Supporting information

Exploiting the reactivity of 2-diazo-1,1,3,3,3-pentafluoropropyl phosphonate in [2,3]-sigmatropic rearrangement reactions

Ita Hajdin[a, b]*, Romana Pajkert[a], Antonija Mravak[b], Jianlin Han[c] and Gerd-Volker Röschenthaler[a]

[a] School of Science, Constructor University Bremen gGmbH, 28759 Bremen, Germany

[b] Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21000 Split, Croatia

[c] Jiangsu Co-Innovation Centre of Efficient Processing and Utilization of Forest Resources, International Innovation Center for Forest Chemicals and Materials, College of Chemical Engineering, Nanjing Forestry University, Nanjing 210037, China

* Corresponding author's e-mail address: ihajdin@ktf-split.hr

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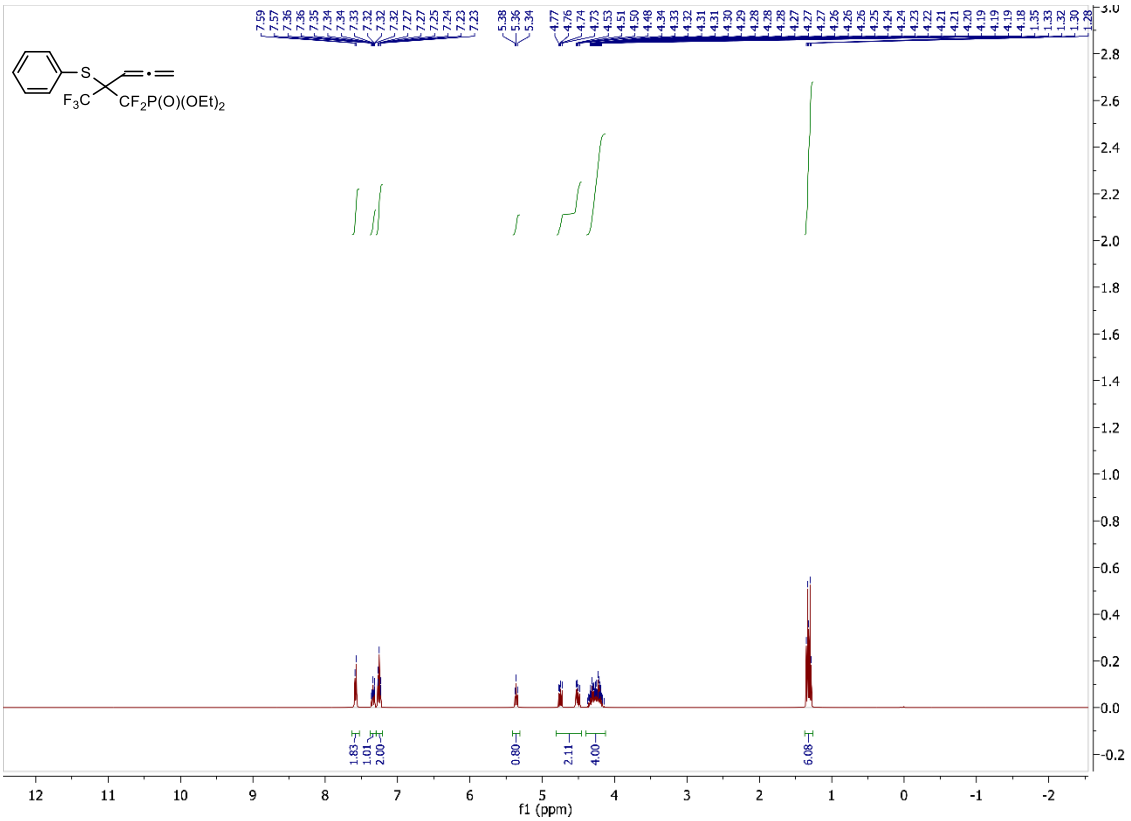
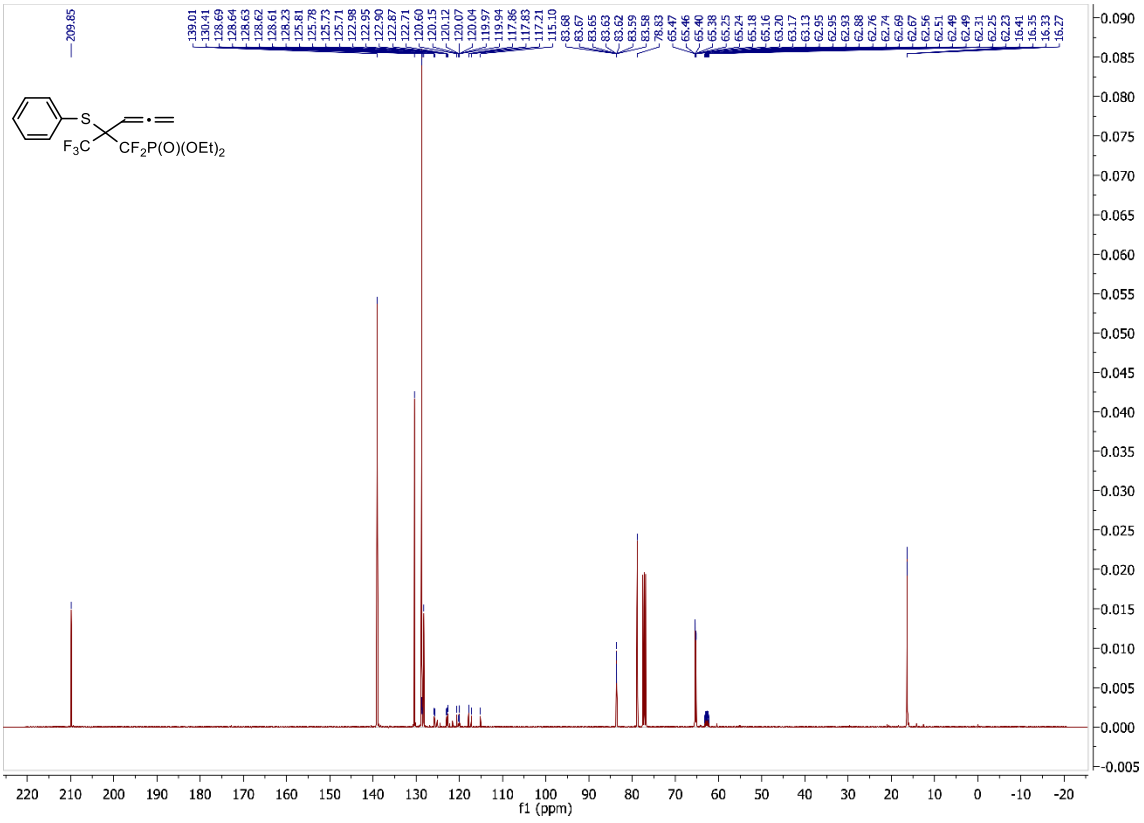
1. Copies of ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR, and ^{31}P-NMR spectra

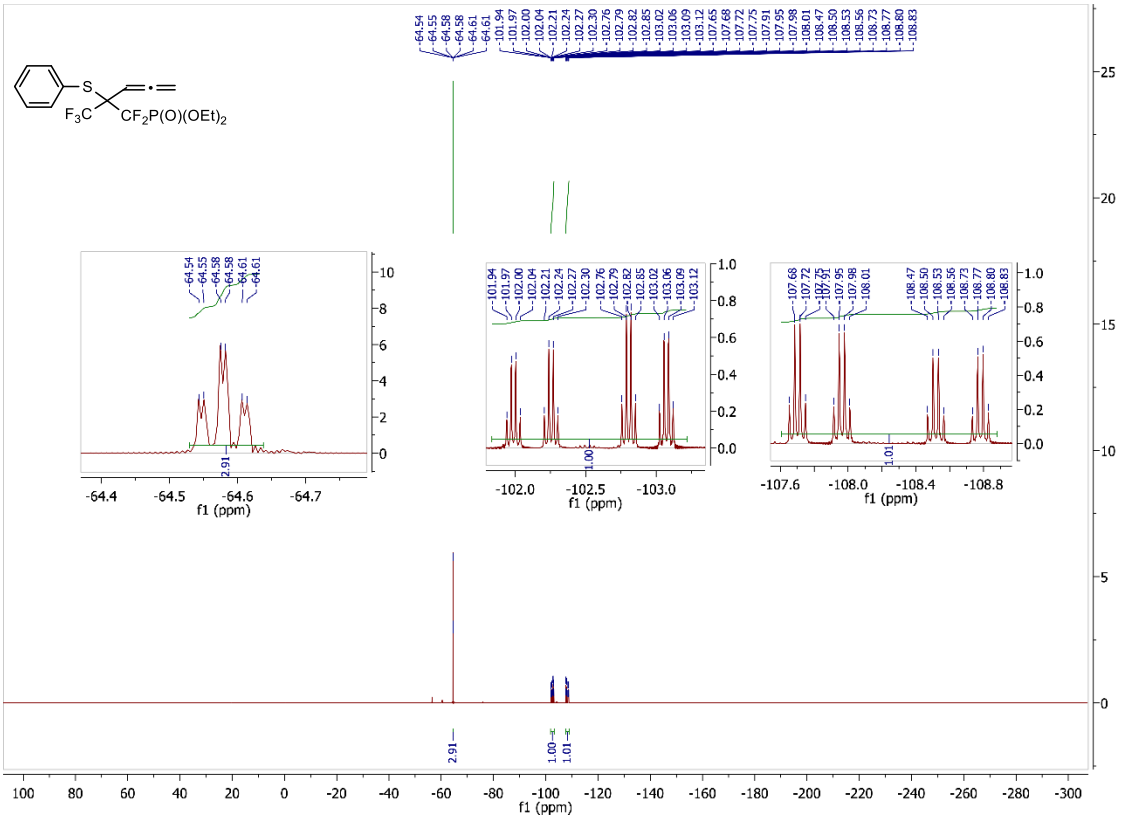
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2**:



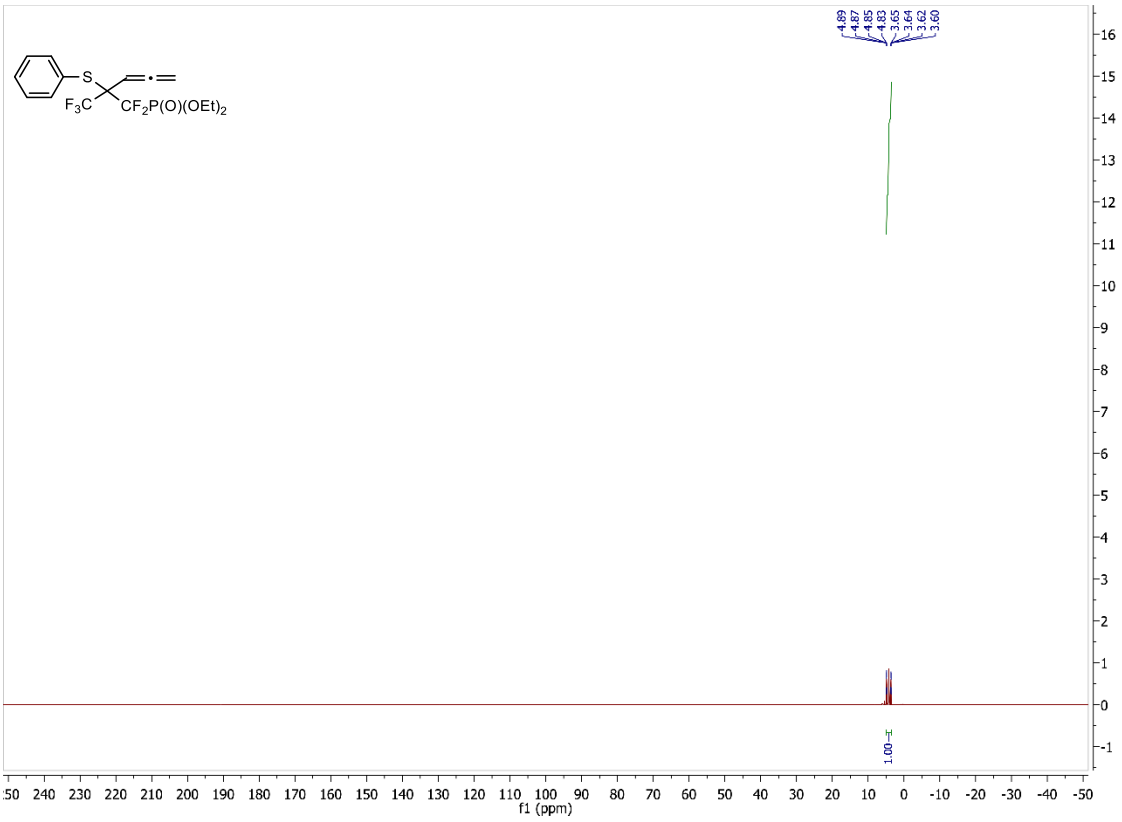
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **2**:



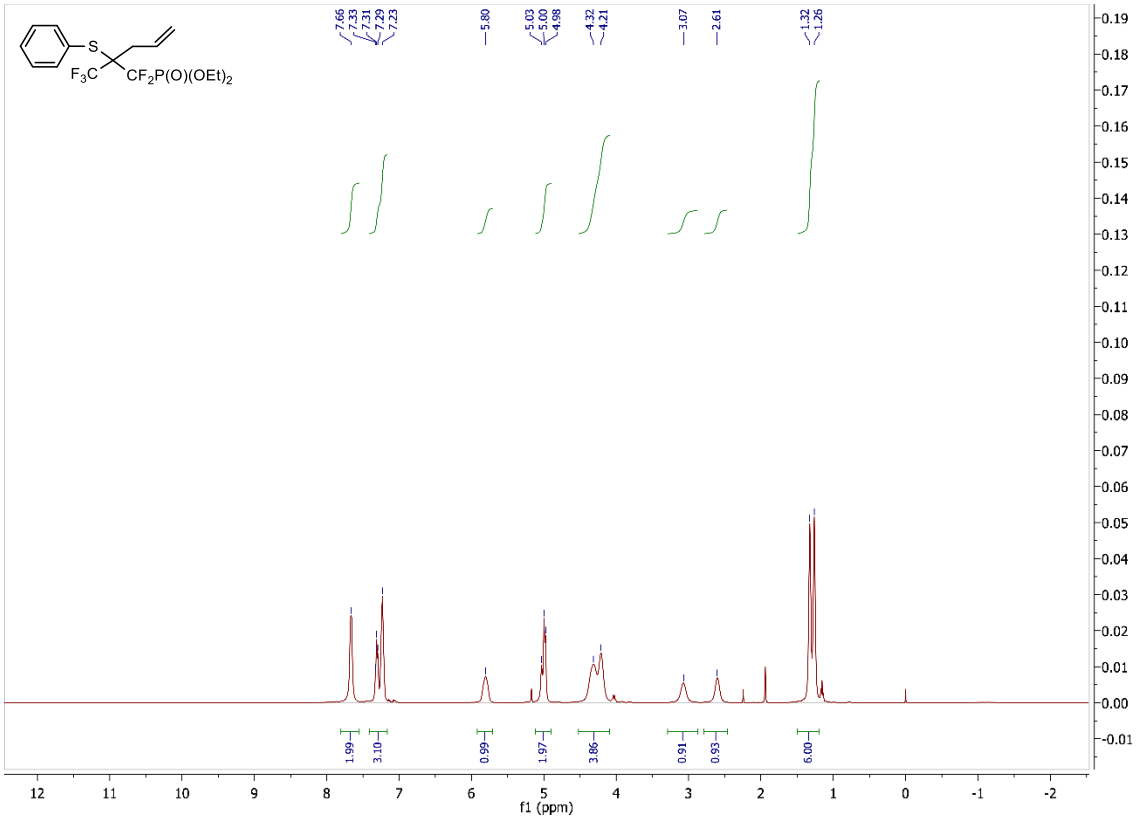
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **2**:



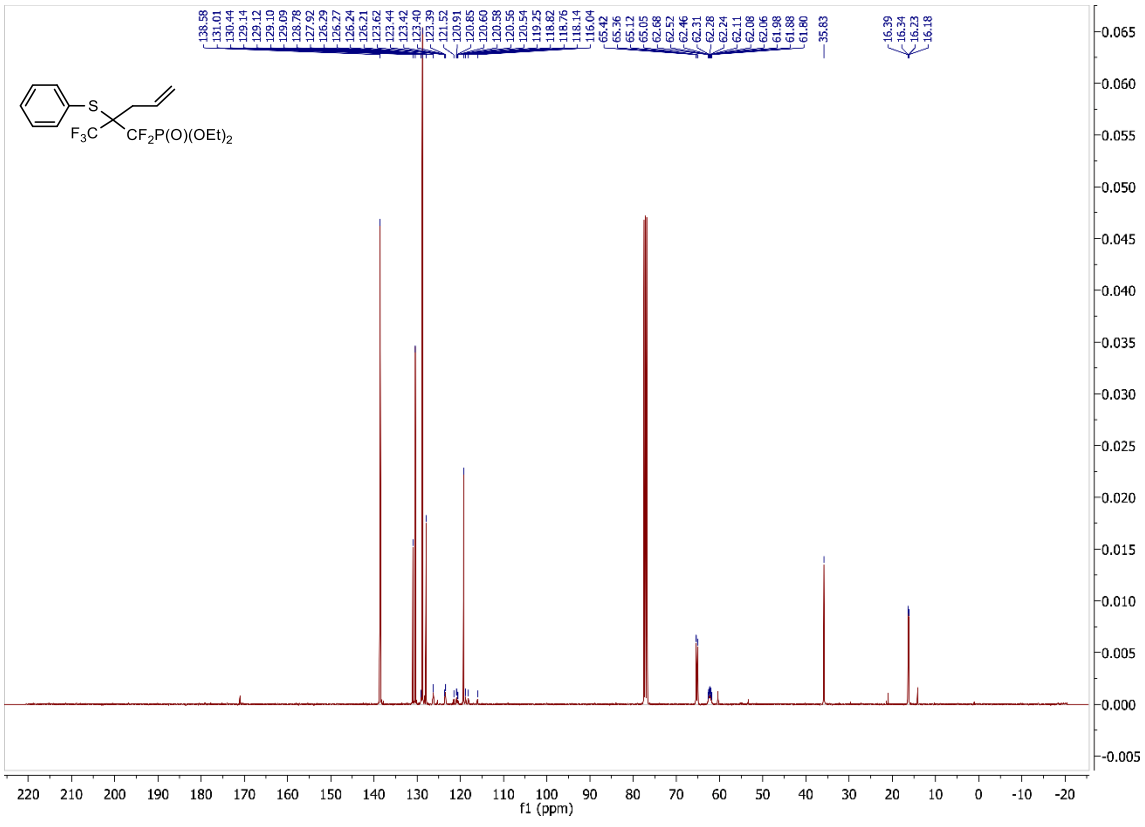
^{31}P {^{1}H} NMR (161 MHz, $CDCl_3$) spectrum of **2**:



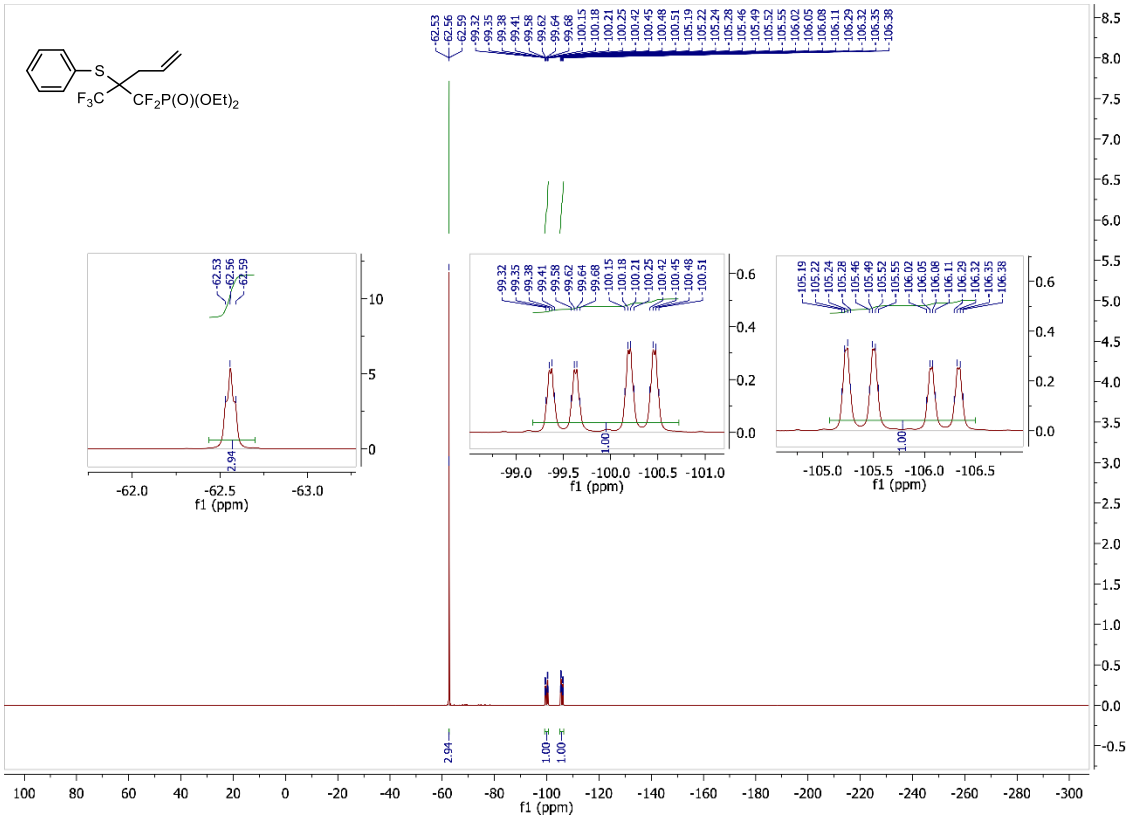
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3a**:



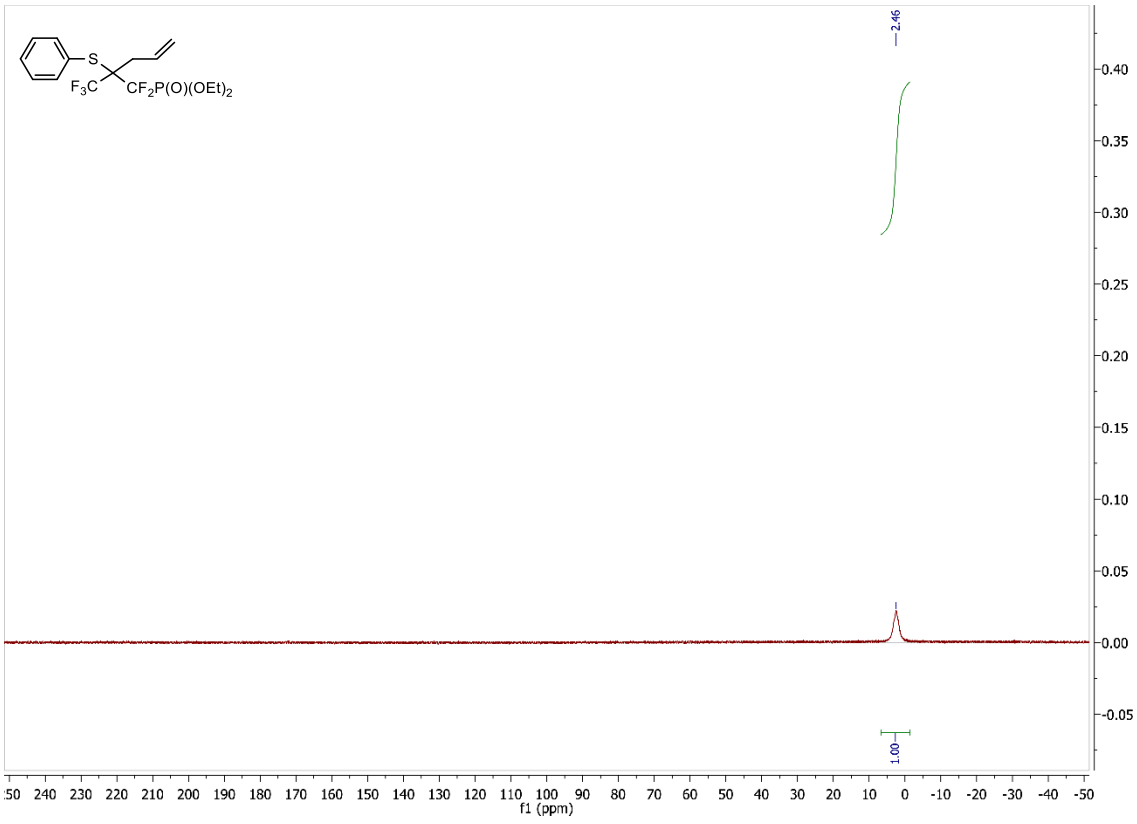
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3a**:



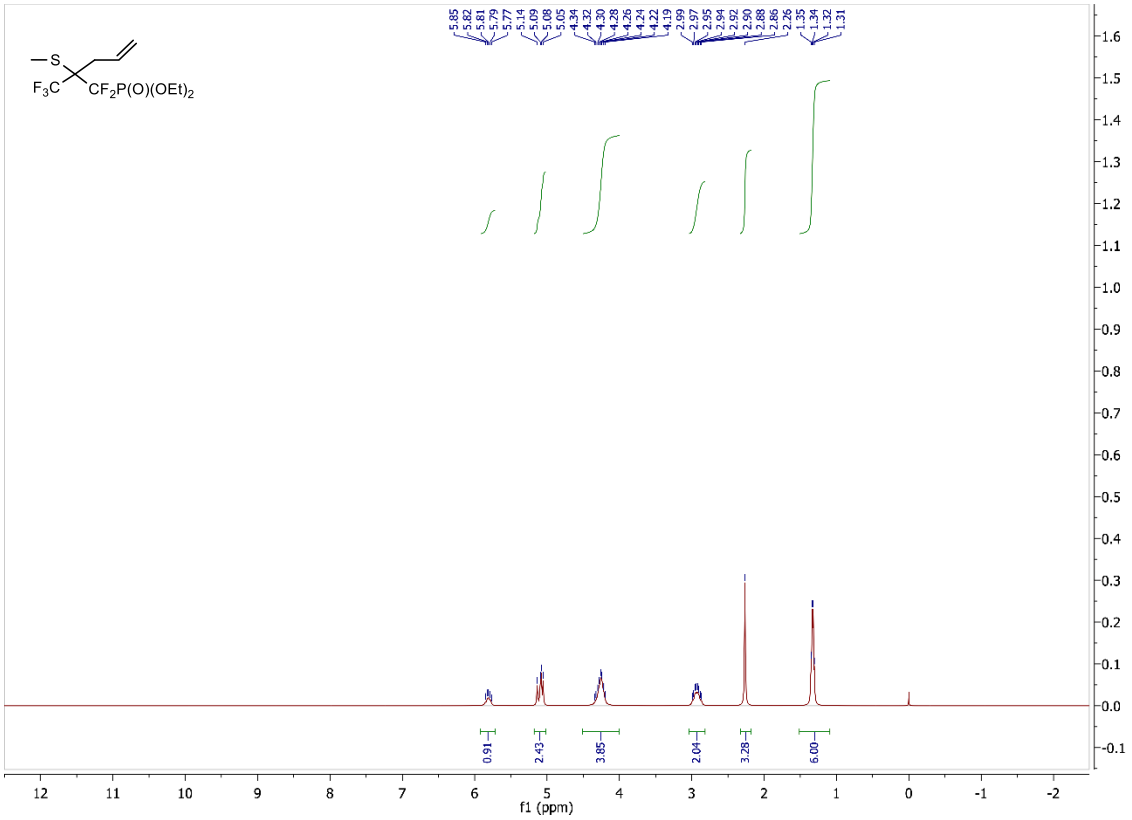
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3a**:



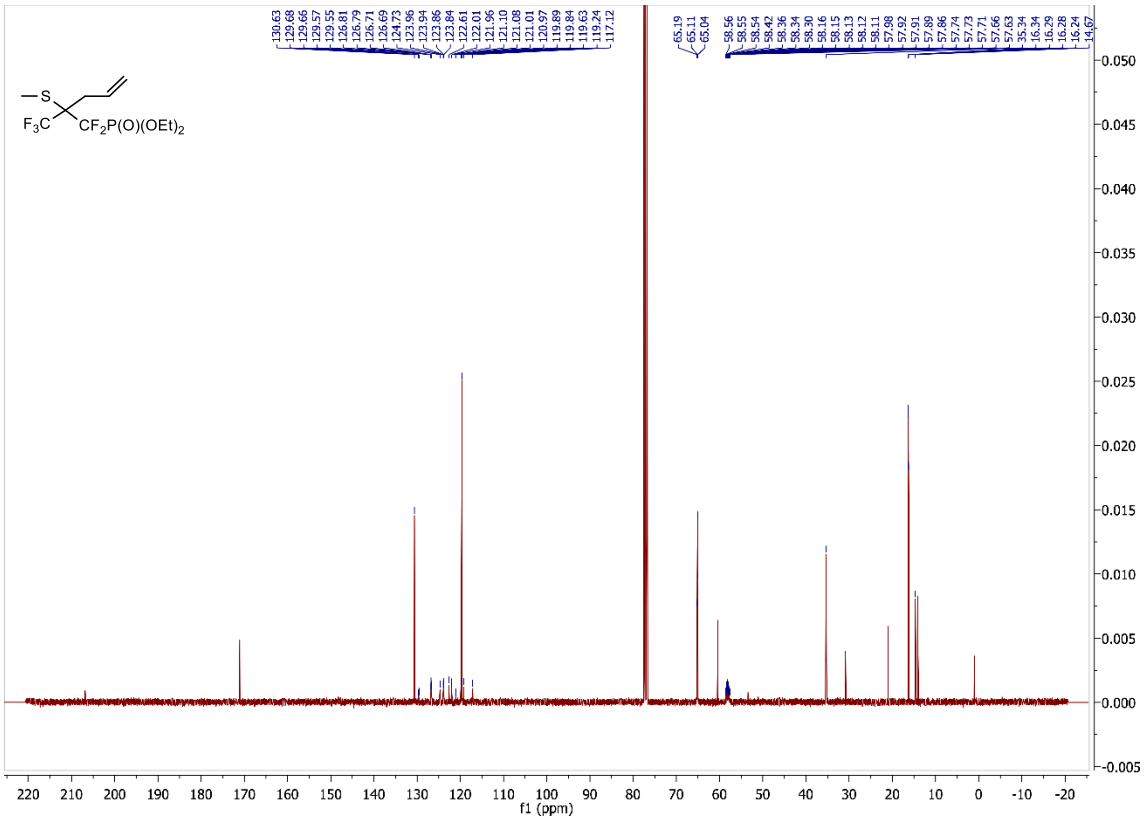
^{31}P {^{1}H} NMR (161 MHz, $CDCl_3$) spectrum of **3a**:



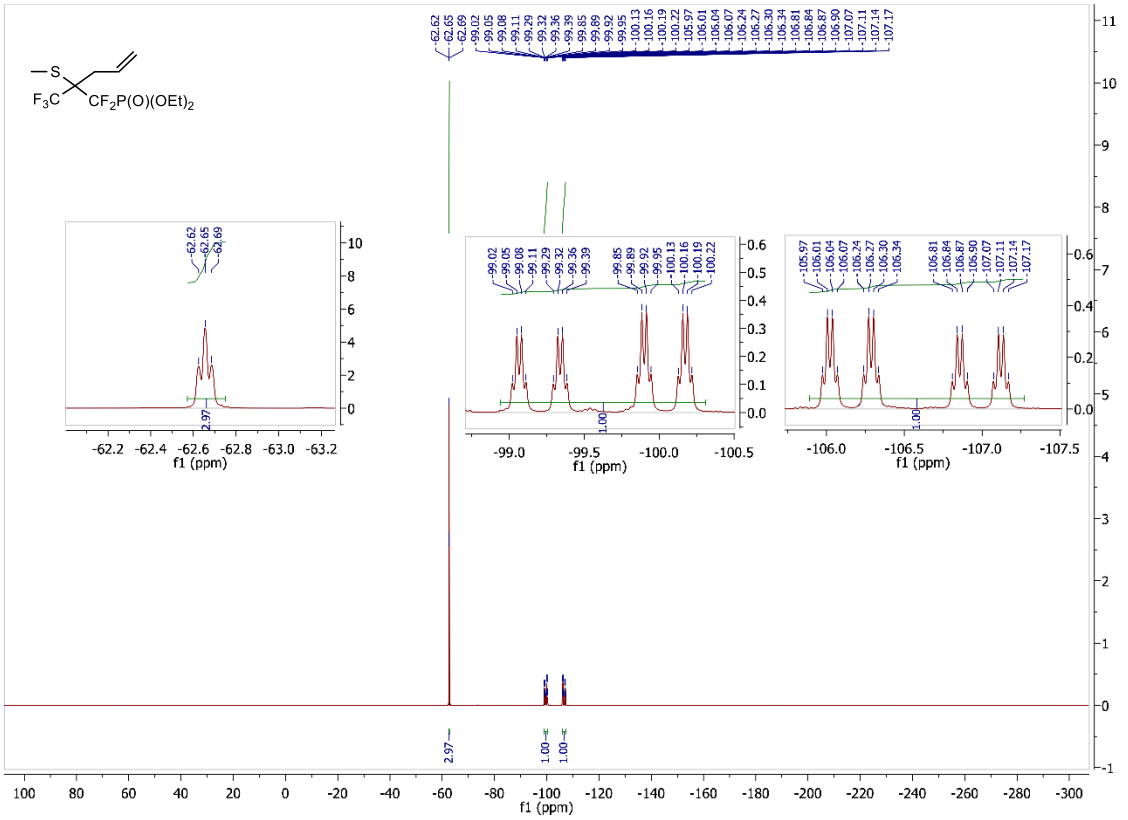
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3b**:



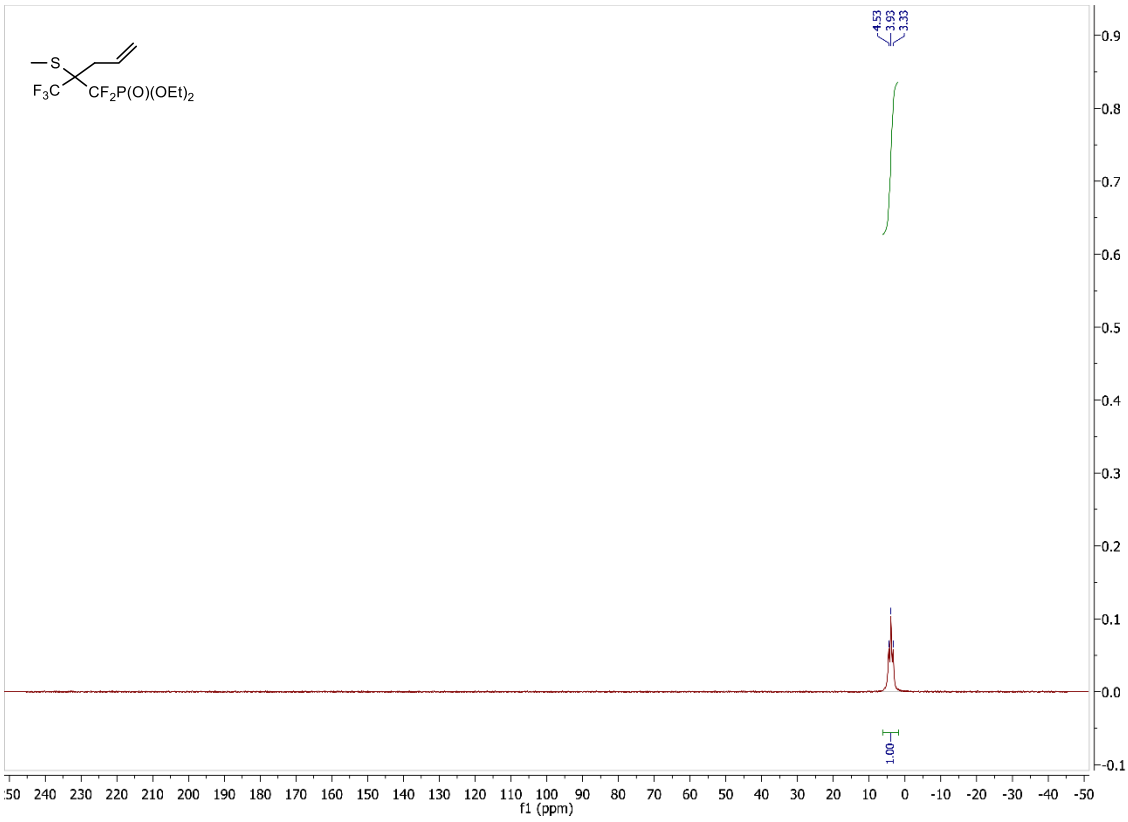
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3b**:



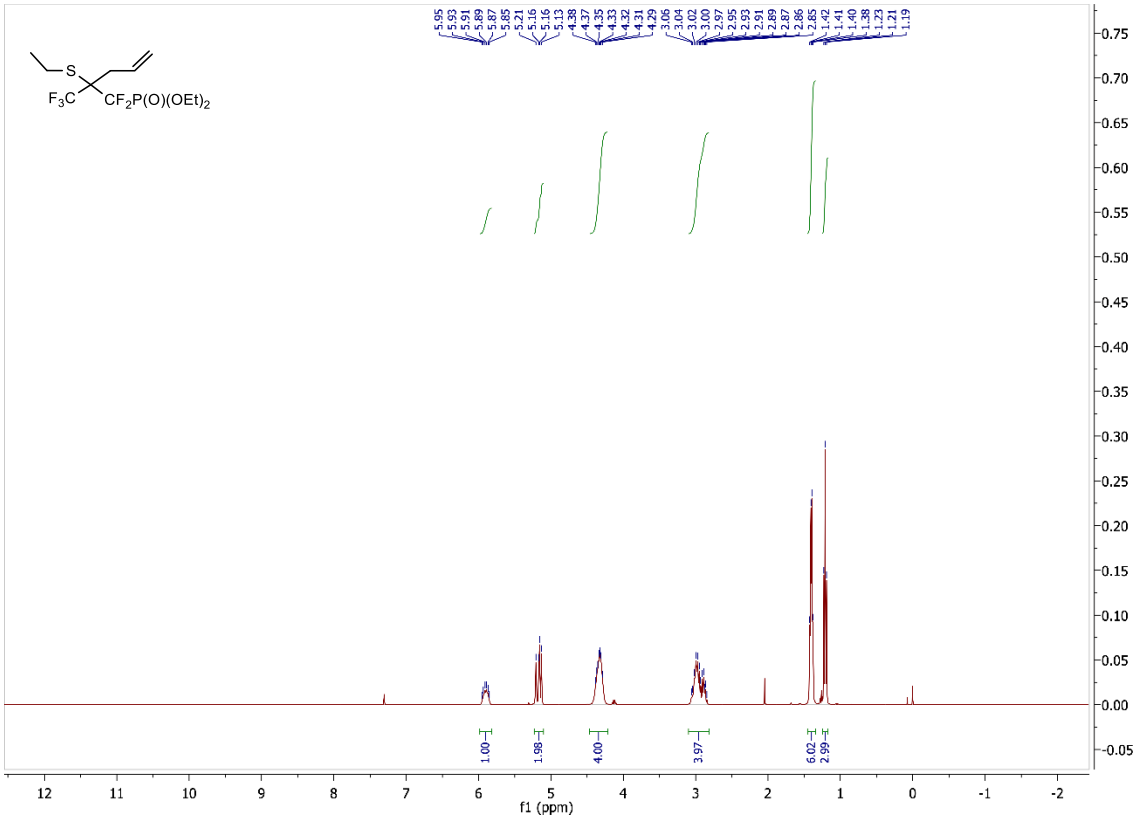
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3b**:



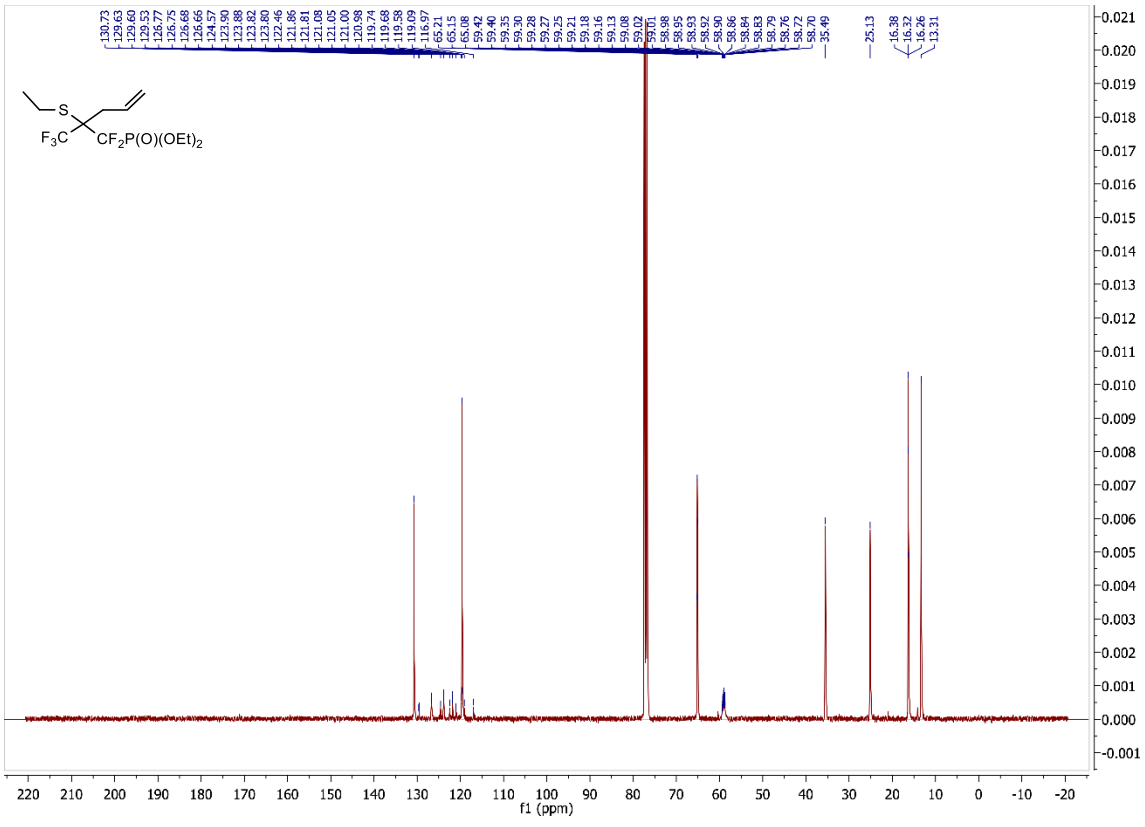
^{31}P {^{1}H} NMR (161 MHz, $CDCl_3$) spectrum of **3b**:



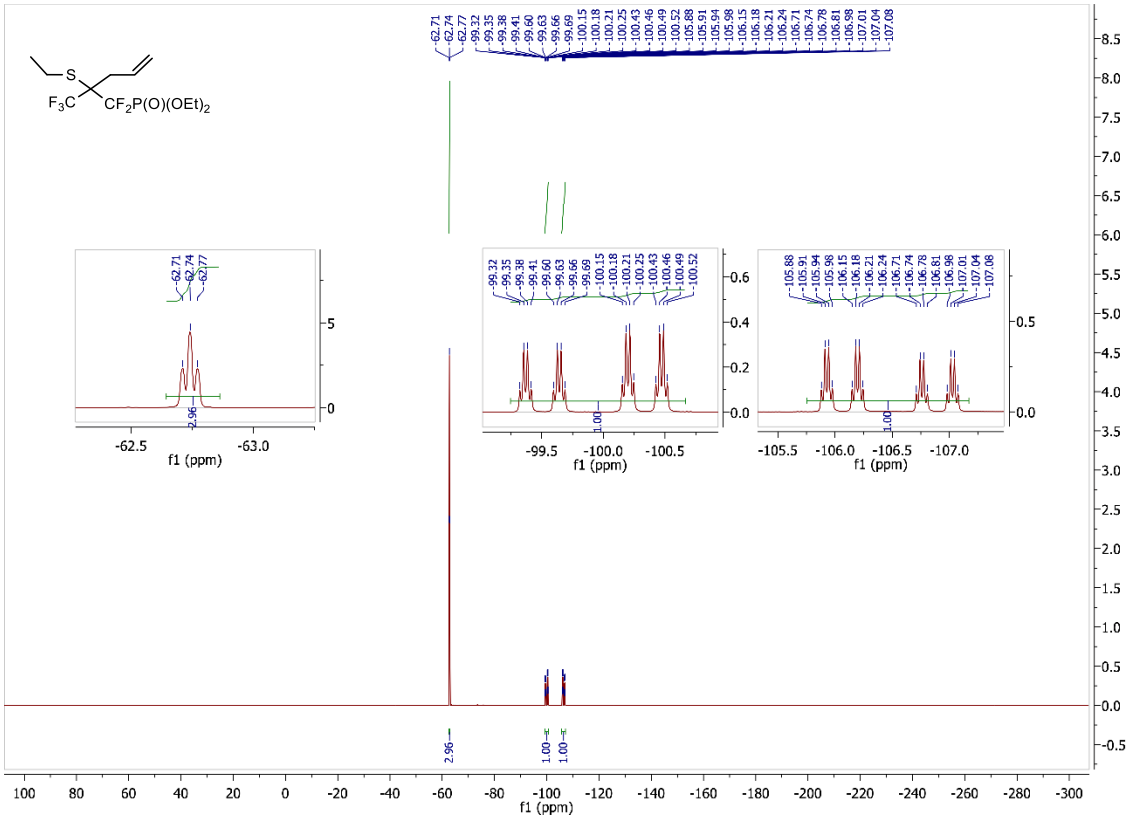
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3c**:



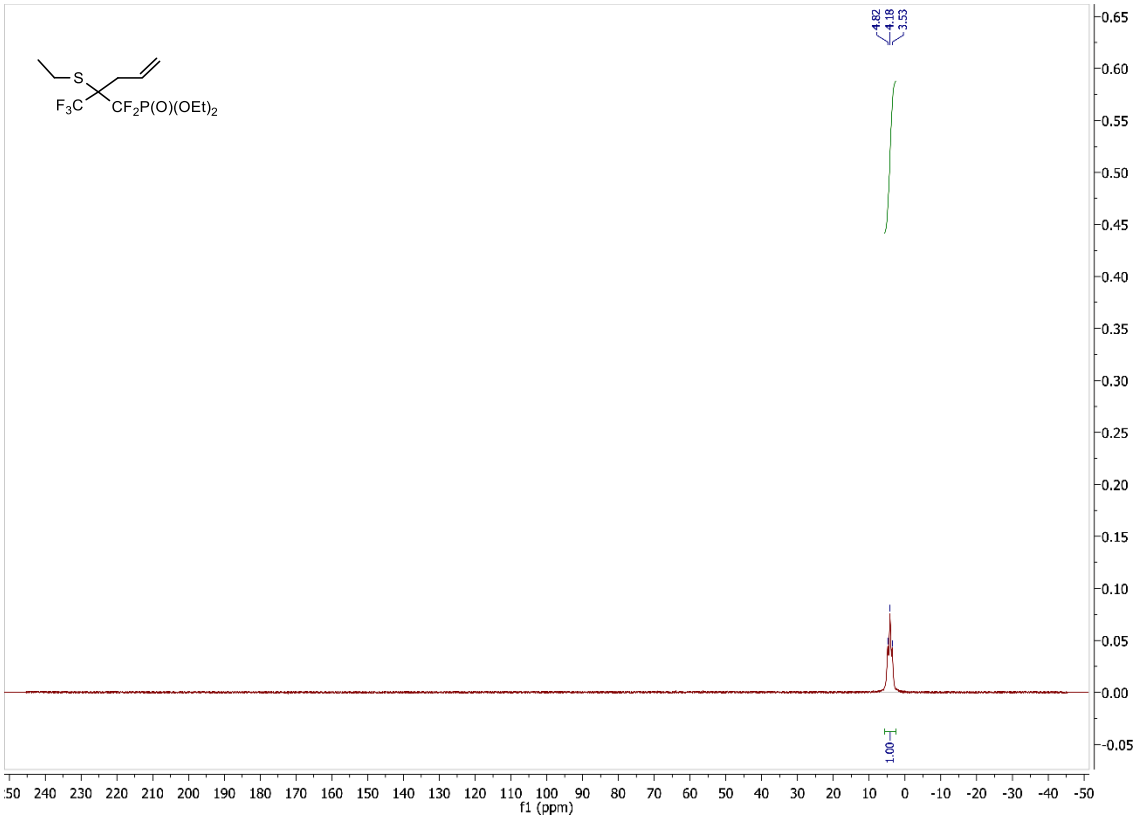
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3c**:



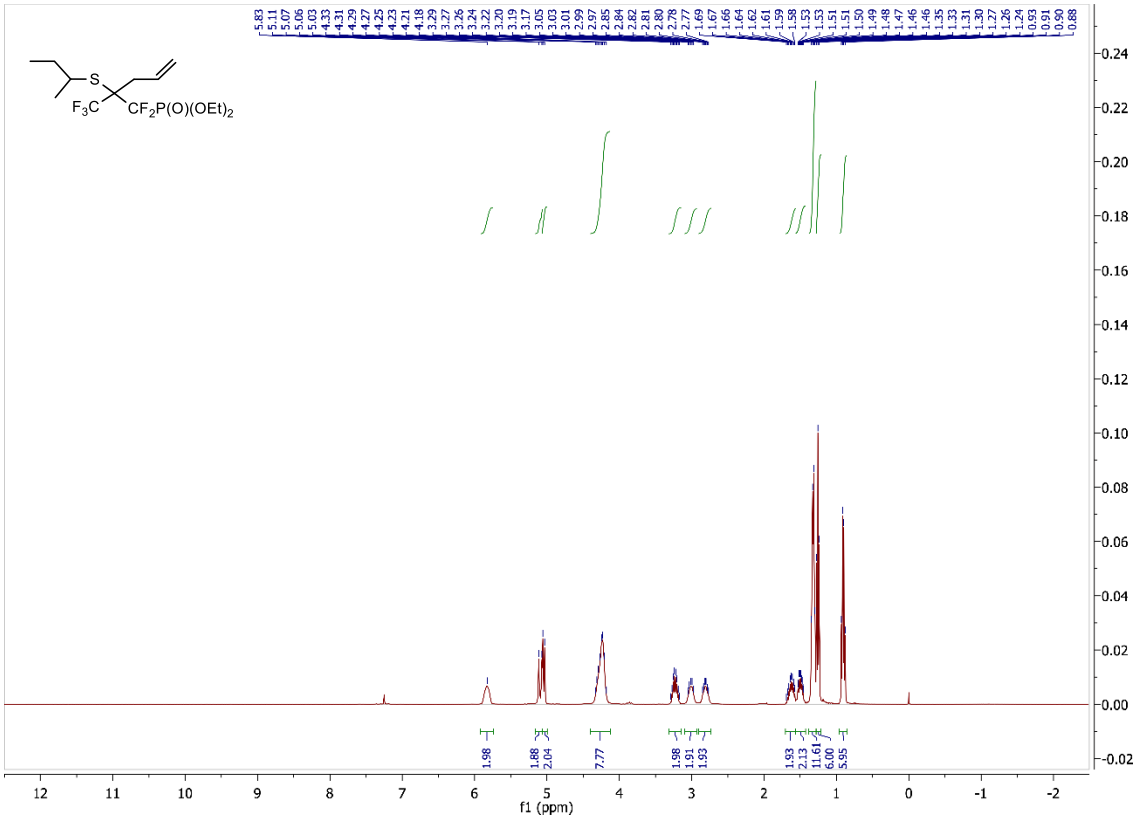
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3c**:



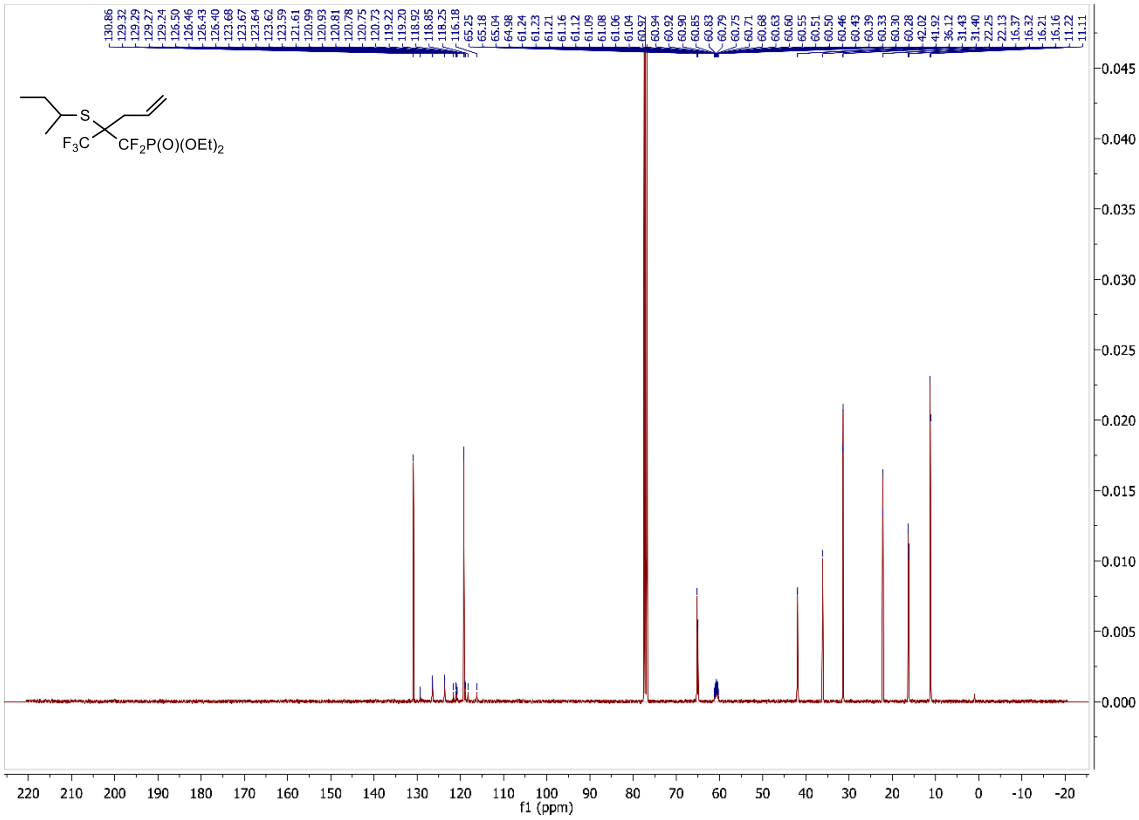
^{31}P {^{1}H} NMR (161 MHz, $CDCl_3$) spectrum of **3c**:



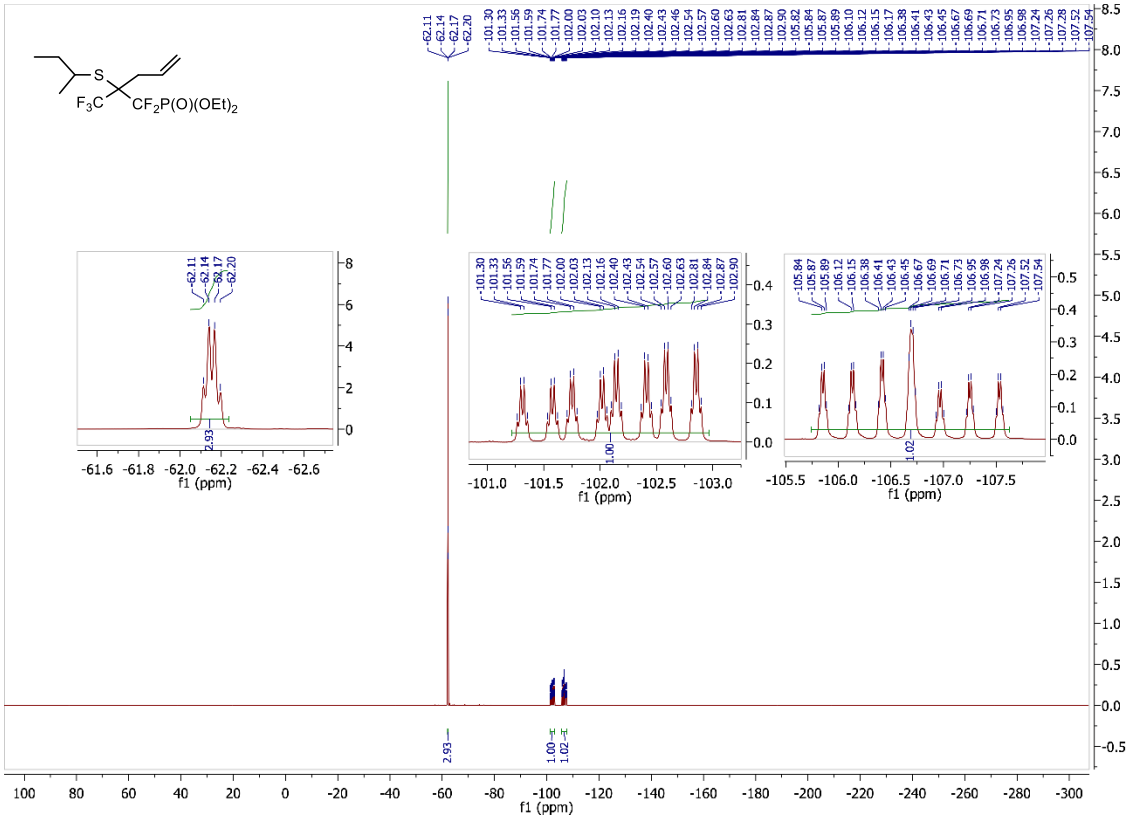
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3d (two stereoisomers in 1:1 ratio)**:



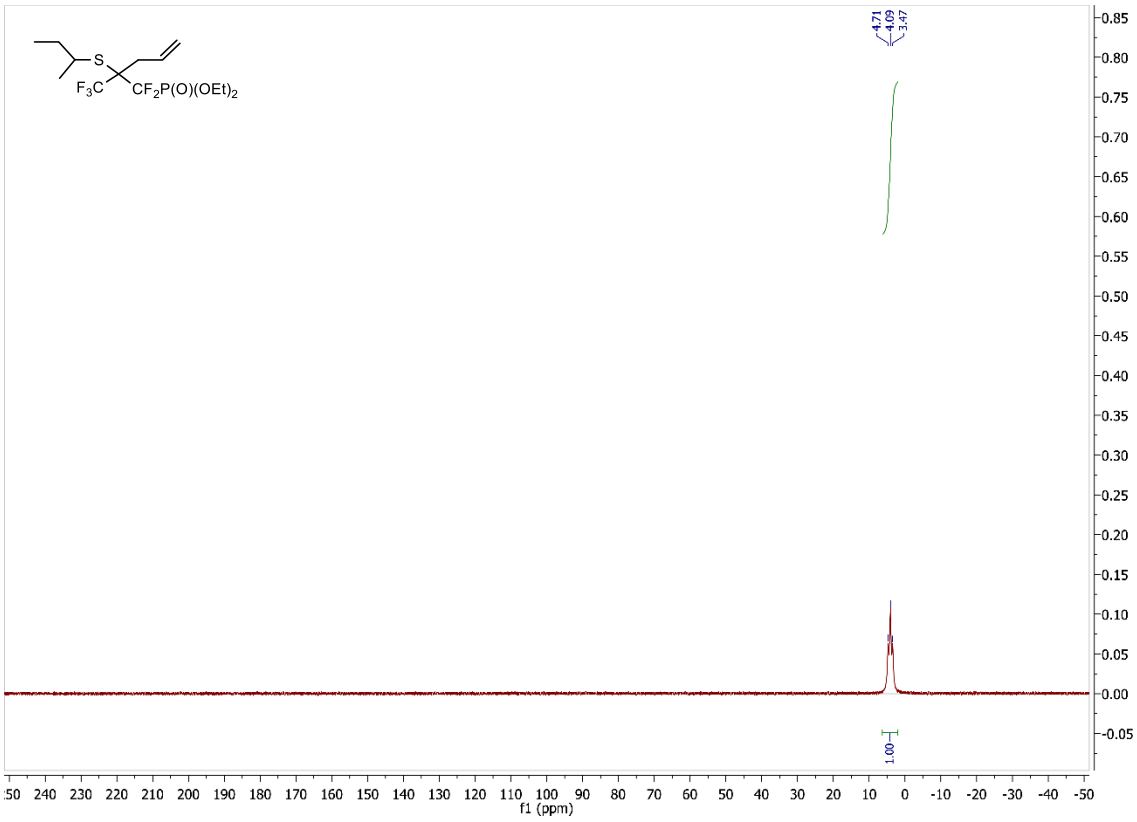
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3d (two stereoisomers in 1:1 ratio)**:



^{19}F NMR (376 MHz, $CDCl_3$) spectrum of **3d (two stereoisomers in 1:1 ratio)**:



^{31}P {^{1}H} NMR (161 MHz, $CDCl_3$) spectrum of **3d (two stereoisomers in 1:1 ratio)**:



2. DFT calculations

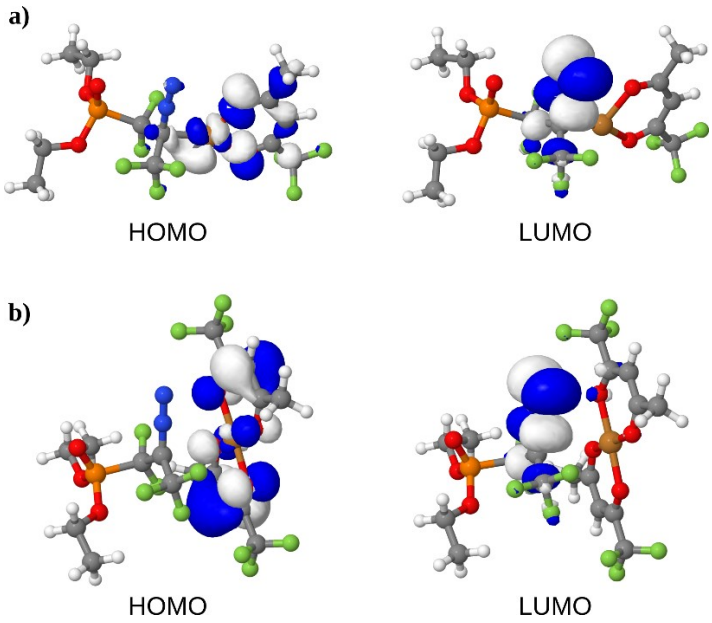


Figure S1. HOMO and LUMO frontier orbitals illustrating electron delocalization in **a)** the diazo complex with CuF_3acac and **b)** the diazo complex with $Cu(F_3acac)_2$.

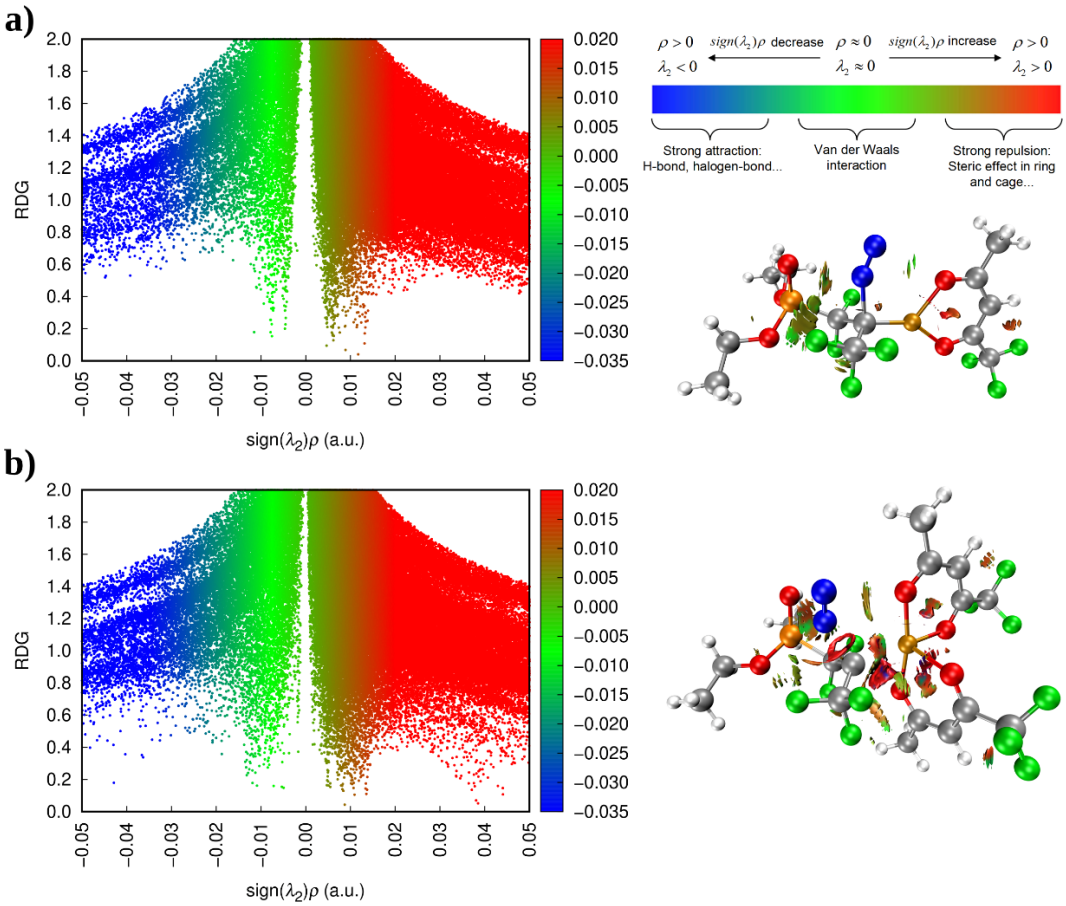
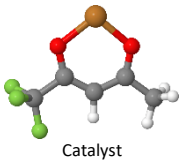
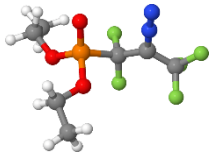
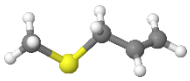
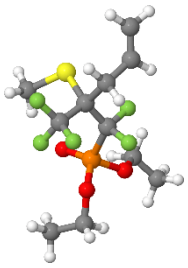


Figure S2. Reduced density gradient (RDG) analysis of TS1 for **a)** the diazo complex with CuF_3acac and **b)** the diazo complex with $Cu(F_3acac)_2$ showing regions of weak and strong noncovalent interactions.

Table S1. Cartesian coordinates with calculated thermochemical values for each reaction step.

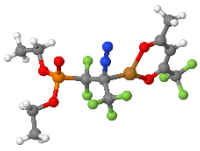
Structure	Coordinates			Thermochemical values / Hartree
Substrates and Catalyst				
 Catalyst	C	5.321993	-0.839957	0.379727	Zero-point correction= 0.087765 (Hartree/Particle)
	C	3.889077	-0.908591	-0.183288	Thermal correction to Energy= 0.105152
	O	3.000665	-0.548628	0.702041	Thermal correction to Enthalpy= 0.106368
	Cu	1.132091	-0.599039	0.089179	Thermal correction to Gibbs Free Energy= 0.031457
	C	3.730317	-1.328658	-1.510690	Sum of electronic and zero-point Energies= -838.989224
	C	2.500601	-1.467725	-2.238669	Sum of electronic and thermal Energies= -838.971837
	O	1.311561	-1.218359	-1.766280	Sum of electronic and thermal Enthalpies= -838.970621
	C	2.553941	-1.943151	-3.676796	Sum of electronic and thermal Free Energies= -839.045532
	F	6.318188	-1.218047	-0.532866	
	F	5.475580	-1.672483	1.498024	
	F	5.646779	0.457557	0.802366	
	H	4.632820	-1.578039	-2.053696	
	H	3.575938	-2.120257	-4.021364	
	H	2.078631	-1.196748	-4.325373	
	H	1.975587	-2.870514	-3.775315	
 Diazo compound	P	1.263987	0.129731	0.492240	Zero-point correction= 0.185031 (Hartree/Particle)
	O	1.315245	-0.074505	2.066682	Thermal correction to Energy= 0.216913
	C	-0.348610	-0.613979	-0.271826	Thermal correction to Enthalpy= 0.218129
	C	-1.631964	-0.226462	0.369364	Thermal correction to Gibbs Free Energy= 0.106878
	N	-1.709434	-0.050049	1.680165	Sum of electronic and zero-point Energies= -1113.303450
	N	-1.798521	0.101592	2.824276	Sum of electronic and thermal Energies= -1113.271569
	C	-2.896534	-0.109182	-0.413468	Sum of electronic and thermal Enthalpies= -1113.270352
	F	-4.004574	-0.015269	0.444443	Sum of electronic and thermal Free Energies= -1113.381603
	F	-2.953506	1.022041	-1.248310	
	F	-3.116841	-1.207686	-1.258422	
	F	-0.146908	-2.048704	-0.213248	
	F	-0.404812	-0.316631	-1.649224	
	O	1.110459	1.685263	-0.131629	
	O	2.547316	-0.519785	-0.396603	
	C	3.436754	-1.609156	0.123797	
	H	4.447743	-1.224246	-0.035901	
	H	3.258687	-1.728016	1.198834	
	C	2.238879	2.665156	-0.196324	
	H	3.042107	2.213689	-0.788397	
	H	2.588941	2.853676	0.825307	
	C	3.183660	-2.896064	-0.653797	
	H	3.327146	-2.734376	-1.727486	
	H	3.895629	-3.663344	-0.320556	
	H	2.167516	-3.267967	-0.487609	
	C	1.677712	3.920429	-0.848842	
	H	0.856462	4.334225	-0.254178	
	H	2.470484	4.676297	-0.923389	
	H	1.307936	3.701232	-1.855881	
 Allyl methyl sulfide	C	0.838494	0.149202	0.325169	Zero-point correction= 0.110012 (Hartree/Particle)
	S	-0.918223	0.505405	0.924722	Thermal correction to Energy= 0.120630
	C	-1.893753	-0.284852	-0.526514	Thermal correction to Enthalpy= 0.121846
	C	-3.321701	-0.512301	-0.114353	Thermal correction to Gibbs Free Energy= 0.066360
	C	-4.380774	0.134326	-0.647248	Sum of electronic and zero-point Energies= -167.183077
	H	-1.819717	0.379500	-1.392163	Sum of electronic and thermal Energies= -167.172459
	H	-1.390466	-1.233428	-0.746898	Sum of electronic and thermal Enthalpies= -167.171243
	H	-3.479590	-1.252012	0.671538	Sum of electronic and thermal Free Energies= -167.226729
	H	-5.396123	-0.071957	-0.316489	
	H	-4.260696	0.886104	-1.425688	
	H	1.517207	0.559325	1.077662	
	H	0.994931	-0.929595	0.237053	
	H	1.017781	0.638915	-0.635792	
Products				
 N_2	N	0.000000	0.000000	0.143496	Zero-point correction= 0.005171 (Hartree/Particle)
	N	0.000000	0.000000	1.276504	Thermal correction to Energy= 0.008214
					Thermal correction to Enthalpy= 0.009430
					Thermal correction to Gibbs Free Energy= -0.019728
					Sum of electronic and zero-point Energies= -109.476167
					Sum of electronic and thermal Energies= -109.473124
					Sum of electronic and thermal Enthalpies= -109.471908
					Sum of electronic and thermal Free Energies= -109.501066
	C	-0.216366	-0.557872	-0.526827	Zero-point correction= 0.290473 (Hartree/Particle)
	P	1.467578	0.011495	0.299397	Thermal correction to Energy= 0.330281
	O	1.653790	1.501175	-0.457810	Thermal correction to Enthalpy= 0.331497
	C	2.955909	2.227415	-0.540351	Thermal correction to Gibbs Free Energy= 0.205778
	C	3.287659	2.944302	0.767765	Sum of electronic and zero-point Energies= -1171.079676



Pr

C	-1.626534	-0.215993	0.039007
S	-1.998343	-1.199143	1.652398
C	-4.049517	-2.801596	-0.987612
C	-2.911425	-2.125533	-1.242255
C	-2.750930	-0.640012	-0.988489
F	-0.081534	-1.976920	-0.568505
F	-0.139210	-0.151553	-1.889019
C	-1.779950	1.304951	0.247705
F	-0.782626	1.860022	1.060611
O	2.615305	-0.930265	-0.530794
C	3.152153	-2.206508	0.031558
C	4.410861	-2.533718	-0.761080
O	1.555277	-0.093338	1.879129
F	-1.741567	2.025001	-0.956177
F	-3.002413	1.629440	0.847497
C	-1.362012	-0.145855	3.098936
H	3.358522	-2.059058	1.097581
H	2.380300	-2.973929	-0.088515
H	2.784384	2.930737	-1.358486
H	3.732132	1.511989	-0.834871
H	5.164083	-1.747329	-0.640829
H	4.834151	-3.480025	-0.399257
H	4.180886	-2.640749	-1.826505
H	3.454071	2.235036	1.586254
H	4.202944	3.535676	0.630825
H	2.476766	3.622668	1.053477
H	-1.933443	0.779072	3.178816
H	-1.558928	-0.781713	3.967667
H	-0.292735	0.033827	2.991602
H	-4.144567	-3.857464	-1.230194
H	-4.912282	-2.324983	-0.525252
H	-2.072736	-2.640649	-1.705227
H	-3.692942	-0.240635	-0.600542
H	-2.535284	-0.134228	-1.937353

Intermediates

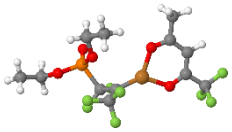
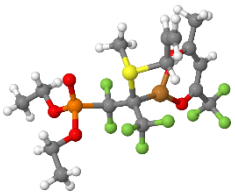


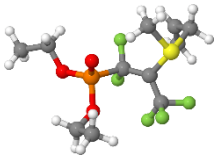
Int1

C	-2.413511	0.619125	0.016150
C	-1.503251	0.054841	1.110423
Cu	0.423205	0.772783	0.715769
O	1.104249	1.937513	2.260790
C	2.273878	2.496342	2.291275
C	2.615971	3.308346	3.525586
F	-2.141535	2.028386	-0.060477
F	-2.062905	0.062919	-1.218237
P	-4.340396	0.546877	0.280113
O	-4.651542	0.859184	1.806569
O	-4.649358	-0.967138	-0.370756
C	-6.020069	-1.470064	-0.712238
C	-5.826918	-2.866884	-1.283403
O	-5.020047	1.588651	-0.869452
C	-5.330419	3.026264	-0.574637
C	-6.208109	3.516989	-1.717226
C	-1.400010	-1.454504	1.289619
F	-0.510498	-1.751431	2.335602
F	-2.613385	-2.079708	1.634325
F	-0.941537	-2.082923	0.142297
O	2.047136	0.965376	-0.348837
C	3.067646	1.663948	0.057470
C	3.245480	2.385066	1.241160
C	4.220857	1.654922	-0.963262
F	4.675644	0.352878	-1.219319
F	5.346084	2.392934	-0.563275
F	3.821744	2.186261	-2.198921
N	-1.684672	0.690613	2.336655
N	-1.744028	1.239253	3.340359
H	-5.837646	3.078630	0.394782
H	-4.379723	3.567252	-0.524268
H	-6.457702	-0.778433	-1.439639
H	-6.617598	-1.478359	0.206342
H	-7.144695	2.951034	-1.762530
H	-6.448496	4.576587	-1.559838
H	-5.688308	3.417700	-2.675774
H	-5.354940	-3.525262	-0.547031
H	-6.805178	-3.286382	-1.552540
H	-5.201247	-2.835517	-2.181259
H	4.186519	2.900567	1.381847

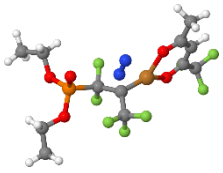
Zero-point correction= 0.272930 (Hartree/Particle)
Thermal correction to Energy= 0.325188
Thermal correction to Enthalpy= 0.326404
Thermal correction to Gibbs Free Energy= 0.162855
Sum of electronic and zero-point Energies= -1952.309583
Sum of electronic and thermal Energies= -1952.257325
Sum of electronic and thermal Enthalpies= -1952.256108
Sum of electronic and thermal Free Energies= -1952.419657

Sum of electronic and thermal Energies= -1171.039868
Sum of electronic and thermal Enthalpies= -1171.038652
Sum of electronic and thermal Free Energies= -1171.164371

	H	3.590863	3.796744	3.447204	
	H	2.616266	2.650971	4.404833	
	H	1.842289	4.068326	3.690348	
 Int2	C	-1.999043	1.495417	-1.871018	Zero-point correction= 0.264287 (Hartree/Particle)
	C	-1.261776	0.393915	-1.207731	Thermal correction to Energy= 0.312825
	Cu	0.080115	0.709303	0.027955	Thermal correction to Enthalpy= 0.314041
	O	-0.007833	1.016182	1.955776	Thermal correction to Gibbs Free Energy= 0.161059
	C	0.975782	1.262845	2.772447	Sum of electronic and zero-point Energies= -1842.839549
	C	0.601441	1.486417	4.219937	Sum of electronic and thermal Energies= -1842.791011
	F	-1.210864	2.673994	-1.926613	Sum of electronic and thermal Enthalpies= -1842.789795
	F	-2.389647	1.239602	-3.217025	Sum of electronic and thermal Free Energies= -1842.942777
	P	-3.619576	1.960193	-0.839517	
	O	-3.689281	3.434228	-0.268437	
	O	-3.374927	0.662315	0.219727	
	C	-4.218730	0.321584	1.404530	
	C	-3.421711	-0.681923	2.228834	
	O	-4.941386	1.440611	-1.756519	
	C	-5.749184	2.361465	-2.622074	
	C	-7.069435	1.651437	-2.887366	
	C	-1.643175	-1.013162	-1.604901	
	F	-1.383926	-1.928797	-0.576945	
	F	-2.969605	-1.233342	-1.995971	
	F	-0.837177	-1.396603	-2.699008	
	O	2.011116	0.870439	0.006900	
	C	2.747801	1.126282	1.049335	
	C	2.344279	1.325279	2.368917	
	C	4.245541	1.203851	0.709203	
	F	4.709920	-0.000103	0.165922	
	F	5.053494	1.480918	1.819985	
	F	4.506245	2.202557	-0.235974	
	H	-5.883953	3.310614	-2.091815	
	H	-5.179756	2.527179	-3.542515	
	H	-5.157000	-0.098747	1.028167	
	H	-4.414537	1.244519	1.962328	
	H	-7.616792	1.480845	-1.954265	
	H	-7.688424	2.273954	-3.546638	
	H	-6.898763	0.688048	-3.378752	
	H	-2.467617	-0.246298	2.543258	
	H	-4.000169	-0.956428	3.120536	
	H	-3.223501	-1.589908	1.649972	
	H	3.092503	1.534107	3.121007	
	H	1.473851	1.698071	4.842669	
	H	0.088932	0.596728	4.606668	
	H	-0.104464	2.323244	4.288583	
 Int3	C	1.401077	-0.646879	0.137288	Zero-point correction= 0.377037 (Hartree/Particle)
	Cu	-1.335189	-0.015621	-0.226365	Thermal correction to Energy= 0.437960
	O	-2.493076	1.018731	1.211459	Thermal correction to Enthalpy= 0.439176
	C	-3.727100	0.766643	1.532070	Thermal correction to Gibbs Free Energy= 0.258424
	C	-4.341864	1.617079	2.629858	Sum of electronic and zero-point Energies= -2010.054702
	F	0.844572	-0.900566	1.455559	Sum of electronic and thermal Energies= -2009.993779
	F	1.226376	-1.854928	-0.575392	Sum of electronic and thermal Enthalpies= -2009.992563
	P	3.294588	-0.520047	0.564587	Sum of electronic and thermal Free Energies= -2010.173315
	O	3.585684	0.740863	1.492621	
	O	3.940908	-0.601845	-0.981993	
	C	5.395241	-0.788980	-1.271949	
	C	5.523144	-0.828884	-2.788277	
	O	3.758437	-2.021414	1.215623	
	C	3.704388	-2.303109	2.682410	
	C	4.470377	-3.601244	2.899644	
	C	0.871823	0.699592	-1.982436	
	F	-0.092162	1.579638	-2.546312	
	F	2.109159	1.335330	-2.291230	
	F	0.837709	-0.454664	-2.755493	
	O	-2.895938	-1.144590	-0.662960	
	C	-4.060922	-1.093021	-0.100901	
	C	-4.521796	-0.247971	0.915836	
	C	-5.043947	-2.133820	-0.673220	
	F	-5.252276	-1.947226	-2.048277	
	F	-6.316339	-2.109137	-0.077720	
	F	-4.564747	-3.442784	-0.517893	
	H	4.156510	-1.459486	3.216168	
	H	2.651055	-2.397434	2.968552	
	H	5.714397	-1.726044	-0.803133	
	H	5.943139	0.053728	-0.834367	
	H	5.515683	-3.494104	2.590125	

	H	4.447222	-3.865232	3.965156
	H	4.016009	-4.418004	2.329070
	H	5.158302	0.103418	-3.231383
	H	6.578432	-0.959898	-3.061896
	H	4.947416	-1.662886	-3.202457
	H	-5.541164	-0.366898	1.258678
	H	-5.377128	1.337163	2.842315
	H	-4.311789	2.674542	2.336717
	H	-3.749109	1.515224	3.547996
	C	0.590550	0.467162	-0.508780
	S	1.002409	2.221033	0.359118
	C	-0.584738	3.288461	-0.103322
	C	-0.518389	4.609167	0.597786
	C	-0.150742	5.755555	-0.016268
	C	0.632871	1.910821	2.189682
	H	-0.525604	3.369385	-1.187435
	H	-1.420799	2.660746	0.212777
	H	-0.828444	4.631528	1.641536
	H	-0.154166	6.704848	0.513322
	H	0.152029	5.777173	-1.061680
	H	1.467133	1.325871	2.570716
	H	0.614314	2.901271	2.647797
	H	-0.328900	1.403947	2.267626
 Int4	C	-0.079072	-0.429191	-0.535543
	P	1.690917	-0.046816	0.202287
	O	1.923719	1.504303	-0.410324
	C	2.985465	2.435128	0.066721
	C	2.510835	3.227380	1.284288
	C	-1.194173	0.374857	-0.046932
	S	-2.270973	-0.134135	1.287709
	C	-3.660373	-1.432202	0.569713
	C	-3.200529	-2.169080	-0.628970
	C	-3.388749	-1.706825	-1.887954
	F	-0.254587	-1.817080	-0.156261
	F	0.073868	-0.444445	-1.958890
	C	-1.484798	1.720097	-0.520777
	F	-1.174672	2.803558	0.387260
	O	2.886984	-0.933369	-0.640690
	C	3.345142	-2.267397	-0.159765
	C	4.617291	-2.593812	-0.932566
	O	1.729209	-0.249374	1.785518
	F	-0.843020	2.067406	-1.710375
	F	-2.891672	1.940673	-0.743865
	C	-1.265863	-1.213764	2.483813
	H	3.520396	-2.212138	0.920847
	H	2.550700	-2.995833	-0.361720
	H	3.155578	3.078589	-0.799923
	H	3.899145	1.864090	0.273759
	H	5.396577	-1.851211	-0.729368
	H	4.988720	-3.582188	-0.630577
	H	4.421021	-2.609059	-2.009978
	H	2.363904	2.572473	2.149813
	H	3.264255	3.984206	1.541734
	H	1.567061	3.736574	1.062600
	H	-0.267685	-0.771816	2.552549
	H	-1.803493	-1.163902	3.431747
	H	-1.211716	-2.228369	2.092802
	H	-3.857718	-2.049048	1.449979
	H	-4.477754	-0.734787	0.379821
	H	-2.654347	-3.095917	-0.468289
	H	-3.911580	-0.773005	-2.084272
	H	-3.022414	-2.256365	-2.751020

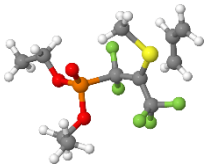
Transition states

 TS1	C	-2.392152	0.655608	-0.074501
	F	-2.181285	2.075395	-0.065637
	F	-2.186388	0.223253	-1.400580
	P	-4.284770	0.491865	0.355534
	O	-4.575697	-1.008042	-0.336982
	C	-5.943890	-1.574026	-0.561023
	C	-5.737653	-2.932215	-1.215624
	C	-1.279154	0.043079	0.774170
	C	-1.315315	-1.467433	1.002458
	F	-2.512109	-1.987480	1.525930
	O	-5.069596	1.541870	-0.721011
	C	-5.415697	2.954223	-0.361378

Zero-point correction= 0.287889 (Hartree/Particle)
Thermal correction to Energy= 0.328779
Thermal correction to Enthalpy= 0.329995
Thermal correction to Gibbs Free Energy= 0.199237
Sum of electronic and zero-point Energies= -1171.021019
Sum of electronic and thermal Energies= -1170.980129
Sum of electronic and thermal Enthalpies= -1170.978913
Sum of electronic and thermal Free Energies= -1171.109671

Zero-point correction= 0.270724 (Hartree/Particle)
Thermal correction to Energy= 0.322850
Thermal correction to Enthalpy= 0.324066
Thermal correction to Gibbs Free Energy= 0.161108
Sum of electronic and zero-point Energies= -1952.297757
Sum of electronic and thermal Energies= -1952.245631
Sum of electronic and thermal Enthalpies= -1952.244415
Sum of electronic and thermal Free Energies= -1952.407373

	C	-6.407112	3.433791	-1.412469
	O	-4.555751	0.743805	1.900125
	N	-1.769963	0.592720	2.434725
	N	-1.614569	1.103209	3.435515
	F	-1.071154	-2.131618	-0.197413
	F	-0.314006	-1.846172	1.909133
	H	-5.841875	2.961346	0.647848
	H	-4.488664	3.536969	-0.374273
	H	-6.491901	-0.879646	-1.206775
	H	-6.442695	-1.656378	0.411361
	H	-7.319586	2.828169	-1.394768
	H	-6.677481	4.477796	-1.206805
	H	-5.966972	3.379856	-2.413680
	H	-5.156820	-3.592472	-0.563483
	H	-6.714825	-3.396116	-1.403786
	H	-5.211220	-2.826597	-2.169758
	C	4.182208	1.879209	-1.068849
	C	3.067311	1.838229	-0.008618
	O	2.033505	1.153915	-0.403651
	Cu	0.438326	0.877262	0.680528
	C	3.275663	2.507406	1.199489
	C	2.316411	2.546260	2.260972
	O	1.158277	1.960011	2.200782
	C	2.635554	3.301475	3.533098
	F	5.319356	2.595233	-0.666114
	F	3.739555	2.475182	-2.258040
	F	4.622390	0.592219	-1.405316
	H	4.212953	3.027069	1.346535
	H	3.630919	3.752142	3.509171
	H	2.568216	2.619360	4.389782
	H	1.887194	4.089019	3.687749



TS2

	C	-1.591771	0.194897	0.294503
	P	-3.381989	-0.587208	0.143337
	O	-3.972058	-0.166643	1.661243
	C	-5.389122	-0.346463	2.088688
	C	-6.244243	0.849266	1.672055
	C	-1.432129	1.660171	0.276286
	S	-1.399336	2.645842	-1.227254
	C	1.018019	2.793272	-1.515564
	C	1.411322	1.655693	-0.765028
	C	1.243276	1.619347	0.608013
	F	-0.907549	-0.399291	-0.831458
	F	-1.019076	-0.418857	1.447108
	C	-1.783061	2.472723	1.458107
	F	-3.159292	2.863818	1.575415
	O	-3.234488	-2.283717	0.288764
	C	-3.136160	-3.161900	-0.912569
	C	-3.391232	-4.585005	-0.431666
	O	-4.174497	-0.115418	-1.156381
	F	-1.484876	1.880839	2.691022
	F	-1.102947	3.726595	1.447151
	C	-1.915539	1.550652	-2.685134
	H	-3.878182	-2.835014	-1.650017
	H	-2.130381	-3.049825	-1.334141
	H	-5.307453	-0.432914	3.174854
	H	-5.768483	-1.292078	1.681860
	H	-4.394719	-4.676189	-0.001932
	H	-3.309050	-5.279646	-1.278211
	H	-2.657260	-4.873376	0.328359
	H	-6.333447	0.914544	0.582351
	H	-7.250421	0.741468	2.099401
	H	-5.804489	1.779817	2.045565
	H	-2.859120	1.061665	-2.431483
	H	-2.041834	2.256781	-3.508566
	H	-1.133295	0.824487	-2.898345
	H	1.096545	2.794400	-2.601215
	H	1.000276	3.772970	-1.044095
	H	1.633071	0.732332	-1.295889
	H	1.068606	2.528473	1.175935
	H	1.418849	0.711709	1.178439

Zero-point correction= 0.287092 (Hartree/Particle)
Thermal correction to Energy= 0.326939
Thermal correction to Enthalpy= 0.328155
Thermal correction to Gibbs Free Energy= 0.202058
Sum of electronic and zero-point Energies= -1171.016749
Sum of electronic and thermal Energies= -1170.976902
Sum of electronic and thermal Enthalpies= -1170.975686
Sum of electronic and thermal Free Energies= -1171.101782