

ELECTRONIC SUPPORTING INFORMATION

Platinum(0)-Mediated C–O Bond Activation of Ethers via S_N2 Mechanism

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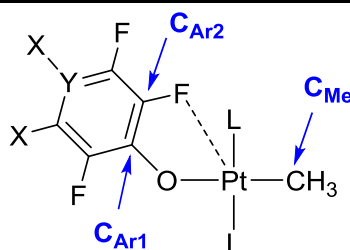
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1. Experimental and computational structural parameters for **1a**, **1b**, **1e**, and **1f**

Table S1. Selected computed bond lengths (Å) and angles (°) of **1a**, **1b**, **1e**, and **1f**.
Experimental values in italics.¹

	1a	1b	1e	1f
Pt–O	2.226 <i>2.1586(15)</i>	2.216 <i>2.1306(15)</i>	2.213 <i>2.1419(14)</i>	2.205 <i>2.1325(13)</i>
Pt–C _{Me}	2.056 <i>2.044(2)</i>	2.058 <i>2.047(2)</i>	2.059 <i>2.0520(19)</i>	2.060 <i>2.0546(19)</i>
Pt···F	3.180 <i>3.110(2)</i>	3.177 <i>3.117(2)</i>	3.181 <i>2.972(1)</i>	3.156 <i>3.046(9)/3.196(20)</i>
C _{Me} –Pt–O	178.5 <i>176.46(9)</i>	178.7 <i>179.56(9)</i>	178.8 <i>176.37(7)</i>	178.6 <i>179.14(8)</i>
C _{Ar1} –O–Pt	128.0 <i>130.10(15)</i>	126.7 <i>126.78(14)</i>	127.3 <i>126.90(13)</i>	126.3 <i>123.3(3)</i>
C _{Ar2} –C _{Ar1} –O–Pt	28.3 <i>21.2(3)</i>	34.1 <i>27.3(3)</i>	33.3 <i>-1.00(14)</i>	33.8 <i>23.8(6)</i>



2. DFT-optimised structures of **1·THF** and **TS_{SN2}1b·THF**

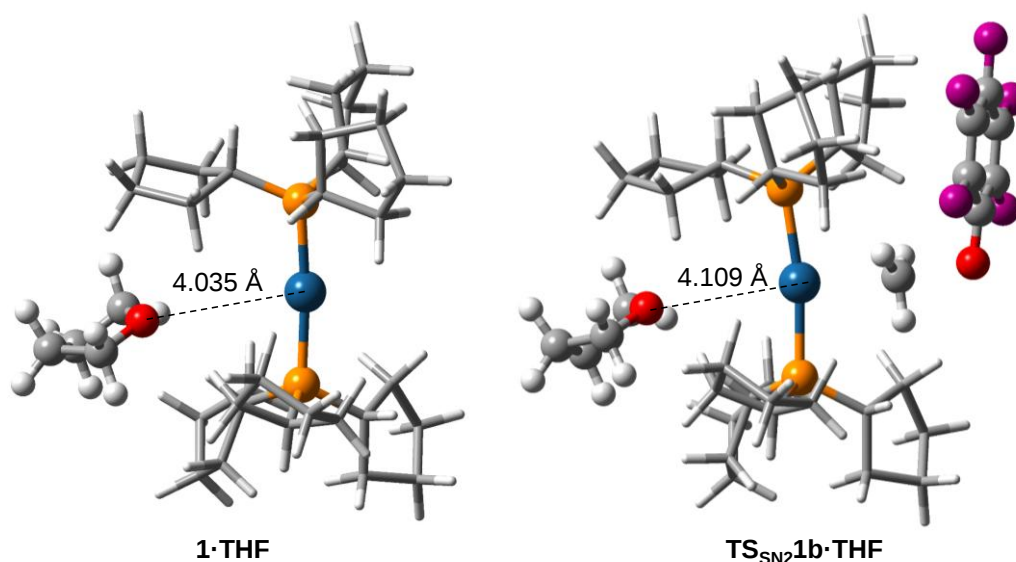


Fig. S1 Structures of **1·THF** and **TS_{SN2}1b·THF**.

¹ N. A. Jasim, R. N. Perutz, B. Procacci and A. C. Whitwood, *Chem. Commun.*, 2014, **50**, 3914.

3. Activation Gibbs energy vs. $q(O)$ for selected substrates

The charges of the oxygen atoms of RO^- have been plotted against the corresponding activation Gibbs energies for all substrates but those including fluorinated aryl groups, i.e., **a**, **b**, $p\text{-CF}_3\text{-b}$, **e**, and **f**.

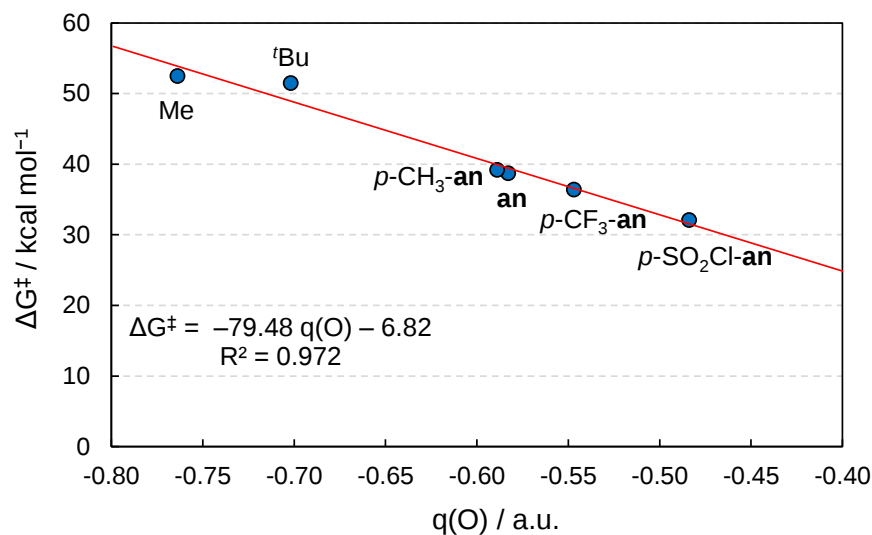


Fig. S2 Plot of activation Gibbs energy vs. $q(O)$ of selected $TS_{SN2}1x$. Regression line in red.

4. XYZ coordinates and energies in THF for all species

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1 E=-1976.954876 G=-1976.240413

C	-3.196079	1.547616	0.053153
H	-2.782256	2.103885	0.906762
C	-4.744679	1.547945	0.142495
H	-5.174454	0.559064	0.341456
H	-5.058088	2.193616	0.974167
C	-5.225319	2.141255	-1.183934
H	-5.293848	1.352383	-1.948886
H	-6.213719	2.609329	-1.109437
C	-4.111372	3.112498	-1.559181
H	-4.155971	3.453873	-2.599897
H	-4.165054	4.002585	-0.914492
C	-2.849219	2.314570	-1.242276
H	-1.949552	2.931276	-1.124721
H	-2.644368	1.618115	-2.070335
C	-3.102815	-1.142796	-1.169906
H	-3.247750	-0.438961	-2.004097
C	-2.173460	-2.285796	-1.671184
H	-1.721083	-1.998438	-2.629382
H	-1.334393	-2.470229	-0.987578
C	-3.073702	-3.522089	-1.820504
H	-2.798630	-4.148901	-2.676235
H	-2.996202	-4.150714	-0.921099
C	-4.487406	-2.956444	-1.910611
H	-5.269483	-3.698068	-1.708943
H	-4.667762	-2.547667	-2.916209
C	-4.454766	-1.820856	-0.892962
H	-4.482189	-2.247854	0.120732
H	-5.301783	-1.129725	-0.980740
C	-2.924770	-0.766412	1.772626
H	-4.020542	-0.827580	1.727007
C	-2.331246	-2.164261	2.090890
H	-3.145424	-2.853585	2.355509
H	-1.796983	-2.613294	1.243272
C	-1.417566	-1.946408	3.297864
H	-1.263107	-2.858225	3.886545
H	-0.429976	-1.596589	2.956162
C	-2.112692	-0.827625	4.064177
H	-1.484106	-0.362757	4.832675
H	-3.011313	-1.221338	4.562769
C	-2.508537	0.142102	2.952577
H	-1.627709	0.745148	2.677217
H	-3.305656	0.839133	3.239362
C	2.823017	2.152951	0.080675
H	3.919507	2.158385	0.013537
C	2.373289	2.767749	1.431566
H	1.986273	2.023875	2.141072
H	3.233278	3.251733	1.914805
C	1.323886	3.817067	1.065179
H	0.343575	3.330004	0.937880
H	1.212888	4.594684	1.830067
C	1.811503	4.342696	-0.279421
H	2.685645	4.993877	-0.128327
H	1.057329	4.922481	-0.824980
C	2.222762	3.067042	-1.013427
H	2.924764	3.244043	-1.837463
H	1.322215	2.600619	-1.445446
C	2.961746	-0.094382	-1.746818
H	2.612754	0.718732	-2.403445
C	2.392897	-1.421831	-2.315049
H	1.995375	-2.076214	-1.528731
H	1.548724	-1.207741	-2.982740
C	3.564802	-2.085802	-3.063218
H	3.993837	-2.890089	-2.448349
H	3.259202	-2.539694	-4.012556
C	4.603731	-0.978128	-3.232573
H	5.615022	-1.356858	-3.422584
H	4.329773	-0.326069	-4.075322
C	4.481560	-0.200718	-1.925636
H	4.977119	0.778371	-1.942376
H	4.933454	-0.789734	-1.114117
C	3.175747	-0.497576	1.236179

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C	4.645781	-0.113116	1.538892
H	5.138230	0.385812	0.696399
H	4.679738	0.594865	2.376588
C	5.353888	-1.438626	1.885728
H	5.955315	-1.775004	1.028982
H	6.038720	-1.343157	2.735927
C	4.226857	-2.442018	2.129683
H	4.548402	-3.485111	2.028780
H	3.818705	-2.317023	3.143546
C	3.177152	-2.026906	1.105256
H	2.182835	-2.460719	1.273116
H	3.508122	-2.335147	0.101740
P	-2.325643	-0.088222	0.157161
P	2.255053	0.397680	-0.104624
Pt	-0.032633	0.132732	0.011194

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b E=-842.571935 G=-842.516566

C	1.669631	0.318878	0.051599
C	1.266175	-1.007481	0.009727
C	-0.079918	-1.320639	-0.079300
C	-1.066044	-0.330795	-0.142209
C	-0.631813	0.996998	-0.116644
C	0.714115	1.319217	-0.009919
O	-2.341570	-0.725272	-0.276652
C	-3.352992	-0.029806	0.466580
H	-4.182010	-0.731959	0.571788
H	-2.983005	0.245163	1.460452
H	-3.694546	0.860333	-0.068733
F	-1.511462	1.997853	-0.217982
F	1.088613	2.596273	0.014238
F	2.175026	-1.977726	0.069840
F	-0.437818	-2.603943	-0.103806
F	2.960886	0.626477	0.145566

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1-b E=-2819.546262 G=-2818.749236

C	0.911114	3.111530	1.597850
C	1.722427	3.527521	0.539529
C	1.191170	4.104666	-0.604301
C	-1.005774	3.886570	0.321368
C	-0.463477	3.325582	1.467921
C	-3.282746	0.876957	-0.048338
H	-2.813624	1.535806	0.696552
C	-4.821559	0.915677	0.133589
H	-5.239765	0.001758	0.572085
H	-5.078084	1.735013	0.819806
C	-5.382370	1.221642	-1.255101
H	-5.456646	0.296630	-1.848359
H	-6.382032	1.670176	-1.223351
C	-4.320230	2.131584	-1.861667
H	-4.418880	2.265258	-2.945131
H	-4.382115	3.127123	-1.397461
C	-3.014070	1.447962	-1.461388
H	-2.146018	2.119560	-1.473463
H	-2.789552	0.642511	-2.177521
C	-3.264411	-1.946632	-0.920908
H	-3.415192	-1.364928	-1.843324
C	-2.398266	-3.185258	-1.286438
H	-1.930640	-3.032762	-2.268291
H	-1.571035	-3.334193	-0.581751
C	-3.362035	-4.383854	-1.293256
H	-3.143958	-5.101543	-2.091956
H	-3.285454	-4.928308	-0.340382
C	-4.751226	-3.761917	-1.398493
H	-5.557423	-4.438372	-1.090582
H	-4.952457	-3.455033	-2.435914
C	-4.627659	-2.526665	-0.513268
H	-4.621795	-2.841824	0.541280
H	-5.449678	-1.811778	-0.639417
C	-2.937483	-1.222134	1.933287
H	-4.031335	-1.317716	1.939091
C	-2.290918	-2.551933	2.404739
H	-3.074276	-3.226716	2.777750

H	-1.761969	-3.086085	1.604163
C	-1.350844	-2.159078	3.546428
H	-1.157928	-2.983660	4.242498
H	-0.380148	-1.837563	3.134146
C	-2.052078	-0.965586	4.183993
H	-1.411272	-0.389870	4.863518
H	-2.922262	-1.309901	4.762865
C	-2.509575	-0.160096	2.969877
H	-1.655857	0.419140	2.586466
H	-3.313372	0.554512	3.187969
C	2.565655	-0.227622	-2.295587
H	3.631903	-0.430897	-2.464081
C	2.301120	1.297663	-2.363824
H	2.045684	1.724136	-1.384767
H	3.203356	1.817707	-2.714107
C	1.164003	1.468398	-3.372012
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H	1.152518	2.460141	-3.840371
C	1.396150	0.327376	-4.355767
H	2.258607	0.561611	-4.997870
H	0.539603	0.128647	-5.010601
C	1.727692	-0.847454	-3.436873
H	2.256045	-1.664144	-3.944120
H	0.787879	-1.261805	-3.035422
C	2.569800	-2.711382	-0.816414
H	2.006224	-3.006071	-1.716869
C	2.092866	-3.625097	0.343319
H	1.936746	-3.070112	1.277102
H	1.122497	-4.070143	0.090444
C	3.190023	-4.695809	0.502558
H	3.821064	-4.459868	1.371381
H	2.781582	-5.698807	0.669539
C	4.031099	-4.594276	-0.769650
H	5.034596	-5.022243	-0.661169
H	3.533422	-5.121823	-1.596930
C	4.036314	-3.095193	-1.051964
H	4.388115	-2.833065	-2.057832
H	4.695206	-2.594394	-0.327088
C	3.328021	-0.120353	0.517169
H	2.835712	0.836219	0.758447
C	4.754584	0.202622	0.014011
H	5.082250	-0.480871	-0.778000
H	4.785259	1.210829	-0.417533
C	5.665528	0.075219	1.255048
H	6.277334	-0.834381	1.176227
H	6.359674	0.916546	1.357363
C	4.713705	-0.060621	2.445000
H	5.173776	-0.549030	3.311877
H	4.367144	0.933645	2.767726
C	3.543459	-0.838668	1.854500
H	2.642762	-0.851487	2.481702
H	3.847181	-1.883861	1.690613
F	3.043213	3.358713	0.616974
F	1.995775	4.485698	-1.593847
F	-2.320073	4.081441	0.235283
F	-1.287324	3.018763	2.473165
O	1.492754	2.586287	2.689254
P	-2.413662	-0.742180	0.222413
P	2.112864	-0.922879	-0.637593
Pt	-0.127158	-0.689755	-0.117719
C	-0.180550	4.270357	-0.724575
F	-0.699797	4.810693	-1.824398
C	0.944632	1.350783	3.181028
H	0.657441	0.703210	2.336468
H	1.738390	0.879455	3.765846
H	0.081666	1.541055	3.827723

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1•b-CC E=-2819.533375 G=-2818.731205

C	1.406062	-3.023668	-0.041888
C	0.472620	-3.855534	0.490695
C	-0.870105	-3.903116	0.006660
C	-0.401719	-2.036963	-1.491246
C	1.008958	-2.039138	-1.037775
C	-3.269873	-0.551438	0.450177
H	-3.054392	-1.348873	-0.271050
C	-4.808253	-0.327229	0.441653

H	-5.107758	0.708356	0.256708
H	-5.246811	-0.925315	-0.367686
C	-5.304825	-0.836013	1.802181
H	-5.349988	-0.006014	2.523367
H	-6.308739	-1.272289	1.749622
C	-4.230521	-1.823524	2.245647
H	-4.276923	-2.074538	3.311502
H	-4.321656	-2.761564	1.676061
C	-2.943111	-1.111773	1.846408
H	-2.060707	-1.764477	1.834123
H	-2.740355	-0.299539	2.563268
C	-2.362542	2.178054	1.120505
H	-1.976220	1.783843	2.073197
C	-1.567670	3.466122	0.760786
H	-0.793906	3.638980	1.520940
H	-1.050091	3.400161	-0.203865
C	-2.589852	4.606983	0.790409
H	-2.141553	5.569720	1.059954
H	-3.052304	4.726937	-0.201080
C	-3.641547	4.116580	1.776565
H	-4.579345	4.683028	1.741404
H	-3.251619	4.176900	2.803834
C	-3.807347	2.658580	1.361824
H	-4.393986	2.633622	0.432741
H	-4.334731	2.042205	2.099694
C	-2.795492	1.411288	-1.683039
H	-3.646284	2.064046	-1.436455
C	-1.775006	2.208705	-2.539598
H	-2.032029	3.276601	-2.537122
H	-0.755111	2.123954	-2.142570
C	-1.860230	1.615612	-3.955996
H	-1.735477	2.370762	-4.740342
H	-1.064240	0.869427	-4.092065
C	-3.212418	0.912601	-3.995343
H	-3.296997	0.176685	-4.803351
H	-4.019972	1.648599	-4.126934
C	-3.302013	0.290577	-2.606771
H	-2.631326	-0.580417	-2.560111
H	-4.308766	-0.050210	-2.338021
C	2.040633	0.829928	2.419322
H	2.984654	1.319649	2.690303
C	2.035096	-0.635393	2.913230
H	2.308279	-1.365017	2.140101
H	2.769939	-0.742625	3.723978
C	0.630056	-0.847013	3.466603
H	-0.071676	-1.005666	2.631039
H	0.555192	-1.711875	4.136270
C	0.330764	0.485577	4.143001
H	0.894835	0.554588	5.084650
H	-0.729680	0.631131	4.385684
C	0.850792	1.513837	3.134536
H	1.139445	2.465894	3.596589
H	0.053985	1.741333	2.412530
C	1.999642	2.768349	0.267646
H	1.156583	3.162855	0.854249
C	1.785934	3.198938	-1.208857
H	1.910017	2.369598	-1.917082
H	0.759576	3.563584	-1.343097
C	2.801404	4.326204	-1.462399
H	3.694453	3.924625	-1.962977
H	2.401587	5.116846	-2.107152
C	3.187407	4.815286	-0.068802
H	4.121013	5.389506	-0.051449
H	2.393420	5.457527	0.341285
C	3.261592	3.516144	0.726924
H	3.294450	3.660235	1.814071
H	4.172385	2.974269	0.435263
C	3.504754	0.197877	-0.003033
H	3.258732	-0.870409	-0.039238
C	4.779539	0.326457	0.865201
H	4.802847	1.244306	1.463728
H	4.831811	-0.507185	1.578051
C	5.952434	0.296971	-0.139787
H	6.392385	1.300556	-0.227540
H	6.758746	-0.376413	0.171733
C	5.328511	-0.094327	-1.480751

H	5.930466	0.213925	-2.343351
H	5.197072	-1.186923	-1.538507
C	3.956852	0.567576	-1.420042
H	3.257761	0.221604	-2.190454
H	4.071730	1.656642	-1.529734
F	0.775813	-4.670947	1.515920
F	-1.722694	-4.766843	0.579852
F	-0.580103	-1.825867	-2.846922
F	1.952539	-1.917104	-2.048080
O	2.700944	-3.034975	0.376937
P	-2.092352	0.782063	-0.084949
P	1.901982	0.941988	0.571099
Pt	0.063194	-0.299265	-0.372779
C	-1.265643	-3.077281	-0.988135
F	-2.488132	-3.205188	-1.530097
C	3.499158	-4.095639	-0.151196
H	4.509510	-3.945488	0.237613
H	3.127646	-5.074741	0.176072
H	3.521931	-4.058820	-1.247261

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TS_{oa}1b E=-2819.460940 G=-2818.671126

C	3.091891	-1.109300	0.099697
C	4.289454	-0.361437	0.143008
C	5.542106	-0.936481	0.015867
C	4.516290	-3.078267	-0.265947
C	3.270484	-2.491518	-0.130142
C	1.216136	-0.314343	-1.633729
H	0.344142	0.173772	-2.075384
H	1.265733	-1.386121	-1.802287
H	2.140939	0.234818	-1.801071
C	-1.209376	-3.223602	0.001505
H	-0.372267	-3.192574	-0.712866
C	-1.958523	-4.571829	-0.178651
H	-3.033960	-4.453457	-0.353013
H	-1.558626	-5.095181	-1.056692
C	-1.672368	-5.374183	1.099948
H	-2.481097	-5.221042	1.830322
H	-1.605131	-6.452691	0.916986
C	-0.384942	-4.764922	1.647083
H	-0.194285	-5.017118	2.696670
H	0.476180	-5.115414	1.058470
C	-0.596108	-3.273059	1.412548
H	0.316851	-2.668163	1.478763
H	-1.304516	-2.889124	2.163275
C	-3.466507	-1.540093	0.923025
H	-2.924978	-1.415266	1.877677
C	-4.391298	-0.327689	0.773394
H	-3.865328	0.632945	0.862552
H	-4.874167	-0.351850	-0.215363
C	-5.430643	-0.567741	1.866531
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H	-6.366517	-0.026462	1.688180
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H	-5.594431	-2.470368	2.935932
C	-4.466106	-2.692075	1.070226
H	-4.836320	-2.989989	0.078409
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C	-2.921703	-1.925035	-1.973617
H	-3.688230	-2.701764	-1.839210
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H	-3.569285	0.040376	-4.665451
H	-2.022216	0.205624	-3.824027
C	-2.459588	-1.839913	-4.344381
H	-1.725127	-1.848793	-5.158149
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C	-0.586212	1.608837	4.349278
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C	-1.931580	3.627476	-1.317054
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C	3.165756	4.745557	-0.735545
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F	4.623863	-4.394982	-0.469197
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C	-1.601618	-3.610232	1.452917
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C	-1.552996	-3.025463	2.859239
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H	-2.483079	-3.261901	3.398035
C	-1.474219	-1.526247	2.589136
H	-0.450527	-1.270906	2.270519
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F	2.955260	2.137413	-1.445239
F	5.015206	2.639283	0.224086
F	5.129682	-1.893458	1.470424
F	3.092008	-2.415315	-0.225741
O	1.941414	-0.464109	-1.707243
P	-1.964845	0.093328	0.331618
Pt	-0.040604	-0.181308	-0.695063
C	5.098000	0.377901	0.863826
F	6.105188	0.630624	1.692687
C	2.057399	-0.129452	-3.112318
H	3.092661	-0.279310	-3.434830
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H	3.833346	-0.088099	1.991133
C	5.206240	-1.700258	1.491455
H	5.561471	-1.932180	0.481000
H	5.921581	-0.982214	1.913305
C	5.123588	-2.951378	2.374371
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C	2.950947	-1.994182	2.444080
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H	2.452797	-2.790464	1.869434
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H	2.601102	-3.071442	-0.249780
C	1.834399	-2.375752	-2.153095
H	1.005482	-3.032131	-1.855739
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H	4.475616	-4.008373	-3.532069
H	3.312163	-4.701547	-2.387550
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H	4.849237	-3.385900	-0.960267
C	4.190656	0.345053	-0.960816
H	5.131319	-0.218476	-1.034778
C	3.739530	0.791178	-2.378373
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H	2.756967	0.391140	-2.662786
C	3.733541	2.324669	-2.342563
H	3.942857	2.773272	-3.320233
H	2.744364	2.686932	-2.020257
C	4.762294	2.670157	-1.273042
H	4.700397	3.706877	-0.922253

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H	0.172990	4.297061	2.855234
C	0.722160	2.394855	3.733970
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H	1.370289	2.918441	4.446139
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C	-1.430349	1.624661	3.067012
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H	-1.149279	0.607838	2.749206
C	-2.532454	1.354898	-0.073686
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C	-2.656780	0.477736	-1.348802
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C	-4.606517	-2.821670	-1.066199
C	-5.382432	-2.052805	-0.209876
C	-4.856334	-1.679378	1.018742
C	-3.575268	-2.066124	1.374861
C	-2.746774	-2.848266	0.540751
C	-3.325034	-3.197055	-0.699600
O	-1.532208	-3.182769	0.863594
F	-3.106605	-1.675061	2.571405
F	-5.590071	-0.934486	1.852716
F	-6.616389	-1.677517	-0.565184
F	-5.099736	-3.178606	-2.256475
F	-2.602594	-3.918411	-1.569362

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1b·OAr E=-2819.545096 G=-2818.749073

C	-0.161259	0.450764	1.534051
H	-0.505485	1.428913	1.174760
H	0.916949	0.489779	1.714949
H	-0.682970	0.189937	2.466230
C	-3.788642	0.491902	1.172037
H	-3.693841	-0.371628	1.848687
C	-5.287701	0.692965	0.830470
H	-5.439440	0.970912	-0.219316
H	-5.839165	-0.242510	0.985699
C	-5.776390	1.819217	1.763888
H	-5.895859	2.748623	1.190260
H	-6.748025	1.596750	2.218262
C	-4.660529	2.003129	2.790514

H	-4.668779	2.990532	3.265065	P	1.473436	-2.047930	0.338564
H	-4.746622	1.250382	3.588141	Pt	-0.628198	-0.978876	0.150769
C	-3.399799	1.742062	1.974984	C	2.713549	4.061522	-0.776686
H	-2.498458	1.601168	2.581805	C	3.473457	3.710237	0.331678
H	-3.210027	2.596573	1.309099	C	2.804706	3.403361	1.509771
C	-2.443801	1.624436	-1.215848	C	1.424307	3.451812	1.574006
H	-2.143376	2.352198	-0.445204	C	0.580804	3.796340	0.471056
C	-1.272371	1.573126	-2.236429	C	1.333323	4.091870	-0.708724
H	-0.410720	2.099970	-1.805376	O	-0.682710	3.830068	0.532997
H	-0.928408	0.553601	-2.458215	F	0.658762	4.454706	-1.822636
C	-1.795373	2.288276	-3.491549	F	3.337994	4.369094	-1.926307
H	-1.021035	2.882268	-3.989777	F	4.819649	3.679575	0.268863
H	-2.159773	1.549896	-4.221560	F	3.518332	3.061702	2.597130
C	-2.971428	3.124760	-2.995649	F	0.842305	3.179932	2.763486
H	-3.643874	3.450692	-3.797735	91			
H	-2.601833	4.023918	-2.481270	1b+	E=-2016.683735	G=-2015.928908	
C	-3.642309	2.200859	-1.983191	C	-0.331327	0.773358	-2.048919
H	-4.192176	1.410105	-2.517687	H	-0.984658	0.044906	-2.546833
H	-4.353848	2.714117	-1.323861	H	0.616778	0.828206	-2.591627
C	-3.694191	-1.133448	-1.252445	H	-0.810999	1.761896	-2.048727
H	-4.631639	-0.637849	-1.532172	C	-3.546928	1.211433	-0.350400
C	-2.930990	-1.640223	-2.480402	H	-3.015132	2.136252	-0.074039
H	-3.651721	-2.107485	-3.167476	C	-4.933196	1.210135	0.337020
H	-2.404814	-0.861516	-3.044757	H	-5.244285	0.197288	0.619765
C	-2.027919	-2.726567	-1.918321	H	-4.903927	1.796585	1.262807
H	-1.583290	-3.377068	-2.681475	C	-5.909695	1.797533	-0.705502
H	-1.135711	-2.265582	-1.415874	H	-6.582453	1.008250	-1.066814
C	-2.921823	-3.464435	-0.921885	H	-6.542405	2.588109	-0.288597
H	-2.354813	-3.915274	-0.098715	C	-5.033455	2.286326	-1.859670
H	-3.433233	-4.284327	-1.440980	H	-5.562523	2.315787	-2.818512
C	-3.951122	-2.421006	-0.429821	H	-4.660562	3.300556	-1.657089
H	-3.870545	-2.255743	0.652321	C	-3.866410	1.306119	-1.847818
H	-4.974789	-2.769175	-0.609970	H	-3.011190	1.624938	-2.453819
C	1.690760	-3.108802	1.835977	H	-4.208091	0.333046	-2.233052
H	2.653377	-3.623003	1.717145	C	-2.946442	-1.682334	-0.697866
C	0.539342	-4.137188	1.954196	H	-3.075880	-1.357371	-1.740712
H	-0.006529	-4.295928	1.014288	C	-1.900985	-2.835743	-0.696343
H	0.956320	-5.110968	2.244950	H	-1.433317	-2.902913	-1.687706
C	-0.345772	-3.600984	3.075566	H	-1.076972	-2.674202	0.012025
H	-0.988417	-2.790373	2.690699	C	-2.700006	-4.106356	-0.368651
H	-0.999644	-4.367304	3.507402	H	-2.323144	-4.989098	-0.896157
C	0.669916	-3.035050	4.060782	H	-2.637591	-4.321538	0.708072
H	1.168124	-3.862255	4.586794	C	-4.141700	-3.755618	-0.724735
H	0.229651	-2.379385	4.820642	H	-4.878252	-4.430816	-0.275154
C	1.667099	-2.301903	3.159362	H	-4.280963	-3.788787	-1.815261
H	2.667388	-2.219173	3.599451	C	-4.267711	-2.316580	-0.234959
H	1.311834	-1.276001	2.995799	H	-4.343215	-2.312663	0.862668
C	2.865060	-0.839201	0.364909	H	-5.144940	-1.787640	-0.628431
H	2.784594	-0.382184	1.364782	C	-2.661261	-0.311401	1.983620
C	2.735998	0.298859	-0.685733	H	-3.723965	-0.526765	2.146301
H	2.056517	0.043230	-1.508753	C	-1.757933	-1.386119	2.596593
H	2.315741	1.195012	-0.210502	H	-2.149469	-1.641598	3.591931
C	4.168469	0.547966	-1.188627	H	-1.699123	-2.318217	2.023089
H	4.326887	0.035229	-2.148338	C	-0.427772	-0.673300	2.773799
H	4.378180	1.610744	-1.356218	H	0.285371	-1.206143	3.414806
C	5.065455	-0.086162	-0.128604	H	0.111628	-0.610335	1.787790
H	6.087845	-0.273048	-0.475801	C	-0.825902	0.703515	3.301590
H	5.125581	0.567410	0.755791	H	-0.094719	1.482328	3.054105
C	4.302839	-1.358427	0.228913	H	-0.883445	0.657637	4.395921
H	4.660199	-1.857310	1.138254	C	-2.223671	0.988431	2.706702
H	4.388712	-2.072473	-0.603029	H	-2.205917	1.858541	2.037760
C	1.685037	-3.225056	-1.074939	H	-2.943879	1.225541	3.497964
H	0.706958	-3.731744	-1.118720	C	2.875354	2.170145	0.011409
C	2.771649	-4.322994	-0.964916	H	3.968824	2.115730	0.093729
H	3.595604	-4.036574	-0.301554	C	2.271126	2.835409	1.272923
H	2.339012	-5.237659	-0.541375	H	1.858894	2.118768	1.996319
C	3.277531	-4.535958	-2.407931	H	3.060091	3.391380	1.797021
H	4.274125	-4.087647	-2.521517	C	1.226106	3.809801	0.736390
H	3.373970	-5.595793	-2.667096	H	0.301613	3.264983	0.476207
C	2.286990	-3.788596	-3.301657	H	0.960591	4.590970	1.457687
H	2.706188	-3.517290	-4.276782	C	1.886517	4.340694	-0.530087
H	1.393342	-4.404603	-3.483707	H	2.693574	5.035518	-0.257157
C	1.906325	-2.583205	-2.450342	H	1.200843	4.877118	-1.195570
H	1.028243	-2.032153	-2.813899	C	2.468350	3.080397	-1.174654
H	2.750843	-1.878932	-2.420063	H	3.316124	3.284492	-1.838556
P	-2.690553	0.073876	-0.258033	H	1.692061	2.605186	-1.789768

C	3.028140	-0.184963	-1.745540
H	2.773102	0.600580	-2.474368
C	2.431309	-1.523881	-2.257664
H	1.940233	-2.097437	-1.460408
H	1.656429	-1.323236	-3.007905
C	3.621121	-2.295689	-2.857992
H	3.965983	-3.061958	-2.149497
H	3.361026	-2.813595	-3.787387
C	4.719889	-1.249638	-3.037633
H	5.721799	-1.684137	-3.126174
H	4.534330	-0.653661	-3.943347
C	4.550946	-0.370828	-1.802592
H	5.090745	0.583009	-1.851955
H	4.914305	-0.917875	-0.921220
C	3.012492	-0.458252	1.267288
H	2.358204	-0.150683	2.098729
C	4.468893	-0.123996	1.678226
H	5.061847	0.284639	0.852547
H	4.465619	0.642659	2.462680
C	5.062637	-1.457044	2.177985
H	5.737215	-1.871927	1.416210
H	5.651229	-1.337189	3.093755
C	3.867023	-2.393401	2.351908
H	4.143189	-3.453450	2.336786
H	3.360792	-2.195273	3.308798
C	2.951804	-1.990423	1.201302
H	1.928426	-2.382246	1.281021
H	3.374157	-2.357640	0.254376
P	-2.388630	-0.142289	0.153644
P	2.278311	0.432491	-0.178650
Pt	-0.074783	0.203514	-0.103517

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1b+' E=-2016.678913 G=-2015.923914

C	-0.211228	0.638093	-2.234894
H	-0.569989	-0.269782	-2.737050
H	0.747222	0.944068	-2.664043
H	-0.943560	1.446873	-2.353915
C	-3.234185	1.482237	0.482796
H	-2.619566	1.904254	1.291183
C	-4.710717	1.384827	0.947652
H	-5.042426	0.362559	1.162069
H	-4.824630	1.950952	1.881346
C	-5.517063	2.059419	-0.161209
H	-5.700589	1.349667	-0.983222
H	-6.491528	2.423346	0.182589
C	-4.582693	3.163479	-0.642052
H	-4.883747	3.614322	-1.594021
H	-4.543212	3.965912	0.108933
C	-3.232627	2.453818	-0.721554
H	-2.372759	3.134289	-0.699888
H	-3.175572	1.902521	-1.672662
C	-3.412224	-1.031435	-1.120278
H	-3.686850	-0.263319	-1.859012
C	-2.651976	-2.170984	-1.859855
H	-2.546463	-1.904522	-2.919084
H	-1.634311	-2.326078	-1.478227
C	-3.530878	-3.417172	-1.707360
H	-3.443396	-4.099721	-2.559463
H	-3.239993	-3.978901	-0.807797
C	-4.934780	-2.855421	-1.518312
H	-5.650785	-3.584745	-1.123326
H	-5.325610	-2.490900	-2.479670
C	-4.703688	-1.677332	-0.576609
H	-4.553983	-2.053816	0.446306
H	-5.540965	-0.970670	-0.546369
C	-2.289672	-0.988482	1.713614
H	-3.241677	-0.866116	2.249346
C	-1.917445	-2.493914	1.639317
H	-2.778011	-3.100618	1.944445
H	-1.653920	-2.814916	0.624142
C	-0.728940	-2.686279	2.599596
H	-0.778423	-3.634192	3.145386
H	0.214992	-2.690914	2.032639
C	-0.757084	-1.463837	3.509817
H	0.194751	-1.273072	4.019920
H	-1.532584	-1.573947	4.281730

C	-1.164301	-0.351153	2.556252
H	-0.268102	-0.112846	1.925007
H	-1.453393	0.591535	3.035248
C	2.737900	2.130072	0.501325
H	3.832071	2.133027	0.593275
C	2.085599	2.443478	1.872644
H	1.682705	1.559560	2.385446
H	2.847565	2.868747	2.539247
C	1.019973	3.494829	1.572449
H	0.107306	3.006384	1.190816
H	0.739191	4.080904	2.454783
C	1.660781	4.321048	0.464074
H	2.451938	4.955034	0.889642
H	0.957561	4.977938	-0.060253
C	2.270473	3.258689	-0.451510
H	3.090071	3.637041	-1.073057
H	1.489754	2.891299	-1.135652
C	3.233341	0.265798	-1.689607
H	2.976033	1.172136	-2.260451
C	2.859038	-0.971863	-2.551703
H	2.251261	-1.705066	-2.006113
H	2.255458	-0.652076	-3.409510
C	4.198762	-1.566182	-3.015635
H	4.493884	-2.395051	-2.355939
H	4.148932	-1.967699	-4.033461
C	5.198431	-0.423386	-2.862024
H	6.242534	-0.755443	-2.854083
H	5.082856	0.295691	-3.686313
C	4.764296	0.223088	-1.550997
H	5.199271	1.214172	-1.374294
H	5.063705	-0.427737	-0.717265
C	2.844136	-0.730576	1.152674
H	2.032670	-0.685361	1.899100
C	4.176088	-0.443501	1.892216
H	4.851192	0.200413	1.317173
H	3.972841	0.084675	2.831453
C	4.804828	-1.830012	2.139277
H	5.621602	-2.000288	1.424071
H	5.233648	-1.923938	3.142651
C	3.685205	-2.834174	1.867023
H	4.052737	-3.842459	1.647365
H	3.014574	-2.905845	2.737382
C	2.937869	-2.194818	0.702776
H	1.954962	-2.640009	0.496131
H	3.543339	-2.284490	-0.211120
P	-2.376053	-0.104786	0.094488
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Pt	-0.071302	0.218078	-0.247667

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1:THF E=-2209.264524 G=-2208.439257

C	3.274773	-0.576228	1.518729
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C	4.784276	-0.270310	1.699871
H	5.215852	0.326441	0.888215
H	4.924393	0.312283	2.620976
C	5.454255	-1.636854	1.850024
H	5.658930	-2.069288	0.857696
H	6.407732	-1.590248	2.388963
C	4.388799	-2.470517	2.552963
H	4.589761	-3.547992	2.537506
H	4.316204	-2.160849	3.606485
C	3.113562	-2.086225	1.806299
H	2.191996	-2.297933	2.362624
H	3.053420	-2.662465	0.870139
C	3.469748	-0.829710	-1.435117
H	3.570455	-1.885275	-1.135349
C	2.728521	-0.792316	-2.798280
H	2.166687	-1.722912	-2.945130
H	1.986603	0.015694	-2.836418
C	3.820689	-0.591616	-3.867045
H	3.681339	-1.236953	-4.741620
H	3.801265	0.445364	-4.231038
C	5.140736	-0.845780	-3.141556
H	6.003284	-0.382124	-3.634984
H	5.337902	-1.926305	-3.079240
C	4.876354	-0.298774	-1.742257

H	4.883553	0.801694	-1.771794
H	5.623049	-0.615257	-1.004219
C	2.812515	1.743730	-0.137018
H	3.905618	1.885243	-0.109472
C	2.259965	2.473361	-1.362488
H	2.787041	2.228042	-2.293981
H	1.199983	2.202141	-1.496556
C	2.392461	3.943171	-0.965909
H	3.426366	4.272233	-1.141177
H	1.745221	4.603303	-1.557131
C	2.072750	3.977696	0.540655
H	1.058571	4.357853	0.722050
H	2.763879	4.638702	1.076981
C	2.178656	2.517102	1.030257
H	1.168555	2.120274	1.222603
H	2.758262	2.418029	1.956708
C	-2.535644	-0.948885	2.031324
H	-3.629858	-1.035518	2.078374
C	-2.078494	0.368107	2.713639
H	-1.702591	1.114778	1.999616
H	-2.930297	0.820610	3.241630
C	-1.006080	-0.053845	3.718794
H	-0.034788	-0.134846	3.204440
H	-0.889219	0.658509	4.544192
C	-1.461508	-1.438999	4.161473
H	-2.326304	-1.348839	4.836323
H	-0.687845	-2.009467	4.689522
C	-1.884625	-2.089934	2.845580
H	-2.560396	-2.943987	2.977946
H	-0.985706	-2.461663	2.327738
C	-2.688550	-2.635823	-0.324215
H	-2.273040	-3.326131	0.427775
C	-2.154603	-3.086203	-1.707598
H	-1.870900	-2.234211	-2.338157
H	-1.242891	-3.682327	-1.579441
C	-3.297731	-3.900541	-2.346832
H	-3.793650	-3.303110	-3.124992
H	-2.944916	-4.818785	-2.829500
C	-4.286006	-4.164458	-1.210249
H	-5.299639	-4.390866	-1.561859
H	-3.948320	-5.017462	-0.603181
C	-4.200112	-2.886329	-0.381698
H	-4.657165	-2.969215	0.612790
H	-4.712050	-2.073448	-0.917935
C	-3.086025	0.351101	-0.503631
H	-2.508949	1.254327	-0.245348
C	-4.536627	0.566568	-0.009633
H	-4.983978	-0.344156	0.405762
H	-4.551726	1.311543	0.797271
C	-5.325507	1.047181	-1.247584
H	-5.987399	0.244747	-1.602478
H	-5.964786	1.911069	-1.030480
C	-4.272243	1.341978	-2.317784
H	-4.670300	1.290071	-3.337895
H	-3.856217	2.351646	-2.177843
C	-3.189259	0.308185	-2.033050
H	-2.228816	0.512726	-2.524500
H	-3.531847	-0.680885	-2.374297
P	2.458783	-0.071902	-0.071775
P	-2.044689	-0.992102	0.243783
Pt	0.216112	-0.617964	-0.042408
C	-1.412404	3.663491	-0.801038
O	-1.205852	3.118628	0.501143
C	-1.884464	3.919591	1.469689
C	-2.332592	5.173317	0.738907
C	-2.579212	4.623250	-0.661199
H	-1.202286	4.112750	2.309008
H	-3.211011	5.639026	1.196206
H	-1.522434	5.915605	0.715839
H	-3.531867	4.071375	-0.687376
H	-2.601484	5.387175	-1.444568
H	-1.590614	2.836350	-1.503040
H	-0.501036	4.194978	-1.128879
H	-2.751667	3.358753	1.859213

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TS_{SN21b}-THF E=-3051.818117 G=-3050.911014

C	1.172506	-1.888589	0.307098
H	1.330138	-1.610561	-0.729220
H	0.472172	-2.677687	0.541341
H	1.593698	-1.307947	1.117409
C	1.662228	2.030568	1.807750
H	0.746630	2.206997	2.391824
C	2.600261	3.260127	1.958622
H	2.804861	3.778826	1.015854
H	2.123069	3.995556	2.619797
C	3.878508	2.720435	2.608475
H	4.578235	2.372583	1.831535
H	4.404819	3.474175	3.204841
C	3.397241	1.520394	3.414992
H	4.207254	0.854771	3.737729
H	2.864525	1.861577	4.315242
C	2.421317	0.853732	2.451436
H	1.745262	0.129238	2.924813
H	3.004681	0.309335	1.691824
C	2.471568	1.321858	-0.967185
H	3.023812	0.517484	-0.453407
C	2.074488	0.798946	-2.377876
H	2.276126	-0.278839	-2.442189
H	1.004576	0.921412	-2.589659
C	2.945442	1.579639	-3.374587
H	3.256017	0.969530	-4.230429
H	2.382083	2.435309	-3.775241
C	4.115521	2.096940	-2.544185
H	4.649379	2.930385	-3.015265
H	4.847627	1.293275	-2.375914
C	3.453620	2.478046	-1.224252
H	2.917374	3.429647	-1.356216
H	4.166577	2.612025	-0.400651
C	0.288590	3.245162	-0.423255
H	1.105427	3.985168	-0.437467
C	-0.390341	3.245047	-1.793228
H	0.312696	3.135048	-2.629300
H	-1.104430	2.406643	-1.842252
C	-1.129388	4.585056	-1.806250
H	-0.447061	5.374048	-2.150209
H	-1.981591	4.582970	-2.496582
C	-1.541942	4.841144	-0.341058
H	-2.628660	4.768039	-0.207275
H	-1.244826	5.848255	-0.024278
C	-0.826486	3.763169	0.494183
H	-1.529685	2.942598	0.707887
H	-0.447676	4.143643	1.450842
C	-2.944477	-1.687159	2.159769
H	-3.852836	-2.306112	2.177972
C	-3.254645	-0.291323	2.766494
H	-3.092298	0.527396	2.050743
H	-4.308517	-0.247428	3.073183
C	-2.332956	-0.159681	3.984337
H	-1.374447	0.286199	3.675777
H	-2.754717	0.477720	4.769952
C	-2.096979	-1.600341	4.421342
H	-2.994695	-1.992419	4.922761
H	-1.252801	-1.718616	5.110444
C	-1.888239	-2.316256	3.090203
H	-1.982763	-3.407007	3.155469
H	-0.872982	-2.091814	2.723441
C	-2.099134	-3.336303	-0.078340
H	-1.410784	-3.691325	0.705362
C	-1.403154	-3.546403	-1.454673
H	-1.341637	-2.627214	-2.051037
H	-0.367976	-3.876601	-1.296526
C	-2.208808	-4.648316	-2.155638
H	-2.994745	-4.203364	-2.785378
H	-1.588926	-5.275074	-2.806199
C	-2.863240	-5.412679	-1.009567
H	-3.686328	-6.062565	-1.328675
H	-2.116685	-6.042206	-0.502630
C	-3.309650	-4.286506	-0.082600
H	-3.585818	-4.618784	0.925893
H	-4.190354	-3.800046	-0.522732
C	-3.860259	-0.898947	-0.490271
H	-3.821303	0.170089	-0.227685

C	-5.278766	-1.430147	-0.142534
H	-5.276561	-2.323898	0.491410
H	-5.825212	-0.658716	0.417747
C	-5.958776	-1.693589	-1.494771
H	-5.826118	-2.747080	-1.785513
H	-7.037340	-1.499699	-1.471464
C	-5.199831	-0.808845	-2.479131
H	-5.360421	-1.084063	-3.527869
H	-5.512487	0.240388	-2.358075
C	-3.754072	-0.971912	-2.024290
H	-3.063625	-0.216535	-2.423818
H	-3.389227	-1.955667	-2.353120
P	0.995756	1.627042	0.121469
P	-2.377878	-1.565473	0.403068
Pt	-0.587591	-0.097851	0.193444
C	-4.423631	2.820795	-1.588428
O	-3.758531	2.451710	-0.380297
C	-4.606584	2.728289	0.735902
C	-5.765908	3.545208	0.191984
C	-5.885838	2.984087	-1.220218
H	-4.020981	3.247098	1.507924
H	-6.675298	3.439734	0.791409
H	-5.500662	4.610841	0.153969
H	-6.387349	2.004629	-1.197948
H	-6.429822	3.633117	-1.913302
H	-4.231915	2.046115	-2.343401
H	-4.006946	3.772273	-1.962704
H	-4.962232	1.774455	1.164006
C	5.570149	-0.931617	0.684923
C	5.925507	-0.714549	-0.639333
C	5.189433	-1.331716	-1.642074
C	4.109098	-2.135376	-1.318623
C	3.708067	-2.387216	0.010491
C	4.494080	-1.748222	0.993436
O	2.660136	-3.101312	0.303188
F	3.415052	-2.697716	-2.319906
F	5.520649	-1.136743	-2.922889
F	6.967171	0.068025	-0.943364
F	6.271461	-0.345607	1.660873
F	4.190959	-1.936778	2.286510

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a E=-759.425487 G=-759.371843

C	1.744035	-0.279801	0.007446
C	0.645805	-1.111460	-0.011893
C	-0.646699	-0.560906	-0.022337
C	-0.706600	0.839479	-0.017058
C	0.478570	1.557632	0.004986
O	-1.650796	-1.424860	-0.043783
C	-3.015274	-0.989595	0.069665
H	-3.600294	-1.908733	0.112356
H	-3.165200	-0.417380	0.989198
H	-3.313758	-0.407042	-0.805688
F	-1.867141	1.504223	-0.041259
F	0.400026	2.887376	0.011350
F	2.959288	-0.823871	0.020061
F	0.792581	-2.436063	-0.018164
N	1.674831	1.030708	0.017379

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TS_{SN2}1a E=-2736.363361 G=-2735.570728

C	-0.440870	-1.823972	0.201166
H	-0.890467	-1.429485	-0.702096
H	-0.742796	-1.467390	1.177708
H	0.455908	-2.422990	0.118851
C	3.575156	-1.099459	1.582734
H	3.554053	-0.151296	2.139458
C	5.007291	-1.694806	1.644567
H	5.510357	-1.737366	0.671755
H	5.632297	-1.062095	2.289048
C	4.839859	-3.078846	2.277335
H	4.605052	-3.823473	1.501009
H	5.741718	-3.422690	2.796362
C	3.630883	-2.907985	3.190263
H	3.207515	-3.855152	3.543338
H	3.913873	-2.318094	4.074812
C	2.667965	-2.109323	2.316935
H	1.863940	-1.611901	2.873920

H	2.185051	-2.795902	1.604897
C	3.050223	-2.124001	-1.158544
H	2.691753	-2.938287	-0.509319
C	2.129002	-2.066680	-2.413886
H	1.306397	-2.784530	-2.297288
H	1.660429	-1.083115	-2.549847
C	3.017648	-2.460062	-3.599607
H	2.464178	-2.982678	-4.387653
H	3.462293	-1.562333	-4.054367
C	4.120884	-3.300133	-2.967897
H	4.993932	-3.440302	-3.615872
H	3.733032	-4.296982	-2.710065
C	4.438994	-2.522781	-1.694349
H	5.030802	-1.634368	-1.959961
H	5.021683	-3.098133	-0.965305
C	4.170026	0.598823	-0.682488
H	5.137444	0.080305	-0.727989
C	3.833457	1.196201	-2.075952
H	4.654044	0.981373	-2.773731
H	2.920384	0.775516	-2.517905
C	3.707366	2.707138	-1.851067
H	3.955996	3.292235	-2.743776
H	2.671688	2.957378	-1.570535
C	4.623111	2.973933	-0.663163
H	4.464812	3.952889	-0.196004
H	5.675193	2.922656	-0.981803
C	4.302291	1.808529	0.267491
H	3.341332	2.006402	0.772947
H	5.055307	1.644241	1.047722
C	-1.251717	2.394282	2.031136
H	-2.088586	3.106171	2.027592
C	0.024584	3.090012	2.577413
H	0.814633	3.201943	1.821823
H	-0.231557	4.101086	2.920950
C	0.481244	2.231588	3.759435
H	1.127950	1.415470	3.399117
H	1.051329	2.800695	4.502749
C	-0.819229	1.646832	4.296997
H	-1.384513	2.424683	4.831994
H	-0.674610	0.807459	4.986938
C	-1.554502	1.248686	3.019947
H	-2.630896	1.087747	3.159532
H	-1.127508	0.302758	2.647997
C	-2.712616	1.116677	-0.121589
H	-2.869612	0.368223	0.673701
C	-2.810454	0.383511	-1.488805
H	-1.932551	0.540882	-2.128428
H	-2.875715	-0.699789	-1.317818
C	-4.105546	0.890408	-2.139823
H	-3.886949	1.734367	-2.811411
H	-4.604002	0.119951	-2.739910
C	-4.945955	1.386675	-0.967486
H	-5.768520	2.045745	-1.268276
H	-5.386616	0.531344	-0.432398
C	-3.910391	2.082783	-0.089584
H	-4.256479	2.287083	0.931391
H	-3.650205	3.045596	-0.550965
C	-0.721473	3.341528	-0.669851
H	0.345396	3.521825	-0.461799
C	-1.490216	4.642888	-0.315780
H	-2.392170	4.468988	0.281312
H	-0.845187	5.294564	0.287148
C	-1.827245	5.295379	-1.668628
H	-2.861136	5.050730	-1.954280
H	-1.752587	6.388198	-1.641829
C	-0.870856	4.642942	-2.664476
H	-1.185195	4.758094	-3.708015
H	0.135482	5.078628	-2.568071
C	-0.846521	3.193529	-2.193831
H	-0.036778	2.588957	-2.623140
H	-1.797983	2.713470	-2.466210
P	2.912549	-0.614125	-0.077604
P	-1.034265	1.787275	0.297310
Pt	0.829448	0.392292	0.072927
C	-4.958664	-2.918179	-0.913879
C	-4.753796	-1.880654	1.051744

C -3.439015 -2.266111 1.192995
 C -2.798574 -3.022031 0.181504
 C -3.650843 -3.353346 -0.898761
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 F -2.750927 -1.919732 2.293295
 F -5.308663 -1.128962 2.011740
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1a E=-2736.429957 G=-2735.634285
 C -0.797040 2.220374 -0.717193
 C -0.476862 2.952376 0.460310
 C -1.034783 4.189941 0.691299
 C -2.165626 4.170419 -1.224576
 C -1.683721 2.931876 -1.574511
 C 0.831602 -2.061320 1.646448
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 H -0.004198 -2.499757 2.203371
 H 1.529573 -1.645365 2.388105
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 H 2.692125 1.881217 0.936592
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 H 5.282717 0.954280 -0.125496
 H 4.796175 2.539790 0.451210
 C 5.573547 1.264072 2.027445
 H 6.032005 0.263664 2.041982
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 H 3.429145 -2.128645 0.910952
 C 3.014110 -2.837467 -1.094961
 H 2.537930 -3.644921 -0.522869
 H 2.246693 -2.459248 -1.780850
 C 4.246305 -3.360415 -1.844135
 H 4.157621 -4.417597 -2.117792
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 H 5.399911 -3.776943 -0.061192
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 H 5.282144 -0.946131 -1.199730
 H 5.636632 -1.358425 0.485863
 C 2.843595 0.518678 -1.839899
 H 3.898178 0.314787 -2.080395
 C 1.954047 -0.080608 -2.961564
 H 2.542463 -0.774283 -3.576189
 H 1.108861 -0.649738 -2.552596
 C 1.451720 1.118932 -3.783869
 H 1.432748 0.915176 -4.860521
 H 0.426971 1.361969 -3.473059
 C 2.379947 2.270730 -3.408015
 H 1.952802 3.257818 -3.621333
 H 3.327906 2.192983 -3.961480
 C 2.637266 2.040280 -1.922735
 H 1.754023 2.343935 -1.344511
 H 3.498250 2.598707 -1.536699
 C -2.864122 -0.445833 2.102747
 H -3.821483 -0.979445 2.193431
 C -3.144054 1.079577 2.000520
 H -2.749717 1.539098 1.084245
 H -4.228481 1.247373 1.986413
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 C -2.516161 0.556877 4.265372
 H -3.534389 0.385179 4.645729
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 H -3.908552 0.111326 -3.308769
 C -2.742330 -1.284770 -2.141633
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 O -0.367361 1.060622 -1.026916
 P 2.554941 -0.193180 -0.155043
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 Pt 0.260995 -0.579087 0.341212
 N -1.865478 4.810579 -0.115214

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e E=-743.372614 G=-743.307710

C 1.655792 1.110035 0.089633
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 C 0.670802 -1.092090 -0.063054
 C -0.623996 -0.564991 -0.128018
 C -0.742919 0.827372 -0.095144
 C 0.380103 1.634114 0.023265
 O -1.638122 -1.431375 -0.266057
 C -2.880106 -1.155320 0.394660
 H -3.378904 -2.120307 0.502185
 H -2.705764 -0.725368 1.387076
 H -3.506004 -0.486768 -0.202502
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 F 0.201152 2.960966 0.055035
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 F 0.838692 -2.417292 -0.095274
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 H 3.591512 -0.194621 2.129888
 C 5.036403 -1.730106 1.586918
 H 5.505058 -1.783353 0.597570
 H 5.681701 -1.087965 2.201282
 C 4.894444 -3.108411 2.239251
 H 4.645532 -3.862307 1.476413
 H 5.811438 -3.440712 2.738970
 C 3.706742 -2.937381 3.179853
 H 3.299202 -3.884280 3.551804
 H 4.005919 -2.336343 4.051544
 C 2.718063 -2.155179 2.320795
 H 1.917162 -1.664366 2.888009
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 C 3.005499 -2.151608 -1.165855

H	2.681560	-2.973674	-0.508923
C	2.035543	-2.095248	-2.384285
H	1.233083	-2.831899	-2.246917
H	1.541347	-1.119742	-2.486593
C	2.886656	-2.451063	-3.608336
H	2.313179	-2.964578	-4.387988
H	3.303140	-1.536972	-4.057528
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16

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103

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H	2.716615	-2.431012	-1.686576	H	2.310602	-1.800167	2.884974
C	2.224507	-3.159545	0.286395	H	2.451320	-3.038687	1.632357
H	1.710859	-2.665795	1.122234	C	3.240246	-2.463947	-1.183057
H	1.444925	-3.689993	-0.274643	H	2.841409	-3.233441	-0.504368
C	3.320931	-4.121714	0.778557	C	2.250577	-2.311048	-2.377098
H	3.639318	-3.842888	1.793358	H	1.385432	-2.968900	-2.220495
H	2.979627	-5.161770	0.825778	H	1.849197	-1.292644	-2.467391
C	4.486131	-3.912258	-0.186412	C	3.030681	-2.748799	-3.621013
H	5.447105	-4.260955	0.209296	H	2.386819	-3.189770	-4.390064
H	4.300073	-4.449077	-1.128593	H	3.537512	-1.884035	-4.075201
C	4.445494	-2.408177	-0.437100	C	4.076148	-3.711728	-3.072241
H	5.055198	-2.082447	-1.289049	H	4.892761	-3.922612	-3.772569
H	4.814915	-1.886847	0.457163	H	3.602853	-4.670453	-2.812780
C	3.128939	0.423232	0.905600	C	4.544169	-3.003190	-1.804611
H	2.562196	1.361740	0.981050	H	5.216794	-2.180343	-2.087636
C	4.636764	0.779539	0.817674	H	5.097321	-3.655934	-1.118896
H	5.174491	0.225495	0.039521	C	4.687342	0.121976	-0.773895
H	4.746316	1.842692	0.570140	H	5.591538	-0.495690	-0.858984
C	5.204796	0.476833	2.216410	C	4.344674	0.749173	-2.151772
H	5.702956	-0.503890	2.214601	H	5.159206	0.540454	-2.859100
H	5.950381	1.213158	2.537104	H	3.425286	0.346748	-2.597411
C	3.982395	0.413034	3.129860	C	4.245396	2.254236	-1.893920
H	4.175329	-0.103425	4.077369	H	4.433677	2.855007	-2.791353
H	3.634689	1.429907	3.368275	H	3.233495	2.502917	-1.532327
C	2.945519	-0.284416	2.256334	C	5.249479	2.486060	-0.771959
H	1.912155	-0.192958	2.614452	H	5.144793	3.460779	-0.280720
H	3.192435	-1.354563	2.186857	H	6.273490	2.421403	-1.169104
O	0.171064	1.114317	1.246773	C	4.974454	1.315052	0.168111
P	-2.362298	-0.374689	0.052648	H	4.083312	1.548261	0.775017
P	2.319968	-0.411623	-0.531240	H	5.795361	1.104429	0.864125
Pt	-0.027366	-0.351659	-0.334879	C	-0.315099	2.685003	2.013863
C	0.308002	5.235129	0.738904	H	-1.030002	3.518912	1.991190
H	0.348916	6.315496	0.620060	C	1.069157	3.193269	2.500117
H	0.821844	5.266538	2.833055	H	1.838640	3.178230	1.715469
H	0.739235	2.802965	3.100251	H	0.976424	4.235588	2.833472
H	-0.207582	4.847130	-1.317908	C	1.436433	2.295896	3.683470
H	-0.299938	2.385231	-1.044958	H	1.919776	1.375124	3.317352
19				H	2.128511	2.777570	4.383827
<i>p</i> -CF ₃ -b E=-1080.315375 G=-1080.250274				C	0.083826	1.949414	4.293686
C	-0.975887	-0.081279	-0.010612	H	-0.320120	2.824464	4.824492
C	-0.386133	1.185355	-0.030659	H	0.119493	1.116903	5.005810
C	0.980837	1.354819	-0.068330	C	-0.764743	1.643275	3.061925
C	1.856232	0.260489	-0.090371	H	-1.845625	1.674323	3.248230
C	1.268226	-1.006558	-0.089561	H	-0.523035	0.625417	2.715493
C	-0.110415	-1.170158	-0.042505	C	-2.002156	1.552860	-0.062987
O	3.157406	0.537083	-0.147756	H	-2.263924	0.879267	0.770193
C	4.120793	-0.401837	0.355129	C	-2.230901	0.775800	-1.390475
H	5.038475	0.172907	0.487917	H	-1.347744	0.762374	-2.042195
H	3.799723	-0.804703	1.320785	H	-2.461439	-0.274080	-1.162170
H	4.295875	-1.209873	-0.359408	C	-3.439916	1.446122	-2.058320
F	2.022016	-2.108799	-0.162973	H	-3.104026	2.217050	-2.768152
F	-0.560114	-2.421519	-0.047549	H	-4.057110	0.736522	-2.622277
F	-1.153402	2.274213	0.002246	C	-4.177439	2.117900	-0.904969
F	1.485088	2.587701	-0.072675	H	-4.904323	2.871877	-1.228130
C	-2.470182	-0.178508	0.047542	H	-4.721759	1.362853	-0.316221
F	-2.956266	0.432474	1.142399	C	-3.035215	2.693883	-0.073921
F	-2.916901	-1.434263	0.072136	H	-3.331034	3.000735	0.937023
F	-3.041993	0.422536	-1.010367	H	-2.638530	3.580383	-0.588116
106				C	0.296701	3.411669	-0.740483
TS_{SN2}1p -CF ₃ -b E=-3057.254000 G=-3056.451289				H	1.383244	3.431007	-0.556200
C	-0.169378	-1.668530	0.385522	C	-0.249504	4.833561	-0.443045
H	-0.581105	-1.275164	-0.535956	H	-1.162448	4.831519	0.162362
H	-0.412240	-1.224069	1.341331	H	0.496320	5.399211	0.129476
H	0.634127	-2.390560	0.335001	C	-0.490187	5.471435	-1.823481
C	4.014178	-1.504723	1.520409	H	-1.554051	5.390382	-2.091586
H	4.138170	-0.561861	2.072982	H	-0.233692	6.536386	-1.848191
C	5.364944	-2.268904	1.511693	C	0.329983	4.623861	-2.793647
H	5.788501	-2.400903	0.509704	H	0.023412	4.741519	-3.839187
H	6.105733	-1.699088	2.088326	H	1.396616	4.889025	-2.725954
C	5.075790	-3.605905	2.201172	C	0.121613	3.214154	-2.253688
H	4.721406	-4.341727	1.462752	H	0.813289	2.464649	-2.660873
H	5.958938	-4.033868	2.688919	H	-0.900503	2.885960	-2.493092
C	3.940248	-3.274784	3.163321	P	3.330958	-0.945973	-0.106951
H	3.431455	-4.158284	3.565121	P	-0.234190	1.973476	0.307362
H	4.330337	-2.697428	4.014879	Pt	1.397612	0.315317	0.105292
C	3.032468	-2.394243	2.310140	C	-4.798954	-2.378561	-0.801053

C	-5.325587	-1.448686	0.104449
C	-4.496636	-1.096639	1.173263
C	-3.234308	-1.640431	1.317302
C	-2.676796	-2.562332	0.403642
C	-3.534913	-2.908865	-0.665808
O	-1.480552	-3.043225	0.509311
F	-2.508153	-1.274953	2.387853
F	-4.887616	-0.216165	2.099133
F	-5.535436	-2.760855	-1.851119
F	-3.100311	-3.782353	-1.582870
C	-6.696040	-0.905554	-0.131803
F	-6.784462	-0.271746	-1.319033
F	-7.088851	-0.032532	0.799479
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p-CF₃-an E=-683.493303 G=-683.392585

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C	1.984755	0.292545	-0.000036
C	1.388224	-0.972697	0.000010
C	0.003559	-1.070999	0.000010
O	3.319093	0.500159	-0.000025
C	4.171466	-0.634028	-0.000026
H	5.192799	-0.249107	-0.000083
H	4.018960	-1.247264	0.897193
H	4.018884	-1.247320	-0.897193
H	1.987758	-1.877633	0.000049
H	-0.464674	-2.053848	0.000052
H	-0.800466	2.235480	-0.000117
H	1.674798	2.415644	-0.000126
C	-2.267384	-0.087183	0.000028
F	-2.710149	-0.778166	1.075089
F	-2.710212	-0.778613	-1.074708
F	-2.927090	1.081909	-0.000186

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TS_{SN21}*p*-CF₃-an E=-2660.412399 G=-2659.574928

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H	-0.684165	-1.440339	1.116958
H	0.578883	-2.450200	0.184991
C	3.786825	-1.406445	1.499072
H	3.788555	-0.497564	2.118712
C	5.208342	-2.030069	1.506498
H	5.687323	-2.044382	0.520746
H	5.860328	-1.433863	2.158696
C	5.028218	-3.436266	2.086566
H	4.782773	-4.146945	1.282374
H	5.928666	-3.809575	2.587257
C	3.824604	-3.290865	3.011290
H	3.392512	-4.247610	3.325669
H	4.116648	-2.741266	3.918635
C	2.868892	-2.445553	2.175463
H	2.062856	-1.971736	2.750312
H	2.389302	-3.094148	1.425954
C	3.202261	-2.254293	-1.284744
H	2.861719	-3.101674	-0.669978
C	2.236769	-2.121594	-2.499918
H	1.406284	-2.830483	-2.386087
H	1.781244	-1.124835	-2.569602
C	3.075461	-2.467224	-3.736527
H	2.487581	-2.949483	-4.525321
H	3.509490	-1.552354	-4.166750
C	4.196101	-3.342692	-3.188344
H	5.042760	-3.455923	-3.875426
H	3.811224	-4.348704	-2.963972
C	4.567460	-2.629873	-1.892029
H	5.152706	-1.730992	-2.135927
H	5.175111	-3.242296	-1.215144
C	4.398350	0.409709	-0.672111
H	5.354787	-0.124560	-0.752599
C	4.059089	1.082433	-2.030085
H	4.882859	0.913939	-2.736987
H	3.151043	0.679587	-2.498249
C	3.924066	2.576865	-1.720399
H	4.155895	3.212590	-2.582506

H	2.890134	2.803078	-1.412327
C	4.855954	2.783493	-0.532851
H	4.699356	3.734386	-0.010130
H	5.903145	2.756941	-0.869860
C	4.555878	1.567199	0.338074
H	3.607388	1.737142	0.876065
H	5.325925	1.359803	1.090790
C	-0.891620	2.279110	2.167767
H	-1.670264	3.053534	2.201526
C	0.431219	2.843290	2.753066
H	1.236020	2.916379	2.008295
H	0.257536	3.858276	3.134383
C	0.801954	1.902441	3.902691
H	1.389712	1.054420	3.515813
H	1.402050	2.393678	4.677188
C	-0.547660	1.396598	4.398187
H	-1.060959	2.191683	4.959475
H	-0.477311	0.520093	5.052566
C	-1.290111	1.111995	3.095597
H	-2.377194	1.021763	3.213925
H	-0.922865	0.157524	2.684782
C	-2.419616	1.213299	-0.053439
H	-2.645861	0.454381	0.714596
C	-2.556481	0.518740	-1.435470
H	-1.710857	0.725455	-2.104020
H	-2.587071	-0.570434	-1.296986
C	-3.888721	1.020409	-2.019313
H	-3.708661	1.831620	-2.739799
H	-4.433755	0.232092	-2.552222
C	-4.650286	1.574888	-0.818178
H	-5.471699	2.247010	-1.092667
H	-5.075602	0.745565	-0.231535
C	-3.548881	2.253954	-0.011255
H	-3.842887	2.519209	1.012133
H	-3.248161	3.179633	-0.523531
C	-0.297472	3.327276	-0.484761
H	0.785846	3.421908	-0.300631
C	-0.962194	4.654474	-0.041029
H	-1.919612	4.501569	0.469731
H	-0.312785	5.175751	0.673056
C	-1.152469	5.467296	-1.338938
H	-2.208508	5.440815	-1.642781
H	-0.882321	6.522382	-1.219599
C	-0.311587	4.746960	-2.393199
H	-0.625848	4.966992	-3.419726
H	0.747194	5.033345	-2.301150
C	-0.473322	3.281383	-2.008069
H	0.239669	2.603003	-2.495306
H	-1.487531	2.946287	-2.273515
P	3.118954	-0.805276	-0.119199
P	-0.709089	1.750374	0.403749
Pt	1.071646	0.265463	0.106352
C	-4.840912	-2.825157	-1.095136
C	-5.414478	-2.111811	-0.034289
C	-4.647062	-1.825988	1.097284
C	-3.326730	-2.239674	1.166425
C	-2.717214	-2.954510	0.103780
C	-3.522431	-3.232686	-1.031401
O	-1.469657	-3.339940	0.147289
H	-3.069914	-3.781240	-1.855380
H	-5.440038	-3.052390	-1.976827
H	-5.085887	-1.278861	1.929501
H	-2.737218	-2.030617	2.058874
C	-6.832854	-1.697975	-0.144579
F	-7.681392	-2.752324	-0.252703
F	-7.263471	-0.978245	0.907326
F	-7.078485	-0.945229	-1.245548

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p-SO₂Cl-an E=-1354.606217 G=-1354.510445

C	-0.264938	0.128234	-0.305516
C	0.312051	1.372632	-0.030824
C	1.679202	1.444371	0.128775
C	2.463896	0.283577	0.037091
C	1.868729	-0.958642	-0.219622
C	0.495176	-1.036311	-0.383881
O	3.782161	0.459492	0.211260

H	2.464032	-1.862813	-0.293323
H	0.023045	-1.995854	-0.579976
H	-0.301117	2.266966	0.045275
H	2.170294	2.392652	0.329855
S	-2.001820	0.015750	-0.476475
O	-2.572450	1.309308	-0.806097
O	-2.372570	-1.177849	-1.215144
Cl	-2.630394	-0.364315	1.508741
C	4.629388	-0.683611	0.178809
H	5.641921	-0.313743	0.346031
H	4.365804	-1.391389	0.974131
H	4.583685	-1.183566	-0.796137
106			
TS_{SN2}1p-SO₂Cl-an E=-3331.530480 G=-3330.699734			
C	-0.108522	-1.747163	0.281919
H	-0.652126	-1.238475	-0.503655
H	-0.270179	-1.506656	1.324948
H	0.685941	-2.431599	0.020732
C	4.001821	-1.693863	1.388260
H	4.094219	-0.823111	2.054286
C	5.374753	-2.412788	1.297042
H	5.808798	-2.405994	0.290598
H	6.094816	-1.898955	1.947635
C	5.121358	-3.833500	1.810508
H	4.795646	-4.481371	0.982242
H	6.013625	-4.292732	2.250944
C	3.969859	-3.659191	2.794423
H	3.484146	-4.600475	3.075544
H	4.337469	-3.184478	3.716459
C	3.041646	-2.702698	2.051940
H	2.304630	-2.206423	2.695332
H	2.477241	-3.271423	1.296562
C	3.256291	-2.345685	-1.409739
H	2.892214	-3.202332	-0.822174
C	2.245851	-2.090164	-2.567930
H	1.396376	-2.779068	-2.470352
H	1.822073	-1.076957	-2.543265
C	3.017531	-2.374309	-3.860853
H	2.374440	-2.752125	-4.663397
H	3.491809	-1.452134	-4.228748
C	4.100112	-3.356345	-3.430043
H	4.910679	-3.467450	-4.159727
H	3.659937	-4.351174	-3.265327
C	4.567546	-2.768707	-2.101834
H	5.206702	-1.897411	-2.306489
H	5.154593	-3.469044	-1.495882
C	4.662269	0.194090	-0.704237
H	5.576043	-0.398246	-0.845882
C	4.319676	0.956197	-2.012478
H	5.131872	0.816903	-2.739129
H	3.398094	0.601365	-2.492826
C	4.223398	2.428635	-1.606241
H	4.423011	3.115056	-2.437187
H	3.208647	2.644933	-1.232913
C	5.214101	2.544573	-0.454790
H	5.104288	3.465719	0.129659
H	6.243091	2.517233	-0.843376
C	4.926507	1.285351	0.358821
H	4.022711	1.453307	0.969110
H	5.735833	1.007296	1.044596
C	-0.432315	2.396543	2.244107
H	-1.118260	3.253621	2.279377
C	0.941648	2.792310	2.846289
H	1.737320	2.879449	2.093134
H	0.855437	3.773022	3.333254
C	1.247698	1.717640	3.889599
H	1.704929	0.842328	3.398680
H	1.940500	2.062557	4.665815
C	-0.131820	1.343857	4.418459
H	-0.510744	2.148061	5.066462
H	-0.145917	0.415414	5.000822
C	-0.968400	1.258693	3.143131
H	-2.048532	1.339407	3.318603
H	-0.789151	0.279738	2.669035
C	-2.044139	1.499335	0.014838
H	-2.347578	0.789292	0.801639

C	-2.254735	0.785277	-1.347673
H	-1.397624	0.892271	-2.025093
H	-2.390718	-0.292437	-1.180617
C	-3.538606	1.394519	-1.938119
H	-3.287773	2.162245	-2.684311
H	-4.163849	0.646837	-2.440847
C	-4.232782	2.053933	-0.749574
H	-4.989327	2.792578	-1.040133
H	-4.736272	1.287713	-0.137893
C	-3.064632	2.647358	0.029651
H	-3.323320	2.971816	1.045439
H	-2.680212	3.522529	-0.513878
C	0.256831	3.414660	-0.400994
H	1.341160	3.425385	-0.201147
C	-0.312253	4.787646	0.037515
H	-1.271926	4.706128	0.559854
H	0.379659	5.268674	0.740118
C	-0.458177	5.601305	-1.264529
H	-1.513484	5.625310	-1.571377
H	-0.136148	6.642267	-1.150327
C	0.347882	4.832658	-2.311303
H	0.055525	5.069239	-3.340617
H	1.420714	5.057784	-2.210334
C	0.098008	3.379169	-1.927029
H	0.778532	2.661366	-2.404649
H	-0.929398	3.100208	-2.206756
P	3.318825	-0.958693	-0.167747
P	-0.288412	1.872398	0.474284
Pt	1.365613	0.252544	0.150135
C	-4.864779	-3.007519	-0.677571
C	-5.298710	-2.010364	0.212035
C	-4.408450	-1.394837	1.103029
C	-3.095159	-1.811073	1.133985
C	-2.613210	-2.820515	0.251681
C	-3.549330	-3.405074	-0.650073
O	-1.377622	-3.209234	0.238168
H	-3.190917	-4.178230	-1.325627
H	-5.563662	-3.459937	-1.378635
H	-4.758122	-0.620107	1.782823
H	-2.411010	-1.369321	1.856139
S	-6.949314	-1.499437	0.158141
O	-7.830935	-2.591936	-0.222776
O	-7.272619	-0.640150	1.286375
Cl	-7.042624	-0.193621	-1.538448

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p-Me-an E=-385.819086 G=-385.694785

C	-1.825918	-0.094852	0.000011
C	-1.272083	1.189006	-0.000034
C	0.101372	1.384955	-0.000044
C	0.964811	0.287754	-0.000010
C	0.436074	-1.004055	0.000036
C	-0.946136	-1.177118	0.000044
O	2.296445	0.571519	-0.000028
C	3.197693	-0.517804	-0.000021
H	4.202308	-0.089502	-0.000084
H	3.075789	-1.141436	0.896022
H	3.075711	-1.141513	-0.895998
H	1.084506	-1.875750	0.000062
H	-1.350131	-2.189733	0.000077
H	-1.933624	2.055000	-0.000064
H	0.526850	2.386363	-0.000083
C	-3.310196	-0.310955	0.000041
H	-3.853620	0.640181	-0.000218
H	-3.636540	-0.878447	0.880950
H	-3.636508	-0.878913	-0.880577

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TS_{SN2}1p-Me-an E=-2362.732925 G=-2361.872684

C	-0.316409	-1.932552	0.334494
H	-0.762547	-1.798923	-0.644414
H	-0.850470	-1.639371	1.228756
H	0.640185	-2.427379	0.426859
C	3.633528	-0.742631	1.479344
H	3.474610	0.185308	2.048658
C	5.150917	-1.069145	1.450911
H	5.584343	-1.059603	0.444154
H	5.694388	-0.309533	2.028404

C 5.281780 -2.437627 2.127036
 H 5.159331 -3.238923 1.382107
 H 6.256290 -2.584603 2.606412
 C 4.106417 -2.472261 3.097719
 H 3.889227 -3.471864 3.490839
 H 4.311209 -1.812606 3.954428
 C 2.970211 -1.897594 2.257562
 H 2.104171 -1.559182 2.840049
 H 2.608015 -2.680717 1.573704
 C 3.121663 -1.862877 -1.221791
 H 2.998331 -2.718707 -0.540738
 C 2.088262 -2.014464 -2.377109
 H 1.429562 -2.867618 -2.168314
 H 1.433215 -1.138275 -2.473760
 C 2.914886 -2.267317 -3.643730
 H 2.400559 -2.915233 -4.362136
 H 3.124363 -1.316153 -4.155564
 C 4.221599 -2.852486 -3.121049
 H 5.035928 -2.835135 -3.854905
 H 4.069314 -3.898488 -2.815719
 C 4.501943 -1.990204 -1.894101
 H 4.872058 -1.009340 -2.227119
 H 5.258507 -2.416035 -1.224279
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 H 2.439985 0.906635 -2.588626
 C 2.818768 2.967822 -1.945699
 H 2.860345 3.583536 -2.851441
 H 1.778685 2.984891 -1.580765
 C 3.745084 3.440483 -0.832419
 H 3.417016 4.369033 -0.350724
 H 4.755324 3.611999 -1.233363
 C 3.754744 2.246540 0.117991
 H 2.823407 2.253643 0.710186
 H 4.591625 2.251207 0.826777
 C -1.725853 1.957933 2.165682
 H -2.637783 2.570634 2.171489
 C -0.539386 2.779821 2.737939
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 H -0.912973 3.738002 3.123360
 C 0.022207 1.935691 3.883427
 H 0.746363 1.205698 3.487004
 H 0.538515 2.535986 4.641323
 C -1.202723 1.198352 4.410802
 H -1.842700 1.894151 4.973965
 H -0.961892 0.358751 5.073037
 C -1.903187 0.761813 3.126214
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 H -1.385550 -0.126348 2.731035
 C -3.002679 0.569712 -0.040176
 H -3.091634 -0.208721 0.737168
 C -2.986355 -0.155339 -1.412864
 H -2.198109 0.214649 -2.081134
 H -2.792416 -1.224970 -1.260828
 C -4.389332 0.057363 -2.008625
 H -4.370027 0.864473 -2.755725
 H -4.764905 -0.840755 -2.514443
 C -5.253006 0.485980 -0.824759
 H -6.182836 0.986172 -1.120132
 H -5.518316 -0.395996 -0.220752
 C -4.307585 1.378990 -0.028083
 H -4.656966 1.606166 0.987049
 H -4.181517 2.333960 -0.559804
 C -1.312769 3.036681 -0.503002
 H -0.266120 3.332879 -0.320188
 C -2.214196 4.223396 -0.078709
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 C -2.557087 4.963266 -1.388373
 H -3.587900 4.727807 -1.688953
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 C -1.592152 4.401621 -2.432582
 H -1.940964 4.541965 -3.462020
 H -0.608350 4.887746 -2.346089

C -1.472756 2.937760 -2.025619
 H -0.643126 2.400486 -2.504247
 H -2.403872 2.412683 -2.286156
 P 2.797718 -0.386968 -0.133816
 P -1.429468 1.427384 0.417197
 Pt 0.587958 0.283159 0.136228
 C -4.416793 -3.740663 -1.242486
 C -5.274995 -3.236183 -0.256687
 C -4.709222 -2.907086 0.978353
 C -3.349638 -3.070825 1.226658
 C -2.476701 -3.581697 0.238828
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 O -1.186956 -3.730925 0.452376
 H -2.403874 -4.293823 -1.791547
 H -4.831539 -4.004986 -2.217527
 H -5.353891 -2.511542 1.766073
 H -2.933281 -2.816009 2.202546
 C -6.741654 -3.065702 -0.525446
 H -6.925405 -2.469328 -1.429962
 H -7.246599 -4.029528 -0.678539
 H -7.246817 -2.563516 0.308248

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Bu E=-272.793293 G=-272.662068

C 2.020102 -0.005364 -0.145792
 H 2.795486 -0.109055 -0.911539
 H 2.203662 0.935801 0.394357
 H 2.130527 -0.842010 0.560985
 O 0.783589 -0.013759 -0.813811
 C -0.397347 0.000285 0.007092
 C -1.536839 0.114517 -0.988916
 H -1.515757 -0.724373 -1.695085
 H -2.503747 0.107354 -0.472278
 H -1.456065 1.047141 -1.560269
 C -0.519355 -1.299075 0.792143
 H -0.477637 -2.162140 0.116274
 H 0.272245 -1.407582 1.543073
 H -1.477655 -1.328071 1.325100
 C -0.400207 1.200446 0.944365
 H -0.233505 2.129092 0.383720
 H -1.371084 1.277497 1.448548
 H 0.366698 1.121564 1.724251

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TS_{SN2}1^{Bu} E=-2249.683825 G=-2248.820397

C -0.253492 1.926860 0.269327
 H 0.734844 2.161512 -0.103704
 H -0.437456 2.002047 1.336055
 H -1.091058 2.013424 -0.411817
 C -3.351632 -0.420052 1.548763
 H -2.859770 -1.050985 2.303732
 C -4.861922 -0.776328 1.490815
 H -5.176047 -1.211494 0.535337
 H -5.084488 -1.527290 2.260672
 C -5.596121 0.529646 1.805484
 H -5.743145 1.112265 0.882988
 H -6.584990 0.366323 2.248904
 C -4.626544 1.271372 2.717912
 H -4.867817 2.332142 2.849341
 H -4.622374 0.803470 3.713867
 C -3.283285 1.045122 2.030214
 H -2.419074 1.224658 2.680251
 H -3.195321 1.742796 1.183583
 C -3.164044 0.200872 -1.352496
 H -3.406460 1.172215 -0.894306
 C -2.221975 0.464833 -2.565373
 H -1.941330 1.526698 -2.583936
 H -1.280393 -0.097109 -2.501324
 C -3.036893 0.097687 -3.811929
 H -2.785664 0.717950 -4.679436
 H -2.845533 -0.948372 -4.093612
 C -4.486418 0.237145 -3.361522
 H -5.203836 -0.253238 -4.029908
 H -4.760324 1.300985 -3.300051
 C -4.457927 -0.369817 -1.962416
 H -4.404518 -1.465369 -2.050127
 H -5.345719 -0.131571 -1.364594
 C -2.633939 -2.537990 -0.287469

H	-3.714961	-2.687427	-0.416466
C	-1.886813	-3.083450	-1.535021
H	-2.616614	-3.447891	-2.270098
H	-1.281409	-2.318938	-2.040291
C	-1.017889	-4.239158	-1.020387
H	-0.864519	-5.022189	-1.771532
H	-0.023415	-3.861149	-0.734151
C	-1.743797	-4.718345	0.230764
H	-1.128989	-5.353904	0.878619
H	-2.638833	-5.293962	-0.049448
C	-2.155719	-3.407823	0.892318
H	-1.270974	-2.951288	1.369914
H	-2.924449	-3.523048	1.665934
C	2.960512	0.038155	2.108089
H	4.041796	-0.148933	2.067278
C	2.308275	-0.840365	3.206438
H	1.756932	-1.702588	2.806027
H	3.092342	-1.240437	3.864034
C	1.410970	0.114068	3.991442
H	0.456715	0.249776	3.456477
H	1.178058	-0.249444	4.998987
C	2.199630	1.417655	3.974507
H	3.054294	1.339996	4.662722
H	1.611995	2.293172	4.273607
C	2.688911	1.504019	2.528482
H	3.575857	2.137079	2.405820
H	1.894294	1.951652	1.913950
C	3.117267	0.837678	-0.692601
H	2.929768	1.806111	-0.199364
C	2.513827	0.915647	-2.119071
H	2.007637	-0.014277	-2.408047
H	1.746739	1.700775	-2.163462
C	3.704009	1.222322	-3.050085
H	3.997819	0.313525	-3.594316
H	3.465448	1.981162	-3.803206
C	4.841466	1.640150	-2.118252
H	5.833661	1.538138	-2.572873
H	4.719592	2.691981	-1.817879
C	4.632732	0.739149	-0.905209
H	5.206975	1.041259	-0.020407
H	4.927984	-0.288958	-1.162816
C	2.891714	-2.069199	0.095233
H	2.180659	-2.699638	0.655286
C	4.320333	-2.452249	0.547771
H	4.991127	-1.586096	0.587257
H	4.297820	-2.871352	1.561215
C	4.816296	-3.479022	-0.494934
H	5.582476	-3.018495	-1.133807
H	5.276784	-4.359225	-0.032862
C	3.592241	-3.824671	-1.345592
H	3.853507	-4.195925	-2.342993
H	2.987942	-4.600238	-0.851315
C	2.811416	-2.516207	-1.369577
H	1.778435	-2.612186	-1.729861
H	3.326085	-1.795749	-2.023402
P	-2.344825	-0.739518	0.027669
Pt	2.270030	-0.355900	0.436130
Pt	-0.056208	-0.340509	0.271022
O	-0.507525	4.043873	0.487545
C	0.088669	4.824600	-0.482457
C	-0.373110	6.274681	-0.276613
H	-0.093217	6.619246	0.727743
H	0.067323	6.964226	-1.012612
H	-1.466344	6.334249	-0.360296
C	-0.319090	4.394071	-1.900148
H	0.085253	5.064164	-2.673142
H	0.038965	3.378505	-2.123567
H	-1.414872	4.393775	-1.988273
C	1.623081	4.796252	-0.377926
H	1.933107	5.094031	0.633134
H	2.015806	3.784804	-0.561833
H	2.107803	5.470738	-1.099527

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Me E=-154.930444 G=-154.876749

C	-1.159282	-0.196387	-0.000001
H	-2.026619	0.470269	0.000161

H	-1.208110	-0.840749	-0.893527
H	-1.207962	-0.840977	0.893370
O	0.000000	0.597444	0.000000
C	1.159282	-0.196387	0.000001
H	1.207972	-0.840962	-0.893380
H	2.026619	0.470269	-0.000141
H	1.208100	-0.840763	0.893518

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TS_{SN2}1Me E=-2131.820506 G=-2131.033457

C	0.239384	2.048957	1.035843
H	-0.480406	1.774629	1.799773
H	-0.070584	2.693271	0.217169
H	1.287223	2.050127	1.307090
C	3.325145	0.607381	-1.362602
H	2.812975	0.342852	-2.299817
C	4.839316	0.294178	-1.501982
H	5.192718	-0.484619	-0.816218
H	5.039178	-0.073064	-2.517393
C	5.548921	1.632707	-1.277655
H	5.733701	1.786086	-0.203317
H	6.517545	1.691785	-1.786955
C	4.533818	2.661244	-1.763285
H	4.762964	3.686928	-1.453083
H	4.486818	2.646579	-2.862630
C	3.226155	2.136331	-1.178521
H	2.326891	2.550300	-1.650336
H	3.180161	2.407890	-0.112996
C	3.250050	-0.065640	1.531609
H	3.494725	1.007434	1.514236
C	2.347661	-0.335383	2.773375
H	2.128679	0.614808	3.277469
H	1.374634	-0.768918	2.504646
C	3.167315	-1.250546	3.689269
H	2.942171	-1.097073	4.750494
H	2.956294	-2.305879	3.459558
C	4.611990	-0.936440	3.319655
H	5.331210	-1.681837	3.678654
H	4.902746	0.038004	3.739556
C	4.551463	-0.847602	1.797792
H	4.492656	-1.865696	1.385543
H	5.429706	-0.364809	1.352805
C	2.651216	-2.098298	-0.578913
H	3.733728	-2.284112	-0.570907
C	1.937195	-3.113357	0.354527
H	2.672021	-3.833553	0.739280
H	1.465495	-2.643445	1.228030
C	0.914142	-3.827296	-0.533575
H	0.665021	-4.832550	-0.174675
H	-0.022331	-3.245908	-0.565041
C	1.561566	-3.803617	-1.912339
H	0.871503	-4.048475	-2.728207
H	2.390427	-4.526441	-1.948650
C	2.103500	-2.379709	-1.996381
H	1.269526	-1.694373	-2.229019
H	2.866519	-2.239792	-2.771561
C	-2.815525	0.946311	-1.911556
H	-3.897412	0.774291	-1.991171
C	-2.095648	0.369042	-3.159714
H	-1.512229	-0.537803	-2.947767
H	-2.844140	0.095343	-3.915664
C	-1.221568	1.510059	-3.679916
H	-0.271242	1.534745	-3.121113
H	-0.978863	1.410216	-4.744164
C	-2.039846	2.751698	-3.348002
H	-2.897370	2.824095	-4.033485
H	-1.474641	3.687624	-3.424340
C	-2.522491	2.464132	-1.927662
H	-3.393943	3.058881	-1.629254
H	-1.711309	2.707476	-1.224729
C	-3.215831	0.976785	0.974976
H	-2.943383	2.035725	0.834262
C	-2.828780	0.584434	2.430033
H	-2.186995	-0.304202	2.484050
H	-2.257603	1.403495	2.887654
C	-4.160856	0.391723	3.168832
H	-4.459970	-0.667231	3.145826

H	-4.105398	0.689337	4.221722
C	-5.157831	1.209156	2.353616
H	-6.205044	0.971121	2.573009
H	-5.008686	2.282651	2.546648
C	-4.749700	0.882189	0.920896
H	-5.186171	1.548878	0.167135
H	-5.074897	-0.141737	0.687063
C	-2.800143	-1.621795	-0.539945
H	-2.017891	-2.041887	-1.194310
C	-4.170598	-1.918436	-1.202803
H	-4.856608	-1.064579	-1.174682
H	-4.023200	-2.157661	-2.263458
C	-4.745342	-3.119535	-0.426972
H	-5.494020	-2.768686	0.298202
H	-5.245826	-3.844238	-1.078674
C	-3.556796	-3.706071	0.332735
H	-3.852353	-4.336941	1.178712
H	-2.937026	-4.319240	-0.339629
C	-2.782090	-2.460552	0.746128
H	-1.763358	-2.658292	1.105686
H	-3.325809	-1.951414	1.555466
P	2.375161	-0.337713	-0.087393
P	-2.236739	0.137237	-0.351191
Pt	0.091924	0.114479	-0.106208
O	0.236974	3.886874	2.129342
C	-1.042313	4.342630	2.030805
H	-1.386788	4.536610	0.982111
H	-1.816927	3.658687	2.469105
H	-1.187853	5.309278	2.560944

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g E=-836.759792 G=-836.676223

C	1.021572	-1.552022	-0.024911
C	-0.132815	-0.912775	-0.444522
C	-0.152594	0.486146	-0.491404
C	1.038220	1.126948	-0.123030
C	2.125036	0.369592	0.265432
O	-1.160529	1.251513	-0.903752
F	1.107311	2.456976	-0.143799
F	3.247049	0.993295	0.619296
F	1.023965	-2.883239	0.018208
F	-1.189172	-1.635926	-0.824064
C	-2.533613	0.883710	-0.590103
H	-3.100851	1.734438	-0.980693
H	-2.824750	-0.011320	-1.149440
C	-2.731145	0.719923	0.875276
H	-2.422216	1.561812	1.497639
C	-3.282738	-0.362929	1.416116
H	-3.598681	-1.206785	0.803020
H	-3.456630	-0.439968	2.486811
N	2.124776	-0.940255	0.321255

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1.g E=-2813.733381 G=-2812.908577

C	-1.302924	-3.115678	0.886457
C	-2.126516	-3.320556	-0.229061
C	-1.582893	-3.838670	-1.388660
C	0.454548	-4.000708	-0.485260
C	0.036891	-3.493964	0.733105
C	3.306179	-1.283882	-0.161314
H	2.746065	-2.007490	0.449230
C	4.825653	-1.486211	0.074431
H	5.299163	-0.670741	0.633787
H	4.977036	-2.398203	0.668078
C	5.427426	-1.675583	-1.318698
H	5.630460	-0.696904	-1.781012
H	6.371712	-2.232002	-1.304625
C	4.311990	-2.376520	-2.085826
H	4.459177	-2.383586	-3.171978
H	4.239873	-3.423308	-1.753683
C	3.067523	-1.603692	-1.655568
H	2.130923	-2.151013	-1.816749
H	2.990564	-0.680655	-2.251078
C	3.564934	1.626504	-0.587405
H	3.717322	1.175038	-1.579766
C	2.823299	2.977318	-0.798875
H	2.406902	3.014706	-1.814462
H	1.968005	3.092015	-0.121388

C	3.877659	4.074170	-0.576352
H	3.760709	4.922380	-1.260132
H	3.793072	4.469963	0.446589
C	5.216267	3.357028	-0.721536
H	6.056494	3.906431	-0.280618
H	5.446354	3.194611	-1.785270
C	4.948583	2.017460	-0.043842
H	4.916313	2.169056	1.045722
H	5.715609	1.260898	-0.248772
C	3.043614	0.516816	2.106787
H	4.139936	0.500243	2.162898
C	2.504773	1.822484	2.749338
H	3.329282	2.349098	3.250043
H	2.073861	2.521712	2.020555
C	1.472189	1.365498	3.781416
H	1.319933	2.095298	4.585066
H	0.500094	1.208361	3.284785
C	2.024826	0.027900	4.259845
H	1.302543	-0.574820	4.825220
H	2.893164	0.197892	4.913911
C	2.466343	-0.635331	2.957372
H	1.583045	-1.062698	2.459630
H	3.186132	-1.451828	3.095970
C	-2.166564	0.798480	-2.585121
H	-3.163426	1.193991	-2.821035
C	-2.129766	-0.728086	-2.849518
H	-2.039791	-1.311675	-1.923324
H	-3.061773	-1.044591	-3.337715
C	-0.938858	-0.949748	-3.783214
H	-0.013604	-1.034154	-3.191308
H	-1.032697	-1.860578	-4.386325
C	-0.895647	0.334498	-4.603477
H	-1.719135	0.338113	-5.333788
H	0.040223	0.471478	-5.157931
C	-1.124757	1.412754	-3.545614
H	-1.456989	2.372178	-3.960911
H	-0.177604	1.594276	-3.011284
C	-1.974160	3.035498	-0.762297
H	-1.262626	3.348801	-1.544007
C	-1.519355	3.696620	0.566616
H	-1.540819	2.997471	1.412485
H	-0.477725	4.030475	0.476745
C	-2.479017	4.881504	0.787691
H	-3.244247	4.612223	1.529908
H	-1.969099	5.774259	1.166609
C	-3.152182	5.101561	-0.566342
H	-4.092852	5.660587	-0.497066
H	-2.482508	5.660377	-1.236970
C	-3.327810	3.679430	-1.089243
H	-3.576771	3.625368	-2.156728
H	-4.140115	3.189287	-0.532664
C	-3.272288	0.452853	0.081063
H	-2.965921	-0.596960	0.214629
C	-4.660260	0.447306	-0.605682
H	-4.772772	1.254571	-1.338864
H	-4.800582	-0.491913	-1.155751
C	-5.684710	0.600904	0.538792
H	-6.093809	1.621266	0.539121
H	-6.535162	-0.082633	0.438542
C	-4.884633	0.378139	1.821846
H	-5.358855	0.805504	2.713653
H	-4.748406	-0.700073	2.003126
C	-3.533459	0.998593	1.489998
H	-2.736402	0.740770	2.201182
H	-3.627372	2.094969	1.477064
F	-3.420120	-3.002816	-0.167331
F	-2.376797	-4.014277	-2.443277
F	1.727764	-4.371284	-0.607996
F	0.901363	-3.424085	1.748549
O	-1.866747	-2.652801	1.998532
P	2.560720	0.345035	0.326993
P	-1.815781	1.188035	-0.807234
Pt	0.304896	0.566486	-0.131312
C	-1.141529	-1.716016	2.821860
H	-0.779894	-0.894004	2.172436
H	-0.263353	-2.205777	3.263536

N	-0.320145	-4.163371	-1.527881
C	-2.036113	-1.217572	3.897266
H	-1.583693	-0.433991	4.507757
C	-3.266498	-1.648229	4.160304
H	-3.741177	-2.431700	3.573691
H	-3.842179	-1.223413	4.978868

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TS_{SN2}1g E=-2813.702302 G=-2812.881289

C	0.988459	1.440982	1.310902
H	1.554760	0.536576	1.143244
H	0.819906	2.096009	0.460469
C	-2.734948	2.720626	0.249612
H	-2.389578	2.741089	1.294035
C	-4.083913	3.483675	0.154214
H	-4.936954	2.847374	-0.106164
H	-4.315212	3.925253	1.133010
C	-3.847069	4.592751	-0.873094
H	-4.028054	4.210299	-1.889909
H	-4.504936	5.457018	-0.726972
C	-2.365563	4.911414	-0.712842
H	-1.950517	5.513532	-1.528959
H	-2.204899	5.464688	0.225505
C	-1.735122	3.525883	-0.607281
H	-0.730125	3.539897	-0.168313
H	-1.633393	3.093224	-1.614354
C	-3.403796	0.787933	-1.878406
H	-2.857811	1.574680	-2.421096
C	-3.098874	-0.567364	-2.580657
H	-2.289246	-0.425087	-3.307951
H	-2.746771	-1.335083	-1.879373
C	-4.403105	-0.982529	-3.276293
H	-4.230630	-1.499223	-4.227020
H	-4.969516	-1.670727	-2.631831
C	-5.182368	0.319388	-3.423629
H	-6.250360	0.171266	-3.621897
H	-4.769481	0.914384	-4.251910
C	-4.908550	1.023609	-2.098615
H	-5.503566	0.543791	-1.306858
H	-5.171830	2.087994	-2.108960
C	-4.040829	0.239346	0.970492
H	-4.965344	0.804286	0.782678
C	-4.324868	-1.272855	0.773561
H	-5.301998	-1.410076	0.292440
H	-3.580773	-1.756058	0.124841
C	-4.301931	-1.891327	2.182850
H	-5.056936	-2.674791	2.313119
H	-3.321109	-2.353558	2.368572
C	-4.484289	-0.710649	3.131975
H	-4.150711	-0.924188	4.154935
H	-5.544454	-0.420638	3.180950
C	-3.677473	0.392660	2.456496
H	-2.601975	0.199134	2.601543
H	-3.890701	1.398269	2.841314
C	0.986283	-2.949215	1.704275
H	1.612255	-3.828939	1.504124
C	-0.396527	-3.398060	2.244253
H	-1.208720	-3.272540	1.513900
H	-0.358389	-4.465831	2.499418
C	-0.619111	-2.569829	3.509603
H	-1.021214	-1.579521	3.238895
H	-1.328340	-3.034460	4.205427
C	0.788050	-2.416321	4.074681
H	1.113525	-3.368084	4.519607
H	0.872874	-1.644321	4.848878
C	1.622176	-2.104257	2.832617
H	2.690060	-2.319367	2.958656
H	1.540046	-1.029364	2.611527
C	2.585202	-1.568987	-0.288876
H	2.932954	-1.080695	0.638104
C	2.742687	-0.545571	-1.441765
H	1.900315	-0.578781	-2.143879
H	2.760676	0.476034	-1.038075
C	4.070274	-0.910064	-2.138195
H	3.866165	-1.407960	-3.096357
H	4.683634	-0.028849	-2.363277
C	4.761891	-1.895604	-1.195202

H	5.501683	-2.528274	-1.699034
H	5.284856	-1.354848	-0.391573
C	3.595278	-2.679698	-0.603343
H	3.861783	-3.275736	0.278498
H	3.196862	-3.365521	-1.365230
C	0.261197	-3.324311	-1.084457
H	-0.823372	-3.363693	-0.888704
C	0.814701	-4.764328	-0.951086
H	1.802314	-4.795357	-0.477379
H	0.150693	-5.365264	-0.317490
C	0.882323	-5.310971	-2.393460
H	1.927864	-5.342833	-2.730199
H	0.491497	-6.331162	-2.475906
C	0.110792	-4.303545	-3.247132
H	0.393442	-4.330407	-4.305683
H	-0.970229	-4.499159	-3.187517
C	0.422632	-2.974769	-2.569133
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H	1.462098	-2.689706	-2.791441
P	-2.727059	0.911146	-0.146345
P	0.831622	-2.018997	0.107821
Pt	-0.758196	-0.313003	0.095032
C	4.280229	3.145244	-1.256801
C	5.538146	1.663684	-0.154205
C	4.655389	1.596319	0.902509
C	3.477830	2.383001	0.901510
C	3.327793	3.176251	-0.261970
O	2.617395	2.362263	1.861061
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F	4.107053	3.910151	-2.341614
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H	-0.984254	2.882429	3.722954
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106

1g·OAr E=-2813.743561 G=-2812.918362

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H	4.756843	2.350485	-2.033635
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H	5.482518	4.685554	-0.603347
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C	2.877712	3.465497	0.521899
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H	2.865937	1.404176	2.202621
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H	2.539165	-1.509234	1.833359
C	4.168368	-1.203772	3.275612
H	3.913699	-1.651236	4.242394
H	4.706041	-1.968579	2.695711
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H	2.031745	-1.672277	-3.366367
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C	-1.552745	-1.299196	2.388050
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C	-4.526295	2.502549	-0.327732
C	-3.691794	3.657641	-0.133135
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F	-5.395328	0.440975	0.358604
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F	-2.079378	4.529569	1.413608
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C	-0.106376	3.316320	-1.340428
H	-0.315034	3.854482	-2.262379
H	-1.137189	1.600932	-1.940212
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H	-2.545410	-4.499735	0.737248

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H	-0.524855	-3.551780	3.856428
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H	-0.743056	-1.295443	2.828719
H	-2.473942	-1.583664	2.566271
C	-3.391213	-1.469727	-0.231332
H	-3.580323	-0.712408	0.540428
C	-3.912996	-0.925011	-1.593016
H	-4.159272	0.139500	-1.499877
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H	-5.945350	-1.131726	-2.414137
H	-4.937393	-2.572058	-2.580686
C	-5.622188	-2.284353	-0.561591
H	-6.327818	-3.119225	-0.638249
H	-6.101807	-1.494150	0.034996
C	-4.293108	-2.679570	0.069496
H	-3.924383	-3.580646	-0.442260
H	-4.353784	-2.905040	1.140419
C	-1.308120	-2.839374	-1.704656
H	-2.320003	-3.172570	-1.978505
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5. Spectra of 2,3,5,6-tetrafluoro-4-allyloxy pyridine

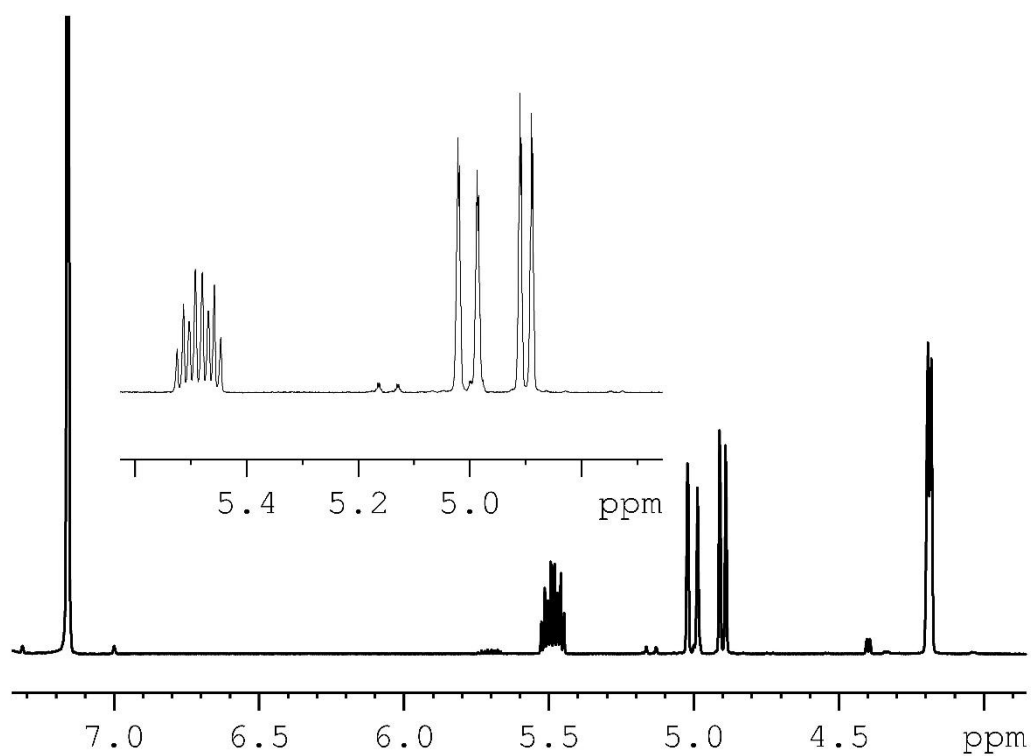


Fig. S3 ^1H NMR spectra (500 MHz) of 2,3,5,6-tetrafluoro-4-allyloxy pyridine in C_6D_6 at room temperature.

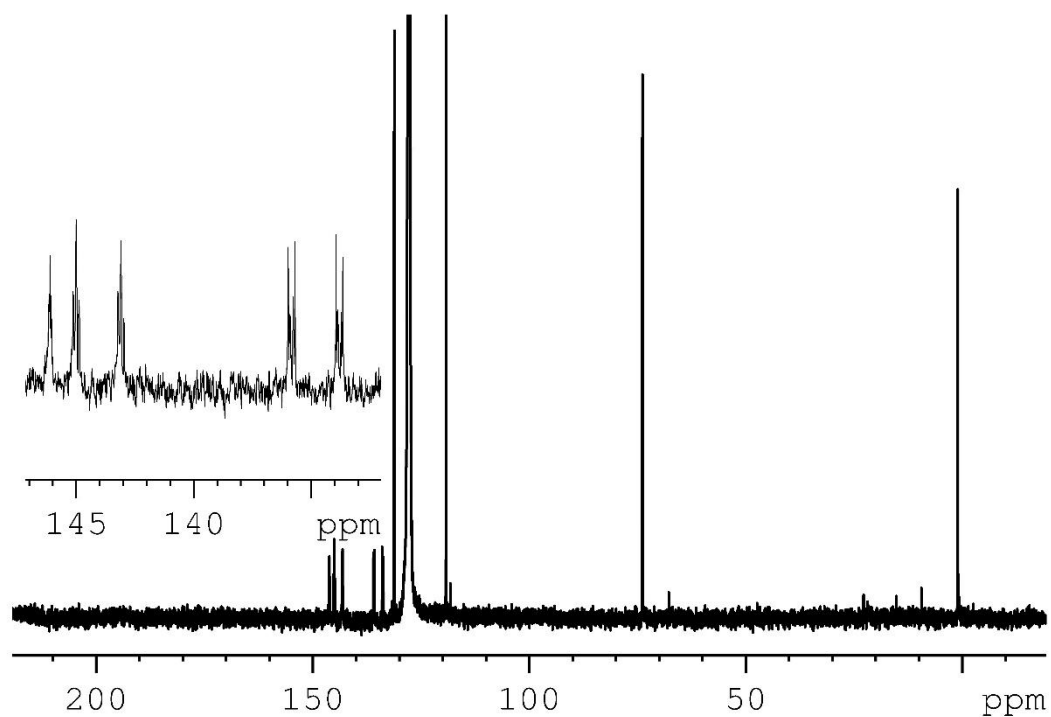


Fig. S4 ^{13}C NMR spectra (125.7 MHz) for 2,3,5,6-tetrafluoro-4-allyloxy pyridine in C_6D_6 . Aromatic carbon fluorine resonances expanded.

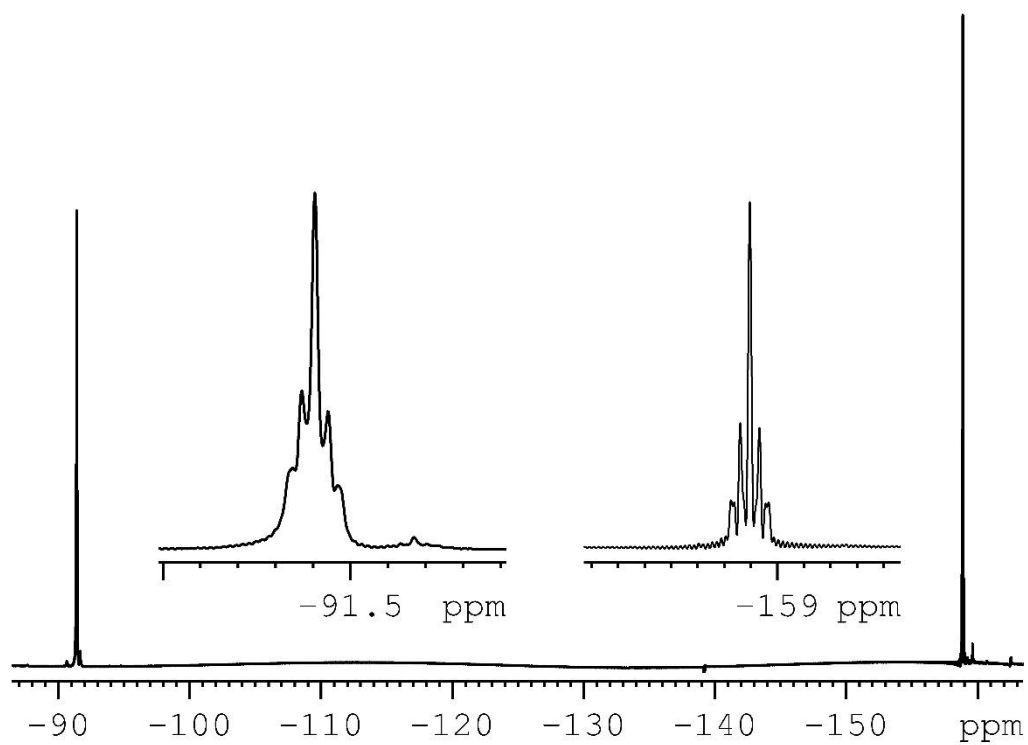


Fig. S5. ^{19}F NMR spectra (407.4 MHz) of 2,3,5,6-tetrafluoro-4-allyloxypyridine in C_6D_6 .

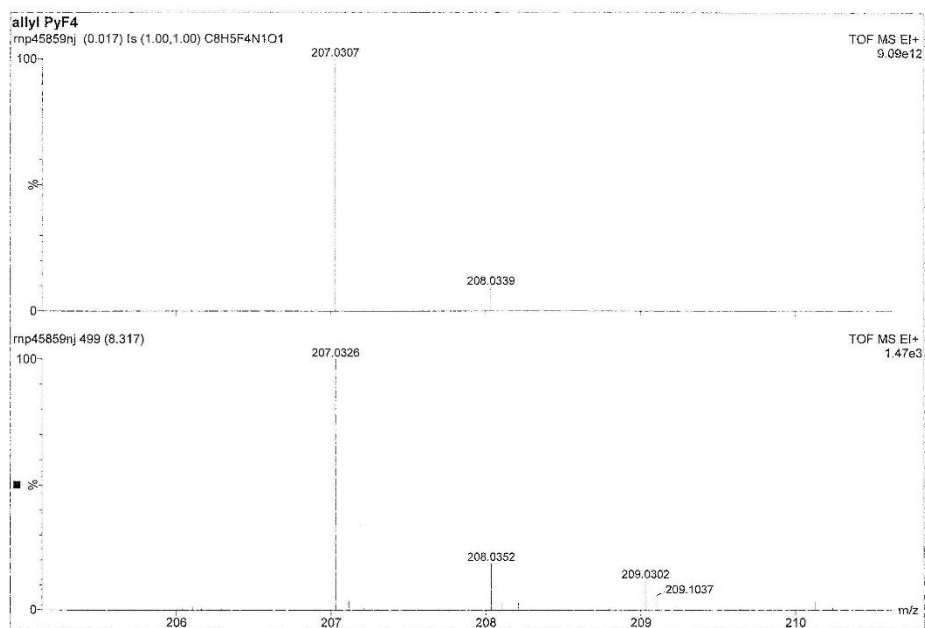


Fig. S6 Below: mass spectrum (LIFDI, M⁺) of 2,3,5,6-tetrafluoro-4-allyloxypyridine.
Above: calcd pattern for C₈H₅F₄NO.

6. Spectra of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$

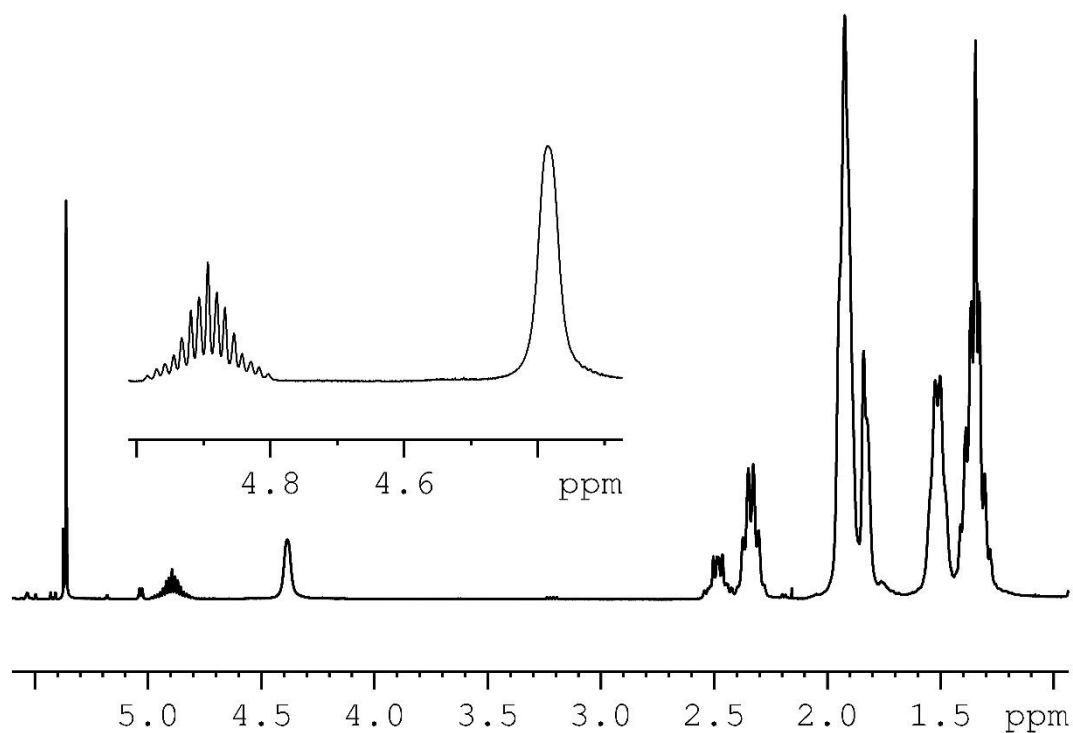


Fig. S7 ^1H NMR spectrum (500 MHz) of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$ in CD_2Cl_2 . Allyl sym and central proton resonances expanded.

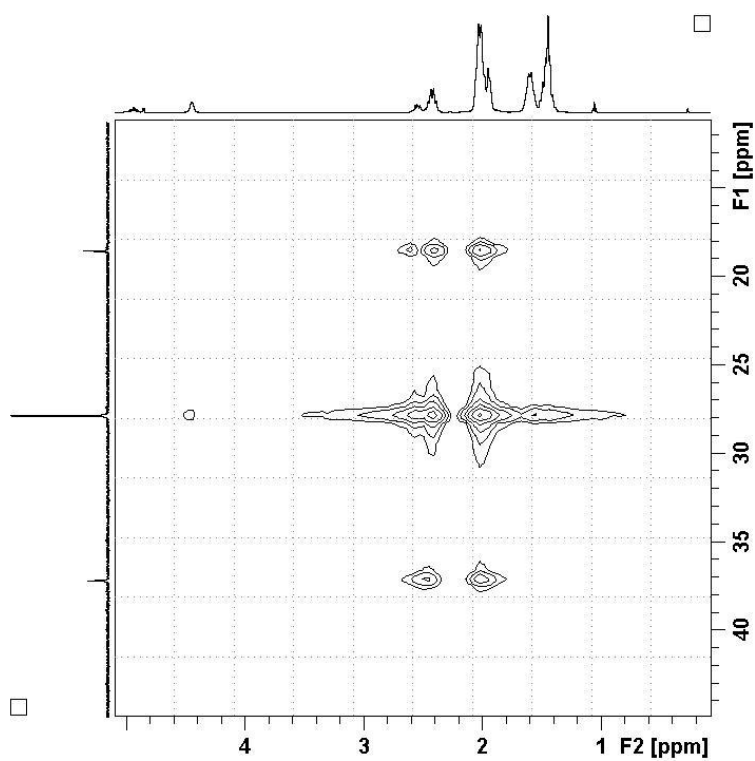


Fig. S8 ^{31}P - ^1H HSQC spectrum (500 MHz) of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$ in CD_2Cl_2 .

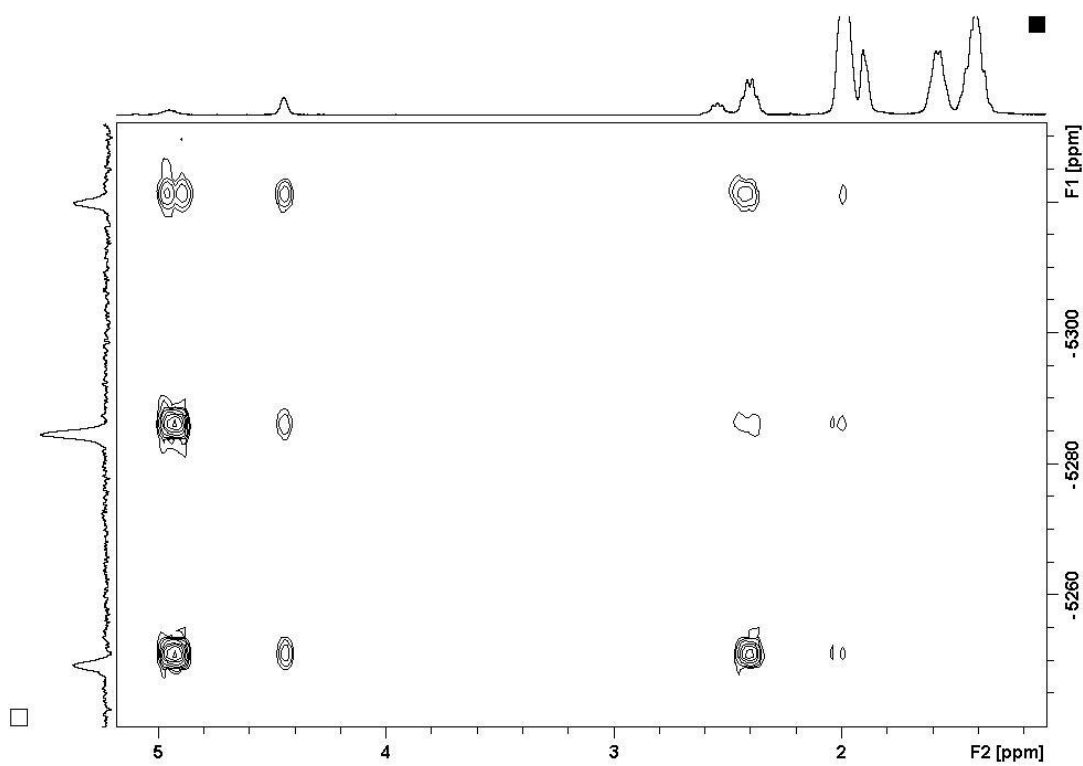


Fig. S9 ^{195}Pt - ^1H HSQC spectrum (500 MHz) of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$ in CD_2Cl_2 .

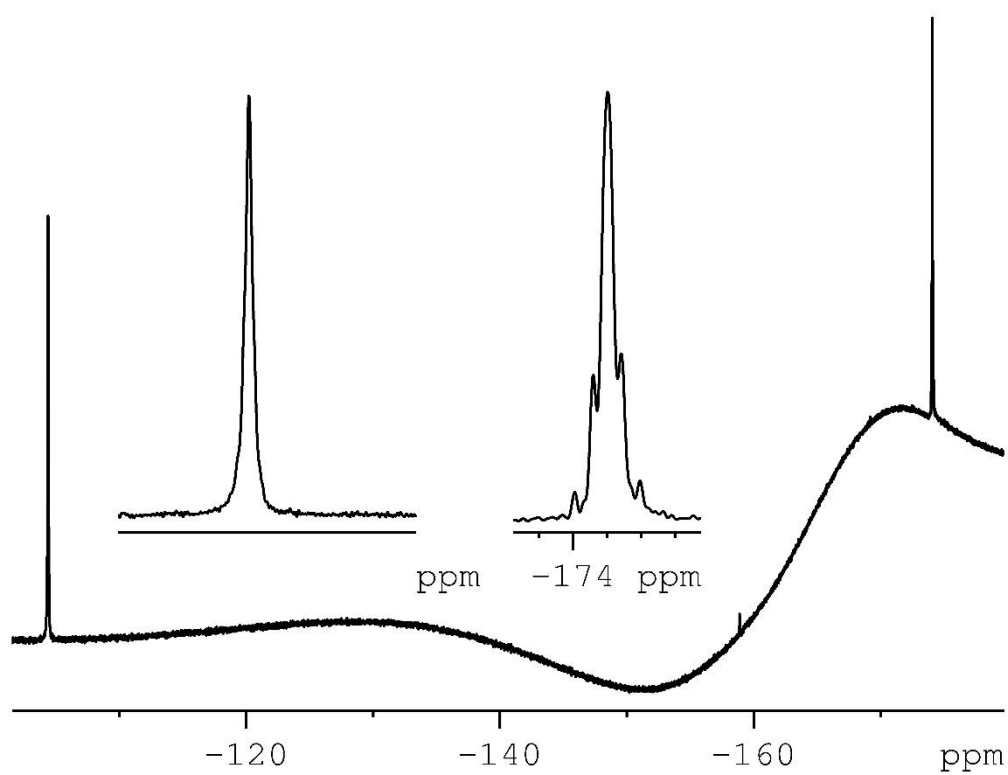


Fig. S10 ^{19}F NMR spectrum (407.4 MHz) of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$ in CD_2Cl_2 .

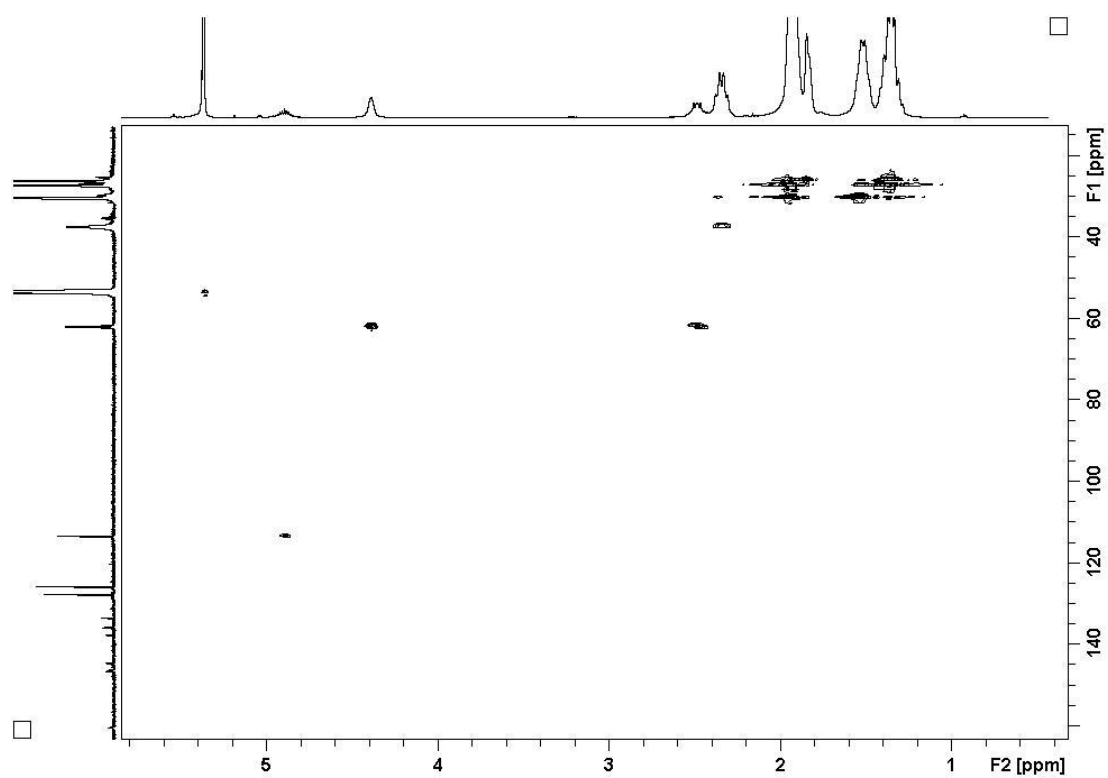


Fig. S11 ^{13}C - ^1H HSQC spectrum of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$ in CD_2Cl_2 .

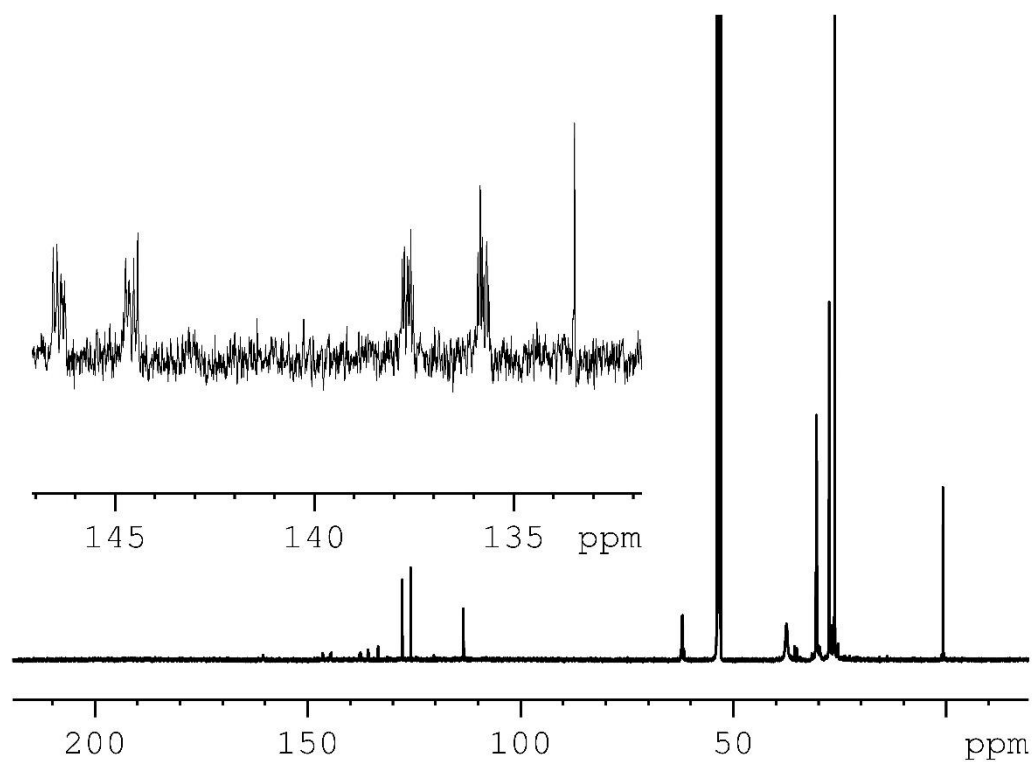


Fig. S12 $^{13}\text{C}\{^1\text{H}\}$ spectrum of $[\text{Pt}(\text{PCy}_3)_2(\eta^3\text{-allyl})][\text{OC}_5\text{NF}_4]$ in CD_2Cl_2 . Aromatic carbon fluorine resonances expanded. The resonances at δ 126 and 128 are due to traces of naphthalene impurity.

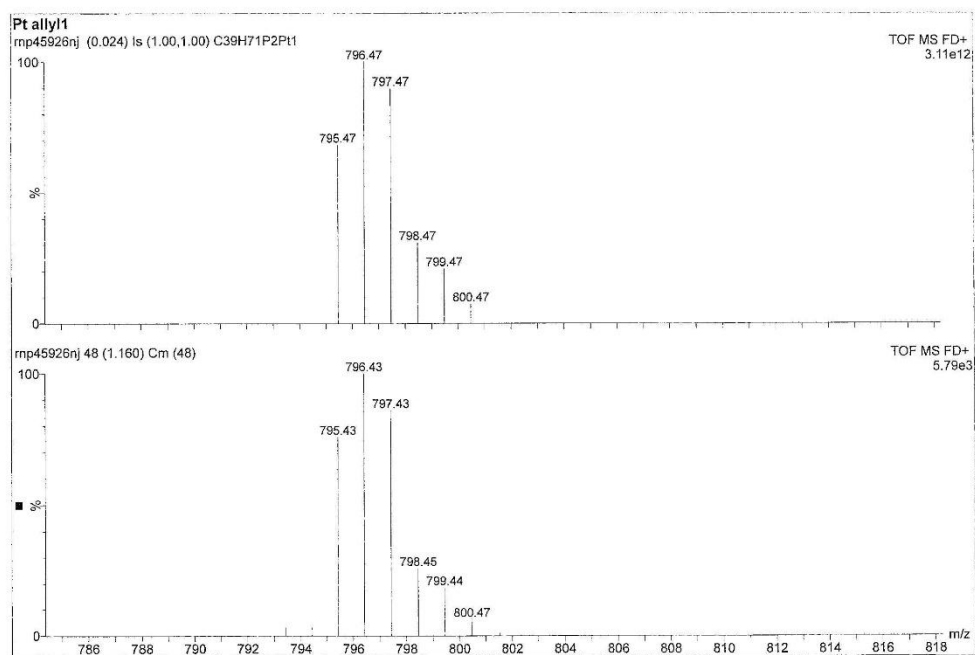


Fig. S13 Below: mass spectrum (LIFDI, M^+) of $[Pt(PCy_3)_2(\eta^3\text{-allyl})]^+$. Above: calcd isotope pattern for $C_{39}H_{72}P_2Pt$.