Nucleophilic Substitution of Bromonorbornenes and Derivatives by Electron Transfer Reactions

*Karina F. Crespo Andrada, Lucas E. Peisino, Arif Daştan,[†] Murat Güney, [†] Adriana B. Pierini**

INFIQC, Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina.

[†]Department of Chemistry, Atatürk University, 25240 Erzurum, Turkey

adriana@fcq.unc.edu.ar

Supporting Info

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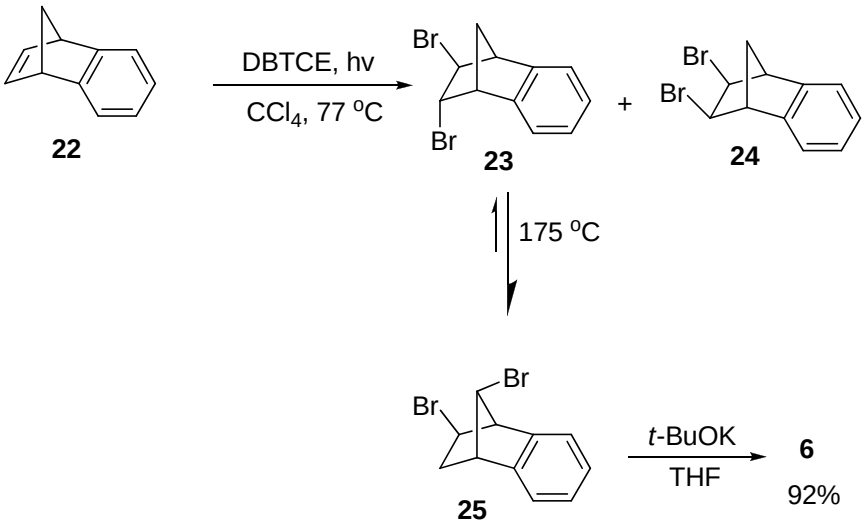
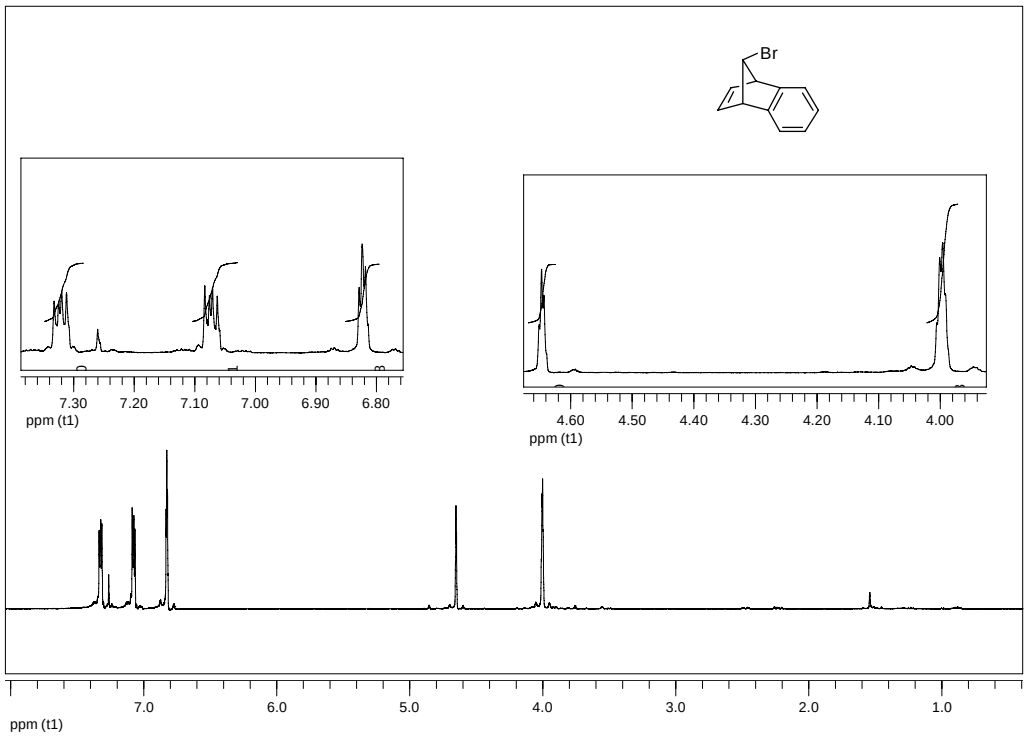
PART 1. SYNTHESIS OF COMPOUND syn-7-Bromobenzonorbornadiene (6)



To obtain 2-*exo*-7-*syn*-Dibromobenzonorborn-5-ene (**25**) we proceed as descript in litetarure.[24a,b] Next synthesized **6** as indicate in experimental section of this paper.

PART 2. CHARACTERIZATION DATA – NMR SPECTRUMS

^{1}H-RMN of **6**



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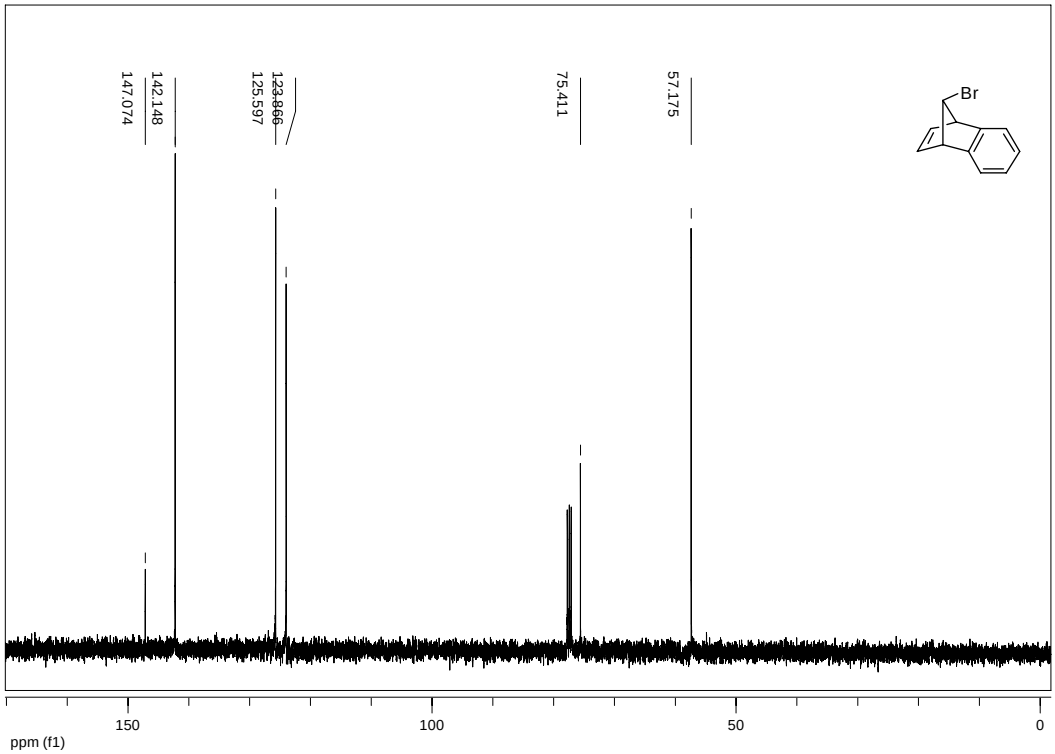

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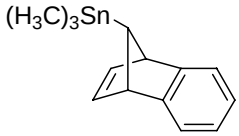

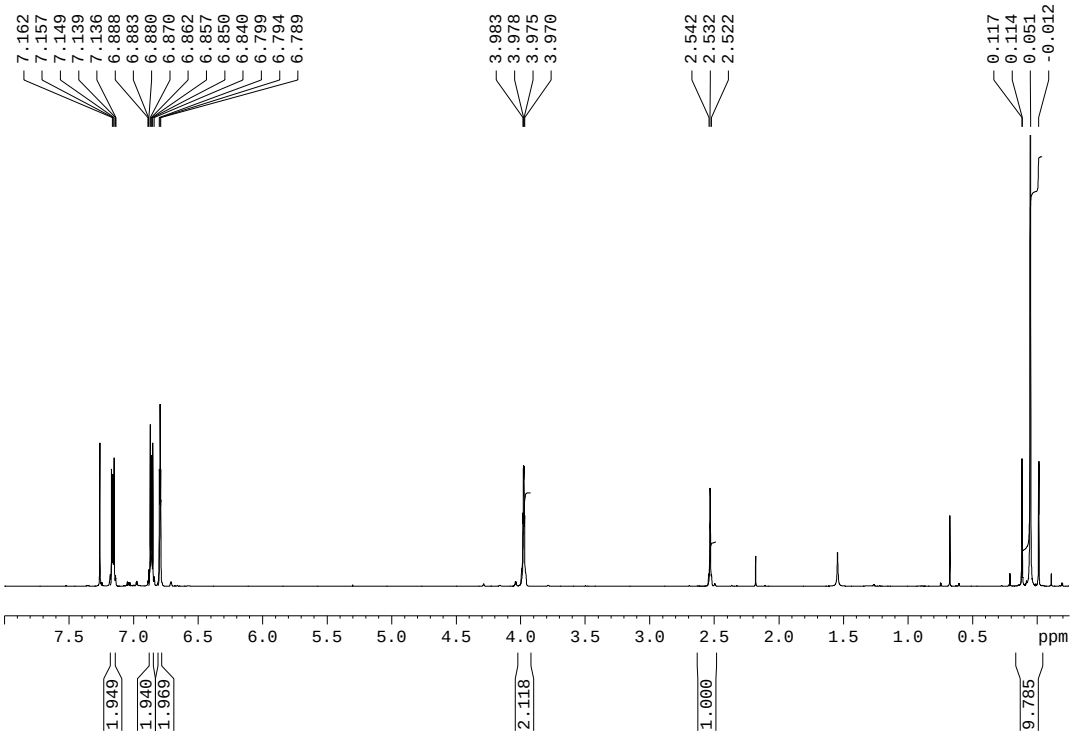

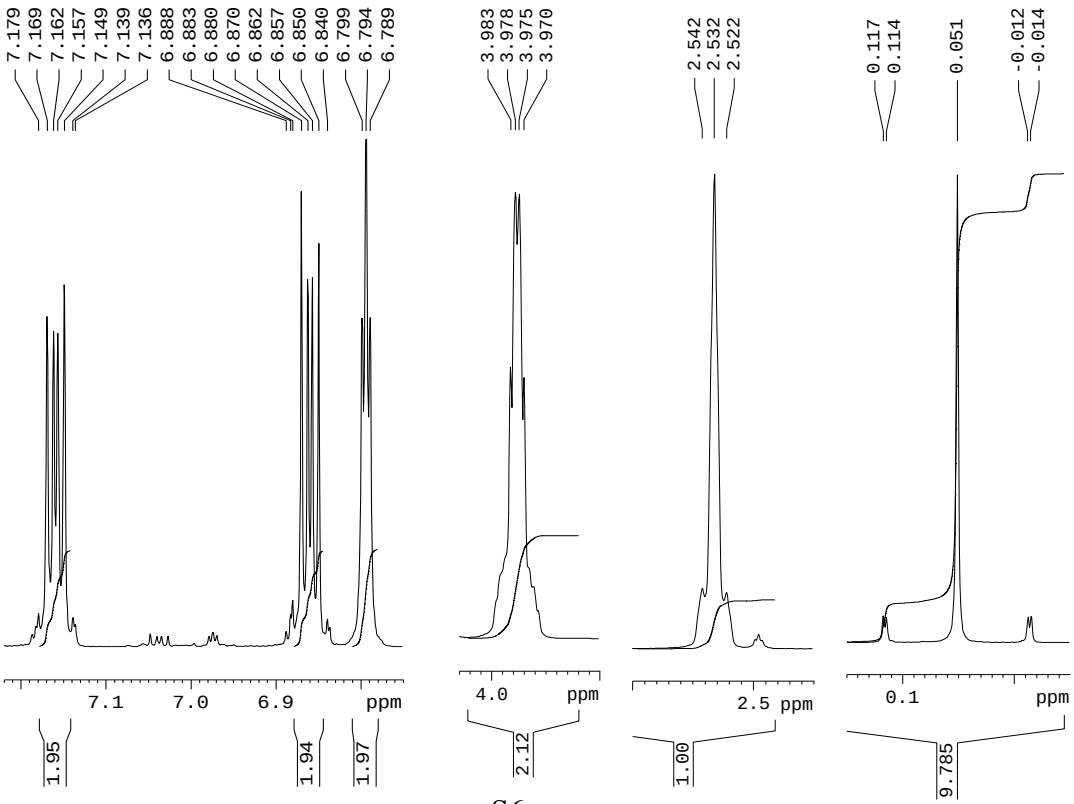

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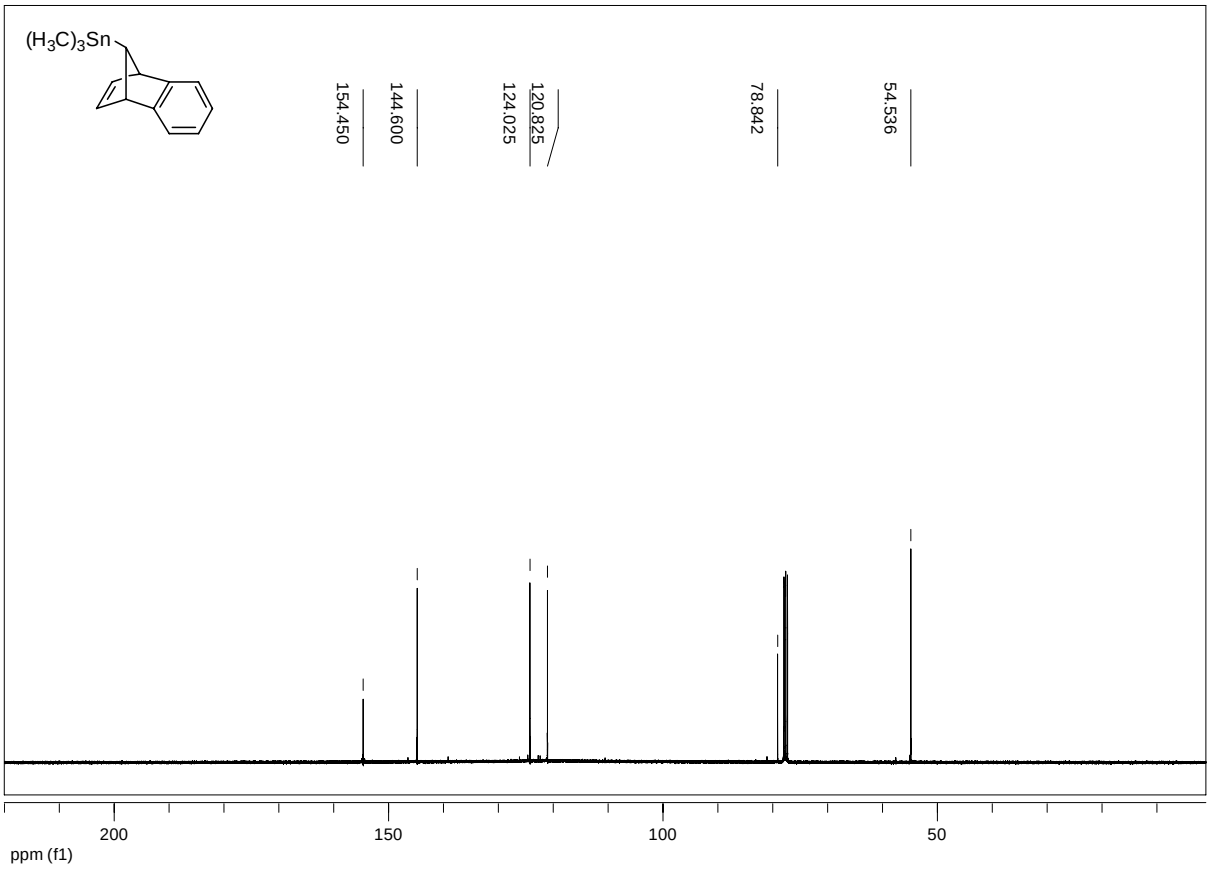

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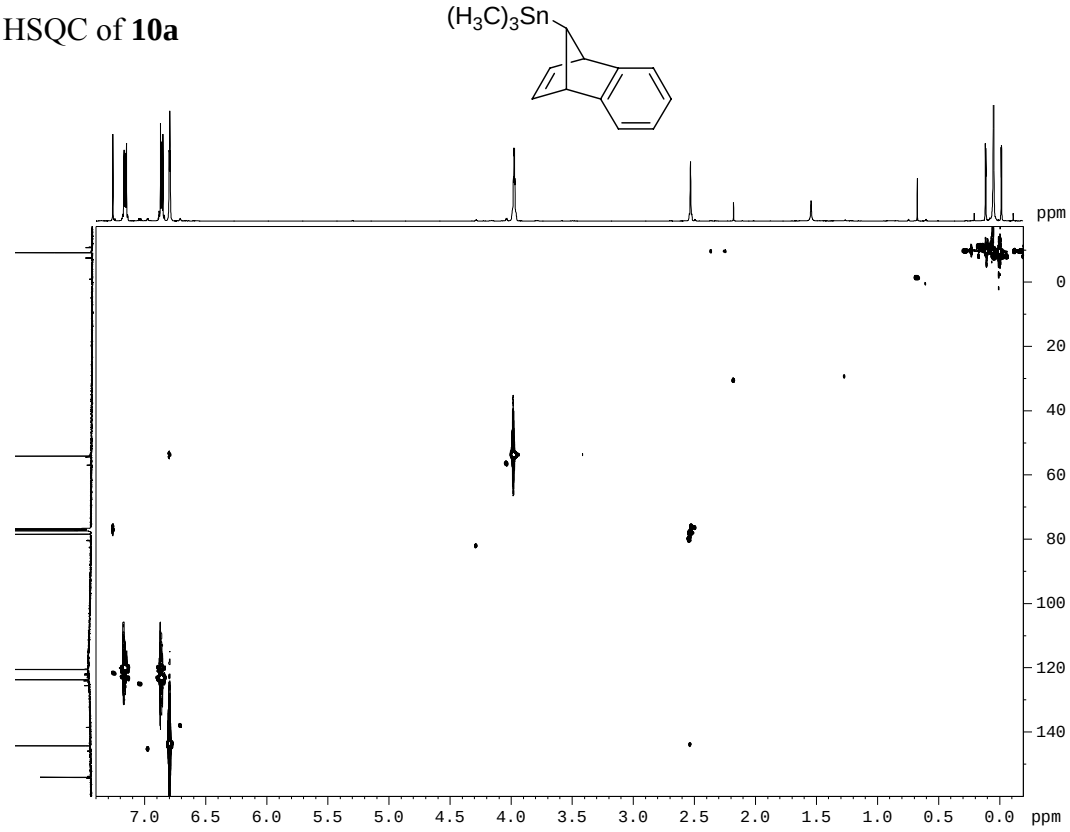

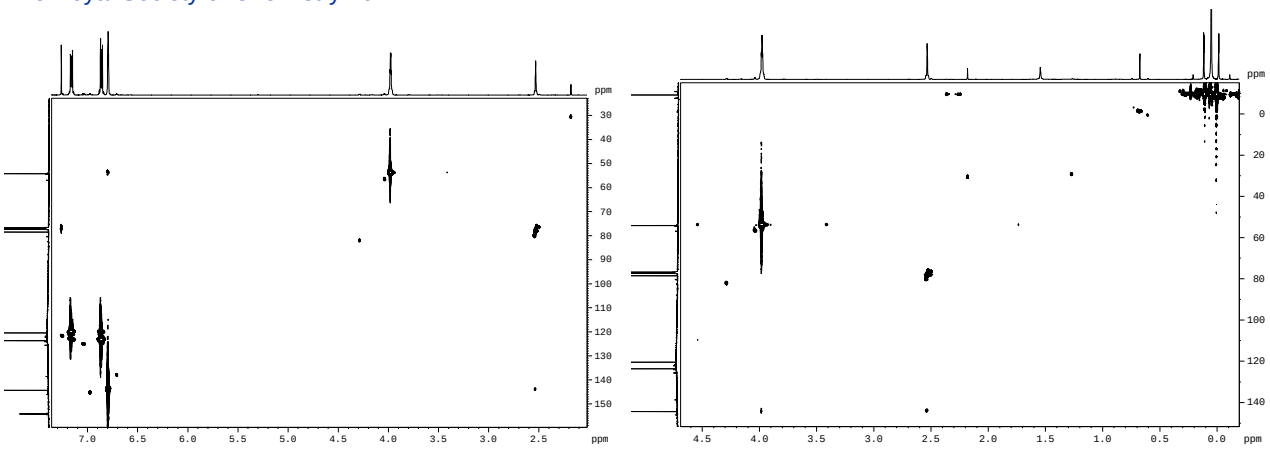

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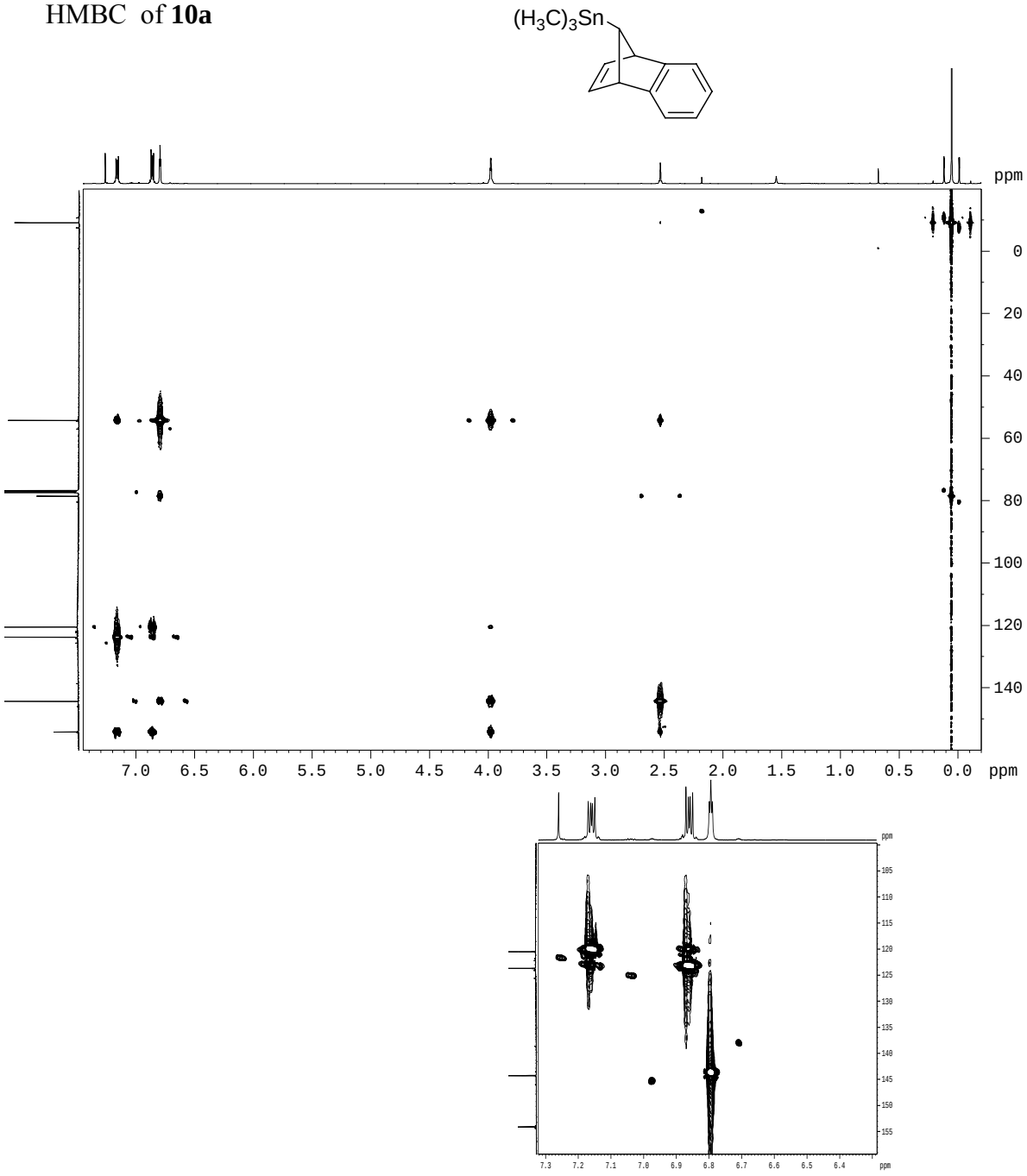

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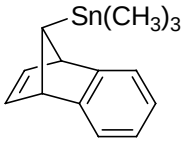

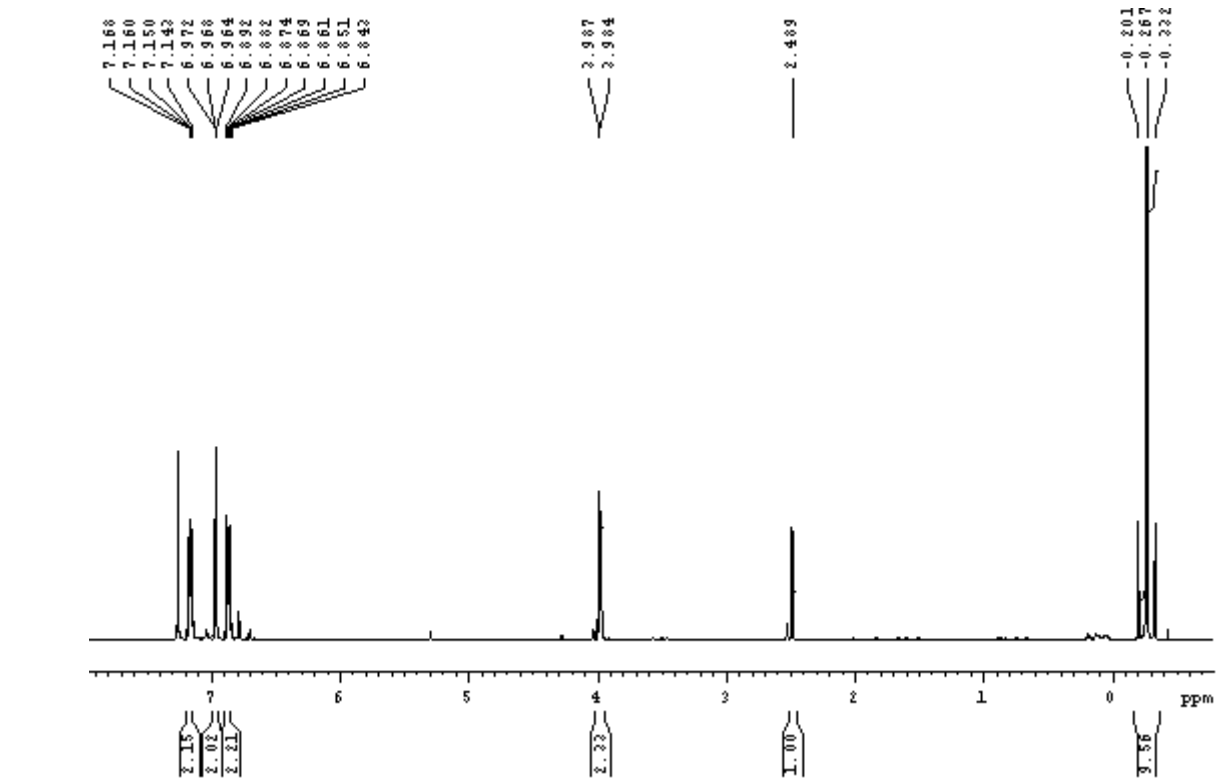

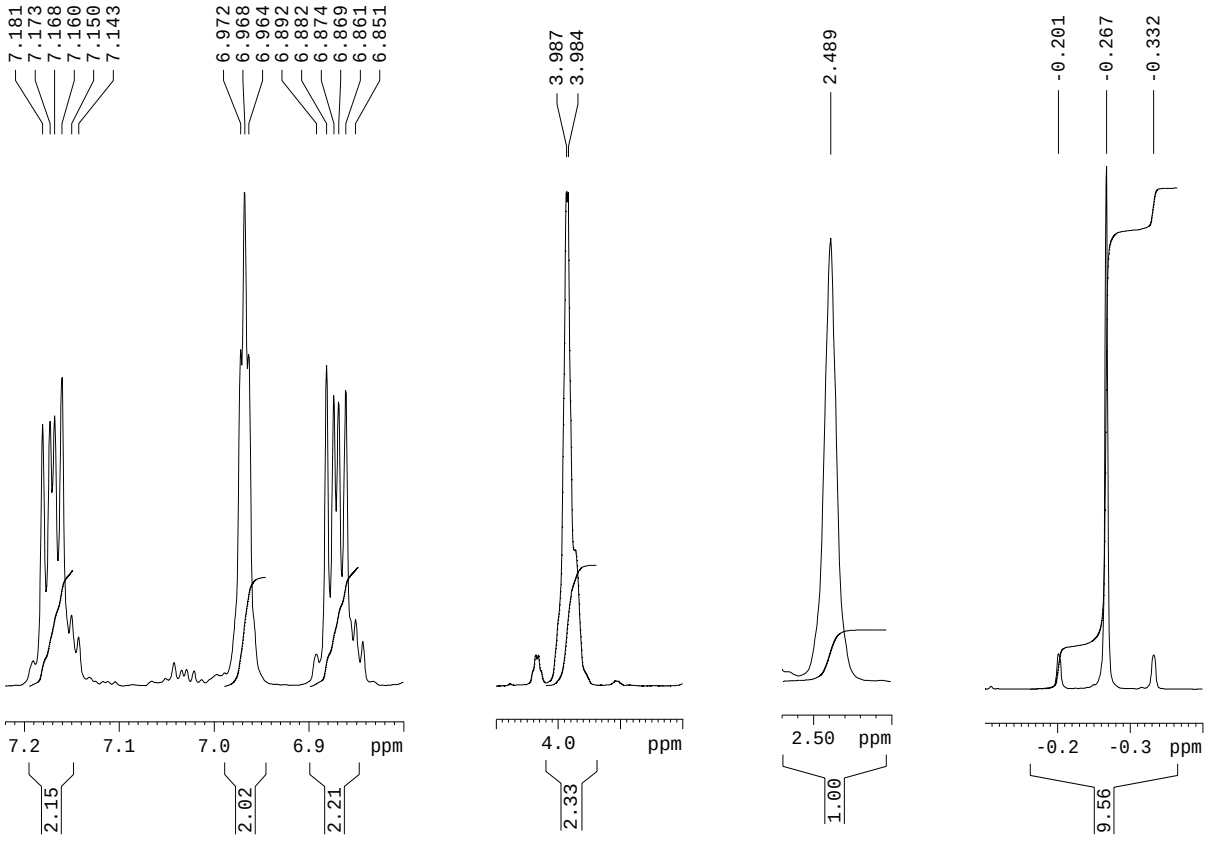

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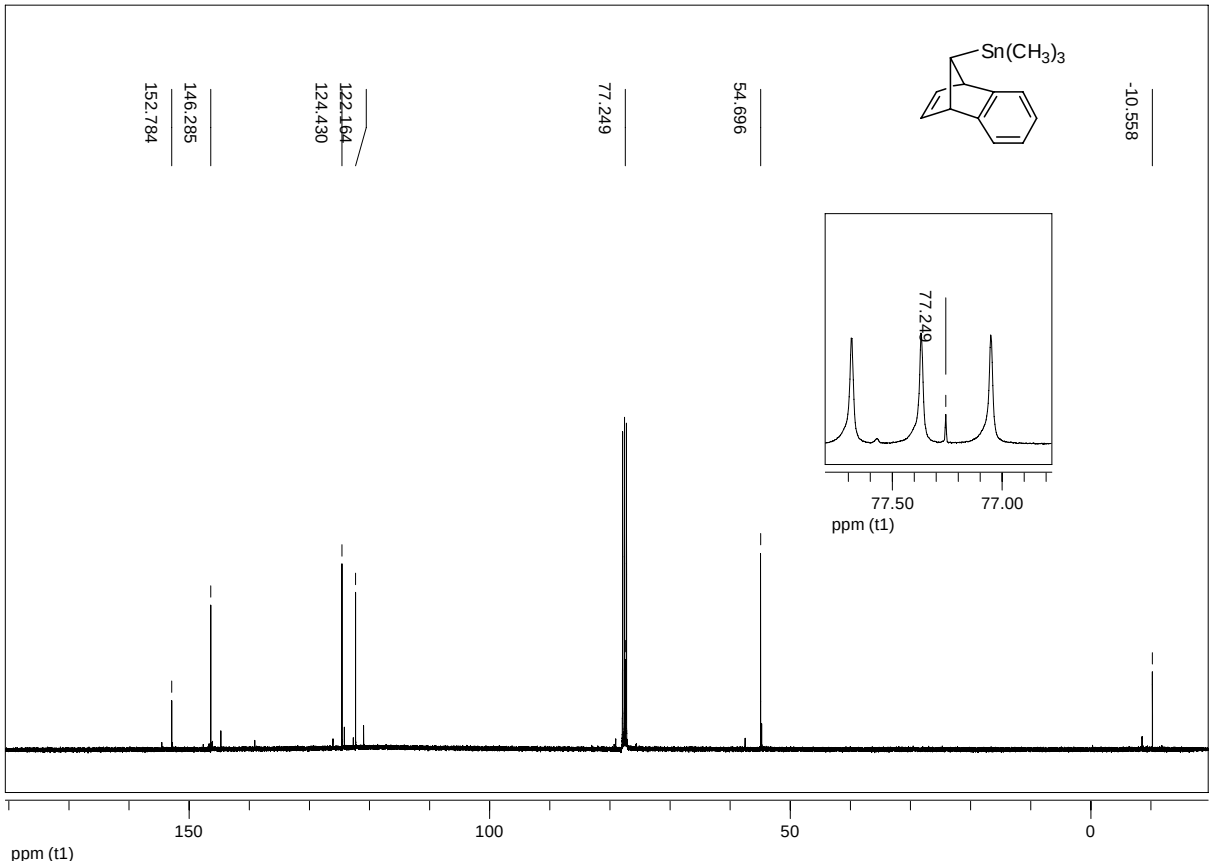

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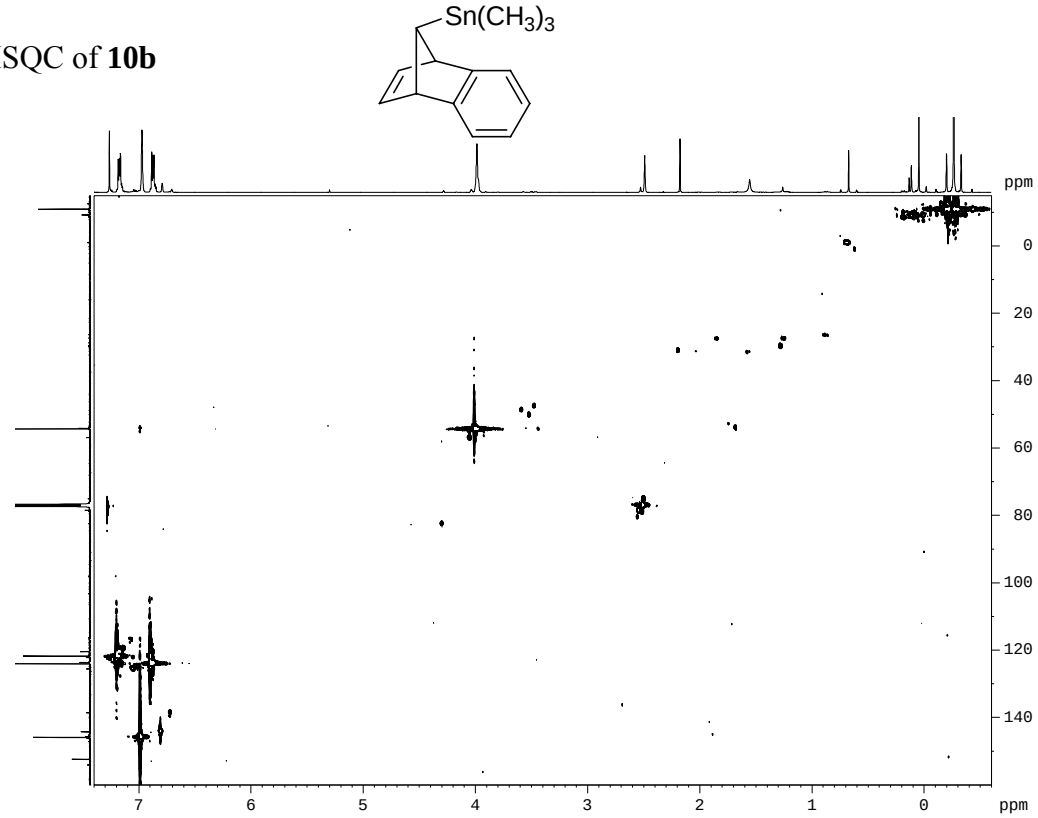

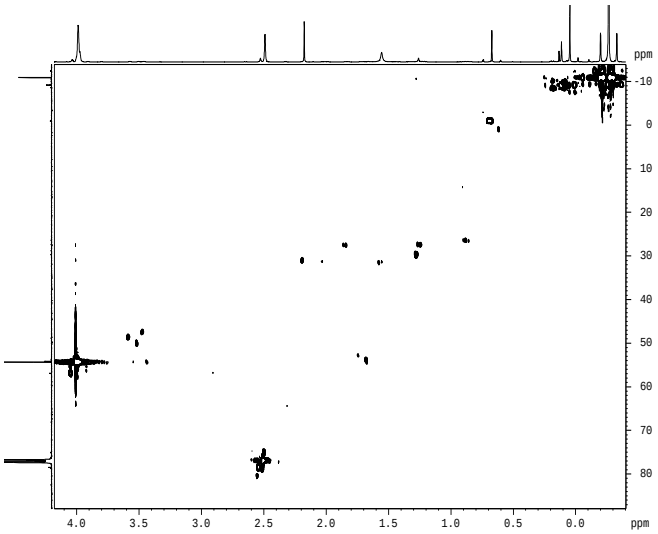

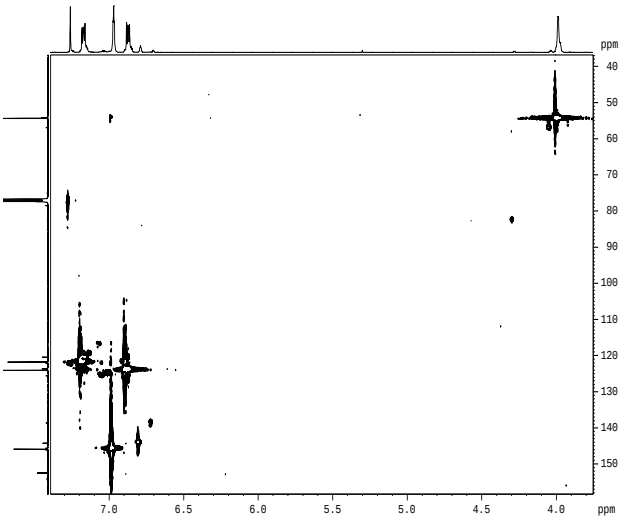

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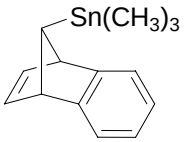

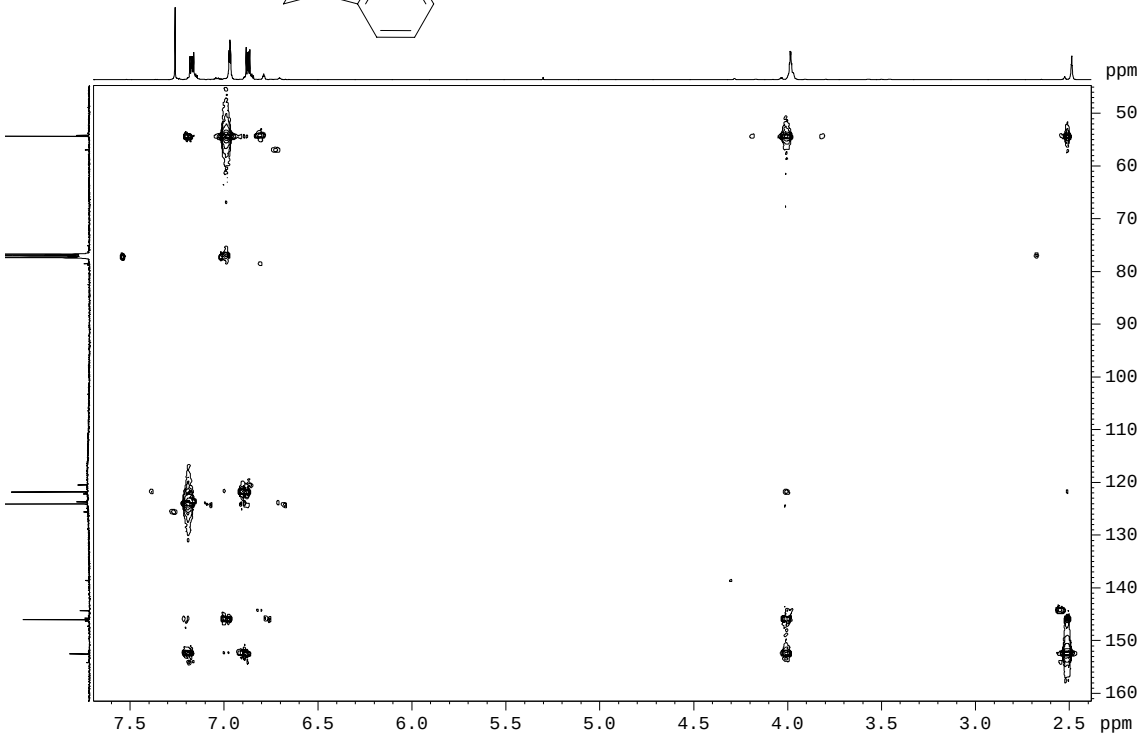

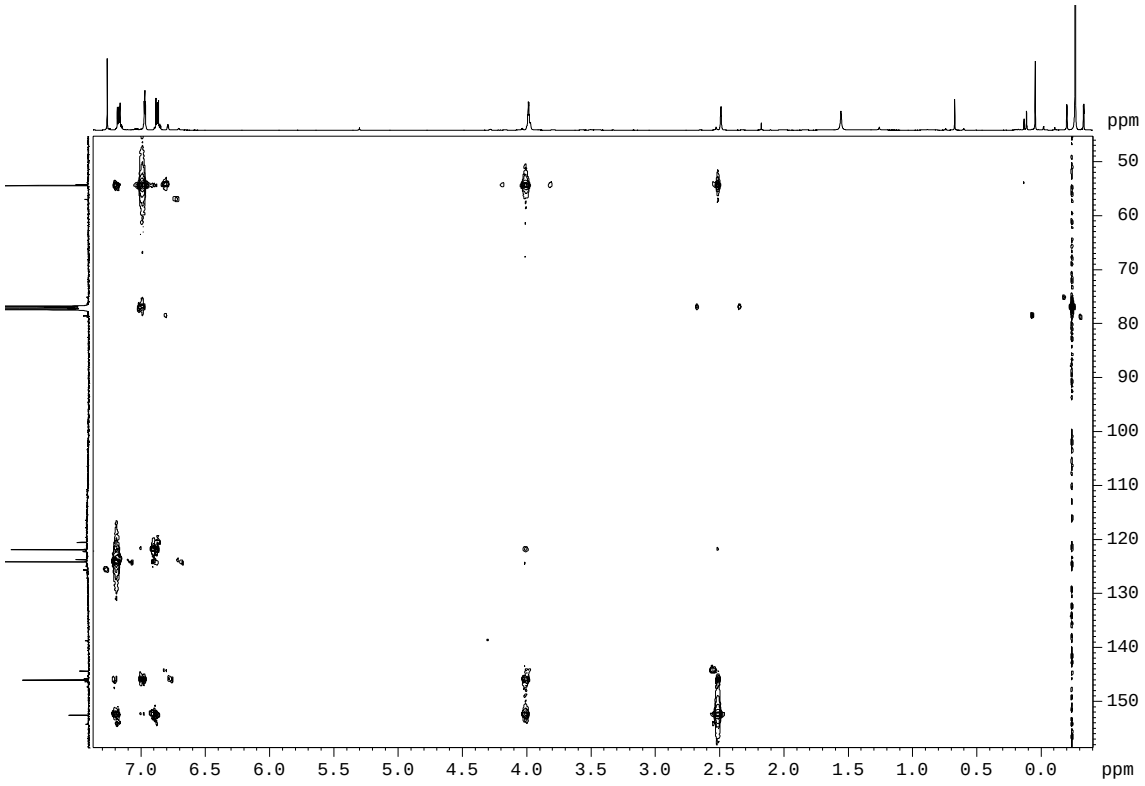

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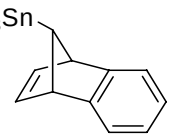

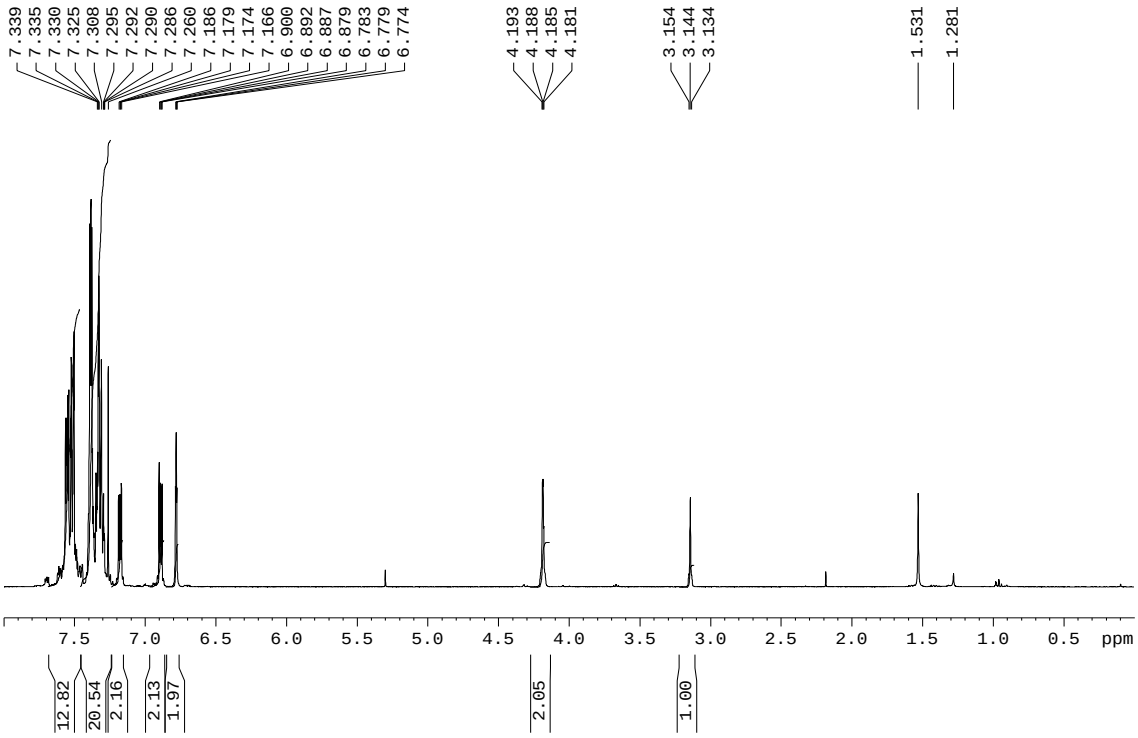

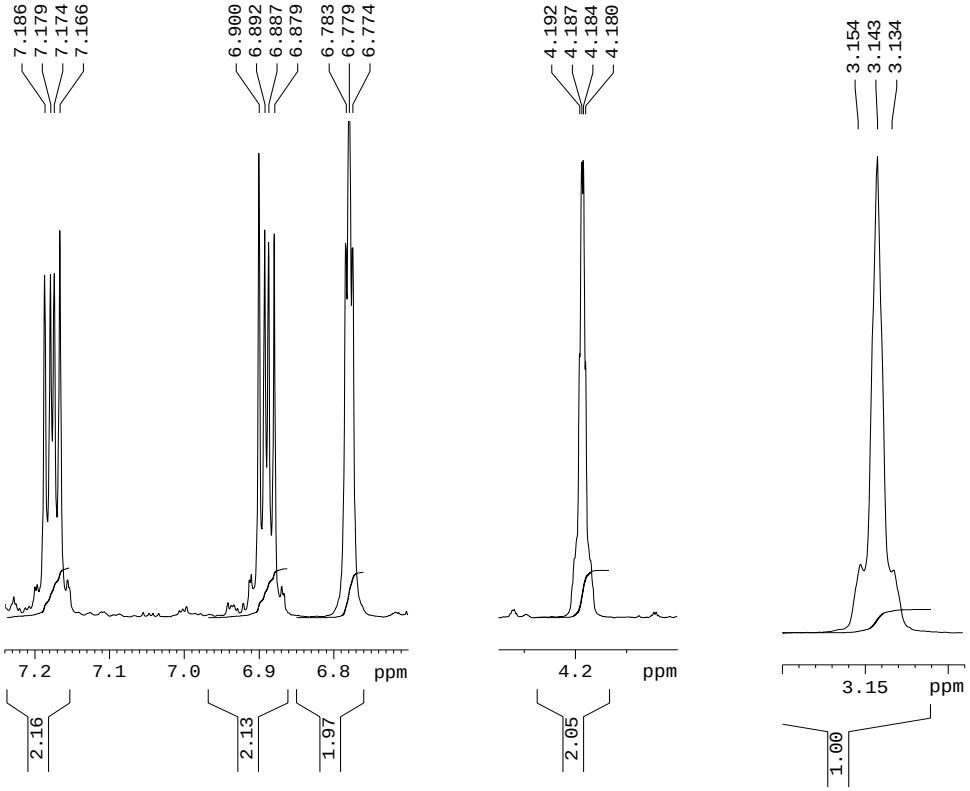

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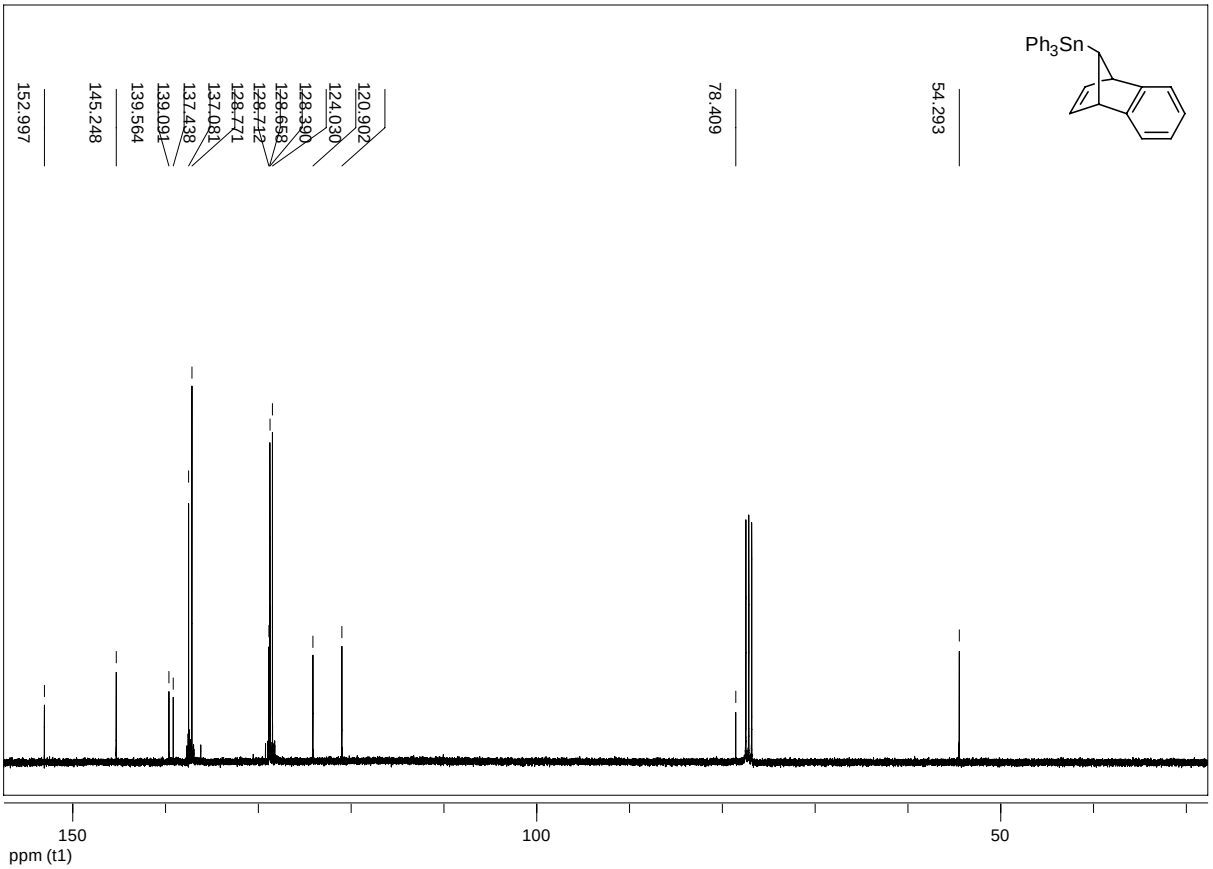

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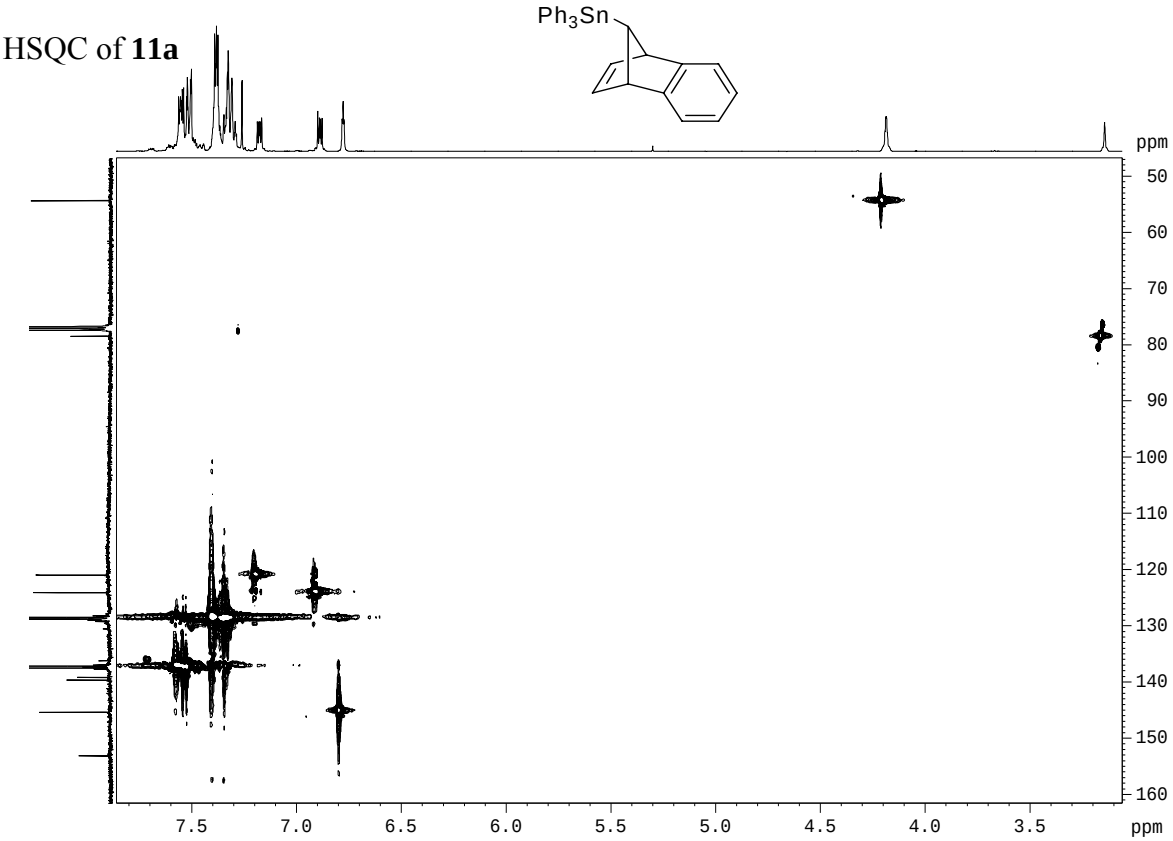

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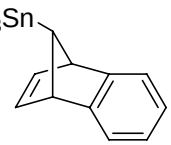

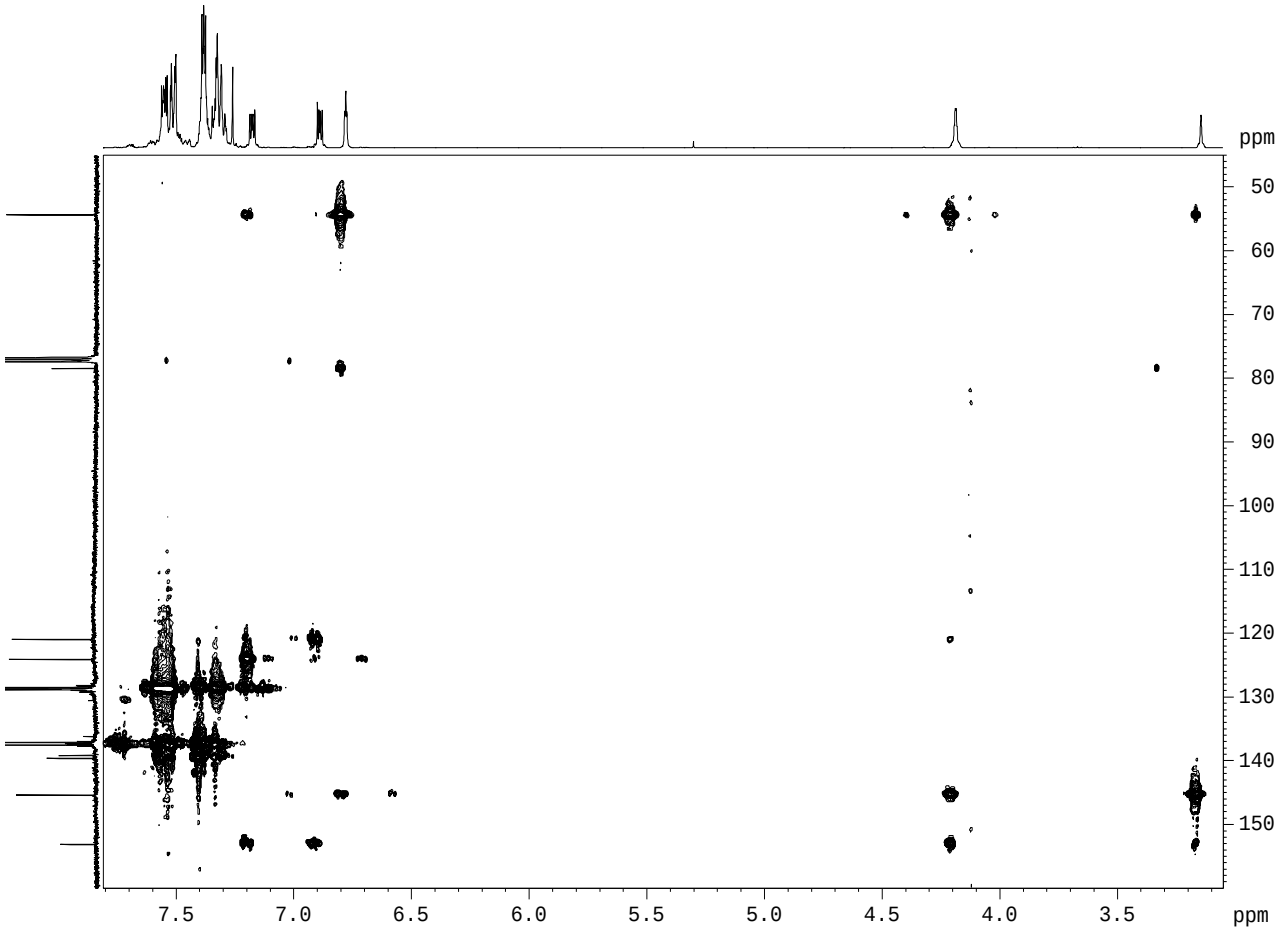

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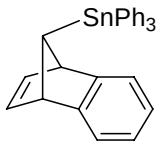

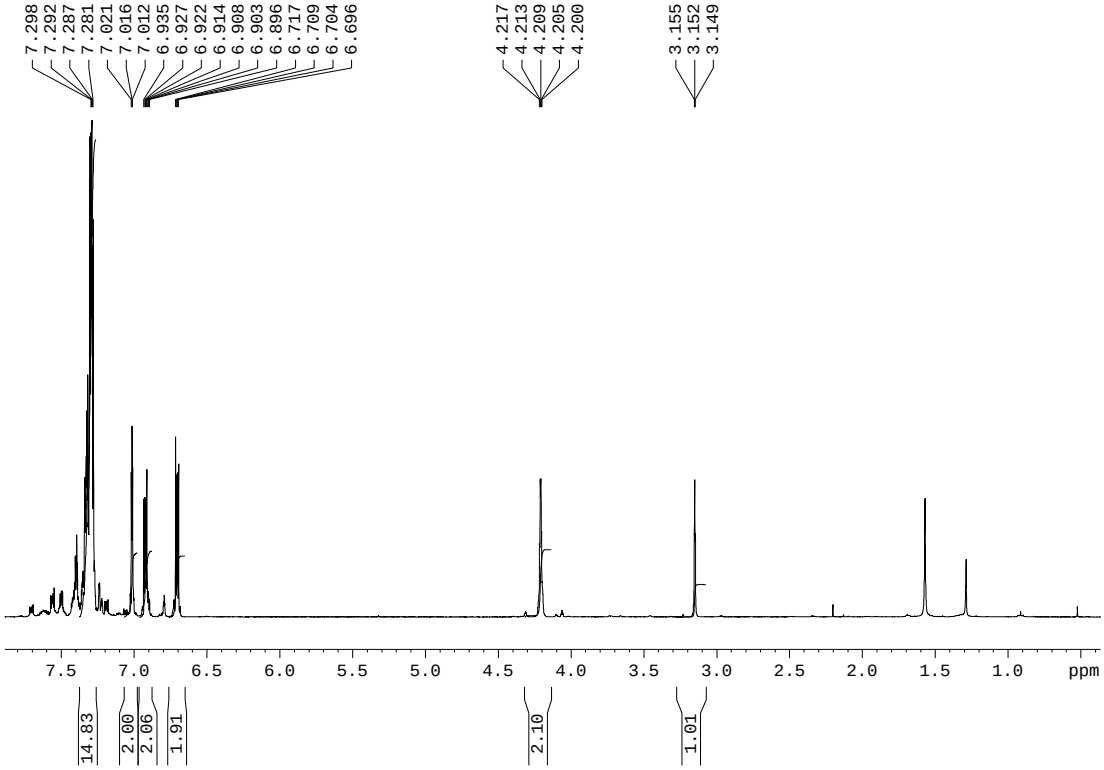

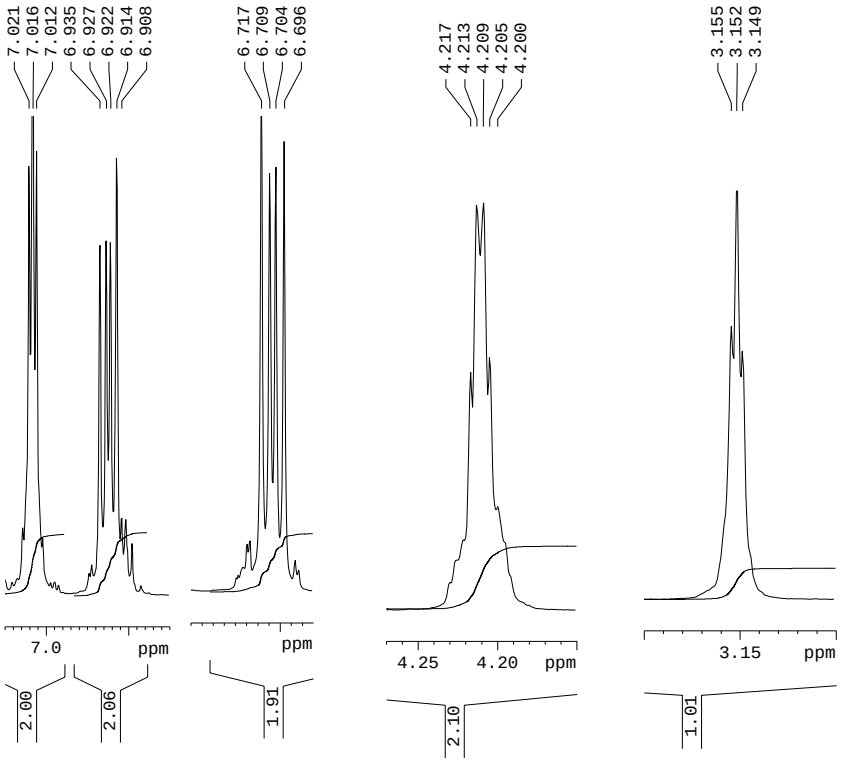

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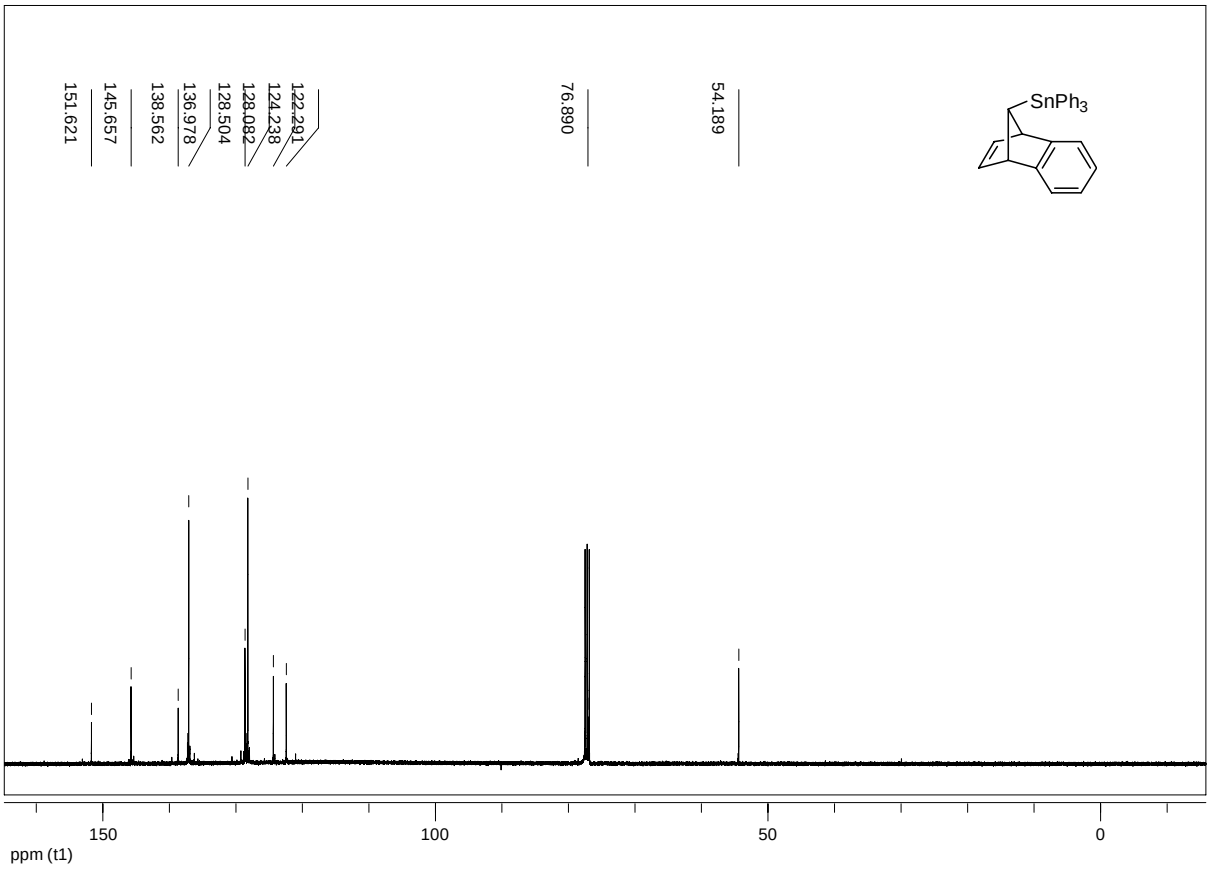

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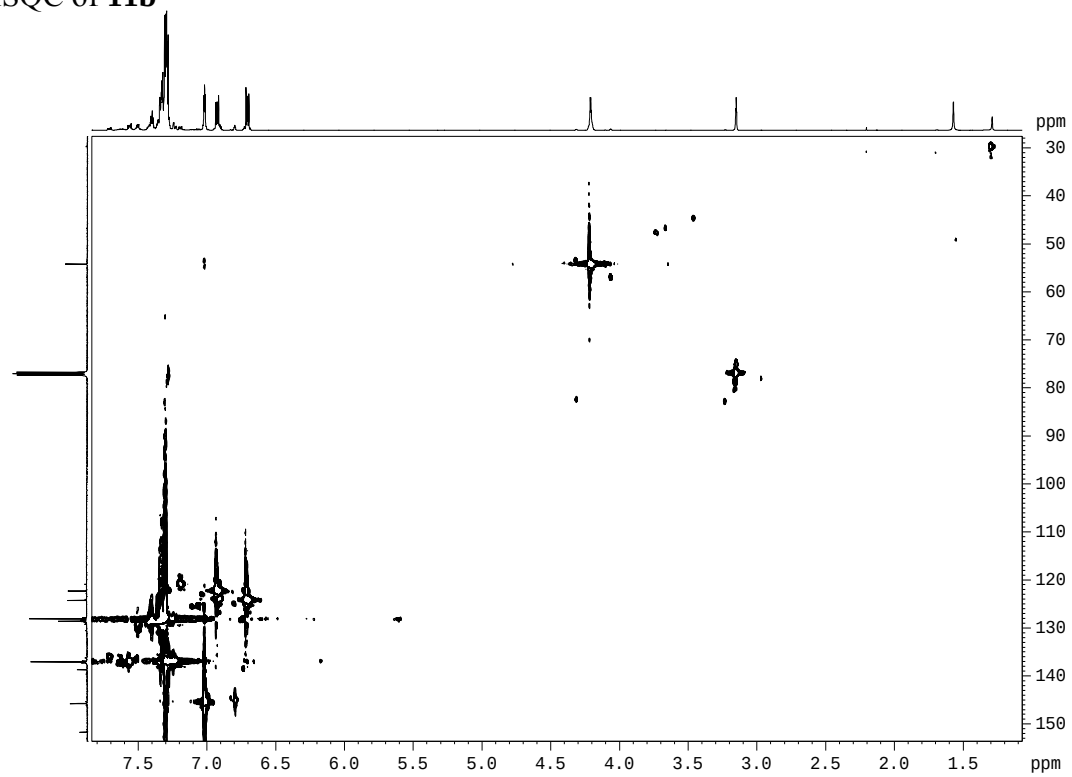

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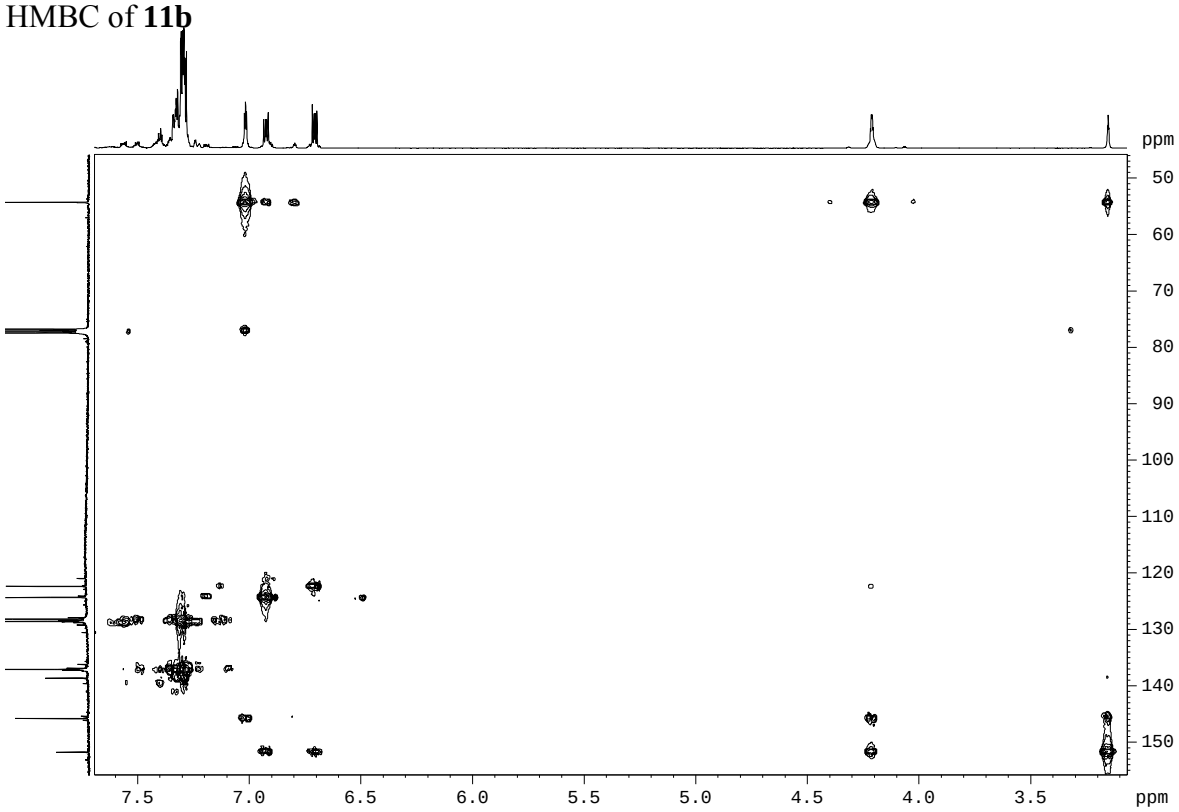

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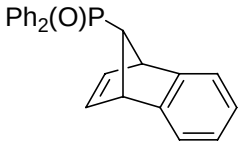

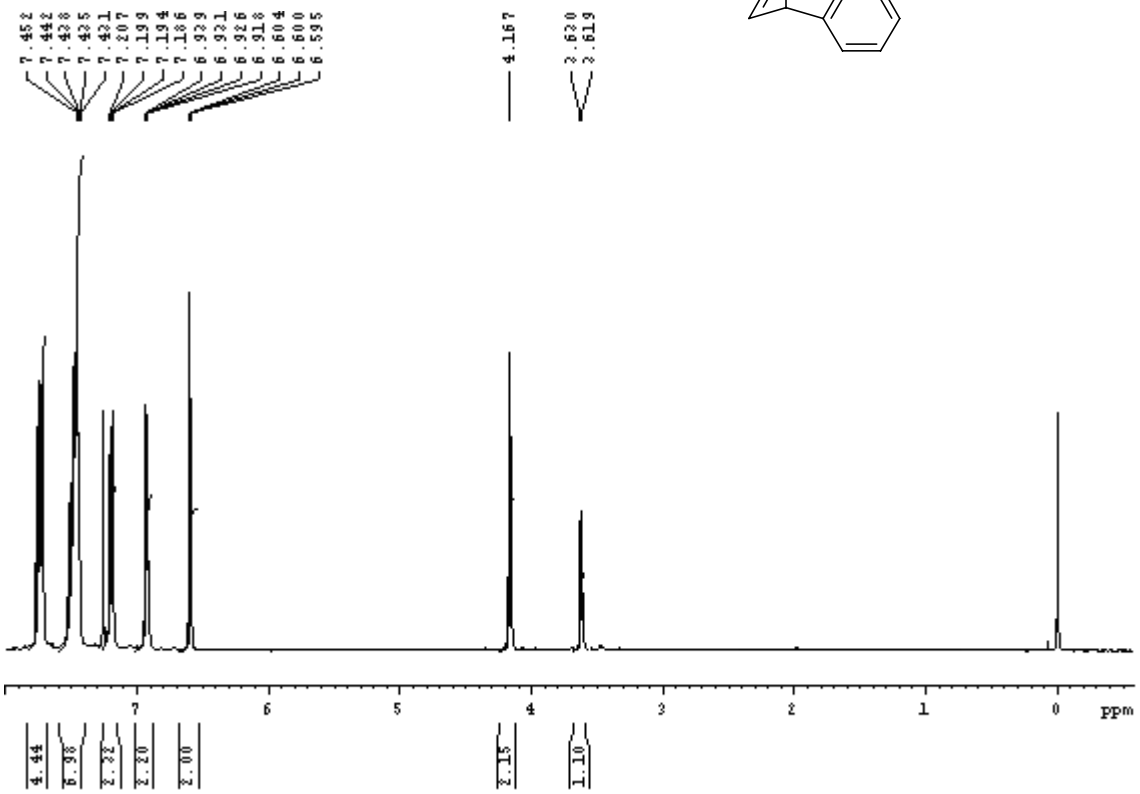

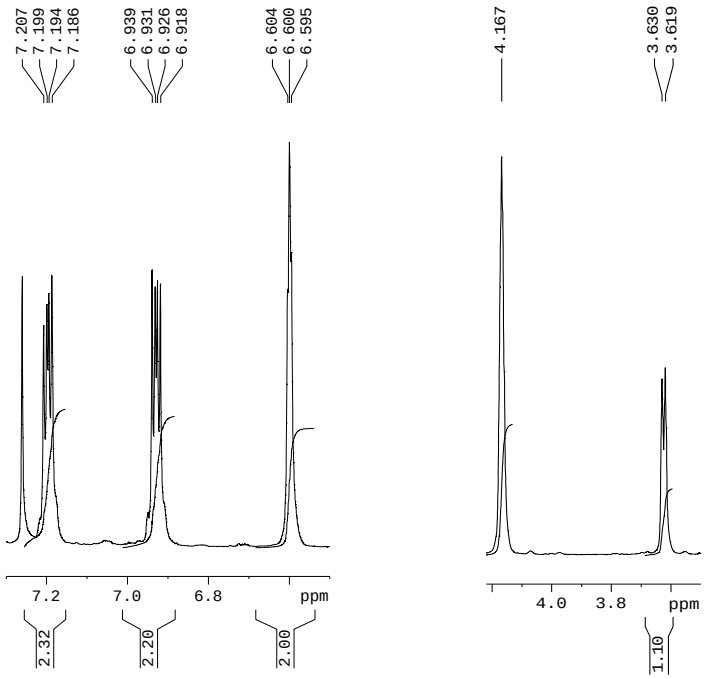

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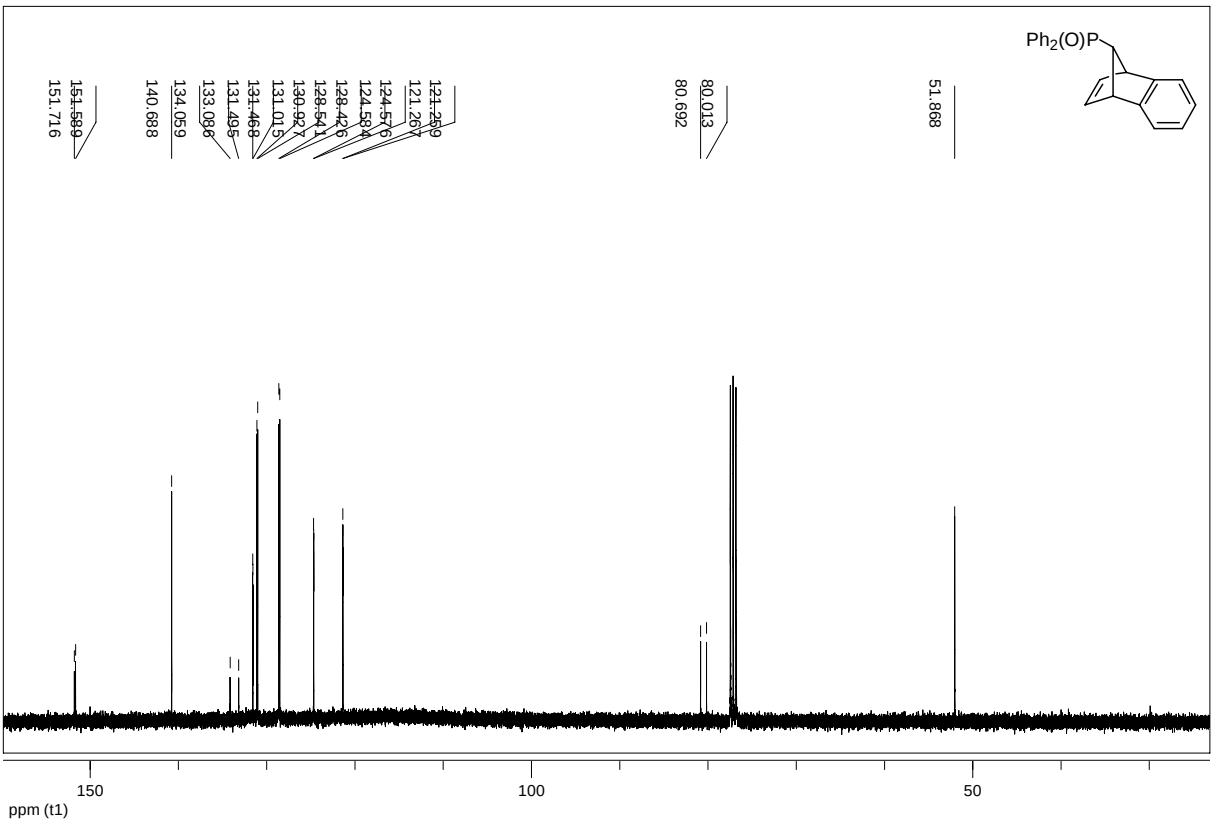

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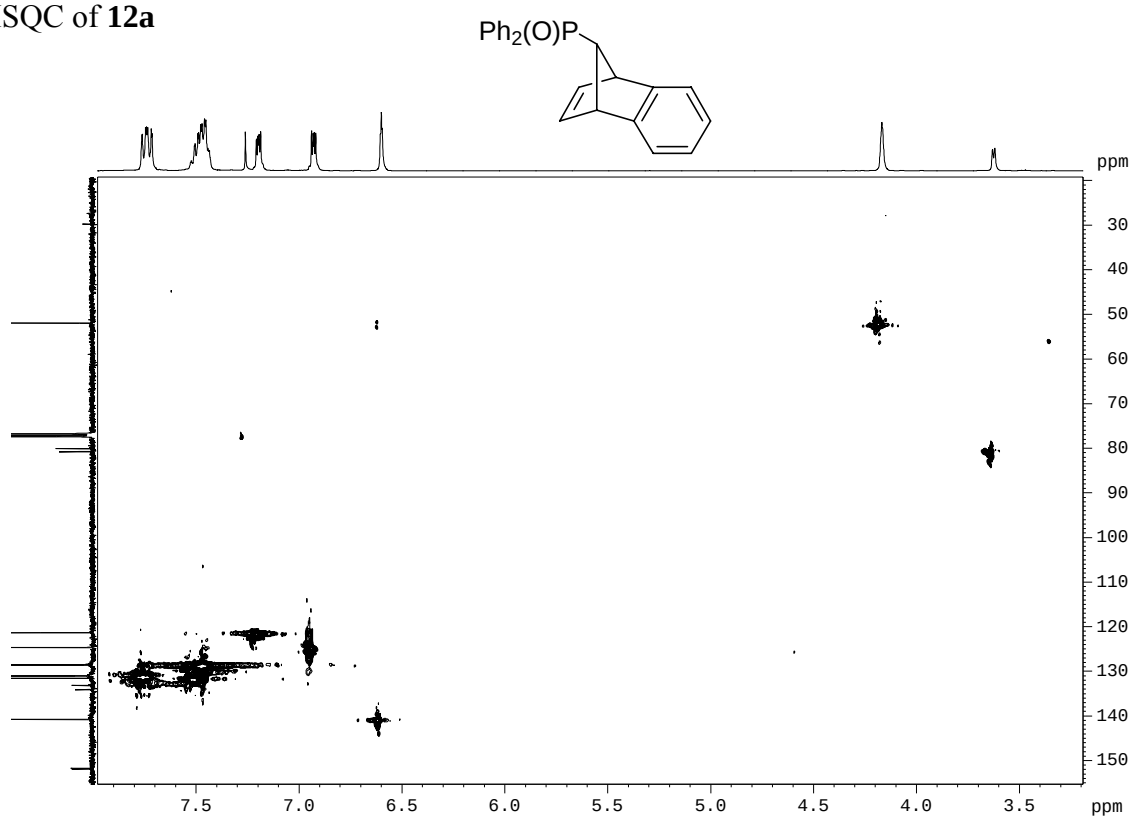

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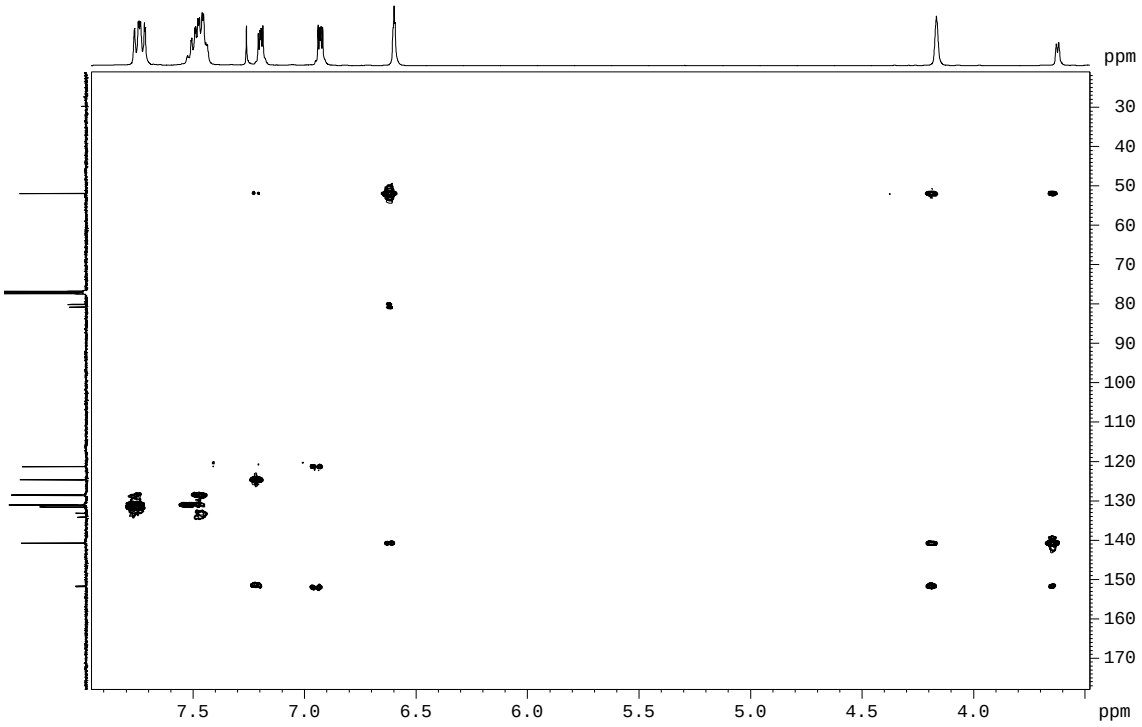

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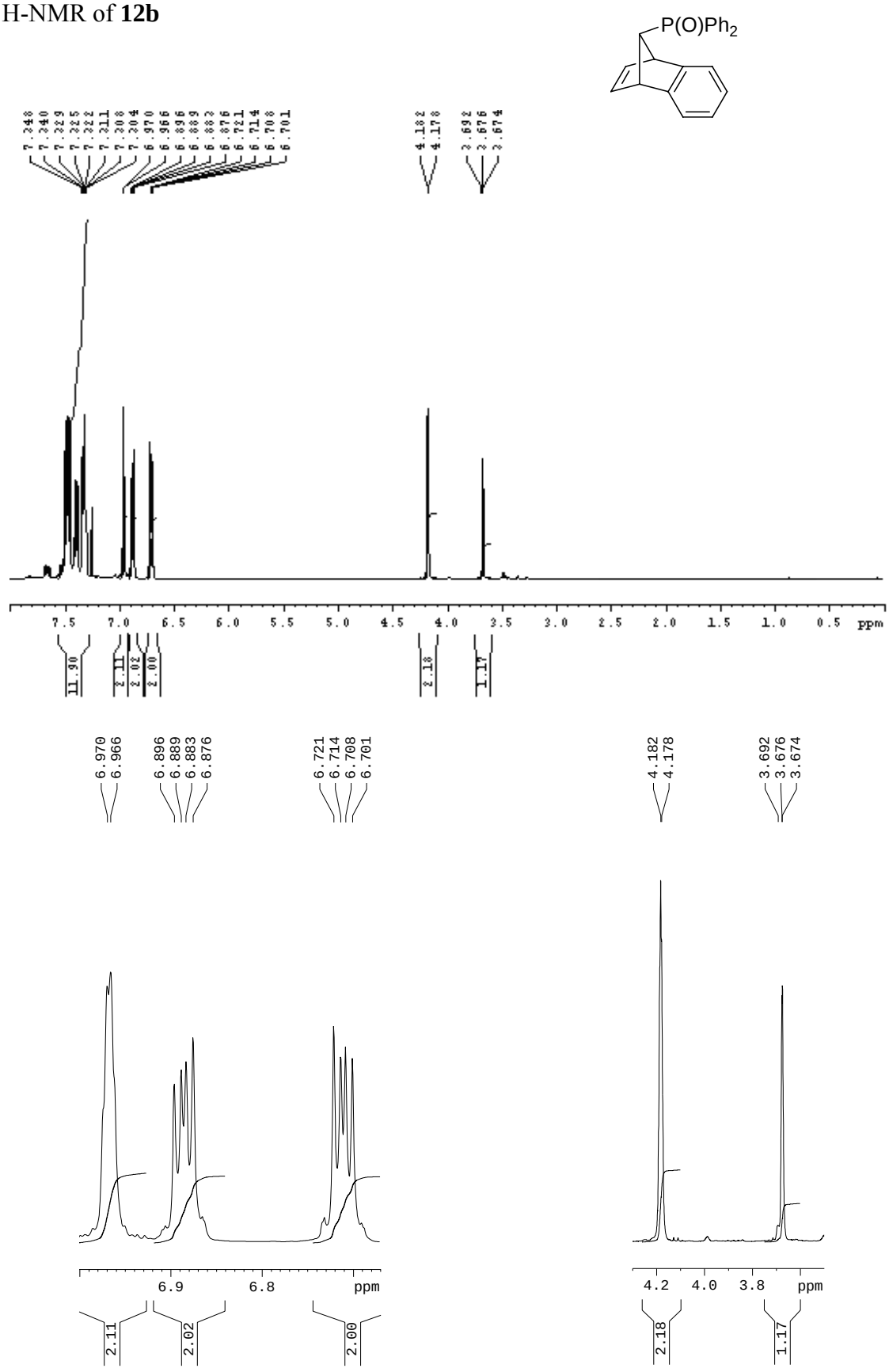

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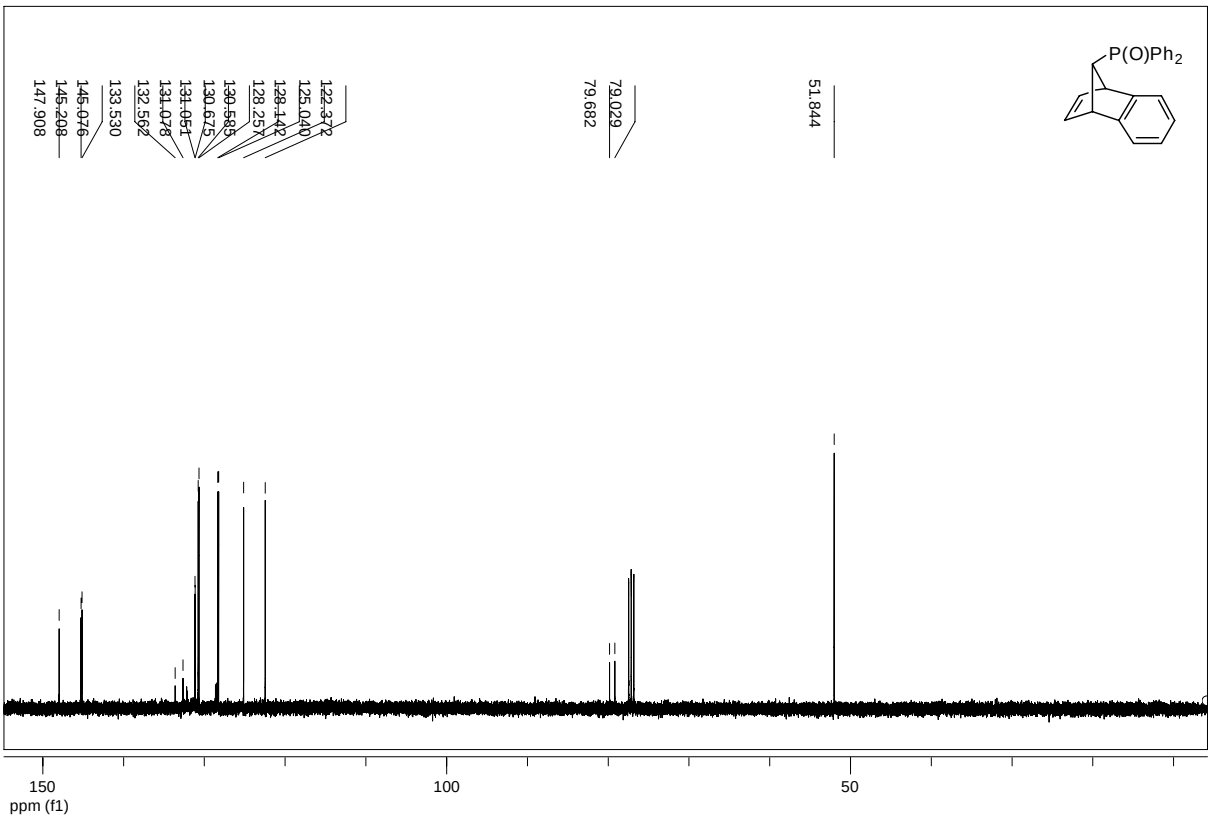

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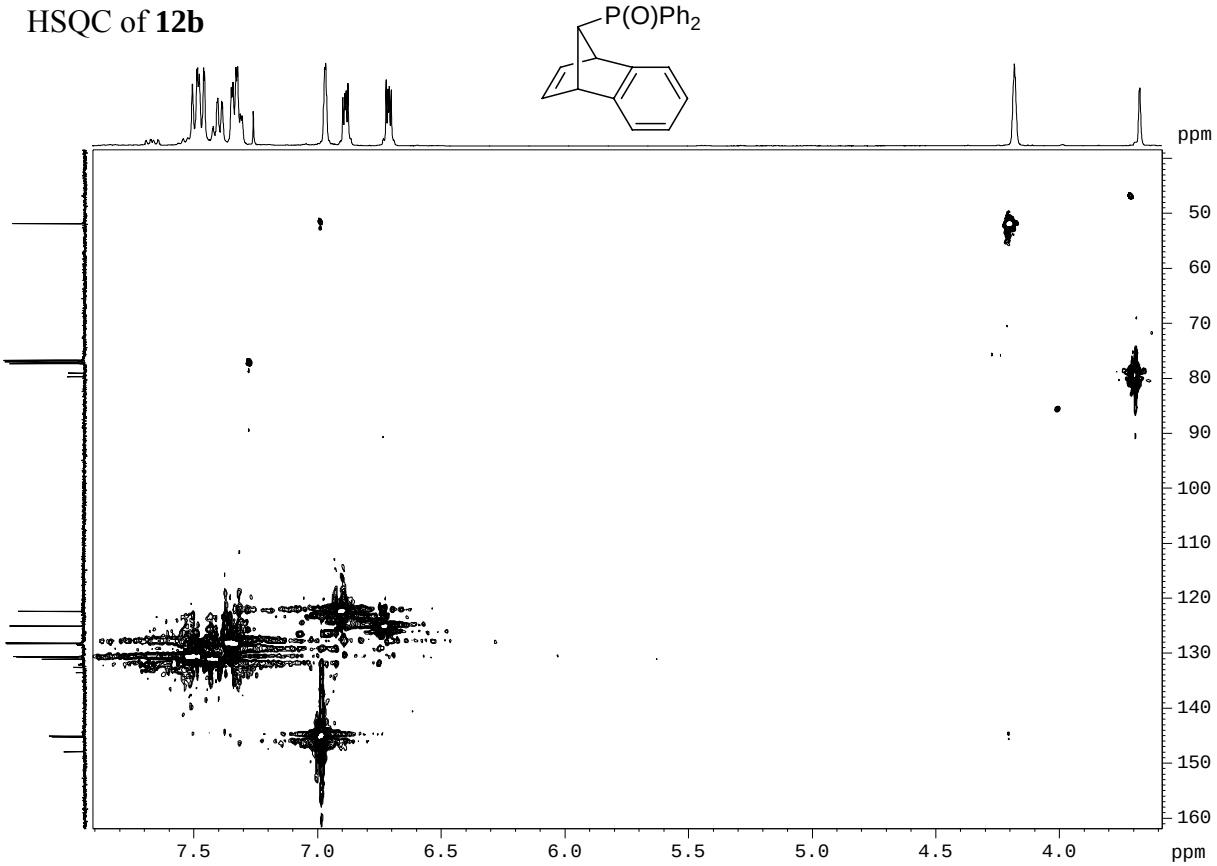

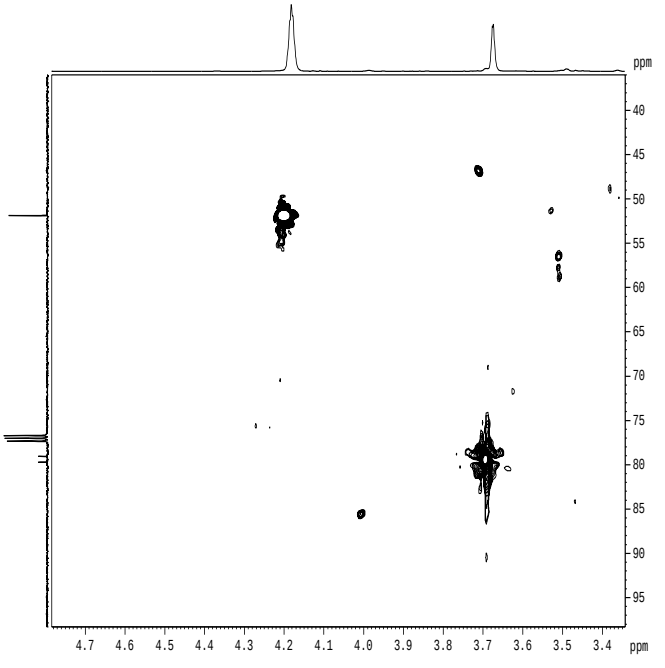
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45
50
55
60
65
70
75
80
85
90
95
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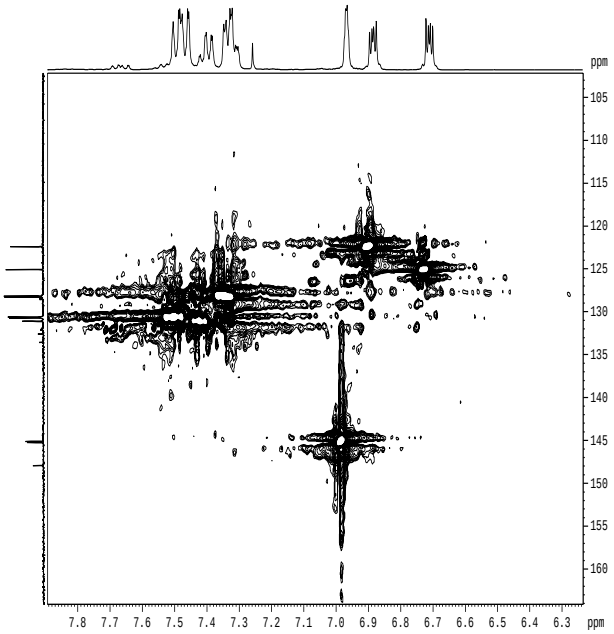
ppm


ppm
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110
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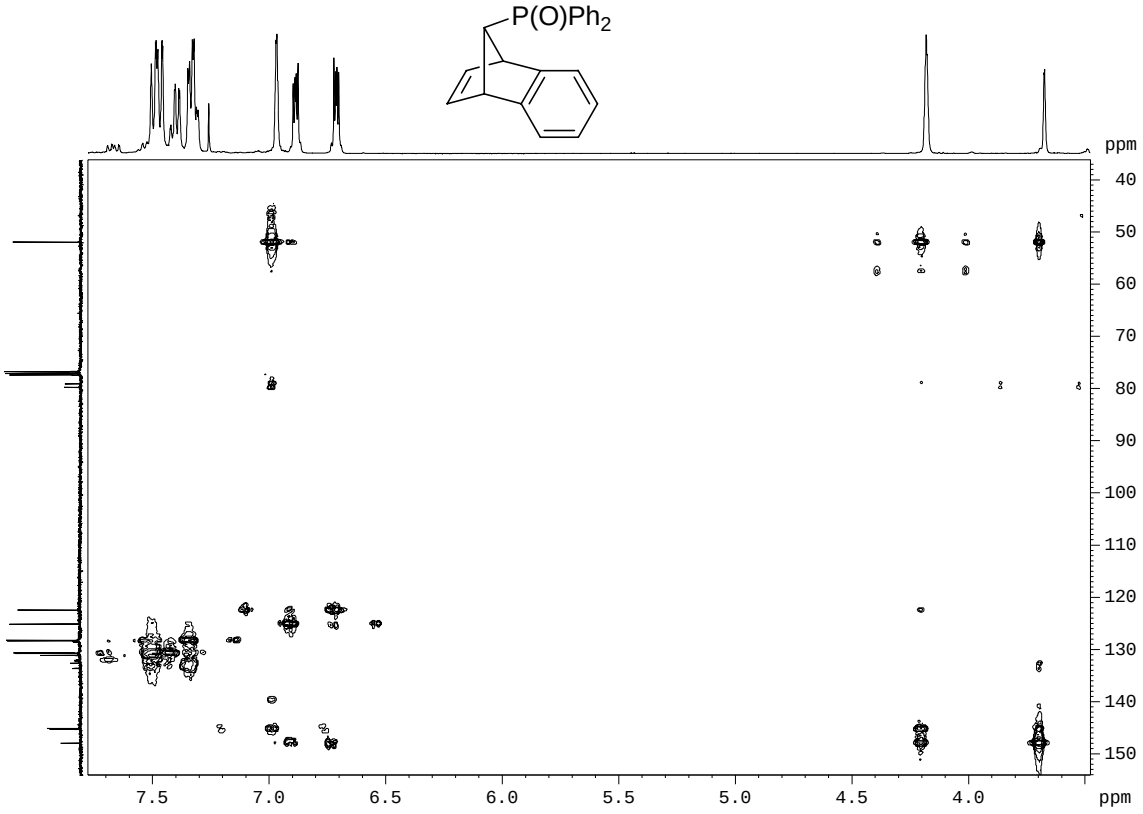
120
125
130
135
140
145
150
155
160
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3
ppm

HMBC of **12b**


P(O)Ph2
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140
150
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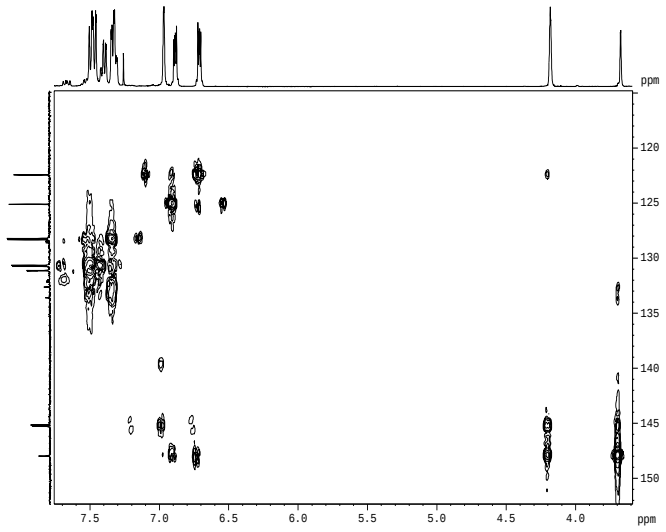

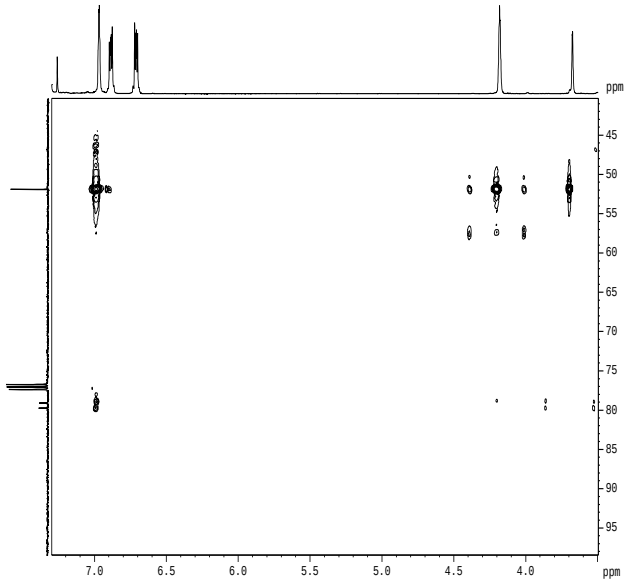

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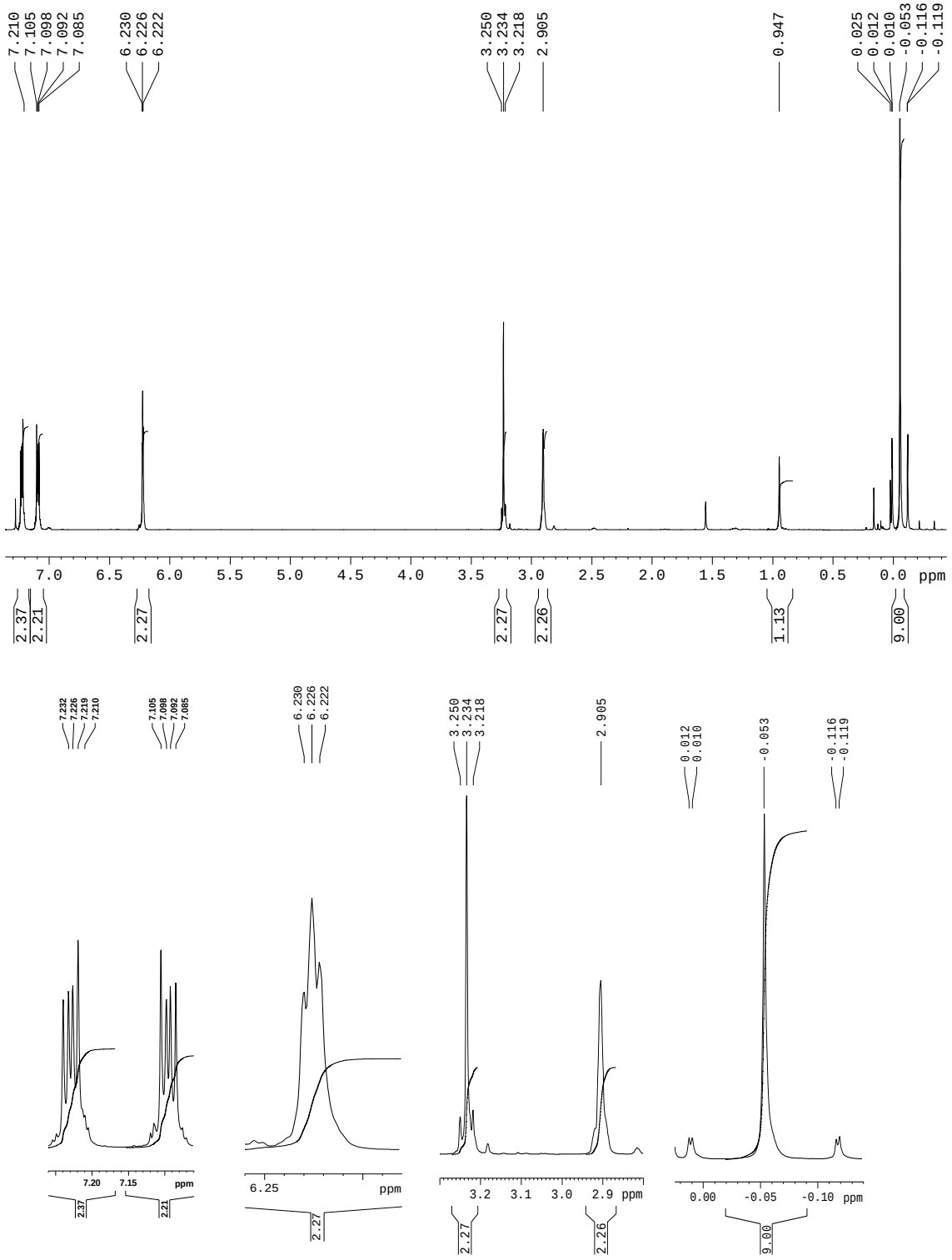

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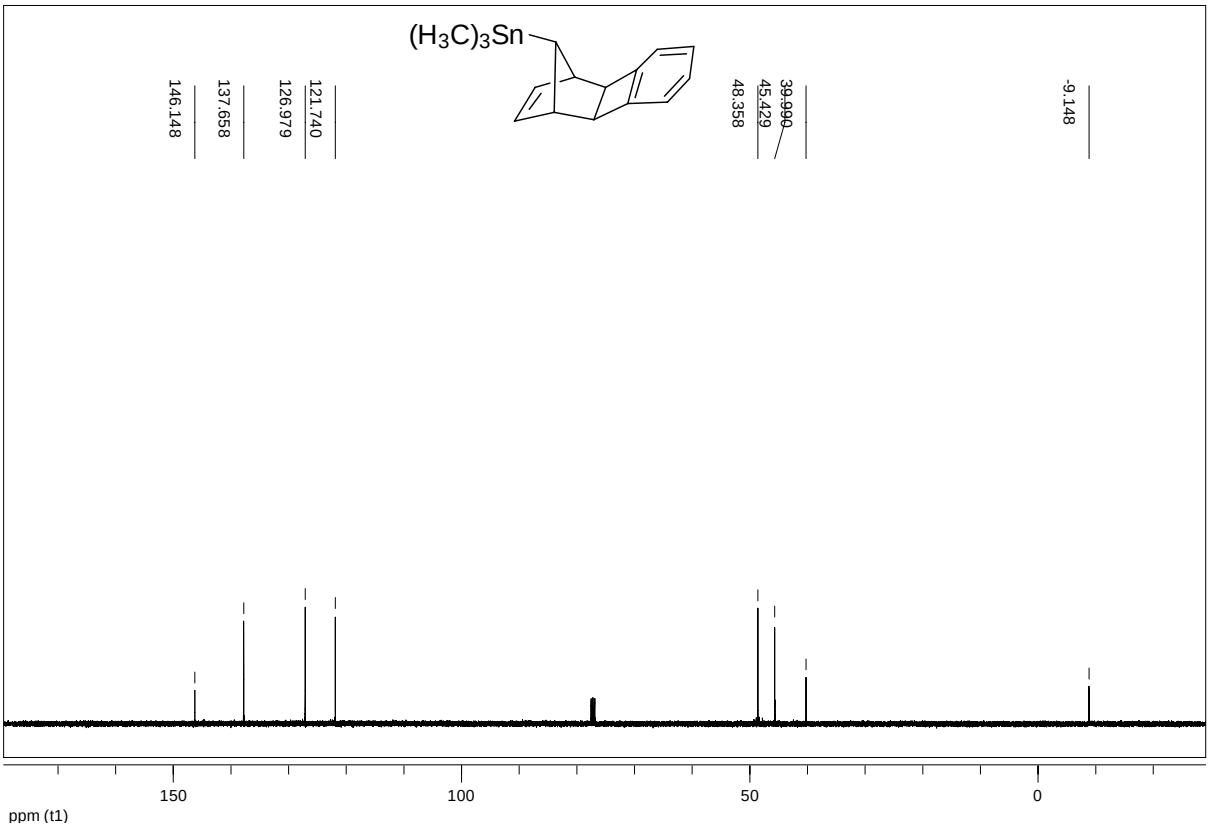

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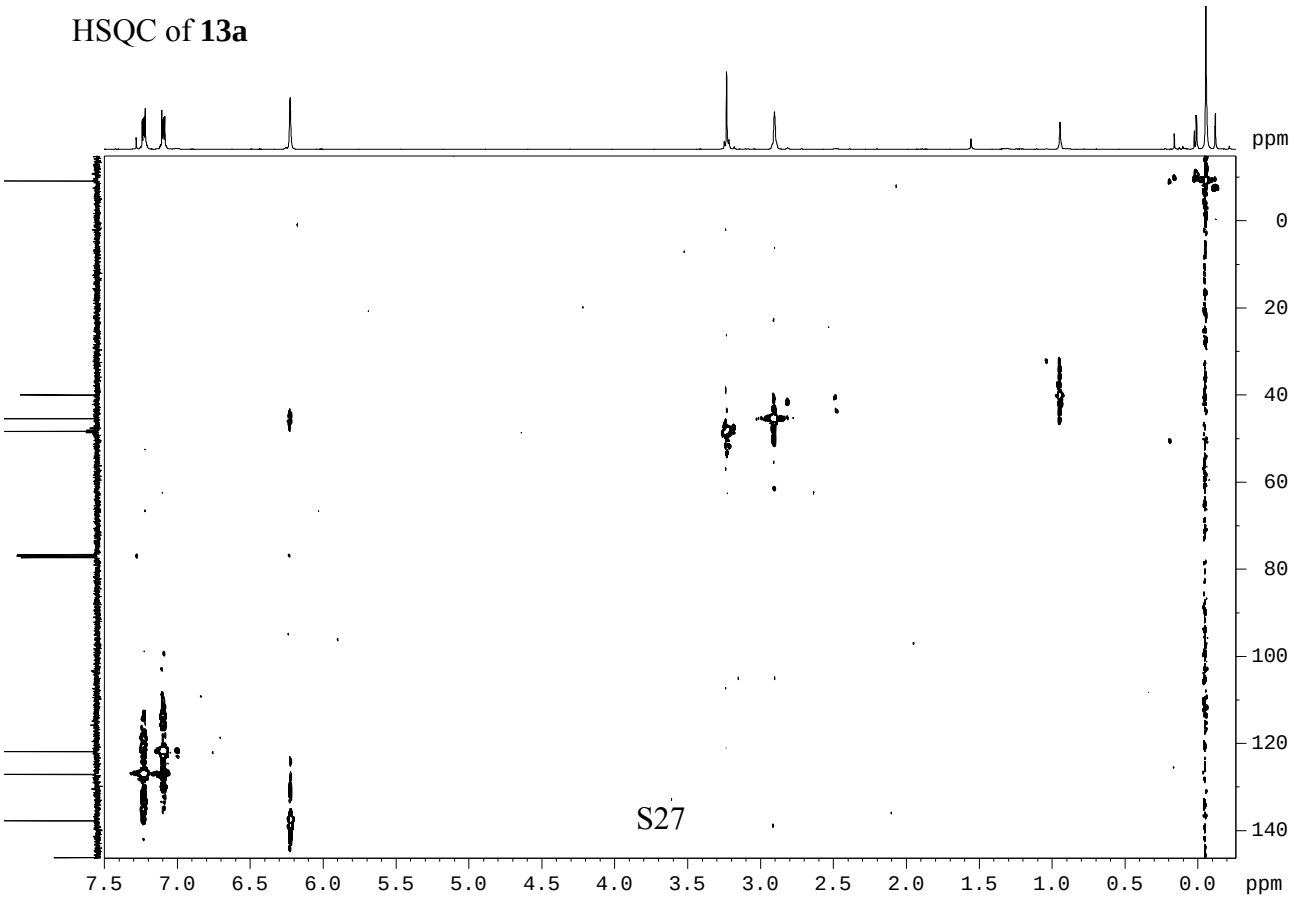

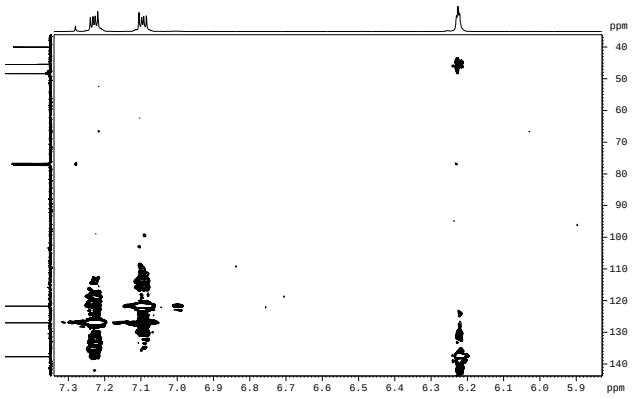

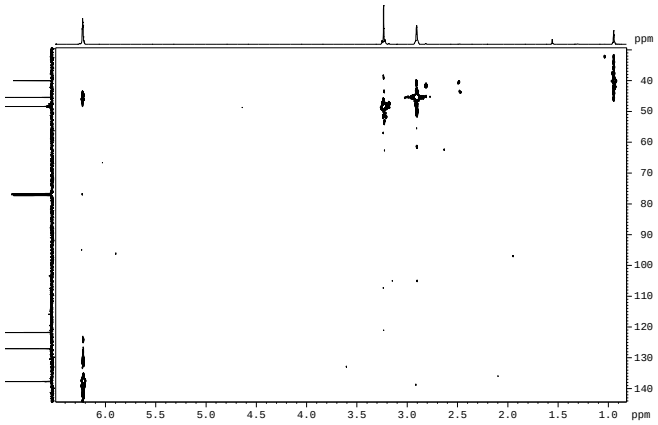

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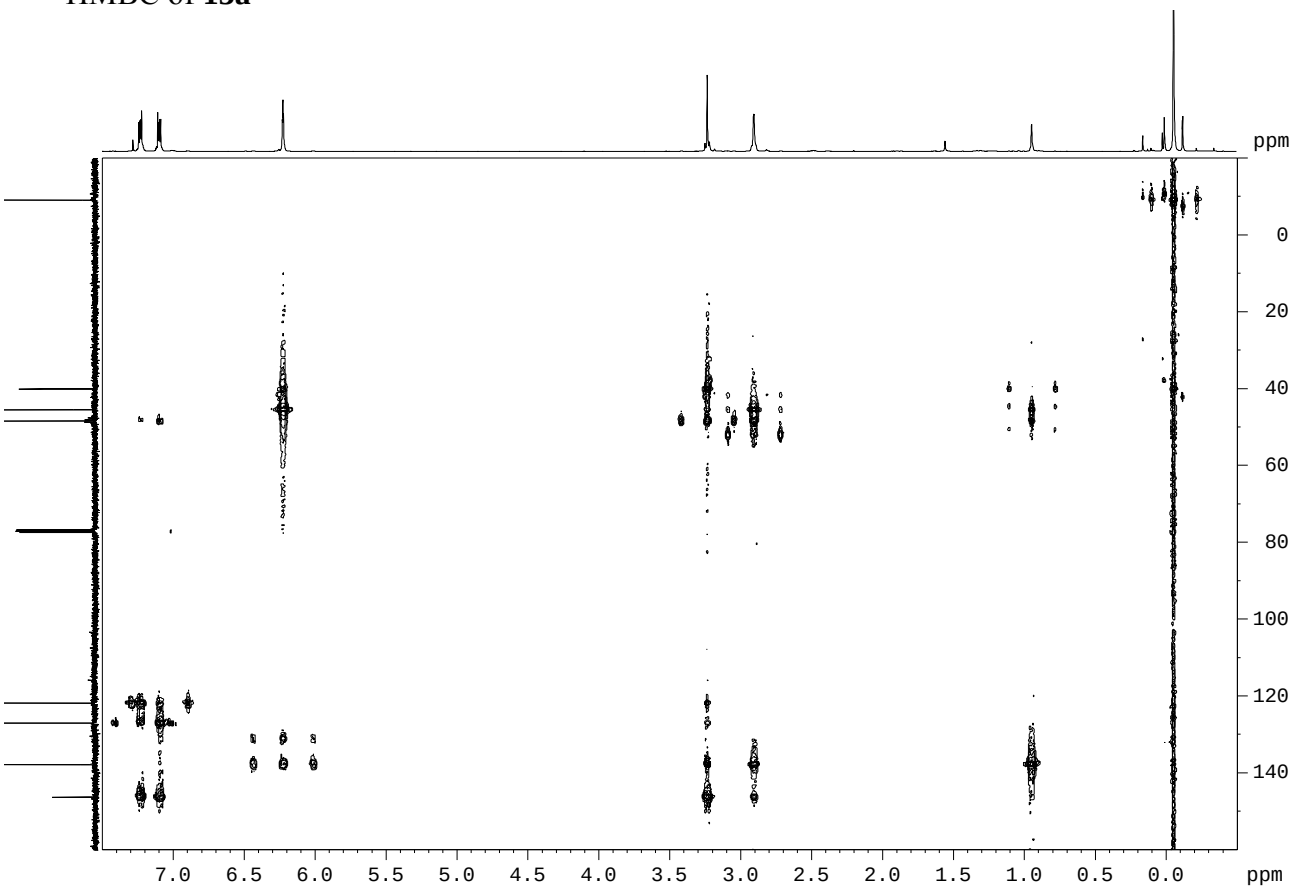

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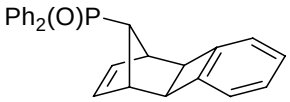
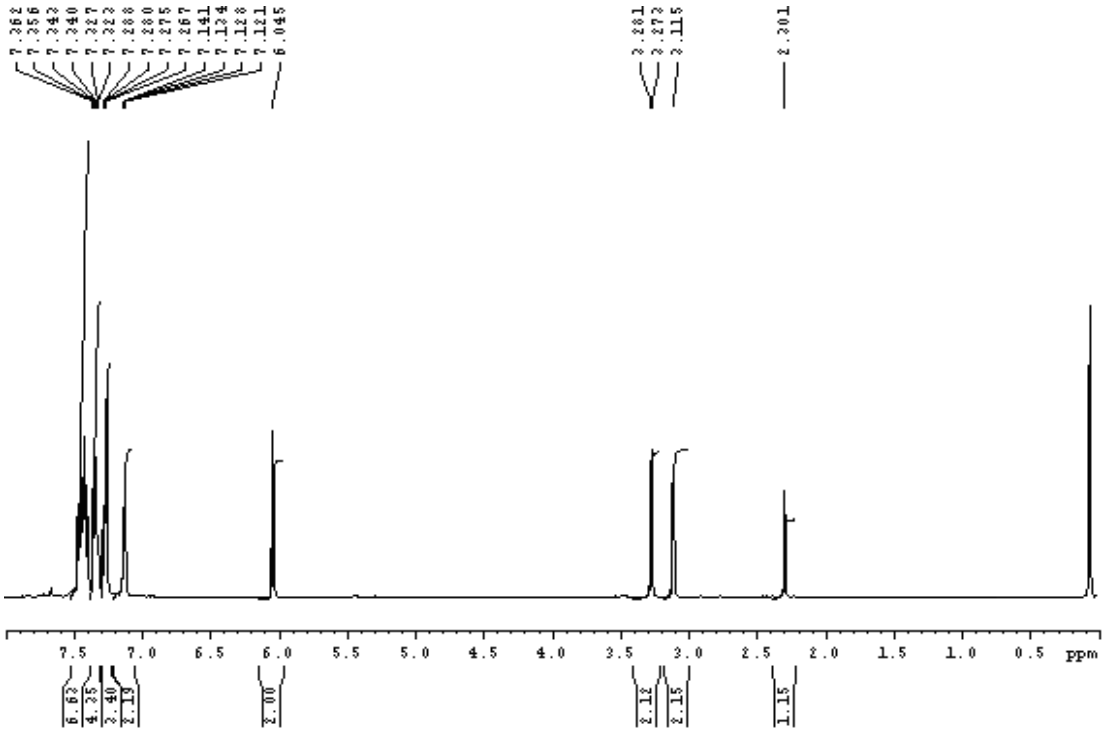
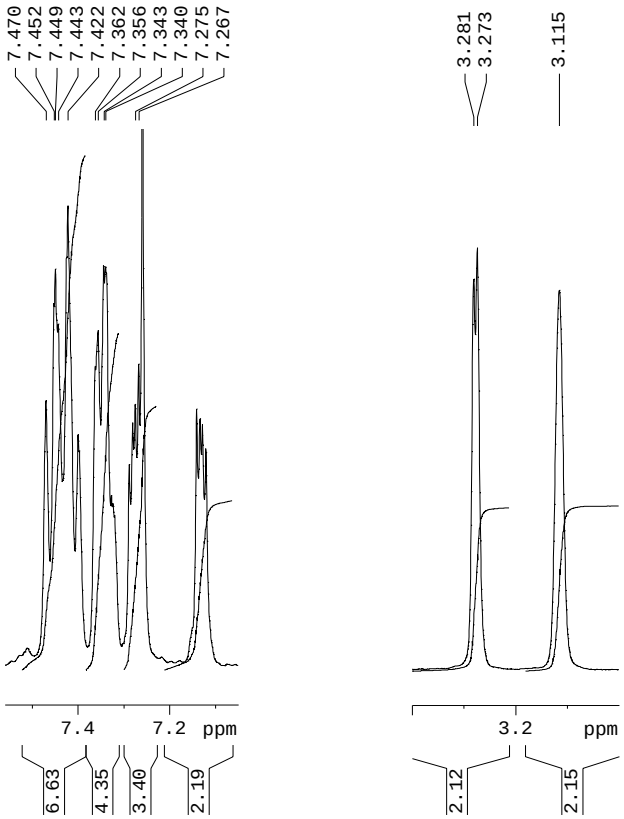
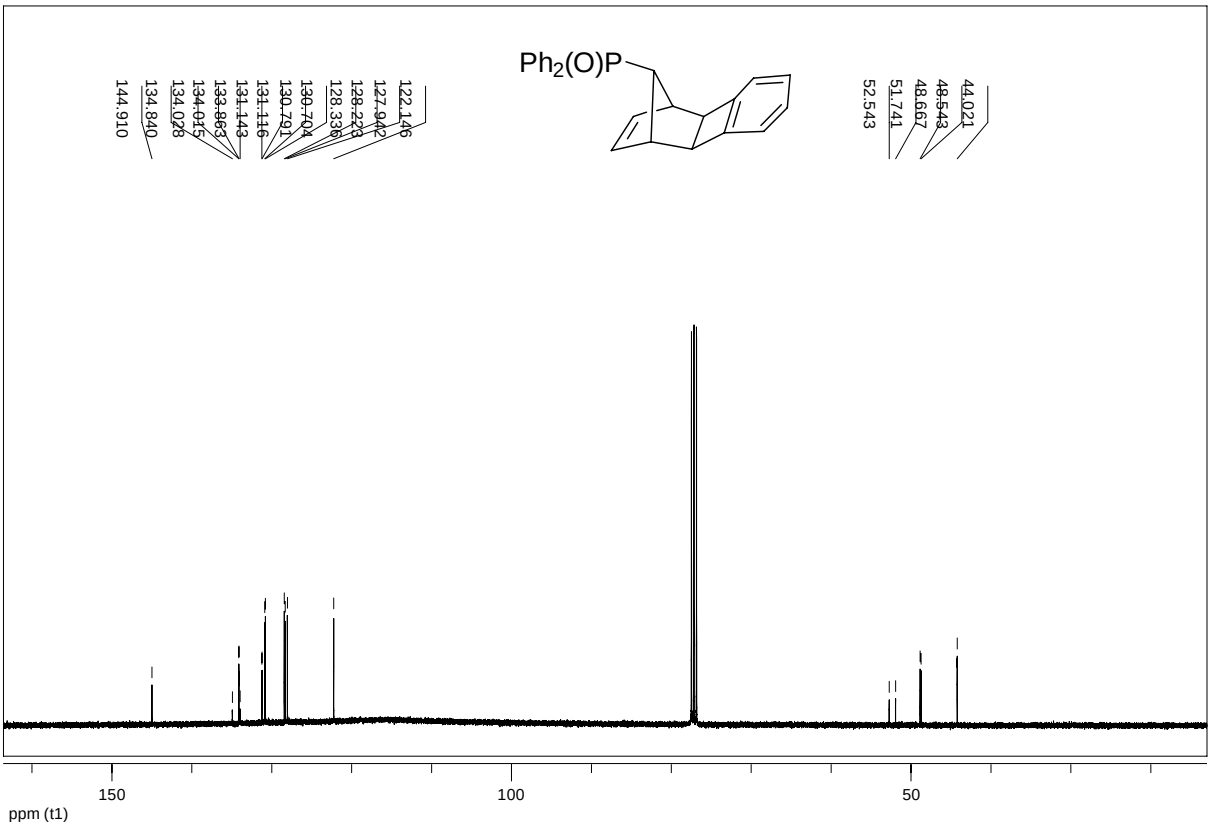


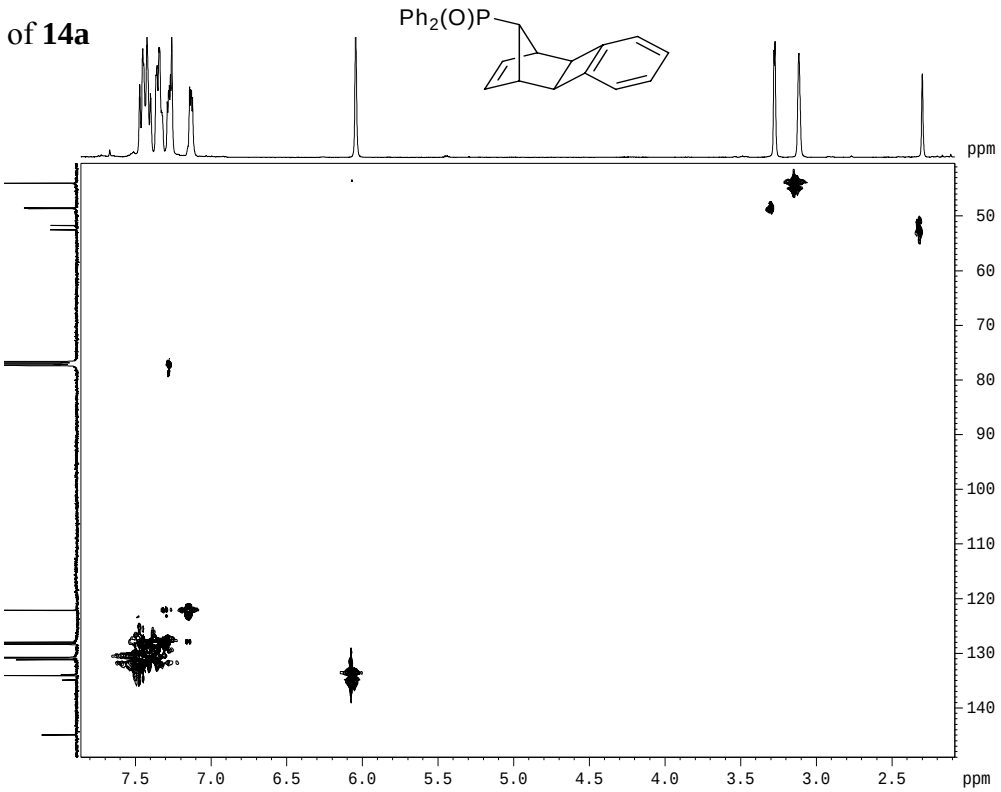


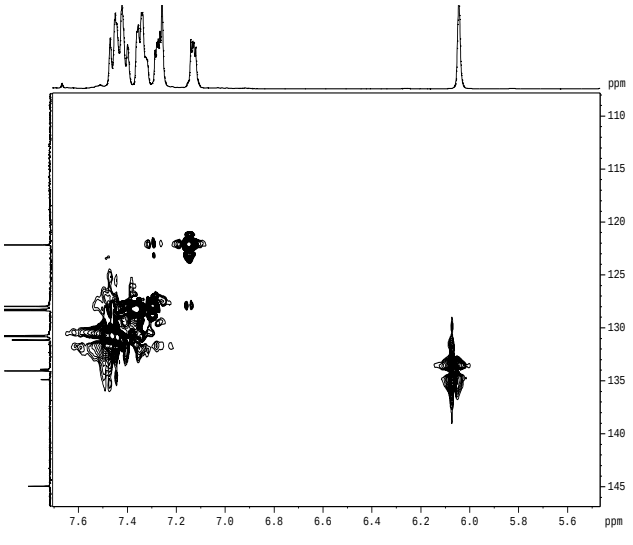


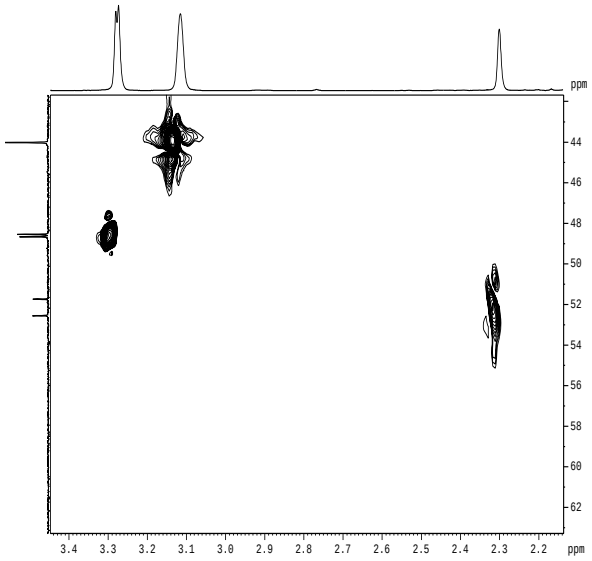
^{13}C-NMR of **14a**



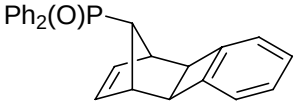
HSQC of **14a**

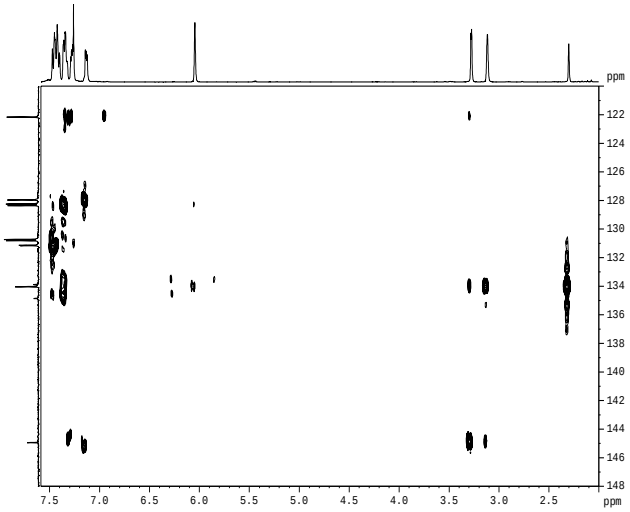


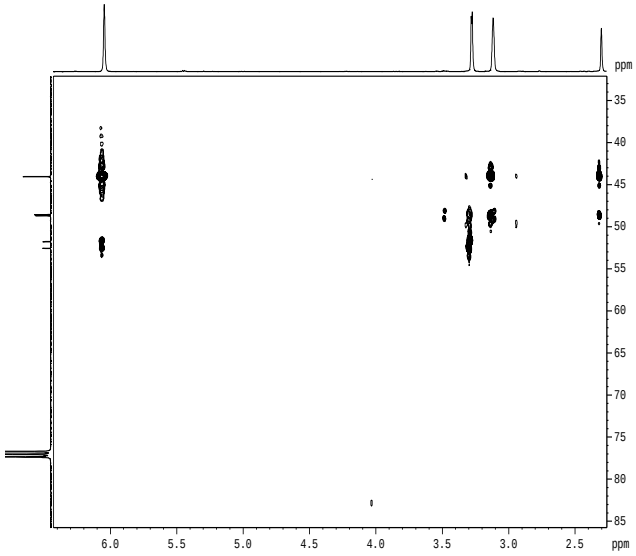




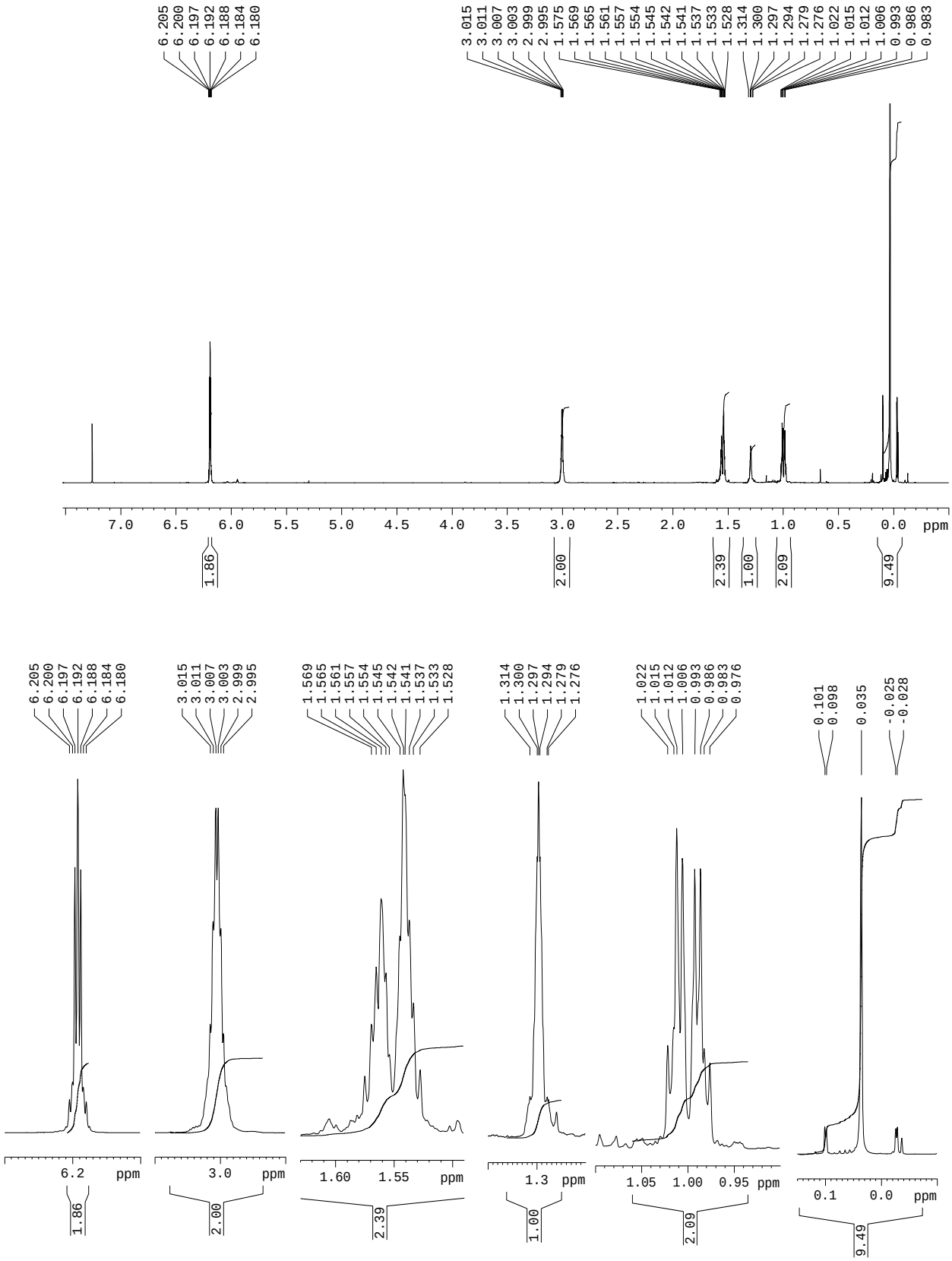
HMBC of **14a**



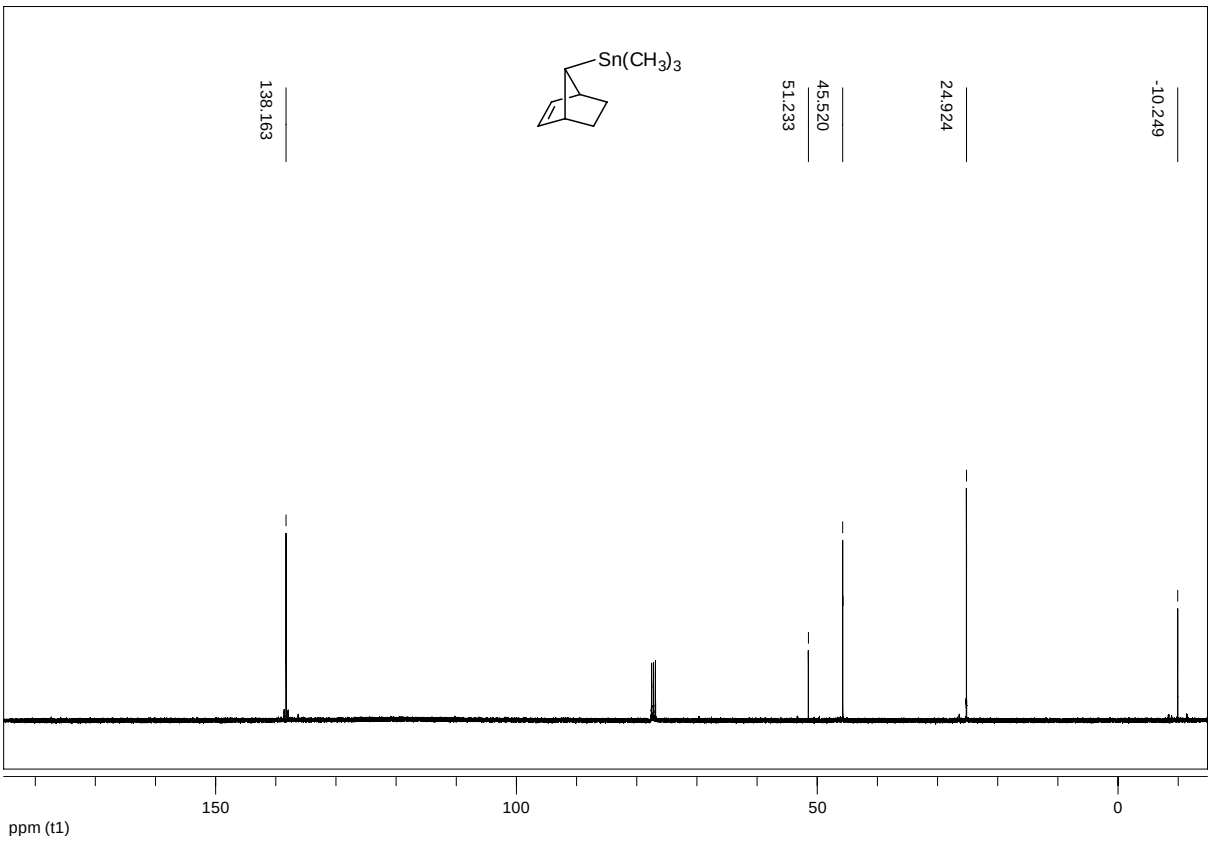




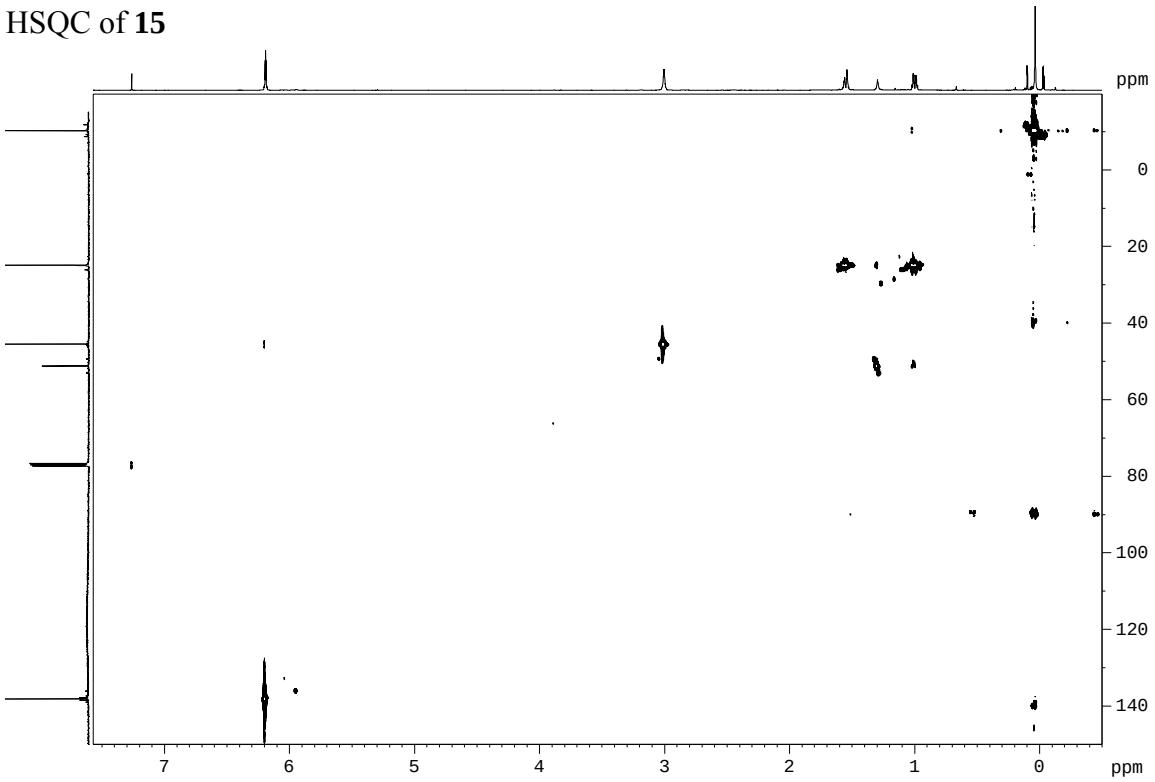
^{1}H-NMR of **15**


6.205
6.200
6.197
6.192
6.188
6.184
6.180
3.015
3.011
3.007
3.003
2.999
2.995
1.575
1.569
1.565
1.561
1.557
1.554
1.545
1.542
1.541
1.537
1.533
1.528
1.314
1.300
1.297
1.294
1.279
1.276
1.022
1.015
1.012
1.006
0.993
0.986
0.983
0.976
0.101
0.098
0.035
-0.025
-0.028
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.86
2.00
2.39
1.00
2.09
9.49
6.2 ppm
3.0 ppm
1.60 1.55 ppm
1.3 ppm
1.05 1.00 0.95 ppm
0.1 0.0 ppm

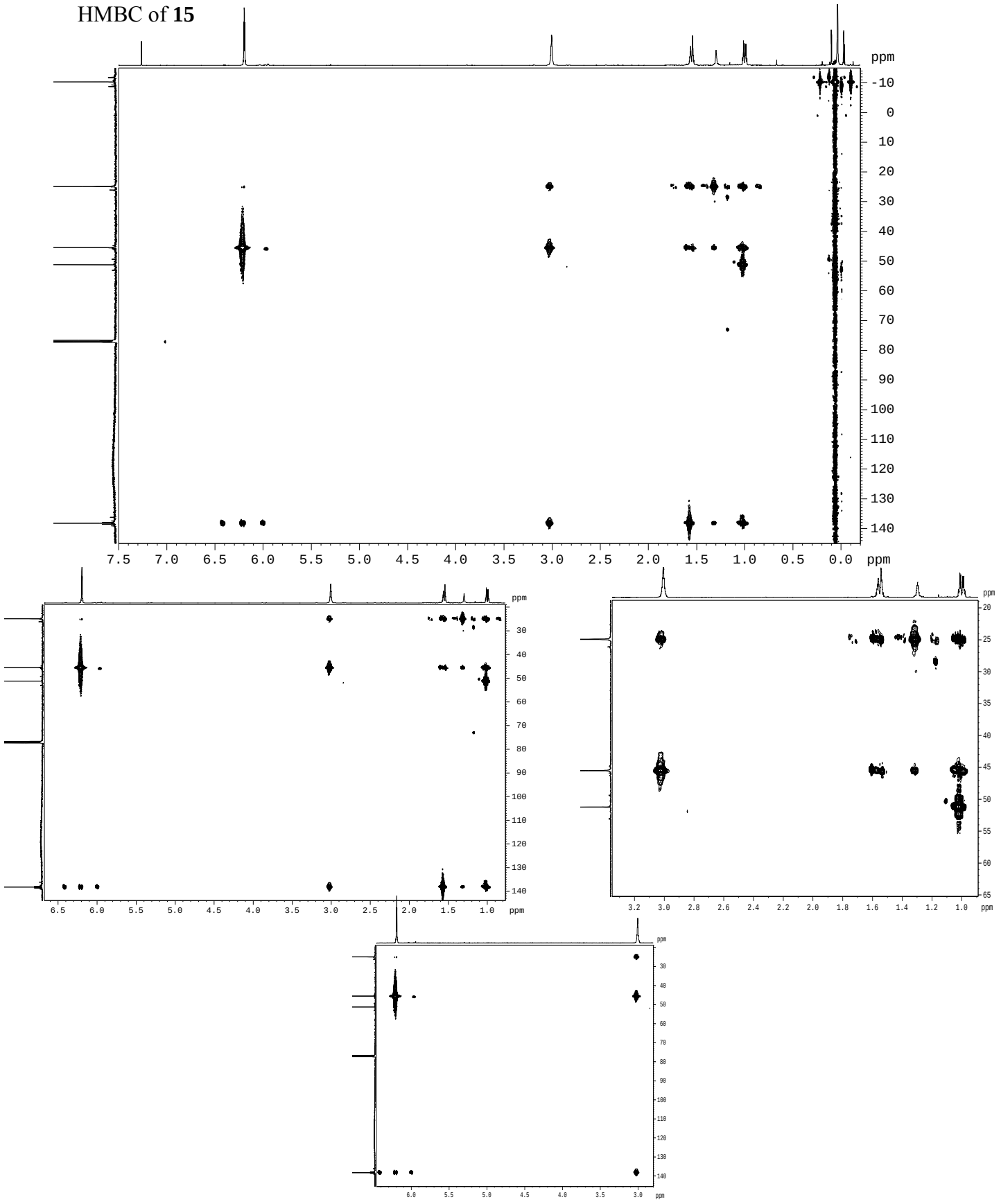
^{13}C-RMN of **15**



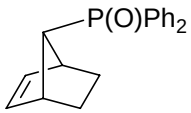
HSQC of **15**

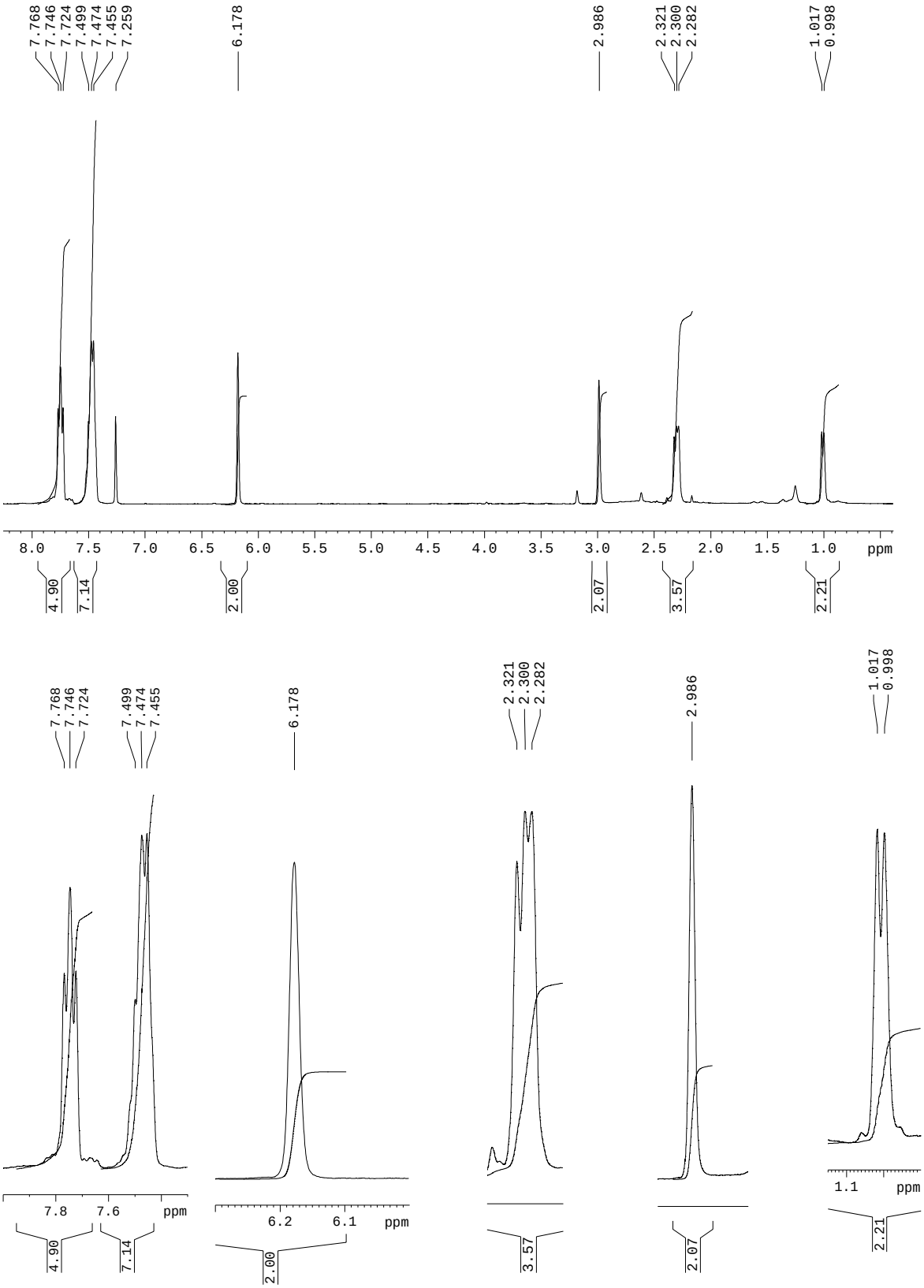


HMBC of **15**

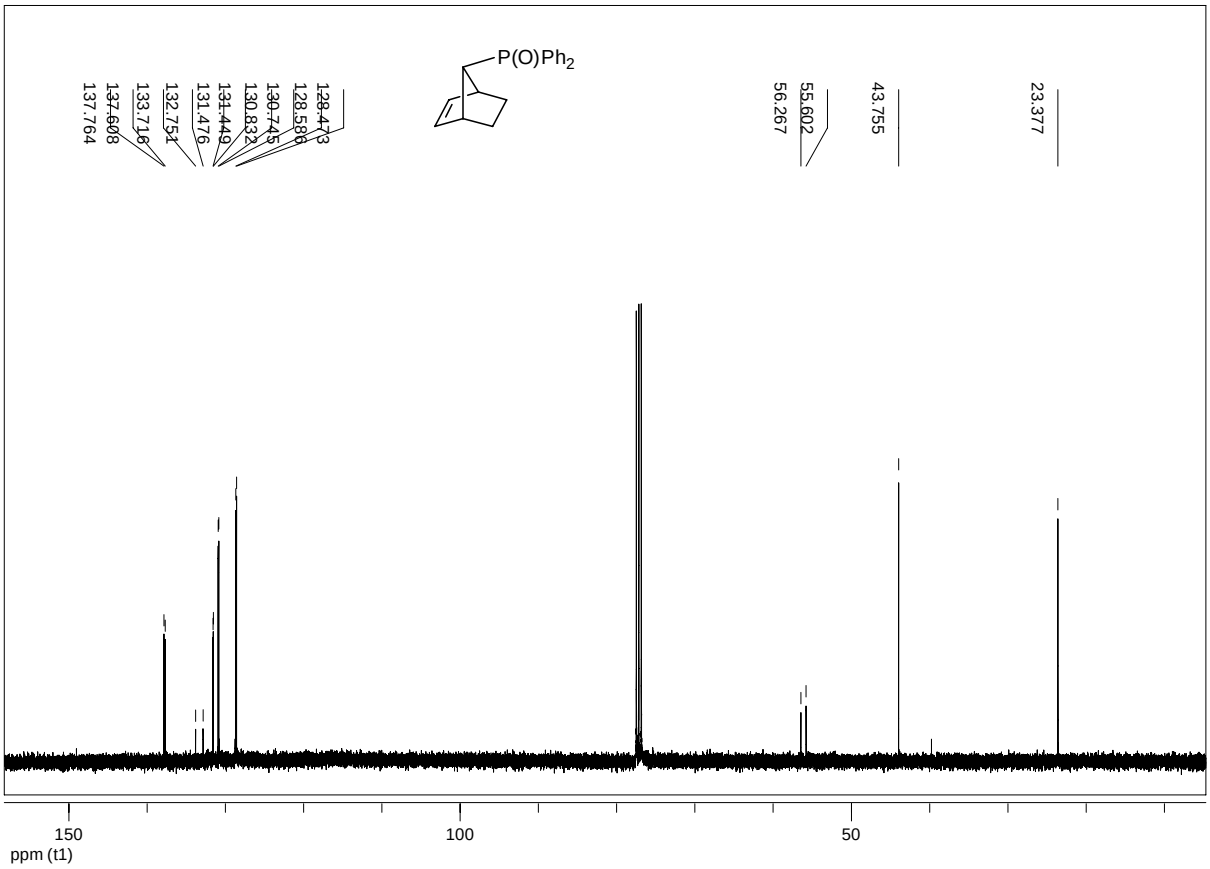


^{1}H-NMR of **16**

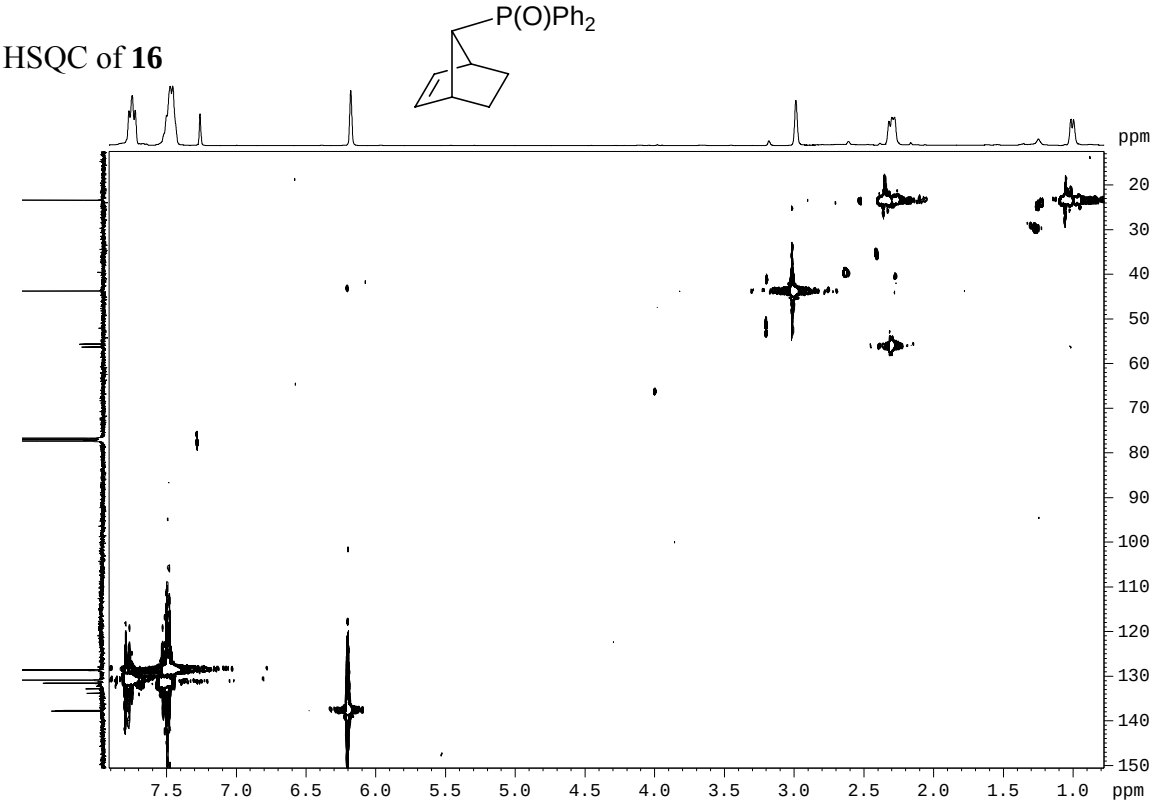


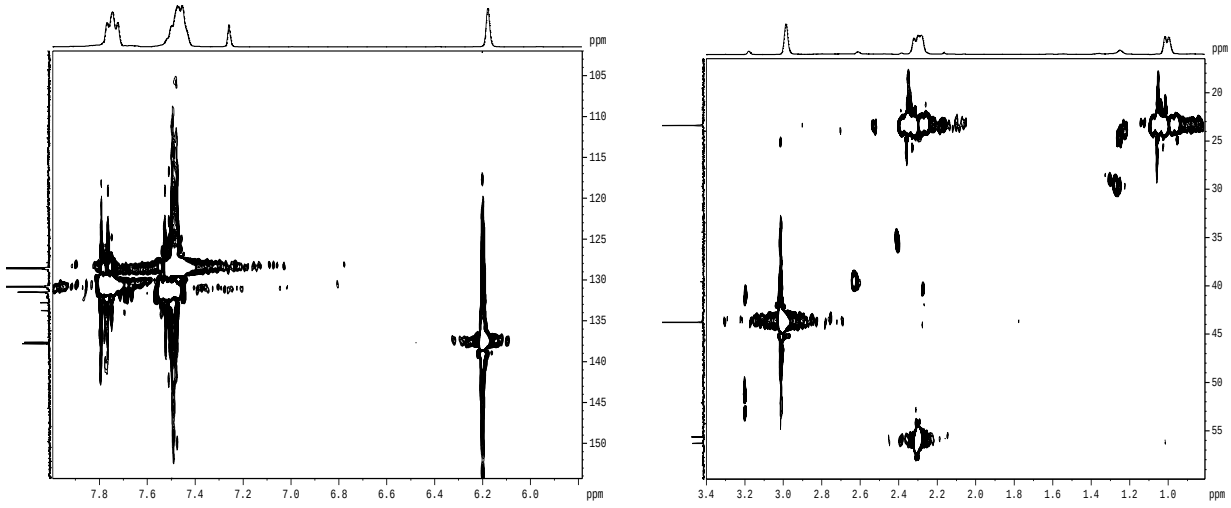


^{13}C-NMR of **16**

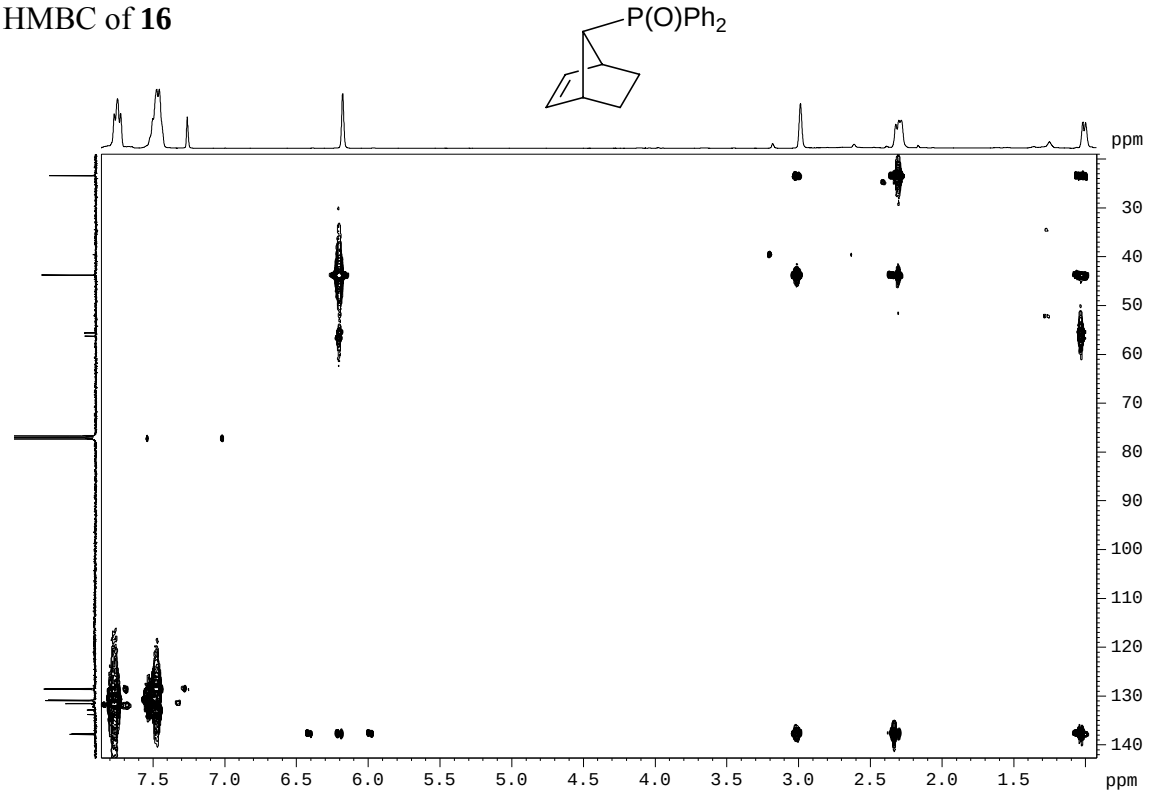


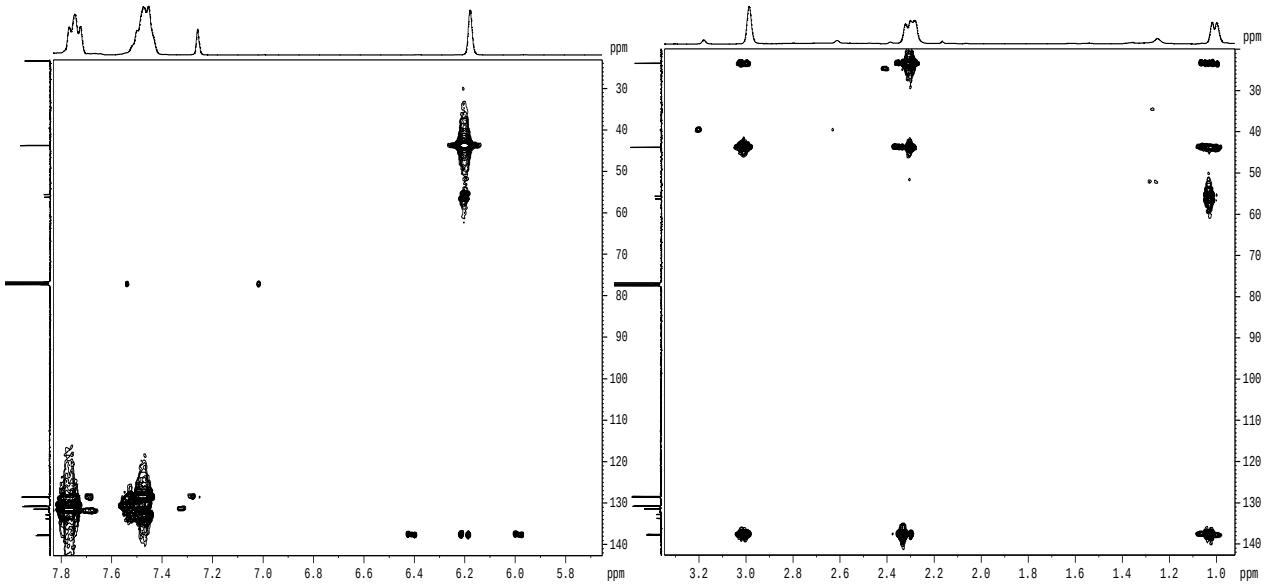
HSQC of **16**



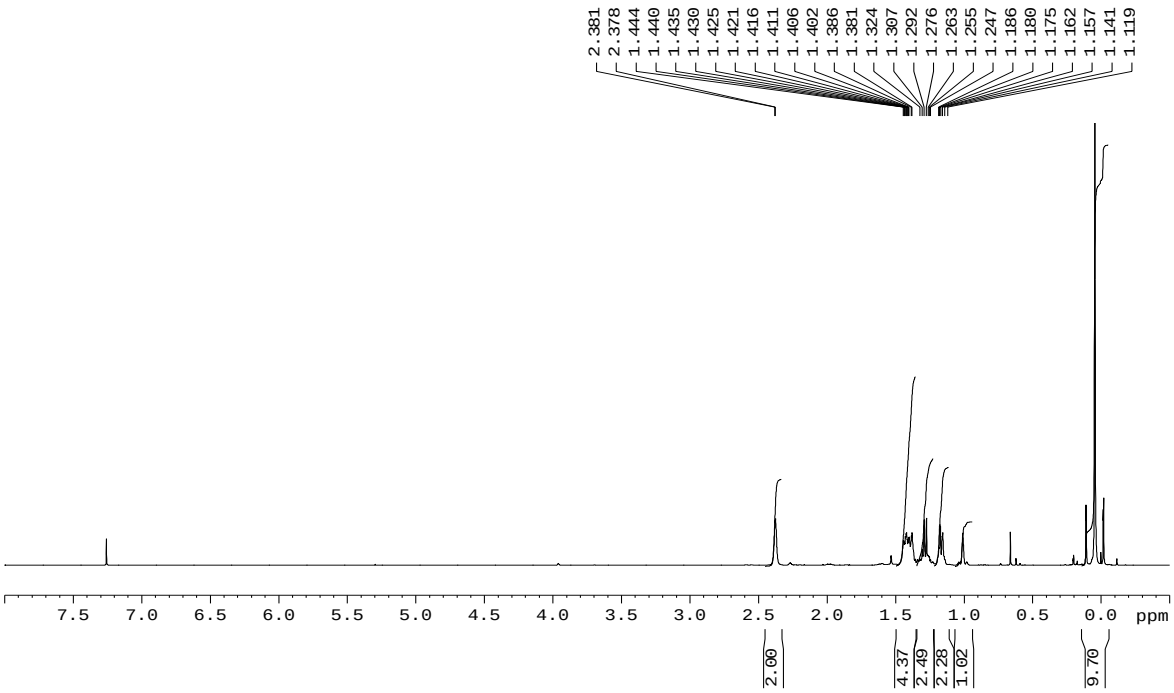


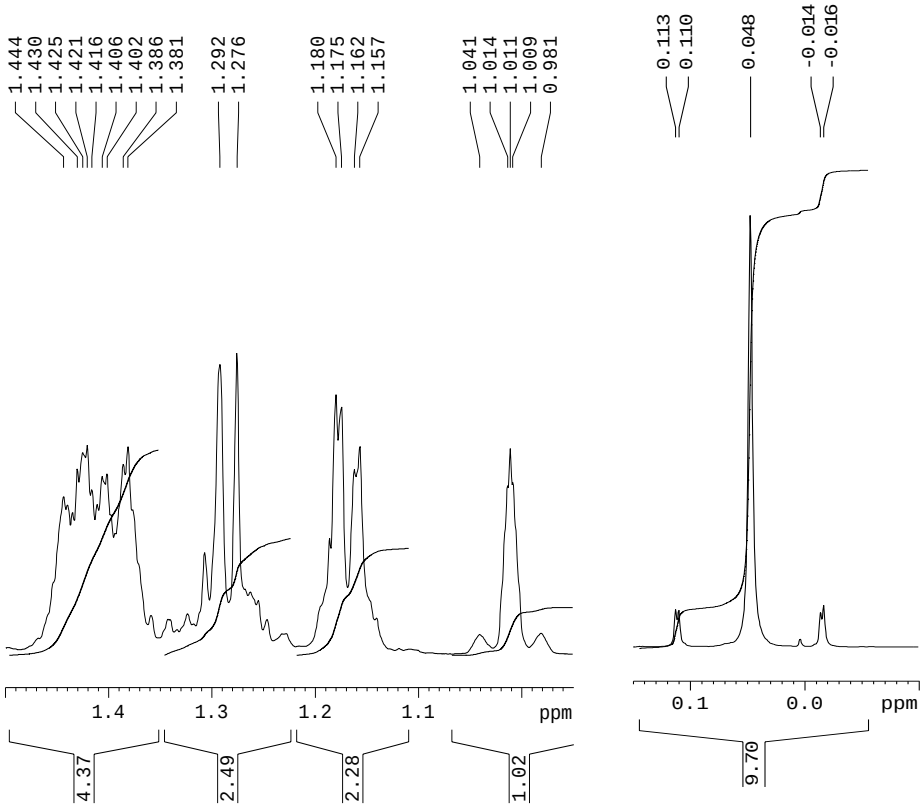
HMBC of **16**



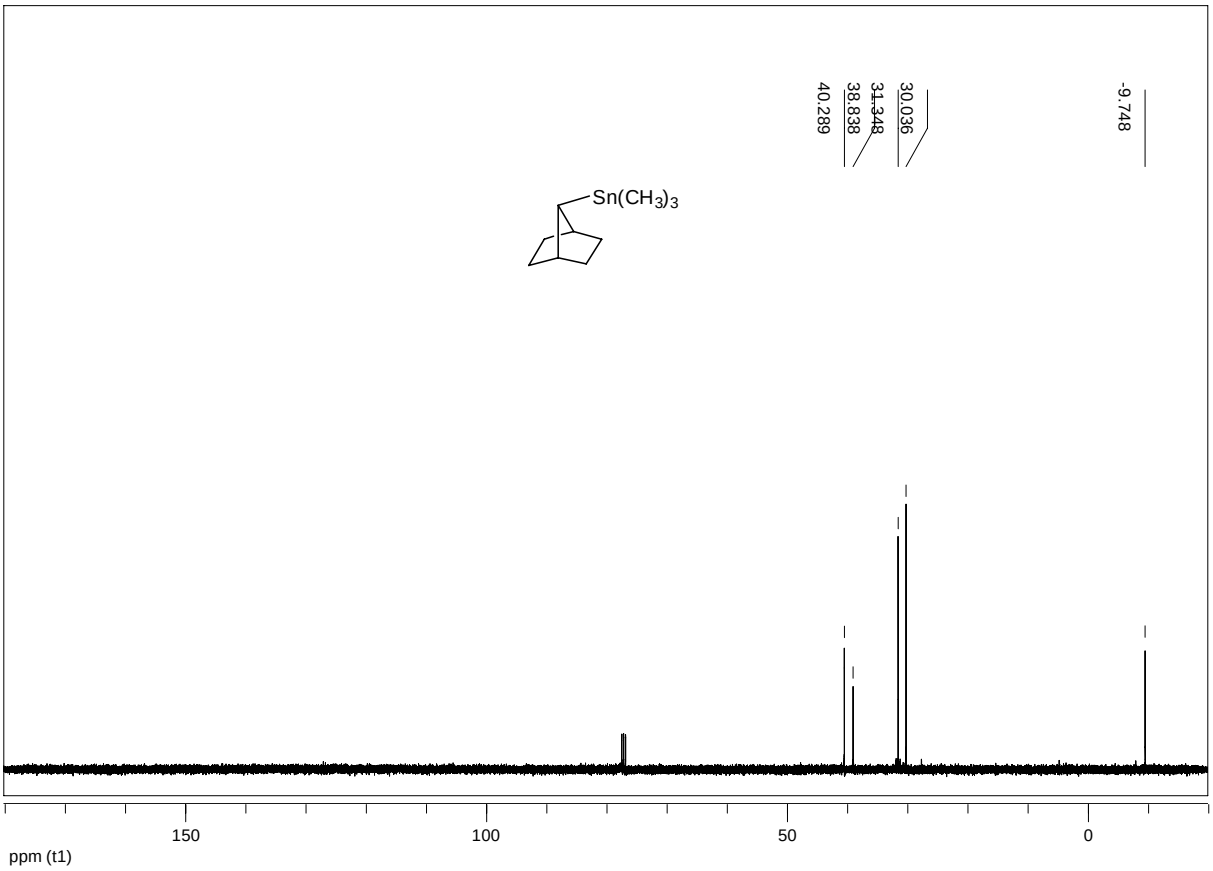


^{1}H-NMR of **17**

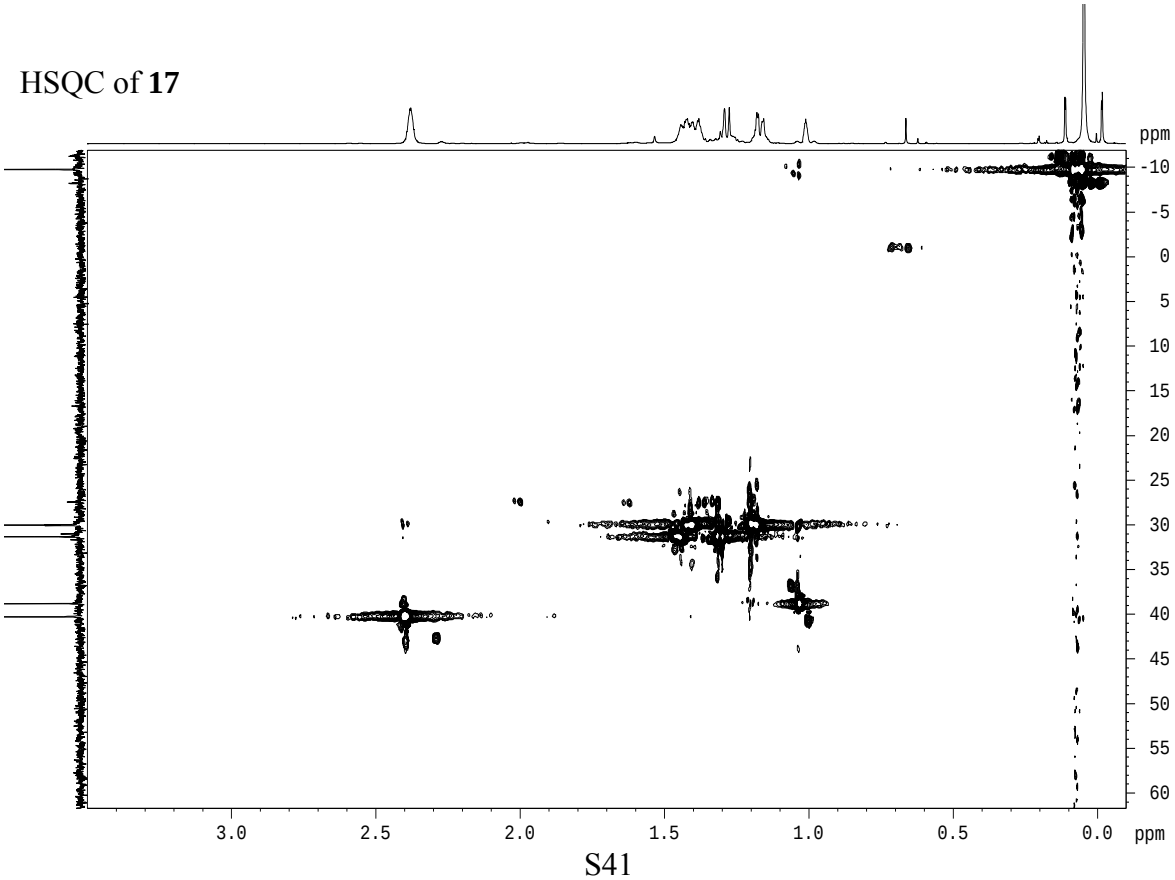


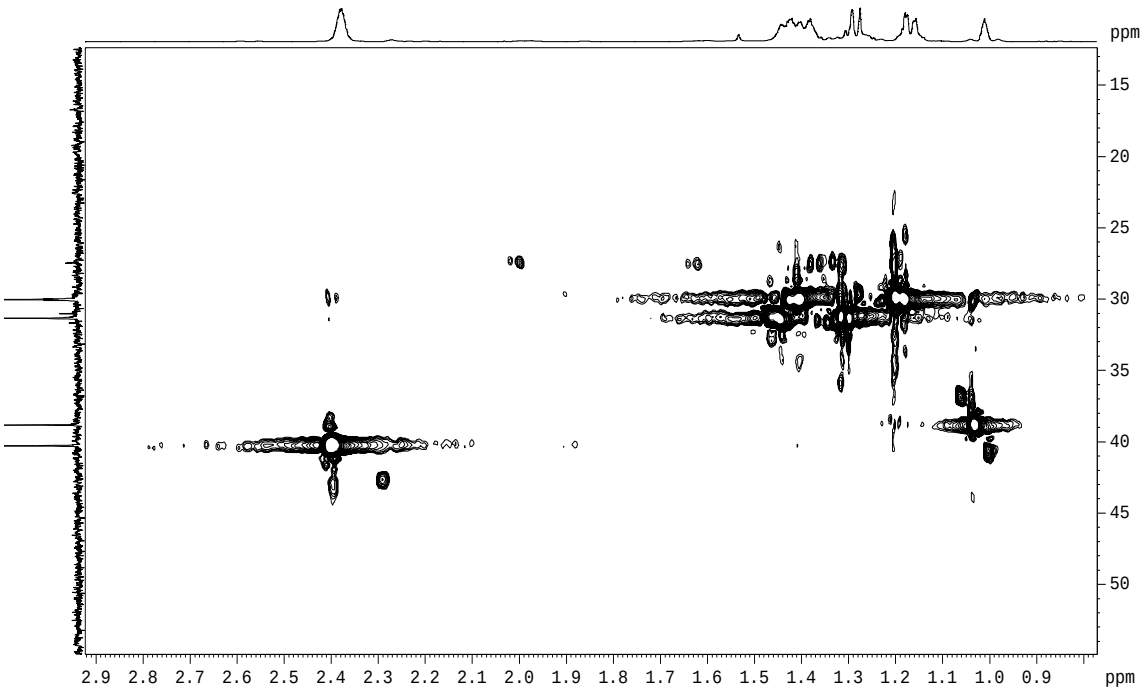


^{13}C-NMR of **17**

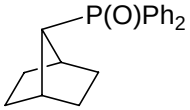


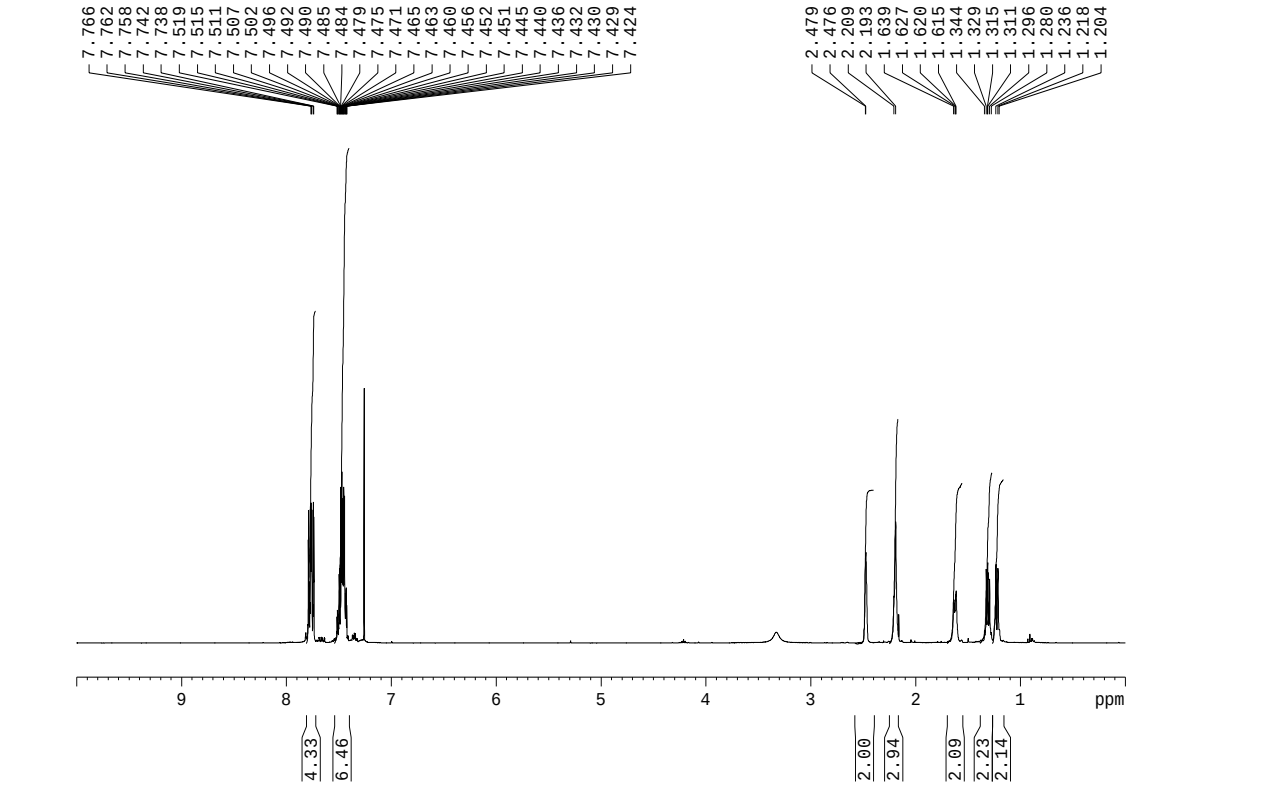
HSQC of **17**

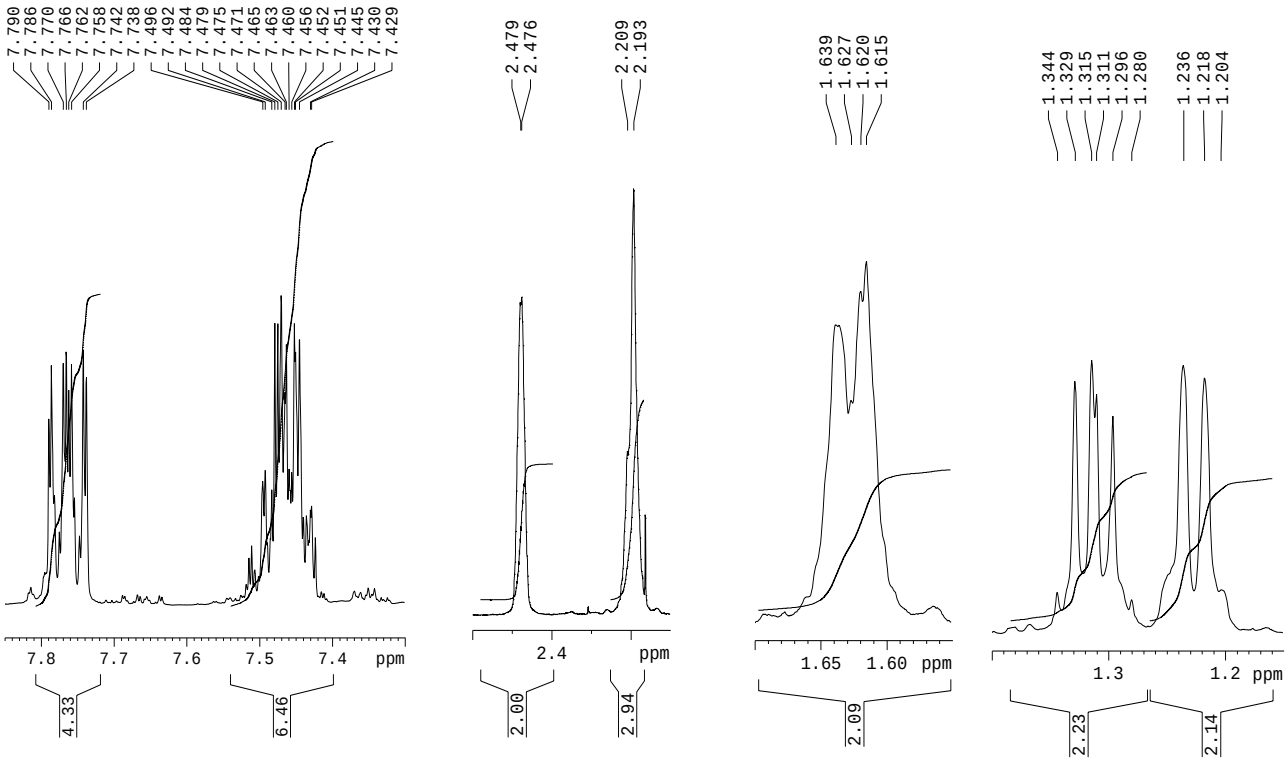




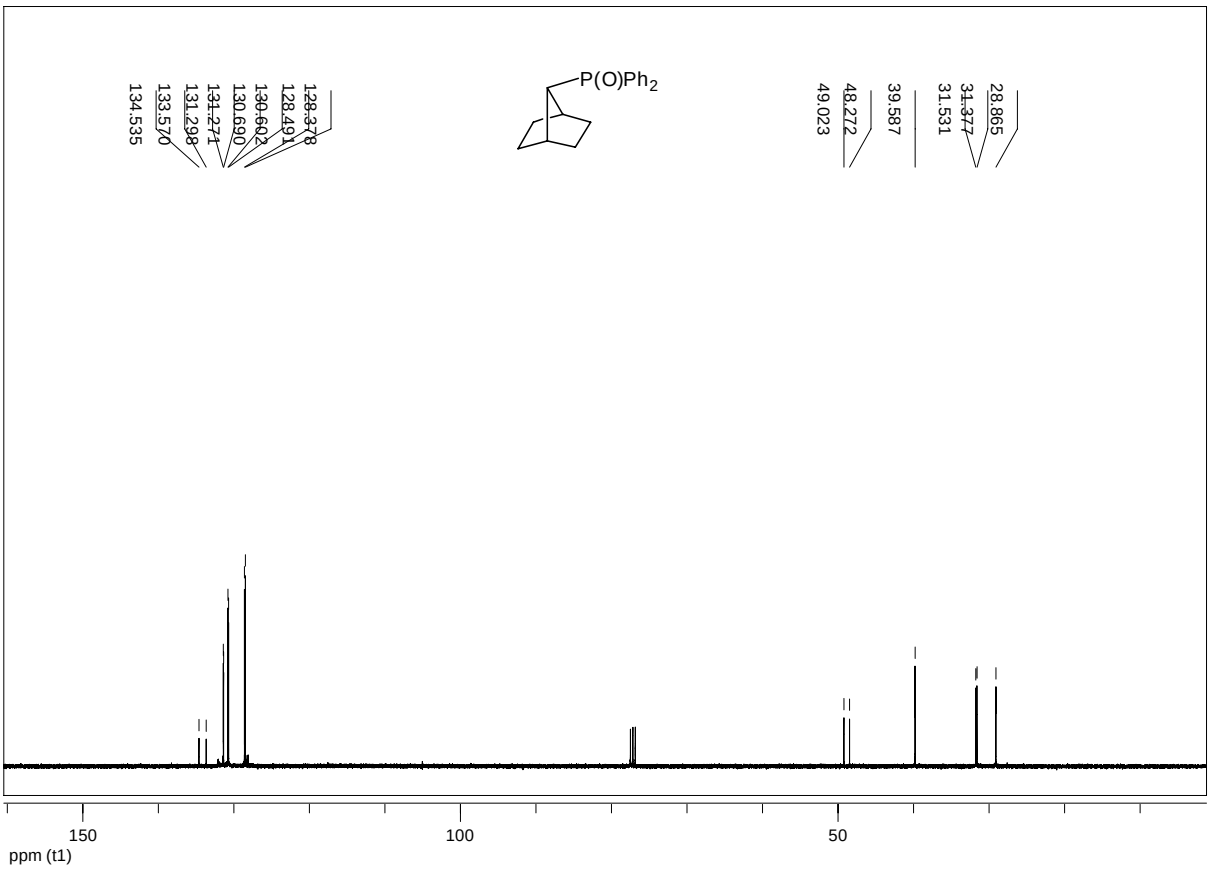
^{1}H-NMR of **18**


P(O)Ph2

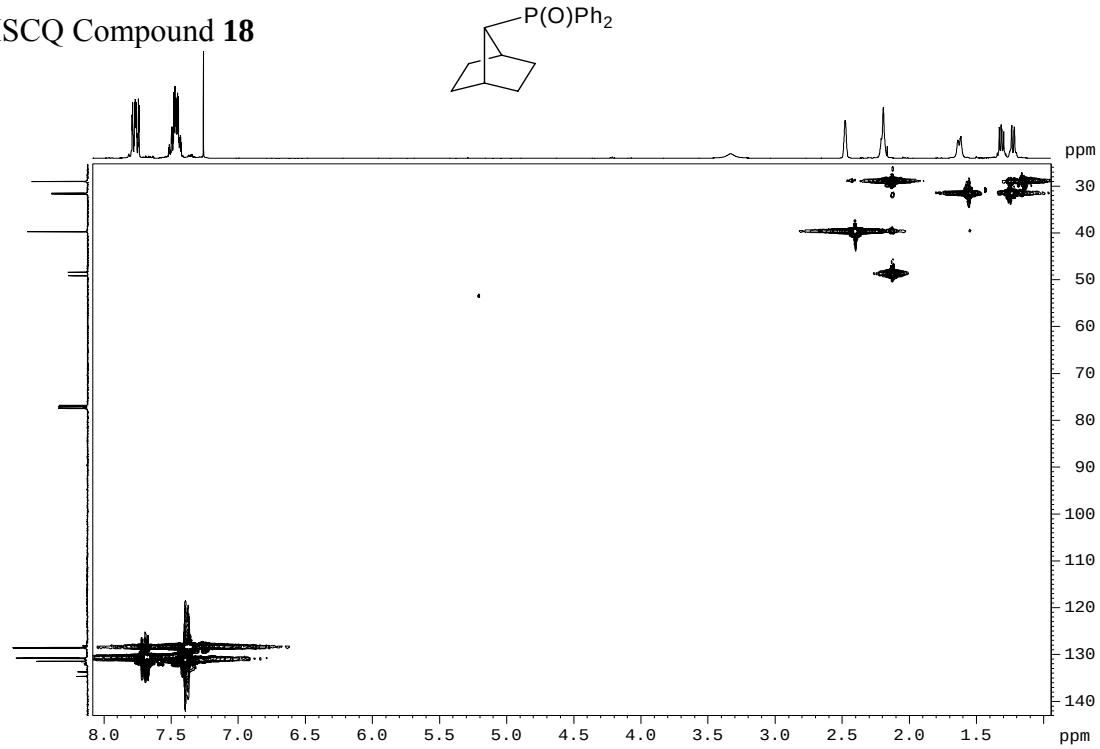

7.766
7.762
7.758
7.742
7.738
7.519
7.515
7.511
7.507
7.502
7.496
7.492
7.490
7.485
7.484
7.479
7.475
7.471
7.465
7.463
7.460
7.456
7.452
7.451
7.445
7.440
7.436
7.432
7.430
7.429
7.424
2.479
2.476
2.209
2.193
1.639
1.627
1.620
1.615
1.344
1.329
1.315
1.311
1.296
1.280
1.236
1.218
1.204
9
8
7
6
5
4
3
2
1
ppm
4.33
6.46
2.00
2.94
2.09
2.23
2.14

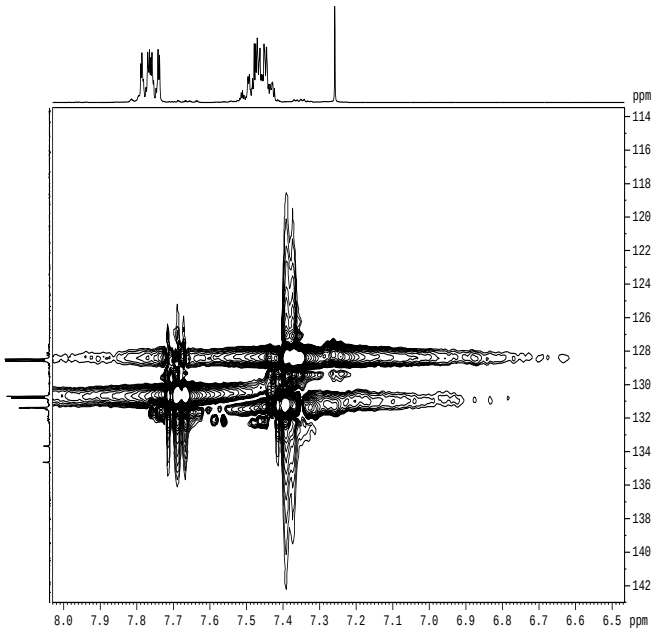

7.790
7.786
7.770
7.766
7.762
7.758
7.742
7.738
7.496
7.492
7.484
7.479
7.475
7.471
7.465
7.463
7.460
7.456
7.452
7.451
7.445
7.430
7.429
2.479
2.476
2.209
2.193
1.639
1.627
1.620
1.615
1.344
1.329
1.315
1.311
1.296
1.280
1.236
1.218
1.204
7.8
7.7
7.6
7.5
7.4
ppm
4.33
6.46
2.4
ppm
2.00
2.94
1.65
1.60
ppm
2.09
1.3
1.2
ppm
2.23
2.14

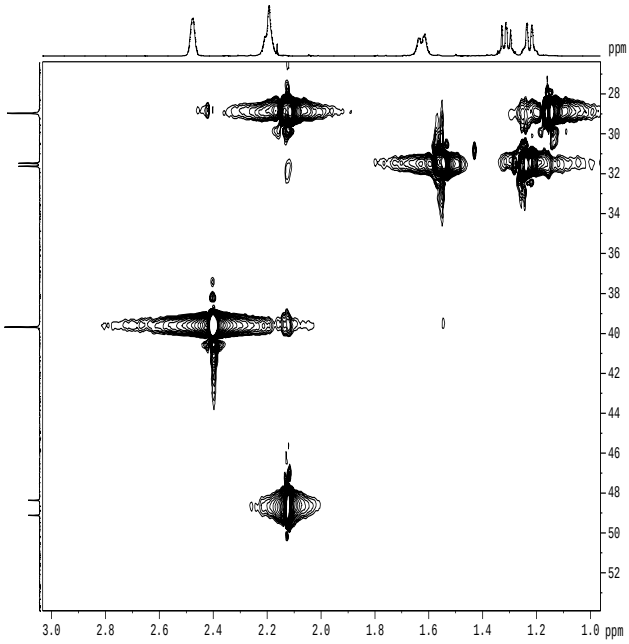
^{13}C-NMR of **18**



HSCQ Compound **18**







PART 3. XYZ COORDINATES OF THE SOLUTION PHASE STRUCTURES

coordinates in Angstrom, energies in kcal/mol

Gaussian03 data

7-anti-bromobenzonorbornene (**5**)

neutral

B3LYP/6-31+G*, -1880204.05
Zero Point Energy Correction 102.91
xyz coordinates:

C	0.044070	0.001446	0.024306
C	-0.010943	0.016376	1.576154
C	1.512900	-0.002759	1.776285
C	2.060348	0.797743	0.750754
C	0.873558	1.309921	-0.081449
C	3.429640	0.999948	0.654244
C	4.259274	0.392203	1.617308
C	3.716611	-0.400862	2.633533
C	2.326412	-0.612633	2.720266
C	-0.461380	1.467039	1.820288
C	0.057786	2.226736	0.846357
Br	-1.717957	0.026700	-0.894620
H	4.376513	-0.861421	3.368394
H	1.909053	-1.237336	3.510318
H	-0.577147	-0.775268	2.072843
H	0.003222	3.307254	0.736011
H	3.858438	1.611402	-0.140047
H	5.337514	0.542666	1.568869
H	-1.036646	1.785953	2.686297
H	1.105721	1.685790	-1.080856
H	0.538113	-0.876687	-0.397273

---

radical anion

B3LYP/6-31+G*, -1880231.34
Zero Point Energy Correction 99.57
xyz coordinates:

C	-0.019734	-0.022801	-0.028725
C	-0.041241	-0.040707	1.523129
C	1.472589	-0.079928	1.717180
C	2.032532	0.739254	0.668227
C	0.847765	1.259184	-0.141955
C	3.398694	1.023306	0.654704
C	4.226703	0.482041	1.652984
C	3.674642	-0.324231	2.687297
C	2.294911	-0.589186	2.722914
C	-0.431115	1.409485	1.829470
C	0.109861	2.200371	0.816864

Br	-1.812468	0.084228	-0.902705
H	4.326740	-0.744861	3.452699
H	1.877997	-1.196417	3.529581
H	-0.617387	-0.837491	2.004028
H	0.345854	3.262265	0.879946
H	3.828984	1.653680	-0.126785
H	5.299216	0.674966	1.630681
H	-0.698849	1.736359	2.833790
H	1.066556	1.624743	-1.150188
H	0.422848	-0.910049	-0.485154

---

radical (anti-19)

B3LYP/6-31+G*, -266373.77
Zero Point Energy Correction 100.97
xyz coordinates:

C	0.037708	0.044084	-0.036006
C	-0.041178	-0.056500	1.499068
C	1.457269	-0.099991	1.808576
C	1.795248	-1.221851	0.823575
C	1.120149	-0.643322	-0.434191
C	-0.323009	-1.536883	1.831329
C	0.817435	-2.260440	1.411645
C	-1.388195	-2.178577	2.448565
C	-1.308579	-3.573913	2.636207
C	-0.181130	-4.289258	2.220746
C	0.903859	-3.632572	1.604491
H	-0.137616	-5.366758	2.378848
H	1.785447	-4.193938	1.293575
H	2.833948	-1.547108	0.723193
H	-0.713439	0.528819	-0.656227
H	-2.265147	-1.625036	2.785571
H	-2.134492	-4.099790	3.114968
H	1.448908	-0.844110	-1.451752
H	-0.669693	0.676108	2.011992
H	1.864810	-0.044353	2.820660

TS

B3LYP/6-31+G*, -1880230.58, 1 imaginary freq.
Zero Point Energy Correction 99.71
xyz coordinates:

C	0.001895	0.022784	-0.004748
C	0.006694	-0.015592	1.528727
C	1.535968	-0.022759	1.814325
C	1.860096	-1.151771	0.809004
C	1.109730	-0.674260	-0.433625
C	-0.248367	-1.483005	1.879363
C	0.942814	-2.181917	1.461674
C	-1.340721	-2.170278	2.380233

C	-1.262054	-3.576247	2.539082
C	-0.081271	-4.265540	2.144913
C	1.013914	-3.579551	1.608027
Br	2.414520	1.809693	1.482193
H	-0.026092	-5.347863	2.268316
H	1.905398	-4.129805	1.300311
H	2.908773	-1.440598	0.691772
H	-0.875406	0.299568	-0.586281
H	-2.245405	-1.636882	2.680698
H	-2.096272	-4.125132	2.974152
H	1.300901	-1.061151	-1.432826
H	-0.596860	0.729700	2.056031
H	1.821858	-0.223215	2.847748

****

****

7-syn-bromobenzonorbornene (**6**)

neutral

B3LYP/6-31+G*, -1880206.02
Zero Point Energy Correction 103.25
xyz coordinates:

C	0.010483	0.010103	-0.007616
C	0.011933	-0.001192	1.533112
C	1.556789	0.016180	1.682998
C	1.778571	-1.260557	0.828253
C	1.051077	-0.732327	-0.422793
C	-0.281897	-1.442887	1.960302
C	0.809132	-2.220454	1.525294
C	-1.375390	-2.027342	2.579009
C	-1.366182	-3.425375	2.764875
C	-0.283920	-4.196666	2.333117
C	0.824184	-3.594807	1.701607
Br	2.213442	-0.116199	3.563081
H	2.041190	0.912994	1.294290
H	-0.295153	-5.275764	2.484884
H	1.666867	-4.200512	1.367013
H	2.804936	-1.607520	0.685713
H	-0.734219	0.524117	-0.611693
H	-2.221736	-1.429572	2.918557
H	-2.213700	-3.908469	3.250606
H	1.349883	-0.962453	-1.443315
H	-0.557902	0.789650	2.027128

---

radical anion

B3LYP/6-31+G*, -1880233.13
Zero Point Energy Correction 99.86
xyz coordinates:

C	-0.000681	0.030072	0.034743
C	0.059575	0.050233	1.573633
C	1.600261	0.072619	1.695028
C	1.833629	-1.212716	0.868825
C	1.096086	-0.747931	-0.401123
C	-0.240005	-1.380816	1.996724
C	0.870460	-2.172144	1.553498
C	-1.366855	-1.993866	2.539188
C	-1.390283	-3.394194	2.676928
C	-0.296982	-4.175210	2.234707
C	0.828898	-3.560461	1.655928
Br	2.265673	-0.055596	3.595298
H	2.087806	0.969390	1.314800
H	-0.321588	-5.258615	2.352759
H	1.664707	-4.171365	1.307951
H	2.868080	-1.549447	0.749019
H	-0.945297	0.161098	-0.495613
H	-2.221012	-1.399355	2.870563
H	-2.253010	-3.878970	3.134068
H	1.143014	-1.327415	-1.324787
H	-0.494087	0.845637	2.082282

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radical (syn-19)

B3LYP/6-31+G*, -266373.98
Zero Point Energy Correction 101.01
xyz coordinates:

C	-0.002240	-0.008262	-0.000213
C	-0.003824	-0.051598	1.386507
C	1.204613	-0.051801	2.114803
C	2.429829	-0.007479	1.465319
C	2.437450	0.040522	0.055863
C	1.240255	0.039911	-0.665633
C	-1.134003	-0.115393	2.422301
C	-1.015746	-1.488601	3.127947
C	0.137081	-1.488804	3.822918
C	0.816989	-0.115856	3.597959
C	-0.472068	0.708634	3.531045
H	-1.009039	1.040689	4.422414
H	1.265899	0.078880	-1.754492
H	-0.932935	-0.005383	-0.568475
H	-2.132406	0.163466	2.075687
H	0.562350	-2.297740	4.414553
H	3.367102	-0.003688	2.022630
H	3.388066	0.080756	-0.475583
H	-1.737459	-2.297545	3.028174
H	1.590072	0.162554	4.318752

TS

B3LYP/6-31+G*, -1880232.30, 1 imaginary freq
Zero Point Energy Correction 99.30
xyz coordinates:

C	-0.291247	-0.642524	-2.373517
C	-0.294888	-0.651545	-0.982479
C	0.936543	-0.644356	-0.255514
C	2.152834	-0.606137	-0.932671
C	2.154473	-0.557239	-2.339095
C	0.938189	-0.579338	-3.057177
C	-1.395178	-0.841462	0.051305
C	-1.192711	-2.244144	0.630967
C	0.036392	-2.274600	1.310104
C	0.577170	-0.834159	1.214572
C	-0.789115	-0.111864	1.265768
Br	-0.560056	1.970877	1.050182
H	-1.344522	-0.178750	2.200017
H	0.950377	-0.535037	-4.146234
H	-1.227423	-0.664926	-2.935381
H	-2.413798	-0.577870	-0.247755
H	0.686677	-3.145390	1.433881
H	3.097830	-0.603790	-0.385546
H	3.100545	-0.498205	-2.877351
H	-1.818904	-3.088151	0.348655
H	1.330975	-0.532983	1.949376

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anti radical (anti-**19**) <-> syn radical (syn-**19**)
isomerization TS

B3LYP/6-31+G*, -266372.02, 1 imaginary freq
Zero Point Energy Correction 100.24
xyz coordinates:

C	1.682852	-0.000006	1.261427	-0.396866
C	1.272113	-1.137052	0.338594	-0.108188
C	-0.195679	-0.706159	0.139468	-0.340215
C	-0.195682	0.706191	0.139475	-0.342110
C	1.272121	1.137052	0.338596	-0.107935
C	-1.375400	1.418397	-0.004144	-0.020749
C	-2.577731	0.697674	-0.149717	-0.090086
C	-2.577722	-0.697692	-0.149715	-0.089967
C	-1.375377	-1.418395	-0.004142	-0.021007
C	2.032417	-0.671207	-0.926279	-0.214974
C	2.032424	0.671208	-0.926275	-0.214859
H	-3.515809	-1.236124	-0.260661	0.209044
H	-1.383731	-2.506324	0.000647	0.213629
H	1.435443	-2.167811	0.656154	0.217554
H	2.417820	1.336752	-1.691984	0.220721
H	-1.383781	2.506327	0.000654	0.213657
H	-3.515826	1.236092	-0.260663	0.209044
H	2.417805	-1.336750	-1.691993	0.220742
H	1.435477	2.167806	0.656162	0.217540
H	2.126577	-0.000035	2.247945	0.224919

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exo-anti-7-bromobenzocyclobutanorbornene (**7**)

neutral

B3LYP/6-31+G*, -1928767.87
Zero Point Energy Correction 125.17
xyz coordinates:

C	-0.144201	0.222298	0.211625
C	0.047704	-0.340868	1.467765
C	1.307948	-0.423550	2.066783
C	2.457848	0.054853	1.449725
C	2.278069	0.638906	0.180230
C	1.010880	0.720542	-0.422795
C	-0.660231	-1.043946	2.624810
C	-1.476058	-0.195462	3.665699
C	-0.369094	0.763097	4.135975
C	0.580147	-0.334960	4.643782
C	0.781960	-1.139719	3.309668
C	-0.383498	-1.203928	5.450889
C	-1.594097	-1.120971	4.875768
H	0.042969	1.409191	3.362496
Br	-0.941422	2.062569	5.525239
H	-2.397263	0.255280	3.285531
H	-0.084472	-1.844848	6.278063
H	-2.491175	-1.680393	5.134074
H	1.498902	-0.008936	5.139640
H	3.448929	-0.011523	1.899889
H	3.142538	1.034172	-0.353785
H	0.924851	1.175854	-1.409691
H	-1.119437	0.283931	-0.272542
H	1.184896	-2.141984	3.496678
H	-1.165333	-1.986293	2.382729

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radical anion

B3LYP/6-31+G*, -1928789.60
Zero Point Energy Correction 121.23
xyz coordinates:

C	-0.105229	-0.201984	-3.259194
C	0.112411	-0.712759	-1.948585
C	1.358770	-0.797679	-1.357499
C	2.563396	-0.386699	-1.994283
C	2.345982	0.240757	-3.278418
C	1.091418	0.327679	-3.872809
C	-0.597318	-1.413456	-0.797894
C	-1.427945	-0.587212	0.253798

C	-0.320277	0.372214	0.720548
C	0.633565	-0.720219	1.231571
C	0.837619	-1.508149	-0.115907
C	-0.326327	-1.595311	2.035170
C	-1.538111	-1.517581	1.459782
H	0.088009	1.017446	-0.053114
Br	-0.903119	1.676459	2.130205
H	-2.353060	-0.134580	-0.115309
H	-0.027150	-2.241469	2.858123
H	-2.428847	-2.086907	1.718146
H	1.545900	-0.386079	1.734498
H	3.536779	-0.370378	-1.507266
H	3.204351	0.646919	-3.818113
H	1.015147	0.798610	-4.855374
H	-1.088941	-0.050620	-3.700060
H	1.225646	-2.523531	0.076936
H	-1.096459	-2.370353	-1.030278

---

anti radical (anti-**20**)

B3LYP/6-31+G*, -314935.90
Zero Point Energy Correction 122.37
xyz coordinates:

C	-0.007095	-0.005691	0.019728
C	0.018830	-0.002683	1.553485
C	1.559909	0.013131	1.900787
C	2.037090	-1.431837	1.412247
C	0.699715	-2.060725	0.854294
C	0.395643	-1.221523	-0.393319
C	-0.315708	-1.458501	1.802969
C	1.989833	-0.427724	3.297647
C	2.084183	-0.022668	4.624312
C	2.621271	-0.966367	5.522035
C	3.038214	-2.238319	5.093134
C	2.940449	-2.632588	3.744045
C	2.405316	-1.692259	2.870982
H	-0.664967	-1.892251	2.738011
H	-0.573785	0.765719	2.058596
H	0.584298	-1.545182	-1.415561
H	-0.214929	0.868052	-0.595653
H	0.720159	-3.147298	0.728745
H	3.276781	-3.619728	3.425489
H	3.451283	-2.932568	5.825089
H	2.721204	-0.706158	6.575914
H	1.772905	0.963198	4.971069
H	2.858504	-1.474801	0.686171
H	2.077010	0.885736	1.482581

---

syn radical (syn-**20**)

B3LYP/6-31+G*, -314937.12

Zero Point Energy Correction 122.58
xyz coordinates:

C	-0.022050	0.004461	0.001306
C	-0.023006	0.014466	1.399193
C	1.151230	-0.008869	2.143224
C	2.350614	-0.048392	1.404936
C	2.351506	-0.058566	-0.000600
C	1.153074	-0.029248	-0.740893
C	-1.545889	0.066825	1.497045
C	-2.298550	-1.257998	1.849677
C	-3.744986	-1.031739	1.379686
C	-3.743416	-1.041756	0.031076
C	-2.296214	-1.275806	-0.432431
C	-1.544635	0.054658	-0.099368
C	-1.858626	-2.171667	0.716112
H	-2.036752	-3.247879	0.724228
H	-2.173675	-1.607526	2.878866
H	-4.586511	-0.850978	-0.631992
H	-4.589502	-0.830897	2.037944
H	-2.169461	-1.641440	-1.455783
H	1.170740	-0.028306	-1.831230
H	3.305554	-0.084891	-0.527353
H	3.303987	-0.067200	1.933229
H	1.167572	0.007557	3.233460
H	-1.972851	0.926569	-0.608075
H	-1.974275	0.946756	1.991568

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anti radical (anti-**20**) <-> syn radical (syn-**20**)
isomerization TS

B3LYP/6-31+G*, -314935.47, 1 imaginary freq
Zero Point Energy Correction 121.69
xyz coordinates:

C	-0.003056	-0.000603	-0.002385
C	-0.001485	-0.003014	1.508612
C	1.545281	-0.001163	1.808050
C	2.130047	0.870780	0.602146
C	0.831945	1.241177	-0.210747
C	0.072123	2.193354	0.729129
C	-0.421002	1.458464	1.744115
C	2.380857	-1.150039	1.249462
C	2.891637	-0.388055	0.194928
C	3.782919	-0.910544	-0.735702
C	4.141635	-2.261290	-0.558206
C	3.627894	-3.027630	0.502323
C	2.728788	-2.482707	1.440120
H	-0.421059	-0.704121	-0.714266
H	-0.575034	-0.771220	2.035009
H	0.042864	3.276574	0.620674
H	-0.935194	1.818963	2.633810
H	1.008401	1.593073	-1.231149

H	4.197172	-0.327027	-1.558509
H	4.837980	-2.726453	-1.256112
H	3.938427	-4.067960	0.600286
H	2.345456	-3.087936	2.262235
H	2.735146	1.748075	0.862104
H	1.781734	0.326683	2.827845

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syn-7-bromonorbornene (**8**)

neutral

B3LYP/6-31+G*, -1784554.09
Zero Point Energy Correction 89.23
xyz coordinates:

C	0.041974	0.054022	-0.054562
C	-0.029357	-0.013579	1.464772
C	1.456798	-0.137584	1.835489
C	1.773605	-1.227295	0.799174
C	1.108095	-0.662222	-0.447756
C	-0.449261	-1.489830	1.814369
C	0.792495	-2.326776	1.352336
Br	2.512137	1.536529	1.644866
H	2.815827	-1.545303	0.711333
H	-0.719131	0.510565	-0.684416
H	1.400319	-0.911785	-1.465958
H	-0.608729	0.760540	1.974737
H	1.638241	-0.435552	2.871408
H	-0.619215	-1.596170	2.891934
H	-1.371937	-1.770688	1.297484
H	0.549382	-3.062403	0.579663
H	1.247577	-2.858679	2.195700

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radical anion

B3LYP/6-31+G*, -1784571.79
Zero Point Energy Correction 87.71
xyz coordinates:

C	-0.004833	-0.006676	-0.001003
C	0.012547	0.004580	1.573328
C	1.535913	0.002066	1.818995
C	1.761045	-1.328139	1.069760
C	1.209271	-0.932067	-0.350428
C	-0.358325	-1.412711	1.993688
C	0.683510	-2.206633	1.693843
Br	2.137219	0.085347	3.692072
H	-0.566976	0.816963	2.024912
H	0.728503	-3.292704	1.760448

H	-1.339500	-1.716650	2.355506
H	2.778795	-1.732913	1.061410
H	2.035044	0.844351	1.322367
H	1.973419	-0.386837	-0.917315
H	0.917091	-1.810053	-0.942421
H	-0.955091	-0.382965	-0.403676
H	0.144373	1.007478	-0.390619

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anti radical (anti-**21**)

B3LYP/6-31+G*, -170723.88
Zero Point Energy Correction 86.68
xyz coordinates:

C	-0.026688	-0.022914	-0.037290
C	0.007853	0.019168	1.547194
C	1.509070	-0.006662	1.749373
C	1.766059	-1.321047	1.040638
C	1.186304	-0.947293	-0.386265
C	-0.344715	-1.395536	2.000863
C	0.698966	-2.190592	1.701107
H	-0.567241	0.838837	1.987373
H	0.750409	-3.275128	1.785011
H	-1.320010	-1.697674	2.379577
H	2.785647	-1.716571	1.022049
H	2.157360	0.868937	1.683046
H	1.942041	-0.407670	-0.969242
H	0.899320	-1.841407	-0.951791
H	-0.983412	-0.407144	-0.409610
H	0.113055	0.985970	-0.443250

---

syn radical (syn-**21**)

B3LYP/6-31+G*, -170722.93
Zero Point Energy Correction 86.46
xyz coordinates:

C	0.006578	0.002991	-0.011703
C	0.024937	0.013238	1.558001
C	1.519971	-0.063695	1.820935
C	1.772369	-1.339255	1.033961
C	1.208674	-0.927939	-0.372268
C	-0.340276	-1.406345	2.005683
C	0.697998	-2.209812	1.694399
H	-0.545009	0.824884	2.019751
H	0.751386	-3.292781	1.803497
H	-1.303927	-1.702129	2.419739
H	2.785190	-1.752577	1.020965
H	1.963459	0.130247	2.799672
H	1.974515	-0.385116	-0.938956
H	0.910141	-1.802173	-0.961417
H	-0.949100	-0.361968	-0.404148
H	0.162872	1.018437	-0.394760

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anti radical <-> syn radical
isomerization TS

B3LYP/6-31+G*, -170722.00, 1 imaginary freq
Zero Point Energy Correction 85.80
xyz coordinates:

C	0.000261	-0.000009	-0.000007	-0.493156
C	-0.000224	0.000026	1.580743	-0.080256
C	1.487513	0.000005	1.836859	-0.275190
C	1.814666	-1.262587	1.076681	-0.079588
C	1.252109	-0.870932	-0.347628	-0.493091
C	-0.315197	-1.443763	1.987072	-0.220094
C	0.761250	-2.192592	1.687888	-0.220291
H	-0.611786	0.781068	2.036746	0.201980
H	0.850962	-3.273366	1.751829	0.209501
H	-1.280904	-1.790332	2.344199	0.209414
H	2.844982	-1.623744	1.076676	0.201838
H	2.127285	0.726153	2.321171	0.214217
H	1.999043	-0.288727	-0.899365	0.207614
H	1.005197	-1.755462	-0.945456	0.204770
H	-0.931300	-0.408186	-0.407834	0.204780
H	0.113136	1.023586	-0.375172	0.207622

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7-bromonorbornane (**9**)

neutral

B3LYP/6-31+G*, -1785331.59
Zero Point Energy Correction 104.58
xyz coordinates:

C	-0.166027	-0.113555	-0.158846
C	-0.087951	-0.017869	1.388136
C	1.438747	-0.045723	1.543443
C	1.648686	-1.404316	0.860778
C	1.028009	-1.068116	-0.521136
C	-0.521099	-1.379678	1.983692
C	0.670600	-2.329016	1.625667
Br	2.090481	0.054019	3.424853
H	-0.598494	0.853036	1.811723
H	0.363322	-3.178912	1.005476
H	-1.471772	-1.713468	1.552429
H	2.681610	-1.764240	0.815073
H	1.955491	0.786174	1.057606
H	1.755617	-0.560711	-1.165159
H	0.701445	-1.975784	-1.041267
H	-1.135869	-0.507029	-0.483772

H	-0.035795	0.871968	-0.620888
H	-0.658631	-1.311653	3.068463
H	1.135898	-2.734726	2.530614

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radical anion

B3LYP/6-31+G*, -1785349.64
Zero Point Energy Correction 103.09
xyz coordinates

C	0.001240	-0.000830	0.007114
C	0.009928	-0.003791	1.557830
C	1.516447	0.029253	1.878335
C	1.850121	-1.216062	1.035247
C	1.269816	-0.842976	-0.354263
C	-0.366373	-1.431463	2.035147
C	0.909673	-2.270850	1.675812
Br	2.475170	1.690778	1.402695
H	2.904793	-1.516647	1.013911
H	-0.923732	-0.435034	-0.392177
H	1.030563	-1.737069	-0.943402
H	-0.597086	0.789795	2.010444
H	1.720058	-0.122306	2.946092
H	-0.556490	-1.444597	3.115320
H	-1.271537	-1.811436	1.538119
H	0.686070	-3.101240	0.989313
H	1.363677	-2.703967	2.575531
H	1.982761	-0.247535	-0.935331
H	0.083808	1.018735	-0.385215

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radical

B3LYP/6-31+G*, -171500.21
Zero Point Energy Correction 101.82
xyz coordinates:

C	0.004633	-0.000417	0.021742
C	-0.005590	-0.022637	1.575267
C	1.475340	-0.034401	1.879109
C	1.844703	-1.243275	1.049700
C	1.277456	-0.841459	-0.339913
C	-0.393136	-1.467233	2.027981
C	0.881590	-2.307891	1.666448
H	2.896430	-1.548472	1.039708
H	-0.915823	-0.425330	-0.397319
H	1.043033	-1.720452	-0.953027
H	-0.611058	0.764653	2.036753
H	1.922748	0.231329	2.837485
H	-0.590873	-1.494404	3.106216
H	-1.296756	-1.823312	1.516553
H	0.669583	-3.120410	0.959434
H	1.325157	-2.757506	2.562891

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 H     2.004441    -0.236113    -0.894352
 H     0.093517     1.027415    -0.349691

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anti-7-Trimethylstannylbenzonorbornene (**10a**)

neutral

B3LYP/6-31+G*, -343670.24
Zero Point Energy Correction 170.52
xyz coordinates:

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 C     0.482723    -0.882778    -3.723050
 C     0.554240    -0.745587    -2.345121
 C     1.789059    -0.516148    -1.701024
 C     2.966249    -0.421469    -2.427569
 C     2.900004    -0.558164    -3.832126
 C     1.678204    -0.785016    -4.469443
 C    -0.507451    -0.784608    -1.233182
 C     0.091284     0.322834    -0.291591
 C     1.475790    -0.416117    -0.198730
 C     0.987089    -1.814776     0.223283
 C    -0.187284    -2.032973    -0.389155
Sn    -0.956664     0.702935     1.583726
 C     0.272217     0.214117     3.284781
 C    -2.812643    -0.386701     1.688049
 C    -1.400765     2.814177     1.645882
 H    -0.221963     0.519679     4.214918
 H    -1.544497    -0.678281    -1.564965
 H     2.260455     0.028733     0.420428
 H    -0.785417    -2.942199    -0.383530
 H     1.558702    -2.506799     0.838790
 H    -0.468806    -1.055746    -4.227482
 H     3.923156    -0.240007    -1.936472
 H     1.644506    -0.884615    -5.554379
 H     3.812467    -0.482033    -4.423528
 H     0.194378     1.277120    -0.829353
 H    -2.037834     3.105300     0.801887
 H    -1.925701     3.075055     2.572756
 H    -0.481193     3.409978     1.597631
 H    -3.384899    -0.084637     2.573489
 H    -3.430354    -0.194067     0.802862
 H    -2.630056    -1.465401     1.748788
 H     0.460688    -0.864175     3.334586
 H     1.239275     0.727915     3.229769
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radical anion

B3LYP/6-31+G*, -343692.36
Zero Point Energy Correction 167.61

xyz coordinates:

C	3.585109	-1.419996	-0.243359
C	2.400038	-0.723001	-0.036239
C	2.400114	0.722574	-0.049484
C	3.585498	1.415278	-0.269010
C	4.780590	0.706776	-0.495402
C	4.780317	-0.716125	-0.482658
C	0.975050	-1.133083	0.293227
C	0.182611	-0.003829	-0.464228
C	0.974999	1.138691	0.273224
C	0.786681	0.706692	1.727910
C	0.787448	-0.675166	1.739915
Sn	-1.958605	-0.003123	-0.189748
C	-2.686412	1.762303	0.819258
C	-2.686162	-1.758964	0.835646
C	-2.878709	-0.011542	-2.154374
H	-3.782626	1.800197	0.813252
H	0.705860	-2.172383	0.070148
H	0.706291	2.173860	0.031348
H	0.945217	-1.328360	2.596889
H	0.946028	1.374580	2.573277
H	3.596161	-2.513357	-0.233713
H	3.597096	2.508666	-0.279233
H	5.699968	-1.265506	-0.681255
H	5.700370	1.252220	-0.703976
H	0.417129	-0.013671	-1.539340
H	-2.584044	-0.903168	-2.721384
H	-3.973388	-0.003685	-2.081229
H	-2.572229	0.867692	-2.734321
H	-3.782023	-1.804189	0.818688
H	-2.299962	-2.666523	0.356519
H	-2.349160	-1.757812	1.877441
H	-2.339161	1.777638	1.857650
H	-2.311476	2.665779	0.323797

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syn-7-Trimethylstannylbenzonorbornene (**10b**)

neutral

B3LYP/6-31+G*, -343669.39
Zero Point Energy Correction 170.53
xyz coordinates:

C	-1.920527	1.118303	-2.965646
C	-2.165236	1.257664	-1.582557
C	-1.079768	1.423296	-0.735447
C	0.236681	1.457911	-1.240651
C	0.483884	1.323728	-2.598875
C	-0.616357	1.150052	-3.465951

C	-0.960973	1.627488	0.782086
C	0.373835	0.837657	1.039960
C	1.153093	1.686318	-0.029568
C	-0.435019	3.067798	0.967876
C	0.816949	3.102743	0.486317
Sn	0.363416	-1.338290	0.830946
C	1.860207	-1.991253	-0.576004
H	1.875686	-3.085930	-0.635933
C	0.847559	-2.149366	2.771966
H	2.214967	1.474621	-0.185720
H	-1.843596	1.360618	1.371091
H	1.471690	3.966001	0.380100
H	-1.033377	3.896048	1.343613
H	1.499696	1.345802	-2.995440
H	-3.185239	1.226722	-1.197714
H	-0.445199	1.038288	-4.536702
H	-2.758529	0.981961	-3.649358
H	0.754760	1.061106	2.046828
H	0.099463	-1.851476	3.516441
H	0.878223	-3.244930	2.739631
H	1.826663	-1.790771	3.111650
C	-1.564424	-2.100841	0.243522
H	-2.346571	-1.747576	0.925704
H	-1.823188	-1.774254	-0.768878
H	-1.560750	-3.197164	0.266275
H	2.856820	-1.652585	-0.268948
H	1.656650	-1.593562	-1.576052

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radical anion

B3LYP/6-31+G*, -343691.98
Zero Point Energy Correction 168.14
xyz coordinates:

C	-1.822514	1.217791	-3.022633
C	-2.106115	1.274802	-1.645312
C	-1.058324	1.363896	-0.734832
C	0.297748	1.416366	-1.198167
C	0.573749	1.386592	-2.561556
C	-0.487400	1.274061	-3.479204
C	-0.992850	1.548834	0.773359
C	0.340467	0.793454	1.083375
C	1.154307	1.628531	0.041304
C	-0.530433	3.006029	0.945346
C	0.799002	3.055781	0.491823
Sn	0.341595	-1.358614	0.850366
C	1.737836	-2.050851	-0.645499
H	1.810423	-3.145691	-0.628909
C	0.976928	-2.219204	2.738078
H	2.220147	1.396014	-0.068490
H	-1.885588	1.244980	1.332984
H	1.267489	3.926383	0.029276
H	-1.240813	3.832237	0.883411

H	1.602599	1.433913	-2.924434
H	-3.142298	1.238483	-1.302623
H	-0.274249	1.217495	-4.546228
H	-2.638422	1.118338	-3.737787
H	0.680687	1.008087	2.106475
H	0.300097	-1.935978	3.553438
H	0.996429	-3.315156	2.682528
H	1.984295	-1.878774	3.007899
C	-1.616234	-2.157992	0.410078
H	-2.352503	-1.778536	1.128312
H	-1.940248	-1.862791	-0.593428
H	-1.616681	-3.253927	0.468278
H	2.736968	-1.640433	-0.461184
H	1.421872	-1.740145	-1.646565

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anti-7-Diphenylphosphineoxidebenzonorbornene (**12a-desoxy**)

neutral

B3LYP/6-31+G*, -771357.47
Zero Point Energy Correction 217.30
xyz coordinates:

C	0.018359	-0.013011	0.000033
C	0.010329	-0.006447	1.386281
C	1.214475	0.011297	2.120439
C	2.443098	0.022686	1.478052
C	2.458458	0.012243	0.066888
C	1.265724	-0.005116	-0.660257
C	-1.124670	-0.025274	2.422142
C	-0.457748	0.923406	3.485835
C	0.813696	0.003834	3.603832
C	0.138962	-1.358237	3.849308
C	-1.004785	-1.375888	3.151447
P	-1.453601	1.201532	5.058974
C	-2.755969	2.352466	4.391069
C	-4.072945	1.865782	4.319764
C	-5.107294	2.661273	3.811803
C	-4.838405	3.961551	3.374270
C	-3.531748	4.460764	3.445438
C	-2.500223	3.662721	3.949212
C	-0.360078	2.355015	6.021916
C	0.735789	3.068853	5.505226
C	1.507198	3.895067	6.331138
C	1.193491	4.028874	7.687480
C	0.105711	3.324855	8.216419
C	-0.653806	2.489043	7.392547
H	-2.116482	0.243206	2.048462
H	1.594013	0.295180	4.311891
H	-1.706137	-2.198908	3.032935

H	0.583659	-2.163383	4.430102
H	-0.909430	-0.020638	-0.572987
H	3.377376	0.041906	2.040157
H	1.297041	-0.009759	-1.749652
H	3.412389	0.020865	-0.460063
H	-4.294548	0.856419	4.667914
H	-1.493035	4.072608	4.001063
H	-6.121758	2.265463	3.764910
H	-3.315572	5.475220	3.110046
H	-5.641875	4.585888	2.983892
H	1.000845	2.996343	4.453031
H	-1.487687	1.931041	7.820873
H	2.353292	4.437596	5.909142
H	-0.145259	3.416462	9.273119
H	1.794851	4.673082	8.328532
H	-0.209696	1.890152	3.028613

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radical anion

B3LYP/6-31+G*, -771387.85
Zero Point Energy Correction 214.10
xyz coordinates:

P	0.218904	-0.169276	0.015751
C	0.027022	0.138664	1.880192
C	1.296553	-0.171760	2.757451
C	-0.864547	-0.856619	2.707491
C	1.298375	-1.709657	2.693742
C	0.704656	0.185814	4.128730
H	2.232758	0.328954	2.494292
C	0.020726	-2.114739	2.661909
C	-0.641859	-0.239308	4.095905
H	-1.905884	-0.981782	2.401316
H	2.194790	-2.324647	2.739623
C	1.234586	0.791008	5.258022
H	-0.359463	-3.134040	2.679678
C	-1.472748	-0.059756	5.192197
C	0.393957	0.973758	6.378316
H	2.271960	1.126523	5.287380
C	-0.938175	0.555156	6.345474
H	-2.515421	-0.379068	5.171301
H	0.789399	1.449754	7.275545
H	-1.574070	0.706824	7.217650
C	0.963694	1.428350	-0.498389
C	2.016565	1.393472	-1.458907
C	0.449246	2.726086	-0.166065
C	2.531615	2.547933	-2.038964
H	2.433303	0.425676	-1.744969
C	0.957121	3.881072	-0.761456
H	-0.346322	2.826657	0.569292
C	2.001707	3.820504	-1.702060
H	3.353959	2.471381	-2.751832
H	0.539639	4.850444	-0.481548

H	2.396624	4.727953	-2.156480
C	-1.531098	-0.103642	-0.540637
C	-2.510565	0.825370	-0.066273
C	-1.905106	-0.912235	-1.648188
C	-3.765527	0.925731	-0.673547
H	-2.294859	1.455322	0.794386
C	-3.158787	-0.818785	-2.245473
H	-1.183420	-1.631904	-2.040192
C	-4.112446	0.114507	-1.764983
H	-4.489596	1.643531	-0.282862
H	-3.409441	-1.474704	-3.080182
H	-5.092890	0.198750	-2.231780
H	-0.302340	1.171184	2.048987

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syn-7-Diphenylphosphineoxidebenzonorbornene (**12b-desoxy**)

neutral

B3LYP/6-31+G*, -771357.58
Zero Point Energy Correction 217.33
xyz coordinates:

P	-0.181851	-0.021347	-0.155577
C	-0.022500	-0.040836	1.699522
C	1.171185	-0.340257	2.379711
C	-1.164643	0.275885	2.455407
C	1.222401	-0.317412	3.776709
H	2.068913	-0.599477	1.820956
C	-1.114963	0.304675	3.854453
H	-2.104132	0.496608	1.947987
C	0.079330	0.007219	4.518151
H	2.155916	-0.554930	4.287432
H	-2.011252	0.553160	4.423039
H	0.119953	0.023087	5.607291
C	0.871095	-1.471613	-0.645170
C	0.229539	-2.725841	-0.667673
C	2.223286	-1.410950	-1.023928
C	0.920310	-3.883986	-1.033665
H	-0.825069	-2.797108	-0.396312
C	2.913693	-2.568366	-1.405621
H	2.759596	-0.464816	-1.024277
C	2.267567	-3.808038	-1.407715
H	0.403542	-4.843814	-1.037131
H	3.961573	-2.496657	-1.697836
H	2.806838	-4.707720	-1.703784
C	0.939667	1.442443	-0.540156
C	1.088886	1.848034	-2.053884
C	0.365560	2.854250	-0.151570
C	1.931001	3.123932	-1.854585

C	-0.340274	2.329212	-2.337236
H	1.492698	1.107145	-2.748996
C	1.503203	3.718564	-0.730599
C	-0.789427	2.954481	-1.157163
H	0.112256	3.031026	0.896902
H	2.677380	3.480080	-2.562058
C	-1.144717	2.267295	-3.464166
H	1.819911	4.671514	-0.311087
C	-2.049395	3.527610	-1.087198
C	-2.429450	2.847957	-3.400525
H	-0.803550	1.781121	-4.378961
C	-2.874844	3.467832	-2.230303
H	-2.404115	4.008997	-0.175081
H	-3.080773	2.809711	-4.273682
H	-3.871062	3.908971	-2.197879
H	1.921314	1.295739	-0.073881

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radical anion

B3LYP/6-31+G*, -771387.70
Zero Point Energy Correction 213.97
xyz coordinates:

P	-0.197433	0.064463	-0.065856
C	0.019512	0.118628	1.755986
C	1.271391	0.277293	2.438327
C	-1.103231	-0.218088	2.565214
C	1.369972	0.099607	3.820291
H	2.164266	0.558771	1.883889
C	-1.005245	-0.382117	3.942827
H	-2.074358	-0.348943	2.083525
C	0.246416	-0.231313	4.596830
H	2.339799	0.231409	4.304568
H	-1.898665	-0.618532	4.522508
H	0.332618	-0.364884	5.674233
C	0.804330	-1.370857	-0.636224
C	0.112319	-2.495577	-1.167266
C	2.211160	-1.532641	-0.417663
C	0.758471	-3.690078	-1.470969
H	-0.961696	-2.413766	-1.346136
C	2.855140	-2.737500	-0.708260
H	2.803928	-0.706065	-0.031467
C	2.150511	-3.831740	-1.238033
H	0.189976	-4.517130	-1.898661
H	3.928952	-2.822884	-0.529718
H	2.662164	-4.765222	-1.468309
C	0.930757	1.489422	-0.605398
C	1.015397	1.775158	-2.148696
C	0.446684	2.952658	-0.296739
C	1.916612	3.025566	-2.101300
C	-0.404828	2.301342	-2.394429
H	1.347238	0.961655	-2.799384
C	1.580288	3.722531	-1.004534

C	-0.757842	3.034266	-1.243164
H	0.258361	3.217734	0.747073
H	2.629015	3.299454	-2.877451
C	-1.275600	2.195848	-3.467419
H	1.957090	4.692417	-0.684574
C	-1.984754	3.672220	-1.151843
C	-2.528688	2.840539	-3.380571
H	-1.010934	1.624520	-4.358015
C	-2.877660	3.568239	-2.240585
H	-2.265458	4.236852	-0.261884
H	-3.230523	2.767083	-4.211303
H	-3.849684	4.058666	-2.188387
H	1.938827	1.344376	-0.201173

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anti-7-Trimethylstannylcyclobutebenzonorbornene (**13a**)

neutral

B3LYP/6-31+G*, -392232.07
Zero Point Energy Correction 192.31
xyz coordinates:

C	1.860921	2.272677	-0.637735
C	1.477798	2.523666	0.683662
C	2.404610	2.704200	1.704568
C	3.761042	2.616589	1.331392
C	4.146044	2.365502	0.003137
C	3.194748	2.188091	-1.021716
C	-0.014317	2.508477	0.356525
C	-0.867649	1.237124	0.709609
C	-0.116666	0.108853	-0.056112
C	-0.244189	0.825951	-1.431636
C	0.422264	2.220851	-1.147844
C	-1.740326	1.144413	-1.439995
C	-2.109980	1.389040	-0.169842
Sn	-0.981701	-1.881469	0.077587
C	0.577899	-3.204627	0.771788
C	-1.662602	-2.605986	-1.835646
H	0.929600	0.029392	0.263798
H	-1.045790	1.094118	1.780665
H	-2.344058	1.263072	-2.338480
H	-3.076972	1.747815	0.179541
H	0.147493	0.309081	-2.314025
H	3.509789	2.003874	-2.049367
H	5.208137	2.312259	-0.237067
H	4.534208	2.751536	2.088085
H	2.122603	2.910145	2.737677
H	0.153667	2.974109	-1.898994
H	-0.554642	3.443726	0.549313

C	-2.604231	-1.969574	1.494848
H	-2.919143	-3.009269	1.645061
H	-2.298980	-1.563604	2.466483
H	-3.468946	-1.396994	1.141698
H	0.208637	-4.233627	0.858134
H	1.427325	-3.205856	0.077919
H	0.945940	-2.892308	1.756661
H	-1.948337	-3.662110	-1.760320
H	-2.532528	-2.039520	-2.185817
H	-0.872673	-2.521166	-2.591237

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radical anion

B3LYP/6-31+G*, -392250.95
Zero Point Energy Correction 192.31
xyz coordinates:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.527092
C	1.526755	0.000000	1.899388
C	1.998718	-1.426029	1.419352
C	0.676580	-2.050067	0.842231
C	0.396127	-1.217887	-0.406515
C	-0.396199	-1.476328	1.808990
C	1.992045	-0.423029	3.279858
C	2.406461	-1.665089	2.859554
C	3.046899	-2.614441	3.706999
C	3.193905	-2.156831	5.068642
C	2.774665	-0.905099	5.492766
C	2.155680	0.056842	4.611300
Sn	-2.453230	-2.011460	1.373270
C	-3.589597	-0.443608	0.422384
C	-3.445871	-2.464695	3.239460
C	-2.546507	-3.780579	0.141077
H	-0.181211	-1.753085	2.847844
H	-0.596848	0.781312	2.011087
H	0.601846	-1.536686	-1.427155
H	-0.187693	0.873354	-0.622361
H	0.696971	-3.136608	0.705077
H	3.342751	-3.616587	3.399620
H	3.658678	-2.822242	5.798528
H	2.925886	-0.635610	6.539687
H	1.787728	1.016477	4.971999
H	2.811179	-1.449574	0.671576
H	2.047067	0.866226	1.453474
H	-4.663612	-0.640517	0.521792
H	-3.376106	0.526989	0.884313
H	-3.346844	-0.374127	-0.643210
H	-4.497952	-2.726622	3.074058
H	-2.962346	-3.309819	3.743384
H	-3.412901	-1.606770	3.921786
H	-3.588221	-4.071163	-0.039691
H	-2.062772	-3.615566	-0.828445

H	-2.042023	-4.620291	0.632573

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syn-7-Trimethylstannylcyclobutebenzonorbornene (**13b**)

neutral

B3LYP/6-31+G*, -392226.23
Zero Point Energy Correction 192.55
xyz cordinates:

C	0.161331	1.835499	-1.131087
C	0.455427	2.101428	0.210552
C	1.745328	2.389638	0.644580
C	2.749274	2.377083	-0.343310
C	2.453634	2.110204	-1.691693
C	1.139033	1.842285	-2.120673
C	-1.012988	2.098505	0.633392
C	-1.667867	0.884503	1.372360
C	-1.481005	-0.310008	0.384978
C	-2.144266	0.451523	-0.805449
C	-1.347418	1.795427	-0.892884
C	-3.448889	0.890482	-0.124776
C	-3.166623	1.147174	1.165405
Sn	0.324037	-1.529427	0.233853
H	-2.184847	-1.094749	0.694726
H	-1.344049	0.741938	2.408763
H	-4.389789	1.067010	-0.644545
H	-3.829664	1.576350	1.915602
H	-2.254365	-0.085750	-1.753379
H	0.921469	1.665641	-3.174352
H	3.263216	2.123701	-2.421702
H	3.780608	2.590850	-0.061922
H	1.985901	2.626924	1.681201
H	-1.911007	2.566982	-1.432289
H	-1.370594	3.056620	1.030916
C	1.877601	-1.067697	1.653856
C	-0.414536	-3.487300	0.786670
C	1.133582	-1.746978	-1.751249
H	0.389892	-4.232631	0.759423
H	-0.832325	-3.478217	1.801301
H	-1.204637	-3.817921	0.100718
H	1.730513	-2.665940	-1.800442
H	0.329692	-1.824051	-2.492877
H	1.769348	-0.899946	-2.022332
H	2.510681	-1.951806	1.798297
H	2.503690	-0.239592	1.311325
H	1.448431	-0.794859	2.625212

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radical anion

B3LYP/6-31+G*, -392245.80
Zero Point Energy Correction 190.41
xyz coordinates:

C	0.185262	1.763820	-1.104409
C	0.473257	2.015566	0.222001
C	1.761787	2.396436	0.683084
C	2.779745	2.322160	-0.333528
C	2.490049	2.069181	-1.666539
C	1.149260	1.854227	-2.143035
C	-0.987658	2.032009	0.637408
C	-1.696229	0.849082	1.379247
C	-1.532900	-0.345449	0.394549
C	-2.165081	0.428055	-0.799990
C	-1.315938	1.741598	-0.876332
C	-3.457780	0.905657	-0.132848
C	-3.180024	1.155381	1.157944
Sn	0.309861	-1.482930	0.223154
H	-2.238590	-1.132102	0.697768
H	-1.389202	0.686303	2.418665
H	-4.386380	1.119270	-0.660356
H	-3.836198	1.613662	1.896579
H	-2.283599	-0.118049	-1.742740
H	0.949367	1.597041	-3.181644
H	3.309005	2.070991	-2.388597
H	3.817088	2.513394	-0.051819
H	2.023098	2.489525	1.735659
H	-1.872789	2.534184	-1.404818
H	-1.342716	3.002421	1.024804
C	1.865552	-1.034453	1.643186
C	-0.346847	-3.480108	0.791332
C	1.089676	-1.744319	-1.766988
H	0.487475	-4.192684	0.763923
H	-0.761527	-3.491584	1.807609
H	-1.125512	-3.852378	0.113143
H	1.819306	-2.563376	-1.768143
H	0.282846	-2.010490	-2.460514
H	1.570175	-0.830508	-2.126725
H	2.530744	-1.901146	1.741452
H	2.447383	-0.162876	1.333026
H	1.433521	-0.824541	2.628922

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anti-7-Diphenylphosphineoxidecyclobutebenzonorbornene (**14a-desoxy**)

neutral

B3LYP/6-31+G*, -819919.81
Zero Point Energy Correction 239.19
xyz coordinates:

C	0.000119	-0.001277	-0.000091
C	0.002207	0.001178	1.405865
C	1.239234	-0.002129	2.073949
C	2.442994	0.006805	1.359648
C	2.426050	0.007126	-0.038411
C	1.200987	0.001129	-0.716275
P	-1.536289	0.028061	2.455593
C	-2.714597	-0.979624	1.431180
C	-2.672587	-2.374174	1.623552
C	-3.521925	-3.227913	0.914889
C	-4.450853	-2.700114	0.010462
C	-4.517338	-1.316662	-0.179255
C	-3.654596	-0.465322	0.521631
C	-2.108850	1.787453	2.125665
C	-1.246492	2.896452	2.799023
C	-1.647938	2.730060	4.263698
C	-2.931237	2.335909	4.292070
C	-3.418039	2.230797	2.847367
C	-3.533059	3.727434	2.388805
C	-2.009285	4.193955	2.353982
C	-2.230394	4.470358	0.867863
C	-1.622479	4.936930	-0.291746
C	-2.432117	4.968921	-1.444036
C	-3.774797	4.555301	-1.414171
C	-4.378628	4.088886	-0.229864
C	-3.566733	4.060312	0.898224
H	-2.160608	1.938272	1.043277
H	-0.175133	2.899208	2.580000
H	-3.566573	2.210917	5.166617
H	-1.017850	2.994985	5.110455
H	-4.316199	1.629060	2.679539
H	-5.423920	3.779361	-0.220833
H	-4.361716	4.601915	-2.331296
H	-2.011131	5.325762	-2.383815
H	-0.584271	5.267030	-0.329861
H	-4.217915	4.301226	3.024189
H	-1.738558	5.061140	2.967765
H	-1.967171	-2.797177	2.339958
H	-3.465575	-4.303996	1.077047
H	-5.121877	-3.361681	-0.536285
H	-5.239282	-0.894285	-0.877934
H	-3.728352	0.604510	0.350646
H	1.262894	-0.014423	3.163909
H	3.391294	0.004867	1.896484
H	3.360905	0.007626	-0.598025
H	1.179777	-0.003267	-1.805904
H	-0.941232	-0.010558	-0.545574

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radical anion

B3LYP/6-31+G*, -819949.42
Zero Point Energy Correction 235.86
xyz coordinates:

C	0.106861	0.611099	0.005796
C	0.092760	0.160950	1.363650
C	1.259657	-0.507589	1.820715
C	2.368104	-0.712764	1.002570
C	2.356366	-0.267268	-0.340692
C	1.212879	0.392930	-0.818976
P	-1.393313	0.133442	2.461520
C	-2.619583	-0.911228	1.590808
C	-2.867712	-2.216625	2.105448
C	-3.648137	-3.147175	1.428553
C	-4.219381	-2.825382	0.168412
C	-3.985015	-1.545907	-0.363939
C	-3.211615	-0.605984	0.319166
C	-2.083819	1.865731	2.145253
C	-1.348368	3.026051	2.878200
C	-1.817644	2.805403	4.316327
C	-3.065232	2.309872	4.266287
C	-3.457895	2.196017	2.793642
C	-3.664773	3.691292	2.359613
C	-2.180961	4.274321	2.416773
C	-2.345530	4.569052	0.926722
C	-1.717882	5.112343	-0.188428
C	-2.469274	5.117559	-1.380728
C	-3.776743	4.605171	-1.430639
C	-4.401491	4.061160	-0.290374
C	-3.646990	4.060094	0.877347
H	-2.112391	2.042460	1.066823
H	-0.268098	3.110732	2.722753
H	-3.735440	2.119593	5.103036
H	-1.258276	3.100600	5.202620
H	-4.292561	1.528630	2.559166
H	-5.419105	3.672967	-0.343582
H	-4.319199	4.634067	-2.375824
H	-2.029771	5.531510	-2.288472
H	-0.706709	5.519863	-0.164833
H	-4.423949	4.199522	2.967232
H	-2.012906	5.148235	3.058562
H	-2.432487	-2.490032	3.069051
H	-3.829162	-4.125866	1.875170
H	-4.827238	-3.551105	-0.369824
H	-4.424623	-1.272897	-1.325569
H	-3.084133	0.381896	-0.116846
H	1.287674	-0.869515	2.850530
H	3.250958	-1.210938	1.405607
H	3.217484	-0.427333	-0.988214
H	1.188963	0.754117	-1.848843
H	-0.743437	1.151273	-0.401596

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syn-7-Diphenylphosphineoxidecyclobutebenzonorbornene (**14b-desoxy**)

neutral

B3LYP/6-31+G*, -819913.96
Zero Point Energy Correction 239.07
xyz coordinates:

C	0.072506	-0.091933	0.001577
C	0.045129	0.014967	1.402708
C	1.268844	0.114847	2.087958
C	2.482300	0.113758	1.393294
C	2.493662	0.014148	-0.003721
C	1.284992	-0.088244	-0.699088
P	-1.628953	0.022830	2.231598
C	-1.283289	-0.992252	3.757028
C	-1.499673	-2.378338	3.628105
C	-1.282716	-3.250463	4.698679
C	-0.864348	-2.748199	5.936481
C	-0.660543	-1.372892	6.086789
C	-0.863882	-0.504019	5.007058
C	-1.563311	1.782140	2.924680
C	-1.662946	2.998802	1.945335
C	-3.181470	3.095363	1.576438
C	-3.893188	2.626757	2.919738
C	-2.683397	2.334917	3.866946
C	-2.102025	3.732850	4.107491
C	-1.500272	4.125797	2.971010
C	-3.918132	1.942233	0.898641
C	-4.156450	1.325427	-0.322653
C	-5.047861	0.235286	-0.299184
C	-5.666704	-0.186494	0.890078
C	-5.429960	0.462577	2.117386
C	-4.537679	1.526196	2.080079
H	-0.603596	1.861382	3.446976
H	-0.971479	3.013944	1.097536
H	-2.260473	4.318484	5.011752
H	-1.064414	5.099400	2.752354
H	-2.923828	1.752424	4.760904
H	-5.928560	0.132313	3.029186
H	-6.353668	-1.032337	0.855540
H	-5.271595	-0.293412	-1.226037
H	-3.692186	1.647002	-1.255413
H	-4.596920	3.333483	3.376585
H	-3.438142	4.094760	1.204101
H	-1.845788	-2.780216	2.674682
H	-1.451369	-4.319538	4.569153
H	-0.704046	-3.422210	6.777701
H	-0.337567	-0.969874	7.046878
H	-0.685580	0.557775	5.158547
H	-0.862628	-0.185301	-0.548603
H	1.282738	-0.170806	-1.786000
H	3.439835	0.011591	-0.544562
H	3.420561	0.188948	1.943337
H	1.282839	0.189302	3.173594

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radical anion

B3LYP/6-31+G*, -819942.21
Zero Point Energy Correction 235.67
xyz coordinates:

C	0.303599	-0.544247	0.129507
C	0.125770	0.150163	1.359971
C	1.319217	0.663142	1.972336
C	2.573674	0.476093	1.388434
C	2.720049	-0.212509	0.171553
C	1.552345	-0.719646	-0.458348
P	-1.550422	0.091652	2.122946
C	-1.318042	-0.913503	3.654657
C	-1.936508	-2.193176	3.695053
C	-1.698776	-3.104464	4.720698
C	-0.802287	-2.781597	5.771186
C	-0.179603	-1.522552	5.755714
C	-0.429253	-0.603054	4.733688
C	-1.605556	1.828423	2.901969
C	-1.788009	3.103863	2.017239
C	-3.317797	3.143646	1.682692
C	-3.975319	2.538834	3.000045
C	-2.728775	2.250501	3.900436
C	-2.229814	3.662708	4.230094
C	-1.670828	4.167895	3.114891
C	-4.013519	2.010586	0.932212
C	-4.267254	1.491944	-0.330624
C	-5.120525	0.372448	-0.378516
C	-5.690318	-0.170452	0.785892
C	-5.438748	0.380216	2.057635
C	-4.583800	1.474071	2.089422
H	-0.654482	1.940840	3.430370
H	-1.118962	3.215520	1.158201
H	-2.408105	4.179309	5.172521
H	-1.300753	5.180955	2.961378
H	-2.909477	1.588687	4.752749
H	-5.900383	-0.043280	2.950131
H	-6.350105	-1.033903	0.696845
H	-5.353233	-0.083255	-1.341343
H	-3.841799	1.908651	-1.244148
H	-4.708155	3.172094	3.516122
H	-3.638303	4.152325	1.392445
H	-2.623845	-2.465824	2.892151
H	-2.212991	-4.066636	4.718089
H	-0.605727	-3.490667	6.574319
H	0.504977	-1.249180	6.561358
H	0.053732	0.370806	4.783437
H	-0.578101	-0.950909	-0.369714
H	1.629978	-1.241482	-1.413356
H	3.702254	-0.347158	-0.279253
H	3.456634	0.882822	1.886211

H	1.262113	1.222470	2.903369

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anti-7-Trimethylstannylnorbornene (**15a**)

neutral

B3LYP/6-31+G*, -248020.80
Zero Point Energy Correction 156.56
xyz coordinates:

C	-0.634288	-0.893648	0.289026
C	-0.603787	-0.890738	1.845525
C	0.897377	-0.923441	2.106181
C	1.461776	-1.644761	1.120323
C	0.342622	-2.102007	0.192276
C	-0.463150	-3.185276	0.999954
C	-1.118568	-2.347265	2.142775
Sn	-0.021219	0.941228	-0.702583
C	-1.664878	1.567949	-1.955820
C	0.388304	2.523188	0.703565
C	1.703467	0.633532	-1.958625
H	0.186471	-3.984572	1.374977
H	-1.166937	-0.107125	2.363426
H	0.647561	-2.430713	-0.806743
H	1.381890	-0.538802	3.002732
H	2.499689	-1.967989	1.050542
H	-1.634379	-1.163054	-0.085699
H	-2.213452	-2.378678	2.083497
H	-0.828964	-2.688895	3.143204
H	-1.222713	-3.646826	0.357097
H	-1.425769	2.497815	-2.486389
H	-1.900810	0.802484	-2.705381
H	-2.567376	1.743283	-1.357397
H	0.591272	3.462812	0.175111
H	-0.466104	2.687831	1.370722
H	1.260661	2.281851	1.321096
H	1.936839	1.546066	-2.520774
H	2.581935	0.366467	-1.360364
H	1.525199	-0.172326	-2.680465

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radical anion

B3LYP/6-31+G*, -248033.34
Zero Point Energy Correction 156.02
xyz coordinates:

C	-0.562182	-0.912364	0.208221
C	-0.791672	-0.894506	1.742328
C	0.637805	-0.788005	2.248332
C	1.420427	-1.459721	1.386767

C	0.515667	-2.024983	0.303244
C	-0.307050	-3.170100	0.994714
C	-1.215739	-2.386340	1.990912
Sn	0.012463	0.967640	-0.742962
C	-1.775661	1.674940	-1.756134
C	0.648475	2.449560	0.710427
C	1.576968	0.502110	-2.173182
H	0.341780	-3.899138	1.493791
H	-1.499198	-0.159471	2.142560
H	1.011283	-2.334787	-0.623075
H	0.933219	-0.340168	3.196131
H	2.480948	-1.685703	1.493967
H	-1.457287	-1.281889	-0.318478
H	-2.277626	-2.521373	1.749101
H	-1.068699	-2.693837	3.033078
H	-0.904226	-3.710551	0.250265
H	-1.568475	2.603553	-2.302417
H	-2.143911	0.931772	-2.480059
H	-2.579263	1.881314	-1.031981
H	0.691454	3.436035	0.233947
H	-0.063392	2.505174	1.548398
H	1.643516	2.213621	1.112850
H	1.872051	1.390897	-2.742684
H	2.467678	0.108168	-1.661361
H	1.224430	-0.255580	-2.889533

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syn-7-Trimethylstannylnorbornene (**15b**)

neutral

B3LYP/6-31+G*, -248022.43
Zero Point Energy Correction 156.33
xyz coordinates:

C	1.479426	-1.323097	-1.568773
C	1.347259	-1.731799	-0.059278
C	2.778878	-1.844931	0.460583
C	3.279180	-0.598505	0.534104
C	2.187515	0.359619	0.061318
C	2.073164	0.118431	-1.486681
C	0.919091	-0.379847	0.584591
Sn	-1.075633	0.405447	0.197725
H	0.966542	-0.462499	1.680871
H	4.305710	-0.308972	0.756556
H	3.312606	-2.782700	0.611080
H	2.316776	1.409798	0.344574
H	1.406499	0.854376	-1.949101
H	3.047656	0.204087	-1.979645
H	2.119889	-2.017678	-2.123193
H	0.496665	-1.325791	-2.057796

H	0.706208	-2.601760	0.115321
C	-1.340291	1.440419	-1.677888
C	-2.488151	-1.224089	0.274756
C	-1.530692	1.790912	1.787334
H	-2.551905	2.176694	1.683904
H	-1.448338	1.302318	2.765539
H	-0.842197	2.644244	1.774554
H	-3.511170	-0.847052	0.157717
H	-2.300067	-1.950639	-0.524372
H	-2.427105	-1.750645	1.234501
H	-2.374853	1.797454	-1.751864
H	-0.676637	2.309400	-1.752345
H	-1.146396	0.784531	-2.534061

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radical anion

B3LYP/6-31+G*, -248032.86
Zero Point Energy Correction 156.69
xyz coordinates:

C	1.469635	-1.412850	-1.506590
C	1.379234	-1.723631	0.024043
C	2.821211	-1.765558	0.513864
C	3.287170	-0.504367	0.502047
C	2.161377	0.387669	-0.008167
C	2.022129	0.043032	-1.531043
C	0.924159	-0.347339	0.584850
Sn	-1.106643	0.371505	0.196298
H	0.995353	-0.357869	1.683726
H	4.307501	-0.171668	0.691191
H	3.387772	-2.674704	0.712009
H	2.265343	1.457637	0.204518
H	1.322615	0.727319	-2.020875
H	2.980647	0.124789	-2.055232
H	2.118642	-2.123406	-2.029775
H	0.477314	-1.476282	-1.974010
H	0.760186	-2.592997	0.269590
C	-1.275454	1.545998	-1.621205
C	-2.531770	-1.275007	0.197247
C	-1.505396	1.744699	1.826442
H	-2.442049	2.289968	1.659658
H	-1.594827	1.201998	2.774868
H	-0.697193	2.481046	1.928842
H	-3.569082	-0.907704	0.180034
H	-2.396766	-1.925095	-0.678116
H	-2.417652	-1.903255	1.092302
H	-2.273213	1.998980	-1.673551
H	-0.534849	2.355649	-1.650266
H	-1.141855	0.922788	-2.512474

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anti-7-Diphenylphosphineoxidenorbornene (**16a-desoxy**)

neutral

B3LYP/6-31+G*, -675707.94
Zero Point Energy Correction 203.31
xyz coordinates:

C	-0.018909	-0.037620	-0.003494
C	-0.012001	-0.025022	1.568188
C	1.525986	0.012644	1.817724
C	1.762591	-1.333514	1.068319
C	1.207609	-0.940975	-0.348681
C	0.698976	-2.223065	1.696942
C	-0.355745	-1.446123	1.992972
P	2.032841	0.060137	3.626233
C	1.607579	1.828999	4.027307
C	0.471423	2.058718	4.823456
C	0.072505	3.360224	5.150458
C	0.813596	4.454941	4.694367
C	1.952144	4.240333	3.908228
C	2.344344	2.939159	3.577764
C	3.887994	0.116487	3.537355
C	4.643910	0.371918	2.379806
C	6.043494	0.358600	2.418567
C	6.714219	0.098487	3.617751
C	5.976000	-0.157083	4.779087
C	4.578844	-0.157903	4.733721
H	0.937059	-1.826835	-0.933046
H	-0.611063	0.775946	2.011064
H	2.781291	-1.731664	1.055475
H	-1.332625	-1.763634	2.354108
H	0.763653	-3.307825	1.765394
H	-0.106575	1.212604	5.196824
H	3.235253	2.794780	2.970060
H	-0.812248	3.516020	5.767774
H	2.538075	5.087872	3.552081
H	0.509956	5.469160	4.953075
H	4.153467	0.587473	1.433717
H	4.015649	-0.378093	5.641826
H	6.608475	0.556447	1.507517
H	6.487161	-0.367375	5.718550
H	7.803624	0.089251	3.646261
H	1.982920	0.858660	1.285528
H	0.112860	0.979190	-0.392595
H	-0.963078	-0.428071	-0.397777
H	1.965384	-0.384836	-0.913905

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radical anion

B3LYP/6-31+G*, -675737.73
Zero Point Energy Correction 199.98

xyz coordinates:

C	0.106172	-0.163987	-0.180243	-0.546131
C	-0.016821	-0.078647	1.385080	-0.124180
C	1.492480	-0.054818	1.765618	0.033212
C	1.765962	-1.434386	1.098054	-0.116146
C	1.339639	-1.103174	-0.379112	-0.545197
C	0.635805	-2.279790	1.669190	-0.320617
C	-0.424719	-1.473190	1.839959	-0.309036
P	1.899967	0.095793	3.604975	-0.333057
C	1.458659	1.852618	3.924295	0.376554
C	0.924877	2.180066	5.203429	-0.397336
C	0.735060	3.494629	5.616673	-0.319836
C	1.090652	4.573380	4.765452	-0.364596
C	1.622674	4.276319	3.498261	-0.525358
C	1.801810	2.957849	3.076746	0.025271
C	3.739175	0.065067	3.556745	0.394357
C	4.553034	0.772130	2.612697	0.038717
C	5.939282	0.845333	2.763653	-0.555219
C	6.589993	0.227284	3.844987	-0.357962
C	5.803742	-0.479936	4.790211	-0.327210
C	4.421173	-0.546432	4.645736	-0.388695
H	1.099660	-2.009222	-0.947083	0.202391
H	-0.634163	0.751298	1.742427	0.200640
H	2.776628	-1.842225	1.193497	0.201151
H	-1.433370	-1.760243	2.133769	0.202801
H	0.671428	-3.361212	1.793089	0.203084
H	0.654131	1.367247	5.880558	0.181771
H	2.195623	2.779314	2.078339	0.177909
H	0.301443	3.693887	6.597746	0.183341
H	1.893152	5.091142	2.823493	0.185011
H	0.951503	5.605323	5.084204	0.182887
H	4.098269	1.246608	1.745438	0.178601
H	3.836525	-1.090297	5.390508	0.182791
H	6.526835	1.387640	2.019966	0.186100
H	6.283061	-0.984812	5.630113	0.184504
H	7.672086	0.287259	3.952333	0.184140
H	2.008079	0.740640	1.211972	0.205286
H	0.291796	0.831809	-0.601571	0.208990
H	-0.808120	-0.555625	-0.640480	0.202297
H	2.153456	-0.586227	-0.902723	0.208917

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syn-7-Diphenylphosphineoxidenorbornene (**16b-desoxy**)

neutral

B3LYP/6-31+G*, -675708.18
Zero Point Energy Correction 203.24
xyz coordinates:

C	-0.230400	-0.121215	0.293761
C	0.015399	0.033418	1.790368
C	1.567643	-0.121159	1.811122
C	1.770003	0.967365	0.711836
C	0.813164	0.433749	-0.347528
C	1.047649	2.207034	1.349381
C	-0.162800	1.563360	2.091710
P	2.401707	0.176853	3.470783
C	4.190088	-0.161177	3.097338
C	4.676609	-0.814086	1.951252
C	6.051559	-0.995364	1.759332
C	6.965097	-0.532971	2.712114
C	6.496086	0.120603	3.857310
C	5.123306	0.311651	4.040119
C	1.879125	-1.364139	4.373877
C	1.027007	-1.211291	5.481128
C	0.574867	-2.324744	6.200072
C	0.977214	-3.609787	5.824307
C	1.830963	-3.775726	4.726381
C	2.276416	-2.662425	4.007620
H	1.844869	-1.112634	1.431184
H	4.771293	0.839321	4.927628
H	0.924401	0.595929	-1.418815
H	-1.150196	-0.506540	-0.144136
H	2.794661	1.162069	0.381499
H	1.712338	2.727924	2.048464
H	0.744971	2.926361	0.581255
H	-1.129862	1.928948	1.730766
H	-0.115244	1.754989	3.169882
H	3.992190	-1.188153	1.193067
H	6.406982	-1.501918	0.861924
H	8.034894	-0.675052	2.560453
H	7.198422	0.492026	4.603497
H	-0.559794	-0.629577	2.443713
H	2.942682	-2.812893	3.160093
H	2.151902	-4.774444	4.429925
H	0.631905	-4.478297	6.384863
H	-0.085856	-2.185090	7.055620
H	0.716207	-0.212497	5.788594

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radical anion

B3LYP/6-31+G*, -675737.52
Zero Point Energy Correction 199.84
xyz coordinates:

C	0.050092	-0.556884	0.016139
C	0.031947	-0.158116	1.393526
C	1.226513	0.431218	1.897214
C	2.358752	0.607692	1.108291
C	2.352237	0.213136	-0.255018
C	1.183108	-0.366336	-0.777538
P	-1.463618	-0.112158	2.460703

C	-2.610486	1.070036	1.645636
C	-3.148541	0.917713	0.325843
C	-3.840355	1.957954	-0.298426
C	-4.045420	3.189336	0.346998
C	-3.529724	3.358155	1.658165
C	-2.828396	2.327684	2.276428
C	-2.270560	-1.765660	2.018060
C	-1.597870	-3.055588	2.576246
C	-2.617118	-4.097538	2.130843
C	-3.833259	-3.524910	2.196236
C	-3.638238	-2.095568	2.687684
C	-3.229372	-2.224684	4.198229
C	-1.819895	-2.885816	4.121551
H	-2.367047	-1.844816	0.928589
H	-2.431714	2.485853	3.281431
H	-4.799825	-4.007424	2.052950
H	-2.388777	-5.142676	1.923126
H	-4.463646	-1.401691	2.500641
H	-3.177401	-1.235324	4.667206
H	-3.953569	-2.824364	4.760619
H	-1.770025	-3.848571	4.642041
H	-1.051797	-2.232000	4.550474
H	-3.038208	-0.026087	-0.204347
H	-4.237327	1.803794	-1.303965
H	-4.590433	3.993181	-0.145947
H	-3.690892	4.296420	2.190961
H	-0.558430	-3.239698	2.286749
H	-0.821578	-1.034820	-0.426675
H	1.160371	-0.686016	-1.821453
H	3.233014	0.352355	-0.880326
H	3.258449	1.042758	1.545884
H	1.252975	0.752390	2.940597

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7-Trimethylstannylnorbornane (**17**)

neutral

B3LYP/6-31+G*, -248798.16
Zero Point Energy Correction 172.05
xyz coordinates:

C	3.136645000	-0.878898000	0.773929000
C	1.806265000	-0.157979000	1.124787000
C	1.974435000	1.344479000	0.791223000
C	2.009805000	1.357403000	-0.773117000
C	1.821328000	-0.136439000	-1.140922000
C	3.138093000	-0.879661000	-0.792227000
C	0.875898000	-0.649868000	-0.018971000
Sn	-1.214752000	-0.060734000	-0.002075000
C	-2.304527000	-1.541189000	-1.130089000

C	-1.629561000	1.872704000	-0.864905000
C	-1.938306000	-0.071531000	2.031267000
H	4.019556000	-0.381999000	-1.215793000
H	1.464095000	-0.348413000	2.148431000
H	1.489691000	-0.300197000	-2.173297000
H	1.127671000	1.930562000	1.173501000
H	2.955077000	1.750088000	-1.167933000
H	0.841528000	-1.751119000	-0.032213000
H	3.140310000	-1.900663000	1.172944000
H	4.006941000	-0.359733000	1.195265000
H	3.118130000	-1.903282000	-1.186514000
H	2.882600000	1.765960000	1.239425000
H	1.206818000	1.976986000	-1.186260000
H	-1.153935000	2.678130000	-0.293286000
H	-1.271890000	1.930557000	-1.900012000
H	-2.711299000	2.053876000	-0.871060000
H	-3.379017000	-1.322687000	-1.130964000
H	-1.963981000	-1.569671000	-2.172422000
H	-2.161879000	-2.540577000	-0.700806000
H	-1.781018000	-1.052980000	2.494573000
H	-1.420261000	0.677598000	2.642102000
H	-3.012000000	0.150125000	2.062197000

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radical anion

B3LYP/6-31+G*, -248816.47
Zero Point Energy Correction 169.10
xyz coordinates:

C	-0.187508000	0.271123000	0.032955000
C	-0.178202000	0.189291000	1.580806000
C	1.269192000	-0.132379000	2.020416000
C	2.018853000	1.211383000	1.763197000
C	0.912565000	2.117147000	1.177292000
C	0.583083000	1.602220000	-0.246967000
C	-0.336328000	1.676641000	1.981828000
Sn	-0.613160000	2.330714000	4.087690000
C	0.714308000	0.931033000	5.376841000
C	-2.461896000	1.217827000	4.578203000
C	-1.810475000	4.225784000	3.501676000
H	1.481931000	1.446343000	-0.859249000
H	-0.923719000	-0.505136000	1.985700000
H	1.162061000	3.185484000	1.208397000
H	1.308876000	-0.414717000	3.076794000
H	2.865788000	1.097022000	1.073850000
H	-1.239574000	2.091992000	1.503706000
H	-1.214832000	0.320039000	-0.350478000
H	0.294131000	-0.596968000	-0.437819000
H	-0.050237000	2.321759000	-0.781033000
H	1.695095000	-0.962922000	1.442233000
H	2.411665000	1.632582000	2.696343000
H	-2.969754000	1.645574000	5.453792000

H	-3.170024000	1.262332000	3.738705000
H	-2.253443000	0.161614000	4.797124000
H	1.771556000	1.026693000	5.097062000
H	0.600235000	1.229376000	6.427313000
H	0.390017000	-0.115533000	5.264125000
H	-2.222566000	4.720618000	4.390663000
H	-1.163241000	4.936874000	2.972744000
H	-2.639225000	3.927021000	2.838936000

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7-Diphenylphosphineoxidenorbornane (**18-desoxy**)

neutral

B3LYP/6-31+G*, -676484.83
Zero Point Energy Correction 218.61
xyz coordinates:

C	-0.038050	-0.127573	0.055448
C	0.005356	-0.065732	1.603057
C	1.543125	-0.009566	1.841654
C	1.807476	-1.346608	1.089331
C	1.200481	-1.017949	-0.298356
C	0.861063	-2.339980	1.807712
C	-0.384972	-1.461518	2.149970
P	2.069283	0.059905	3.643983
C	1.635166	1.825006	4.045293
C	0.523784	2.051390	4.876356
C	0.120059	3.352544	5.199464
C	0.832332	4.449541	4.704516
C	1.947256	4.237973	3.883981
C	2.343820	2.937319	3.557285
C	3.922639	0.126924	3.546601
C	4.669225	0.376356	2.381928
C	6.069156	0.378697	2.414170
C	6.748498	0.139491	3.612933
C	6.018930	-0.110224	4.781175
C	4.621656	-0.125505	4.743092
H	0.925241	-1.928963	-0.843927
H	-0.577377	0.760051	2.025555
H	2.849552	-1.681145	1.045620
H	-0.563091	-1.430685	3.231127
H	0.614709	-3.192760	1.163619
H	-0.031091	1.203769	5.279888
H	3.215272	2.794994	2.920929
H	-0.745616	3.506361	5.843893
H	2.510971	5.087580	3.497871
H	0.524660	5.463630	4.959385
H	4.170577	0.574812	1.436346
H	4.065043	-0.339927	5.656726
H	6.627651	0.572486	1.498140

H	6.537128	-0.303340	5.720594
H	7.838180	0.141482	3.635900
H	1.980714	0.844887	1.305570
H	0.058639	0.875740	-0.377289
H	-0.982322	-0.552672	-0.306059
H	1.919469	-0.468673	-0.918618
H	-1.303873	-1.829807	1.678138
H	1.324204	-2.741672	2.716763

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radical anion

B3LYP/6-31+G*, -676514.27
Zero Point Energy Correction 215.35
xyz coordinates:

C	0.015739	0.030861	0.004520
C	0.012043	0.001826	1.427569
C	1.294393	-0.055130	2.066230
C	2.474386	-0.081972	1.320185
C	2.451414	-0.046168	-0.084702
C	1.192920	0.016713	-0.737214
P	-1.602129	-0.220472	2.279644
C	-1.543569	-1.918180	2.979159
C	-2.363061	-2.915661	2.378730
C	-2.262034	-4.262351	2.713787
C	-1.308140	-4.694196	3.671804
C	-0.483814	-3.728536	4.275487
C	-0.592110	-2.375450	3.949176
C	-1.354460	0.834262	3.827134
C	-2.521853	0.853667	4.852723
C	-1.946949	1.807341	5.931580
C	-1.154883	2.861071	5.084794
C	-1.372974	2.375474	3.628570
C	-2.847313	2.658206	3.246598
C	-3.639694	1.610044	4.092843
H	-1.520758	3.885144	5.235162
H	-2.831874	-0.121325	5.244959
H	-0.643739	2.775705	2.915282
H	-4.205504	0.928982	3.446577
H	-3.132456	3.692275	3.478396
H	-3.098268	-2.609823	1.631445
H	0.049548	-1.662663	4.463394
H	-2.928350	-4.986505	2.242797
H	0.249965	-4.037848	5.022720
H	-1.219519	-5.746982	3.936051
H	1.364271	-0.059359	3.152085
H	-0.940618	0.069277	-0.521075
H	3.432561	-0.121160	1.842481
H	1.144895	0.063785	-1.826102
H	3.377110	-0.062739	-0.658178
H	-0.423572	0.530575	4.325773
H	-1.279761	1.266024	6.614130
H	-2.738496	2.263099	6.540532

H	-0.088140	2.854356	5.341947
H	-4.352854	2.076284	4.784352
H	-3.012681	2.505160	2.173908

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Trimethyltin anion

B3LYP/6-31+G*, -77315.18
Zero Point Energy Correction 66.10
xyz coordinates:

C	-0.209063	0.247651	-2.027557
Sn	-0.230869	0.259723	0.206832
C	1.992015	0.240093	0.423566
C	-0.468106	-1.950873	0.431573
H	2.433760	1.205309	0.138350
H	2.294686	0.036434	1.460401
H	2.428942	-0.539056	-0.219274
H	-1.476752	-2.286015	0.149934
H	0.259377	-2.474715	-0.206611
H	-0.294664	-2.260934	1.471926
H	0.132539	1.215361	-2.421762
H	0.476245	-0.531440	-2.393938
H	-1.206726	0.053048	-2.446750

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Diphenyl phosphorus anion

B3LYP/6-31+G*, -505005.46
Zero Point Energy Correction 112.70
xyz coordinates:

C	-0.27540421	-0.15099061	-0.28932360
P	-0.53821536	-0.40250322	1.51671515
C	0.98065927	-0.06209158	-0.93842677
C	1.08726690	0.24045206	-2.29925226
C	-0.05657337	0.48687665	-3.07082859
C	-1.31134130	0.41919655	-2.45007636
C	-1.41599108	0.09672123	-1.09428670
H	1.89383648	-0.21664944	-0.36730770
H	2.07550880	0.29606821	-2.75795772
H	0.02814975	0.72744665	-4.13007142
H	-2.21714514	0.60270721	-3.02933381
H	-2.40718221	0.02881630	-0.64349044
C	0.87542062	-1.43189423	2.09251496
C	1.22944665	-1.35465314	3.46383582
C	2.21144855	-2.17569879	4.02368975
C	2.90422498	-3.10094860	3.23050014

C	2.57820429	-3.19331273	1.87057004
C	1.58159220	-2.38430252	1.31672998
H	0.72136370	-0.63046839	4.10250668
H	2.45013833	-2.07964424	5.08368763
H	3.67843514	-3.73462441	3.66181133
H	3.09499237	-3.91375436	1.23489248
H	1.33847902	-2.50641421	0.26356889

Gaussian09 data

radical (anti-**19**)

B3LYP/6-31+G*, -266370.85
Zero Point Energy Correction 101.86
xyz coordinates:

C	-0.001775	0.000632	-0.000308
C	-0.001342	0.000406	1.387578
C	1.211699	-0.000101	2.114288
C	2.435525	0.000136	1.459624
C	2.438494	-0.010724	0.050295
C	1.239361	-0.010534	-0.668056
C	-1.131992	0.049240	2.436461
C	-1.060199	-1.270969	3.225632
C	0.090936	-1.270734	3.915572
C	0.820764	0.049392	3.606010
C	-0.399630	0.955280	3.428741
H	1.263507	-0.014642	-1.755066
H	-0.931108	0.012673	-0.565400
H	-2.112607	0.350827	2.066557
H	0.503627	-2.067476	4.525719
H	3.372283	0.011983	2.012328
H	3.385493	-0.014810	-0.483914
H	-1.792369	-2.068168	3.149505
H	1.609620	0.351386	4.295824
H	-0.332238	2.037032	3.316115

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radical (syn-**19**)

B3LYP/6-31+G*, -266371.05
Zero Point Energy Correction 101.89
xyz coordinates:

C	-0.003096	0.001626	0.000374
C	0.000365	-0.001517	1.531684
C	1.518095	-0.001974	1.754992
C	2.075025	0.760510	0.707065
C	0.899146	1.228392	-0.160327
C	3.444320	0.964773	0.622712
C	4.268239	0.387204	1.609987

C	3.716527	-0.368447	2.647747
C	2.323770	-0.569773	2.730722
C	-0.477327	1.459693	1.713469
C	0.053425	2.186354	0.713115
H	-0.908930	-0.144585	-0.587207
H	4.367804	-0.808039	3.399259
H	1.900682	-1.161081	3.539851
H	-0.571853	-0.763613	2.061784
H	-0.041965	3.253951	0.540822
H	3.880125	1.549309	-0.184596
H	5.344955	0.530198	1.561218
H	-1.098916	1.806665	2.533094
H	1.141499	1.580722	-1.163500

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anti radical (anti-**20**)

B3LYP/6-31+G*, -314932.73
Zero Point Energy Correction 123.36
xyz coordinates:

C	-0.001379	0.005824	0.000019
C	-0.000897	0.003840	1.397660
C	1.174192	-0.002146	2.139959
C	2.372690	-0.009925	1.400527
C	2.372206	-0.007879	-0.004534
C	1.173198	0.002023	-0.743107
C	-1.523939	0.012640	1.498204
C	-2.257966	-1.344328	1.836473
C	-3.699621	-1.105441	1.371164
C	-3.699976	-1.103715	0.025955
C	-2.258560	-1.341517	-0.440666
C	-1.524485	0.014683	-0.099442
C	-1.779734	-2.219053	0.696703
H	-0.897852	-2.852403	0.695727
H	-2.120175	-1.697695	2.860203
H	-4.530705	-0.872296	-0.634022
H	-4.530004	-0.875700	2.032157
H	-2.121278	-1.692357	-1.465335
H	1.189471	0.010683	-1.830686
H	3.323779	-0.010552	-0.531118
H	3.324625	-0.014087	1.926446
H	1.191233	0.003500	3.227546
H	-1.975897	0.876049	-0.602787
H	-1.974846	0.872823	2.004038

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syn radical (syn-**20**)

B3LYP/6-31+G*, -314934.05
Zero Point Energy Correction 123.67
xyz coordinates:

C	0.005965	-0.002289	0.000083
C	0.003213	-0.001026	1.520917
C	1.534214	0.001990	1.838676
C	2.138437	0.868122	0.641106
C	0.866336	1.237074	-0.190307
C	0.061027	2.185140	0.712024
C	-0.449373	1.453825	1.722795
C	2.373191	-1.151395	1.295530
C	2.901986	-0.393405	0.246997
C	3.804317	-0.921104	-0.669237
C	4.155143	-2.272280	-0.483967
C	3.623650	-3.034233	0.570197
C	2.713606	-2.484431	1.493627
H	-0.890558	-0.189828	-0.587929
H	-0.579764	-0.764749	2.039573
H	-0.010736	3.260733	0.575809
H	-1.019606	1.814856	2.574301
H	1.057861	1.585038	-1.207340
H	4.231063	-0.342406	-1.485478
H	4.858109	-2.740338	-1.169248
H	3.928356	-4.073039	0.674481
H	2.317126	-3.085283	2.309141
H	2.740986	1.741277	0.909807
H	1.758105	0.332397	2.857707

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anti radical (anti-**21**)

B3LYP/6-31+G*, -170722.37
Zero Point Energy Correction 87.19
xyz coordinates:

C	-0.000089	0.001846	-0.001325
C	0.000878	0.004133	1.525178
C	1.493178	0.000213	1.785365
C	1.839521	-1.132411	0.840703
C	1.090543	-0.672814	-0.407326
C	-0.327306	-1.486325	1.952862
C	0.941188	-2.270445	1.480412
H	2.888797	-1.406329	0.714568
H	-0.812400	0.376012	-0.617972
H	1.348494	-0.961006	-1.422461
H	-0.614751	0.758601	2.018827
H	1.948699	0.148302	2.763350
H	-0.449807	-1.546962	3.040115
H	-1.253179	-1.843579	1.488677
H	0.715282	-3.060277	0.755571
H	1.462912	-2.729584	2.327684

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syn radical (syn-**21**)

B3LYP/6-31+G*, -170721.42
Zero Point Energy Correction 86.99
xyz coordinates:

C	-0.000089	0.001846	-0.001325
C	0.000878	0.004133	1.525178
C	1.493178	0.000213	1.785365
C	1.839521	-1.132411	0.840703
C	1.090543	-0.672814	-0.407326
C	-0.327306	-1.486325	1.952862
C	0.941188	-2.270445	1.480412
H	2.888797	-1.406329	0.714568
H	-0.812400	0.376012	-0.617972
H	1.348494	-0.961006	-1.422461
H	-0.614751	0.758601	2.018827
H	1.948699	0.148302	2.763350
H	-0.449807	-1.546962	3.040115
H	-1.253179	-1.843579	1.488677
H	0.715282	-3.060277	0.755571
H	1.462912	-2.729584	2.327684

TS
anti-7-Diphenylphosphinebenzonorbornadiene (**12a-desoxy**)

B3LYP/6-31+G*, -771370.05, 1 imaginary freq.
Zero Point Energy Correction 215.14
xyz coordinates

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38708900
C	1.21563900	0.00000000	2.11282100
C	2.43629000	-0.00075100	1.45415000
C	2.44053400	0.00632800	0.03973100
C	1.24281300	0.00695900	-0.67512100
C	-1.12235500	0.06732600	2.44153600
C	-0.40465100	1.00372000	3.44717800
C	0.81995400	0.06945500	3.60131300
C	0.10057000	-1.25325500	3.91000700
C	-1.05049100	-1.25483200	3.22217700
P	-1.53904700	1.89637100	5.81517800
C	-2.29753300	3.32132700	4.94904700
C	-3.32684100	3.03747500	4.01468300
C	-4.04959600	4.04928200	3.37920300
C	-3.76611000	5.39686800	3.63767800
C	-2.74881300	5.70453300	4.55250100
C	-2.03400000	4.69101200	5.19514900
C	0.06538000	2.48895700	6.45760700
C	0.92185900	3.42079700	5.81629800
C	2.18556600	3.72874900	6.32567800
C	2.66353200	3.10587400	7.48673600
C	1.84609400	2.16253700	8.12771100
C	0.57780200	1.86747700	7.62630200
H	-2.10523600	0.35458500	2.06075500
H	1.61828800	0.36117700	4.28685400
H	-1.77892100	-2.05656900	3.14293100
H	0.51679000	-2.05363600	4.51484600

H	-0.93039400	0.00623000	-0.56505500
H	3.37524900	0.00522000	2.00484800
H	1.26311100	0.01779800	-1.76278000
H	3.38815200	0.01689700	-0.49449700
H	-3.56107000	1.99891400	3.78665900
H	-1.27017100	4.96847700	5.91637400
H	-4.83276800	3.78415300	2.67098200
H	-2.51576900	6.74450100	4.77525800
H	-4.32222800	6.18719900	3.13951400
H	0.59665200	3.90262000	4.89836700
H	-0.04270000	1.14259200	8.15193200
H	2.80831300	4.45371000	5.80377900
H	2.19540000	1.66333000	9.02980000
H	3.64767400	3.34688900	7.88095000
H	-0.19251700	2.01659000	3.08923300

TS
syn-7-Diphenylphosphinebenzonorbornadiene (**12b-desoxy**)

B3LYP/6-31+G*, -771369.65, 1 imaginary freq.
Zero Point Energy Correction 215.22
xyz coordinates

C	0.32623200	0.00405100	-0.29193400
C	0.12210900	-0.00432000	1.10580700
C	1.23154000	0.00019500	1.93662200
C	2.53735600	0.01781900	1.40068500
C	2.74406300	0.03105100	0.03024600
C	1.61736400	0.02147000	-0.82168300
C	1.39814600	-0.00376900	3.46063900
C	2.66805800	-0.88319600	3.55163800
C	3.48946600	0.02325700	2.60219400
C	2.02321500	1.36629300	3.82053200
C	3.26734100	1.38198000	3.31104900
P	2.26972900	-3.57190000	3.09883400
C	3.93530400	-3.95098600	3.76165000
C	5.04914700	-3.50214100	3.00540700
C	6.36130500	-3.82843600	3.35410500
C	6.62442800	-4.60769100	4.48860700
C	5.54157300	-5.05850400	5.25714000
C	4.22900500	-4.74068100	4.90023900
C	1.11100400	-3.75760400	4.49775500
C	1.38201500	-3.42777500	5.85168600
C	0.39514500	-3.50032900	6.83781500
C	-0.91438800	-3.88364700	6.51764500
C	-1.21627600	-4.18970700	5.18125500
C	-0.22654600	-4.13122600	4.20016800
H	2.37874400	-3.10030200	6.13387800
H	-0.48421300	-4.38880200	3.17348500
H	0.64906500	-3.24399000	7.86528600
H	-2.22665400	-4.48727800	4.90615300
H	-1.68046000	-3.94007400	7.28704700

H	4.87570200	-2.88633200	2.12457000
H	3.41586500	-5.13059500	5.50617800
H	7.18432200	-3.46417200	2.74149600
H	5.72002800	-5.67224500	6.13862900
H	7.64530700	-4.85753600	4.76692300
H	4.52837600	-0.23916400	2.39035000
H	0.51609800	-0.29239200	4.03678000
H	3.97855700	2.20424100	3.32000300
H	1.50457800	2.17371000	4.33130600
H	3.74828900	0.04208500	-0.38966200
H	-0.88779000	-0.02139600	1.51163900
H	1.75869100	0.02543100	-1.90020000
H	-0.53176900	-0.00552900	-0.96049000
H	3.08286000	-1.01809300	4.55569200

TS
anti-7-Diphenylphosphineoxidecyclobutebenzonorbornene (**14a-desoxy**)

B3LYP/6-31+G*, -819930.77, 1 imaginary freq.
Zero Point Energy Correction 236.91
xyz coordinates:

C	-3.353381000	-0.999546000	0.265886000
C	-3.280146000	0.269754000	-0.316743000
C	-3.631614000	0.498182000	-1.641824000
C	-4.065097000	-0.625681000	-2.373217000
C	-4.138686000	-1.900434000	-1.788174000
C	-3.782773000	-2.116003000	-0.441770000
C	-2.774873000	0.935330000	0.960449000
C	-1.231401000	1.269772000	1.089094000
C	-0.587572000	-0.102779000	0.891603000
C	-1.352162000	-0.779042000	2.031246000
C	-2.859308000	-0.512360000	1.625557000
C	-1.121127000	0.229157000	3.157861000
C	-1.049185000	1.448510000	2.597123000
P	2.131335000	-0.189687000	1.037027000
C	2.207748000	-1.391252000	-0.344760000
C	1.536427000	-2.627835000	-0.160569000
C	1.622144000	-3.663302000	-1.093719000
C	2.371067000	-3.504363000	-2.266952000
C	3.038847000	-2.288755000	-2.476523000
C	2.961605000	-1.258600000	-1.536535000
C	2.525524000	1.438953000	0.320549000
C	2.192998000	1.882280000	-0.988129000
C	2.440052000	3.191662000	-1.405961000
C	3.008857000	4.131404000	-0.534567000
C	3.321266000	3.727956000	0.773963000
C	3.088278000	2.416425000	1.186025000
H	-0.655707000	-0.556469000	-0.098914000
H	-0.897788000	2.095659000	0.454977000
H	-1.131111000	-0.009313000	4.218397000
H	-0.988437000	2.406390000	3.107589000
H	-1.129404000	-1.825855000	2.259214000

H	-3.853222000	-3.108649000	-0.001526000
H	-4.482293000	-2.738055000	-2.391184000
H	-4.353849000	-0.506635000	-3.415234000
H	-3.587810000	1.480408000	-2.108153000
H	-3.559144000	-0.638848000	2.460621000
H	-3.420998000	1.716534000	1.379219000
H	0.937704000	-2.773935000	0.736798000
H	1.093237000	-4.596659000	-0.908104000
H	2.434362000	-4.305914000	-2.998804000
H	3.634448000	-2.145039000	-3.376562000
H	3.514434000	-0.341757000	-1.721960000
H	3.354666000	2.127359000	2.202166000
H	3.760420000	4.438567000	1.472131000
H	3.200616000	5.149797000	-0.863345000
H	2.174560000	3.485199000	-2.420578000
H	1.723734000	1.192634000	-1.684444000

TS
syn-7-Diphenylphosphineoxidecyclobutebenzonorbornene (**14b-desoxy**)

B3LYP/6-31+G*, -819927.95, 1 imaginary freq.
Zero Point Energy Correction 237.21
xyz coordinates:

C	0.019307	0.187239	0.099261
C	0.061508	0.101570	1.634113
C	1.594124	-0.001707	1.939117
C	1.955217	-1.447652	1.375945
C	0.578826	-1.949939	0.831094
C	0.326615	-1.034309	-0.378576
C	-0.433932	-1.344783	1.828277
P	-1.190154	-2.075490	4.168599
C	-2.520304	-0.844324	4.315825
C	-2.402497	0.138479	5.339690
C	-3.297846	1.198872	5.458194
C	-4.368886	1.336514	4.556146
C	-4.500280	0.392557	3.526884
C	-3.596182	-0.663595	3.400662
C	-1.984251	-3.590355	3.503642
C	-1.128802	-4.587544	2.966683
C	-1.612456	-5.828405	2.545376
C	-2.978581	-6.126528	2.628263
C	-3.846474	-5.154910	3.149912
C	-3.359741	-3.918031	3.578678
H	-0.460924	0.898017	2.172217
H	0.526466	-3.024420	0.633800
H	-0.129759	1.098049	-0.477643
H	0.471758	-1.312471	-1.421010
H	-1.465084	-1.474692	1.486468
H	-0.062996	-4.383483	2.887917
H	-4.058558	-3.200068	3.998725

H	-0.918453	-6.565224	2.144161
H	-4.911515	-5.365945	3.231329
H	-3.358414	-7.089919	2.296885
H	-1.589715	0.050206	6.059840
H	-3.718595	-1.359067	2.574881
H	-5.312841	0.485753	2.807496
H	-5.075441	2.157157	4.652382
H	-3.170471	1.919544	6.264372
C	2.080931	-0.514608	3.291442
C	2.390219	-1.785395	2.799235
C	2.958156	-2.771230	3.596861
C	3.201946	-2.420532	4.940133
C	2.898394	-1.141013	5.432296
C	2.330392	-0.149037	4.608088
H	3.218153	-3.760892	3.226171
H	3.644974	-3.152516	5.612132
H	3.113639	-0.912356	6.473959
H	2.113480	0.842009	5.001915
H	2.160762	0.842230	1.529160
H	2.750269	-1.496076	0.622931

TS
anti-7-Diphenylphosphineoxidenorbornene (**16a-desoxy**)

B3LYP/6-31+G*, -675719.69, 1 imaginary freq.
Zero Point Energy Correction 200.58
xyz coordinates:

C	-0.000709	0.058329	0.019861
C	-0.019909	0.019530	1.440586
C	1.248652	-0.039049	2.079781
C	2.443432	-0.040722	1.360935
C	2.433186	0.024525	-0.042244
C	1.195924	0.071612	-0.700038
P	-1.504194	-0.154584	2.484058
C	-2.839873	0.766284	1.633088
C	-2.676785	1.825577	0.706493
C	-3.767480	2.539224	0.204743
C	-5.075191	2.232268	0.609281
C	-5.264283	1.189268	1.525838
C	-4.173625	0.469617	2.017933
C	-2.337330	-2.518995	1.421808
C	-1.320982	-3.657831	1.563591
C	-2.119282	-4.819119	0.963117
C	-3.415666	-4.606968	1.263864
C	-3.486364	-3.304036	2.066831
C	-2.856572	-3.635181	3.466939
C	-1.355935	-3.879851	3.118134
H	-2.513209	-2.151679	0.405328
H	-4.350497	-0.341987	2.721306
H	-4.250127	-5.282718	1.082869
H	-1.691841	-5.702003	0.490586

H	-4.471426	-2.830934	2.117198
H	-2.970305	-2.779029	4.141282
H	-3.331861	-4.503357	3.939241
H	-1.010232	-4.881606	3.400351
H	-0.711257	-3.146456	3.615064
H	-1.677509	2.109866	0.388367
H	-3.594273	3.349875	-0.501290
H	-5.922781	2.790696	0.219551
H	-6.269425	0.929006	1.853641
H	-0.317622	-3.507028	1.154203
H	-0.939086	0.067706	-0.527779
H	1.161933	0.107104	-1.788031
H	3.363158	0.035294	-0.605308
H	3.390524	-0.080896	1.896443
H	1.287411	-0.074587	3.168016

TS
syn-7-Diphenylphosphineoxidenorbornene (**16b-desoxy**)

B3LYP/6-31+G*, -675719.08, 1 imaginary freq.
Zero Point Energy Correction 200.49
xyz coordinates:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.421058
C	1.276572	0.000000	2.045781
C	2.462373	0.017347	1.311979
C	2.432740	0.043059	-0.092041
C	1.186741	0.032155	-0.735241
P	-1.467619	-0.191491	2.484631
C	-2.312633	-2.544511	1.465299
C	-3.245945	-3.455467	2.270628
C	-2.277053	-4.050094	3.283581
C	-1.078998	-4.147623	2.680877
C	-1.241783	-3.619604	1.262211
C	-2.096832	-4.723142	0.509889
C	-3.489603	-4.608520	1.209588
C	-2.827607	0.692985	1.633602
C	-4.153902	0.374762	2.026175
C	-5.259831	1.067489	1.528950
C	-5.093307	2.104040	0.601085
C	-3.792838	2.432075	0.189421
C	-2.687248	1.745206	0.695686
H	-1.657659	-5.726025	0.594879
H	-4.169757	-3.029486	2.673634
H	-0.323050	-3.341254	0.738532
H	-2.556559	-4.436544	4.261034
H	-0.184486	-4.630522	3.067675
H	-4.313705	-0.433308	2.737878
H	-1.694416	2.044355	0.370918
H	-6.258854	0.790760	1.861840

H	-3.637400	3.237975	-0.526096
H	-5.952517	2.641999	0.208019
H	-0.945078	-0.036253	-0.535136
H	1.328980	-0.004264	3.133984
H	1.138931	0.036643	-1.823282
H	3.416610	0.023029	1.836080
H	3.354943	0.068245	-0.667305
H	-2.737286	-2.109945	0.553169
H	-4.269241	-4.304270	0.500761
H	-3.812235	-5.548804	1.676288
H	-2.164556	-4.478977	-0.557161

Diphenyl phosphorus anion

B3LYP/6-31+G*, -505002.38
Zero Point Energy Correction 113.24
xyz coordinates:

C	0.006660	0.012201	-0.007110
C	-0.003226	-0.003258	1.410725
C	1.268886	-0.010946	2.040435
C	2.460289	-0.011284	1.312560
C	2.439678	0.016562	-0.088700
C	1.197478	0.029857	-0.737544
P	-1.485210	-0.162057	2.486665
C	-2.877014	0.579600	1.541247
C	-2.780881	1.639470	0.604237
C	-3.912086	2.209831	0.015323
C	-5.198187	1.761352	0.345879
C	-5.324036	0.723153	1.278977
C	-4.190860	0.142745	1.852559
H	-1.802984	2.035536	0.343103
H	-3.787962	3.021249	-0.700231
H	-6.077464	2.207549	-0.112206
H	-6.311085	0.353240	1.551405
H	-4.319391	-0.675764	2.560036
H	1.317205	-0.012853	3.128891
H	3.411263	-0.019138	1.842631
H	3.365287	0.028731	-0.658927
H	1.154175	0.042417	-1.825582
H	-0.935317	-0.005583	-0.549093

PART 4. ADDITIONAL CALCULATIONS

Stepwise ET mechanism using Marcus – Hush Theory

According to Marcus equation, the solvent reorganization energy λ_o may be calculated from the following equation:

$$\lambda_o = 331.2kcal/mol\left(\frac{1}{2a_1}+\frac{1}{2a_2}-\frac{1}{(a_1+a_2)}\right)\left(\frac{1}{\epsilon_{op}}-\frac{1}{\epsilon}\right)$$

here a_1 and a_2 are the radii of the molecules involved in ET, ε_{op} is the optical dielectric constant (ε_{op} = 1.8), and ε is the static dielectric constant for the NH_3 solvent (ε = 22.4). We calculated the radii of the donor (radical anion) and acceptor (RBr) with B3LYP/6-31+G*
As there is not sufficient data to calculate the inner reorganization energy for the reactants, λ_i is estimate $\lambda i \approx 0$, since the inner reorganization energies in stepwise electron transfer reactions are usually small. Thus, the total reorganization energy $\lambda = \lambda_0 + \lambda_i$
According to Marcus theory,

$$\Delta G_{ET}^{\ddagger} = \Delta G_0^{\ddagger}\left(1+\frac{\Delta G_r}{4\Delta G_0^{\ddagger}}\right)^2$$

where ΔG_r is the reaction energy, and $\Delta G^{\ddagger}_0$ is the intrinsic barrier (i.e. the activation energy at zero driving force) for the outer-sphere electron transfer. $\Delta G^{\ddagger}_0$ is related to the reorganization energy (λ) by:

$$\Delta G_0^{\ddagger} = \frac{\lambda}{4}$$

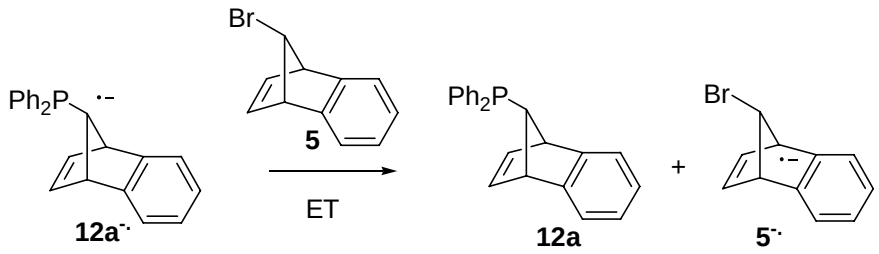
The concerted DET mechanism using Savéant's model

Savéant's model is used for concerted inter-DET. In Savéant's model, the intrinsic barrier $\Delta G^{\ddagger}_0$ includes contribution from bond dissociation free energy (BDFE):

$$\Delta G_0^{\ddagger} = \frac{\lambda}{4} = \frac{\lambda_o + \lambda_i + BDE}{4}$$

λ_0 and λ_i are the same as in the Marcus-Hush theory.

Estimation of activation barrier for ET from 12a(desoxi) to 5 in NH_3(l) as solvent



Marcus-Hush

RA (a_1= 5.89 Å); RBr (a_2= 4.56 Å); λo=16,76638469; $\Delta G^{\ddagger}_0$=4,19159617
$E_{RPPh2^{-\cdot}}$ (zero point corrected)= -1228,9445152H(Hartree); E_{RBr} (zero point corrected)= -2996,1341230H
E_{RPPh2} (zero point corrected)= -1228,8909958H; $E_{RBr^{-\cdot}}$ (zero point corrected)= -2996,1829421H

ΔG_p =0,0047003H=2,9494806kcal/mol

$$\Delta G_{ET}^{\ddagger} = 4{,}19\left(1 + \frac{2{,}95}{16{,}77}\right)^2 = 5{,}77 \text{ kcal/mol}$$

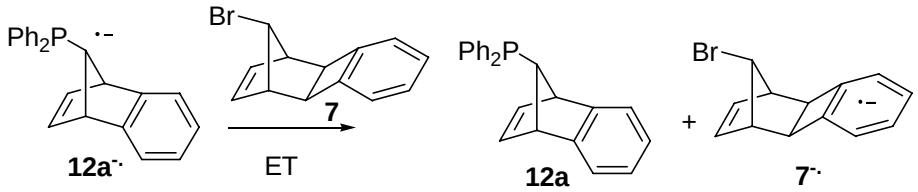
Savéant's model

E_{RBr} (zero point corrected)= -2996,1341230H; $E_{R^{\cdot}}$ (zero point corrected)= -424,3330419H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 79,99710008 kcal/mol

λo= 96,76348477kcal/mol; $\Delta G^{\ddagger}_0$= 24,1908712kcal/mol; ΔG_p =-32,64kcal/mol

$$\Delta G_{ET}^{\ddagger} = 24{,}19\left(1 + \frac{-32{,}64}{96{,}76}\right)^2 = 10{,}62 \text{ kcal/mol}$$

Estimation of activation barrier for ET from 12a(desoxi) to 7 in NH_3(l) as solvent



Marcus-Hush

RA (a_1= 5.89 Å); RBr (a_2= 4.81 Å); λo= 16,17894917; $\Delta G^{\ddagger}_0$= 4,04473729

$E_{RPPh2^{\cdot}}$ (zero point corrected)= -1228,9445152; E_{RBr} (zero point corrected)= -3073,4901025

E_{RPPh2} (zero point corrected)= -1228,8909958; $E_{RBr^{\cdot}}$ (zero point corrected)= -3073,5310025

ΔG_p =0,0126194H= 7,9187871kcal/mol

$$\Delta G_{ET}^{\ddagger} = 4{,}04\left(1 + \frac{7{,}92}{16{,}18}\right)^2 = 8{,}97 \text{ kcal/mol}$$

Savéant's model

RA (a_1= 5.89 Å); RBr (a_2= 4.81 Å); λo´= 16,17894917

$E_{RPPh2^{\cdot}}$ (zero point corrected)= -1228,9445152; E_{RBr} (zero point corrected)= -3073,4901025

E_{RPPh2} (zero point corrected)= -1228,8909958; $E_{anti\text{-}R^{\cdot}}$ (zero point corrected)= -501,687673H

E_{Br^-} = -2571,906612H

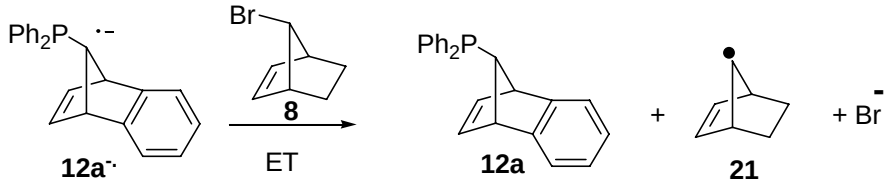
ΔG_p = -31,79kcal/mol

E_{RBr} (zero point corrected)= -3073,4901025H; $E_{anti\text{-}R^{\cdot}}$ (zero point corrected)= -501,687673H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 79,837782 kcal/mol

λo= 96,016731kcal/mol; $\Delta G^{\ddagger}_0$= 24,0041828 kcal/mol; ΔG_p = -31,79kcal/mol

$$\Delta G_{ET}^{\ddagger} = 24{,}004\left(1 + \frac{-31{,}79}{96{,}02}\right)^2 = 10{,}74 \text{ kcal/mol}$$

Estimation of activation barrier for ET from 12a(desoxi) to 8 in NH_3(l) as solvent



Savéant's model

RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol

$E_{RPPh_2^{-\cdot}}$ (zero point corrected)= -1228,9445152; E_{RBr} (zero point corrected)= -2843,7279126

E_{RPPh2} (zero point corrected)= -1228,8909958; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,9267293

E_{Br^-} = -2571,906612H

ΔG_r° = -32,57kcal/mol

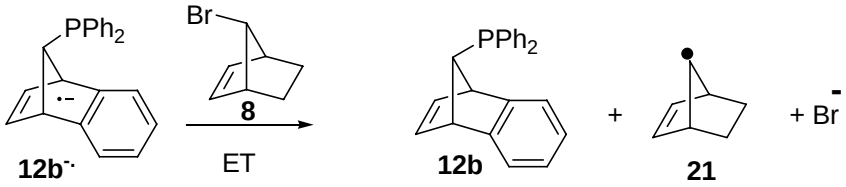
E_{RBr} (zero point corrected)= -2843,72791 H; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,926729H;

$E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,06 kcal/mol

λo= 97,69kcal/mol; $\Delta G^{\ddagger}_0$= 24,42 kcal/mol; ΔG_r° = -32,57 kcal/mol

$$\Delta G_{ET}^{\ddagger} = 24{,}42\left(1+\frac{-32{,}57}{97{,}69}\right)^2 = 10{,}85 \text{ kcal/mol}$$

Estimation of activation barrier for ET from 12b(desoxi)$^{-\cdot}$ to 8 in NH_3(l) as solvent



RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol

$E_{RPPh_2^{-\cdot}}$ (zero point corrected)= -1228,9445178; E_{RBr} (zero point corrected)= -2843,7279126

E_{RPPh2} (zero point corrected)= -1228,8911805; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,9267293

E_{Br^-} = -2571,906612H

ΔG_r° = -0,0520914H

ΔG_r° = -32,69kcal/mol

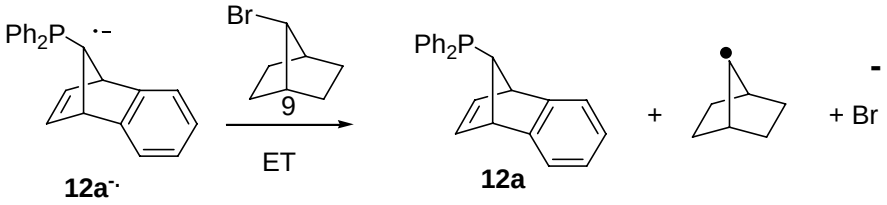
E_{RBr} (zero point corrected)= -2843,72791 H; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,926729H;

$E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,06 kcal/mol

λo= 97,69kcal/mol; $\Delta G^{\ddagger}_0$= 24,42 kcal/mol; ΔG_r° = -32,69 kcal/mol

$$\Delta G_{ET}^{\ddagger} = 24{,}42\left(1+\frac{-32{,}69}{97{,}69}\right)^2 = 10{,}81 \text{ kcal/mol}$$

Estimation of activation barrier for ET from 12a(desoxi) to 9 in NH_3(l) as solvent



Savéant's model

RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol

$E_{RPPh2^{-\cdot}}$ (zero point corrected)= -1228,9445152; E_{RBr} (zero point corrected)= -2844,942479H

E_{RPPh2} (zero point corrected)= -1228,8909958; $E_{anti\text{-}R^{\cdot}}$ (zero point corrected)= -273,1409174

E_{Br^-} = -2571,906612H

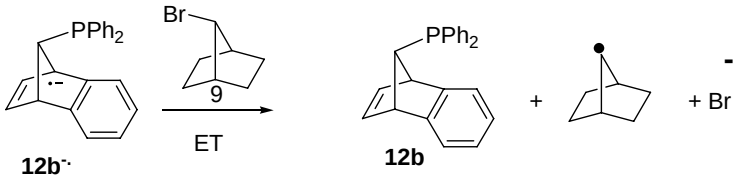
ΔG_r = -32,34kcal/mol

E_{RBr} (zero point corrected)= -2844,942479H; $E_{R^{\cdot}}$ (zero point corrected)= -273,1409271H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,29 kcal/mol

λo= 97,92kcal/mol; $\Delta G^{\ddagger}_0$= 24,48 kcal/mol; ΔG_r = -32,34 kcal/mol

$$\Delta G^{\ddagger}_{ET} = 24{,}48\left(1+\frac{-32{,}34}{97{,}92}\right)^2 = 10{,}98 \text{ kcal/mol}$$

Estimation of activation barrier for ET from 12b(desoxi) to 9 in NH_3(l) as solvent



Savéant's model

RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol

$E_{RPPh2^{-\cdot}}$ (zero point corrected)= -1228,9445178; E_{RBr} (zero point corrected)= -2844,942479H

E_{RPPh2} (zero point corrected)= -1228,8911805; $E_{anti\text{-}R^{\cdot}}$ (zero point corrected)= -273,1409174

E_{Br^-} = -2571,906612H

ΔG_r = -0.0517131kcal/mol

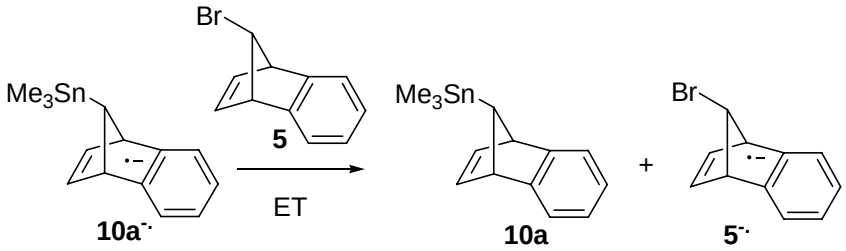
ΔG_r = -32,45kcal/mol

E_{RBr} (zero point corrected)= -2844,942479H; $E_{R^{\cdot}}$ (zero point corrected)= -273,1409271H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,29 kcal/mol

λo= 97,92kcal/mol; $\Delta G^{\ddagger}_0$= 24,48 kcal/mol; ΔG_r = -32,34 kcal/mol

$$\Delta G^{\ddagger}_{ET} = 24{,}48\left(1+\frac{-32{,}45}{97{,}92}\right)^2 = 10{,}94 \text{ kcal/mol}$$

Estimation of activation barrier for ET from 10a to 5 in NH_3(l) as solvent



Marcus-Hush

RA (a_1= 5.89 Å); RBr (a_2= 4.56 Å); λo=16,76638469; $\Delta G^{\ddagger}_0$=4,19159617

$E_{RSnMe3^{-\cdot}}$ (zero point corrected)= -547,4419490H(Hartree); E_{RBr} (zero point corrected)= -2996,1341230H

E_{RSnMe3} (zero point corrected)= -547,4020612; $E_{RBr^{-\cdot}}$ (zero point corrected)= -2996,1829421H

ΔG_r =-0,0089312H=-5,6kcal/mol

$$\Delta G_{ET}^{\ddagger} = 4{,}19\left(1+\frac{-5{,}6}{16{,}77}\right)^2 = 1{,}89\ \text{kcal/mol}$$

Savéant's model

$E_{RSnMe3^{-\cdot}}$ (zero point corrected)= -547,4419490H(Hartree); E_{RBr} (zero point corrected)= -2996,1341230H

E_{RSnMe3} (zero point corrected)= -547,4020612; $E_{R^{\cdot}}$ (zero point corrected)= -424,3330419H

E_{Br^-} = -2571,906612H

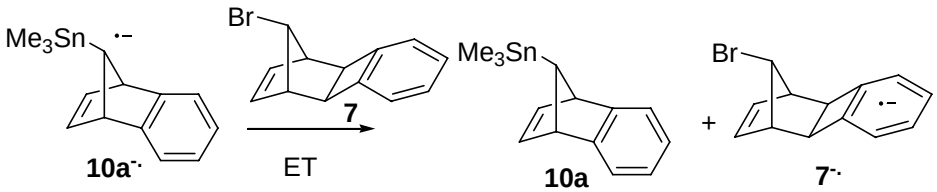
ΔG_r =-41,20kcal/mol

E_{RBr} (zero point corrected)= -2996,1341230H; $E_{R^{\cdot}}$ (zero point corrected)= -424,3330419H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 79,99710008 kcal/mol

λo= 96,76348477kcal/mol; $\Delta G^{\ddagger}_0$= 24,1908712kcal/mol;

$$\Delta G_{ET}^{\ddagger} = 24{,}19\left(1+\frac{-41{,}20}{96{,}76}\right)^2 = 7{,}97\ \text{kcal/mol}$$

Estimation of activation barrier for ET from 10a to 7



Marcus-Hush

RA (a_1= 5.89 Å); RBr (a_2= 4.81 Å); λo= 16,17894917; $\Delta G^{\ddagger}_0$= 4,04473729

$E_{RSnMe3^{-\cdot}}$ (zero point corrected)= -547,4419490H; E_{RBr} (zero point corrected)= -3073,4901025H

E_{RSnMe3} (zero point corrected)= -547,4020612; $E_{RBr^{-\cdot}}$ (zero point corrected)= -3073,5310025

ΔG_r =-0,0010121H= -0,6351181kcal/mol

$$\Delta G_{ET}^{\ddagger} = 4{,}04\left(1+\frac{-0{,}635}{16{,}18}\right)^2 = 3{,}73\ \text{kcal/mol}$$

Savéant's model

RA (a_1= 5.89 Å); RBr (a_2= 4.81 Å); λo´= 16,17894917

$E_{RSnMe3}^{\cdot-}$ (zero point corrected)= -547,4419490H; E_{RBr} (zero point corrected)= -3073,4901025H

E_{RSnMe3} (zero point corrected)= -547,4020612; $E_{R^{\cdot}}$ (zero point corrected)= -501,6876730

E_{Br^-} = -2571,906612H

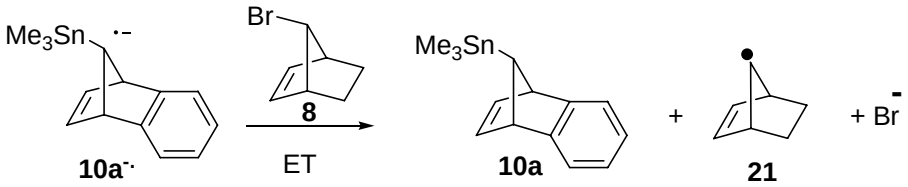
ΔG_r = -40,34kcal/mol

E_{RBr} (zero point corrected)= -3073,4901025H; $E_{anti\text{-}R^{\cdot}}$ (zero point corrected)= -501,687673H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 79,837782 kcal/mol

λo= 96,016731kcal/mol; $\Delta G^{\ddagger}_0$= 24,0041828 kcal/mol; ΔG_r = -40,34kcal/mol

$$\Delta G_{ET}^{\ddagger} = 24{,}004\left(1+\frac{-40{,}34}{96{,}02}\right)^2 = 8{,}07\ \text{kcal/mol}$$

Estimation of activation barrier for ET from 10a to 8 in NH_3(l) as solvent



Savéant's model

RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol

$E_{RSnMe3}^{\cdot-}$ (zero point corrected)= -547,4419490H; E_{RBr} (zero point corrected)= -2843,7279126

E_{RSnMe3} (zero point corrected)= -547,4020612H; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,9267293

E_{Br^-} = -2571,906612H

ΔG_r = -0.0655414

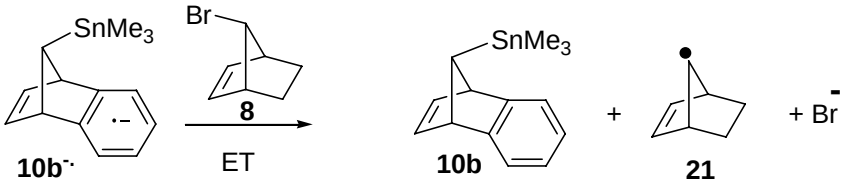
ΔG_r = -41.12kcal/mol

E_{RBr} (zero point corrected)= -2843,72791 H; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,926729H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,06 kcal/mol

λo= 97,69kcal/mol; $\Delta G^{\ddagger}_0$= 24,42 kcal/mol; ΔG_r = -41,12 kcal/mol

$$\Delta G_{ET}^{\ddagger} = 24{,}42\left(1+\frac{-41{,}12}{97{,}69}\right)^2 = 8{,}20\ \text{kcal/mol}$$

Estimation of activation barrier for ET from 10b to 8 in NH_3(l) as solvent



Savéant's model

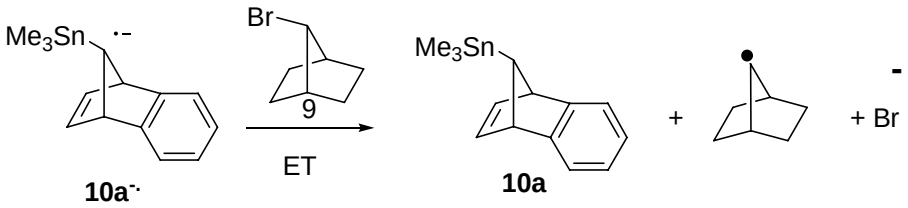
RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol

$E_{RSnMe3}^{\cdot-}$ (zero point corrected)= -547,4404989H; E_{RBr} (zero point corrected)= -2843,7279126

E_{RSnMe3} (zero point corrected)= -547,4006907H; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,9267293
E_{Br^-} = -2571,906612H
ΔG_v = -0.06562
ΔG_v = -41.18kcal/mol
E_{RBr} (zero point corrected)= -2843,72791 H; $E_{syn\text{-}R^{\cdot}}$ (zero point corrected)= -271,926729H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,06 kcal/mol
λo= 97,69kcal/mol; $\Delta G^{\ddagger}_0$= 24,42 kcal/mol; ΔG_v = -41,12 kcal/mol

$$\Delta G^{\ddagger}_{ET} = 24{,}42\left(1+\frac{-41{,}18}{97{,}69}\right)^2 = 8{,}17\ \text{kcal/mol}$$

Estimation of activation barrier for ET from 10a to 9 in NH_3(l) as solvent

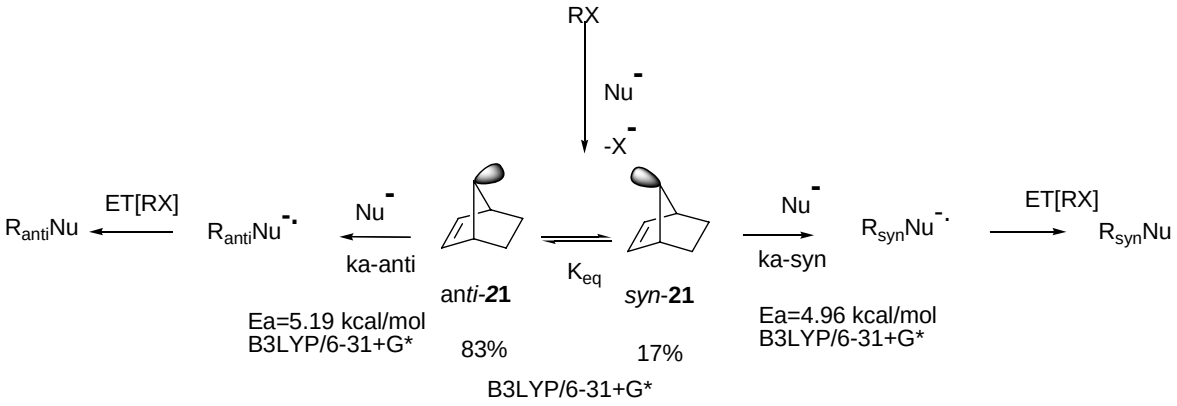


Savéant's model
RA (a_1= 5.89 Å); RBr (a_2= 4.25 Å); λo´= 17,62677819 kcal/mol
$E_{RSnMe3^{-\cdot}}$ (zero point corrected)= -547,4419490H; E_{RBr} (zero point corrected)= -2844,942479H
E_{RSnMe3} (zero point corrected)= -547,4020612H;; $E_{R^{\cdot}}$ (zero point corrected)= -273,1409174
E_{Br^-} = -2571,906612H
ΔG_v = -40,89kcal/mol
E_{RBr} (zero point corrected)= -2844,942479H; $E_{R^{\cdot}}$ (zero point corrected)= -273,1409271H; $E_{Br^{\cdot}}$= -2571,67359756H; BDE= 80,29 kcal/mol
λo= 97,92kcal/mol; $\Delta G^{\ddagger}_0$= 24,48 kcal/mol; ΔG_v = -40,89 kcal/mol

$$\Delta G^{\ddagger}_{ET} = 24{,}48\left(1+\frac{-40{,}89}{97{,}92}\right)^2 = 8{,}3\ \text{kcal/mol}$$

Kinetic Calculations

Estimated **16**-*syn*/*anti* Ratio



$$\frac{d[R_{syn}Nu]}{dt} = kET[RX][RsynNu]-.$$

$$\frac{d[R_{anti}Nu]}{dt} = kET[RX][RantiNu]-.$$

$$\frac{d[R_{syn}Nu]}{d[R_{anti}Nu]} = \frac{k_{ET}[RX][R_{syn}Nu]-.}{k_{ET}[RX][R_{syn}Nu]-.} = \frac{[R_{syn}Nu]-.}{[R_{anti}Nu]-.} =$$

Assuming steady-state

$$\frac{d[R_{syn}Nu-.]}{dt} = ka(syn)[syn(21)][Nu-] - kET\,[RX][RsynNu-.] = 0$$

$$\frac{d[R_{anti}Nu-.]}{dt} = ka(anti)[anti(21)][Nu-] - kET\,[RX][RantiNu-.] = 0$$

$$[R_{syn}Nu-.] = \frac{ka(syn)[syn(21)][Nu^-]}{k_{ET}[RX]}$$

$$[RantiNu-.] = \frac{ka(anti)[anti(21)][Nu^-]}{k_{ET}[RX]}$$

$$\frac{d[R_{syn}Nu]}{d[R_{anti}Nu]} = \frac{k_{a(syn)}}{k_{a(anti)}}K_{eq} = \frac{k_{a(syn)}}{k_{a(anti)}}e^{-\frac{\Delta E(syn-anti)}{RT}} = \frac{Ae^{\frac{(-4.96)1000}{240x1.98}}}{Ae^{\frac{(-5.19)1000}{240x1.98}}}e^{\frac{-0.78x1000}{240x1.98}} = 0.33$$

$$= 24.8/75.2$$