Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Sigma-hole interactions in the molecular and crystal structures of N-boryl benzo-2,1,3-selenadiazoles

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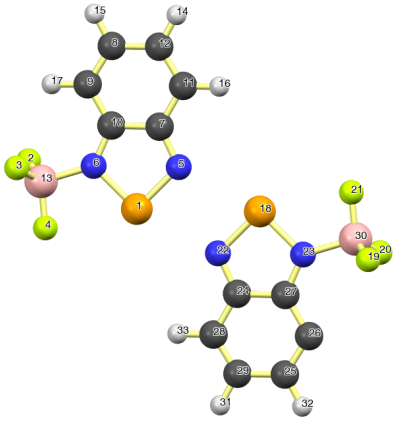
Supplementary Information

Table S1. Cartesian coordinates (Å) of all optimized structures.

($\mathbf{2}^{Se}$-BF_3)$_2$



1.Se	1.121209	1.124011	-0.957267
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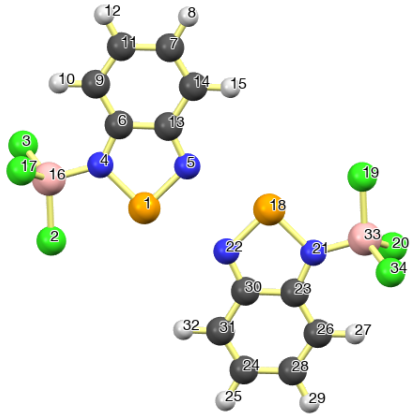
4.F	2.428698	2.719824	-2.890773
5.N	1.103119	0.504592	0.728177
6.N	2.654090	2.047177	-0.615514
7.C	2.157695	0.984031	1.395074
8.C	4.436042	2.112696	2.570473
9.C	4.196724	2.423034	1.255623
10.C	3.045145	1.859313	0.645389
11.C	2.450706	0.692808	2.758690
12.C	3.570078	1.254158	3.317290
13.B	3.326650	2.942060	-1.839742
14.H	3.812594	1.044938	4.359456
15.H	5.312041	2.530954	3.066933
16.H	1.788102	0.038312	3.323412
17.H	4.847473	3.075220	0.675883
18.Se	-1.121209	-1.124011	0.957267
19.F	-4.580827	-2.411038	2.060488
20.F	-3.348998	-4.247979	1.395295
21.F	-2.428698	-2.719824	2.890773
22.N	-1.103119	-0.504592	-0.728177
23.N	-2.654090	-2.047177	0.615514
24.C	-2.157695	-0.984031	-1.395074
25.C	-4.436042	-2.112696	-2.570473
26.C	-4.196724	-2.423034	-1.255623
27.C	-3.045145	-1.859313	-0.645389
28.C	-2.450706	-0.692808	-2.758690
29.C	-3.570078	-1.254158	-3.317290
30.B	-3.326650	-2.942060	1.839742
31.H	-3.812594	-1.044938	-4.359456
32.H	-5.312041	-2.530954	-3.066933
33.H	-1.788102	-0.038312	-3.323412
34.H	-4.847473	-3.075220	-0.675883

$(\mathbf{2}^{Se}\text{-}BCl_3)_2$



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10.H	-3.729180	4.425507	0.000000
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14.C	0.175767	3.743195	-0.000000
15.H	1.246563	3.542975	-0.000000
16.B	-4.463337	1.591474	0.000000
17.Cl	-5.141475	2.338789	1.536604
18.Se	1.817209	-0.295231	-0.000000
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31.C	-0.175767	-3.743195	0.000000
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33.B	4.463337	-1.591474	-0.000000
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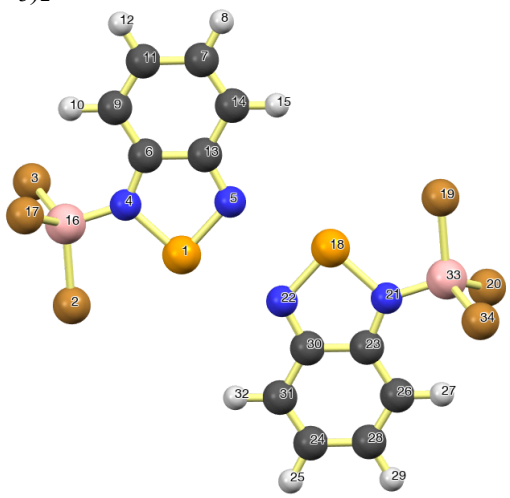

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9.C	-2.603781	4.252687	-0.000014
10.H	-3.673167	4.449306	-0.000029
11.C	-1.672375	5.263040	-0.000009
12.H	-2.014270	6.298321	-0.000027
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14.C	0.222194	3.724945	0.000005
15.H	1.290452	3.511581	0.000007
16.B	-4.417802	1.624827	0.000001
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21.N	2.874308	-1.798439	0.000001
22.N	0.350672	-1.355650	-0.000001
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26.C	2.603781	-4.252687	0.000014
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28.C	1.672375	-5.263040	0.000009
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31.C	-0.222194	-3.724945	-0.000005
32.H	-1.290452	-3.511581	-0.000007
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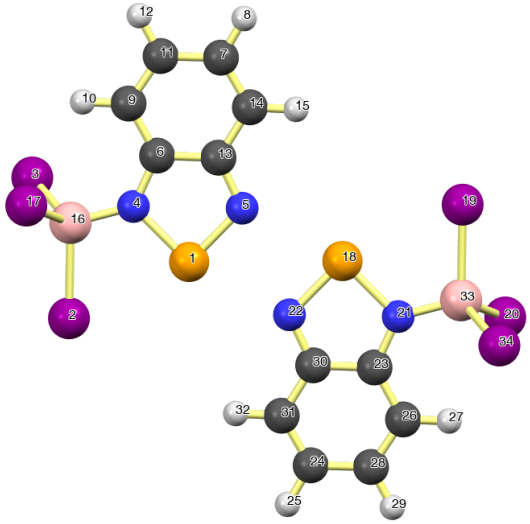
$(\mathbf{2}^{Se}\text{-}BI_3)_2$



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5.N	-0.340780	1.351652	0.000000
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15.H	1.307224	3.490520	0.000000
16.B	-4.404517	1.648530	-0.000000
17.I	-5.242700	2.544835	1.880800
18.Se	1.791485	-0.276490	0.000000
19.I	4.819290	0.608602	0.000000
20.I	5.242700	-2.544835	-1.880800
21.N	2.871939	-1.800434	0.000000
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29.H	1.977609	-6.300683	-0.000000
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31.C	-0.240689	-3.714110	-0.000000
32.H	-1.307224	-3.490520	-0.000000
33.B	4.404517	-1.648530	0.000000
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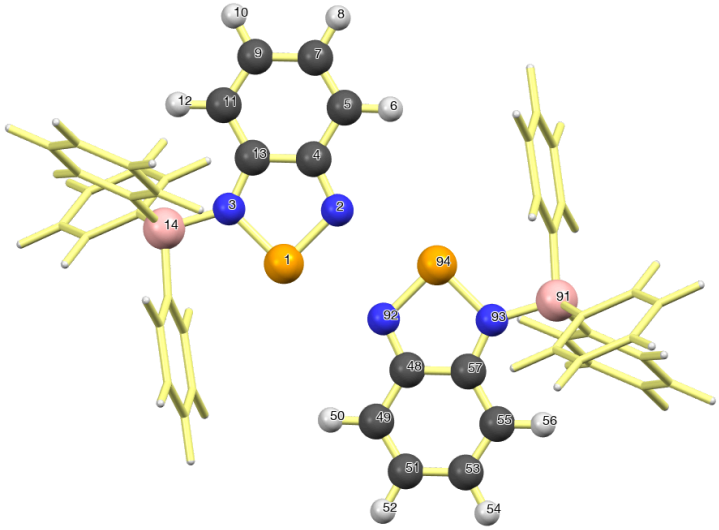
($\mathbf{2}^{Se}$-BPh_3)$_2$



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12.H	-4.330508	3.802578	0.179832
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23.H	-5.318093	2.751706	-4.154817
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27.C	-6.520589	2.236466	1.603915
28.H	-7.157446	2.170645	0.720605
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32.H	-6.583546	3.541417	4.757693
33.C	-4.925392	2.472226	3.869530
34.H	-4.287782	2.562111	4.751129
35.C	-4.455272	1.809460	2.735073
36.H	-3.443035	1.396088	2.759536
37.C	-4.547786	-0.763098	0.497381
38.C	-4.336631	-1.613800	-0.610775
39.H	-4.356441	-1.185845	-1.615986

40.C	-4.115273	-2.985379	-0.460716
41.H	-3.953917	-3.610490	-1.341047
42.C	-4.118768	-3.555716	0.813804
43.H	-3.957223	-4.627955	0.938415
44.C	-4.356718	-2.745357	1.926540
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46.C	-4.567314	-1.373838	1.765715
47.H	-4.756801	-0.760023	2.647903
48.C	1.114695	-2.499647	0.030285
49.C	0.378527	-3.718746	0.106647
50.H	-0.708509	-3.680339	0.181065
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55.C	3.246243	-3.784519	-0.093892
56.H	4.330508	-3.802578	-0.179832
57.C	2.565324	-2.537049	-0.057864
58.C	5.465417	-1.173526	1.111221
59.C	4.978707	-1.936248	2.183919
60.H	3.979874	-2.374750	2.138768
61.C	5.734067	-2.154473	3.341144
62.H	5.318093	-2.751706	4.154817
63.C	7.010645	-1.607406	3.458391
64.H	7.603628	-1.775596	4.358584
65.C	7.516120	-0.831167	2.412474
66.H	8.509475	-0.385543	2.492752
67.C	6.750491	-0.615573	1.267056
68.H	7.154858	0.015559	0.472210
69.C	5.236886	-1.666430	-1.571326
70.C	6.520589	-2.236466	-1.603915
71.H	7.157446	-2.170645	-0.720605
72.C	7.004630	-2.899107	-2.735297
73.H	8.008077	-3.329014	-2.721965
74.C	6.209354	-3.020712	-3.874907
75.H	6.583546	-3.541417	-4.757693
76.C	4.925392	-2.472226	-3.869530
77.H	4.287782	-2.562111	-4.751129
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79.H	3.443035	-1.396088	-2.759536
80.C	4.547786	0.763098	-0.497381
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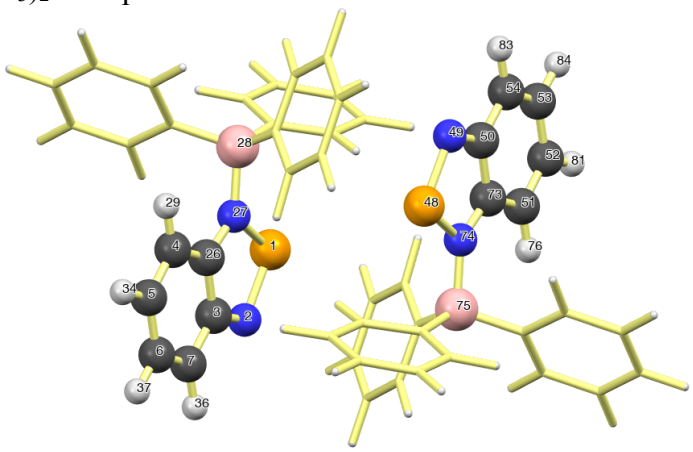
82.H	4.356441	1.185845	1.615986
83.C	4.115273	2.985379	0.460716
84.H	3.953917	3.610490	1.341047
85.C	4.118768	3.555716	-0.813804
86.H	3.957223	4.627955	-0.938415
87.C	4.356718	2.745357	-1.926540
88.H	4.384740	3.185664	-2.924994
89.C	4.567314	1.373838	-1.765715
90.H	4.756801	0.760023	-2.647903
91.B	4.663632	-0.860815	-0.271497
92.N	0.552736	-1.289122	0.025373
93.N	3.129073	-1.322163	-0.111728
94.Se	1.824122	-0.019323	-0.087920

($\mathbf{2}^{Se}$-BPh_3)$_2$ Se-Cpi



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5.C	-3.636766	-3.002967	-2.559115
6.C	-2.598285	-3.803114	-3.121225
7.C	-1.338210	-3.299482	-3.316070
8.C	-3.829312	1.570547	-2.276800
9.C	-5.118628	1.782239	-1.761433
10.C	-6.215257	2.018091	-2.594488
11.C	-6.053498	2.044970	-3.979481
12.C	-4.784836	1.829924	-4.521040
13.C	-3.698137	1.594089	-3.678723
14.C	-1.434386	2.546431	-1.365773
15.C	-1.446868	3.578225	-2.322328
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17.C	0.618105	4.512297	-1.465198
18.C	0.648397	3.516674	-0.488590
19.C	-0.367879	2.560440	-0.440850
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22.C	-3.698352	1.807107	2.386539
23.C	-3.673311	0.519805	2.927985
24.C	-3.264824	-0.543442	2.123436
25.C	-2.890124	-0.315204	0.792681
26.C	-2.126055	-1.154504	-2.334183
27.N	-1.733679	0.081551	-1.983899
28.B	-2.528664	1.322306	-1.323639
29.H	-4.219348	-1.088674	-1.749264
30.H	-2.558360	-1.174368	0.210009
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33.H	-4.001947	2.652677	3.005560
34.H	-4.629906	-3.436912	-2.441337
35.H	-3.232981	-1.558496	2.525280
36.H	-0.531761	-3.890891	-3.746947
37.H	-2.819469	-4.832162	-3.404898
38.H	-0.485128	5.333863	-3.128776
39.H	-0.348246	1.804637	0.346263
40.H	-2.267027	3.627986	-3.039897
41.H	1.404953	5.266739	-1.506798

42.H	1.456698	3.494063	0.244256
43.H	-5.273360	1.758564	-0.681547
44.H	-2.718238	1.419019	-4.131142
45.H	-6.908074	2.227608	-4.632390
46.H	-4.642559	1.842377	-5.603146
47.H	-7.202647	2.178622	-2.157792
48.Se	-0.041256	-0.289506	2.440326
49.N	-0.120774	1.365348	3.091781
50.C	1.071478	1.952600	2.936360
51.C	3.425307	1.703278	2.167542
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53.C	2.598285	3.803114	3.121225
54.C	1.338210	3.299482	3.316070
55.C	3.829312	-1.570547	2.276800
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57.C	6.215257	-2.018091	2.594488
58.C	6.053498	-2.044970	3.979481
59.C	4.784836	-1.829924	4.521040
60.C	3.698137	-1.594089	3.678723
61.C	1.434386	-2.546431	1.365773
62.C	1.446868	-3.578225	2.322328
63.C	0.440764	-4.545618	2.375193
64.C	-0.618105	-4.512297	1.465198
65.C	-0.648397	-3.516674	0.488590
66.C	0.367879	-2.560440	0.440850
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69.C	3.698352	-1.807107	-2.386539
70.C	3.673311	-0.519805	-2.927985
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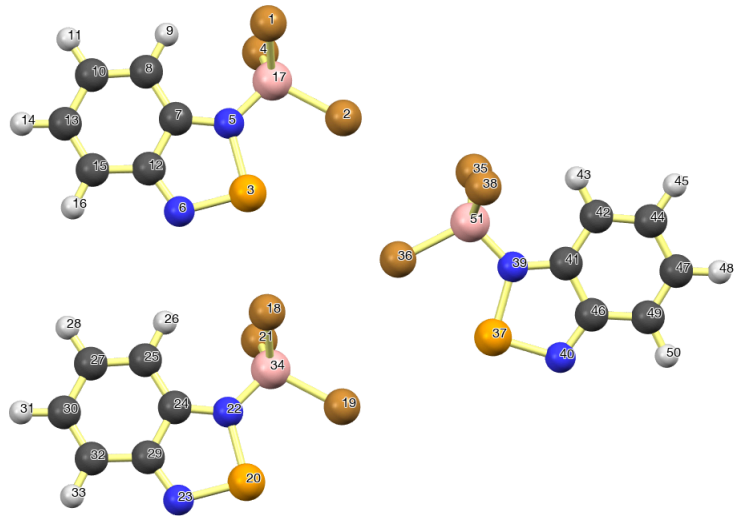
72.C	2.890124	0.315204	-0.792681
73.C	2.126055	1.154504	2.334183
74.N	1.733679	-0.081551	1.983899
75.B	2.528664	-1.322306	1.323639
76.H	4.219348	1.088674	1.749264
77.H	2.558360	1.174368	-0.210009
78.H	3.961172	-0.350070	-3.966039
79.H	3.339542	-3.035607	-0.662840
80.H	4.001947	-2.652677	-3.005560
81.H	4.629906	3.436912	2.441337
82.H	3.232981	1.558496	-2.525280
83.H	0.531761	3.890891	3.746947
84.H	2.819469	4.832162	3.404898
85.H	0.485128	-5.333863	3.128776
86.H	0.348246	-1.804637	-0.346263
87.H	2.267027	-3.627986	3.039897
88.H	-1.404953	-5.266739	1.506798
89.H	-1.456698	-3.494063	-0.244256
90.H	5.273360	-1.758564	0.681547
91.H	2.718238	-1.419019	4.131142
92.H	6.908074	-2.227608	4.632390
93.H	4.642559	-1.842377	5.603146
94.H	7.202647	-2.178622	2.157792

$(\mathbf{2}^{Se}\text{-}BBr_3)_3$



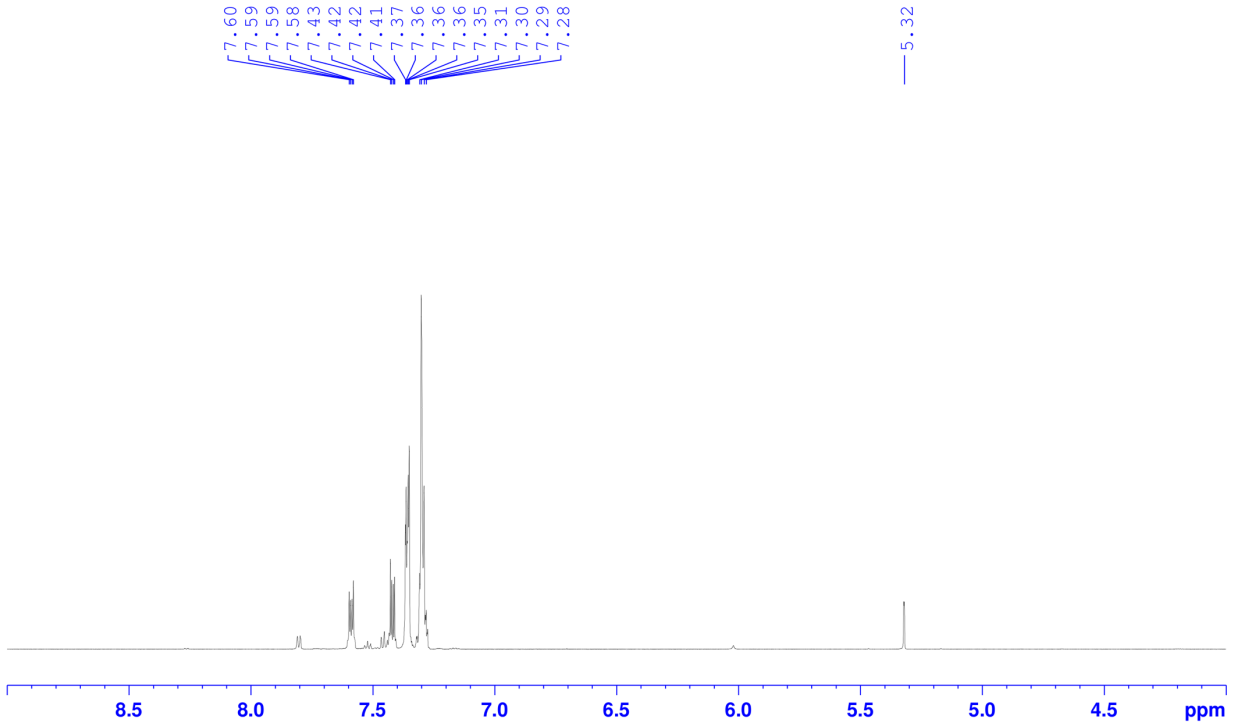
1.Br	2.646247	-0.512140	-6.065531
2.Br	0.653476	0.738669	-3.764282
3.Se	3.074370	0.545849	-1.823086
4.Br	2.622253	2.801275	-5.514687
5.N	3.543386	0.810381	-3.602064
6.N	4.799386	0.559205	-1.349452
7.C	4.882283	0.870507	-3.709647
8.C	5.626155	1.048913	-4.902736
9.H	5.106908	1.147738	-5.852651
10.C	6.996218	1.088298	-4.808783
11.H	7.584948	1.224115	-5.716248
12.C	5.562198	0.732832	-2.434699
13.C	7.676374	0.956354	-3.562685
14.H	8.765799	0.993271	-3.549847
15.C	6.985421	0.782175	-2.392253
16.H	7.485571	0.673607	-1.430743
17.B	2.440806	0.956354	-4.699094
18.Br	2.639940	-0.526385	1.241652
19.Br	0.647168	0.724424	3.542902
20.Se	3.068063	0.531605	5.484097
21.Br	2.614398	2.773347	1.768292
22.N	3.528973	0.781522	3.702015
23.N	4.782294	0.494966	5.954282
24.C	4.870830	0.806438	3.593687
25.C	5.616942	0.958710	2.398603
26.H	5.114897	1.054809	1.438097
27.C	6.987462	0.962008	2.498200
28.H	7.578430	1.075550	1.588986
29.C	5.551096	0.648400	4.870550
30.C	7.666564	0.819874	3.744258
31.H	8.756336	0.833446	3.756154
32.C	6.974991	0.662722	4.915893
33.H	7.470431	0.546885	5.878546
34.B	2.440806	0.956354	2.599654
35.Br	-2.638928	0.528671	-2.414456
36.Br	-0.650129	-0.731108	-0.114664
37.Se	-3.074370	-0.545849	1.823086
38.Br	-2.655474	-2.777759	-1.847486
39.N	-3.547257	-0.761921	0.048529

40.N	-4.783775	-0.472825	2.312167
41.C	-4.890006	-0.765424	-0.049303
42.C	-5.645900	-0.911873	-1.238214
43.H	-5.137249	-1.038062	-2.190514
44.C	-7.015936	-0.885291	-1.136677
45.H	-7.614039	-0.995100	-2.041524
46.C	-5.560892	-0.598934	1.230087
47.C	-7.685058	-0.718237	0.111446
48.H	-8.774878	-0.704044	0.127948
49.C	-6.984347	-0.577202	1.280061
50.H	-7.473032	-0.448728	2.244655
51.B	-2.451718	-0.934445	-1.055948

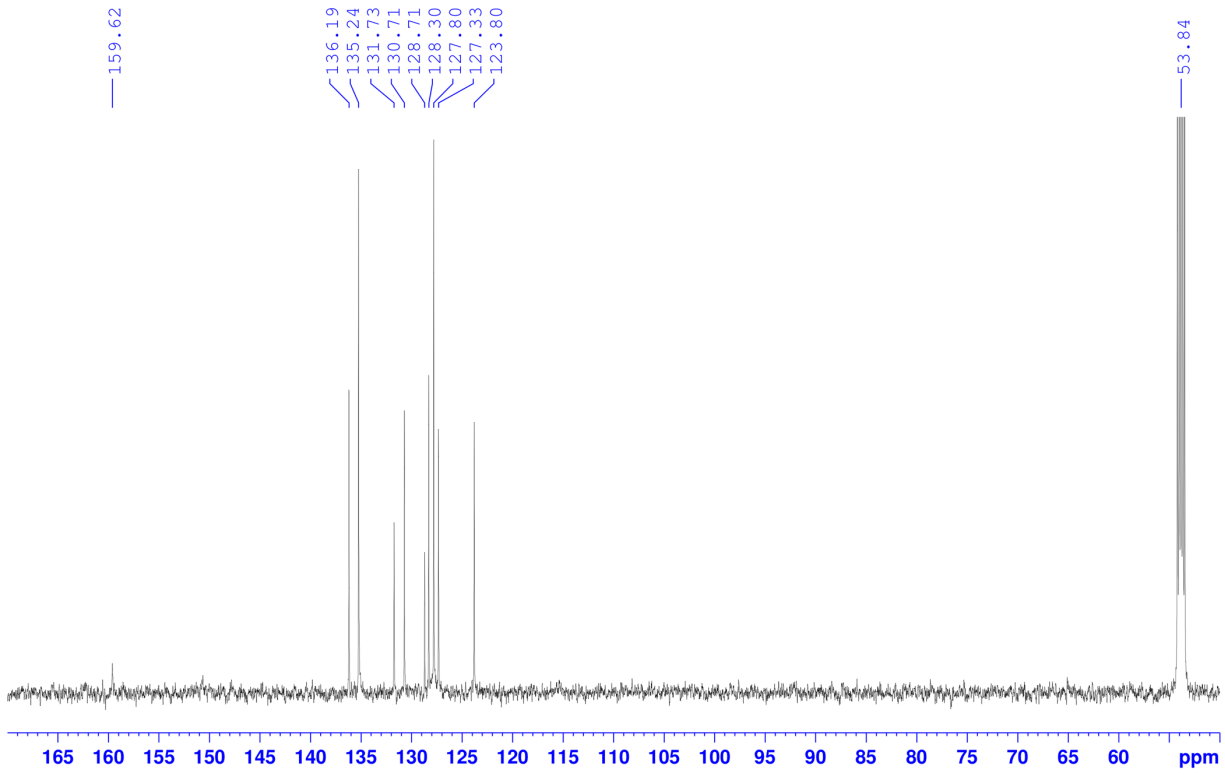
NMR Spectra

2^{Se}-BPh_3

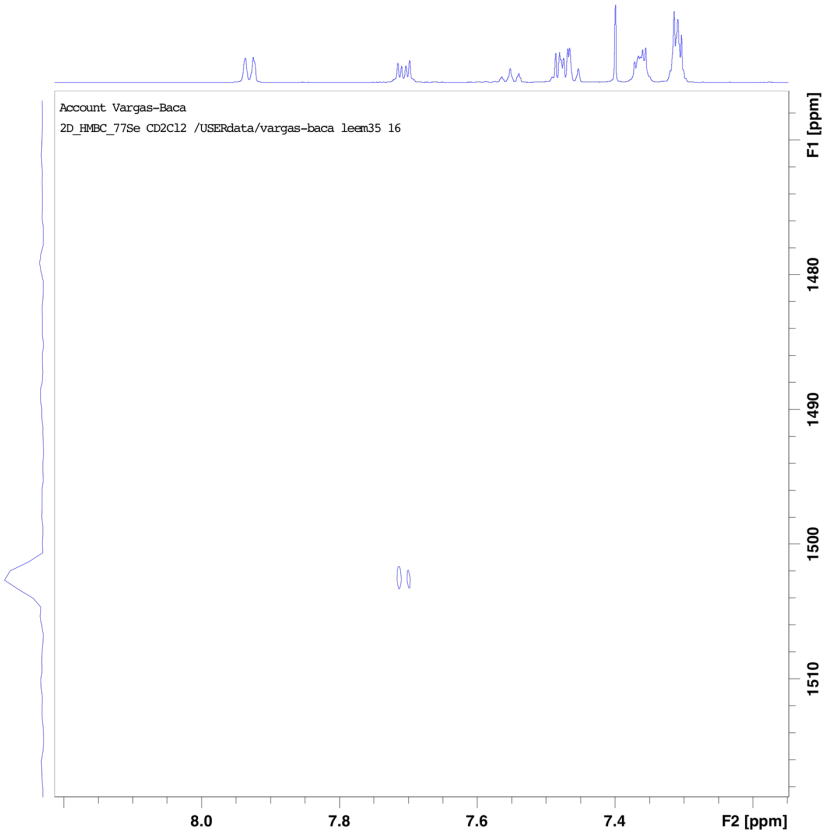
^{1}H NMR



^{13}C NMR

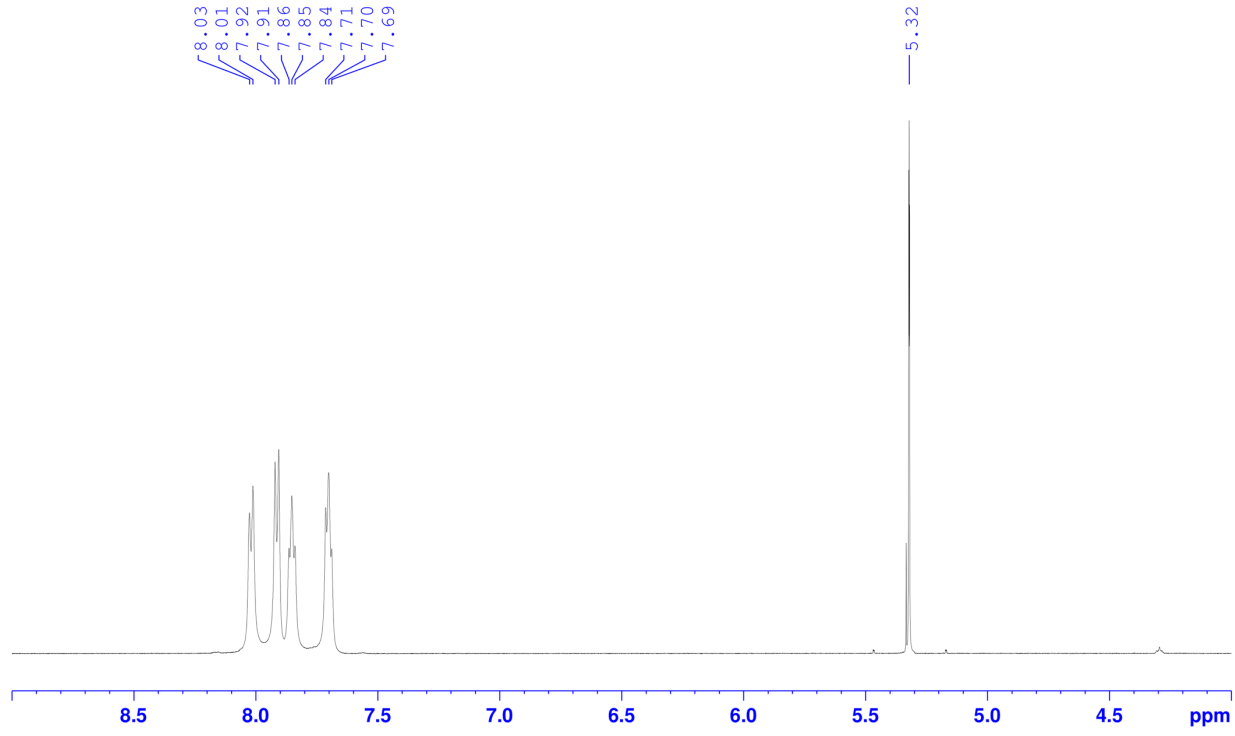


^{77}Se-^{1}H HMBC ^{1}H NMR

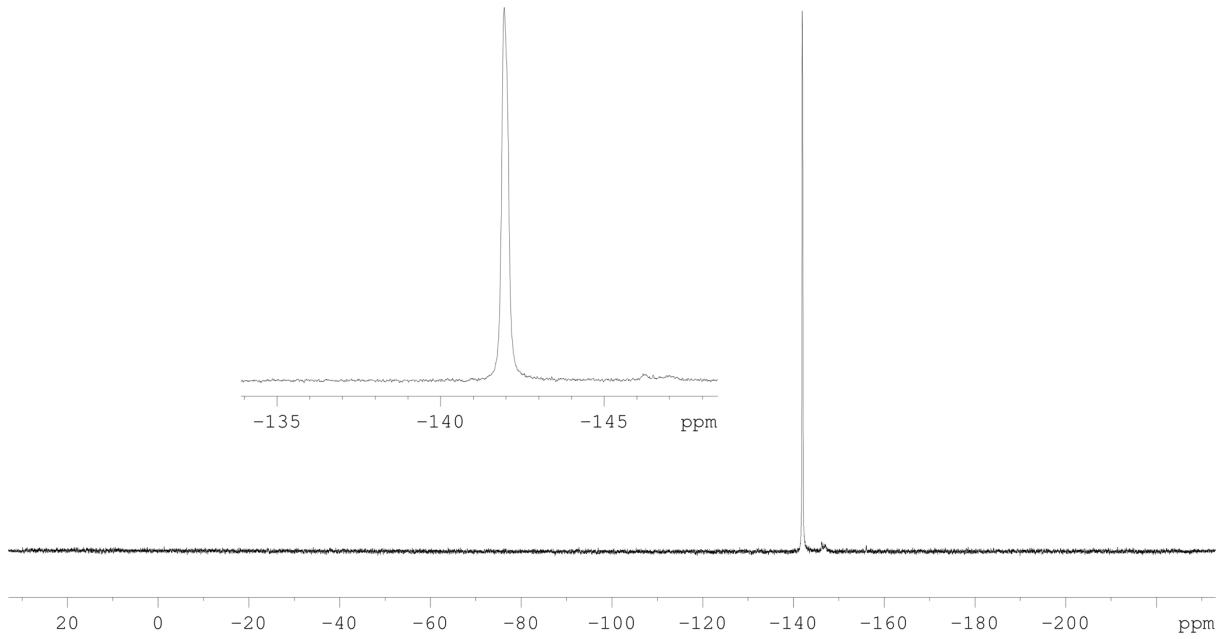


2^{Se}-BF_3

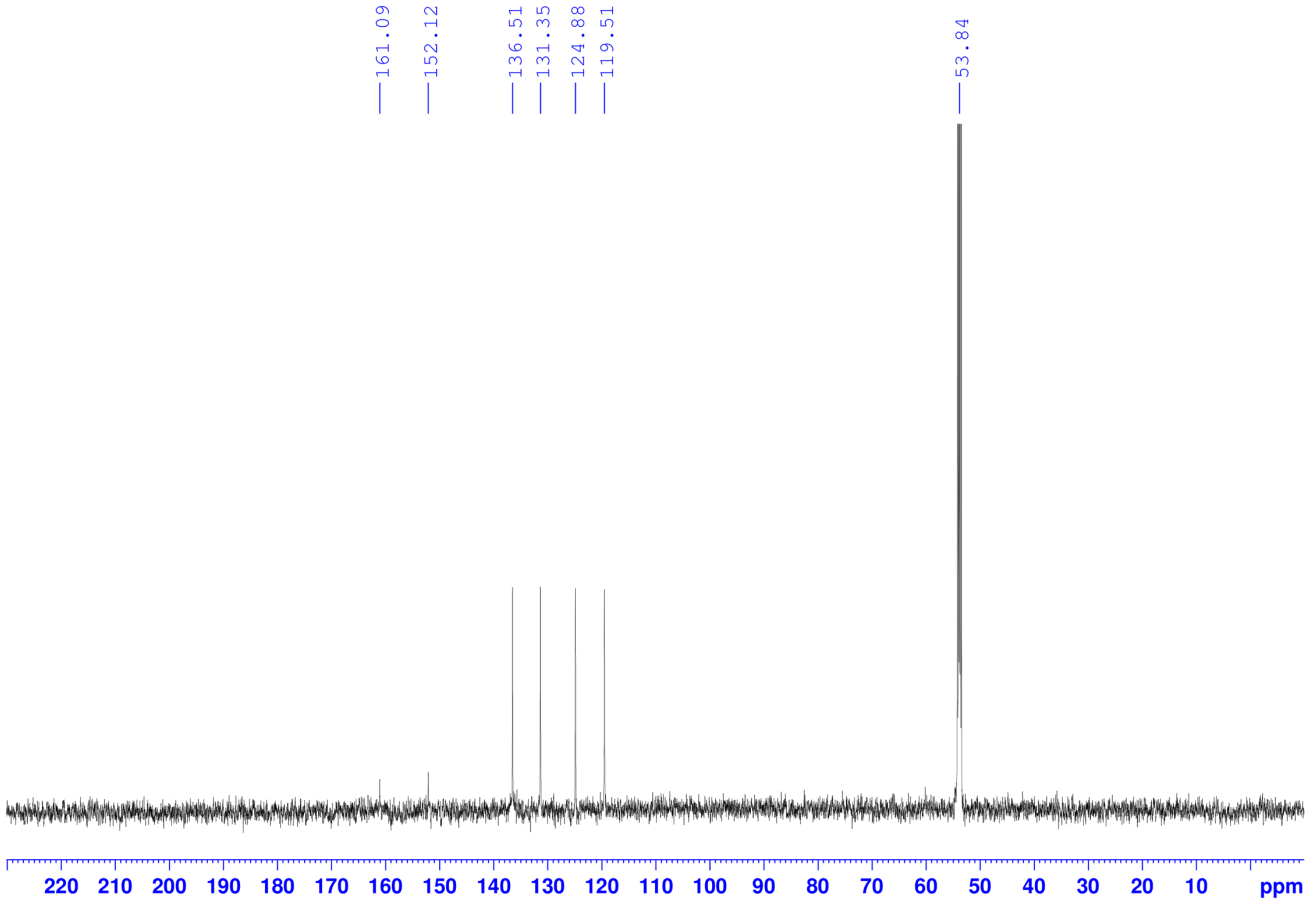
^{1}H NMR



^{19}F NMR

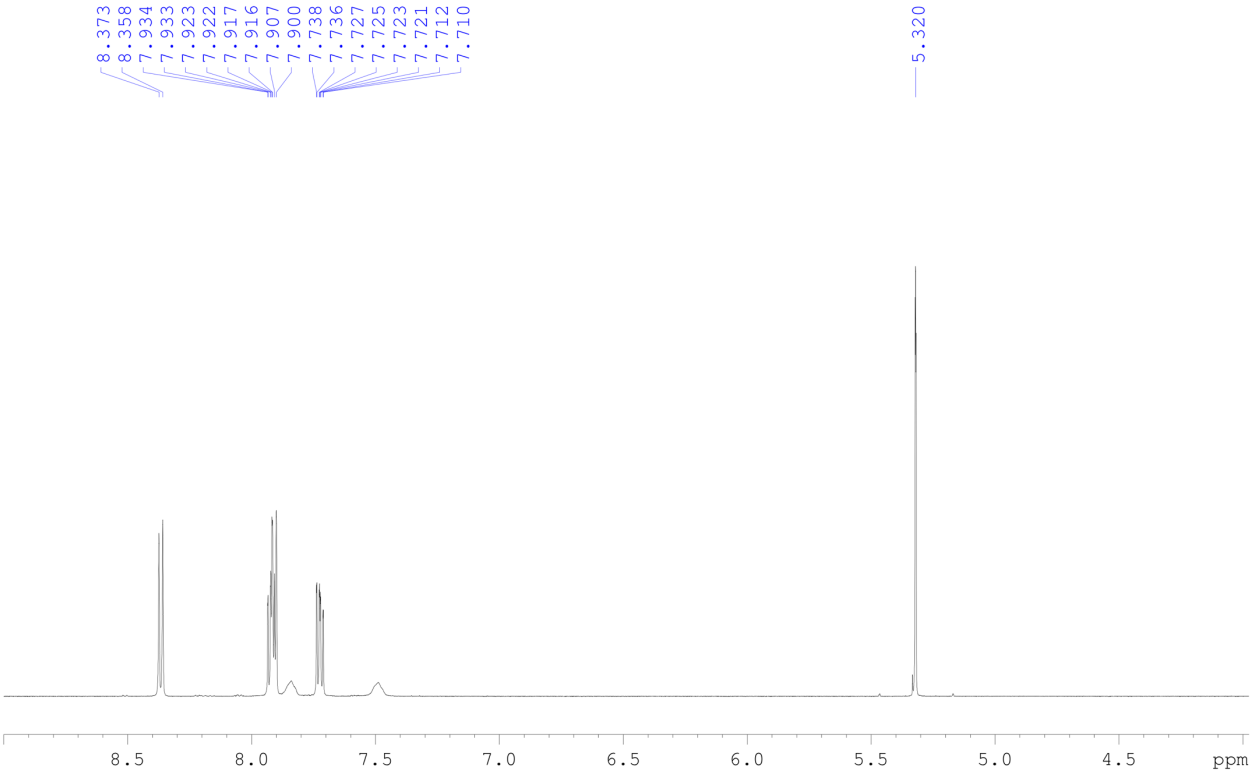


^{13}C NMR

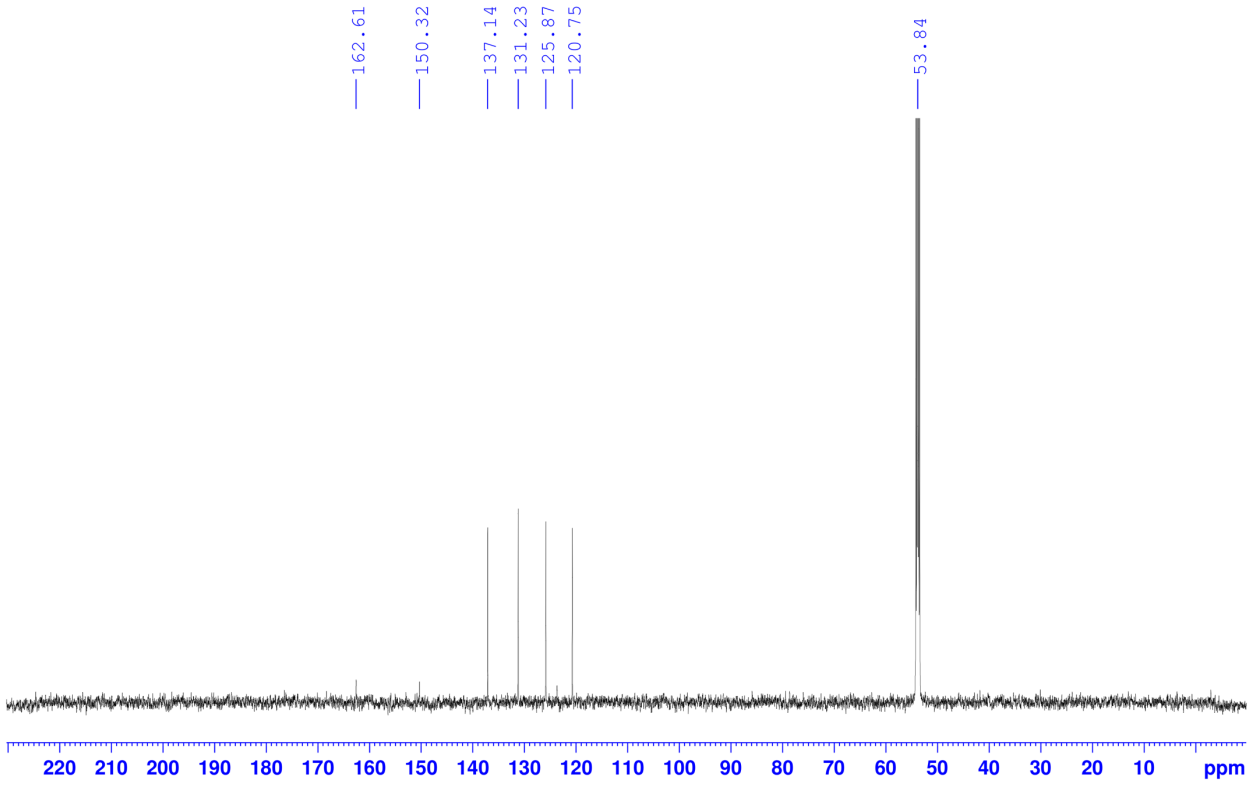


2^{Se}-BCl_3

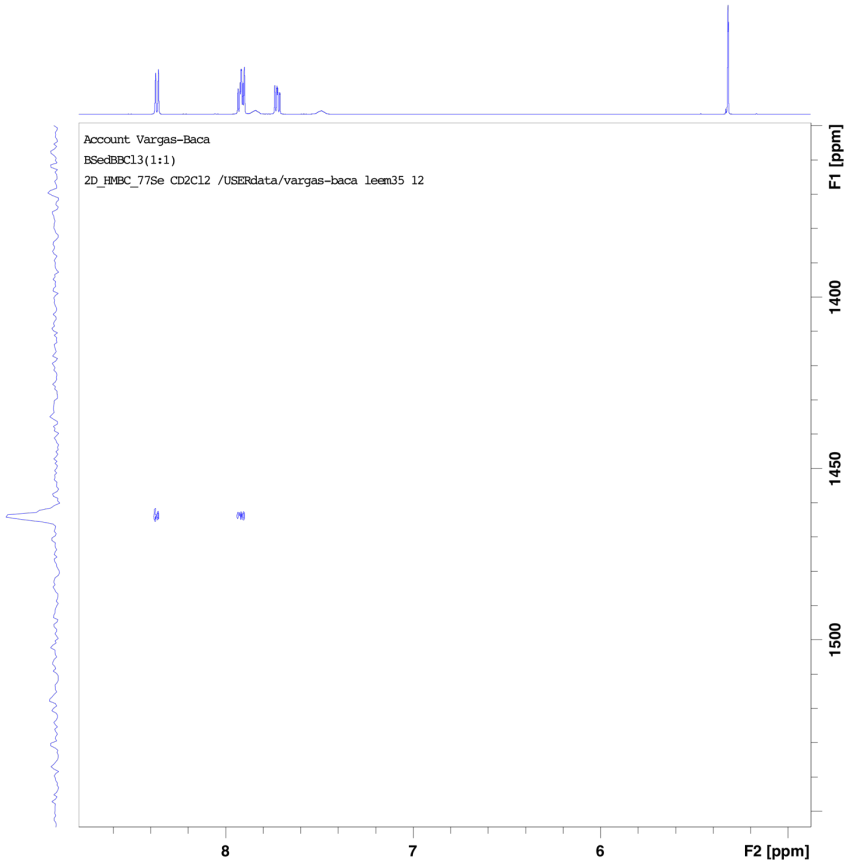
^{1}H NMR



^{13}C NMR

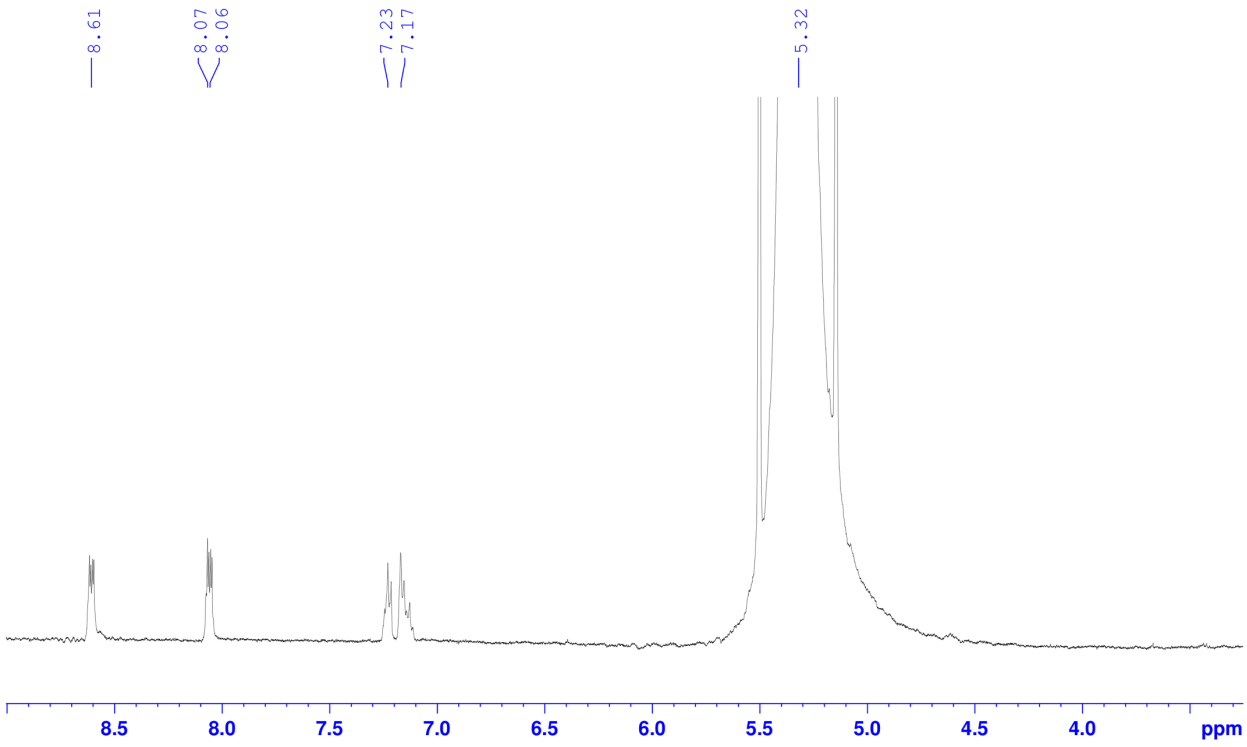


^{77}Se-^{1}H HMBC ^{1}H NMR



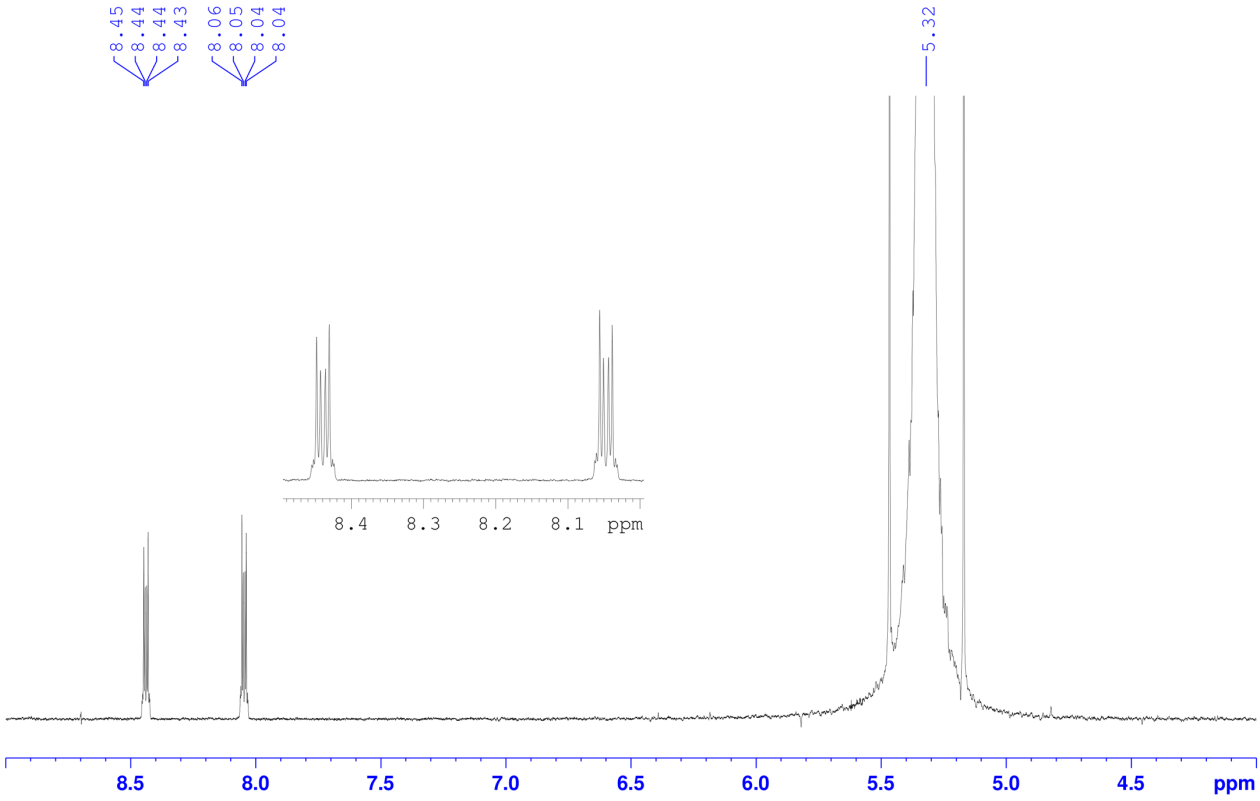
2^{Se}-BBr_3

^{1}H NMR



($\mathbf{2}^{Se}$-BCl_3)$_2$

^{1}H NMR



^{13}C NMR