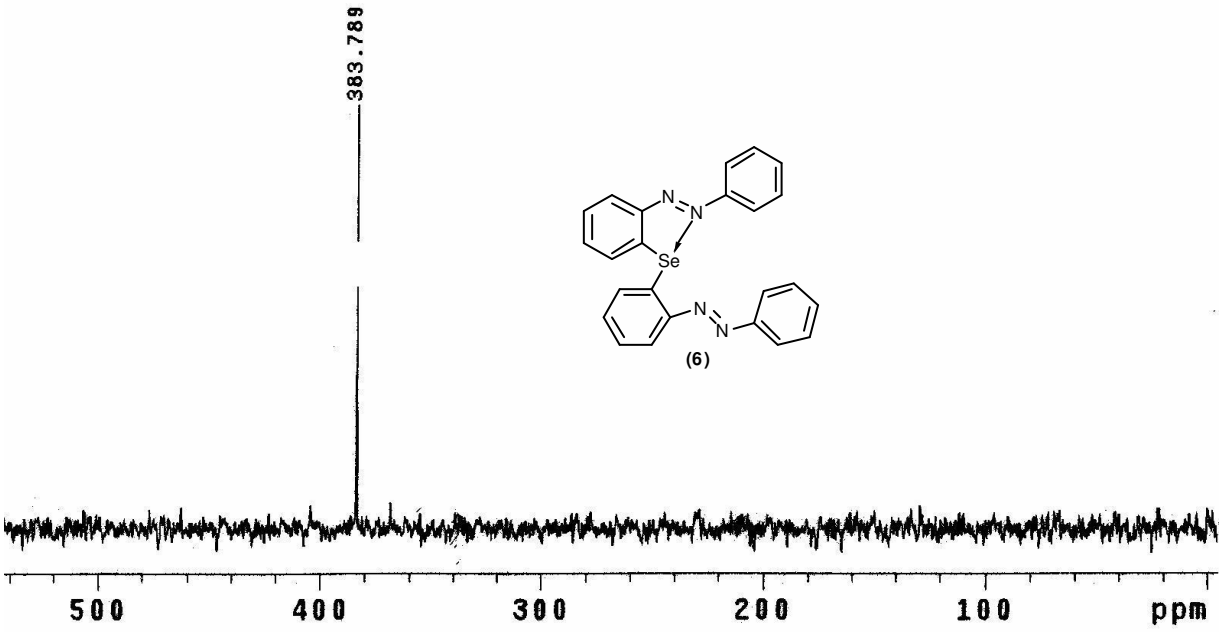
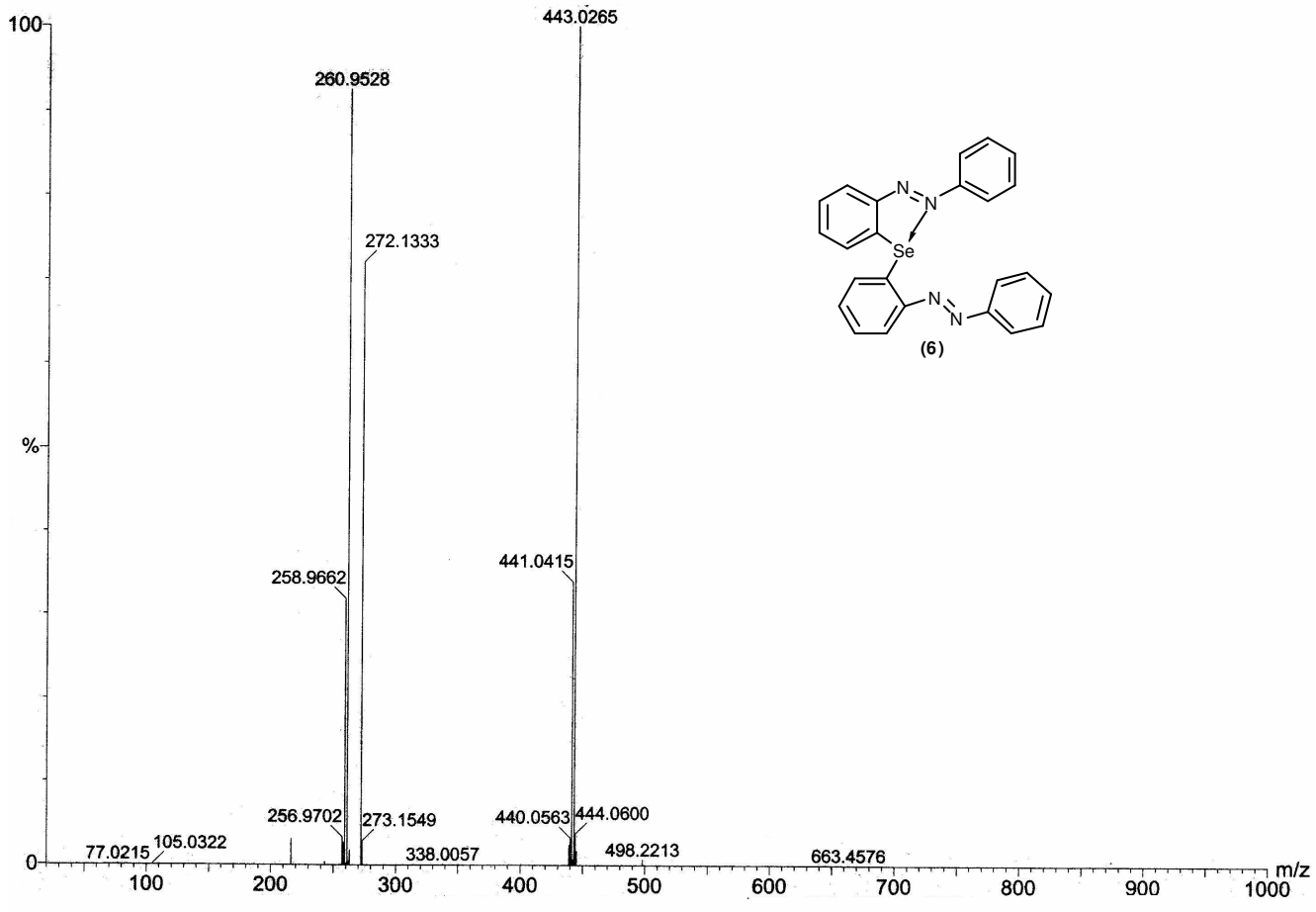
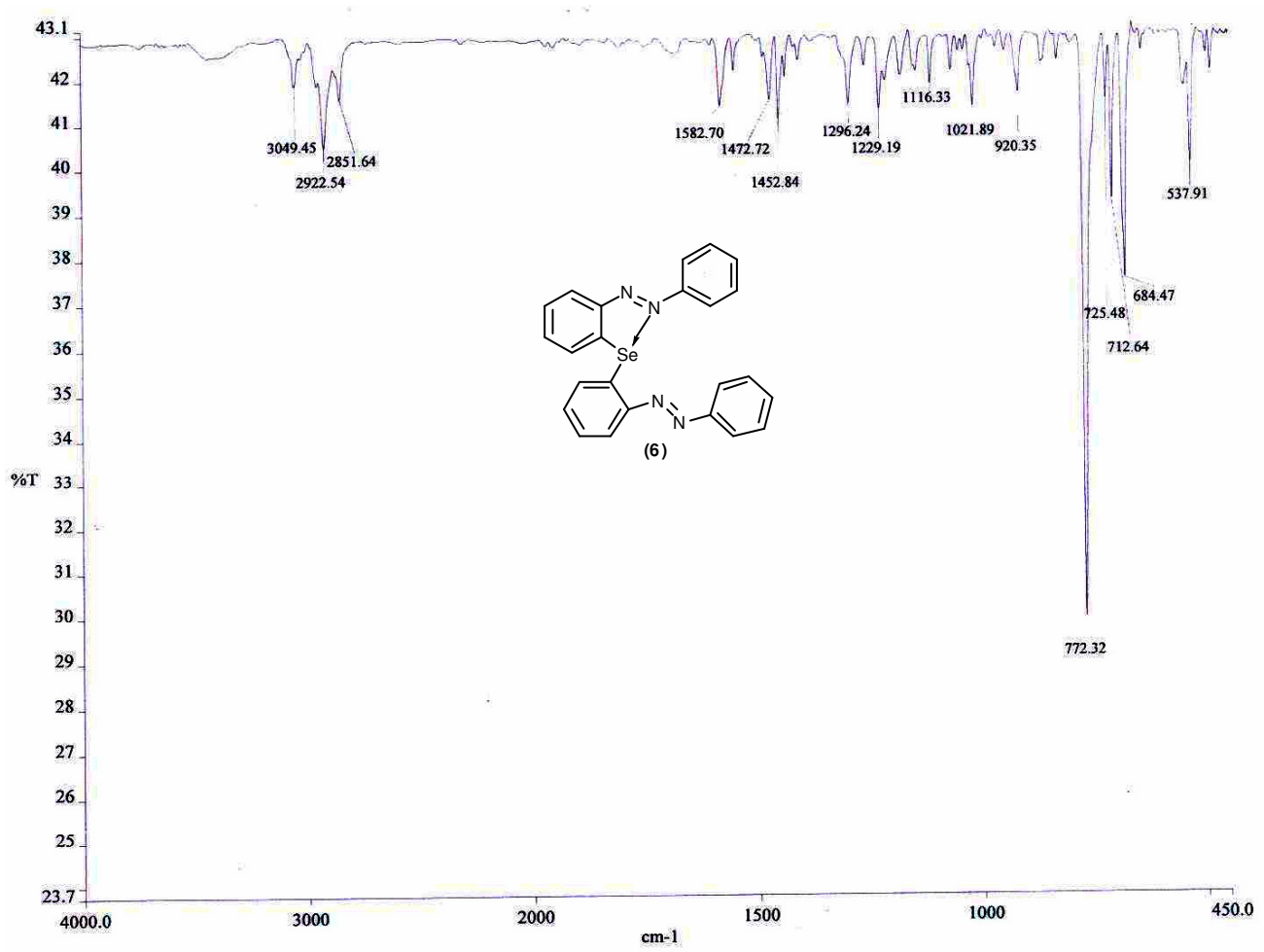


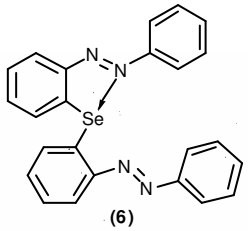
Figure S8: ^{77}Se NMR spectrum of **6**



FigureS9: ES-MS spectrum of **6**



FigureS10: FT-IR spectrum of **6**



(6)

Eager 300 Report

Page: 1 Sample: KRAZOMONOSE (KRAZOMONOSE)

Method Name : sp310807
Method File : G:\eager300\Eager 300 EA1112\SP310807.mth
Chromatogram : KRAZOMONOSE
Operator ID : SP Company Name : C.E. Instruments
Analysed : 08/31/2007 14:03 Printed : 8/31/2007 17:03
Sample ID : KRAZOMONOSE (# 19) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : 1.774

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	12.0590	44	253946	FU	11.381000	.118707E+07
Carbon	65.2080	65	2890161	FU	1.000000	.249843E+07
Hydrogen	3.7823	175	332277	RS	8.698047	.495206E+07
Totals	81.0494		3476384			

FigureS11: Elemental analysis (C, H, N) of **6**

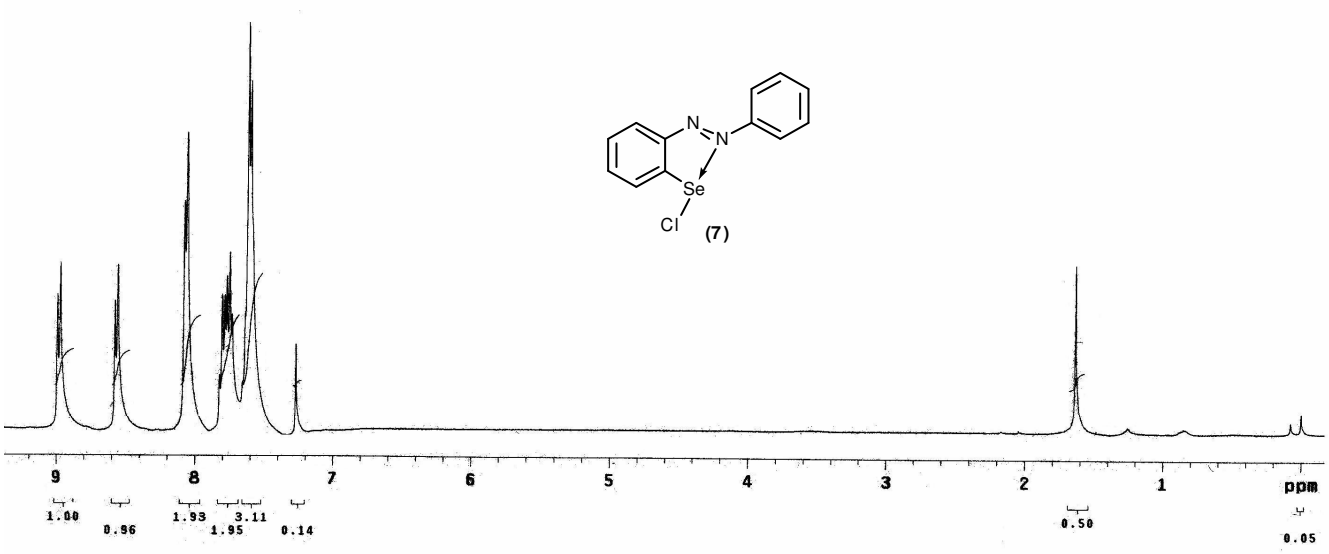


Figure S12: ^{1}H NMR spectrum of **7**

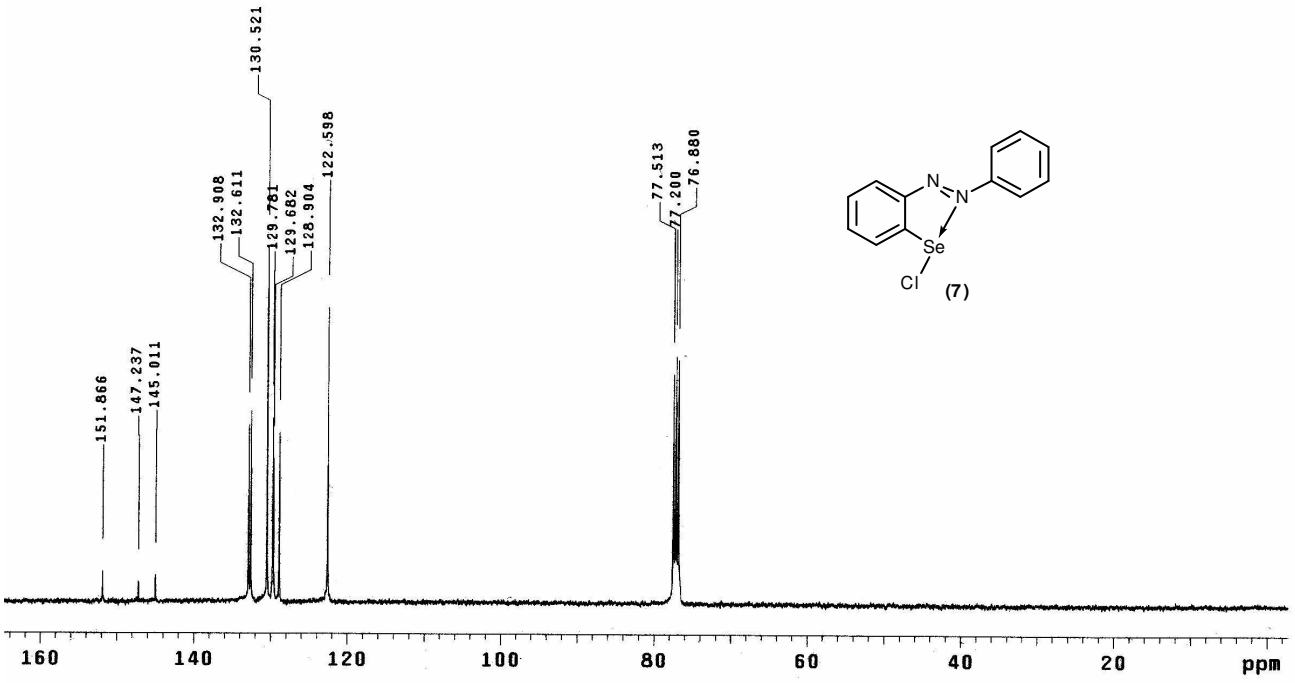


Figure S13: ^{13}C NMR spectrum of **7**

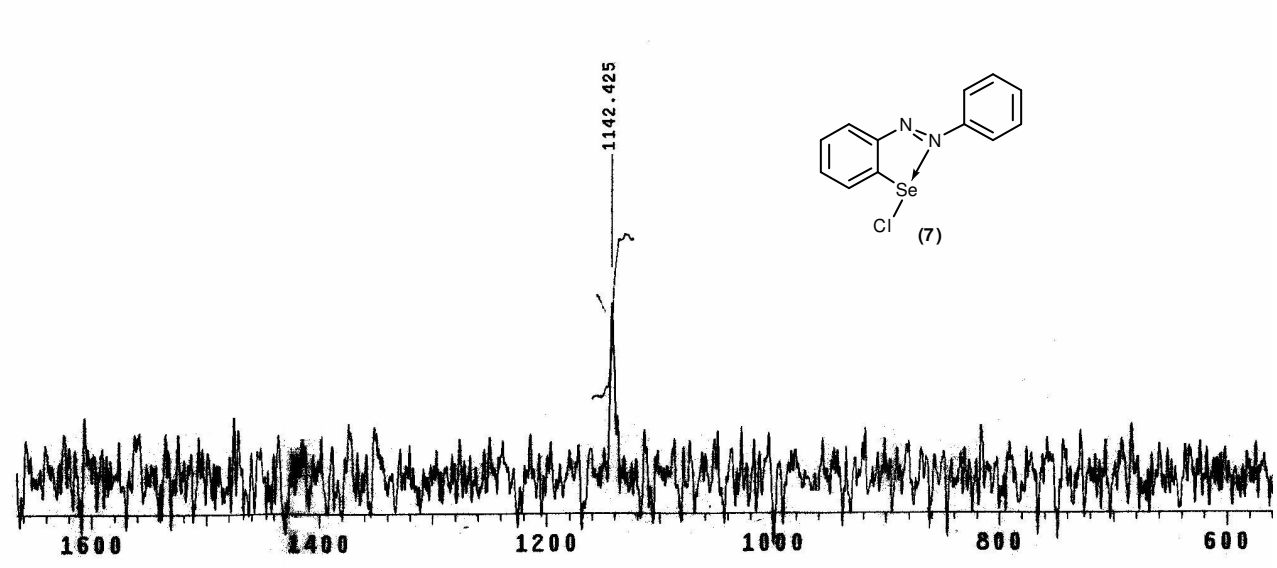


Figure S14: ^{77}Se NMR spectrum of **7**

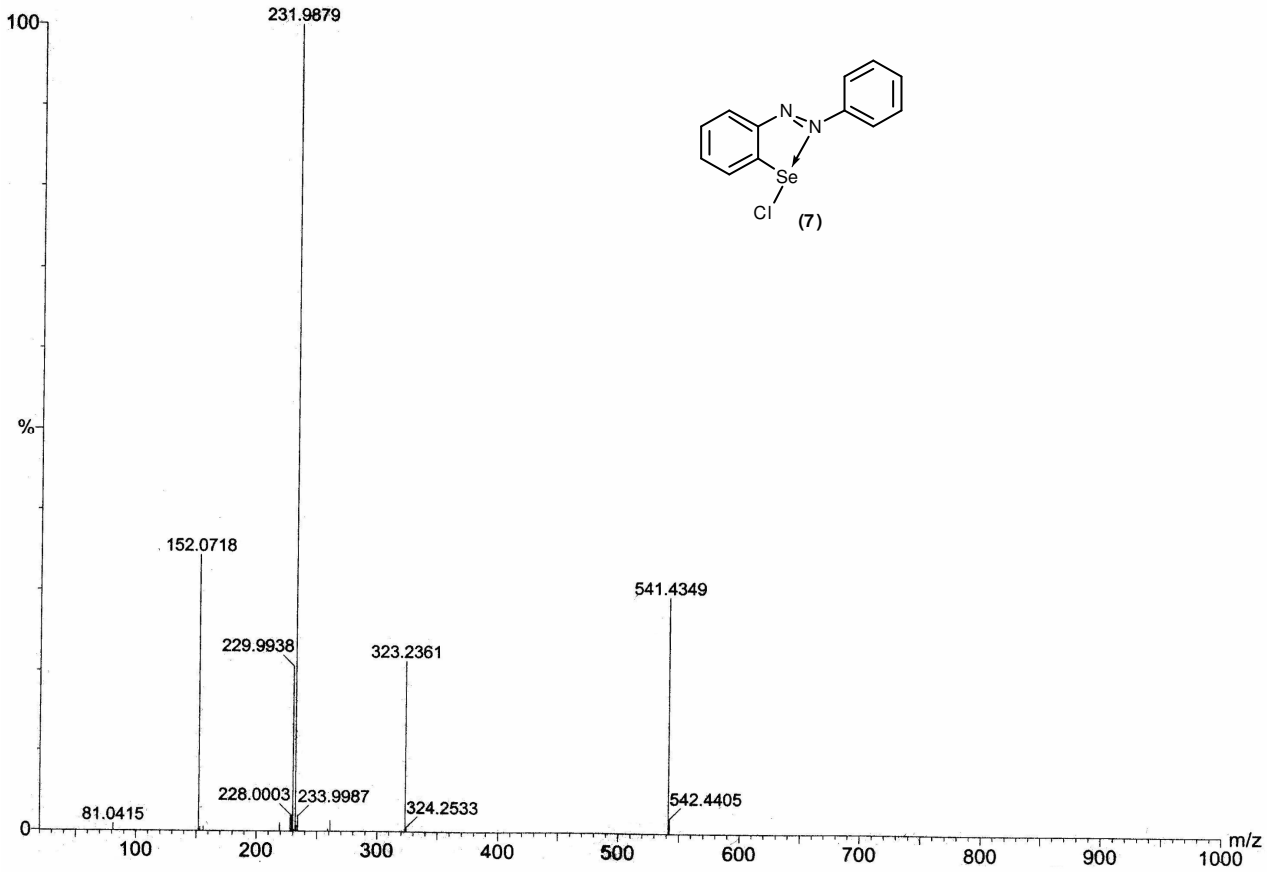


Figure S15: ES-MS spectrum of **7**

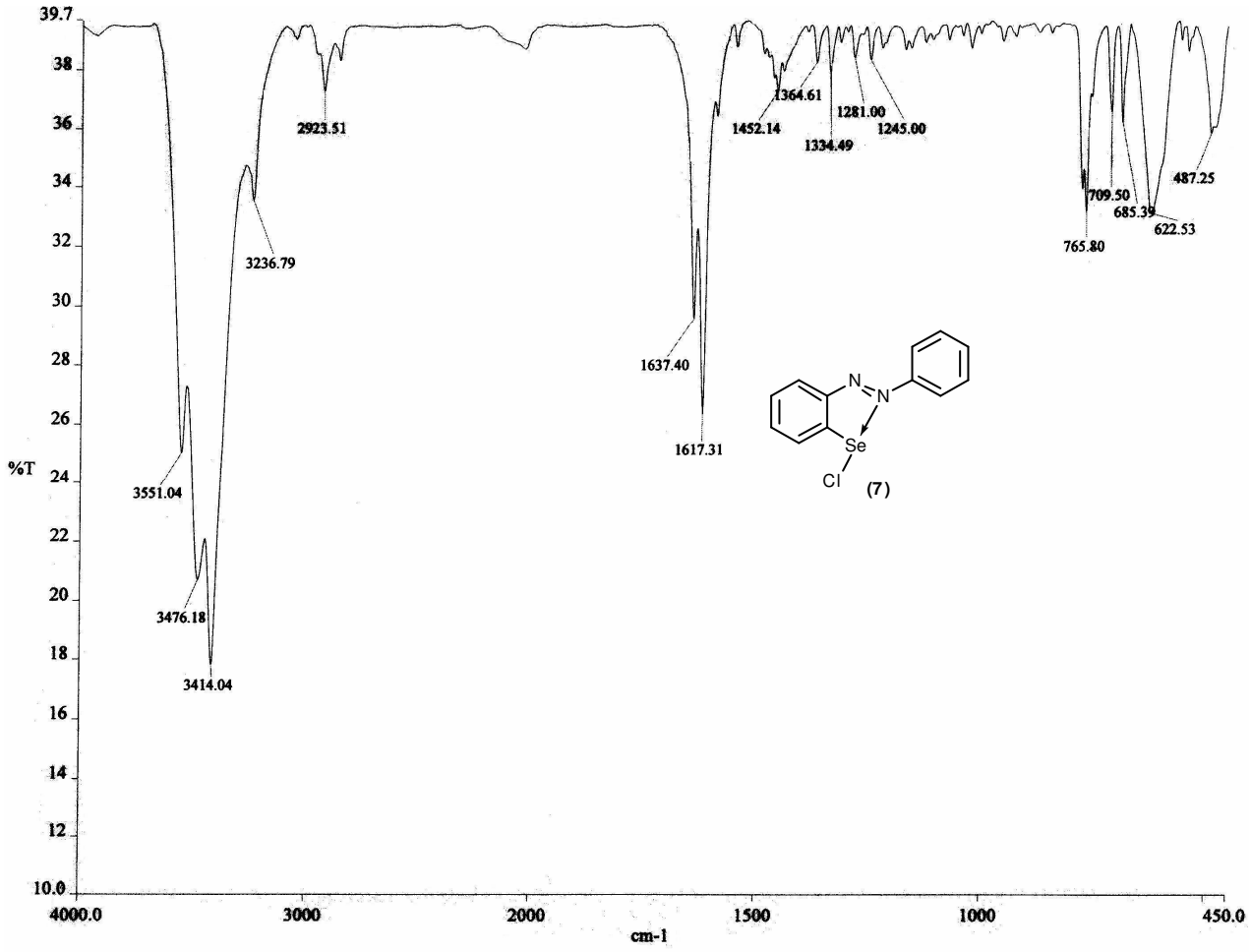
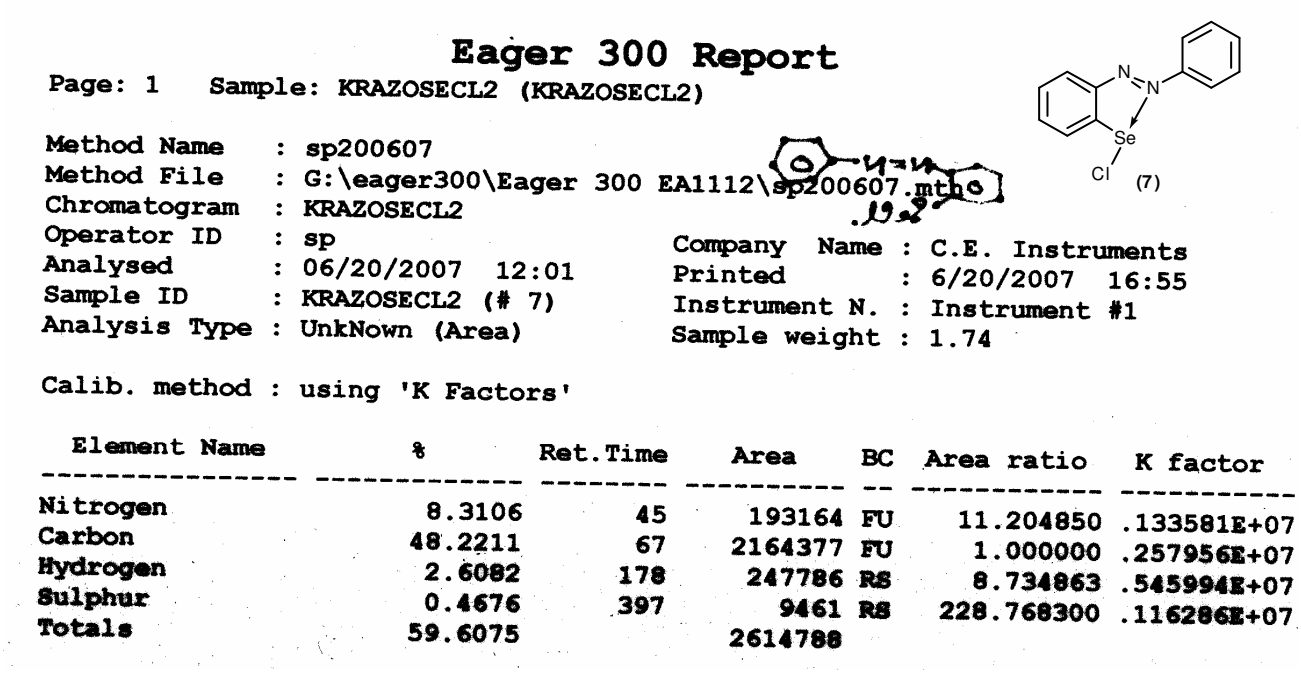


Figure S16: FT-IR spectrum of **7**



Eager 300 Report

Page: 1 Sample: KRAZOSECL2 (KRAZOSECL2)

(7)

Method Name : sp200607
Method File : G:\eager300\Eager 300 EA1112\sp200607.mth
Chromatogram : KRAZOSECL2
Operator ID : sp
Analysed : 06/20/2007 12:01
Sample ID : KRAZOSECL2 (# 7)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 6/20/2007 16:55
Instrument N. : Instrument #1
Sample weight : 1.74

Calib. method : using 'K Factors'

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.3106	45	193164	FU	11.204850	.133581E+07
Carbon	48.2211	67	2164377	FU	1.000000	.257956E+07
Hydrogen	2.6082	178	247786	RS	8.734863	.545994E+07
Sulphur	0.4676	397	9461	RS	228.768300	.116286E+07
Totals	59.6075		2614788			

Figure S17: Elemental analysis (C, H, N) of **7**

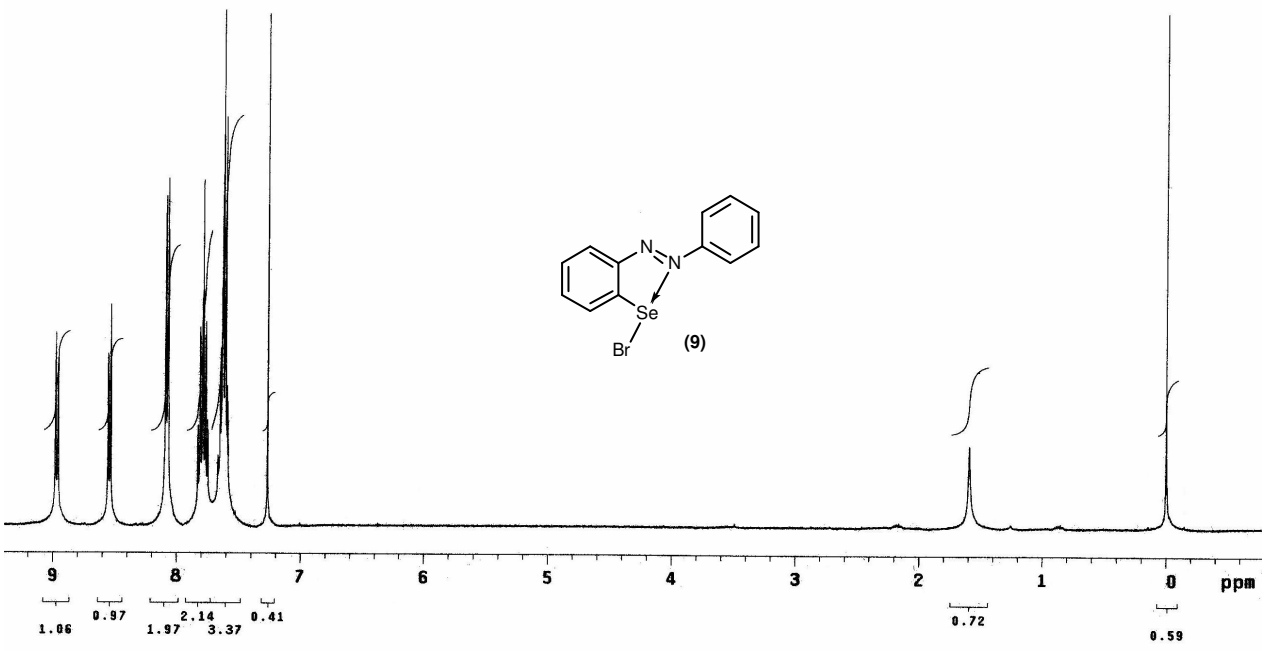


Figure S18: ^{1}H NMR spectrum of **9**

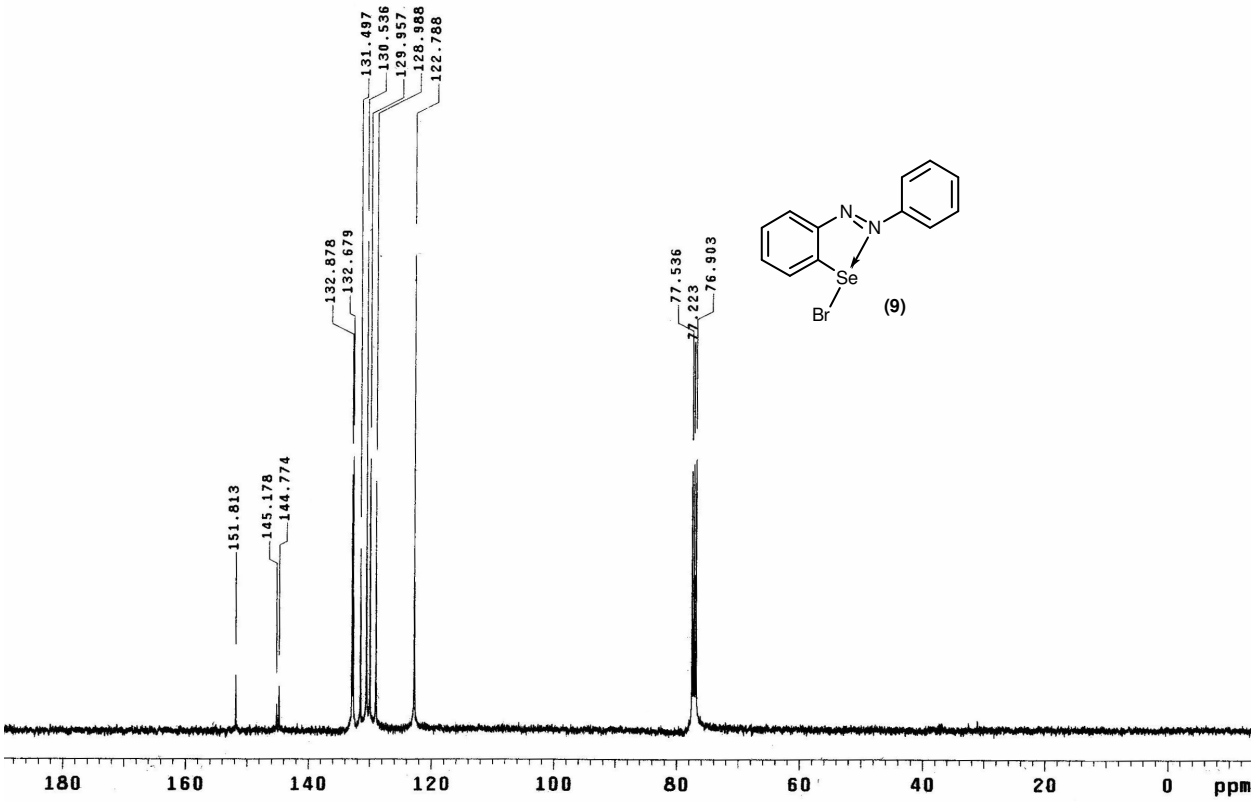


Figure S19: ^{13}C NMR spectrum of **9**

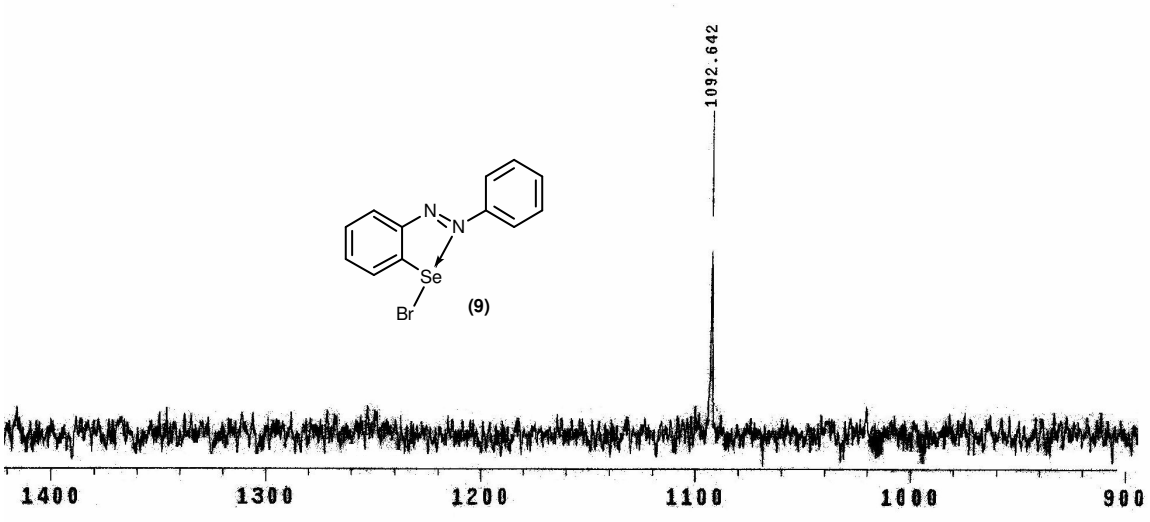


Figure S20: ^{77}Se NMR spectrum of **9**

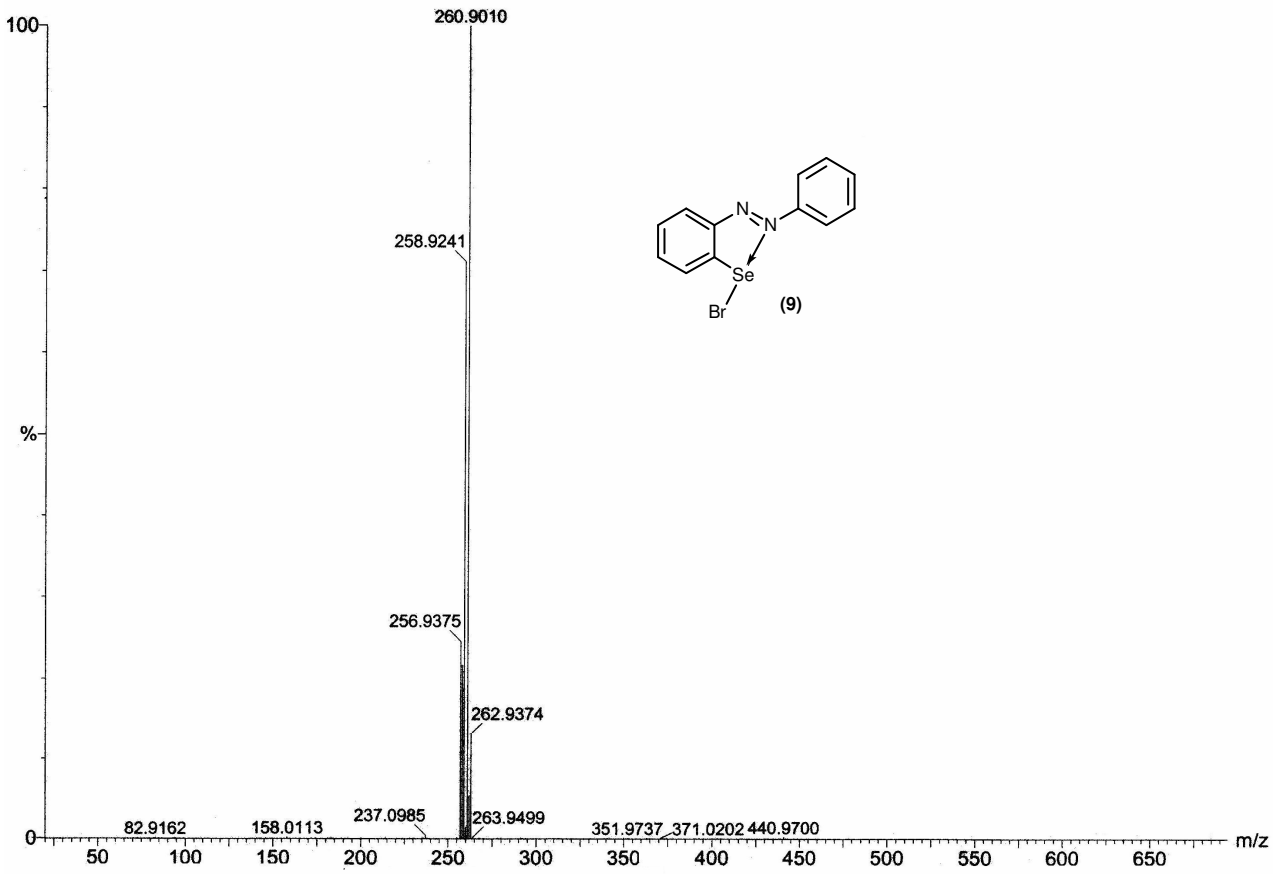


Figure S21: ES-MS spectrum of **9**

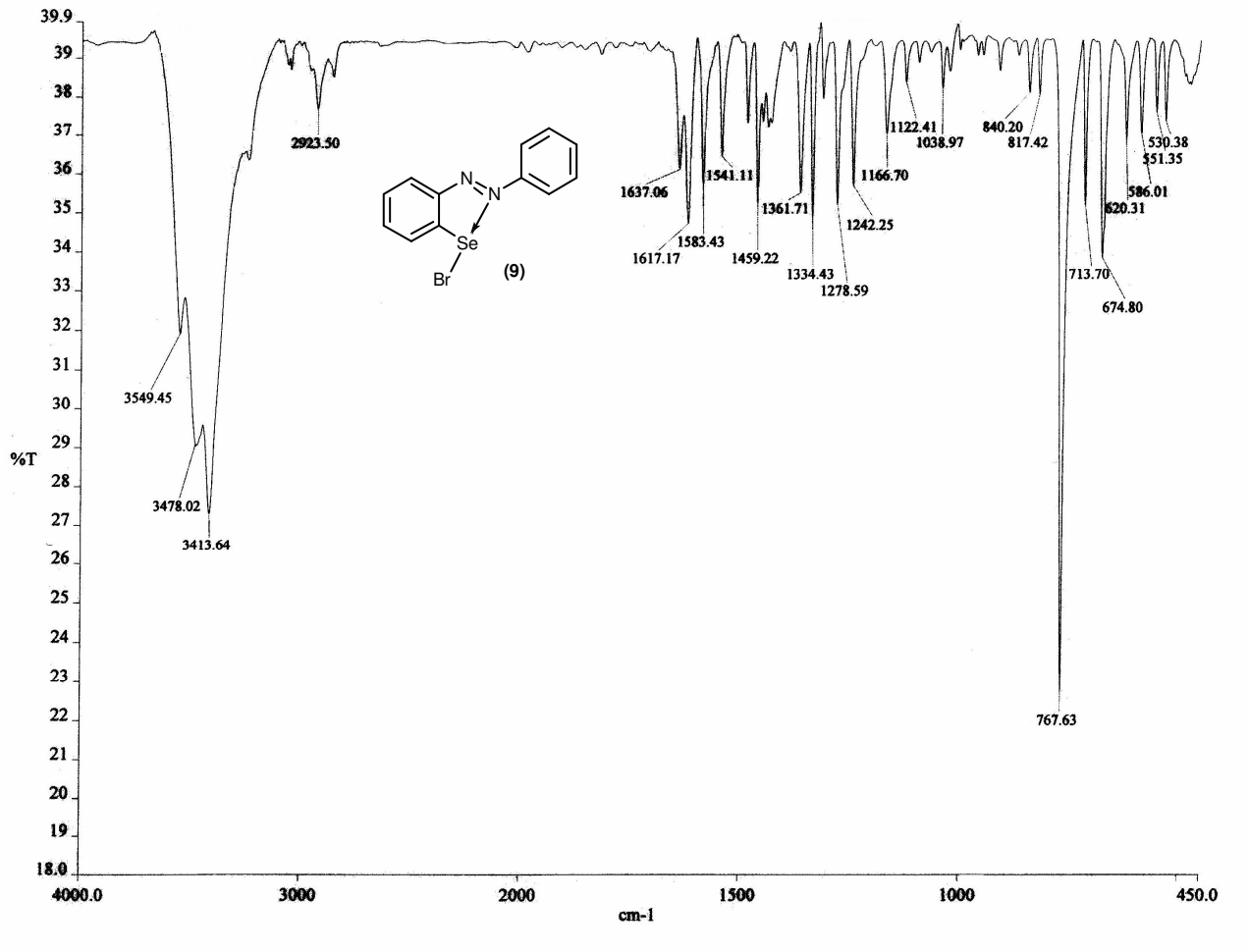
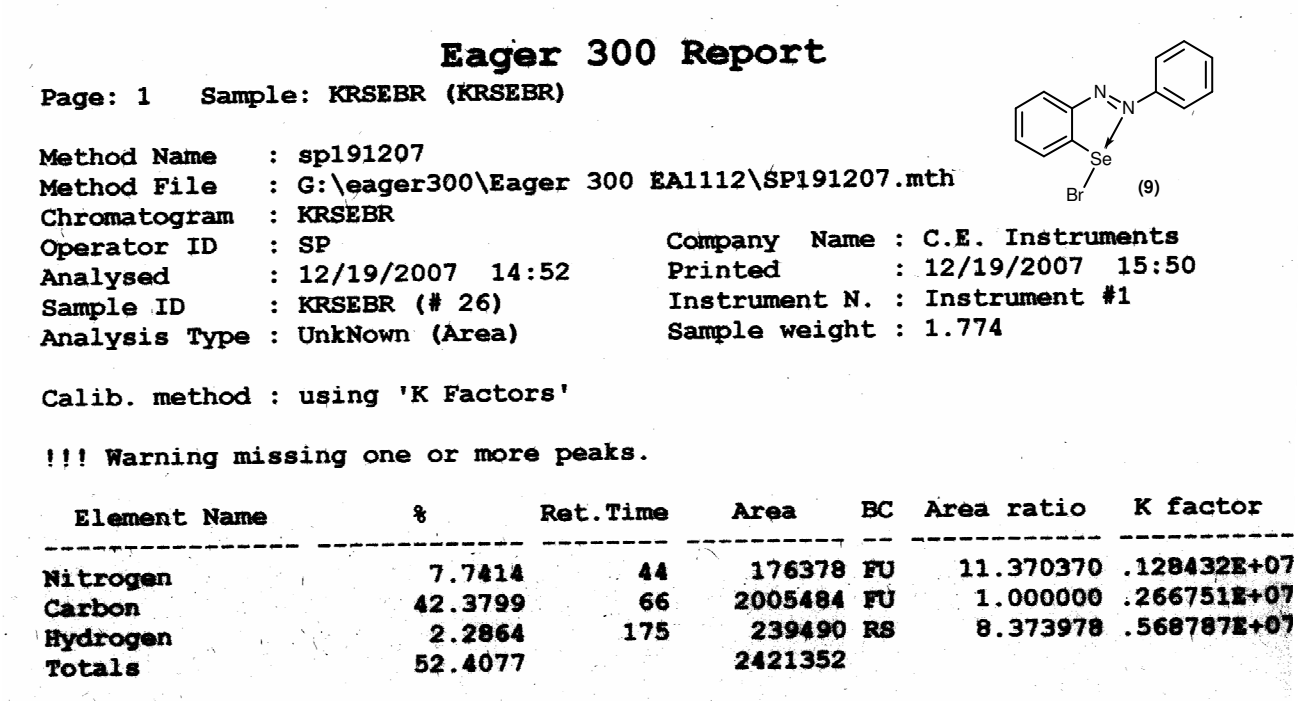


Figure S22: FT-IR spectrum of **9**



Eager 300 Report

Page: 1 Sample: KRSEBR (KRSEBR)

(9)

Method Name : sp191207
Method File : G:\eager300\Eager 300 EA1112\SP191207.mth
Chromatogram : KRSEBR
Operator ID : SP
Analysed : 12/19/2007 14:52
Sample ID : KRSEBR (# 26)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 12/19/2007 15:50
Instrument N. : Instrument #1
Sample weight : 1.774

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	7.7414	44	176378	FU	11.370370	.128432E+07
Carbon	42.3799	66	2005484	FU	1.000000	.266751E+07
Hydrogen	2.2864	175	239490	RS	8.373978	.568787E+07
Totals	52.4077		2421352			

Figure S23: Elemental analysis (C, H, N) of **9**

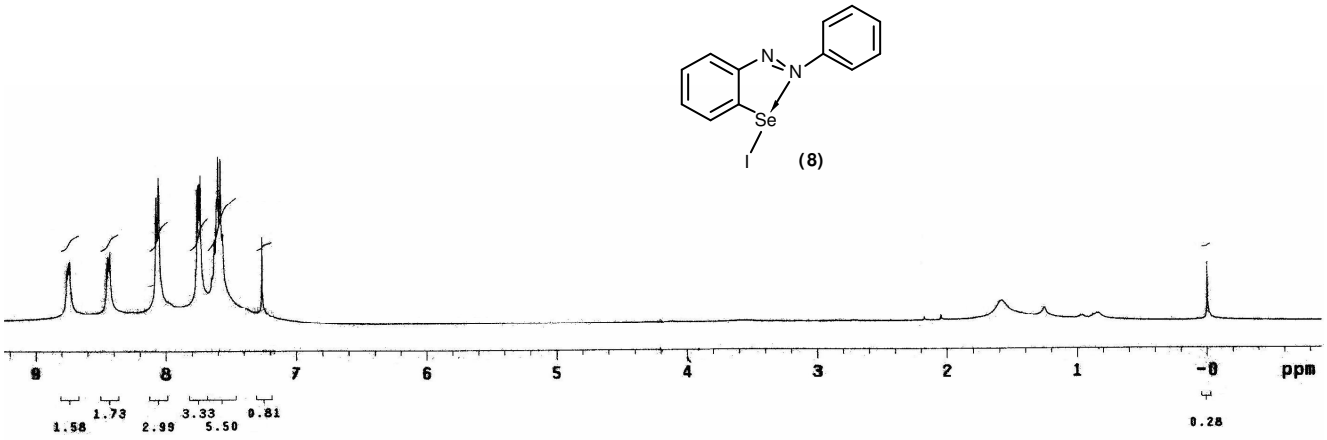


Figure S24: ^{1}H NMR spectrum of **8**

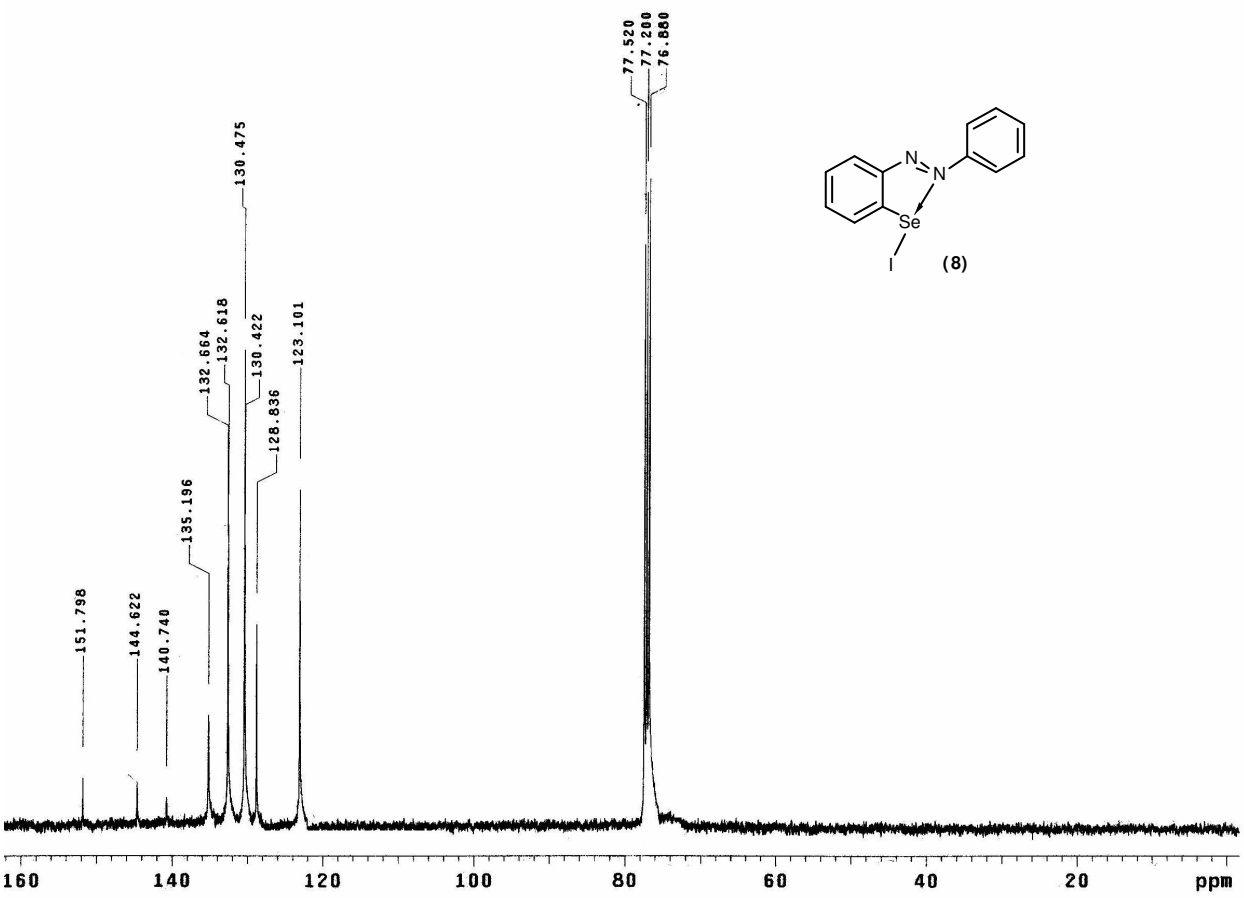


Figure S25: ^{13}C NMR spectrum of **8**

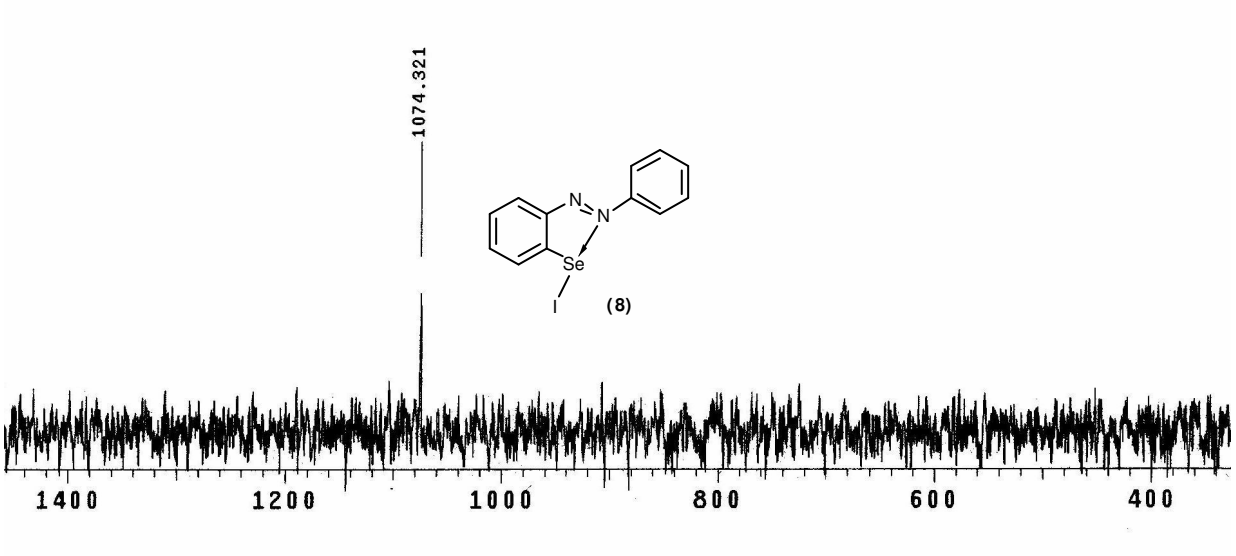


Figure S26: ^{77}Se NMR spectrum of **8**

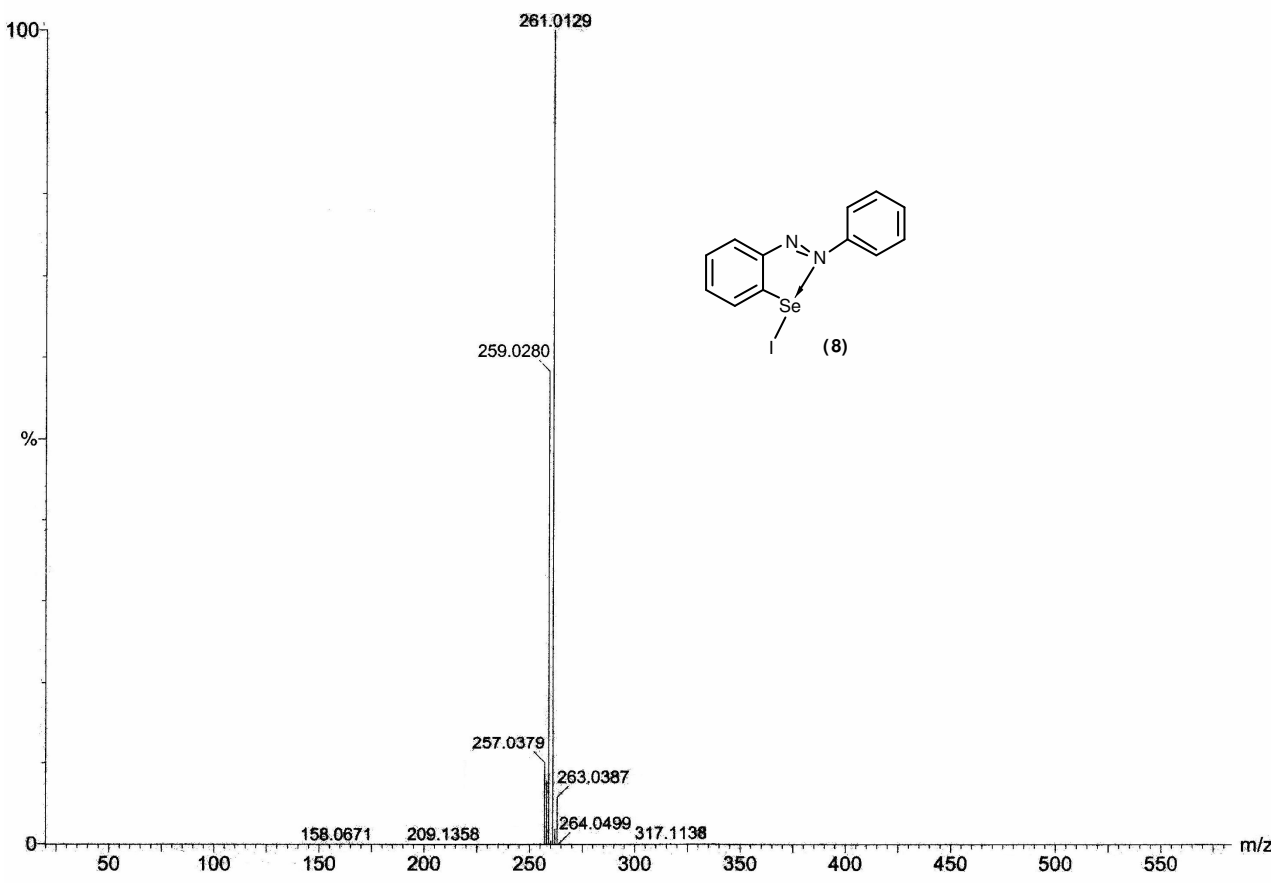
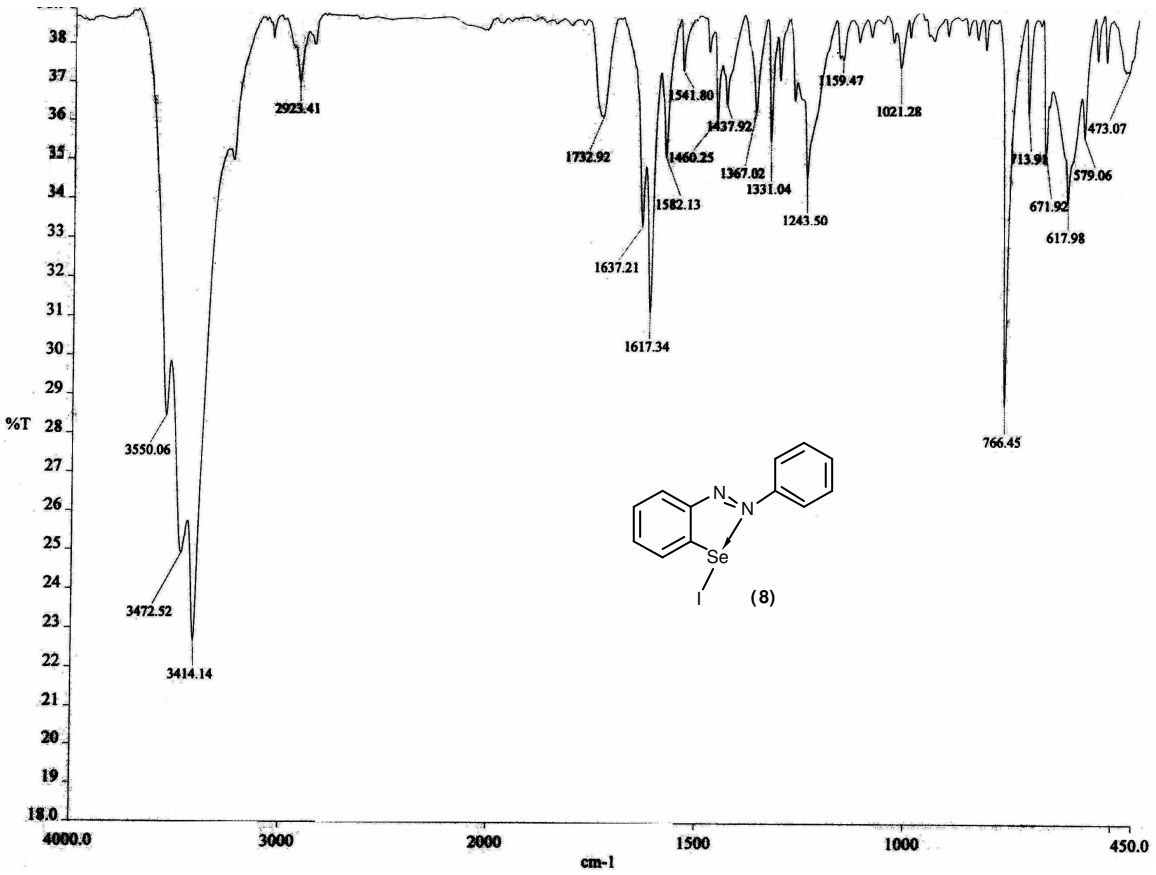
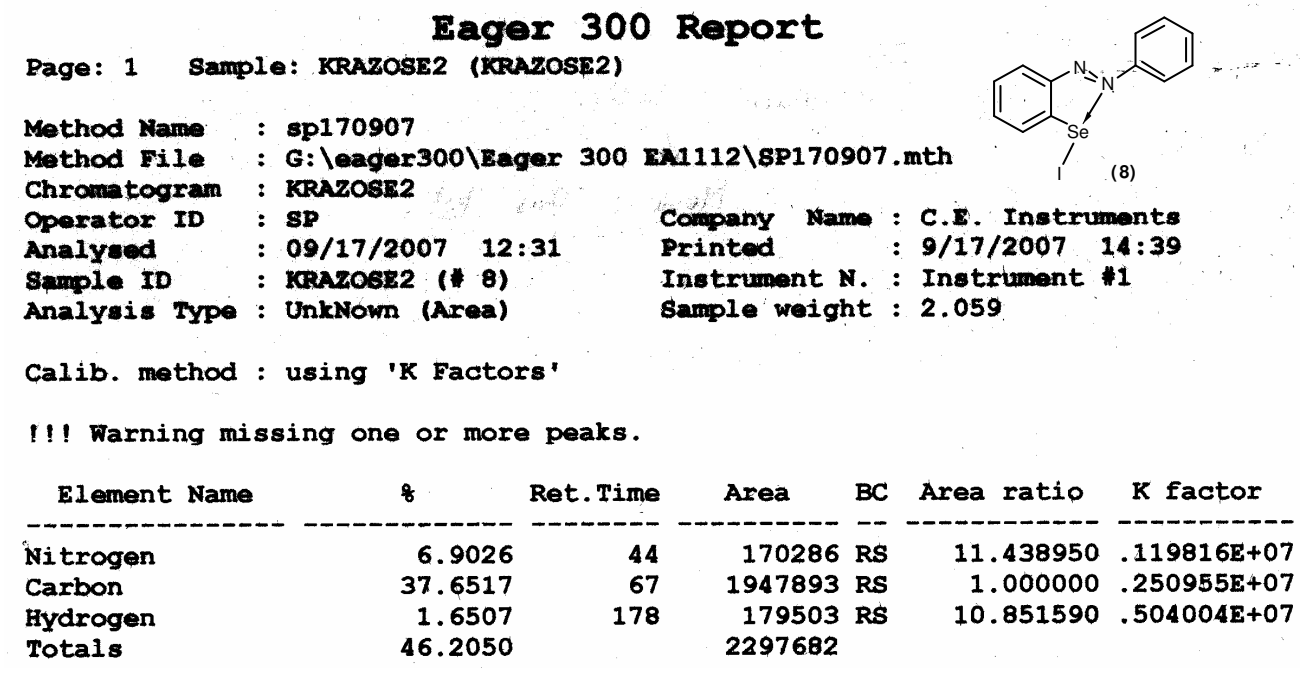


Figure S27: ES-MS spectrum of **8**



FigureS28: FT-IR spectrum of **8**



Eager 300 Report

Page: 1 Sample: KRAZOSE2 (KRAZOSE2)

Method Name : sp170907
Method File : G:\eager300\Eager 300 EA1112\SP170907.mth
Chromatogram : KRAZOSE2
Operator ID : SP
Analysed : 09/17/2007 12:31
Sample ID : KRAZOSE2 (# 8)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 9/17/2007 14:39
Instrument N. : Instrument #1
Sample weight : 2.059

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	6.9026	44	170286	RS	11.438950	.119816E+07
Carbon	37.6517	67	1947893	RS	1.000000	.250955E+07
Hydrogen	1.6507	178	179503	RS	10.851590	.504004E+07
Totals	46.2050		2297682			

FigureS29: Elemental analysis (C, H, N) of **8**

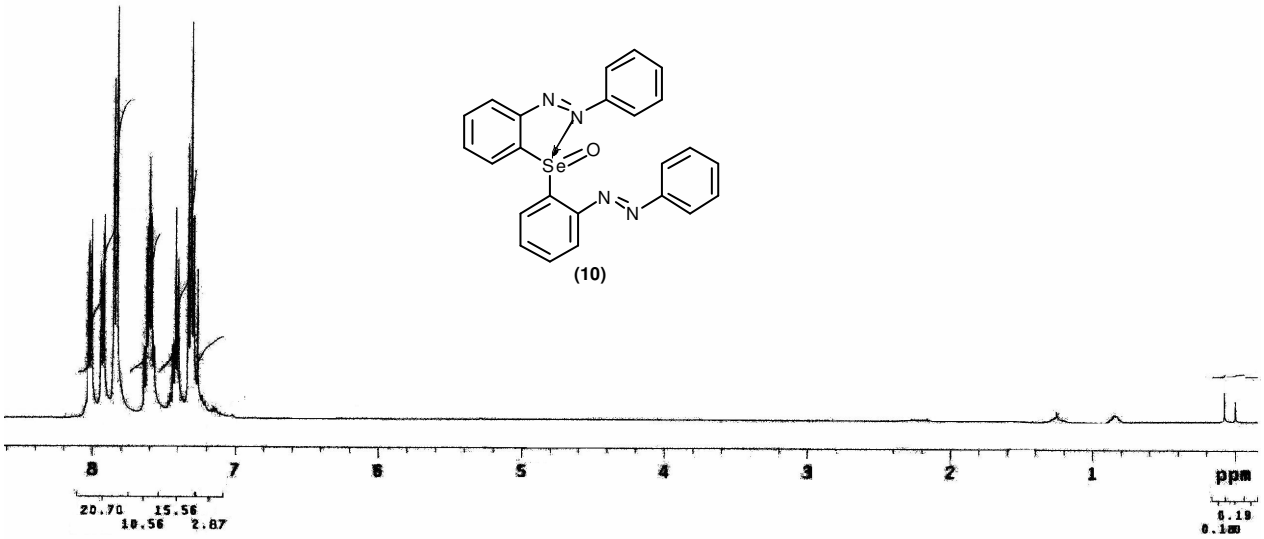


Figure S30: 1H NMR spectrum of **10**

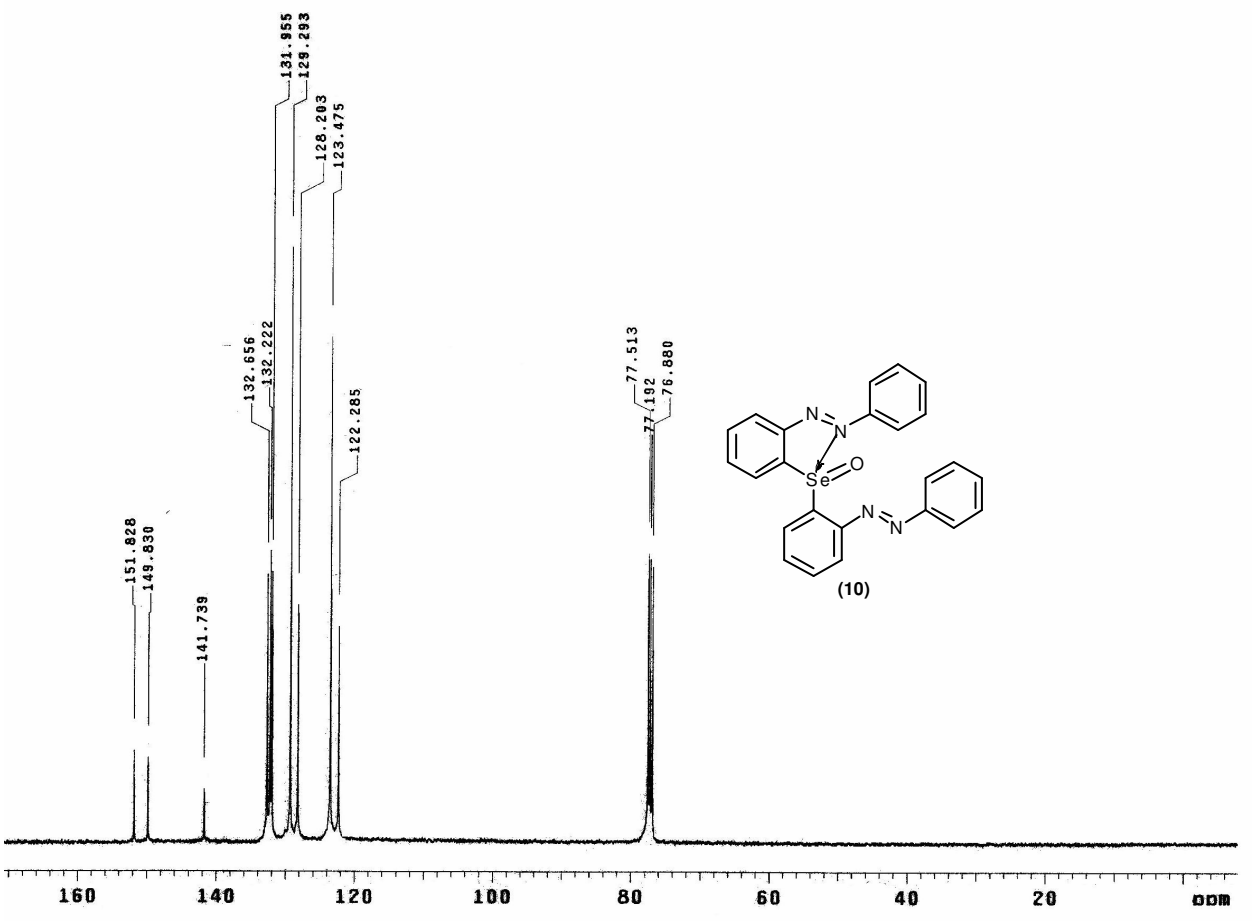


Figure S31: ^{13}C NMR spectrum of **10**

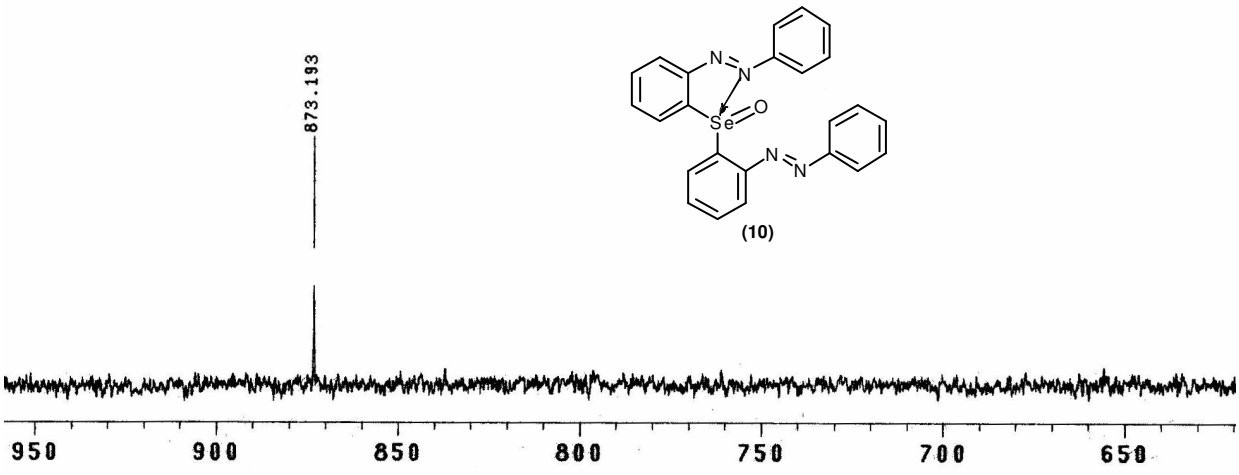
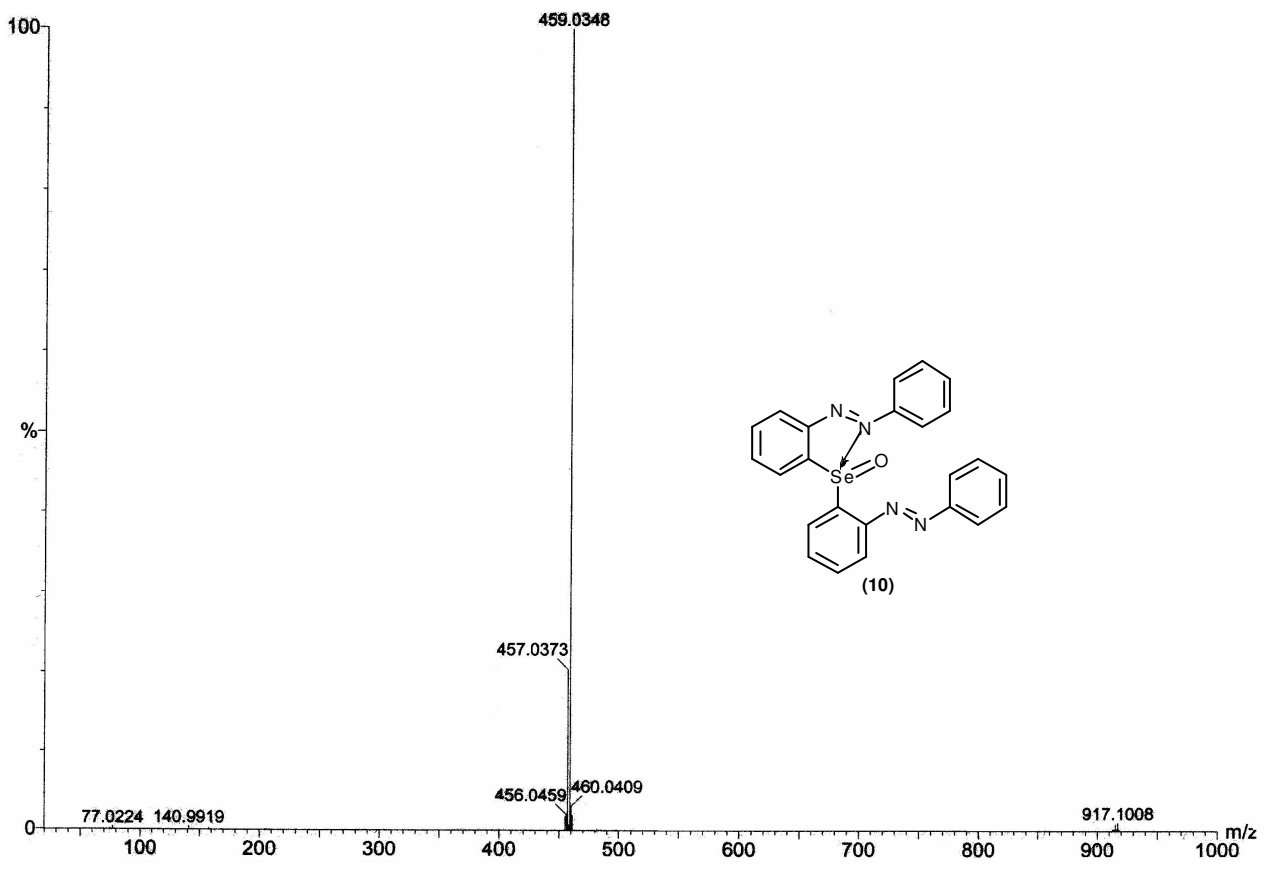


Figure S32: ^{77}Se NMR spectrum of **10**



FigureS33: ES-MS spectrum of **10**

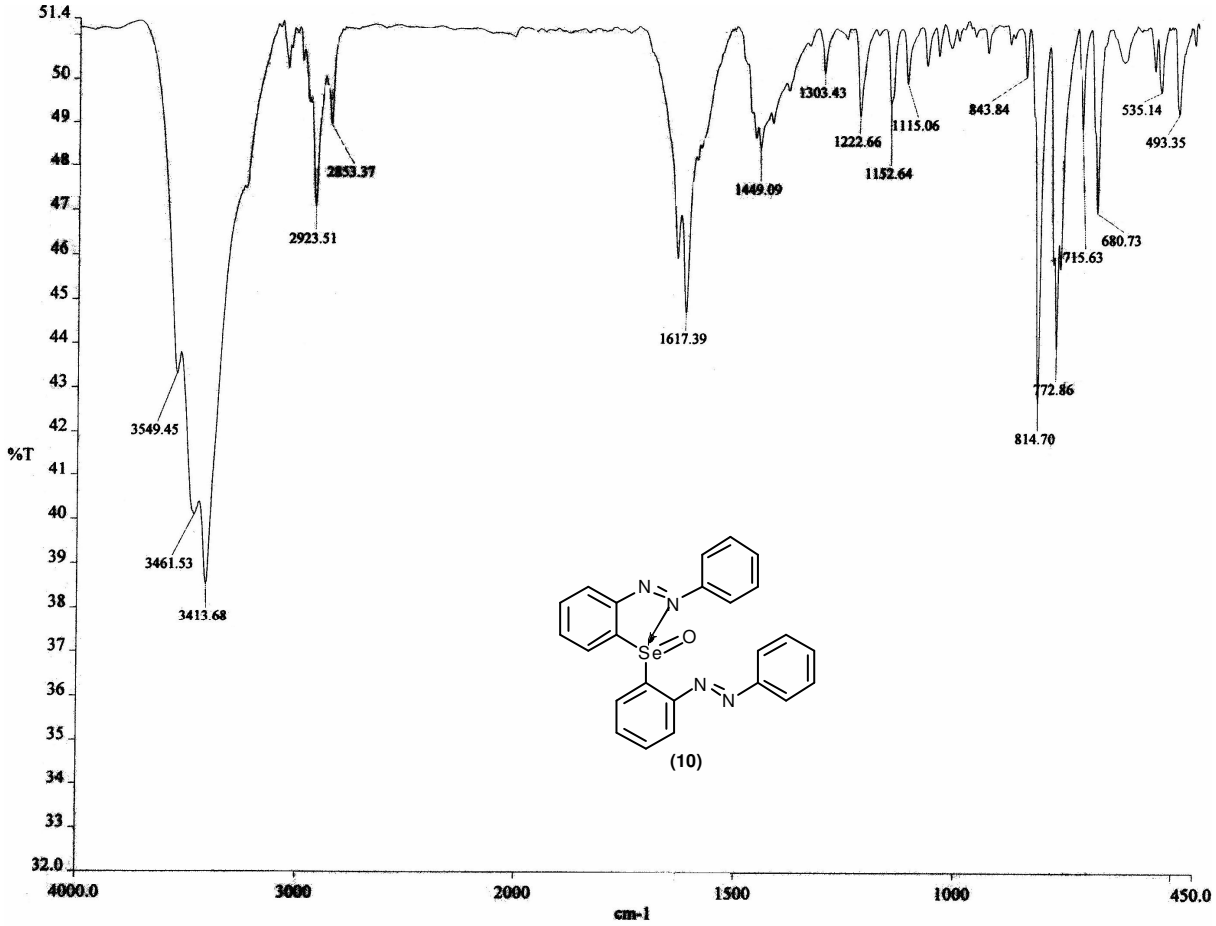
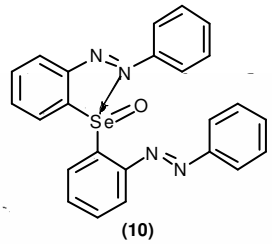


Figure S34: FT-IR spectrum of **10**



(10)

Eager 300 Report

Page: 1 Sample: KRAZOSEO (ARAZOSEO)

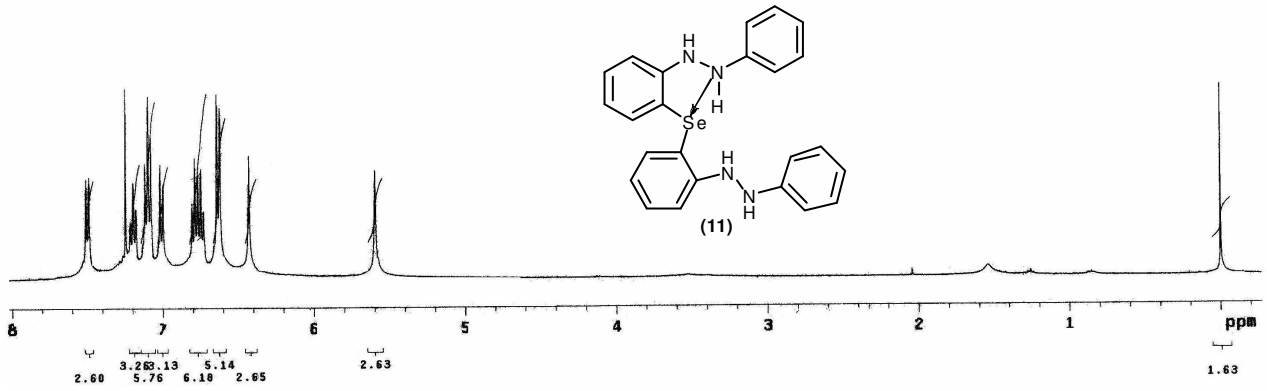
Method Name : sp061107
Method File : G:\eager300\Eager 300 EA1112\SP061107.mth
Chromatogram : ARAZOSEO
Operator ID : SP
Company Name : C.E. Instruments
Analysed : 11/06/2007 14:35
Printed : 11/6/2007 16:16
Sample ID : KRAZOSEO (# 25)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : 1.803

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.5347	44	270825	FU	11.340450	.130223E+07
Carbon	63.4209	65	3071276	FU	1.000000	.268411E+07
Hydrogen	3.7230	169	395587	BB	7.763844	.575777E+07
Totals	78.6785		3737688			

Figure S35: Elemental analysis (C, H, N) of **10**



(11)

Figure S36: ^{1}H NMR spectrum of **11**

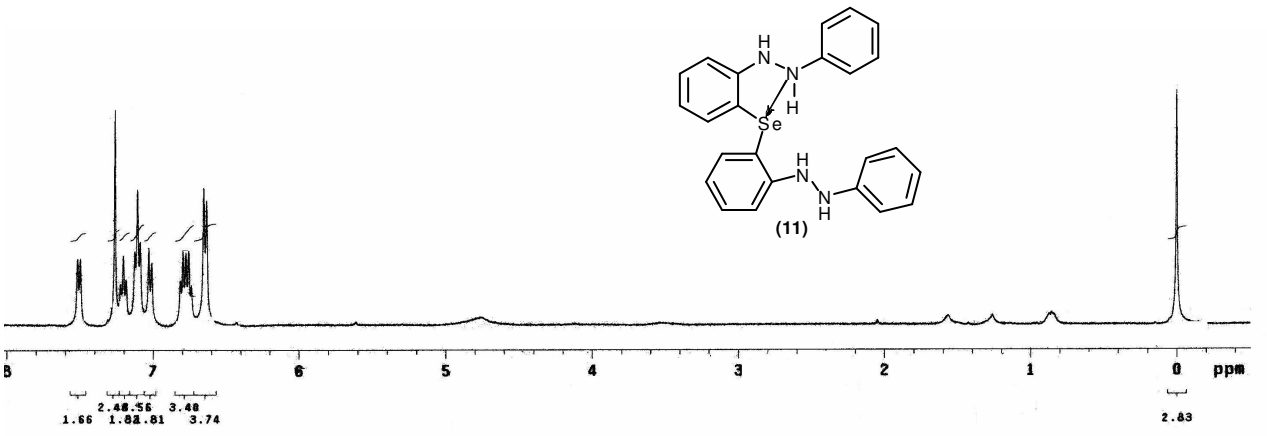


Figure S37: D_2O exchange ^1H NMR spectrum of **11**

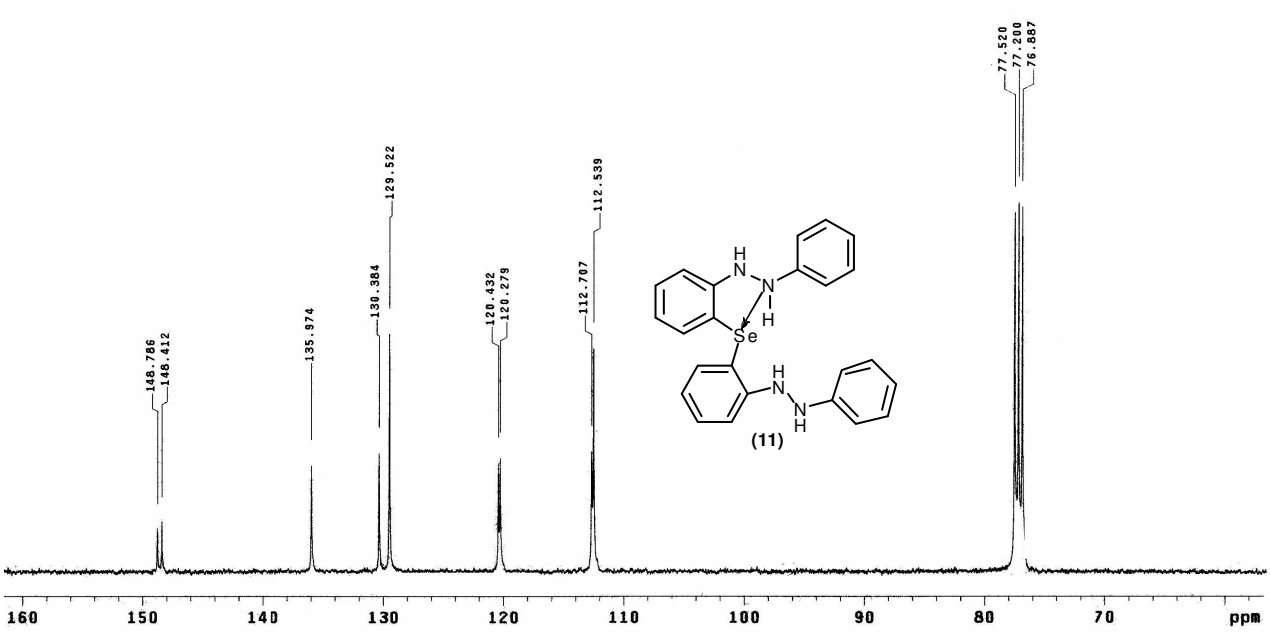


Figure S38: ^{13}C NMR spectrum of **11**

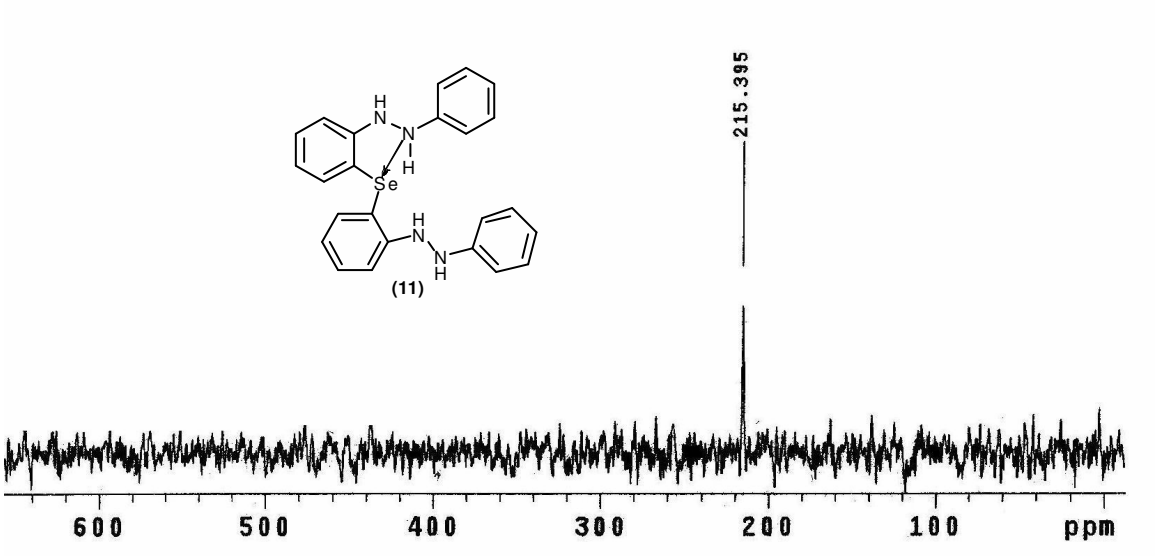


Figure S39: ^{77}Se NMR spectrum of **11**

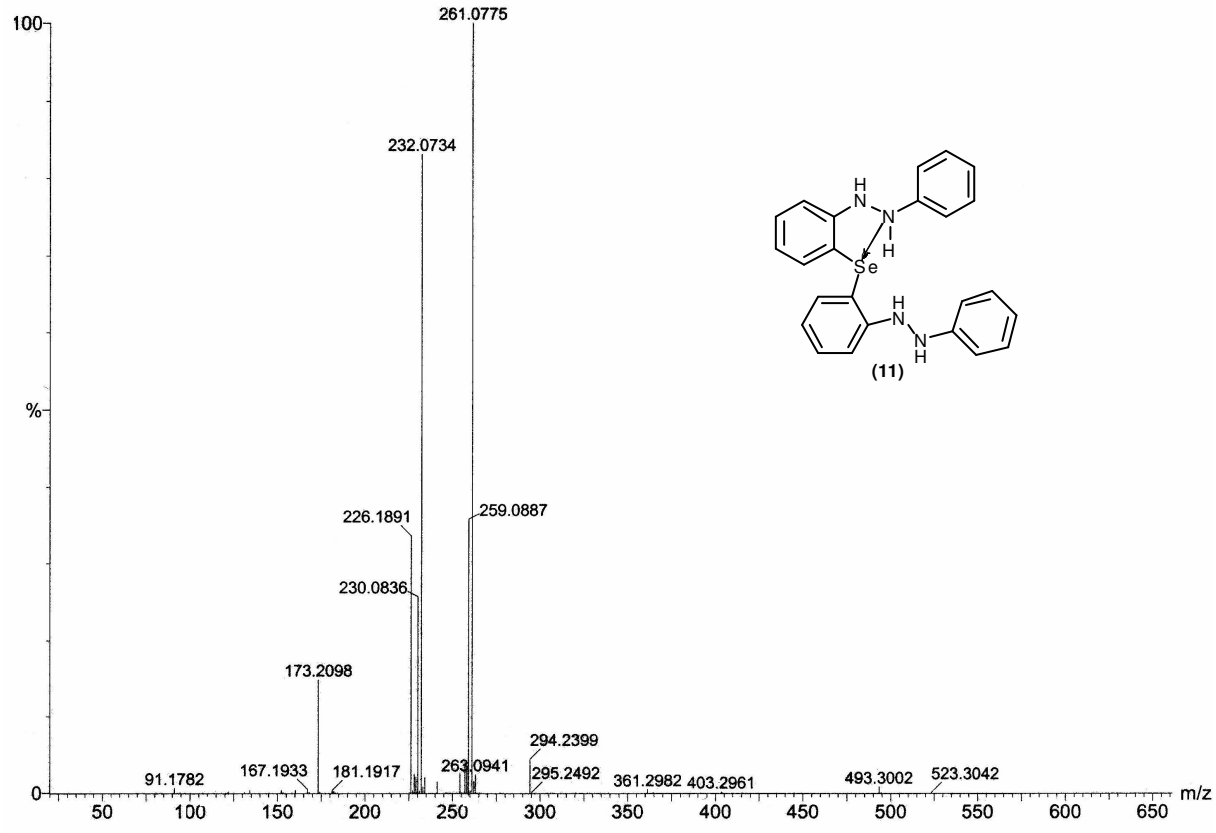


Figure S40: ES-MS of **11**

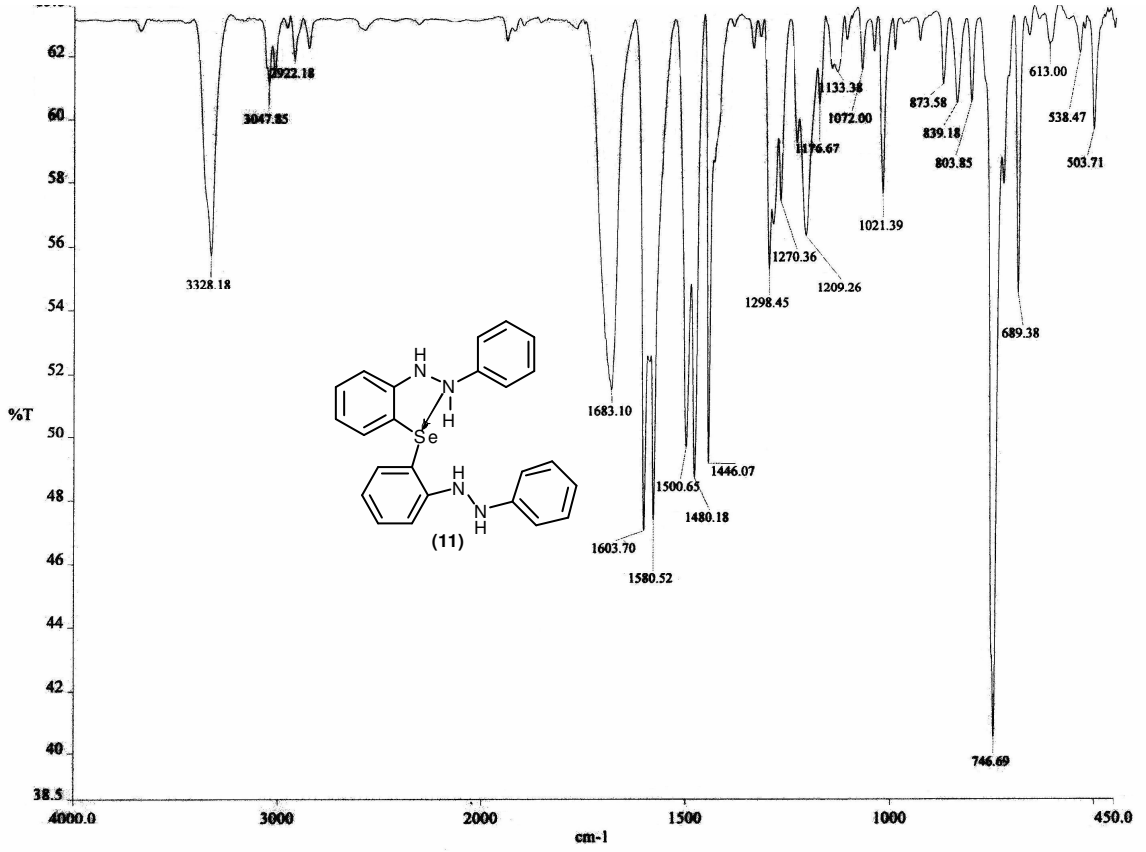
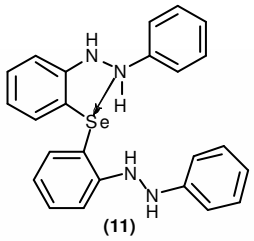


Figure S41: FT-IR spectrum of **11**



Eager 300 Report

Page: 1 Sample: KRAMINE (KRAMINE)

Method Name : sp021107
Method File : G:\eager300\Eager 300 EA1112\SP021107.mth
Chromatogram : KRAMINE
Operator ID : SP
Analysed : 11/02/2007 14:49
Sample ID : KRAMINE (# 30)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 11/2/2007 16:11
Instrument N. : Instrument #1
Sample weight : 1.717

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.7779	43	258744	FU	11.504820	.127947E+0
Carbon	65.1790	64	2976805	FU	1.000000	.265670E+0
Hydrogen	4.9396	169	503643	RS	5.910546	.583662E+0
Totals	81.8965		3739193			

Figure S42: Elemental analysis (C, H, N) of **11**

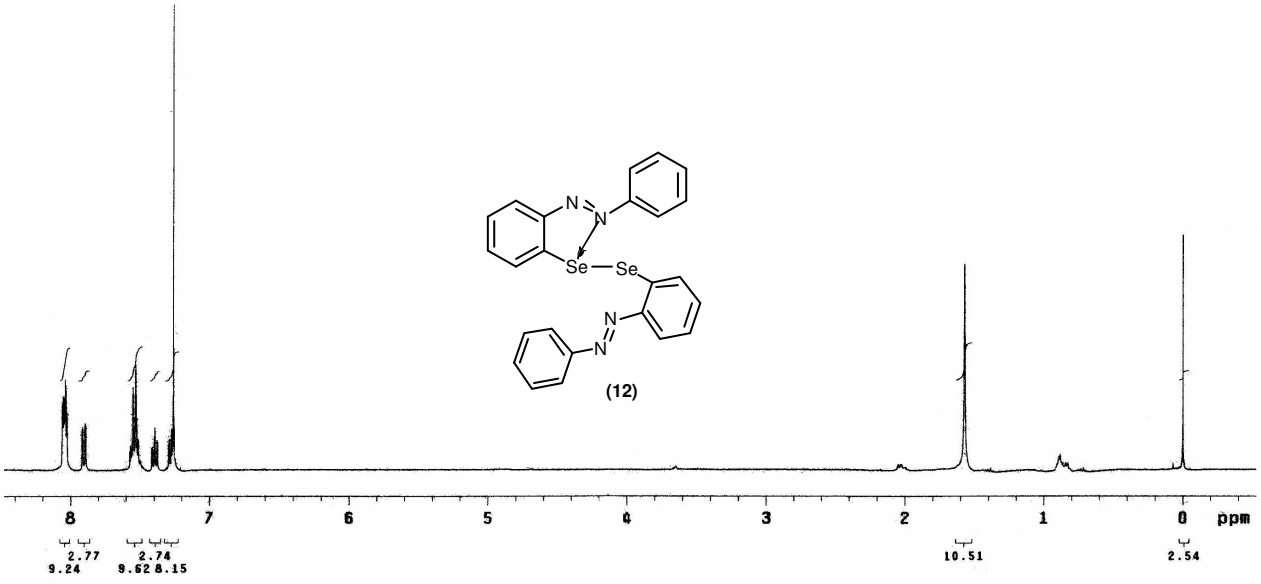


Figure S43: ^{1}H NMR spectrum of **12**

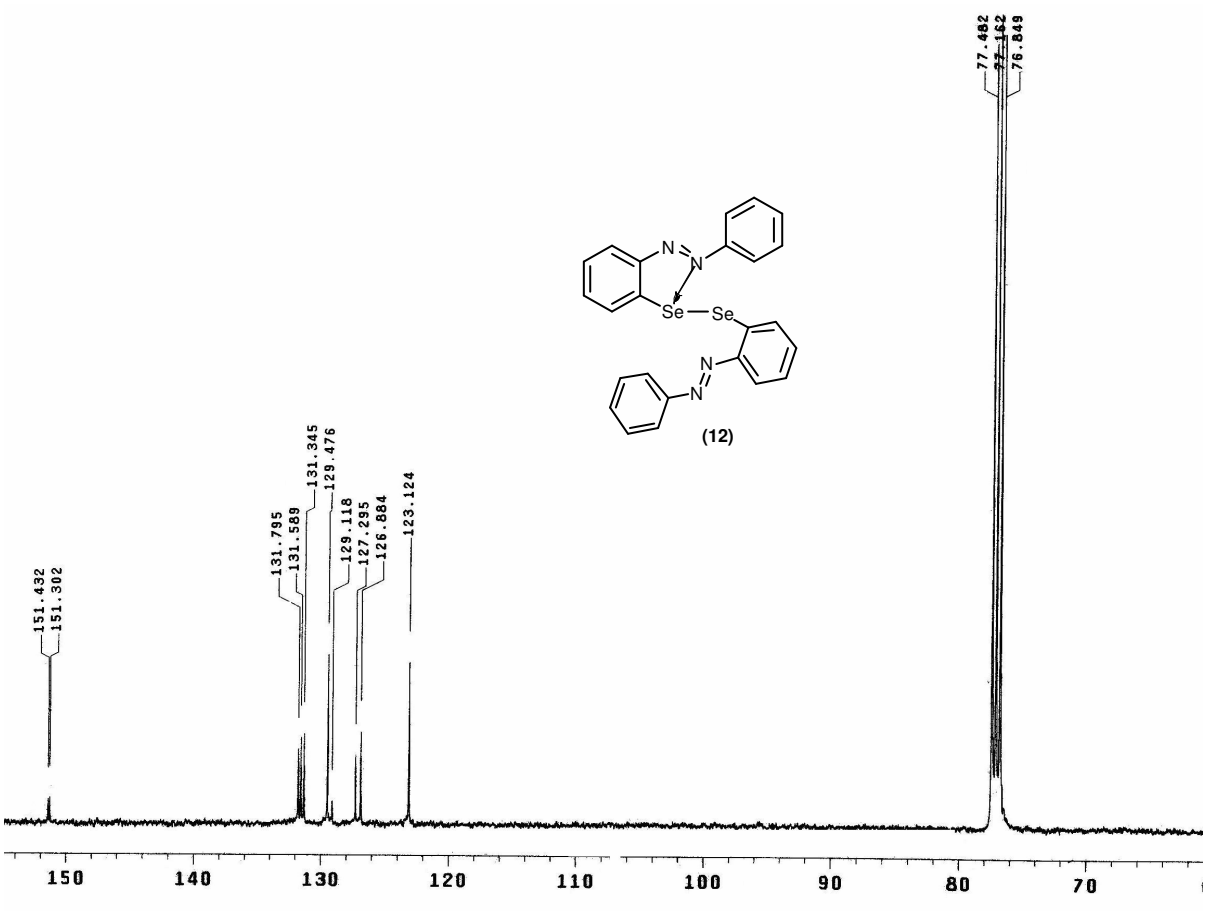


Figure S44: ^{13}C NMR spectrum of **12**

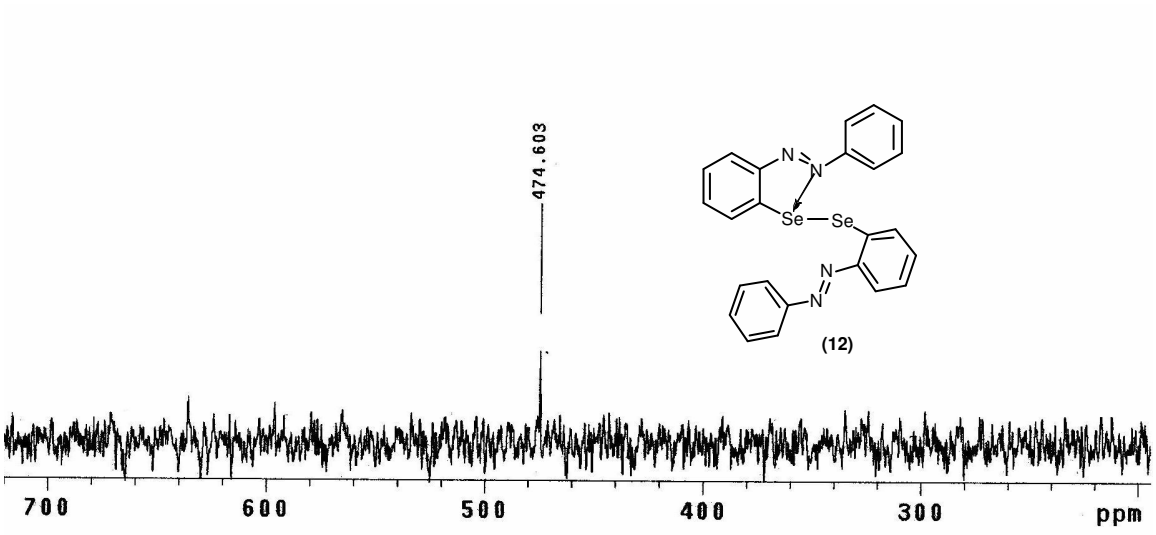


Figure S45: ^{77}Se spectrum of **12**

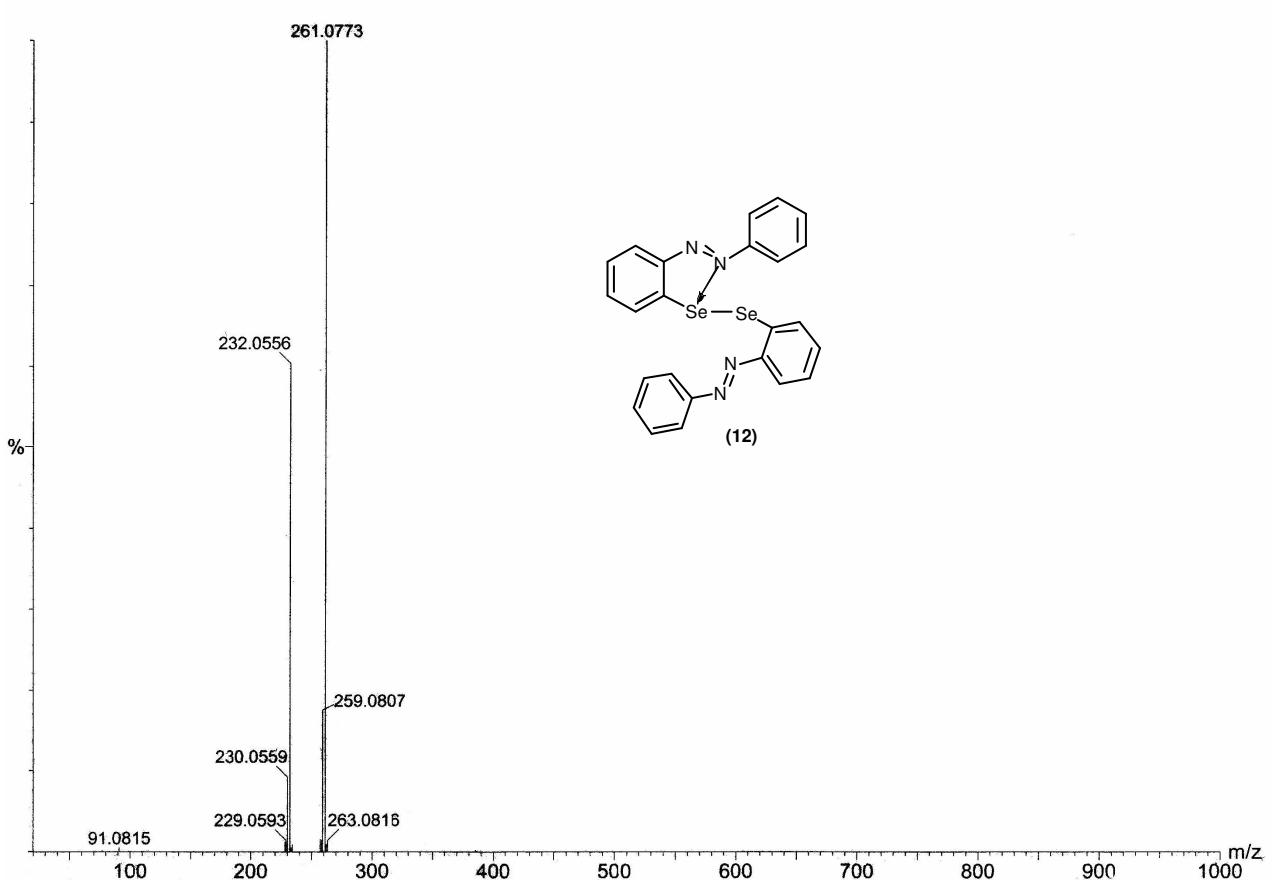


Figure S46: ES-MS of **12**

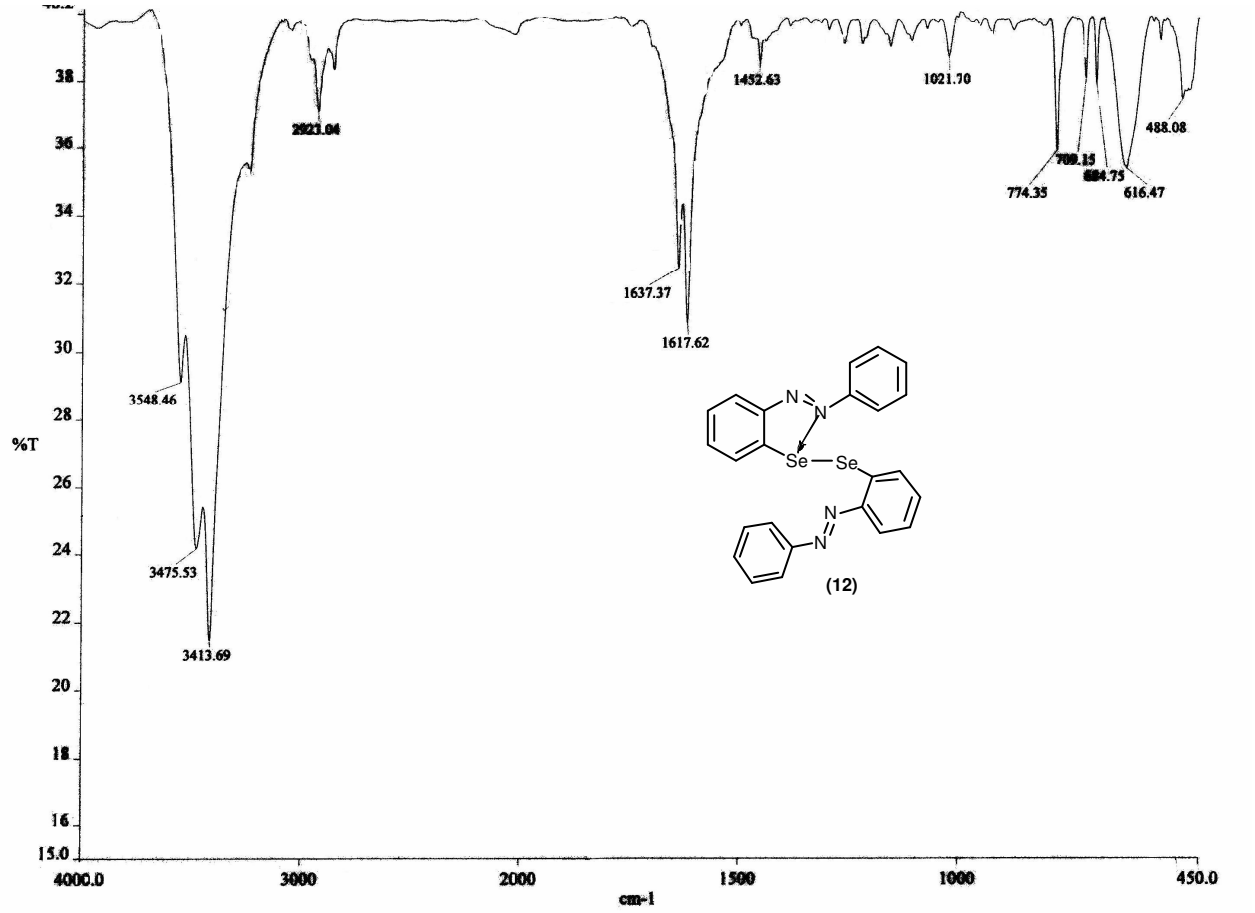
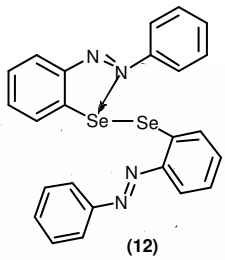


Figure S47: FT-IR of **12**



(12)

Eager 300 Report

Page: 1 Sample: HBSKRAZOSECL (HBSKRAZOSECL)

Method Name	: sp261007		
Method File	: G:\eager300\Eager 300 EA1112\SP261007.mth		
Chromatogram	: HBSKRAZOSECL		
Operator ID	: SP	Company Name	: C.E. Instruments
Analysed	: 10/26/2007 14:18	Printed	: 10/26/2007 15:52
Sample ID	: HBSKRAZOSECL (# 24)	Instrument N.	: Instrument #1
Analysis Type	: UnkNown (Area)	Sample weight	: 1.448

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	9.7754	43	183525	FU	11.577480	.129655E+07
Carbon	54.7260	65	2124752	FU	1.000000	.268131E+07
Hydrogen	3.6939	169	312958	RS	6.789255	.576150E+07
Totals	68.1953		2621234			

Figure S48: Elemental analysis (C, H, N) of **12**

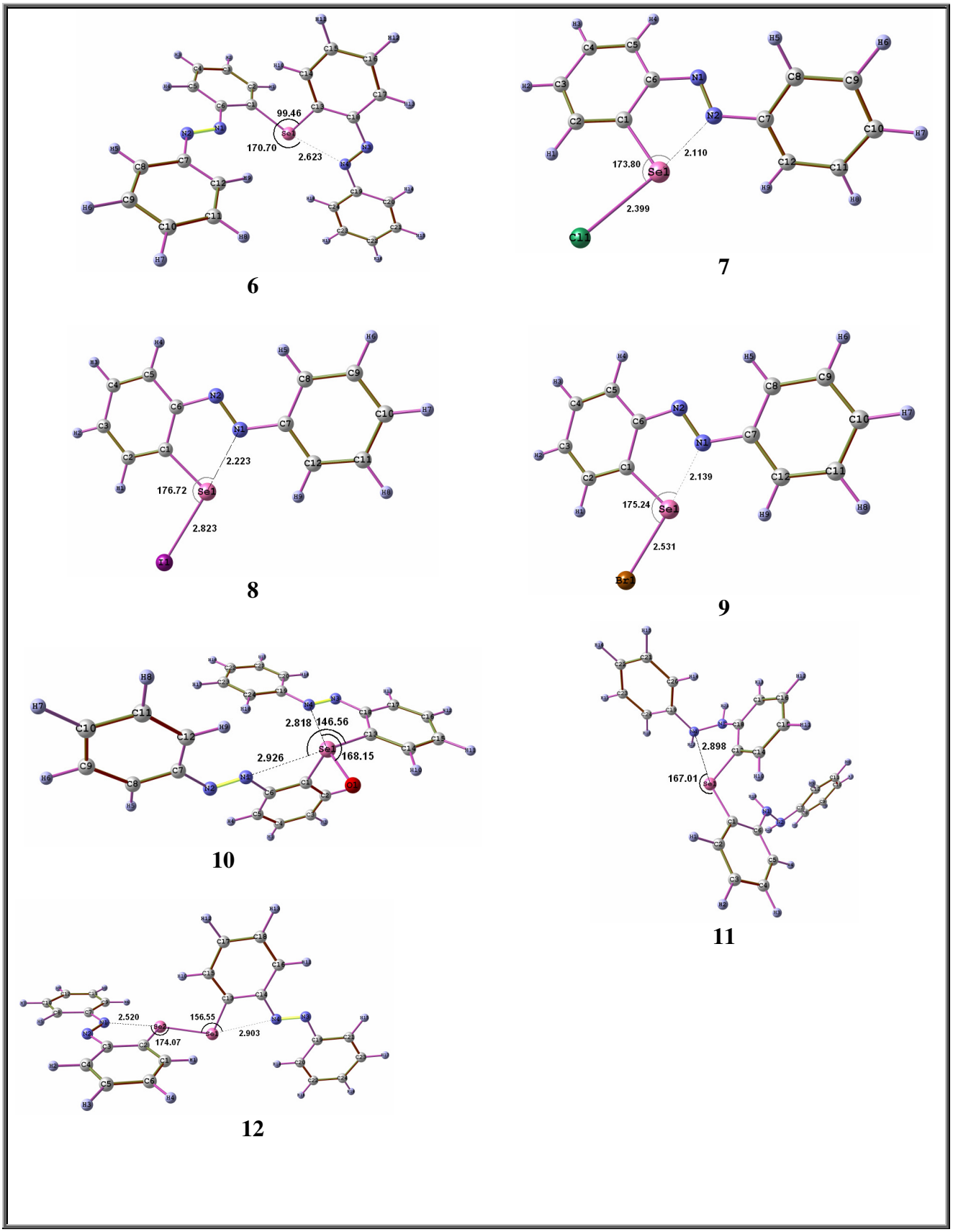


Figure S49 Optimized geometry of compound **6-12** at B3LYP/6-31+G(d)

Optimizide coordinates and Energy of **6**:

34	-0.512931000	-0.924034000	-0.639370000
7	2.461161000	0.027525000	-0.485231000
7	3.566636000	0.613374000	-0.610708000
7	-2.922716000	-0.181369000	1.388894000
7	-2.785647000	0.108025000	0.167670000
6	1.140994000	-1.910185000	-1.012365000
6	1.019456000	-3.214460000	-1.500588000
1	0.037714000	-3.678079000	-1.542057000
6	2.144782000	-3.928292000	-1.915825000
1	2.040006000	-4.947730000	-2.278306000
6	3.407729000	-3.324482000	-1.869375000
1	4.287387000	-3.876169000	-2.191497000
6	3.542329000	-2.018913000	-1.407450000
1	4.512815000	-1.535595000	-1.366846000
6	2.409062000	-1.296165000	-0.992226000
6	3.598955000	1.933941000	-0.091702000
6	4.852532000	2.562161000	-0.115427000
1	5.700547000	2.013757000	-0.515767000
6	4.993923000	3.863386000	0.369391000
1	5.967629000	4.345710000	0.353535000
6	3.880529000	4.543066000	0.870503000
1	3.985635000	5.558111000	1.245038000
6	2.624454000	3.918715000	0.884775000
1	1.759072000	4.453194000	1.268440000
6	2.475865000	2.619523000	0.409063000
1	1.510230000	2.125518000	0.409757000
6	-0.663368000	-1.261017000	1.240095000
6	0.349407000	-1.910346000	1.959718000
1	1.255228000	-2.218311000	1.450352000
6	0.214746000	-2.173985000	3.322477000
1	1.021923000	-2.680077000	3.846066000
6	-0.942145000	-1.790727000	4.013368000
1	-1.046144000	-1.995645000	5.074981000
6	-1.952881000	-1.139721000	3.320168000
1	-2.864894000	-0.819214000	3.815517000
6	-1.834076000	-0.866245000	1.943143000
6	-3.853914000	0.810353000	-0.439873000
6	-5.032761000	1.193458000	0.224245000
1	-5.155690000	0.941621000	1.271934000
6	-6.018437000	1.888086000	-0.471740000
1	-6.930530000	2.185221000	0.039944000
6	-5.841238000	2.207098000	-1.825318000
1	-6.614343000	2.751361000	-2.361469000
6	-4.668411000	1.824944000	-2.483065000
1	-4.527678000	2.070456000	-3.532439000

6	-3.676923000	1.124791000	-1.796006000
1	-2.758932000	0.820239000	-2.288910000

Energy (**E**): -3543.79253191

Optimized coordinates and energy of **7**:

34	-0.525467000	-1.132958000	0.013332000
17	-2.207378000	-2.814824000	0.324481000
7	0.296998000	1.657892000	-0.139511000
7	0.810661000	0.491663000	-0.157825000
6	-1.716919000	0.330655000	-0.043934000
6	-3.117225000	0.277210000	-0.041063000
1	-3.619344000	-0.681984000	0.006019000
6	-3.845635000	1.461216000	-0.083321000
1	-4.931271000	1.410572000	-0.074455000
6	-3.209899000	2.719390000	-0.135626000
1	-3.805030000	3.627409000	-0.163782000
6	-1.829134000	2.790562000	-0.151203000
1	-1.299258000	3.737422000	-0.193466000
6	-1.077002000	1.597609000	-0.119190000
6	2.222425000	0.364631000	-0.081582000
6	2.967567000	1.193283000	0.768047000
1	2.457722000	1.948317000	1.357525000
6	4.352095000	1.045734000	0.823586000
1	4.935494000	1.691481000	1.474216000
6	4.984575000	0.047483000	0.073673000
1	6.062536000	-0.075562000	0.133024000
6	4.231824000	-0.783819000	-0.761513000
1	4.722379000	-1.549977000	-1.355269000
6	2.847142000	-0.631514000	-0.842425000
1	2.255577000	-1.256639000	-1.504620000

Energy (**E**): -3431.82850732

Optimized coordinates and energy of **8**:

34	0.253775000	-0.434026000	-0.029913000
53	2.961673000	-1.468668000	0.060801000
7	-1.769488000	0.473673000	-0.064011000
7	-1.771735000	1.739692000	-0.038277000
6	0.634185000	1.431797000	-0.041696000
6	1.904390000	2.014133000	-0.048268000
1	2.783455000	1.379676000	-0.047885000
6	2.029028000	3.400467000	-0.050049000
1	3.023932000	3.836692000	-0.053453000
6	0.900994000	4.240102000	-0.046417000
1	1.023977000	5.318585000	-0.048073000

6	-0.364152000	3.682415000	-0.040790000
1	-1.263763000	4.289238000	-0.039049000
6	-0.506089000	2.280266000	-0.039100000
6	-3.000590000	-0.222563000	-0.028617000
6	-4.202884000	0.429875000	0.290902000
1	-4.185944000	1.490482000	0.512730000
6	-5.386926000	-0.298626000	0.321998000
1	-6.317316000	0.203127000	0.572089000
6	-5.383774000	-1.669167000	0.039717000
1	-6.312330000	-2.231869000	0.068240000
6	-4.185431000	-2.313101000	-0.276698000
1	-4.177560000	-3.375743000	-0.499614000
6	-2.992280000	-1.595363000	-0.311513000
1	-2.061756000	-2.088889000	-0.571166000

Energy (**E**): -9893.16722435

Optimized coordinates and Energy of **9**:

34	0.458135000	-0.735799000	-0.000153000
35	2.591284000	-2.098352000	0.000055000
7	-1.243010000	0.561416000	0.000121000
7	-0.988074000	1.809699000	0.000070000
6	1.276227000	0.968736000	0.000025000
6	2.650589000	1.235070000	-0.000060000
1	3.356941000	0.413340000	-0.000052000
6	3.092413000	2.554092000	-0.000076000
1	4.161663000	2.748978000	-0.000231000
6	2.188276000	3.635344000	0.000025000
1	2.560078000	4.655719000	0.000007000
6	0.827184000	3.389272000	0.000183000
1	0.097263000	4.193232000	0.000348000
6	0.363027000	2.057135000	0.000111000
6	-2.599279000	0.144268000	0.000085000
6	-3.652399000	1.073000000	-0.000147000
1	-3.425710000	2.132865000	-0.000339000
6	-4.969679000	0.622275000	-0.000135000
1	-5.781839000	1.344184000	-0.000219000
6	-5.248504000	-0.749575000	-0.000016000
1	-6.278068000	-1.096901000	-0.000017000
6	-4.197967000	-1.671745000	0.000129000
1	-4.405326000	-2.738068000	0.000155000
6	-2.875506000	-1.231085000	0.000208000
1	-2.065226000	-1.952382000	0.000321000

Energy (**E**): -5543.36693440

Optimized coordinates and energy of **10**:

34	-0.871615000	-1.209904000	-0.819999000
8	-0.953849000	-2.863379000	-1.097818000
7	1.692394000	-0.970560000	0.570240000
7	2.886669000	-0.983530000	0.963356000
7	-2.551839000	1.716642000	-0.380695000
7	-1.310182000	1.523046000	-0.289364000
6	-0.619267000	-1.150303000	1.137275000
6	-1.659752000	-1.302074000	2.051827000
1	-2.687283000	-1.364886000	1.708303000
6	-1.376951000	-1.359616000	3.418149000
1	-2.189876000	-1.466038000	4.131844000
6	-0.051838000	-1.284789000	3.870209000
1	0.161129000	-1.330626000	4.935065000
6	0.991789000	-1.159472000	2.960571000
1	2.024948000	-1.109594000	3.286646000
6	0.710097000	-1.095870000	1.583982000
6	3.861766000	-0.855432000	-0.056988000
6	5.192600000	-0.843382000	0.387067000
1	5.383487000	-0.931611000	1.452820000
6	6.237146000	-0.725279000	-0.530550000
1	7.266685000	-0.718072000	-0.182824000
6	5.954948000	-0.621265000	-1.895392000
1	6.765795000	-0.534479000	-2.614066000
6	4.624777000	-0.634523000	-2.340487000
1	4.408739000	-0.559068000	-3.403123000
6	3.576966000	-0.745863000	-1.431658000
1	2.545681000	-0.768223000	-1.766208000
6	-2.797870000	-0.742459000	-0.829704000
6	-3.654232000	-1.791984000	-1.139933000
1	-3.220036000	-2.777853000	-1.295734000
6	-5.034646000	-1.571905000	-1.238102000
1	-5.696920000	-2.402261000	-1.469377000
6	-5.556152000	-0.289717000	-1.047256000
1	-6.624975000	-0.113274000	-1.132089000
6	-4.696699000	0.769577000	-0.758193000
1	-5.071855000	1.779698000	-0.620829000
6	-3.313416000	0.557997000	-0.641088000
6	-0.525029000	2.681069000	-0.059454000
6	-1.065356000	3.958571000	0.173226000
1	-2.142327000	4.084183000	0.186506000
6	-0.212187000	5.036258000	0.385588000
1	-0.626205000	6.024387000	0.569710000
6	1.178562000	4.853855000	0.361671000
1	1.839231000	5.701160000	0.526597000
6	1.714199000	3.584618000	0.127654000
1	2.790851000	3.439567000	0.107592000

6	0.864120000	2.496928000	-0.078650000
1	1.257909000	1.501965000	-0.261675000

Energy (**E**): -3618.96747620

Optimized coordinates and geometry of **11**:

34	0.711127000	1.325114000	-0.496227000
7	-2.301710000	0.477999000	-0.659242000
7	-3.487054000	0.079658000	-1.272344000
7	1.890272000	-1.609329000	-0.307603000
7	2.686953000	-0.720977000	-1.053445000
6	-0.872591000	2.348457000	-0.059176000
6	-0.730288000	3.674253000	0.362765000
1	0.270037000	4.072397000	0.511021000
6	-1.846494000	4.483869000	0.582528000
1	-1.722640000	5.512099000	0.910461000
6	-3.121831000	3.946034000	0.381996000
1	-4.003745000	4.558711000	0.553462000
6	-3.285370000	2.629458000	-0.045354000
1	-4.275018000	2.215920000	-0.207693000
6	-2.164468000	1.812049000	-0.275062000
6	-4.026933000	-1.166508000	-0.899475000
6	-4.902612000	-1.818485000	-1.784439000
1	-5.111097000	-1.379660000	-2.758902000
6	-5.518809000	-3.012650000	-1.412231000
1	-6.197488000	-3.500380000	-2.107869000
6	-5.259938000	-3.587135000	-0.163457000
1	-5.736772000	-4.520256000	0.123425000
6	-4.377377000	-2.942561000	0.708213000
1	-4.161338000	-3.377143000	1.681381000
6	-3.755001000	-1.744971000	0.349900000
1	-3.066119000	-1.251315000	1.026774000
6	0.756068000	0.128855000	1.034079000
6	0.218385000	0.516812000	2.264943000
1	-0.223939000	1.503745000	2.360516000
6	0.216514000	-0.347539000	3.360941000
1	-0.219144000	-0.026597000	4.303079000
6	0.772528000	-1.622501000	3.230865000
1	0.779177000	-2.310934000	4.071838000
6	1.346524000	-2.006594000	2.020522000
1	1.799943000	-2.991867000	1.923499000
6	1.353899000	-1.139855000	0.915259000
6	4.089351000	-0.737508000	-0.884610000
6	4.684048000	-1.033152000	0.352251000
1	4.065956000	-1.260526000	1.214510000
6	6.075480000	-1.012344000	0.478742000

1	6.521237000	-1.244006000	1.442906000
6	6.890150000	-0.687128000	-0.608188000
1	7.971028000	-0.670069000	-0.500693000
6	6.295427000	-0.382882000	-1.837476000
1	6.913401000	-0.130847000	-2.695676000
6	4.909463000	-0.417746000	-1.980580000
1	4.456073000	-0.192953000	-2.944327000
1	-1.448802000	0.062434000	-1.034383000
1	-3.509621000	0.259490000	-2.274560000
1	2.326144000	-2.525988000	-0.210770000
1	2.398438000	-0.728938000	-2.025584000

Energy (**E**): -3546.21347415

Optimized coordinates and geometry of **12**:

6	0.800169000	2.417720000	-0.925752000
6	1.813470000	1.482504000	-0.696681000
6	3.161250000	1.924019000	-0.772401000
6	3.451421000	3.268079000	-1.072787000
6	2.431123000	4.182241000	-1.294257000
6	1.101549000	3.746913000	-1.219806000
1	-0.235834000	2.098973000	-0.885309000
1	4.496487000	3.559292000	-1.125147000
1	2.661315000	5.218143000	-1.525678000
1	0.287633000	4.446213000	-1.393635000
7	3.965217000	-0.105354000	-0.331340000
7	4.268054000	1.094290000	-0.578893000
6	5.031795000	-1.011998000	-0.128531000
6	6.387695000	-0.653057000	-0.222628000
6	4.675779000	-2.330494000	0.193551000
6	7.371882000	-1.612632000	-0.004853000
1	6.648151000	0.370438000	-0.469049000
6	5.668353000	-3.285875000	0.412212000
1	3.624778000	-2.591437000	0.268101000
6	7.016715000	-2.931028000	0.312125000
1	8.420240000	-1.335896000	-0.081016000
1	5.389246000	-4.306286000	0.660290000
1	7.789352000	-3.676465000	0.481219000
6	-1.422376000	0.212708000	1.346803000
6	-2.798986000	0.224375000	1.652568000
6	-0.503132000	0.590761000	2.328346000
6	-3.236145000	0.615516000	2.929819000
6	-0.945161000	0.983458000	3.591347000
1	0.559277000	0.577953000	2.109653000
6	-2.313309000	0.994102000	3.897474000
1	-4.301030000	0.612767000	3.136831000

1	-0.216536000	1.277644000	4.342773000
1	-2.651324000	1.295680000	4.885200000
7	-4.885613000	-0.142375000	0.845905000
7	-3.652303000	-0.174585000	0.600832000
6	-5.725297000	-0.545135000	-0.222528000
6	-5.269664000	-0.937671000	-1.495191000
6	-7.099540000	-0.534514000	0.057201000
6	-6.192098000	-1.318615000	-2.464764000
1	-4.204796000	-0.941863000	-1.700312000
6	-8.018627000	-0.916104000	-0.921319000
1	-7.423318000	-0.225500000	1.047023000
6	-7.566570000	-1.308223000	-2.184058000
1	-5.843817000	-1.624262000	-3.448217000
1	-9.082416000	-0.906814000	-0.699450000
1	-8.278533000	-1.606248000	-2.949456000
34	-0.942563000	-0.405613000	-0.415656000
34	1.459382000	-0.373460000	-0.319188000

Energy (**E**): -5943.24056877