Supplementary Information

Computational and experimental investigation on the BCl_3 promoted intramolecular amination of alkenes and alkynes

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CONTENTS

Section 1: Computational details

The DFT calculations were performed with Gaussian 09 (1). Geometry optimizations of all the minima and transition structures were carried out at the M06-2X level of theory (2) with the 6-31G(d) basis set in DCE using the CPCM model (3). Vibrational frequencies were computed at the same level to verify that optimized structures are energy minima or transition states and to evaluate zero-point vibrational energies (ZPVE) and thermal corrections at 298 K. Solvent effects in DCE were evaluated at the more accurate M06-2X/6-311+G(d,p) level with the CPCM model, using the above optimized structures.

References

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DFT-Computed Energies and Cartesian Coordinates

1

G(DCE) = -1149.046955 Hartree

C	4.547584	-0.878434	1.835428
C	4.244996	-1.163387	0.570605
H	5.510273	-0.460779	2.114028
H	3.837466	-1.058469	2.639922
C	2.933683	-1.746577	0.122449
H	4.985547	-0.973713	-0.206285
C	2.062360	-0.813493	-0.751420
H	3.125328	-2.657253	-0.461700
H	2.351561	-2.048746	1.003364
C	1.659780	0.398037	0.100765
H	2.545354	0.909561	0.492792
H	1.083211	0.047594	0.965430
N	0.821067	1.342333	-0.656872
H	1.332693	2.066445	-1.159426
S	-0.457661	2.039123	0.136355
O	-0.127015	2.379149	1.519490
O	-0.937317	3.091649	-0.755731
C	-1.621699	0.705035	0.180236
C	-2.276560	0.347235	-0.998210

C	-1.833522	0.015541	1.367527
C	-3.153444	-0.726776	-0.976268
H	-2.094297	0.902489	-1.913393
C	-2.715162	-1.063807	1.368932
H	-1.318056	0.321851	2.271954
C	-3.382438	-1.448558	0.204492
H	-3.670144	-1.016512	-1.887038
H	-2.885882	-1.612613	2.290415
C	-4.347269	-2.604830	0.207552
H	-4.279927	-3.176000	1.135947
H	-5.376708	-2.246228	0.103706
H	-4.151088	-3.279736	-0.630501
C	0.807837	-1.579415	-1.179690
H	0.232836	-1.914591	-0.307111
H	0.157080	-0.945781	-1.789578
H	1.082035	-2.461562	-1.768509
C	2.832158	-0.352336	-1.993274
H	3.685885	0.281177	-1.728950
H	3.208510	-1.215161	-2.553870
H	2.178265	0.219942	-2.659590

2

G(DCE) = -2554.633255 Hartree

C	-3.309371	3.033156	-1.922731
C	-3.743483	2.535093	-0.766760
H	-3.014707	4.073263	-2.022271
H	-3.240131	2.413616	-2.814533
C	-4.167603	1.105643	-0.571836
H	-3.806050	3.188669	0.102510
C	-3.234787	0.261843	0.335719
H	-5.166644	1.078949	-0.117394
H	-4.248178	0.612836	-1.549315
C	-1.882526	0.191769	-0.399598
H	-1.509046	1.194895	-0.607946
H	-2.006453	-0.326905	-1.352333
N	-0.795576	-0.544548	0.354494
S	0.286393	0.627173	1.336379
O	-0.352790	1.915925	1.165241
O	0.324486	-0.046528	2.619206
H	-1.226138	-1.053585	1.141607
B	-0.066078	-1.725063	-0.513190
Cl	-1.397555	-2.902681	-1.024236
Cl	0.734501	-0.967850	-1.980593
C	1.884683	0.719689	0.616581
C	2.087177	1.625193	-0.426539
C	2.927244	-0.006031	1.186581
C	3.369033	1.766014	-0.932544
H	1.261785	2.203538	-0.827673
C	4.203820	0.160163	0.665200
H	2.741836	-0.673178	2.020137
C	4.439792	1.032133	-0.402723
H	3.547072	2.461315	-1.747156
H	5.030747	-0.392999	1.099177
C	5.818642	1.180852	-0.984918
H	5.898021	0.607519	-1.914833
H	6.032537	2.225635	-1.224445
H	6.582817	0.813780	-0.296845
C	-3.857075	-1.132156	0.476590
H	-3.995119	-1.607958	-0.498681
H	-3.247610	-1.804613	1.092141
H	-4.833433	-1.046349	0.963907
C	-3.129510	0.901754	1.725265
H	-2.714717	1.909746	1.687849
H	-4.127142	0.947745	2.174203
H	-2.503237	0.309164	2.405044
Cl	1.113121	-2.596443	0.600357

3

G(DCE) = -2093.822419 Hartree

C	3.943259	-2.861477	-1.639991
C	4.144636	-2.152718	-0.531058
H	3.874993	-3.944875	-1.622495
H	3.843942	-2.377108	-2.609264
C	4.252458	-0.653646	-0.493501
H	4.244819	-2.674325	0.420426
C	3.103610	0.069226	0.253827
H	5.190708	-0.369865	0.002288
H	4.304613	-0.267946	-1.520285
C	1.809427	-0.236339	-0.526551
H	1.637904	-1.312987	-0.548378
H	1.911198	0.104169	-1.559916
N	0.588657	0.409660	0.022627
S	-0.308248	-0.508499	1.169276
O	0.291123	-1.835172	1.161147
O	-0.391665	0.234243	2.416391
B	0.142481	1.687424	-0.395115

Cl	0.853378	2.477763	-1.810303
Cl	-1.157996	2.566216	0.409967
C	-1.919889	-0.627131	0.445527
C	-2.052148	-1.236404	-0.801959
C	-3.020028	-0.178020	1.163673
C	-3.322567	-1.378266	-1.339553
H	-1.178035	-1.588310	-1.342606
C	-4.286895	-0.337021	0.608383
H	-2.881954	0.296370	2.129405
C	-4.455527	-0.933681	-0.642931
H	-3.442476	-1.843627	-2.313680
H	-5.156422	0.013002	1.156447
C	-5.825659	-1.110753	-1.241431
H	-6.589369	-0.614984	-0.638757
H	-5.863387	-0.700701	-2.254909
H	-6.080726	-2.173239	-1.309637
C	3.411361	1.568796	0.255302
H	3.539388	1.954653	-0.761105
H	2.615825	2.141663	0.746142
H	4.336470	1.755159	0.811017
C	3.015293	-0.418034	1.703558
H	2.752347	-1.476719	1.766171
H	3.978002	-0.265200	2.203768
H	2.259994	0.148706	2.259780

4

G(DCE) = -2093.821934 Hartree

C	1.881185	-1.101258	-0.249205
C	1.491096	0.341348	0.060759
H	1.544334	-1.368687	-1.258405
H	1.337487	-1.770335	0.436888
C	2.062138	1.367826	-0.926978
H	1.797756	0.590650	1.083437
C	1.042518	2.517176	-0.954722
H	3.063184	1.698114	-0.633884
H	2.130273	0.911801	-1.923489
C	-0.277666	1.730754	-0.922667
H	-0.568331	1.399207	-1.926015
H	-1.100234	2.312083	-0.494689
N	0.019404	0.540839	-0.093365
S	-0.923702	0.288457	1.238539
O	-0.298448	-0.815222	1.968712
O	-1.199131	1.523087	1.977078
B	3.385472	-1.474067	-0.075998
Cl	4.484580	-0.530102	0.926661
Cl	4.032993	-2.926033	-0.835308
C	-2.448409	-0.243724	0.507933
C	-2.432110	-1.313221	-0.388470
C	-3.635113	0.376716	0.876585
C	-3.632575	-1.758292	-0.920622
H	-1.489796	-1.775692	-0.667817
C	-4.831315	-0.084410	0.330522
H	-3.617470	1.207723	1.573483
C	-4.847539	-1.151336	-0.569356
H	-3.633922	-2.587988	-1.622119
H	-5.765025	0.395158	0.609132
C	-6.138052	-1.646739	-1.166996
H	-6.997649	-1.116816	-0.751333
H	-6.140741	-1.505099	-2.252475
H	-6.267943	-2.716711	-0.978238
C	1.163626	3.376635	-2.208722
H	1.080126	2.766749	-3.114447
H	0.378249	4.139676	-2.234783
H	2.130922	3.889270	-2.229187
C	1.171066	3.382912	0.302643
H	1.012431	2.800212	1.215799
H	2.165302	3.839403	0.350905
H	0.425904	4.185475	0.290600

5

G(DCE) = -2554.641247 Hartree

C	2.577030	-2.761917	2.556059
C	2.447127	-3.407964	1.399237
H	3.549903	-2.488475	2.952616
H	1.707749	-2.486597	3.149837
C	1.128046	-3.808769	0.798094
H	3.340992	-3.670938	0.834179
C	0.734230	-3.032382	-0.482378
H	1.155725	-4.874180	0.533741
H	0.332845	-3.683636	1.544545
C	0.542412	-1.566216	-0.077995
H	1.451924	-1.167365	0.386429
H	-0.277842	-1.487934	0.644904
N	0.175923	-0.738752	-1.251389
H	0.898025	-0.680273	-1.973194
S	-0.386116	0.755871	-0.958092

O	0.358481	1.373362	0.252751
O	-0.342467	1.537580	-2.174955
B	1.724258	2.029993	0.215348
Cl	1.514179	3.784097	-0.307149
Cl	2.839809	1.113297	-0.962943
Cl	2.341473	1.888530	1.944463
C	-0.578697	-3.605809	-1.021368
H	-1.377059	-3.529716	-0.274070
H	-0.898614	-3.074433	-1.923286
H	-0.451744	-4.662335	-1.278868
C	1.833905	-3.154347	-1.544777
H	1.499779	-2.763079	-2.512348
H	2.742922	-2.617740	-1.251825
H	2.094223	-4.206922	-1.698136
C	-1.981746	0.504867	-0.275759
C	-2.801385	-0.446851	-0.885432
C	-2.421104	1.302262	0.779472
C	-4.093124	-0.603842	-0.405108
H	-2.431375	-1.056676	-1.703189
C	-3.720292	1.123655	1.236874
H	-1.761881	2.030355	1.237707
C	-4.570670	0.176831	0.655515
H	-4.741426	-1.347533	-0.857967
H	-4.077345	1.727978	2.064868
C	-5.983463	0.012297	1.144729
H	-6.663604	0.620590	0.538682
H	-6.309617	-1.027356	1.064751
H	-6.083054	0.334477	2.183428

6

G(DCE) = -2093.838365 Hartree

C	2.718362	-0.256761	-0.149161
C	1.928451	0.898489	0.453698
H	2.788200	-0.106358	-1.235488
H	3.739586	-0.232280	0.244919
C	2.415989	2.305854	0.100343
H	1.855471	0.770270	1.538851
C	1.153562	3.183874	0.044503
H	3.147112	2.668278	0.828664
H	2.893581	2.285264	-0.887134
C	0.170354	2.241503	-0.665752
H	0.349392	2.228445	-1.747989
H	-0.878313	2.486233	-0.470893
N	0.504633	0.928101	-0.063649
S	-0.118616	-0.385888	-0.770218
O	0.032093	-0.476703	-2.212599
O	0.493430	-1.549014	0.029608
Cl	2.591732	-3.044767	-0.924231
Cl	2.245207	-2.142754	1.988806
B	2.033127	-1.662509	0.193309
C	1.368260	4.466897	-0.751739
H	0.433363	5.029648	-0.843540
H	2.098108	5.106882	-0.245802
H	1.741390	4.250068	-1.757873
C	0.645486	3.507106	1.453694
H	1.395947	4.083174	2.004251
H	-0.271302	4.103405	1.401207
H	0.424381	2.599053	2.024744
C	-1.816350	-0.399285	-0.331507
C	-2.758612	-0.607110	-1.331787
C	-2.169815	-0.207841	1.005703
C	-4.103207	-0.625339	-0.973147
H	-2.445357	-0.746444	-2.360774
C	-3.514706	-0.233769	1.335500
H	-1.406956	-0.040208	1.759991
C	-4.496956	-0.442249	0.354424
H	-4.855777	-0.782871	-1.739255
H	-3.814482	-0.087733	2.368975
C	-5.950251	-0.466606	0.743135
H	-6.593927	-0.589759	-0.129840
H	-6.147197	-1.290787	1.435835
H	-6.228976	0.460811	1.252364

7

G(DCE) = -2554.636247 Hartree

C	-1.935430	-0.826593	-0.001089
C	-1.193189	0.416449	-0.449058
H	-1.672882	-1.657866	-0.661973
H	-1.655190	-1.108072	1.019818
C	-1.368553	1.691043	0.360511
H	-1.445253	0.607257	-1.494435
C	-0.213543	2.608220	-0.061212
H	-2.348541	2.130134	0.157280
H	-1.313740	1.464513	1.432533
C	0.960256	1.622741	-0.069324
H	1.330465	1.482475	0.949355

H	1.787243	1.891571	-0.727922
N	0.383262	0.290341	-0.516805
H	0.639143	0.098723	-1.492560
S	1.118644	-1.099839	0.426293
O	0.738906	-0.819053	1.792899
O	0.695638	-2.275991	-0.297370
C	2.831560	-0.817817	0.181963
C	3.418432	-1.261109	-1.005841
C	3.562176	-0.181831	1.183978
C	4.773446	-1.035456	-1.189338
H	2.831566	-1.779691	-1.757399
C	4.919909	0.025733	0.975196
H	3.081996	0.126086	2.107119
C	5.539967	-0.390652	-0.207486
H	5.250316	-1.370820	-2.105301
H	5.506931	0.515790	1.745284
C	7.011891	-0.174011	-0.427343
H	7.445488	0.446432	0.359007
H	7.539042	-1.133434	-0.437779
H	7.191664	0.307699	-1.392625
C	0.039050	3.723886	0.951412
H	0.183428	3.318801	1.958013
H	0.925497	4.306134	0.679893
H	-0.817460	4.404169	0.974804
C	-0.438548	3.210373	-1.452903
H	-0.573632	2.451408	-2.230204
H	-1.330893	3.843232	-1.445767
H	0.417225	3.829702	-1.739170
Cl	-4.211426	0.344271	1.398375
Cl	-4.315164	-2.387976	0.051366
Cl	-4.105396	0.151547	-1.659008
B	-3.546133	-0.669606	-0.048900

8

G(DCE) = -2554.641925 Hartree

C	-1.129509	-0.695977	0.144619
C	-2.126402	0.308878	-0.415922
H	-1.164134	-1.650632	-0.381389
H	-1.278589	-0.857433	1.217204
C	-1.931441	1.671986	0.257804
H	-1.946873	0.400666	-1.496879
C	-0.490081	2.202662	0.172453
H	-2.606364	2.407156	-0.192805
H	-2.211885	1.585866	1.316937
C	0.467241	1.137263	0.721426
H	0.267650	0.927026	1.776151
H	1.510202	1.443215	0.600422
N	0.288617	-0.172338	0.006926
H	0.494305	-0.051203	-0.995055
S	1.463244	-1.458293	0.612177
O	1.262574	-1.422331	2.042956
O	1.127590	-2.604371	-0.200905
C	3.016881	-0.792452	0.164806
C	3.494897	-1.016074	-1.127783
C	3.735609	-0.065936	1.115478
C	4.726159	-0.477357	-1.470371
H	2.922713	-1.604287	-1.837897
C	4.965456	0.458769	0.744278
H	3.342226	0.073724	2.117203
C	5.474608	0.263476	-0.545710
H	5.117401	-0.637430	-2.470184
H	5.541179	1.027305	1.467726
C	6.821522	0.812725	-0.926384
H	7.080345	1.682760	-0.319391
H	7.593839	0.052122	-0.768212
H	6.847515	1.096210	-1.981022
C	-0.336349	3.436426	1.067050
H	-0.580609	3.202382	2.108259
H	0.684969	3.830257	1.029125
H	-1.016579	4.223096	0.726510
C	-0.110824	2.578942	-1.265485
H	-0.216629	1.751703	-1.975613
H	-0.765932	3.381611	-1.617451
H	0.922803	2.937318	-1.314644
Cl	-4.086634	-0.572139	1.527646
Cl	-3.782658	-1.908108	-1.212754
Cl	-4.859217	0.947623	-1.021267
B	-3.634604	-0.270825	-0.279583

9a

G(DCE) = -1378.779620 Hartree

C	-0.229285	-2.771207	-0.309490
C	0.496306	-1.428224	-0.135736
H	0.934753	-1.135922	-1.096700
H	-0.213027	-0.646905	0.159407
C	0.744011	-3.816207	-0.856534

H	1.590368	-3.940535	-0.175328
H	0.243544	-4.783543	-0.970999
H	1.137908	-3.512547	-1.832880
C	-0.808703	-3.236785	1.027720
H	-0.006571	-3.422383	1.748742
H	-1.489049	-2.487103	1.446539
H	-1.367435	-4.169761	0.897279
N	1.573609	-1.519495	0.859814
H	1.321012	-1.226170	1.800770
S	3.080078	-0.971578	0.459661
O	3.452044	-1.639189	-0.781783
O	3.886320	-1.130489	1.664421
C	2.949996	0.764709	0.109483
C	2.958088	1.671660	1.169696
C	2.799874	1.191459	-1.205906
C	2.811322	3.024194	0.896837
H	3.091050	1.319041	2.187776
C	2.652633	2.552967	-1.459217
H	2.816404	0.470584	-2.016811
C	2.654849	3.483658	-0.418106
H	2.821771	3.739812	1.714341
H	2.538969	2.896042	-2.483384
C	2.507171	4.957337	-0.691258
H	3.421829	5.493833	-0.419049
H	2.302618	5.146965	-1.747096
H	1.691512	5.383162	-0.099299
C	-1.362392	-2.573294	-1.344264
H	-1.841855	-3.544098	-1.522966
H	-0.927108	-2.259850	-2.302202
C	-2.380095	-1.600791	-0.934572
C	-3.205456	-0.793443	-0.570430
C	-4.187102	0.161380	-0.137273
C	-5.025363	0.792421	-1.068139
C	-4.316244	0.472268	1.224576
C	-5.973589	1.715752	-0.641336
H	-4.925366	0.551948	-2.121683
C	-5.266340	1.396952	1.643851
H	-3.666887	-0.016707	1.944088
C	-6.096822	2.020450	0.713550
H	-6.618280	2.198868	-1.368733
H	-5.358931	1.631210	2.699637
H	-6.837798	2.741654	1.043459

10

G(DCE) = -2784.369440 Hartree

C	-1.423826	-2.447970	-0.863822
C	-0.901908	-1.029904	-0.590013
H	-0.671257	-0.536158	-1.541447
H	-1.655058	-0.426399	-0.075283
C	-0.391085	-3.240237	-1.666989
H	0.543634	-3.337236	-1.106678
H	-0.768451	-4.245613	-1.879587
H	-0.167123	-2.746856	-2.619251
C	-1.730926	-3.161093	0.454837
H	-0.818371	-3.294403	1.044389
H	-2.455744	-2.596784	1.051377
H	-2.149349	-4.153577	0.258195
N	0.322380	-1.062862	0.236926
H	0.209610	-0.944167	1.242318
S	1.657333	-0.343020	-0.337599
O	1.992233	-0.881583	-1.634143
O	2.594271	-0.604439	0.857069
C	1.488441	1.405907	-0.431432
C	1.574862	2.169833	0.734112
C	1.217822	1.969295	-1.674652
C	1.383607	3.538300	0.633217
H	1.807726	1.707885	1.688390
C	1.025964	3.345365	-1.744951
H	1.177895	1.351648	-2.565674
C	1.104781	4.143780	-0.601289
H	1.456854	4.152963	1.525402
H	0.818768	3.803696	-2.706776
C	0.912361	5.633791	-0.679745
H	1.844235	6.152321	-0.432728
H	0.602902	5.943115	-1.679803
H	0.155163	5.963989	0.037294
C	-2.709567	-2.316776	-1.714928
H	-3.062516	-3.326391	-1.959286
H	-2.466258	-1.832383	-2.669396
C	-3.785824	-1.573917	-1.052740
C	-4.655628	-0.957362	-0.479503
Cl	4.529898	-2.388338	0.122265
Cl	4.792113	0.619704	-0.306806
Cl	4.655916	-0.506104	2.526753
B	4.114283	-0.715634	0.781393
C	-5.693315	-0.233150	0.200063
C	-6.664978	0.468302	-0.528664

C	-5.744357	-0.222754	1.601826
C	-7.668161	1.165267	0.135890
H	-6.625056	0.459781	-1.613138
C	-6.749967	0.477196	2.259268
H	-4.991850	-0.766575	2.164364
C	-7.713561	1.171959	1.529332
H	-8.416664	1.704759	-0.435745
H	-6.781942	0.479733	3.344179
H	-8.497778	1.716896	2.045119

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G(DCE) = -2784.349355 Hartree

C	-0.228961	-2.434343	0.652663
C	1.013914	-1.633134	0.237970
H	1.904377	-2.062581	0.716978
H	1.144439	-1.708728	-0.847056
C	0.116984	-3.915317	0.441775
H	0.963143	-4.204273	1.073188
H	-0.735232	-4.549248	0.704613
H	0.383370	-4.115605	-0.601827
C	-0.574658	-2.197507	2.124899
H	0.284432	-2.428206	2.764698
H	-0.879923	-1.162657	2.311805
H	-1.406148	-2.843563	2.424573
N	0.894054	-0.206260	0.569059
H	1.024465	-0.003644	1.560832
S	1.806870	0.860889	-0.334666
O	1.721269	2.133280	0.370402
O	1.337854	0.730265	-1.709244
C	3.486085	0.295229	-0.276223
C	3.965690	-0.536720	-1.283532
C	4.282889	0.660253	0.808636
C	5.272416	-1.007818	-1.198262
H	3.331166	-0.796136	-2.124885
C	5.583470	0.179771	0.874659
H	3.890342	1.318272	1.577467
C	6.095668	-0.658583	-0.124392
H	5.658878	-1.654579	-1.980392
H	6.215733	0.460347	1.712360
C	7.516466	-1.150962	-0.045816
H	8.215178	-0.344458	-0.292196
H	7.756820	-1.494417	0.964098
H	7.690741	-1.972689	-0.743719
C	-1.438579	-2.134481	-0.249675
H	-2.220483	-2.866394	-0.028037
H	-1.166786	-2.277088	-1.302970
C	-2.078591	-0.764261	-0.152400
C	-1.648258	0.415888	-0.001068
B	-3.776055	-0.744986	-0.286800
Cl	-4.376112	-1.654463	1.222407
Cl	-4.165019	-1.689241	-1.838372
Cl	-4.551455	0.934572	-0.362708
C	-1.418778	1.785834	0.137699
C	-1.199510	2.572746	-1.012944
C	-1.407204	2.367101	1.423801
C	-0.976927	3.931712	-0.870277
H	-1.203652	2.098048	-1.987818
C	-1.179508	3.725240	1.550328
H	-1.580320	1.739959	2.292522
C	-0.964661	4.499913	0.405671
H	-0.809937	4.551624	-1.743830
H	-1.168939	4.188539	2.530435
H	-0.786391	5.565525	0.511492

12

G(DCE) = -2784.377051 Hartree

C	0.970653	2.974153	0.934534
C	-0.417984	2.294263	1.080785
H	-0.655317	2.034422	2.113200
H	-1.232670	2.887833	0.663890
C	0.824882	4.424854	0.481371
H	1.812126	4.872911	0.332744
H	0.271804	4.483210	-0.461693
H	0.293714	5.017149	1.233600
C	1.715203	2.889472	2.270541
H	1.160066	3.412049	3.056462
H	1.853760	1.846194	2.576570
H	2.703754	3.350184	2.182274
N	-0.320827	0.994637	0.314679
H	-0.738052	0.206822	0.830752
S	-1.274375	1.047819	-1.305754
O	-0.602091	0.061470	-2.116640
O	-1.307158	2.451471	-1.657470
C	-2.824146	0.478340	-0.725969
C	-3.850493	1.394416	-0.510565
C	-2.949751	-0.882356	-0.435004

C	-5.050089	0.916240	0.003847
H	-3.714966	2.444419	-0.747710
C	-4.153748	-1.326392	0.087582
H	-2.130141	-1.573679	-0.620519
C	-5.217187	-0.438645	0.310102
H	-5.868395	1.608688	0.173817
H	-4.272655	-2.379381	0.325726
C	-6.522733	-0.949913	0.854025
H	-7.074491	-1.481606	0.071599
H	-6.354668	-1.654315	1.672842
H	-7.150308	-0.133231	1.215784
C	1.700886	2.110979	-0.120628
H	2.782465	2.117195	0.015522
H	1.483694	2.472291	-1.136240
C	1.117488	0.745134	0.063984
C	1.616043	-0.494493	0.075403
C	0.696479	-1.640238	0.336706
C	0.392333	-2.550518	-0.684118
C	0.111871	-1.814588	1.597651
C	-0.484833	-3.604439	-0.448388
H	0.843903	-2.418833	-1.662666
C	-0.778636	-2.865110	1.828089
H	0.371388	-1.133565	2.406373
C	-1.077763	-3.761596	0.806685
H	-0.712392	-4.302315	-1.248039
H	-1.226339	-2.983871	2.809544
H	-1.765110	-4.582295	0.985296
B	3.204854	-0.734161	-0.178641
Cl	3.643022	-2.553654	-0.203524
Cl	4.189002	0.078608	1.213006
Cl	3.714652	0.023992	-1.824395

13

G(DCE) = -2784.367545 Hartree

C	0.165437	-2.452375	0.792113
C	1.133905	-1.380734	0.318164
H	2.068474	-1.391242	0.882565
H	1.349301	-1.518394	-0.746482
C	0.851518	-3.807376	0.607300
H	1.726445	-3.896380	1.259635
H	0.153210	-4.610455	0.862059
H	1.174245	-3.952689	-0.428933
C	-0.205815	-2.257097	2.265707
H	0.690213	-2.228088	2.895005
H	-0.783635	-1.341273	2.431795
H	-0.828624	-3.092333	2.599970
N	0.546084	-0.005182	0.457332
H	0.637221	0.315155	1.433469
S	1.609836	1.225975	-0.512614
O	1.479146	2.452442	0.239278
O	1.124812	1.042671	-1.861315
C	3.238340	0.598444	-0.349247
C	3.757377	-0.199451	-1.368042
C	3.980582	0.946927	0.781842
C	5.058217	-0.666912	-1.236100
H	3.161601	-0.435254	-2.243760
C	5.274135	0.460688	0.889141
H	3.556885	1.587431	1.548169
C	5.828858	-0.349794	-0.111940
H	5.482525	-1.285880	-2.020065
H	5.869226	0.718288	1.759997
C	7.241349	-0.847682	0.021603
H	7.946350	-0.015593	-0.075123
H	7.401761	-1.299104	1.004608
H	7.477545	-1.586647	-0.746128
C	-1.064377	-2.353136	-0.106403
H	-1.838865	-3.034236	0.261028
H	-0.818333	-2.694756	-1.120460
C	-1.648898	-0.955484	-0.186789
C	-0.910249	0.131839	0.074894
B	-3.258768	-0.957535	-0.410739
Cl	-3.985148	-1.451303	1.270362
Cl	-3.697852	-2.296367	-1.674912
Cl	-4.087531	0.606206	-0.982794
C	-1.377230	1.536654	0.255674
C	-1.459807	2.432552	-0.813633
C	-1.721891	1.963605	1.540535
C	-1.882159	3.738844	-0.597606
H	-1.206227	2.094465	-1.812912
C	-2.143126	3.273622	1.756351
H	-1.684229	1.262852	2.371639
C	-2.221505	4.162113	0.687118
H	-1.952795	4.427198	-1.433752
H	-2.416724	3.595139	2.756123
H	-2.552314	5.182646	0.852802

14

G(DCE) = -2323.560922 Hartree

C	0.140953	2.593843	-0.548655
C	0.985479	1.463378	0.029544
H	1.952905	1.440018	-0.476037
H	1.154533	1.641668	1.101098
C	0.856404	3.913774	-0.255599
H	1.833356	3.948229	-0.749622
H	0.258776	4.752994	-0.626234
H	1.008129	4.052593	0.820144
C	-0.023608	2.422000	-2.062460
H	0.955164	2.412863	-2.553950
H	-0.541620	1.492447	-2.316009
H	-0.602342	3.256327	-2.472319
N	0.339082	0.140243	-0.161637
S	1.208029	-1.131106	0.623832
O	0.958654	-2.380088	-0.078007
O	0.933890	-1.045797	2.056381
C	2.892693	-0.679836	0.331722
C	3.636689	-0.119214	1.363561
C	3.444746	-0.931333	-0.923585
C	4.967957	0.205710	1.123306
H	3.179054	0.056528	2.331702
C	4.771877	-0.590599	-1.144043
H	2.843893	-1.381809	-1.707237
C	5.550241	-0.020770	-0.127150
H	5.562723	0.643437	1.919424
H	5.216444	-0.772941	-2.118150
C	6.996322	0.314596	-0.377827
H	7.130521	0.757574	-1.368192
H	7.377650	1.011660	0.371441
H	7.609985	-0.591704	-0.337756
C	-1.213298	2.565695	0.160263
H	-1.873213	3.311329	-0.297347
H	-1.089449	2.868858	1.208861
C	-1.847286	1.185830	0.080065
C	-1.068169	0.075196	-0.044573
B	-3.380583	1.136947	0.130260
Cl	-4.449731	0.037751	-0.749164
Cl	-4.221681	2.395572	1.068215
C	-1.669209	-1.286007	-0.123676
C	-2.270812	-1.849585	1.000352
C	-1.679177	-1.970793	-1.341580
C	-2.894252	-3.092477	0.905842
H	-2.247934	-1.312520	1.944652
C	-2.312941	-3.202247	-1.436901
H	-1.198954	-1.526259	-2.208959
C	-2.921913	-3.764356	-0.312560
H	-3.361389	-3.530403	1.782146
H	-2.335179	-3.727306	-2.386594
H	-3.414704	-4.728576	-0.389343

15

G(DCE) = -3729.151887 Hartree

C	-0.954465	-3.269627	0.703014
C	0.182276	-2.421226	0.140162
H	1.089660	-2.594071	0.720680
H	0.365226	-2.707229	-0.903222
C	-0.563159	-4.738282	0.523347
H	0.341414	-4.975650	1.092752
H	-1.370744	-5.382498	0.885051
H	-0.382863	-4.976699	-0.530043
C	-1.170516	-2.969853	2.190067
H	-0.255690	-3.174630	2.755755
H	-1.454438	-1.927827	2.364623
H	-1.965860	-3.609260	2.586150
N	-0.135507	-0.958251	0.218808
S	1.012136	-0.003228	-0.527425
C	2.541036	-0.836945	-0.322786
C	3.088073	-1.468660	-1.434356
C	3.167065	-0.821038	0.924411
C	4.308943	-2.115503	-1.281092
H	2.578800	-1.444502	-2.392329
C	4.380169	-1.479036	1.047784
H	2.721117	-0.300486	1.766168
C	4.966820	-2.130904	-0.047527
H	4.757535	-2.612482	-2.135327
H	4.888768	-1.481821	2.006975
C	6.299935	-2.809904	0.106360
H	6.354094	-3.354990	1.052183
H	6.488165	-3.506544	-0.712862
H	7.103282	-2.065540	0.109321
C	-2.211187	-2.961416	-0.115366
H	-3.063635	-3.502897	0.311853
H	-2.093257	-3.331534	-1.142623
C	-2.486634	-1.470799	-0.122533
C	-1.503252	-0.558678	0.015620

B	-3.974744	-1.050964	-0.209446
Cl	-4.803344	-0.073447	0.998230
Cl	-4.971503	-1.748481	-1.491665
C	-1.828136	0.892588	0.051210
C	-2.479756	1.469147	-1.041424
C	-1.638905	1.636999	1.221314
C	-2.966857	2.771941	-0.958069
H	-2.602849	0.892303	-1.954779
C	-2.129385	2.932892	1.301977
H	-1.127674	1.186805	2.067676
C	-2.801247	3.498588	0.216024
H	-3.475143	3.213416	-1.809115
H	-1.994612	3.502949	2.215657
H	-3.186178	4.511077	0.286758
O	0.731311	0.281652	-1.919092
O	1.079175	1.209156	0.417935
Cl	0.568555	3.483368	-1.058363
Cl	3.362380	2.358104	-0.654634
Cl	1.775475	3.388590	1.744941
B	1.677522	2.577978	0.091773

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G(DCE) = -2784.391332 Hartree

C	-0.456572	-2.451382	-0.344026
C	-0.537649	-1.702105	0.985793
H	-1.536664	-1.775105	1.416434
H	0.177774	-2.098956	1.712447
C	-0.804266	-3.916530	-0.071003
H	-1.847766	-4.017910	0.245489
H	-0.665132	-4.507857	-0.981330
H	-0.162553	-4.337297	0.709958
C	-1.425120	-1.877972	-1.382644
H	-2.457284	-1.884325	-1.012897
H	-1.177088	-0.850794	-1.672299
H	-1.384590	-2.489474	-2.289380
N	-0.221307	-0.261425	0.793307
S	-1.416743	0.793931	1.644746
O	-1.007667	2.170495	1.516360
O	-1.542302	0.151533	2.934587
C	-2.835699	0.494735	0.652797
C	-3.806976	-0.396791	1.098403
C	-2.934362	1.157921	-0.571749
C	-4.903355	-0.639702	0.277128
H	-3.710351	-0.880211	2.065466
C	-4.033239	0.893277	-1.373439
H	-2.166815	1.860203	-0.886059
C	-5.027568	-0.008413	-0.964219
H	-5.672750	-1.330459	0.607282
H	-4.127671	1.393696	-2.332495
C	-6.215661	-0.268354	-1.849437
H	-6.824548	-1.089757	-1.467203
H	-6.845499	0.624935	-1.911965
H	-5.895048	-0.513852	-2.865790
C	0.995249	-2.331138	-0.796180
H	1.119900	-2.741427	-1.803014
H	1.601369	-2.950765	-0.128130
C	1.533486	-0.883447	-0.783210
C	0.714044	0.113462	-0.050706
B	3.113032	-0.859565	-0.208639
Cl	3.060056	-1.052471	1.663902
Cl	4.039739	-2.304192	-0.963234
C	1.017914	1.543672	-0.293482
C	1.576257	2.327740	0.720533
C	0.850109	2.061198	-1.579523
C	1.952817	3.634205	0.445124
H	1.734268	1.902426	1.706750
C	1.203447	3.382466	-1.839386
H	0.433594	1.443427	-2.370542
C	1.760469	4.164414	-0.830918
H	2.397990	4.240482	1.226736
H	1.054991	3.792726	-2.832441
H	2.051177	5.188888	-1.039975
H	1.636742	-0.478645	-1.798573
Cl	4.051829	0.684028	-0.667202

19

G(DCE) = -1378.809718 Hartree

C	3.721070	0.191033	0.744493
C	2.774036	0.922197	-0.207386
H	2.716682	1.980659	0.051368
H	3.162579	0.838125	-1.232458
C	5.106390	0.825305	0.609856
H	5.092106	1.872878	0.929341
H	5.827168	0.288899	1.236126
H	5.461280	0.785994	-0.425737
C	3.233221	0.321573	2.190730

H	3.138439	1.377024	2.468440	H	-2.344633	1.684191	-0.767887
H	2.261205	-0.158979	2.335045	H	-1.310957	3.004747	-1.353518
H	3.950417	-0.146703	2.873246	C	-2.879327	3.947831	0.668738
N	1.395918	0.370243	-0.138463	H	-3.793611	3.356841	0.550471
S	0.383258	1.122180	-1.276519	H	-2.985907	4.562686	1.568317
O	0.292621	0.315774	-2.491865	H	-2.787074	4.618544	-0.192281
O	0.878105	2.492163	-1.379398	C	-1.860727	2.049351	1.946474
C	-1.207674	1.166179	-0.504419	H	-2.681184	1.355816	1.737450
C	-1.347245	1.835698	0.708732	H	-0.952350	1.466253	2.129274
C	-2.285680	0.559842	-1.136904	H	-2.092313	2.595176	2.866750
C	-2.597785	1.866891	1.310613	N	-0.269271	1.430240	-0.475461
H	-0.488356	2.305041	1.179434	S	-0.428977	-0.173171	-0.710381
C	-3.531467	0.610033	-0.521227	O	-0.460274	-0.574209	-2.100220
H	-2.140047	0.038897	-2.077059	O	-1.743335	-0.445249	0.067805
C	-3.702073	1.248587	0.710206	C	0.840349	-0.995454	0.176169
H	-2.722007	2.376164	2.262016	C	0.869298	-0.908569	1.565473
H	-4.382082	0.130603	-0.997762	C	1.798734	-1.690357	-0.557546
C	-5.042415	1.239665	1.396581	C	1.924859	-1.515368	2.232835
H	-5.149791	0.334802	2.005486	H	0.084639	-0.395291	2.111536
H	-5.155837	2.100877	2.059408	C	2.840270	-2.287692	0.135531
H	-5.859288	1.247054	0.670650	H	1.733545	-1.741817	-1.638881
C	3.771024	-1.282342	0.313914	C	2.927599	-2.194423	1.530565
H	4.302115	-1.871897	1.071264	H	1.970729	-1.460773	3.315904
H	4.351445	-1.377996	-0.614441	H	3.605584	-2.826691	-0.414831
C	2.381094	-1.823970	0.136884	C	4.099108	-2.799365	2.253896
C	1.300240	-1.056719	-0.050659	H	4.978790	-2.155684	2.141786
C	-0.068773	-1.647453	0.006752	H	3.895800	-2.910586	3.320846
C	-0.556625	-2.436672	-1.034432	H	4.353826	-3.778232	1.839620
C	-0.859426	-1.439980	1.143081	C	-0.393276	3.879885	1.049285
C	-1.826872	-3.005750	-0.946723	H	-0.343595	4.159341	2.109183
H	0.056670	-2.585968	-1.917860	H	-0.455184	4.825904	0.492668
C	-2.127262	-2.002540	1.228299	C	0.878958	3.193483	0.639861
H	-0.477224	-0.821178	1.950986	C	0.955647	2.057361	-0.064088
C	-2.613785	-2.786309	0.180582	C	2.231502	1.505207	-0.581916
H	-2.201856	-3.615888	-1.762685	C	2.366386	1.202328	-1.942195
H	-2.738105	-1.828770	2.109285	C	3.309506	1.296813	0.282543
H	-3.605666	-3.223321	0.244659	C	3.565667	0.688853	-2.426401
H	2.210842	-2.887999	0.271069	H	1.529971	1.366912	-2.616553
----------				C	4.506482	0.780888	-0.205566
20				H	3.191245	1.510765	1.341000
G(DCE) = -2784.404385 Hartree				C	4.635367	0.471816	-1.558860
----------				H	3.664520	0.458074	-3.482336
C	-1.655720	3.038951	0.797200	H	5.334672	0.606841	0.474552
C	-1.471055	2.296594	-0.533625	H	5.566461	0.061364	-1.936487

H	1.815554	3.706371	0.838916
Cl	-3.781268	-1.601855	1.301085
Cl	-3.725046	-1.091963	-1.707155
Cl	-1.839300	-3.158351	-0.467244
B	-2.732686	-1.555592	-0.217149

21

G(DCE) = -562.413557 Hartree

C	-1.161331	-0.420885	-0.000231
C	-1.201234	-1.818226	-0.000054
C	0.000006	-2.517307	-0.000045
C	1.201242	-1.818225	-0.000156
C	1.161333	-0.420882	-0.000399
N	0.000002	0.244069	-0.000324
H	0.000006	-3.603405	0.000128
H	-2.143735	-2.351949	0.000083
H	2.143746	-2.351943	-0.000039
C	2.414823	0.454984	-0.000017
C	2.388999	1.344388	-1.252658
C	2.388565	1.343534	1.253269
C	3.701557	-0.373734	-0.000110
H	2.419566	0.736119	-2.163378
H	1.479381	1.950475	-1.272763
H	3.257365	2.012337	-1.257354
H	2.418217	0.734597	2.163567
H	3.257204	2.011125	1.259052
H	1.479180	1.949986	1.273169
H	4.566600	0.297168	-0.000093
H	3.772053	-1.010459	0.888396
H	3.771961	-1.010342	-0.888706
C	-2.414824	0.454981	-0.000007
C	-2.388324	1.344168	1.252807
C	-2.389252	1.343750	-1.253121
C	-3.701557	-0.373740	0.000587
H	-2.418007	0.735709	2.163425
H	-1.478847	1.950495	1.272321
H	-3.256864	2.011889	1.258305
H	-2.419785	0.734998	-2.163517
H	-3.257726	2.011560	-1.258103
H	-1.479733	1.949970	-1.273617
H	-4.566602	0.297159	0.000576
H	-3.772209	-1.010706	-0.887734
H	-3.771800	-1.010109	0.889367

22

G(DCE) = -1023.236323 Hartree

C	-1.203266	0.879178	-0.000014
C	-1.203268	2.267539	0.000149
C	-0.000002	2.959345	0.000358
C	1.203310	2.267457	0.000255
C	1.203342	0.879189	0.000029
H	0.000069	4.044242	0.000587
H	-2.140618	2.804910	0.000093
H	2.140637	2.804888	0.000232
C	2.471023	0.037442	-0.000116
C	2.497064	-0.831945	1.270607
C	2.496561	-0.832458	-1.270546
C	3.717095	0.930571	-0.000627
H	2.489163	-0.201876	2.166063
H	1.655503	-1.527741	1.308112
H	3.419446	-1.421451	1.274320
H	2.488536	-0.202700	-2.166211
H	3.418804	-1.422184	-1.274217
H	1.654884	-1.528137	-1.307564
H	4.600873	0.286833	-0.000956
H	3.766180	1.564540	-0.891683
H	3.766814	1.564491	0.890442
C	-2.471014	0.037475	-0.000112
C	-2.496611	-0.832430	-1.270484
C	-2.496984	-0.831908	1.270642
C	-3.717147	0.930543	-0.000589
H	-2.488747	-0.202713	-2.166184
H	-1.654885	-1.528042	-1.307589
H	-3.418832	-1.422193	-1.274049
H	-2.489207	-0.201810	2.166067
H	-3.419279	-1.421554	1.274266
H	-1.655357	-1.527616	1.308155
H	-4.600874	0.286740	-0.001041
H	-3.767036	1.564392	0.890512
H	-3.766183	1.564570	-0.891619
N	-0.000031	0.247095	0.000005
Cl	-0.000014	-3.056941	0.000294
H	-0.000039	-0.799235	-0.000083

BCl_3

G(DCE) = -1405.582645 Hartree

B	0.000000	0.000000	0.000000
Cl	0.000000	1.744143	0.000000
Cl	1.510472	-0.872071	0.000000
Cl	-1.510472	-0.872071	0.000000

HCl

G(DCE) = -460.810659 Hartree

Cl	0.000000	0.000000	0.071390
H	0.000000	0.000000	-1.213622

TS1

G(DCE) = -2554.616713 Hartree

C	2.884363	-3.162699	-1.889603
C	3.597967	-2.518939	-0.967714
H	2.670931	-4.224252	-1.810097
H	2.493524	-2.645386	-2.763572
C	3.923857	-1.052140	-1.022213
H	3.977590	-3.072540	-0.109542
C	3.196191	-0.184671	0.036679
H	5.003041	-0.912816	-0.874374
H	3.684494	-0.662880	-2.020572
C	1.694740	-0.240524	-0.305009
H	1.374434	-1.284834	-0.341618
H	1.539745	0.180688	-1.305993
N	0.795288	0.482307	0.623421
S	-0.070900	-0.459052	1.743340
O	0.645630	-1.698517	2.021178
O	-0.386940	0.464760	2.825900
H	1.271078	1.202233	1.174074
B	-0.506708	2.195734	-0.744309
Cl	0.969528	3.009646	-1.253642
Cl	-1.257871	1.044308	-1.834239
C	-1.547817	-0.898069	0.878789
C	-1.509182	-1.945238	-0.040871
C	-2.718863	-0.191911	1.131704
C	-2.662991	-2.252167	-0.749877
H	-0.600292	-2.519971	-0.189431
C	-3.865874	-0.523056	0.418914
H	-2.728196	0.593655	1.878701
C	-3.850639	-1.540586	-0.539746
H	-2.646349	-3.063868	-1.471406
H	-4.788410	0.016628	0.612113
C	-5.085005	-1.861830	-1.339842
H	-5.131435	-2.925660	-1.585359
H	-5.992029	-1.588011	-0.795929
H	-5.081454	-1.304687	-2.283056
C	3.723463	1.248481	-0.089698
H	3.589152	1.631945	-1.106518
H	3.222646	1.938134	0.600724
H	4.791879	1.274220	0.148908
C	3.486705	-0.708066	1.446107
H	3.089791	-1.713614	1.598684
H	4.569086	-0.723121	1.615581
H	3.043225	-0.061125	2.211782
Cl	-1.412984	2.870389	0.599569

TS2

G(DCE) = -2554.586502 Hartree

C	-0.343232	4.214005	0.412945
C	0.890672	3.947328	-0.014733
H	-1.053812	4.762969	-0.197836
H	-0.680551	3.899764	1.399181
C	1.919456	3.194191	0.784034
H	1.192783	4.286077	-1.004822
C	2.220446	1.757496	0.271726
H	2.869219	3.743213	0.767081
H	1.601224	3.137654	1.833238
C	0.908787	0.984458	0.494543
H	0.096614	1.553660	0.045507
H	0.692502	0.896707	1.559950
N	0.838041	-0.416348	-0.102222
S	-0.386442	-0.455886	-1.504336
O	-0.020093	0.725517	-2.251394
O	-0.266371	-1.780236	-2.060677
H	1.762369	-0.676806	-0.617151
B	0.874913	-1.603013	0.883335
Cl	3.158038	-1.997664	-0.901768
Cl	1.662284	-1.369312	2.414248
Cl	0.023885	-3.085107	0.603479
C	-1.934777	-0.209355	-0.716683
C	-2.383296	1.099449	-0.516400
C	-2.712859	-1.318400	-0.383668
C	-3.620268	1.286958	0.081566
H	-1.792273	1.949250	-0.844482

C	-3.949935	-1.100156	0.207187
H	-2.369216	-2.322250	-0.604771
C	-4.413289	0.196151	0.460811
H	-3.983137	2.297304	0.243686
H	-4.571056	-1.951734	0.466329
C	-5.739649	0.417773	1.133567
H	-5.595973	0.541724	2.212456
H	-6.225446	1.321705	0.758771
H	-6.408214	-0.432053	0.981004
C	3.371699	1.185917	1.104264
H	3.133377	1.195930	2.172912
H	3.611760	0.159899	0.806682
H	4.266818	1.797072	0.948682
C	2.631774	1.801052	-1.204028
H	1.834682	2.183336	-1.844109
H	3.506337	2.452246	-1.308203
H	2.921243	0.809956	-1.571387

TS3

G(DCE) = -2093.788459 Hartree

C	2.087996	1.861751	-1.376407
C	2.569327	0.536595	-1.204206
H	1.636094	2.071851	-2.341819
H	2.718029	2.656577	-0.983950
C	3.538850	0.161239	-0.145475
H	2.314104	-0.211647	-1.951061
C	3.055615	-1.055889	0.672289
H	4.471830	-0.099835	-0.667343
H	3.742229	1.020704	0.500219
C	1.596505	-0.748239	1.093644
H	1.586265	-0.095991	1.967134
H	1.087774	-1.678813	1.352812
N	0.863433	-0.067627	0.004787
S	-0.196485	-1.007467	-0.896939
O	-0.112606	-0.541077	-2.277929
O	0.111016	-2.406129	-0.610313
B	0.889945	1.518389	-0.198384
Cl	1.373325	2.330373	1.410122
Cl	-0.713461	2.240107	-0.775401
C	-1.825971	-0.684041	-0.272275
C	-2.864443	-0.518302	-1.179361
C	-2.044810	-0.671226	1.102820
C	-4.154019	-0.331117	-0.690685
H	-2.661516	-0.519226	-2.245080
C	-3.337635	-0.477218	1.569965
H	-1.221062	-0.794352	1.800449
C	-4.407976	-0.303660	0.682973
H	-4.975029	-0.198559	-1.389233
H	-3.521783	-0.457511	2.640352
C	-5.799321	-0.068358	1.209350
H	-6.020503	-0.735515	2.046970
H	-5.902959	0.959546	1.572947
H	-6.549377	-0.226544	0.431287
C	3.914061	-1.213501	1.927509
H	3.893364	-0.303120	2.535784
H	3.542194	-2.042840	2.538604
H	4.953620	-1.429642	1.662555
C	3.144982	-2.329904	-0.173839
H	2.574745	-2.263310	-1.103989
H	4.190801	-2.537142	-0.423569
H	2.747264	-3.182994	0.384228

TS4

G(DCE) = -2554.623681 Hartree

C	2.020825	3.640897	-1.734132
C	1.216786	4.009996	-0.739044
H	3.060358	3.951479	-1.776875
H	1.661252	3.012118	-2.546328
C	-0.228207	3.609663	-0.626686
H	1.612311	4.643764	0.054591
C	-0.556659	2.662303	0.551614
H	-0.846912	4.509521	-0.506323
H	-0.542656	3.127653	-1.562057
C	0.233427	1.363585	0.343972
H	1.308972	1.565981	0.293160
H	-0.051301	0.919529	-0.617943
N	-0.039216	0.379182	1.406060
H	0.580605	0.425713	2.213939
S	-0.241117	-1.199134	0.965071
O	0.690597	-1.593871	-0.107177
O	-0.235551	-1.965735	2.205645
B	3.018175	-1.210218	-0.370142
Cl	3.377841	-2.908115	-0.617354
Cl	3.300866	-0.492652	1.215559
Cl	2.807730	-0.156199	-1.758864
C	-2.058179	2.364099	0.533367

H	-2.354591	1.881438	-0.406677
H	-2.330671	1.696448	1.356215
H	-2.631349	3.291763	0.637763
C	-0.174760	3.301157	1.890704
H	-0.491442	2.665180	2.724206
H	0.906668	3.454983	1.972837
H	-0.667704	4.272622	2.006240
C	-1.853700	-1.186942	0.241476
C	-2.958573	-1.107611	1.089288
C	-1.992617	-1.205186	-1.140980
C	-4.224649	-1.040374	0.528326
H	-2.821783	-1.095980	2.166403
C	-3.273513	-1.132256	-1.684394
H	-1.115512	-1.277985	-1.775636
C	-4.399808	-1.047768	-0.863470
H	-5.095316	-0.979365	1.175119
H	-3.396401	-1.142950	-2.763241
C	-5.785350	-0.980508	-1.448994
H	-6.343136	-1.894735	-1.221440
H	-6.346616	-0.142496	-1.025506
H	-5.753206	-0.862782	-2.534125

TS5-A

G(DCE) = -2554.611678 Hartree

C	-2.037694	-1.162589	-0.191383
C	-1.868190	0.113772	-0.580776
H	-2.233257	-1.940967	-0.921133
H	-1.832744	-1.475583	0.828676
C	-1.549990	1.262134	0.324722
H	-2.038860	0.353721	-1.629138
C	-0.486103	2.265303	-0.178849
H	-2.481369	1.835858	0.457550
H	-1.264013	0.884179	1.313800
C	0.912022	1.632641	-0.136836
H	1.136334	1.337005	0.893369
H	1.666198	2.366442	-0.445772
N	0.998326	0.439372	-0.985808
H	1.332225	0.590219	-1.934799
S	1.608322	-0.959016	-0.351441
O	0.961647	-1.145901	0.941777
O	1.483162	-1.957760	-1.406231
C	3.338907	-0.698848	-0.046347
C	4.246436	-0.865933	-1.092631
C	3.756659	-0.285280	1.214476
C	5.590936	-0.611258	-0.861568
H	3.901672	-1.202711	-2.065363
C	5.109948	-0.034018	1.426112
H	3.036347	-0.180400	2.019265
C	6.041374	-0.191035	0.397308
H	6.307364	-0.743404	-1.667685
H	5.446406	0.284431	2.408429
C	7.506990	0.067892	0.628018
H	7.684480	0.490306	1.619325
H	8.080378	-0.861131	0.545759
H	7.902511	0.761839	-0.119589
C	-0.475298	3.462420	0.778162
H	-0.300605	3.140378	1.810781
H	0.311425	4.173266	0.503519
H	-1.434176	3.989424	0.743403
C	-0.804414	2.752545	-1.595700
H	-0.693979	1.957644	-2.339826
H	-1.832772	3.126861	-1.652691
H	-0.130359	3.569528	-1.875098
Cl	-4.202003	-0.016573	1.913679
Cl	-4.897379	-2.272146	0.001139
Cl	-4.932560	0.601340	-0.972157
B	-4.397919	-0.583998	0.242617

TS5-B

G(DCE) = -2554.598692 Hartree

C	-1.746161	-0.854996	-0.247133
C	-2.337179	0.333037	-0.585387
H	-1.797517	-1.729352	-0.888997
H	-1.298503	-0.994438	0.733814
C	-1.903849	1.596651	0.130248
H	-2.678270	0.435984	-1.615460
C	-0.503751	2.096548	-0.299053
H	-2.627414	2.391892	-0.071411
H	-1.903980	1.421428	1.214162
C	0.623349	1.123136	0.102381
H	0.497187	0.826546	1.149750
H	1.588330	1.641437	0.012161
N	0.635776	-0.115786	-0.698592
H	0.838434	0.037690	-1.687227
S	1.577236	-1.376441	-0.129895
O	1.069414	-1.670804	1.205250

O	1.541722	-2.384132	-1.180722
C	3.232934	-0.771616	0.029883
C	4.083075	-0.827154	-1.073426
C	3.639578	-0.207680	1.236878
C	5.365707	-0.308179	-0.954609
H	3.746155	-1.279727	-2.000560
C	4.927576	0.307618	1.333480
H	2.963388	-0.187316	2.085541
C	5.805212	0.264150	0.245434
H	6.039704	-0.348909	-1.805371
H	5.257443	0.748022	2.269800
C	7.208690	0.795203	0.368154
H	7.899024	-0.012218	0.635429
H	7.552365	1.223281	-0.576775
H	7.275873	1.560815	1.144475
C	-0.234351	3.400143	0.463569
H	-0.222822	3.229620	1.545611
H	0.730915	3.827134	0.172537
H	-1.012510	4.137166	0.242904
C	-0.462194	2.377057	-1.805208
H	-0.681282	1.486962	-2.404707
H	-1.205436	3.137323	-2.066560
H	0.523828	2.752629	-2.100860
Cl	-3.819287	-0.714105	1.939038
Cl	-4.562063	-1.774599	-0.845170
Cl	-5.051150	1.120670	-0.130901
B	-3.979906	-0.343967	0.148452

TS6 (located at the B3LYP/6-31G(d) level)

G(DCE) = -2554.625194 Hartree

C	2.392642	-0.734726	-0.365746
C	1.494293	0.230862	0.429844
H	2.007605	-1.762997	-0.273626
H	2.372494	-0.517625	-1.438763
C	1.863851	1.718489	0.254196
H	1.497018	-0.061489	1.481283
C	1.028552	2.275958	-0.943534
H	1.609161	2.260082	1.169607
H	2.938317	1.843886	0.092743
C	-0.049572	1.178461	-1.187523
H	0.153000	0.616279	-2.104748
H	-1.062470	1.583965	-1.245875
N	0.041553	0.268481	-0.004652
S	-0.720122	-1.292722	-0.223774
O	-0.376071	-1.814016	-1.555206
O	-0.361083	-2.053454	0.979668
B	3.879111	-0.861872	0.114300
Cl	5.112996	-1.473970	-0.995670
Cl	4.381083	-0.504553	1.771795
H	-0.644735	0.962522	1.276619
Cl	-1.118394	1.586523	2.437262
C	0.376880	3.619802	-0.570887
H	1.145562	4.360533	-0.321550
H	-0.210924	4.014545	-1.407930
H	-0.285973	3.516607	0.294629
C	1.888970	2.466638	-2.206282
H	1.270768	2.784176	-3.054278
H	2.648307	3.238572	-2.037629
H	2.405495	1.544871	-2.495421
C	-2.462299	-0.919394	-0.203304
C	-3.157634	-0.962115	1.008367
C	-3.116373	-0.642527	-1.407945
C	-4.526211	-0.706153	1.005511
H	-2.639827	-1.195930	1.931231
C	-4.484358	-0.383937	-1.385576
H	-2.569428	-0.641334	-2.344298
C	-5.209741	-0.411976	-0.184427
H	-5.072535	-0.737053	1.944090
H	-4.997585	-0.163665	-2.317450
C	-6.697611	-0.163388	-0.176663
H	-7.247185	-1.106299	-0.295398
H	-7.022200	0.286674	0.766474
H	-6.997075	0.495012	-0.997725

TS7

G(DCE) = -2784.354722 Hartree

C	-1.687421	-2.650451	-0.685669
C	-1.027021	-1.275333	-0.505107
H	-0.757227	-0.875379	-1.489765
H	-1.726993	-0.572183	-0.041590
C	-0.743242	-3.584405	-1.443800
H	0.193435	-3.709201	-0.893303
H	-1.203736	-4.569420	-1.573574
H	-0.501883	-3.181499	-2.433680
C	-2.041646	-3.249420	0.676841
H	-1.135931	-3.424506	1.265676

H	-2.703285	-2.583705	1.241805
H	-2.551854	-4.210069	0.549113
N	0.189757	-1.362023	0.318382
H	0.076316	-1.127588	1.301969
S	1.594727	-0.754451	-0.282748
O	1.822089	-1.373670	-1.579405
O	2.565254	-0.942439	0.809599
C	1.403990	0.989218	-0.536564
C	1.478412	1.846262	0.562368
C	1.167947	1.469152	-1.819948
C	1.312309	3.208131	0.357905
H	1.679671	1.453721	1.554512
C	1.002021	2.839671	-2.002451
H	1.135202	0.783326	-2.660072
C	1.071078	3.723539	-0.923504
H	1.374933	3.887513	1.203341
H	0.822429	3.226587	-3.001069
C	0.899812	5.206590	-1.119834
H	1.803687	5.743423	-0.815276
H	0.693624	5.447943	-2.164628
H	0.074604	5.585601	-0.509174
C	-2.966340	-2.457544	-1.534839
H	-3.409394	-3.444087	-1.720897
H	-2.691778	-2.049519	-2.516333
C	-3.969259	-1.588100	-0.912433
C	-4.780500	-0.868378	-0.374370
Cl	5.402633	-1.901562	0.990686
Cl	4.827927	0.487121	-0.789897
Cl	4.605968	0.754397	2.223644
B	4.781540	-0.268396	0.801959
C	-5.747260	-0.018496	0.262908
C	-6.716059	0.651825	-0.498335
C	-5.731431	0.148602	1.655634
C	-7.650031	1.472078	0.125041
H	-6.728061	0.522476	-1.575792
C	-6.668094	0.971032	2.271885
H	-4.981246	-0.370911	2.243670
C	-7.628944	1.634089	1.509640
H	-8.396468	1.986526	-0.471860
H	-6.648237	1.094362	3.350090
H	-8.359094	2.275205	1.993220

TS8-A

G(DCE) = -2784.343318 Hartree

C	0.185892	-2.055903	1.834394
C	1.504661	-1.321553	1.544785
H	2.141700	-1.348651	2.435422
H	2.039310	-1.849283	0.746402
C	0.539948	-3.514018	2.148890
H	1.257194	-3.567134	2.974726
H	-0.355164	-4.071689	2.441408
H	0.982976	-4.010259	1.278271
C	-0.526826	-1.424551	3.030637
H	0.076096	-1.545345	3.937007
H	-0.704008	-0.356549	2.871355
H	-1.496402	-1.906375	3.198607
N	1.307591	0.074579	1.142463
H	1.479514	0.784658	1.848958
S	1.779851	0.564244	-0.357945
O	1.369254	1.960579	-0.467177
O	1.289292	-0.437103	-1.297674
C	3.554494	0.512913	-0.415614
C	4.190390	-0.614581	-0.926238
C	4.282757	1.587413	0.094689
C	5.581829	-0.663560	-0.919034
H	3.604620	-1.430203	-1.337383
C	5.669126	1.520309	0.091276
H	3.768198	2.464275	0.475073
C	6.337544	0.396680	-0.412887
H	6.086938	-1.538404	-1.317965
H	6.246375	2.353473	0.482444
C	7.842864	0.353253	-0.427981
H	8.237117	0.996964	-1.221495
H	8.254947	0.712463	0.519079
H	8.209012	-0.660526	-0.604282
C	-0.719828	-2.065581	0.575368
H	-1.470314	-2.858240	0.692184
H	-0.120931	-2.310092	-0.307954
C	-1.438935	-0.806759	0.333907
C	-1.932363	0.308406	0.383601
B	-3.199357	-1.216068	-1.137764
Cl	-4.211461	-2.088598	0.057327
Cl	-2.189796	-2.215863	-2.228951
Cl	-3.939374	0.214133	-1.909380
C	-2.491838	1.618915	0.507647
C	-1.873856	2.710761	-0.118078
C	-3.661713	1.802364	1.260250

C	-2.430589	3.978075	0.012523
H	-0.960617	2.553359	-0.682889
C	-4.210510	3.072534	1.380086
H	-4.129475	0.945663	1.735734
C	-3.596299	4.159117	0.756201
H	-1.954968	4.827025	-0.467584
H	-5.116666	3.217009	1.959026
H	-4.027552	5.150615	0.851901

TS8-B

G(DCE) = -2784.334760 Hartree

C	1.517469	2.950941	0.715043
C	0.092042	3.167621	0.195207
H	-0.419153	3.921768	0.804229
H	0.133192	3.553119	-0.828475
C	2.259545	4.288146	0.649249
H	3.282503	4.180022	1.022243
H	2.304835	4.667508	-0.377062
H	1.750034	5.033605	1.267857
C	1.504395	2.425290	2.151012
H	1.001239	3.141959	2.808446
H	0.985890	1.463629	2.225365
H	2.526098	2.283096	2.517073
N	-0.667581	1.906991	0.190550
H	-1.195867	1.748509	1.046504
S	-1.647553	1.646385	-1.153435
O	-0.902660	0.807296	-2.086969
O	-2.153269	2.928550	-1.645302
C	-2.986707	0.727780	-0.455144
C	-4.045241	1.426714	0.128323
C	-2.964490	-0.660054	-0.507826
C	-5.095684	0.705651	0.675757
H	-4.044240	2.512167	0.138918
C	-4.032013	-1.363230	0.044773
H	-2.133938	-1.177139	-0.979079
C	-5.104181	-0.696411	0.641082
H	-5.928560	1.233690	1.131442
H	-4.026847	-2.448876	0.009373
C	-6.260943	-1.456954	1.233279
H	-7.190938	-1.213739	0.709775
H	-6.102967	-2.535376	1.167434
H	-6.401038	-1.191853	2.285650
C	2.247915	1.959601	-0.224804
H	3.297952	1.885720	0.092949
H	2.245169	2.326713	-1.258199
C	1.720995	0.607324	-0.194929
C	1.466612	-0.599649	-0.145488
C	0.485102	-1.674092	-0.068024
C	0.204045	-2.453804	-1.193761
C	-0.163767	-1.916404	1.144849
C	-0.731425	-3.478940	-1.099939
H	0.719112	-2.253820	-2.127746
C	-1.095492	-2.947814	1.229811
H	0.068128	-1.303747	2.010472
C	-1.376073	-3.731177	0.112105
H	-0.953814	-4.084686	-1.972265
H	-1.602823	-3.137084	2.170250
H	-2.099117	-4.537831	0.183187
B	3.370435	-1.043623	0.004266
Cl	3.310142	-2.860780	-0.091673
Cl	3.935585	-0.460327	1.643589
Cl	4.316725	-0.332443	-1.391554

TS9

G(DCE) = -2784.343726 Hartree

C	-0.089692	-2.476057	0.613467
C	1.052726	-1.570058	0.143739
H	1.995918	-1.883137	0.610152
H	1.161298	-1.652808	-0.943269
C	0.358123	-3.920421	0.358053
H	1.248047	-4.156537	0.950424
H	-0.434432	-4.619764	0.641070
H	0.595285	-4.081668	-0.698978
C	-0.371035	-2.286970	2.107296
H	0.541973	-2.432241	2.695213
H	-0.775838	-1.294130	2.330731
H	-1.111348	-3.020352	2.442399
N	0.783997	-0.151446	0.447190
H	0.875932	0.057791	1.444818
S	1.739186	0.962992	-0.415306
O	1.618039	2.212931	0.318870
O	1.308812	0.847732	-1.801059
C	3.407138	0.386644	-0.294124
C	3.934233	-0.403182	-1.311657
C	4.151625	0.718366	0.838246
C	5.239399	-0.868352	-1.186475

H	3.338062	-0.635273	-2.188275
C	5.450732	0.242328	0.942669
H	3.722246	1.346764	1.612087
C	6.011424	-0.555409	-0.064134
H	5.664828	-1.481845	-1.974862
H	6.044390	0.495310	1.816467
C	7.428722	-1.046348	0.063443
H	8.132257	-0.212503	-0.028983
H	7.595030	-1.506552	1.041592
H	7.666724	-1.778975	-0.710378
C	-1.353704	-2.229657	-0.216281
H	-2.122572	-2.944008	0.093179
H	-1.153103	-2.429701	-1.276315
C	-1.965710	-0.846376	-0.139152
C	-1.441122	0.307565	0.035955
B	-3.639480	-0.813375	-0.270865
Cl	-4.257862	-1.640408	1.288295
Cl	-4.070303	-1.837849	-1.769297
Cl	-4.411732	0.862066	-0.435131
C	-1.385689	1.712010	0.177848
C	-1.288025	2.521961	-0.968529
C	-1.456015	2.286907	1.460334
C	-1.271942	3.900752	-0.826110
H	-1.227788	2.054099	-1.945046
C	-1.431930	3.665564	1.589530
H	-1.536617	1.643239	2.330875
C	-1.338811	4.466724	0.448119
H	-1.205696	4.536776	-1.701799
H	-1.489693	4.121754	2.571542
H	-1.321676	5.546871	0.554612

TS10

G(DCE) = -2784.363447 Hartree

C	-0.053580	2.581161	0.764316
C	-0.933767	1.464337	0.206058
H	-1.868098	1.391246	0.771311
H	-1.169730	1.694475	-0.839854
C	-0.819189	3.895685	0.595363
H	-1.738454	3.890561	1.190099
H	-0.199603	4.731702	0.935044
H	-1.084758	4.071439	-0.452349
C	0.269062	2.364148	2.246153
H	-0.651017	2.284463	2.833573
H	0.856163	1.456136	2.415461
H	0.845803	3.214512	2.624150
N	-0.286145	0.114001	0.266185
H	-0.624272	-0.397695	1.585130
S	-1.108492	-1.006318	-0.869336
O	-0.900109	-2.337936	-0.334042
O	-0.636528	-0.639889	-2.195779
C	-2.813741	-0.588023	-0.709609
C	-3.396818	0.250776	-1.657941
C	-3.546076	-1.144040	0.338084
C	-4.746838	0.550481	-1.535082
H	-2.804612	0.649588	-2.475248
C	-4.893658	-0.823601	0.442220
H	-3.070713	-1.808486	1.051639
C	-5.510057	0.023698	-0.486085
H	-5.217152	1.202363	-2.265010
H	-5.478889	-1.242539	1.255219
C	-6.978331	0.335158	-0.378205
H	-7.310866	0.314912	0.662190
H	-7.206587	1.315954	-0.801692
H	-7.563627	-0.409400	-0.928734
C	1.226978	2.610771	-0.073792
H	1.932376	3.329609	0.360255
H	1.009191	2.966353	-1.090057
C	1.857346	1.234647	-0.140249
C	1.144916	0.103066	0.006610
B	3.397019	1.191825	-0.337295
Cl	4.506809	0.435529	0.797316
Cl	4.100632	2.100989	-1.675209
C	1.800006	-1.230509	-0.060336
C	2.470037	-1.598047	-1.230068
C	1.831154	-2.074790	1.054549
C	3.184223	-2.793696	-1.281717
H	2.414732	-0.950763	-2.101732
C	2.547965	-3.263125	1.000405
H	1.309620	-1.790266	1.963962
C	3.227477	-3.623140	-0.165588
H	3.702441	-3.073831	-2.192999
H	2.583618	-3.909807	1.871205
H	3.785924	-4.553144	-0.201323
Cl	-1.113751	-0.822434	2.889092

TS11

G(DCE) = -3729.136204 Hartree

C	1.461362	3.234143	0.543256
C	0.240751	2.478424	0.027177
H	-0.648303	2.816823	0.562710
H	0.106648	2.687066	-1.043553
C	1.259022	4.718405	0.233019
H	0.382762	5.112628	0.758609
H	2.134902	5.289829	0.556888
H	1.122041	4.884567	-0.840796
C	1.615641	3.038417	2.055097
H	0.720627	3.391369	2.578391
H	1.774041	1.988591	2.318759
H	2.472447	3.614071	2.420256
N	0.373043	1.013093	0.242935
S	-0.923640	0.121259	-0.432930
C	-2.319736	1.182162	-0.231168
C	-2.782528	1.905982	-1.324649
C	-2.955268	1.224106	1.008950
C	-3.909010	2.704734	-1.161260
H	-2.273921	1.837480	-2.280873
C	-4.073313	2.033897	1.149822
H	-2.582930	0.630395	1.837767
C	-4.564907	2.781876	0.071294
H	-4.285037	3.275802	-2.004703
H	-4.580115	2.083383	2.109075
C	-5.798092	3.628962	0.236225
H	-5.862399	4.392052	-0.542417
H	-6.697228	3.006756	0.172171
H	-5.808409	4.121556	1.211906
C	2.683279	2.705452	-0.209638
H	3.587665	3.167335	0.202974
H	2.634396	3.014069	-1.262759
C	2.773743	1.191834	-0.107945
C	1.659700	0.436209	0.074849
B	4.187166	0.589518	-0.185374
Cl	4.838420	-0.699444	0.831684
Cl	5.356704	1.348038	-1.287908
C	1.750663	-1.048045	0.162726
C	2.171432	-1.779988	-0.947833
C	1.505082	-1.699373	1.375500
C	2.366464	-3.156039	-0.844321
H	2.344772	-1.266938	-1.890050
C	1.708063	-3.068824	1.478782
H	1.167182	-1.123662	2.232489
C	2.142668	-3.798192	0.369447
H	2.694235	-3.721727	-1.710589
H	1.531567	-3.571179	2.424628
H	2.299972	-4.868997	0.454184
O	-0.681984	-0.097182	-1.854733
O	-1.142259	-1.045557	0.434014
Cl	-1.302444	-3.616379	-1.202456
Cl	-3.807548	-1.965300	-0.749171
Cl	-2.488807	-3.396687	1.582048
B	-2.431496	-2.855488	-0.092693

TS12

G(DCE) = -2784.356590 Hartree

C	0.009677	-2.003751	-1.797421
C	-0.962631	-0.847382	-1.577567
H	-1.286775	-0.412680	-2.529697
H	-1.841924	-1.208094	-1.036834
C	-0.794206	-3.206637	-2.297093
H	-1.322564	-2.966686	-3.225622
H	-0.120557	-4.045653	-2.497259
H	-1.530034	-3.527438	-1.552692
C	1.084976	-1.639619	-2.827165
H	0.632607	-1.511565	-3.815678
H	1.612932	-0.712542	-2.580046
H	1.828287	-2.441569	-2.894072
N	-0.349321	0.257169	-0.790114
S	-1.400929	1.645498	-0.609269
O	-1.587012	2.184111	-1.945184
O	-0.875797	2.462348	0.465011
C	-2.884265	0.863222	-0.065999
C	-2.905119	0.294592	1.208576
C	-3.987342	0.837253	-0.911130
C	-4.074938	-0.316223	1.633683
H	-2.022595	0.314662	1.843247
C	-5.152556	0.227397	-0.455833
H	-3.931206	1.282483	-1.898881
C	-5.212437	-0.354209	0.813232
H	-4.110563	-0.772775	2.618506
H	-6.026092	0.200135	-1.099941
C	-6.477816	-1.000768	1.308953
H	-7.183028	-1.172069	0.493090
H	-6.263743	-1.957212	1.793513
H	-6.966404	-0.360038	2.050597

C	0.619914	-2.321234	-0.424460
H	1.265020	-3.201776	-0.498173
H	-0.186106	-2.572851	0.278129
C	1.412692	-1.111029	0.087668
C	0.862489	0.160718	-0.211056
B	2.944834	-1.326863	0.201252
Cl	4.174951	-0.413264	-0.670953
Cl	3.519576	-2.682654	1.176128
C	1.617124	1.381706	0.123977
C	2.265398	1.500753	1.356937
C	1.787862	2.359939	-0.863979
C	3.077942	2.602946	1.600936
H	2.110914	0.751318	2.129071
C	2.620575	3.443554	-0.620366
H	1.289342	2.252876	-1.824165
C	3.263704	3.566798	0.612105
H	3.569567	2.705819	2.562415
H	2.770262	4.191944	-1.391257
H	3.909475	4.418220	0.801254
Cl	0.283932	-1.225155	2.836630
H	0.981521	-1.089933	1.414048

TS13

G(DCE) = -2784.373200 Hartree

C	-0.779989	-2.258410	-0.700713
C	-0.600807	-1.538507	0.642386
H	-1.516749	-1.590598	1.234444
H	0.195725	-2.021431	1.220028
C	-1.158095	-3.711905	-0.411304
H	-2.143786	-3.772437	0.062959
H	-1.193755	-4.284527	-1.343967
H	-0.426053	-4.186968	0.250885
C	-1.868739	-1.602819	-1.553606
H	-2.827836	-1.567698	-1.024446
H	-1.597004	-0.581529	-1.840670
H	-2.008670	-2.181689	-2.472601
N	-0.228645	-0.120235	0.462850
S	-1.240481	0.998732	1.253598
O	-0.860836	2.340922	0.855554
O	-1.227567	0.606029	2.654829
C	-2.858507	0.687891	0.607357
C	-3.733275	-0.146438	1.295812
C	-3.220289	1.300221	-0.591675
C	-4.989106	-0.394000	0.749284
H	-3.438670	-0.585721	2.243696
C	-4.477306	1.041721	-1.118491
H	-2.523897	1.959896	-1.100348
C	-5.375026	0.188910	-0.461355
H	-5.680175	-1.046732	1.274161
H	-4.771435	1.507464	-2.054637
C	-6.741989	-0.063198	-1.039375
H	-7.205059	-0.946109	-0.593578
H	-7.398592	0.793026	-0.851362
H	-6.689821	-0.204427	-2.122170
C	0.570620	-2.193189	-1.425811
H	0.416960	-2.338154	-2.502699
H	1.205691	-3.023507	-1.099483
C	1.275590	-0.874443	-1.220851
C	0.776943	0.153262	-0.458292
B	3.243942	-1.196933	0.268795
Cl	2.636877	-0.925360	1.921475
Cl	3.552906	-2.885056	-0.199441
C	1.409009	1.494431	-0.544433
C	1.877022	2.162470	0.594217
C	1.651398	2.039842	-1.807225
C	2.584350	3.349141	0.464492
H	1.699943	1.741403	1.578670
C	2.350197	3.238441	-1.934729
H	1.280909	1.527714	-2.690205
C	2.822734	3.890578	-0.800128
H	2.953976	3.854020	1.351143
H	2.524790	3.657876	-2.920243
H	3.374005	4.820689	-0.897069
H	2.041800	-0.597733	-1.938406
Cl	4.314630	0.031249	-0.439800

TS14

G(DCE) = -2784.385370 Hartree

C	0.133138	3.379146	1.196368
C	-0.096837	2.895635	-0.241020
H	-1.159068	2.762824	-0.443627
H	0.302768	3.630883	-0.949944
C	-0.612091	4.699664	1.389963
H	-1.695185	4.550788	1.321337
H	-0.388792	5.120375	2.376143
H	-0.317735	5.435055	0.633013

C	-0.372969	2.337296	2.195554	B	-3.597562	-0.721072	-0.647744
H	-1.408831	2.052780	1.978221	---			
H	0.249181	1.436359	2.168136	**TS15**			
H	-0.330543	2.738871	3.213509	*G*(DCE) = -1023.214329 Hartree			
N	0.600667	1.624932	-0.517317	---			
S	-0.307075	0.233069	-0.766303	C	1.104317	-0.714516	-0.107913
O	-0.100489	-0.258953	-2.121470	C	1.110326	-1.850859	-0.921059
O	-1.682151	0.605207	-0.385340	C	-0.097069	-2.354509	-1.381394
C	0.237128	-1.027595	0.357761	C	-1.284278	-1.749720	-0.984864
C	-0.372728	-1.117904	1.608800	C	-1.229671	-0.611541	-0.180460
C	1.165698	-1.973330	-0.069541	N	-0.045912	-0.090584	0.199826
C	-0.005747	-2.153418	2.458110	H	-0.116928	-3.228252	-2.025503
H	-1.141780	-0.408538	1.896514	H	2.044134	-2.331613	-1.190092
C	1.519413	-3.000354	0.797688	H	-2.235907	-2.162677	-1.296140
H	1.601173	-1.907463	-1.062112	C	-2.501770	-0.007229	0.419723
C	0.949574	-3.100801	2.070636	C	-2.342433	1.474854	0.771861
H	-0.478854	-2.237232	3.432152	C	-3.702934	-0.157755	-0.523997
H	2.246715	-3.739996	0.475462	C	-2.774113	-0.793748	1.717440
C	1.358562	-4.201131	3.013107	H	-1.468499	1.648093	1.405852
H	2.131052	-3.843655	3.702689	H	-2.249740	2.090761	-0.127055
H	0.511571	-4.539838	3.615090	H	-3.231864	1.807586	1.316460
H	1.766725	-5.056599	2.470112	H	-3.992867	-1.202747	-0.666213
C	1.643106	3.582653	1.378023	H	-4.565610	0.361897	-0.095095
H	1.883913	3.640573	2.447614	H	-3.493183	0.281432	-1.504930
H	1.946586	4.548564	0.948553	H	-3.687946	-0.421839	2.193556
C	2.451205	2.494579	0.731172	H	-2.902333	-1.861500	1.511159
C	1.969813	1.573659	-0.119701	H	-1.943504	-0.675364	2.421117
C	2.860262	0.576391	-0.765438	C	2.413388	-0.169149	0.469640
C	2.808756	0.350289	-2.145239	C	3.267934	0.430587	-0.660014
C	3.787864	-0.129406	0.008526	C	2.161345	0.886971	1.551843
C	3.659325	-0.581013	-2.734681	C	3.188555	-1.329840	1.121219
H	2.091179	0.895480	-2.749062	H	3.492378	-0.319277	-1.425866
C	4.639846	-1.056774	-0.582232	H	2.756497	1.270381	-1.139689
H	3.809525	0.029113	1.082996	H	4.217581	0.793693	-0.252219
C	4.572018	-1.290614	-1.955081	H	1.525957	0.488243	2.348678
H	3.610524	-0.751017	-3.805666	H	3.120356	1.182627	1.989419
H	5.345335	-1.608604	0.030986	H	1.685093	1.786263	1.155939
H	5.228082	-2.022281	-2.416106	H	4.105325	-0.941963	1.577193
H	3.523711	2.491733	0.902854	H	2.591890	-1.808257	1.904868
Cl	-4.224844	-0.244606	0.924866	H	3.478791	-2.094439	0.395369
Cl	-4.147431	0.118733	-2.089232	Cl	0.305533	2.710204	-1.019546
Cl	-2.812536	-2.287558	-0.815060	H	0.116122	1.576283	-0.315464

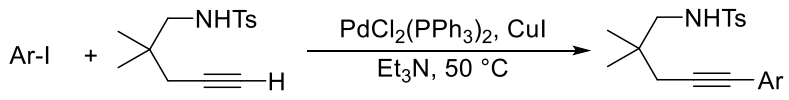
Section 2: Materials and instrumentation

Chemical reagents were obtained from commercial sources (Energy Chemical, Innochem, J&K Scientific) and used without further purification. All reactions were monitored by TLC with silica gel-coated plates with 0.2 mm silica gel-coated HSGF 254 plates. Compounds were purified by column chromatography on silica gel (200-300 mesh) with a gradient (petroleum ether/ethyl acetate).

Nuclear magnetic resonance spectra were recorded on a Bruker Ascend™ 400 or 500 spectrometer at 295.15 K. Chemical shifts for ^{1}H NMR spectra were reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.0) and relative to the signal of chloroform-*d* (δ 7.26, singlet). Multiplicities were given as: s (singlet); d (doublet); t (triplet); q (quartet); dd (doublets of doublet) or m(multiplets). The number of protons (n) for a given resonance is indicated by nH. Coupling constants were reported as a *J* value in Hz. Chemical shifts for ^{13}C NMR spectra were reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.0) and relative to the signal of chloroform-d (δ 77.16, triplet). ^{19}F NMR spectrawere recorded on Bruker Ascend™ 500 (470MHz) or Bruker Ascend™ 400 (376 MHz), and were referenced relative to CF_3COOH (neat) at δ -78.5 ppm. ^{11}B NMR spectra were recorded on Bruker Ascend™ 400 (128 MHz) and were referenced relative to BF_3-Et_2O (47%) at δ 0.0 ppm. High-resolution mass spectra (HRMS) analyses were performed on a Thermo Scientific LTQ-Orbitrap XL mass spectrometer.

Section 3: Preparation of alkyne substrates

General procedure for synthesis of aryl substituted alkyne substrates



S1 **S2** **9**

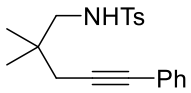
N-(2,2-dimethylpent-4-yn-1-yl)-4-methylbenzenesulfonamide **S2** was prepared according to a literature protocol.[1]

A flask was charged with $PdCl_2(PPh_3)_2$ (2% equiv), CuI (1% equiv), and terminal alkyne **S2** (1.0 equiv). The flask was then evacuated and refilled with N_2 three times before 30 mL of Et_3N and Ar-I **S1** (1.2 equiv) were added in sequence at 0 °C. The

[1]Mo, D. L.; Ding, C. H.; Dai, L. X.; Hou, X. L.; *Chem. Asian J.***2011**, *6*, 3200.

reaction mixture was stirred at 50 °C overnight. After the starting material was consumed completely which was detected by TLC, the mixture was concentrated *in vacuo* and purified by flash chromatography on silica gel (PE/EtOAc = 10:1-3:1) to afford the corresponding Sonogashira coupling products **9**.

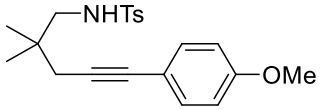
***N-(2,2-dimethyl-5-phenylpent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9a**



Prepared according to general procedure.

1.3 g, yield 76%. **^{1}H NMR** (500 MHz, $CDCl_3$)δ 7.74 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.30 (m, 2H), 7.30 – 7.27 (m, 4H), 7.26 (s, 1H), 4.62 (t, *J* = 7.0 Hz, 1H), 2.87 (d, *J* = 7.0 Hz, 2H), 2.39 (s, 3H), 2.30 (s, 2H), 1.02 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.4, 137.0, 131.6, 129.8, 128.3, 127.9, 127.2, 123.6, 86.9, 83.2, 52.5, 34.8, 30.4, 25.1, 21.6. **HRMS (ESI+):** calcd. for $C_{20}H_{23}NNaO_2S^+$ $[M+Na]^+$: 364.1342, found: 364.1342.

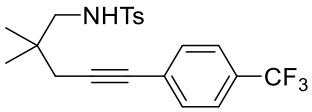
***N-(5-(4-methoxyphenyl)-2,2-dimethylpent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9b**



Prepared according to general procedure.

1.0 g, yield 67%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.25 (m, 4H), 6.83 (d, *J* = 8.5 Hz, 2H), 4.83 (t, *J* = 6.5 Hz, 1H), 3.82 (s, 3H), 2.88 (d, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 2.30 (s, 2H), 1.03 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.3, 143.4, 137.0, 133.0, 129.8, 127.2, 115.7, 114.0, 85.2, 83.0, 55.4, 52.6, 34.8, 30.5, 25.2, 21.7. **HRMS (ESI+):** calcd. for $C_{21}H_{26}NO_3S^+$ $[M+H]^+$: 372.1628, found: 372.1631.

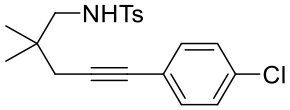
***N-(2,2-dimethyl-5-(4-(trifluoromethyl)phenyl)pent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9c**



Prepared according to general procedure.

630 mg, yield 77%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 2H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 7.2 Hz, 2H), 4.77 (t, *J* = 7.2 Hz, 1H), 2.86 (d, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 2.34 (s, 2H), 1.02 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.5, 137.0, 131.9, 129.8, 127.2, 125.2 (q, J_{C-F} = 3.8 Hz), 124.2 (q, J_{C-F} = 270 Hz), 89.9, 82.0, 52.5, 34.9, 30.3, 25.1, 21.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -65.58 (s, C*F*$_3$). **HRMS (ESI+):** calcd. for $C_{21}H_{23}F_3NO_2S^+$ $[M+H]^+$: 410.1396, found:410.1388.

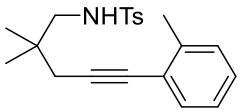
***N-(5-(4-chlorophenyl)-2,2-dimethylpent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9d**



Prepared according to general procedure.

1.1 g, yield 84%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.20 (m, 6H), 4.82 (t, *J* = 6.8 Hz, 1H), 2.85 (d, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 2.30 (s, 2H), 1.00 (s, 6H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.5, 137.0, 133.9, 132.9, 129.8, 128.6, 127.2, 122.1, 88.0, 82.1, 52.5, 34.8, 30.3, 25.1, 21.7. **HRMS (ESI+):** calcd. for $C_{20}H_{23}ClNO_2S^+$ $[M+H]^+$:376.1133, found:376.1131.

***N-(2,2-dimethyl-5-(o-tolyl)pent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9e**

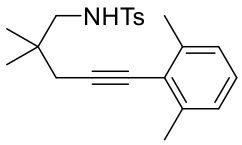


Prepared according to general procedure.

950 mg, yield 67%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.21 – 7.15 (m, 2H), 7.10 (td, *J* = 7.0, 2.0 Hz, 1H), 4.54 (t, *J* = 7.0 Hz, 1H), 2.88 (d, *J* = 7.0 Hz, 2H), 2.39 (s, 3H), 2.36 (s, 2H), 2.33 (s, 3H), 1.03 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.5, 140.0, 137.0, 132.1, 129.8, 129.5, 127.9, 127.2, 125.6, 123.4, 90.6, 82.1, 52.6, 34.8, 30.6, 25.2, 21.6, 21.0. **HRMS**

(ESI+): calcd. for $C_{21}H_{26}NO_2S^+$ $[M+H]^+$: 356.1679, found: 356.1676.

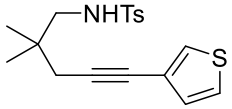
***N-(5-(2,6-dimethylphenyl)-2,2-dimethylpent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9f**



Prepared according to general procedure.

680 mg, yield 46%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.07 (dd,*J* = 8.0, 6.8Hz, 1H), 7.01 (d, *J* = 7.5 Hz, 2H), 4.59 (t, *J* = 7.0 Hz, 1H), 2.88 (d, *J* = 7.0 Hz, 2H), 2.42 (s, 2H), 2.38 (s, 3H), 2.33 (s, 6H), 1.04 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.5, 140.2, 136.9, 129.8, 127.3, 127.2, 126.7, 123.4, 95.1, 80.7, 52.6, 34.8, 30.8, 25.2, 21.6, 21.4.**HRMS (ESI+):** calcd. for $C_{22}H_{28}NO_2S^+$ $[M+H]^+$: 370.1835, found:370.1834.

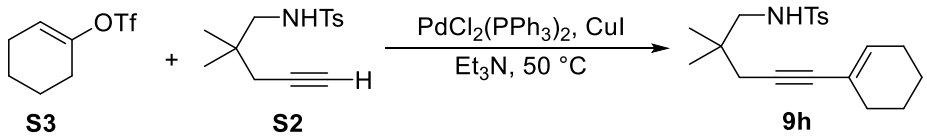
***N-(2,2-dimethyl-5-(thiophen-3-yl)pent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9g**



Prepared according to general procedure.

960 mg, yield 69%.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.31 (dd, *J* = 3.0, 1.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.24 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.01 (dd, *J* = 5.0, 1.0 Hz, 1H), 4.73 (t, *J* = 7.0 Hz, 1H), 2.85 (d, *J* = 7.0 Hz, 2H), 2.41 (s, 3H), 2.28 (s, 2H), 1.00 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.5, 137.0, 130.0, 129.9, 128.1, 127.2, 125.3, 122.5, 86.4, 78.3, 52.6, 34.8, 30.4, 25.2, 21.7. **HRMS (ESI+):** calcd. for $C_{18}H_{22}NO_2S_2^+$ $[M+H]^+$: 348.1086, found: 348.1083.

***N-(5-(cyclohex-1-en-1-yl)-2,2-dimethylpent-4-yn-1-yl)-4-methylbenzenesulfonamide* 9h**



S3 **S2** **9h**

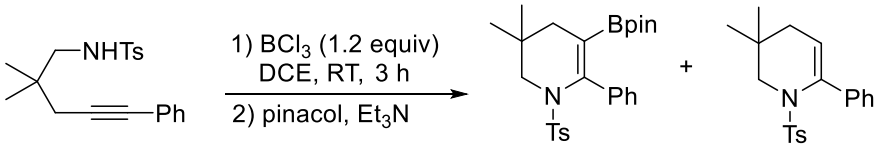
Cyclohex-1-en-1-yl trifluoromethanesulfonate **S3** was prepared according to a literature protocol.[2]

A flask was charged with $PdCl_2(PPh_3)_2$ (0.08 mmol, 2% equiv), CuI (0.04 mmol, 1% equiv), and terminal alkyne **S2** (4.0 mmol, 1.0 equiv). The flask was then evacuated and refilled with N_2 three times before 30 mL of Et_3N and **S3** (4.8 mmol, 1.2 equiv) were added in sequence at 0 °C. The reaction mixture was stirred at 50 °C overnight. After the starting material was consumed completely which was detected by TLC, the mixture was concentrated *in vacuo* and purified by flash chromatography on silica gel (PE/EtOAc = 10:1-3:1) to afford the Sonogashira coupling product **9h**.

1.0 g, yield 72%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.97 – 5.93 (m, 1H), 4.62 (t, *J* = 7.0 Hz, 1H), 2.80 (d, *J* = 6.5 Hz, 2H), 2.43 (s, 3H), 2.17 (s, 2H), 2.09 – 2.00 (m, 4H), 1.64 – 1.52 (m, 4H), 0.95 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.4, 137.1, 133.9, 129.8, 127.2, 120.7, 85.1, 83.8, 52.6, 34.6, 30.5, 30.0, 25.7, 25.1, 22.4, 21.7, 21.6. **HRMS (ESI+):** calcd. for $C_{20}H_{28}NO_2S^+$ $[M+H]^+$: 346.1835, found: 346.1829.

Section 4: Aminoboration and hydroamination of alkyne substrates

Procedure for generation of 16a and 17a



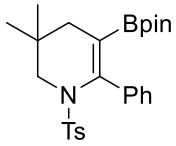
9a **16a** (24%) **17a** (54%)

To a 10 mL Schlenk tube charged with **9a** (0.2 mmol, 1.0 equiv) was added 1.0 mL anhydrous DCE under argon. Then BCl_3 (1M in DCM, 0.24 mmol, 1.2 equiv) was added at 0 °C. After stirring at 0 °C for 5 min, the reaction was allowed to warm up to room temperature and stirred for 3 hours. The reaction was quenched with a solution of

[2]Hioki, Y.; Okano, K.; Mori, A. *Chem. Commun.* **2017**, *53*, 2614.

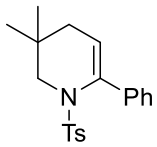
pinacol (0.36 mmol**,** 1.8 equiv) in Et_3N (3 mmol, 15 equiv) at 0 °C and stirred for 5 min. The mixture was concentrated *in vacuo*. The crude product was purified by column chromatography (PE/EtOAc = 50:1-10:1) to afford product **16a** (22.3 mg,24%) and product **17a** (36.9 mg, 54%).

3,3-dimethyl-6-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-tosyl-1,2,3,4-tetrahydropyridine **16a**



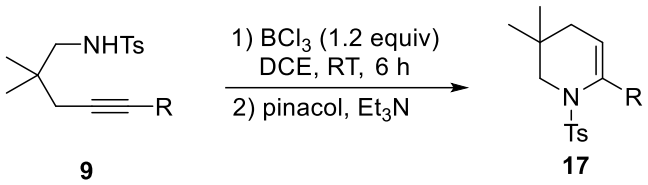
22.3 mg, yield 24%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.13 – 7.06 (m, 3H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.96 – 6.86 (m, 4H), 3.64 (s, 2H), 2.34 (s, 3H), 2.05 (s, 2H), 1.11 (s, 6H), 0.94 (s, 12H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.9, 142.4, 140.0, 136.9, 131.0, 128.9, 127.4, 126.8, 126.7, 83.0, 57.1, 40.4, 29.5, 26.6, 24.5, 21.6. **^{11}B NMR** (128 MHz, $CDCl_3$) δ 31.20 (s). **HRMS (ESI+):** calcd. for $C_{26}H_{34}BNNaO_4S^+$ $[M+Na]^+$: 490.2194, found: 490.2216.

3,3-dimethyl-6-phenyl-1-tosyl-1,2,3,4-tetrahydropyridine **17a**



36.9 mg, yield 54%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.15(d, *J* = 8.5 Hz, 2H), 7.08 – 7.04 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.95 (t, *J* = 8.0 Hz, 2H), 6.87 (dd, *J* = 8.0, 1.0 Hz, 2H), 4.96 (t, *J* = 4.0 Hz, 1H), 3.54 (s, 2H), 2.29 (s, 3H), 1.87 (d, *J* = 4.0 Hz, 2H), 1.04 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.7, 139.5, 137.9, 137.7, 129.0, 128.7, 127.3, 127.0, 115.4, 57.4, 38.1, 29.9, 26.8, 21.5. **HRMS (ESI+):** calcd. for $C_{20}H_{24}NO_2S^+$ $[M+H]^+$: 342.1522, found: 342.1521.

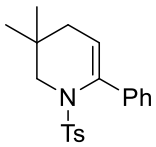
General procedure for hydroamination of alkynes



9 **17**

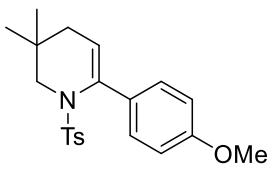
To a 10 mL Schlenk tube with alkyne substrate **9** (0.2 mmol, 1.0 equiv) was added 1.0 mL anhydrous DCE under argon. Then BCl_3 (1M in DCM, 0.24 mmol, 1.2 equiv) was added at 0 °C. The solution was allowed to stir at 0 °C for 5 min, then allowed to warm up to room temperature and stirred for 6 hours. After the starting material was consumed completely which was detected by TLC, the reaction was quenched with a solution of pinacol (0.36 mmol**,** 1.8 equiv) in Et_3N (3 mmol, 15 equiv) at 0 °C. The mixture was concentrated *in vacuo*. The crude product was purified by column chromatography (PE/EtOAc = 50:1-10:1) to afford the corresponding hydroamination product **17**.

3,3-dimethyl-6-phenyl-1-tosyl-1,2,3,4-tetrahydropyridine **17a**



59.4 mg, yield 87%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.15(d, *J* = 8.5 Hz, 2H), 7.08 – 7.04 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.95 (t, *J* = 8.0 Hz, 2H), 6.87 (dd, *J* = 8.0, 1.0 Hz, 2H), 4.96 (t, *J* = 4.0 Hz, 1H), 3.54 (s, 2H), 2.29 (s, 3H), 1.87 (d, *J* = 4.0 Hz, 2H), 1.04 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.7, 139.5, 137.9, 137.7, 129.0, 128.7, 127.3, 127.0, 115.4, 57.4, 38.1, 29.9, 26.8, 21.5. **HRMS (ESI+):** calcd. for $C_{20}H_{24}NO_2S^+$ $[M+H]^+$: 342.1522, found: 342.1521.

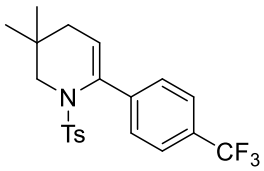
6-(4-methoxyphenyl)-3,3-dimethyl-1-tosyl-1,2,3,4-tetrahydropyridine **17b**



Prepared according to general procedure.

67.6 mg, yield 91%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ7.24 (d, *J* = 8.5 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 2H), 6.55 (d, *J* = 8.5 Hz, 2H), 4.98 (t, *J* = 4.0 Hz, 1H), 3.75 (s, 3H), 3.62 (s, 2H), 2.37 (s, 3H), 1.93 (d, *J* = 4.0 Hz, 2H), 1.11 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.9, 142.6, 139.7, 137.5, 130.2, 130.0, 128.9, 127.1, 114.6, 112.7, 57.4, 55.3, 38.1, 29.9, 26.8, 21.6. **HRMS (ESI+):** calcd. for $C_{21}H_{26}NO_3S^+[M+H]^+$: 372.1628, found: 372.1633.

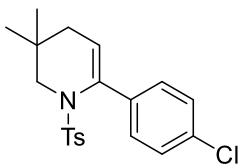
***3,3-dimethyl-1-tosyl-6-(4-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydropyridine* 17c**



Prepared based on general procedure with more BCl_3 (1M in DCM, 0.48 mmol, 2.4 equiv), pinacol (0.72 mmol, 3.6 equiv), and a reaction time of 5 hours at room temperature.

37.5 mg, yield 46%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.5 Hz, 2H),7.22 (d, *J* = 8.5 Hz, 2H),7.11 – 7.03 (m, 4H),5.11 (t, *J* = 4.0 Hz, 1H), 3.63 (s, 2H), 2.38 (s, 3H), 1.97 (d, *J* = 4.0 Hz, 2H), 1.12 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.2, 141.2, 139.2, 136.8, 129.2, 129.0, 127.0, 124.2 (q, $J_{C\text{-}F}$ = 270 Hz), 124.3 (q, $J_{C\text{-}F}$ = 3.8 Hz), 117.0, 57.3, 38.1, 30.0, 26.8, 21.5.**^{19}F NMR** (470 MHz, $CDCl_3$) δ -65.23 (s, CF_3). **HRMS (ESI+):** calcd. for $C_{21}H_{23}F_3NO_2S^+[M+H]^+$: 410.1396, found: 410.1386.

***6-(4-chlorophenyl)-3,3-dimethyl-1-tosyl-1,2,3,4-tetrahydropyridine* 17d**

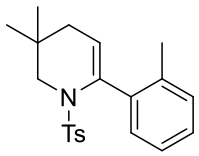


Prepared according to general procedure.

64.5 mg, yield 86%.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.0 Hz,2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 4.96 (t, *J* = 4.0 Hz, 1H), 3.53 (s, 2H), 2.32 (s, 3H), 1.86 (d, *J* = 4.0 Hz, 2H), 1.03 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.0, 139.4, 136.9, 136.2, 133.2, 130.0, 129.1, 127.5, 127.0, 115.9,

57.4, 38.0, 29.9, 26.8, 21.6.**HRMS (ESI+):** calcd. for $C_{20}H_{23}ClNO_2S^+[M+H]^+$: 376.1133, found: 376.1135.

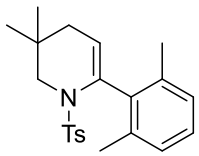
***3,3-dimethyl-6-(o-tolyl)-1-tosyl-1,2,3,4-tetrahydropyridine* 17e**



Prepared according to general procedure.

57.4 mg, yield 81%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.12 – 7.06 (m, 2H), 7.04 – 6.99 (m, 3H), 6.97 (t, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 7.5 Hz, 1H), 4.89 (t, *J* = 3.5 Hz, 1H), 3.59 (s, 2H), 2.34 (s, 3H), 2.00 (d, *J* = 3.5 Hz, 2H), 1.80 (s, 3H), 1.16 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.4, 138.9, 137.8, 136.4, 136.3, 131.5, 129.1, 128.7, 127.9, 126.9, 124.8, 114.0, 56.7, 38.1, 29.5, 26.6, 21.5, 19.2.**HRMS (ESI+):** calcd. for $C_{21}H_{26}NO_2S^+[M+H]^+$: 356.1679, found: 356.1680.

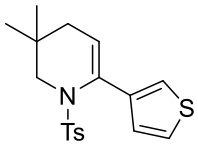
***6-(2,6-dimethylphenyl)-3,3-dimethyl-1-tosyl-1,2,3,4-tetrahydropyridine* 17f**



Prepared based on general procedure with more BCl_3 (1M in DCM, 0.48 mmol, 2.4 equiv), pinacol (0.72 mmol, 3.6 equiv), and a reaction time of 24 hours at room temperature.

38.0 mg, yield 51%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.04 (t, *J* = 7.6 Hz, 1H), 7.00 – 6.94 (m, 4H), 6.79 (d, *J* = 7.6 Hz, 2H), 4.79 (t, *J* = 4.0 Hz, 1H), 3.55 (s, 2H), 2.35 (s, 3H), 2.00 (d, *J* = 4.0 Hz, 2H), 1.94 (s, 6H), 1.19 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.4, 138.7, 138.5, 135.7, 134.7, 128.7, 127.8, 127.0, 127.1, 112.9, 56.6, 38.3, 29.6, 26.5, 21.6, 20.1. **HRMS (ESI+):** calcd. for $C_{22}H_{28}NO_2S^+[M+H]^+$: 370.1835, found: 370.1837.

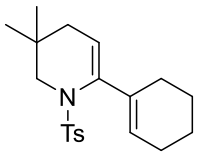
***3,3-dimethyl-6-(thiophen-3-yl)-1-tosyl-1,2,3,4-tetrahydropyridine* 17g**



Prepared according to general procedure.

60.3 mg, yield 87%.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.84 (dd, *J* = 5.0, 2.8 Hz, 1H), 6.73 (dd, *J* = 2.8, 1.2 Hz, 1H), 6.52 (dd, *J* = 4.8, 1.2 Hz, 1H), 5.00 (t, *J* = 4.0 Hz, 1H), 3.53 (s, 2H), 2.30 (s, 3H), 1.85 (d, *J* = 3.6 Hz, 2H), 1.03 (s, 6H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.7, 139.5, 138.2, 132.7, 129.1, 128.7, 126.9, 124.0, 123.5, 114.9, 57.2, 38.0, 29.8, 26.8, 21.6.**HRMS (ESI+):** calcd. for $C_{18}H_{22}NO_2S_2^+$[M+H]$^+$: 348.1086, found: 348.1089.

6-(cyclohex-1-en-1-yl)-3,3-dimethyl-1-tosyl-1,2,3,4-tetrahydropyridine **17h**

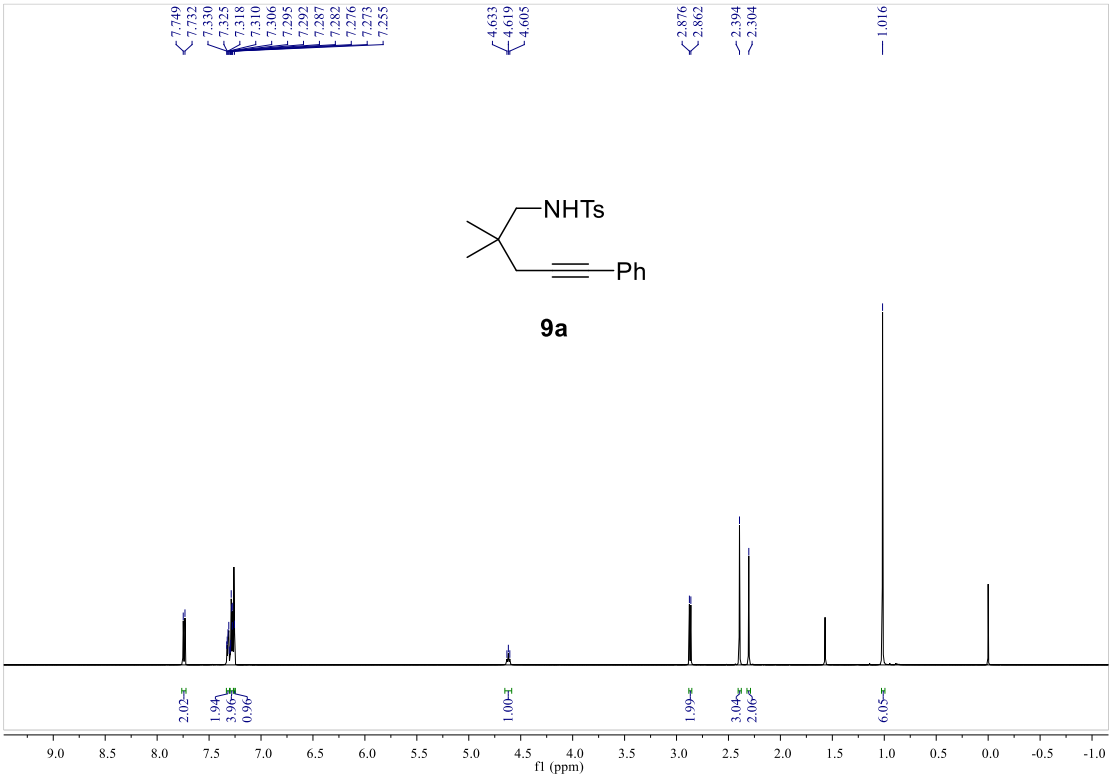


Prepared based on general procedure with a reaction time of 3 hours at room temperature.

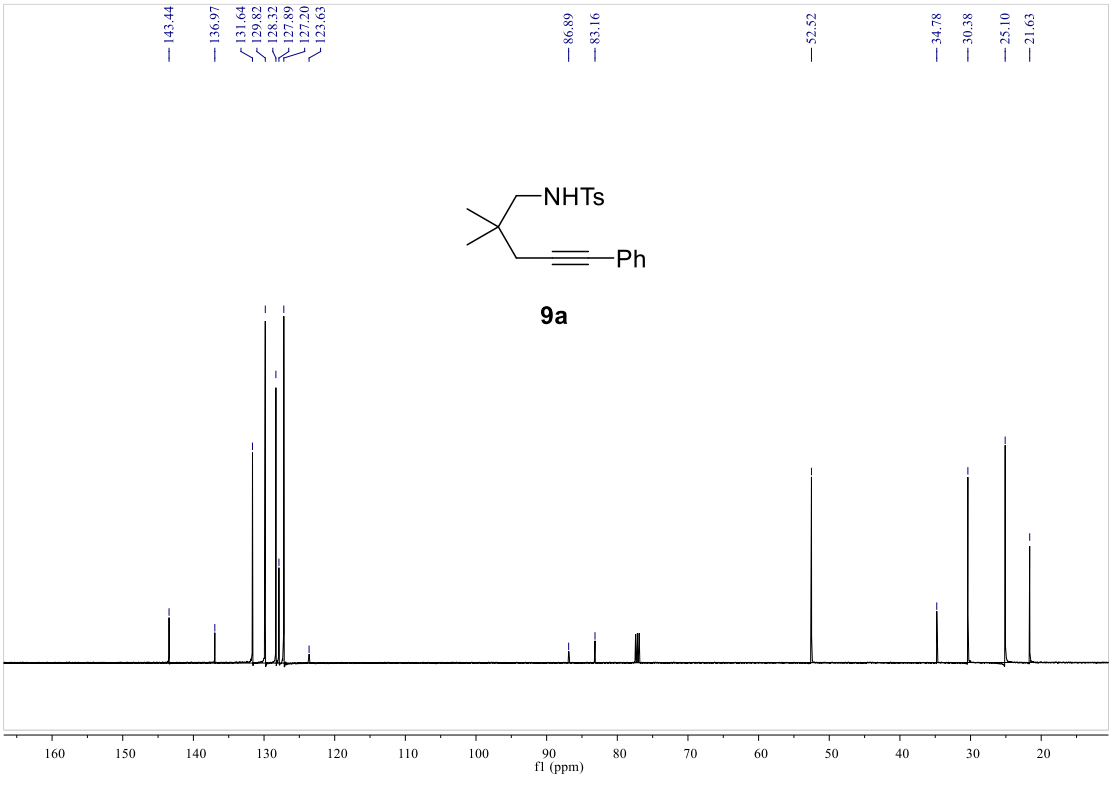
55.7 mg, yield 81%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 5.26 – 5.23 (m, 1H), 4.91 (t, *J* = 4.0 Hz, 1H), 3.40 (s, 2H), 2.39 (s, 3H), 2.05 – 2.00 (m, 2H),1.86 – 1.80 (m, 2H), 1.76 (d, *J* = 4.5 Hz, 2H), 1.51 – 1.44 (m, 4H), 0.97 (s, 6H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.8, 140.0, 139.3, 135.9, 129.1, 127.3, 126.6, 111.5, 57.5, 37.4, 30.1, 28.9, 26.9, 25.3, 22.6, 22.0, 21.6.**HRMS (ESI+):** calcd. for $C_{20}H_{28}NO_2S^+$ [M+H]$^+$: 346.1835, found: 346.1838.

Section 5: NMR spectra

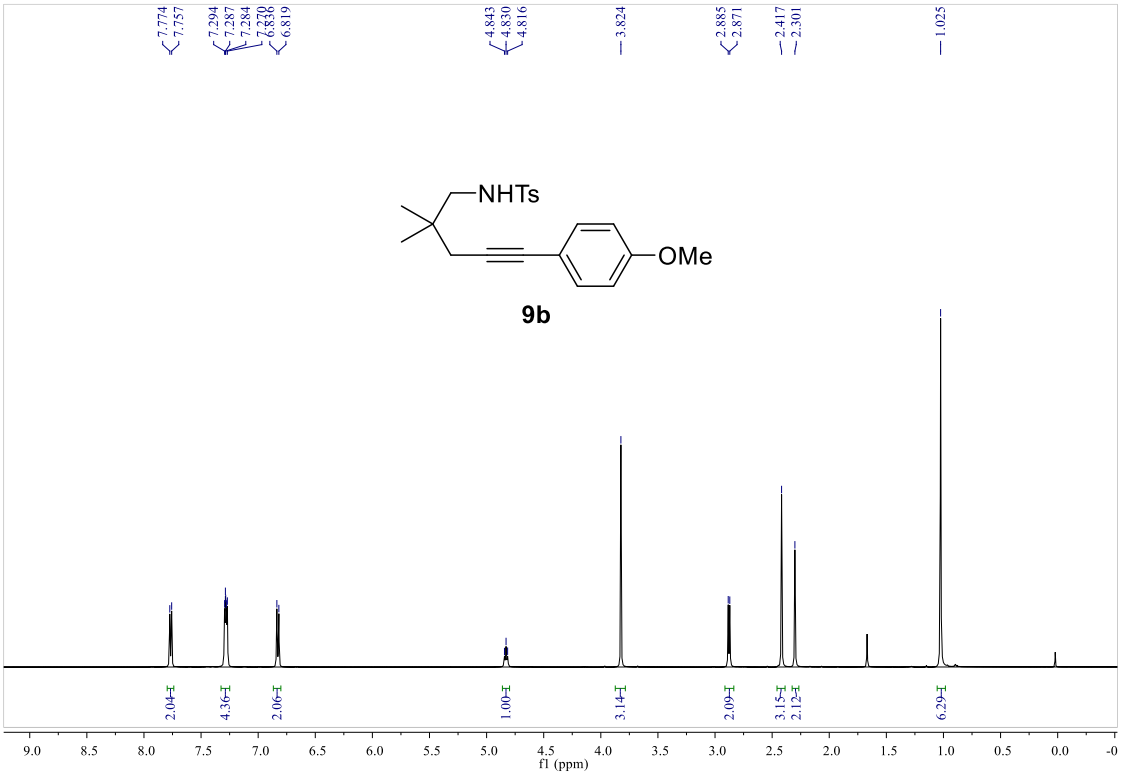
^{1}H NMR spectrum of **9a** (500 MHz, $CDCl_3$)



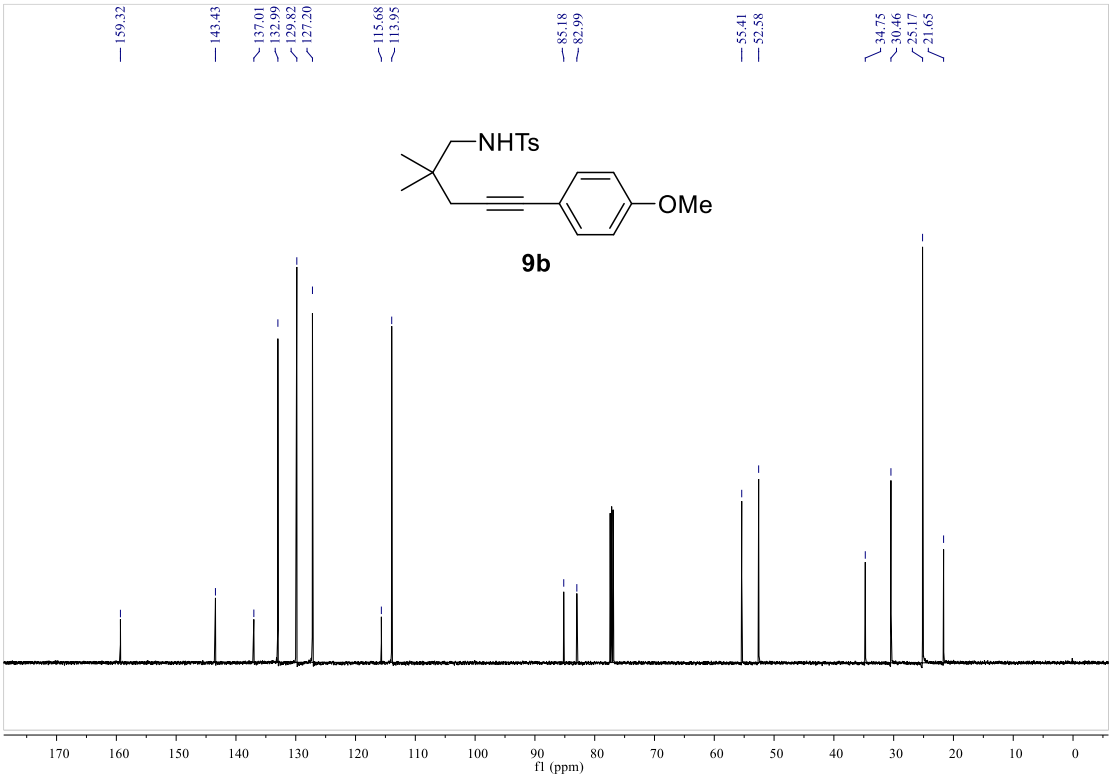
^{13}C NMR spectrum of **9a** (125 MHz, $CDCl_3$)



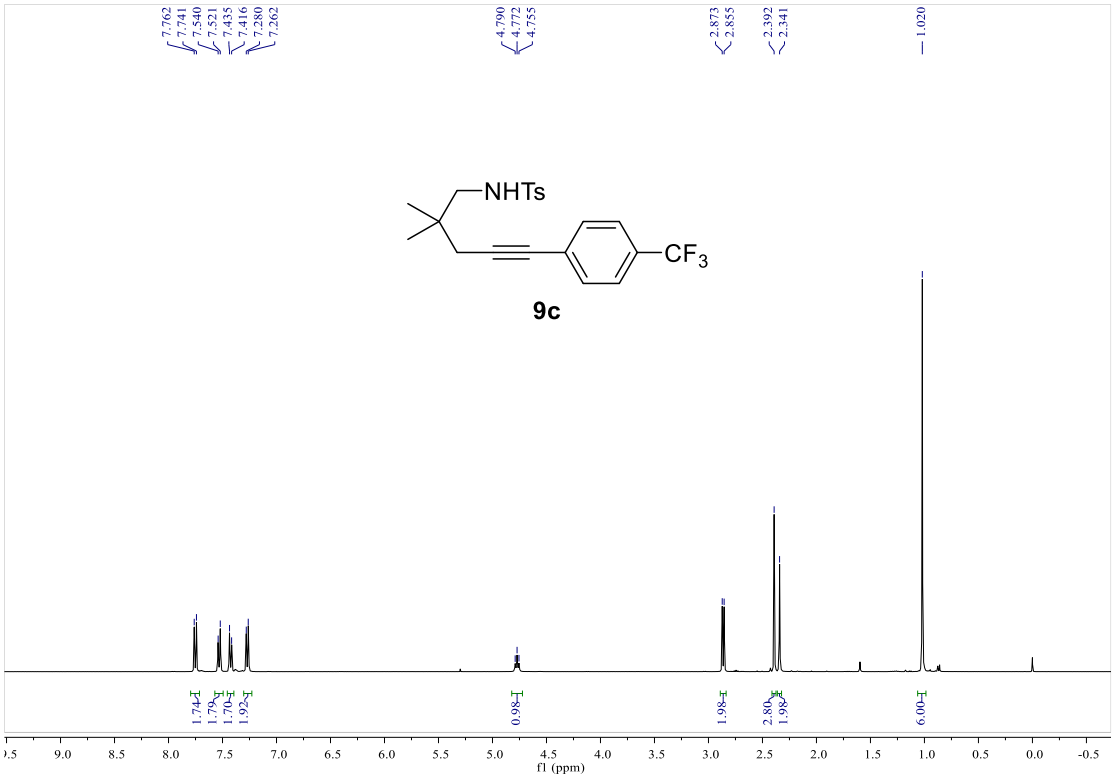
^{1}H NMR spectrum of **9b** (500 MHz, $CDCl_3$)



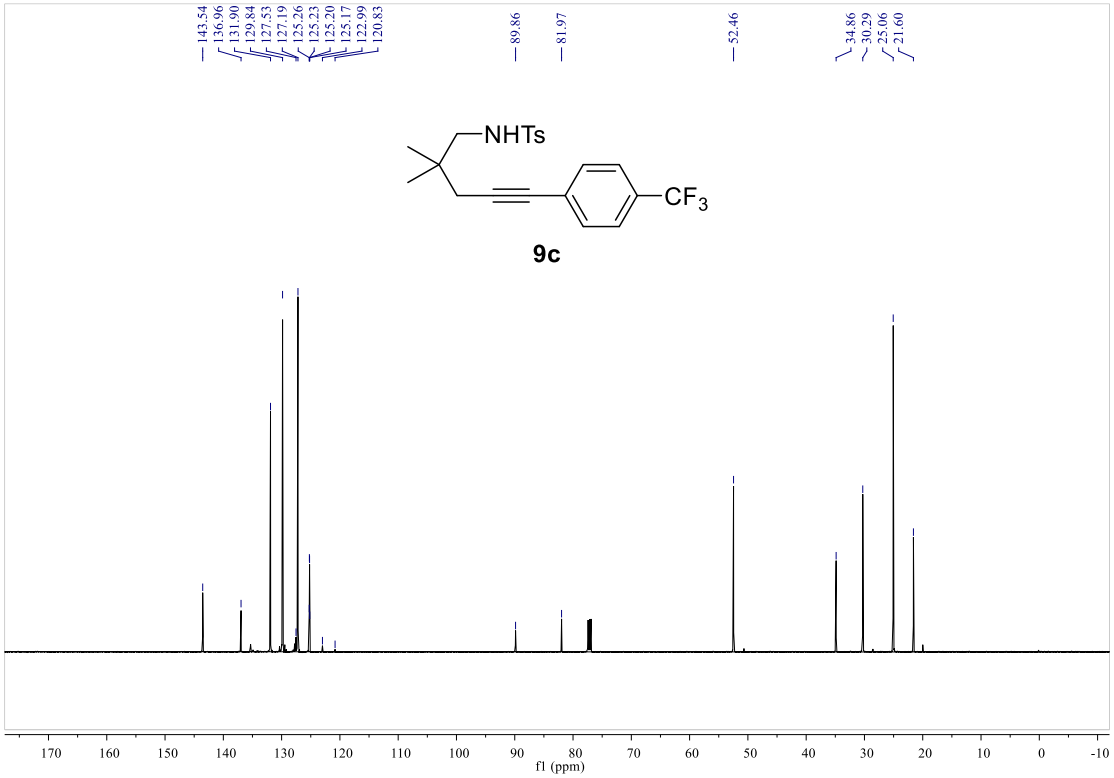
^{13}C NMR spectrum of **9b** (125 MHz, $CDCl_3$)



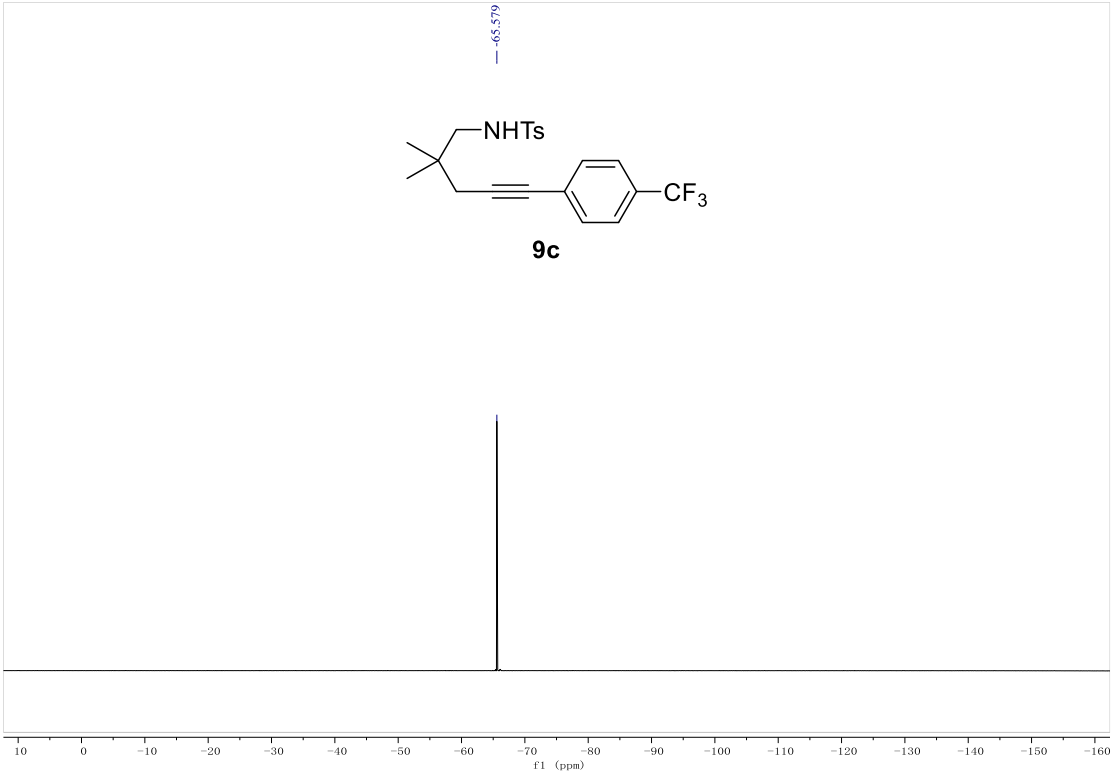
^{1}H NMR spectrum of **9c** (400 MHz, $CDCl_3$)



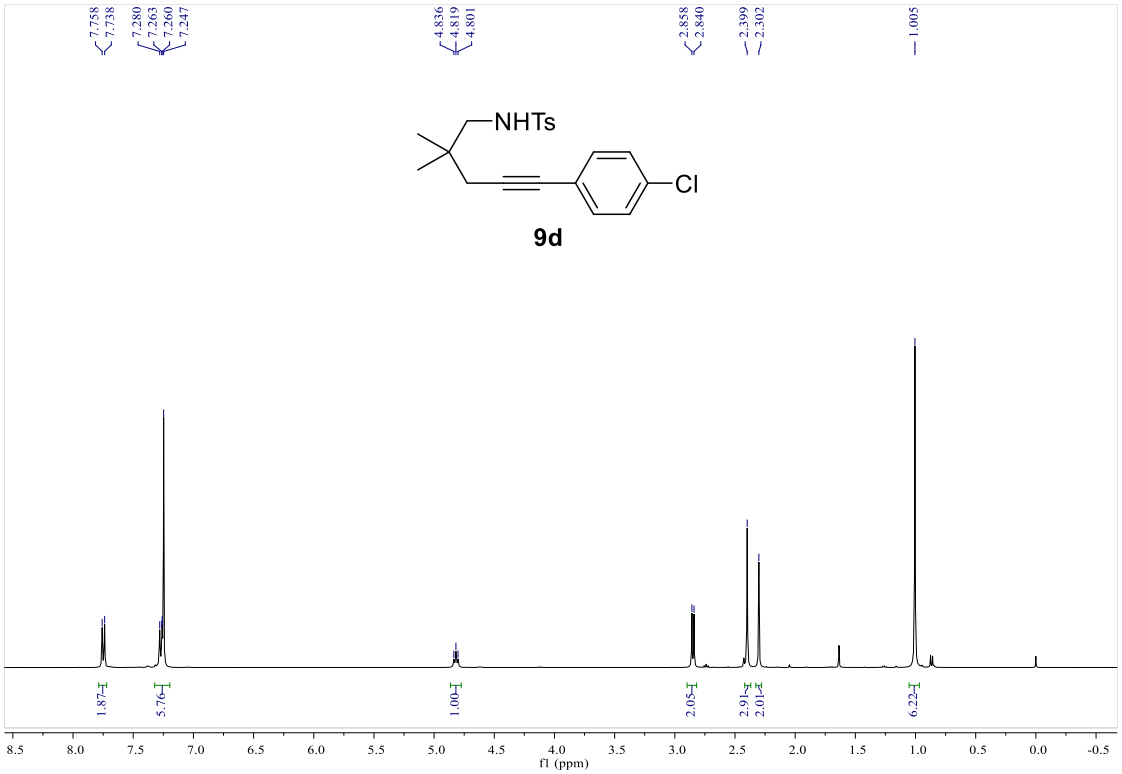
^{13}C NMR spectrum of **9c** (125 MHz, $CDCl_3$)



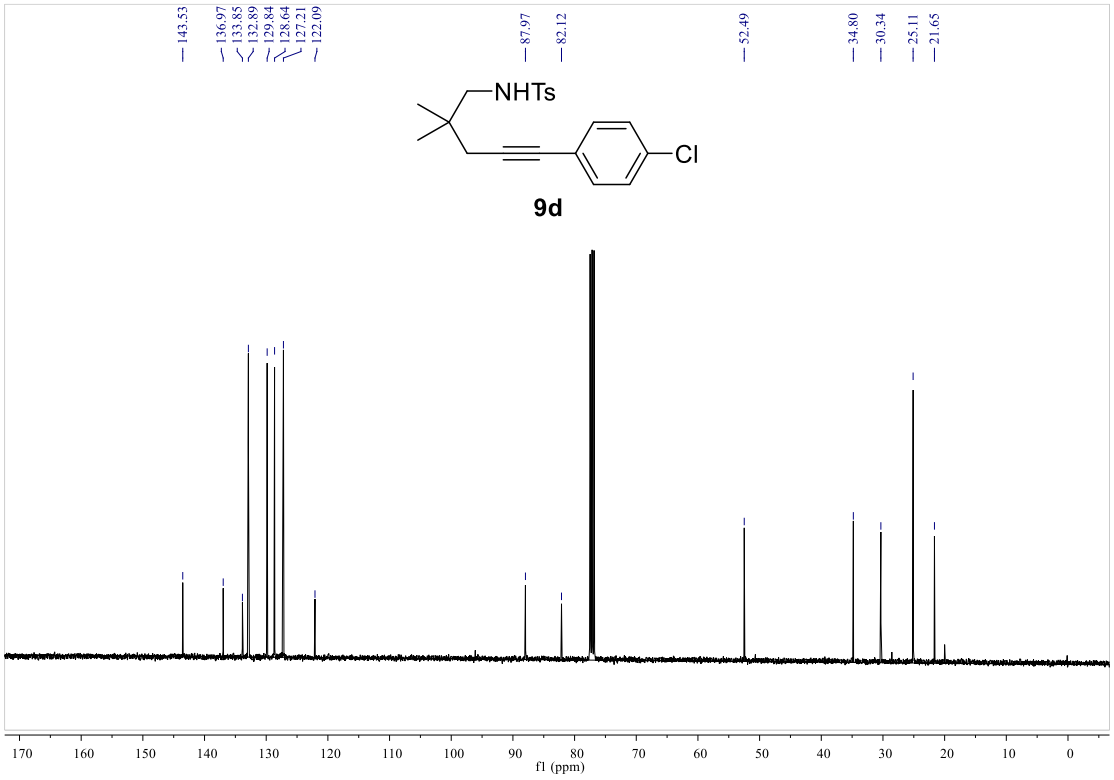
^{19}F NMR spectrum of **9c** (376 MHz, $CDCl_3$)



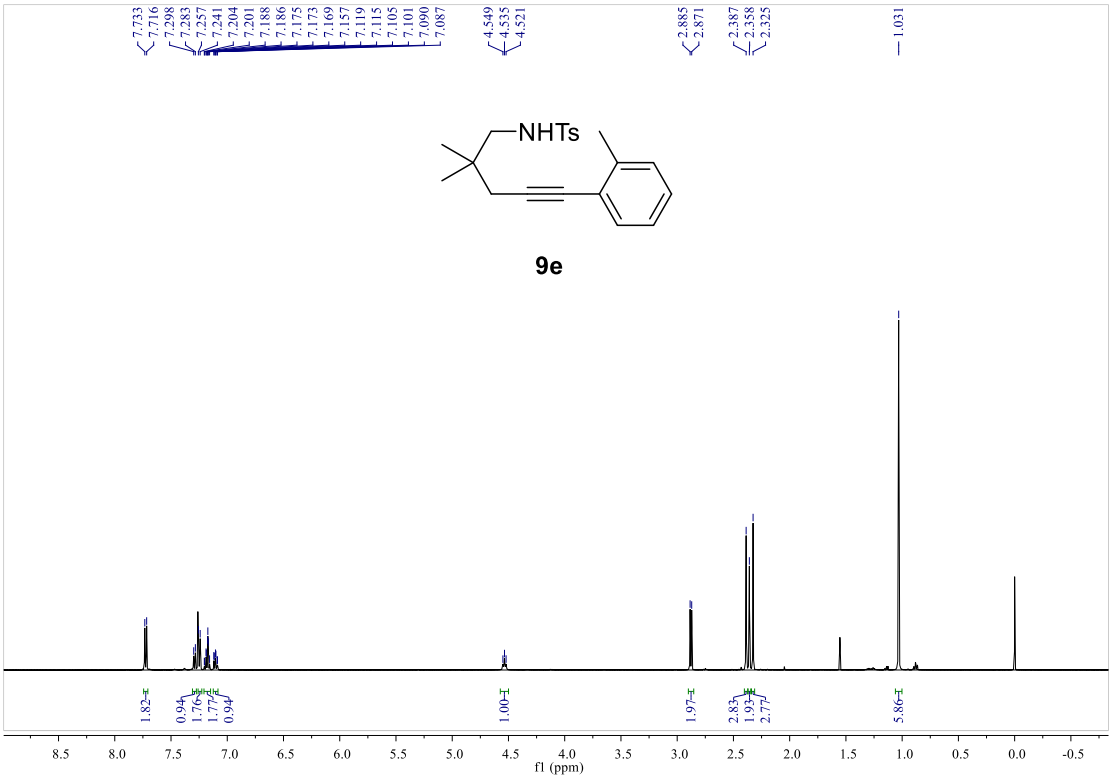
^{1}H NMR spectrum of **9d** (400 MHz, $CDCl_3$)



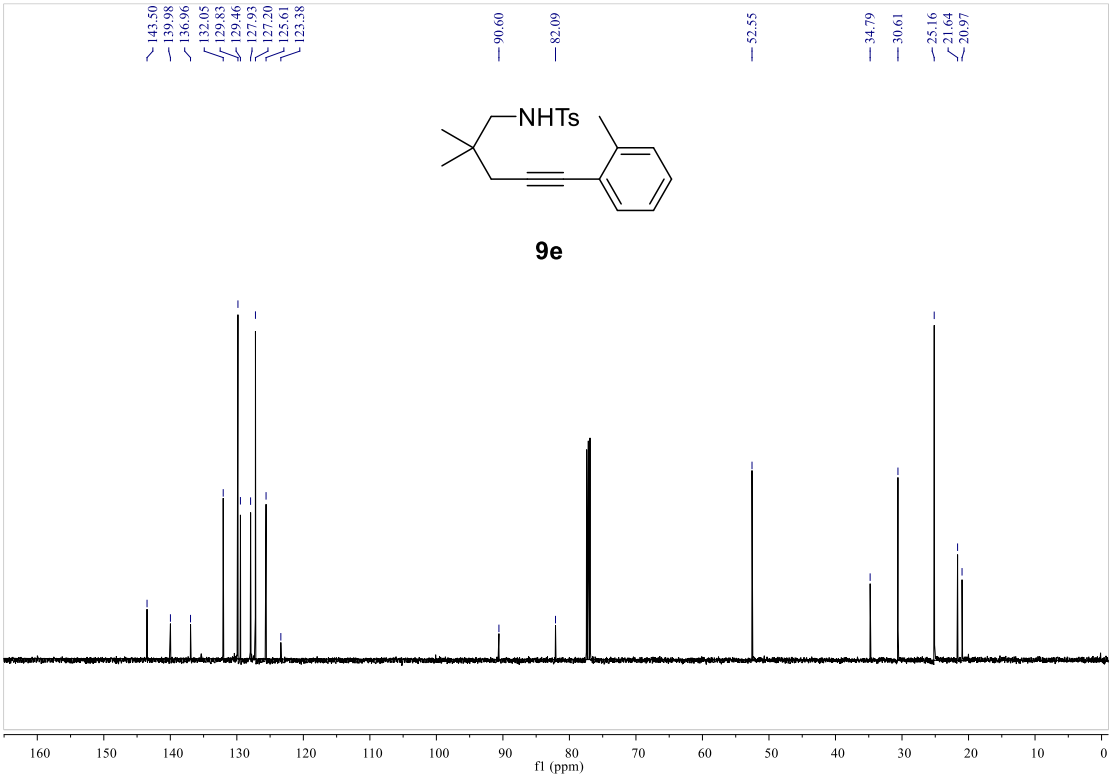
^{13}C NMR spectrum of **9d** (100 MHz, $CDCl_3$)



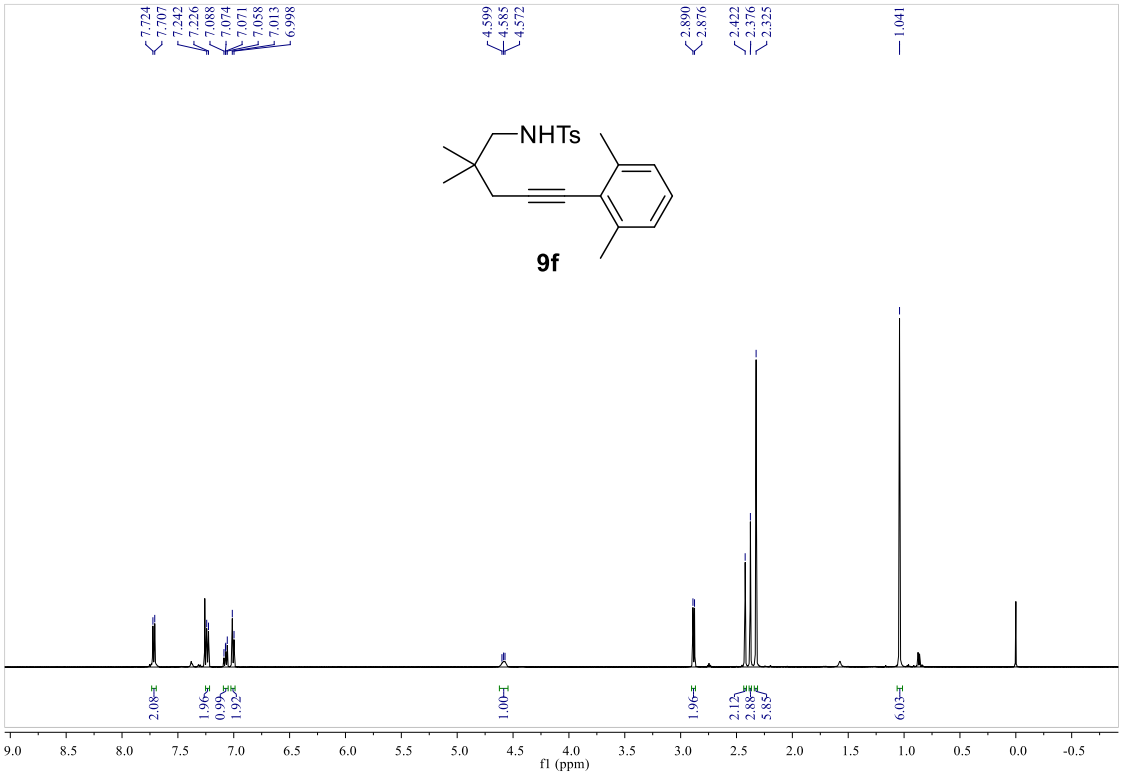
^{1}H NMR spectrum of **9e** (500 MHz, $CDCl_3$)



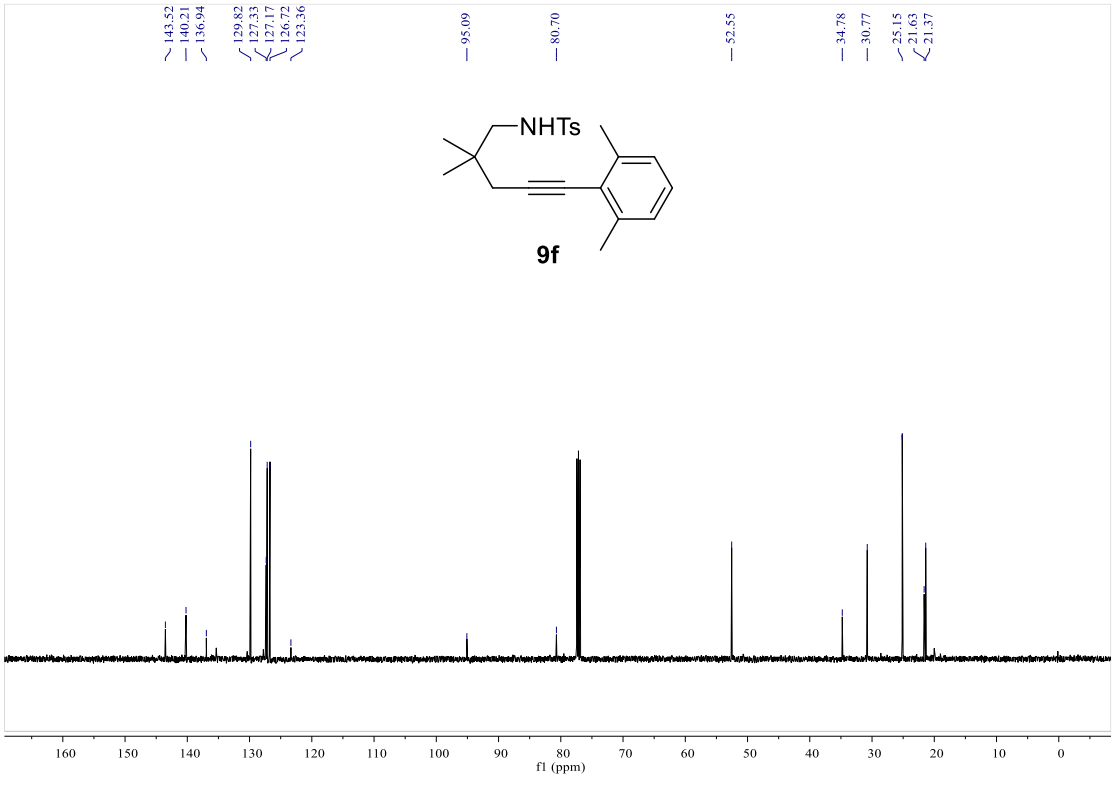
^{13}C NMR spectrum of **9e** (125 MHz, $CDCl_3$)



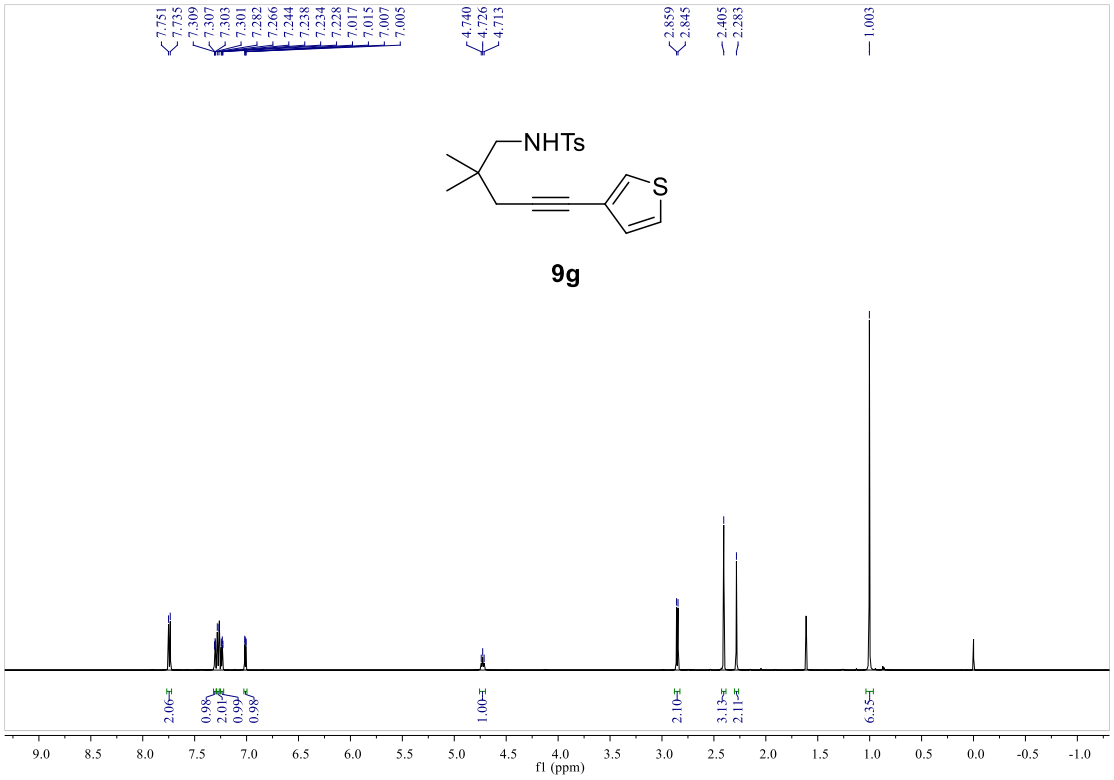
^{1}H NMR spectrum of **9f** (500 MHz, $CDCl_3$)



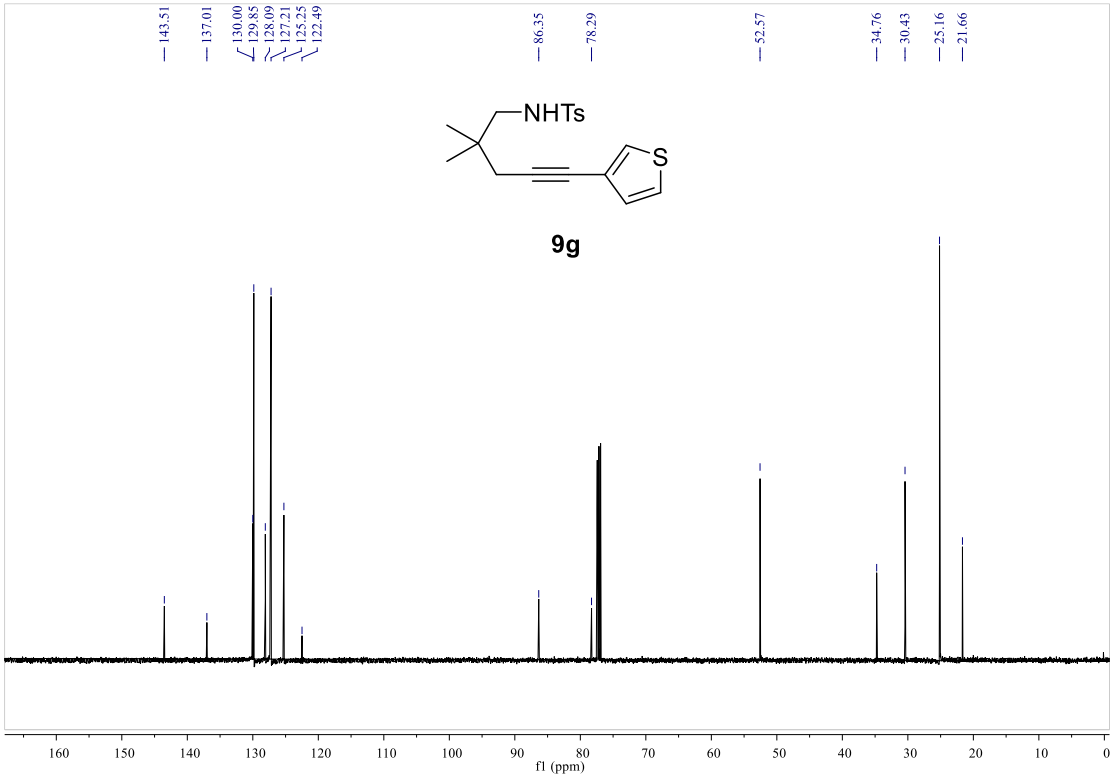
^{13}C NMR spectrum of **9f** (125 MHz, $CDCl_3$)



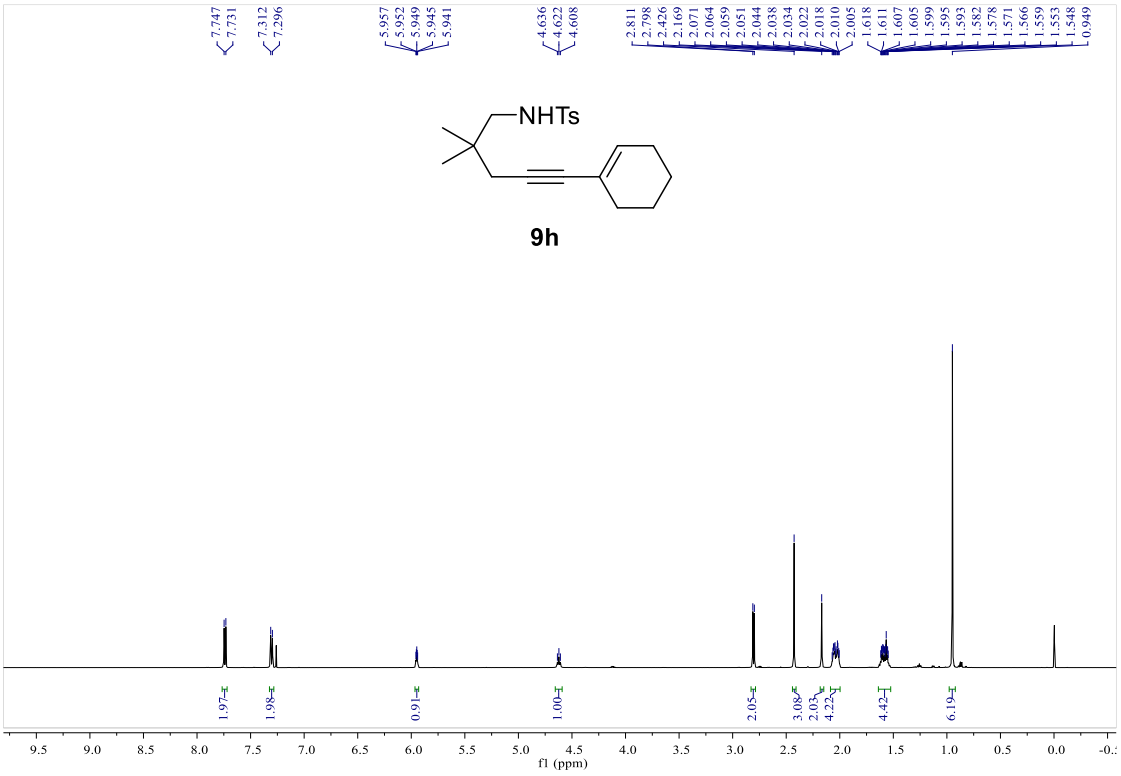
^{1}H NMR spectrum of **9g** (500 MHz, $CDCl_3$)



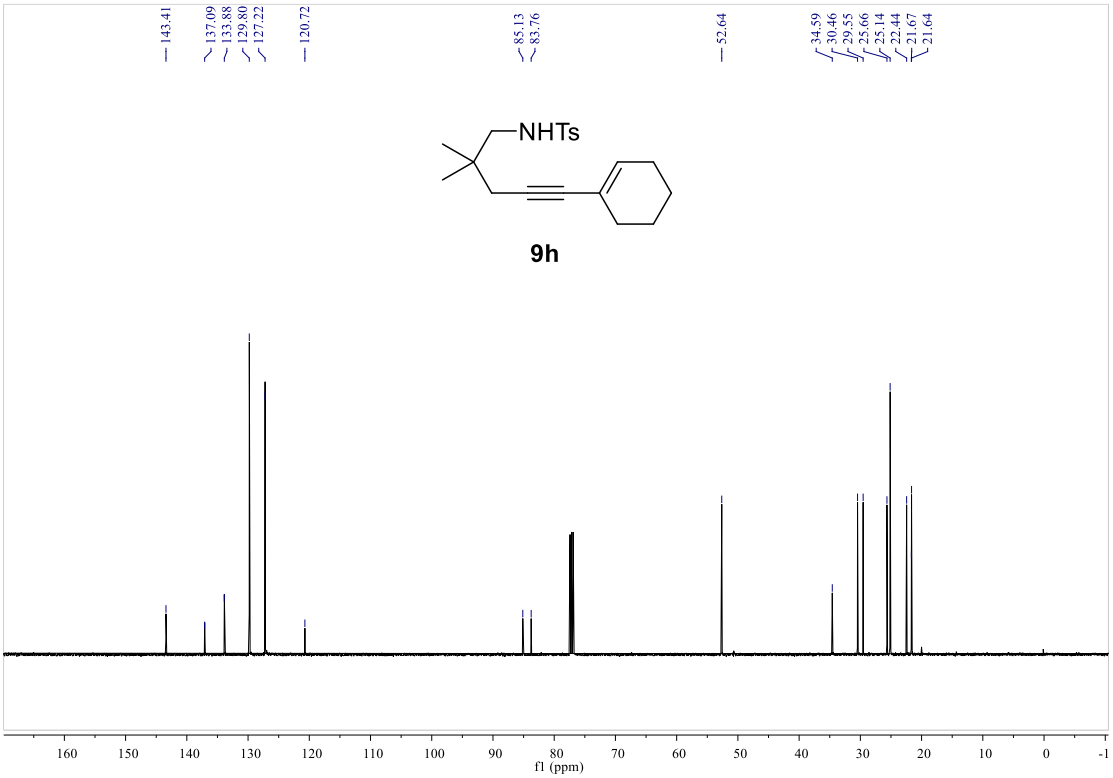
^{13}C NMR spectrum of **9g** (125 MHz, $CDCl_3$)



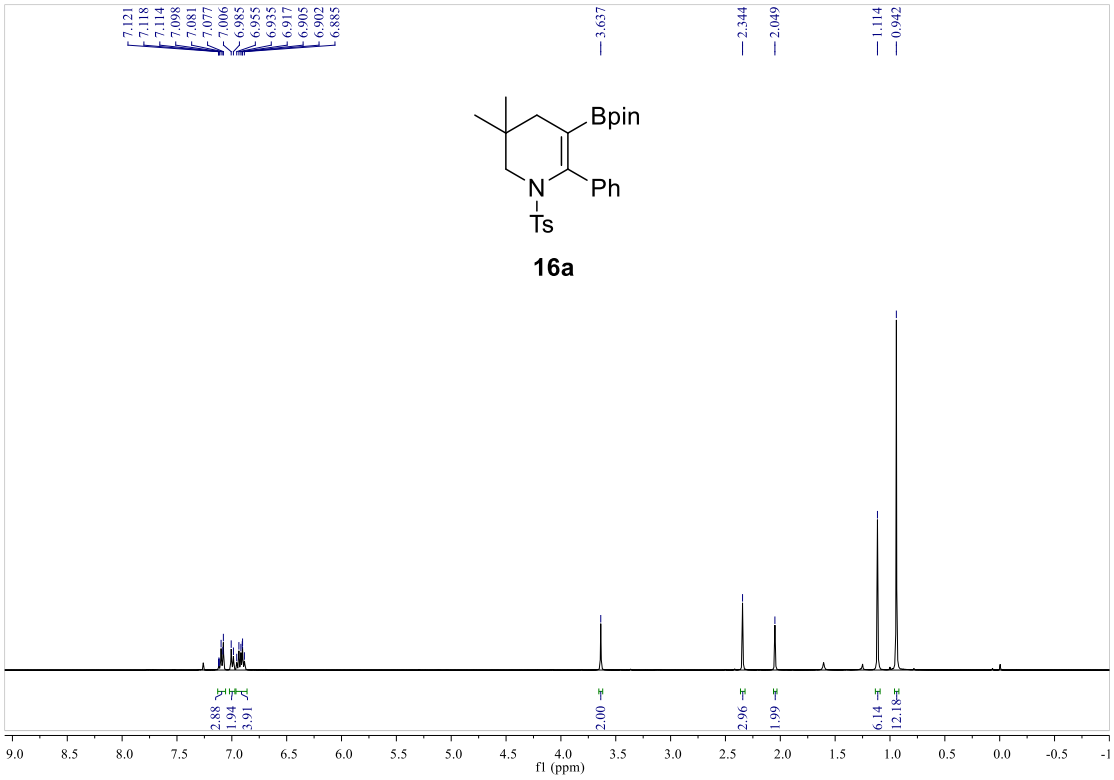
^{1}H NMR spectrum of **9h** (500 MHz, $CDCl_3$)



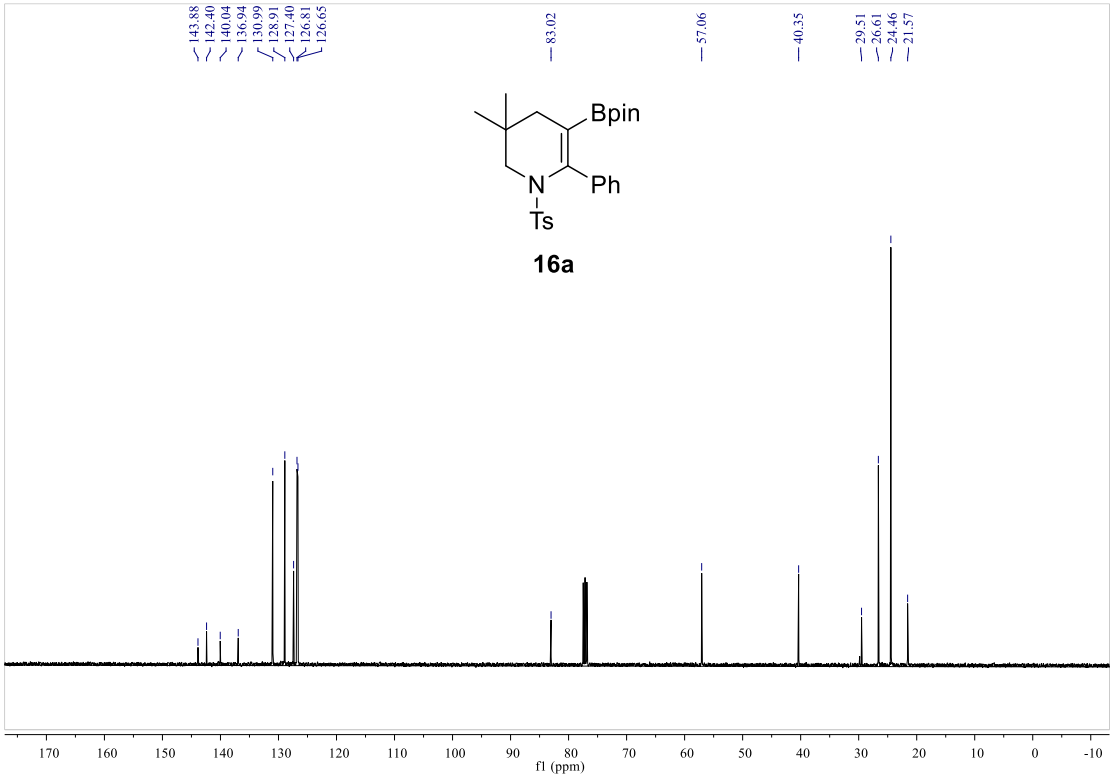
^{13}C NMR spectrum of **9h** (125 MHz, $CDCl_3$)



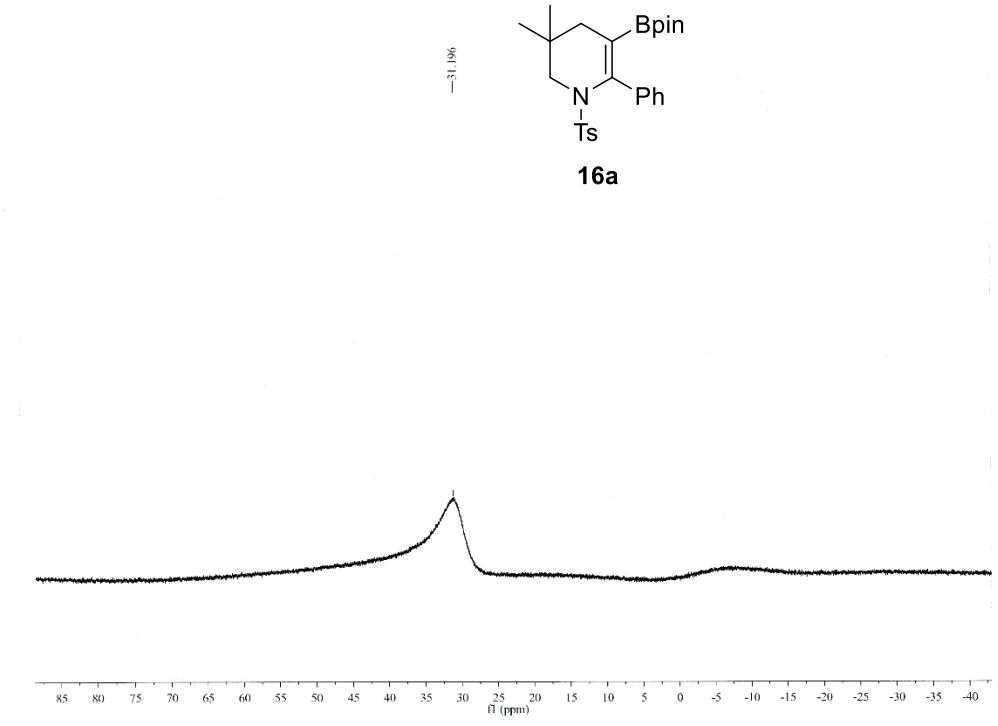
^{1}H NMR spectrum of **16a** (400 MHz, $CDCl_3$)



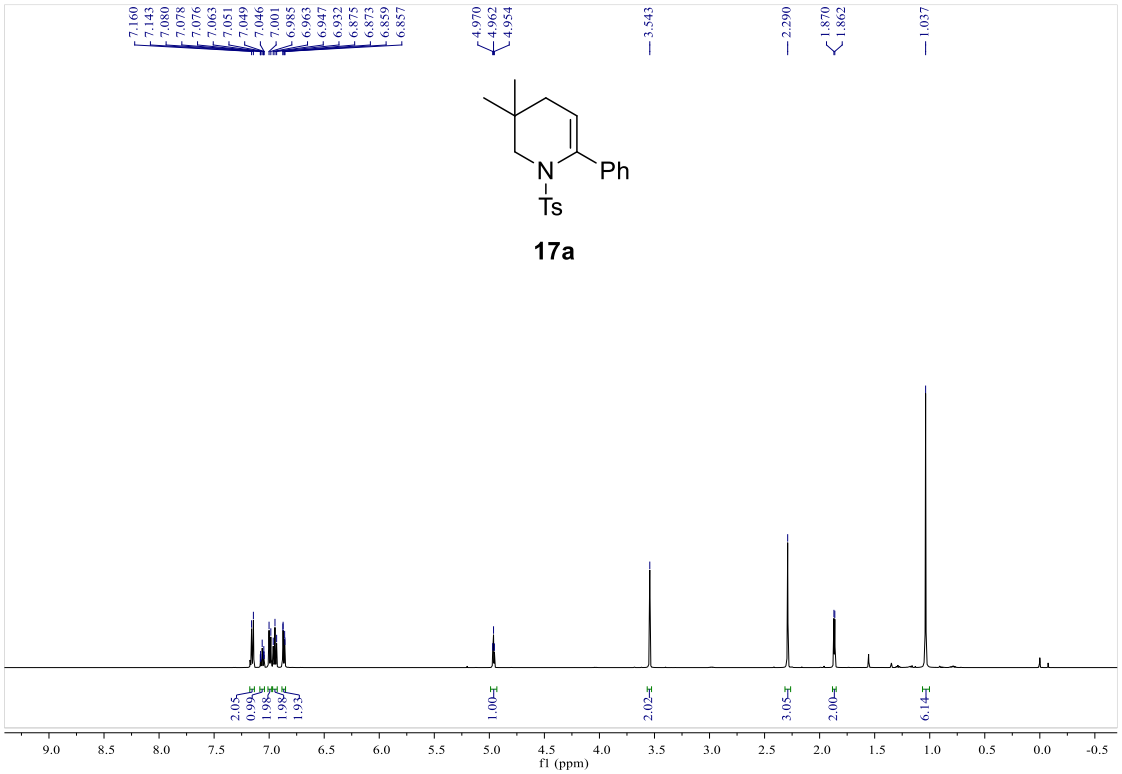
^{13}C NMR spectrum of **16a** (100 MHz, $CDCl_3$)



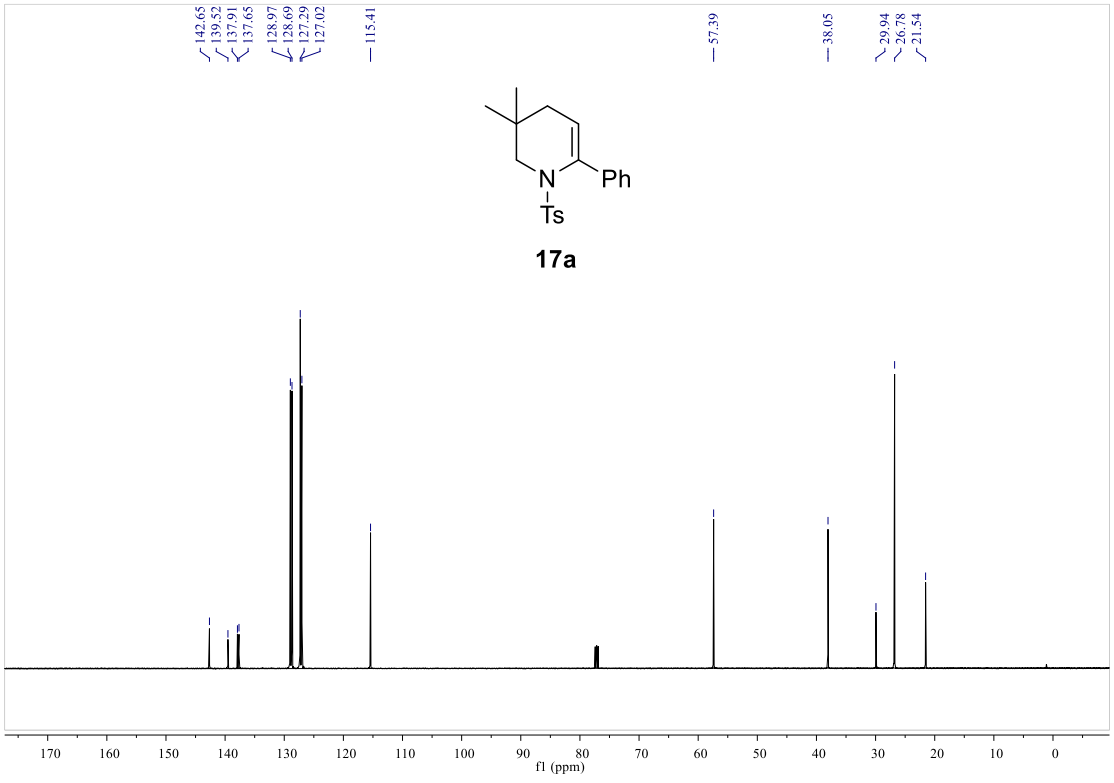
^{11}B NMR spectrum of **16a** (128 MHz, $CDCl_3$)



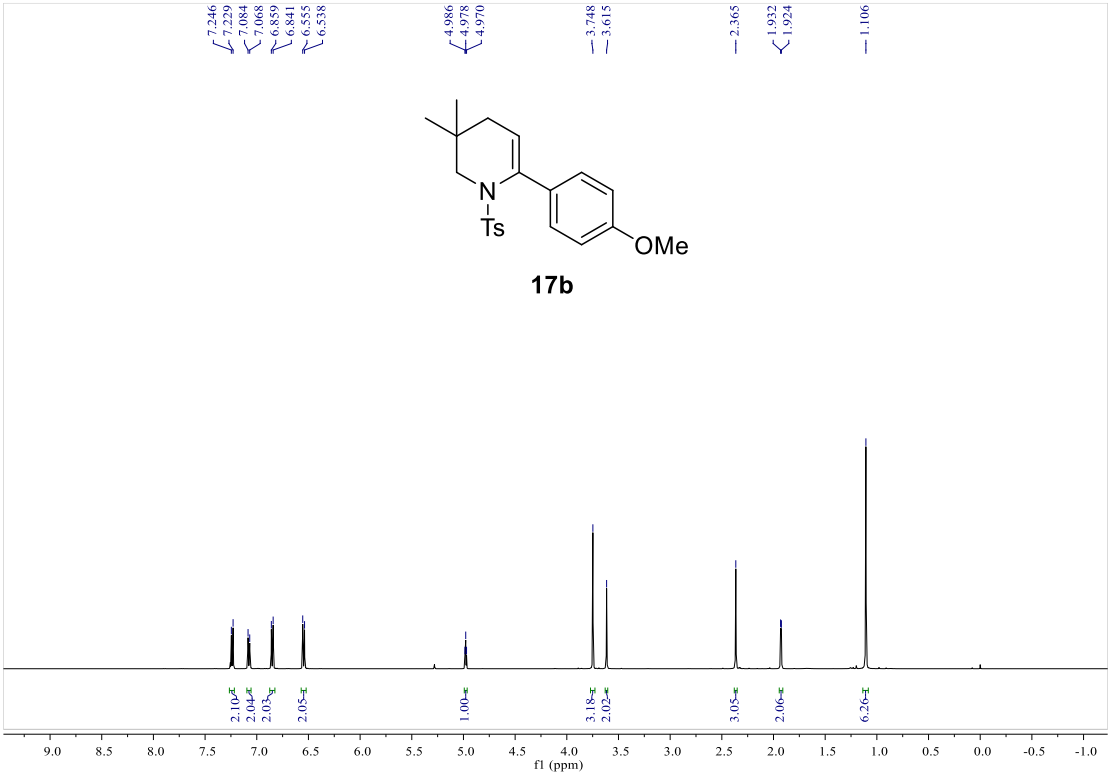
^{1}H NMR spectrum of **17a** (500 MHz, $CDCl_3$)



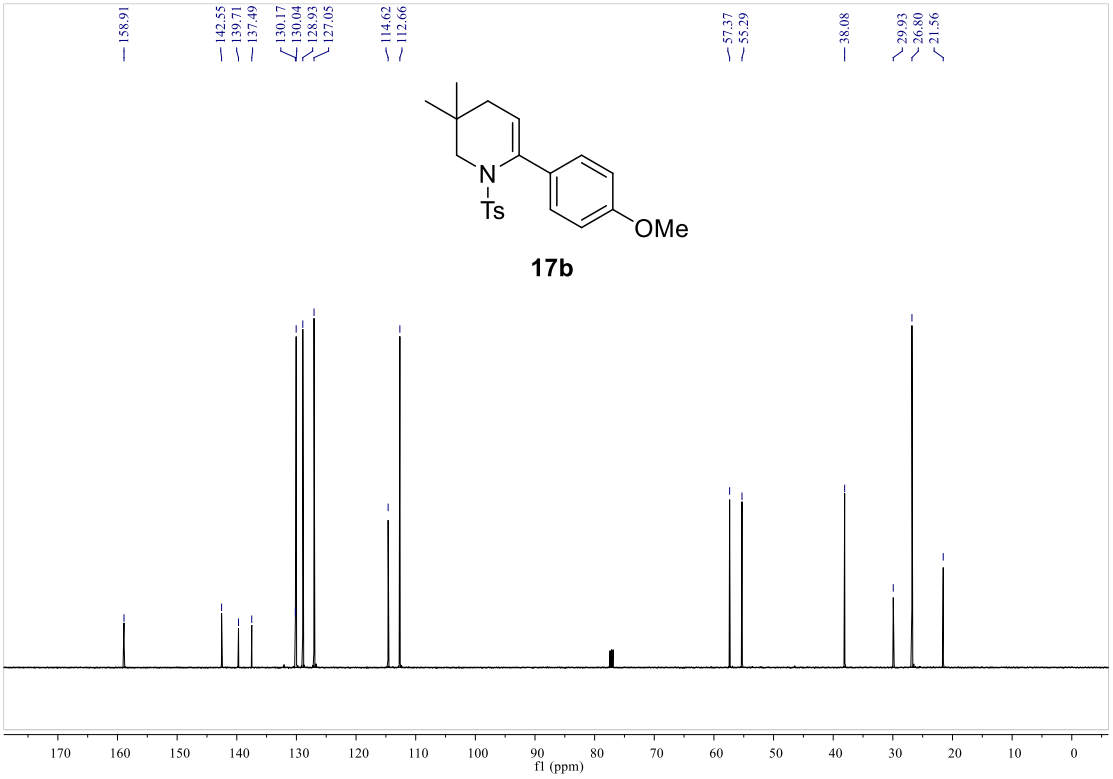
^{13}C NMR spectrum of **17a** (125 MHz, $CDCl_3$)



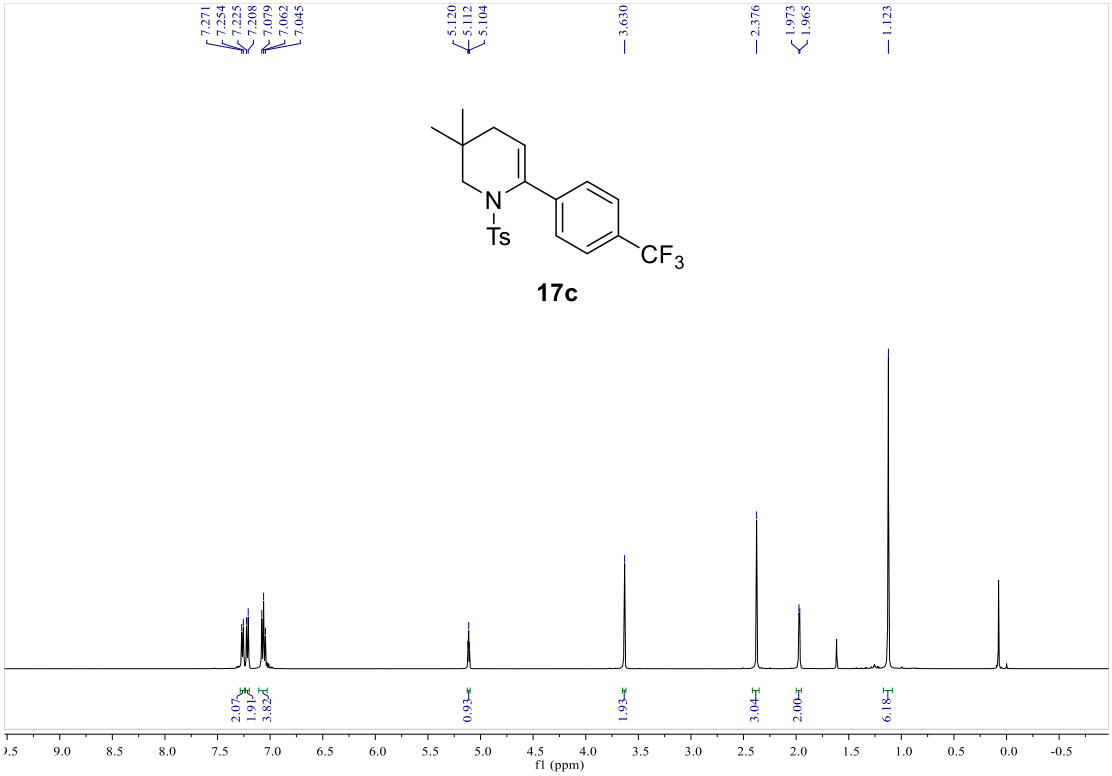
^{1}H NMR spectrum of **17b** (500 MHz, $CDCl_3$)



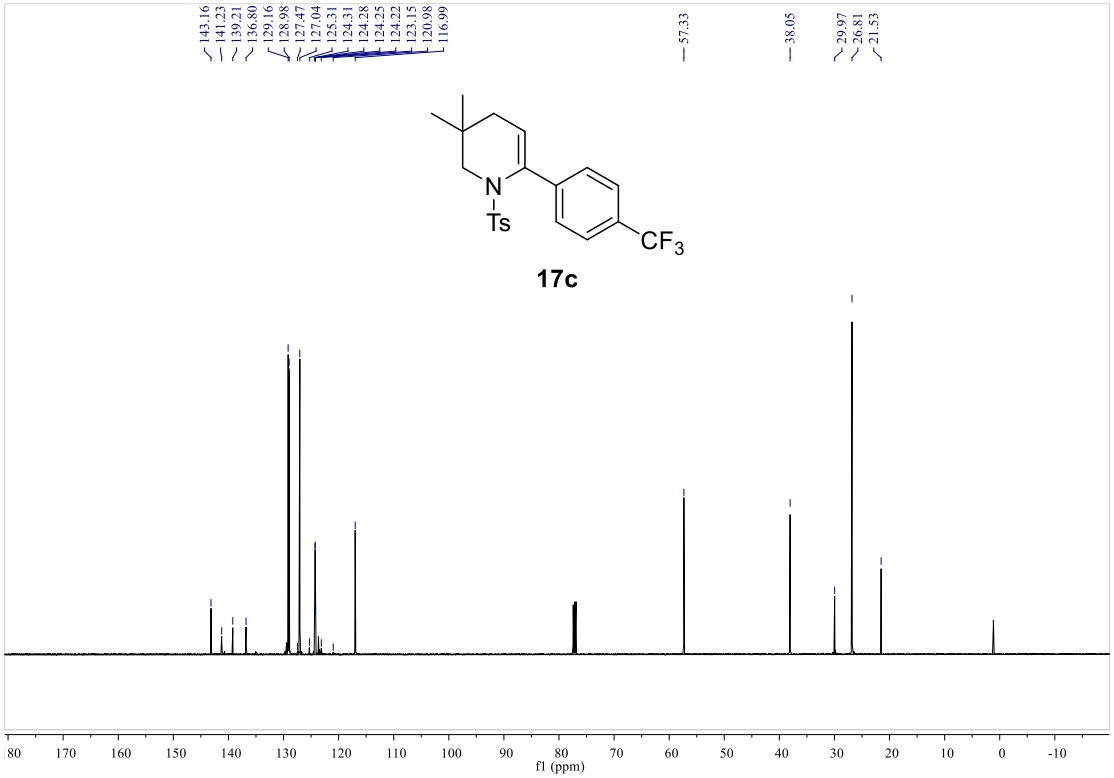
^{13}C NMR spectrum of **17b** (125 MHz, $CDCl_3$)



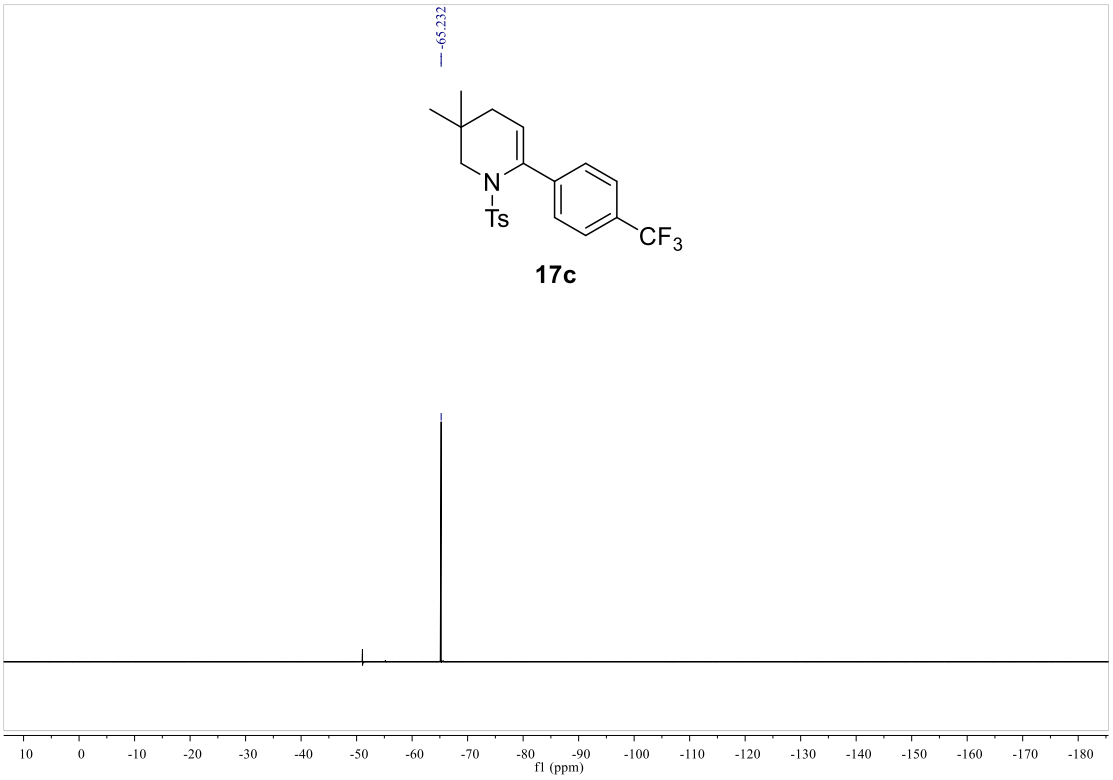
^{1}H NMR spectrum of **17c** (500 MHz, $CDCl_3$)



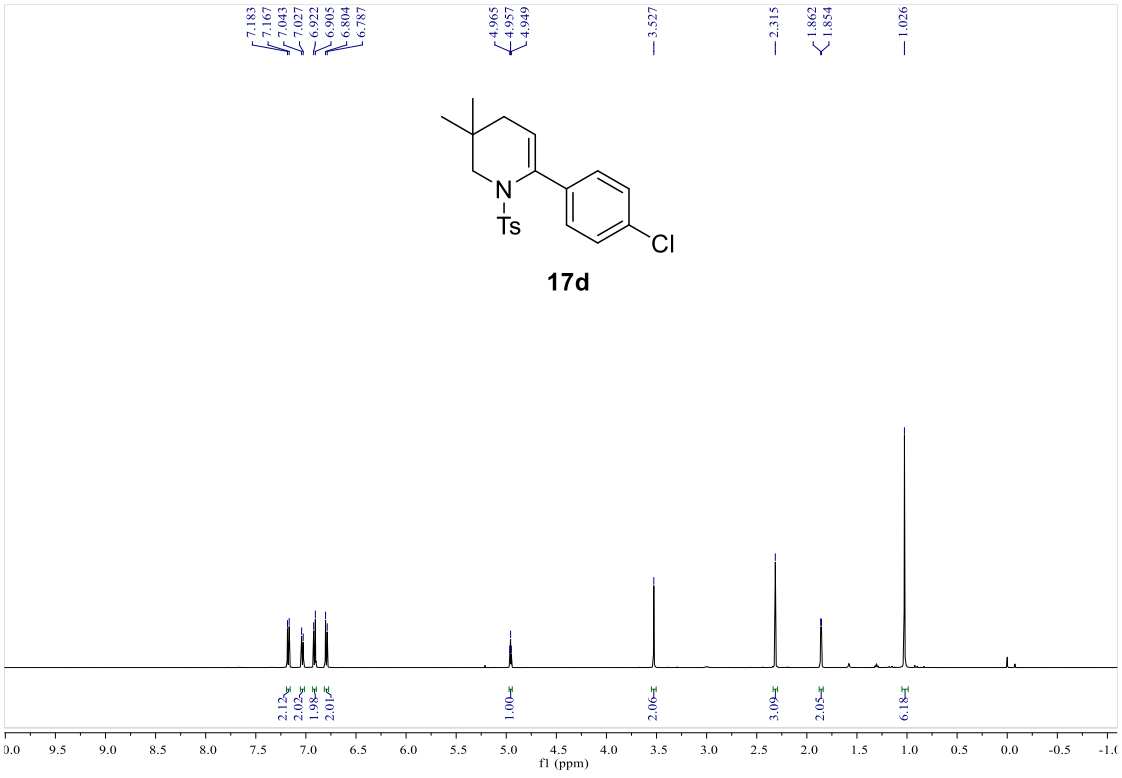
^{13}C NMR spectrum of **17c** (125 MHz, $CDCl_3$)



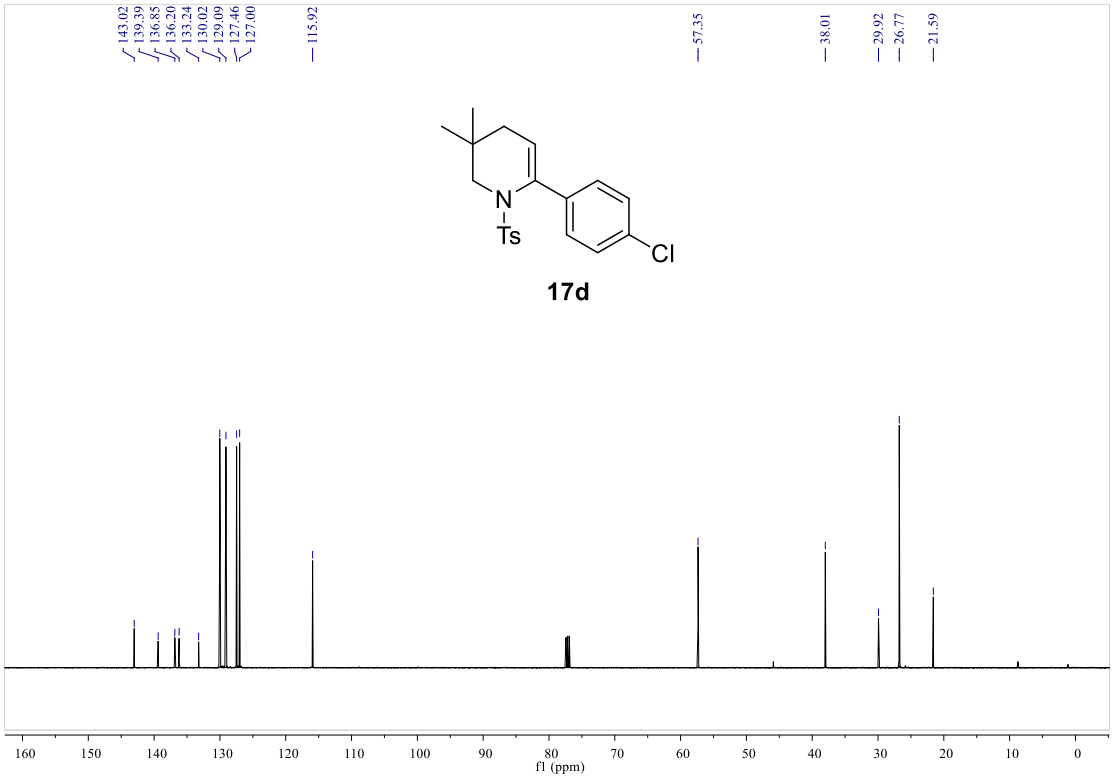
^{19}F NMR spectrum of **17c** (471 MHz, $CDCl_3$)



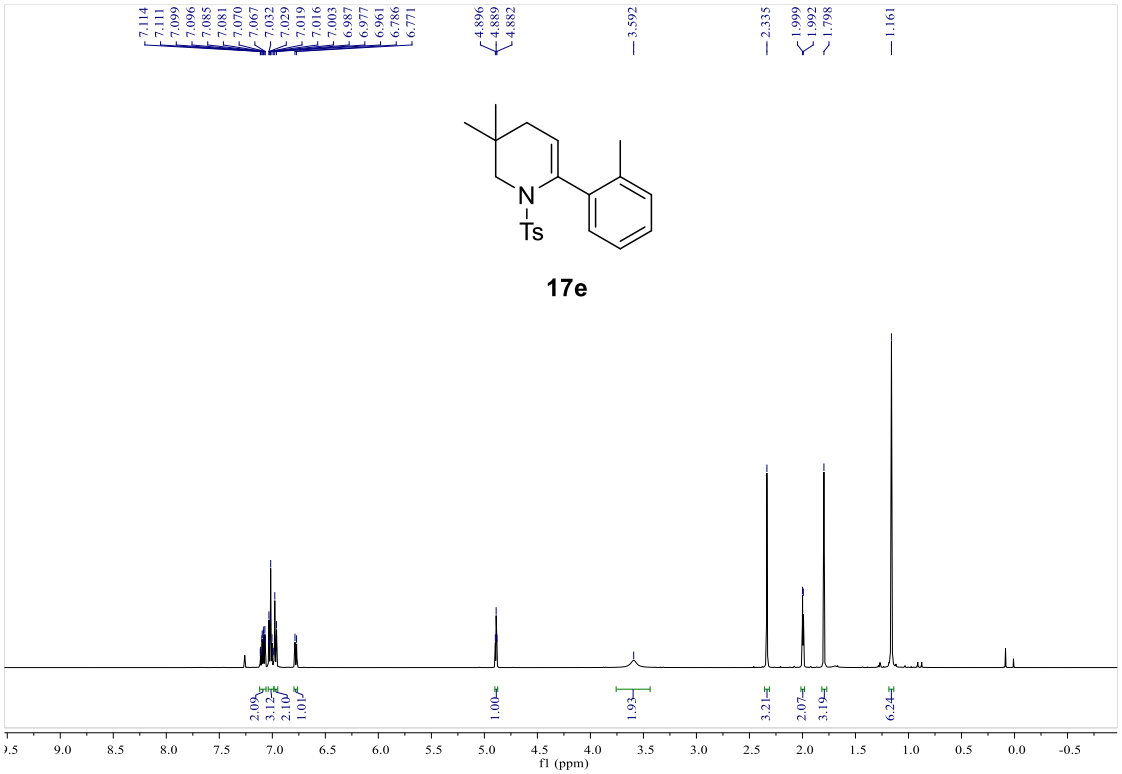
^{1}H NMR spectrum of **17d** (500 MHz, $CDCl_3$)



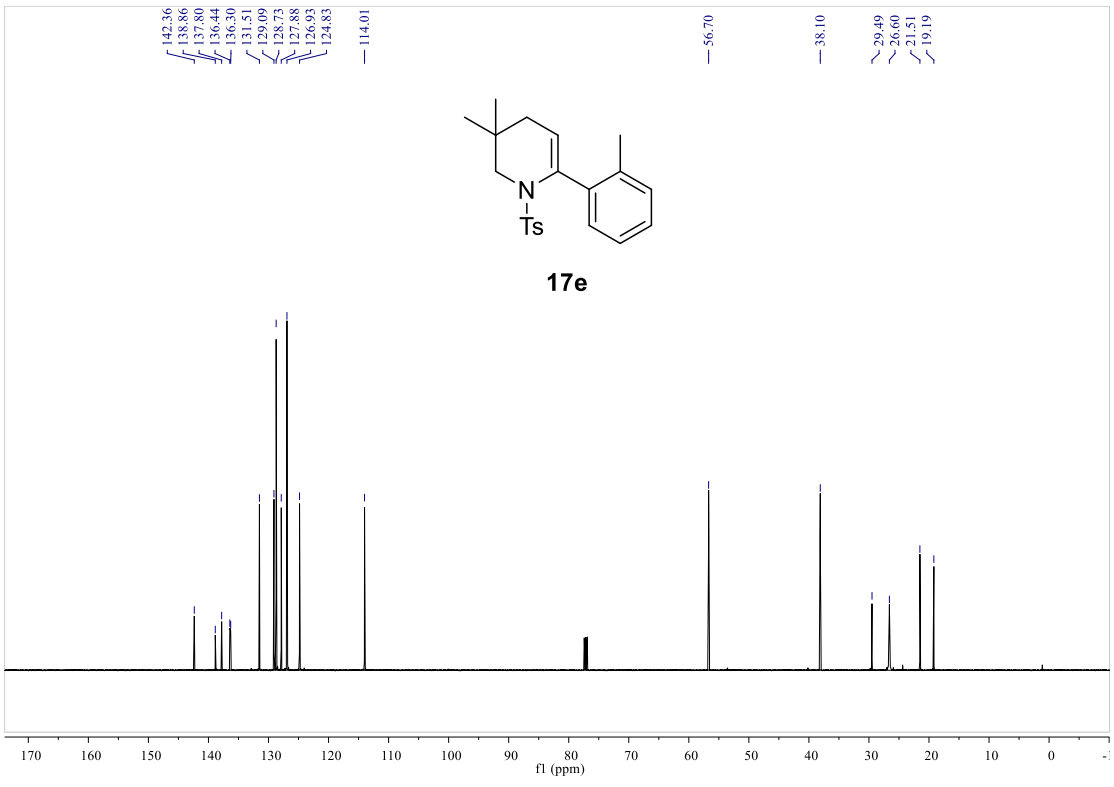
^{13}C NMR spectrum of **17d** (125 MHz, $CDCl_3$)



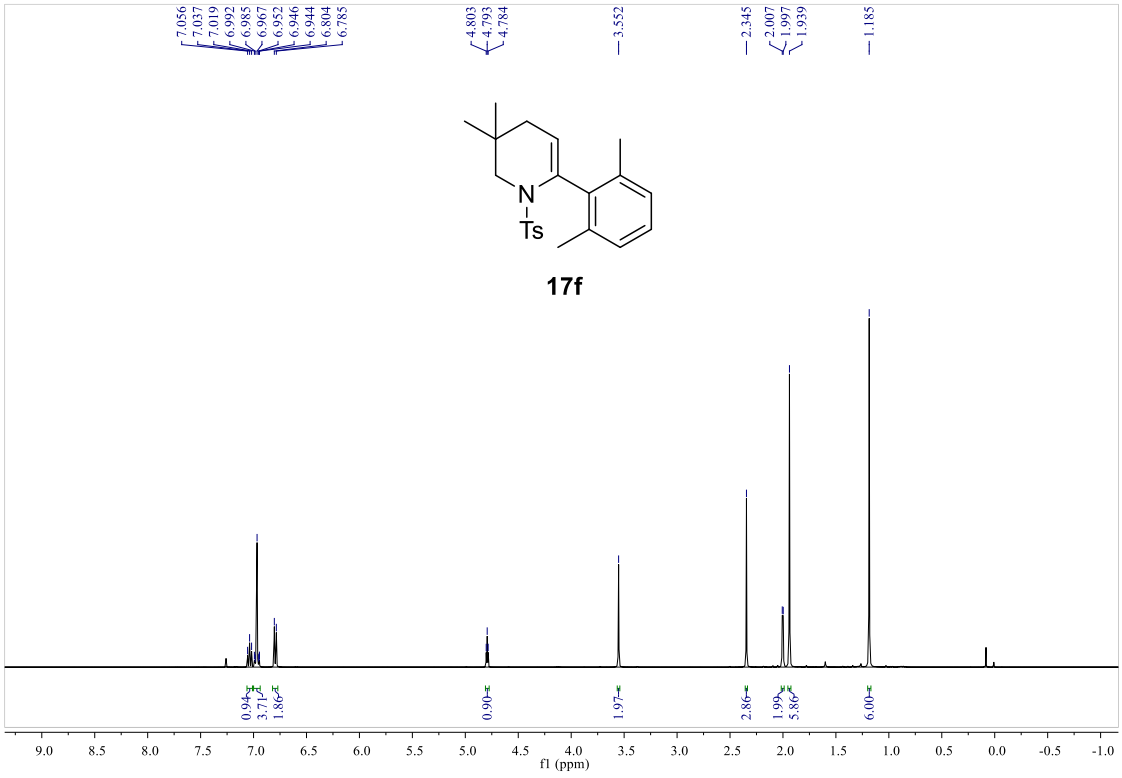
^{1}H NMR spectrum of **17e** (500 MHz, $CDCl_3$)



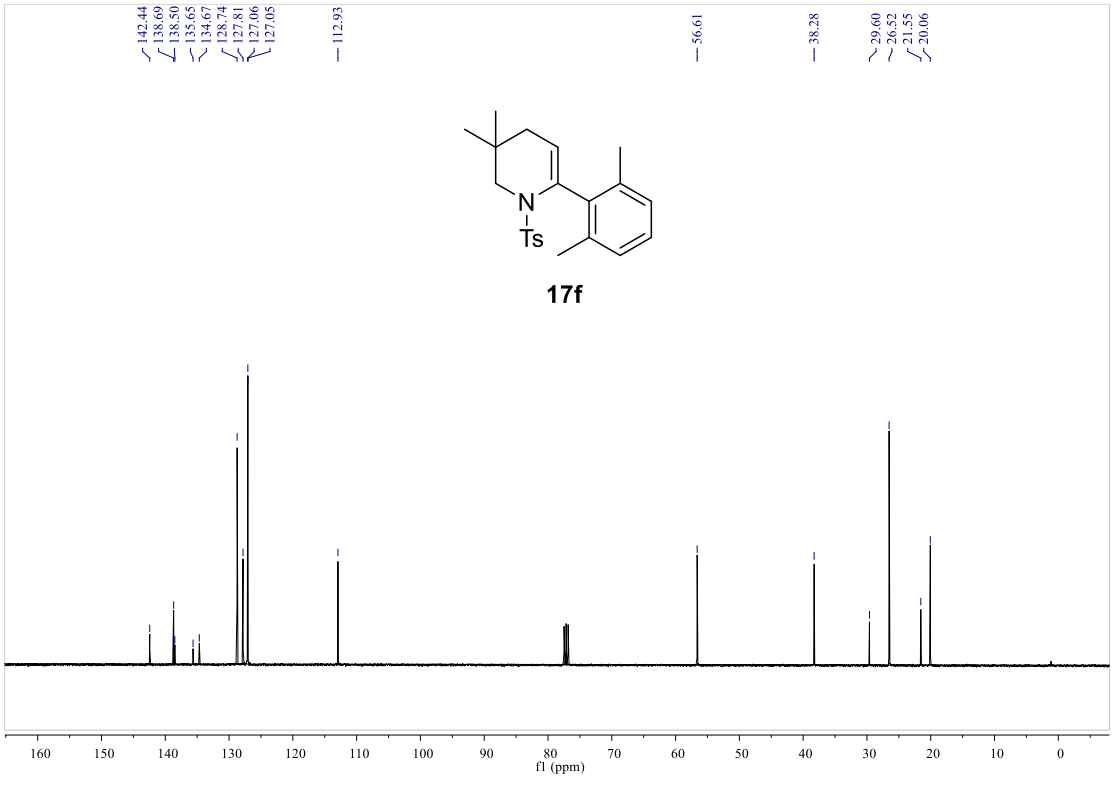
^{13}C NMR spectrum of **17e** (125 MHz, $CDCl_3$)



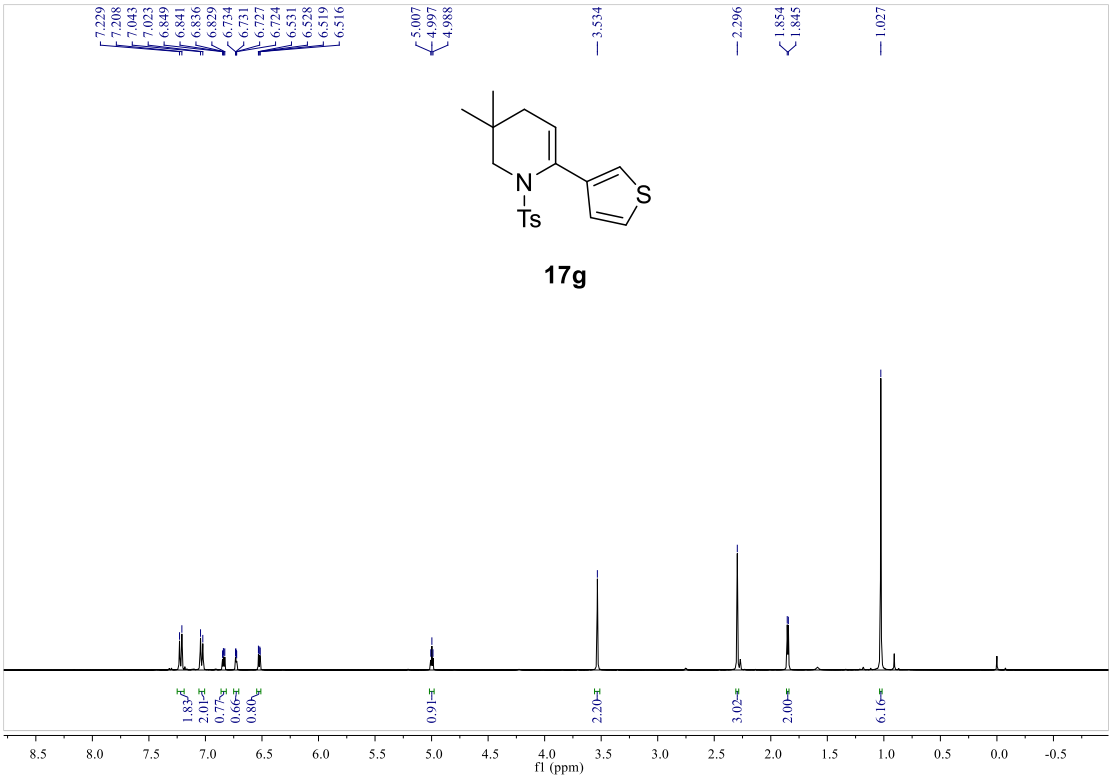
^{1}H NMR spectrum of **17f** (400 MHz, $CDCl_3$)



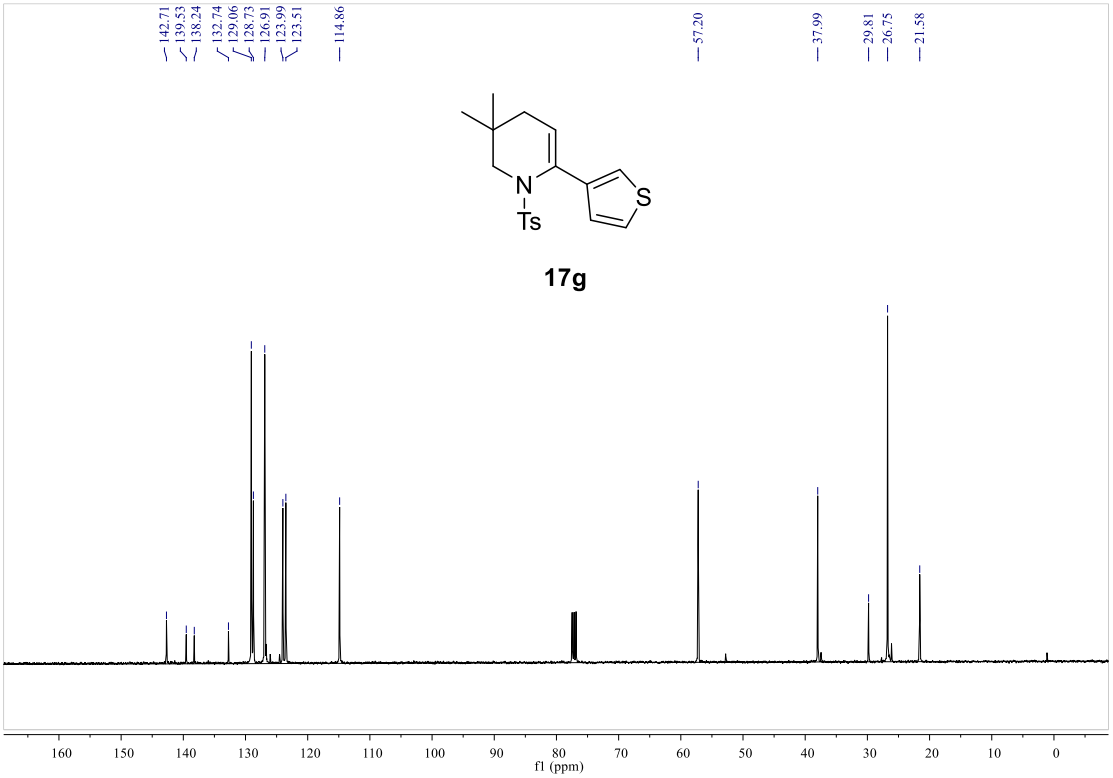
^{13}C NMR spectrum of **17f** (100 MHz, $CDCl_3$)



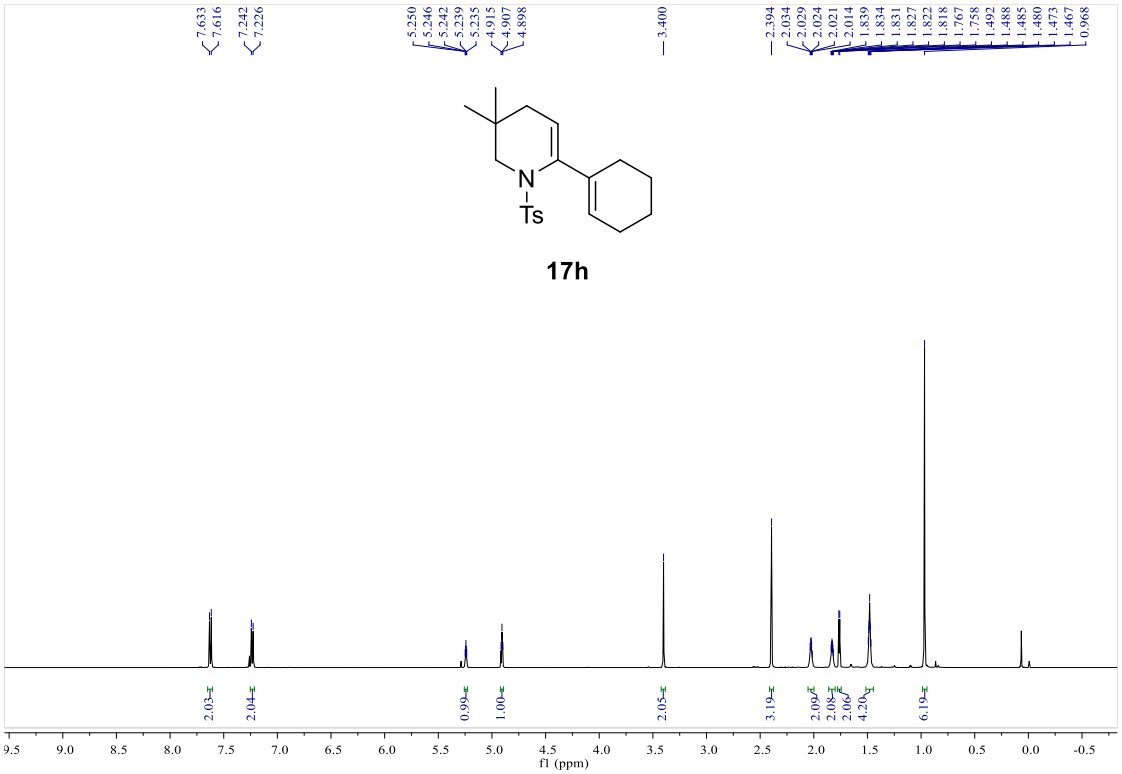
^{1}H NMR spectrum of **17g** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **17g** (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of **17h** (500 MHz, $CDCl_3$)



^{13}C NMR spectrum of **17h** (125 MHz, $CDCl_3$)