

Supporting Information

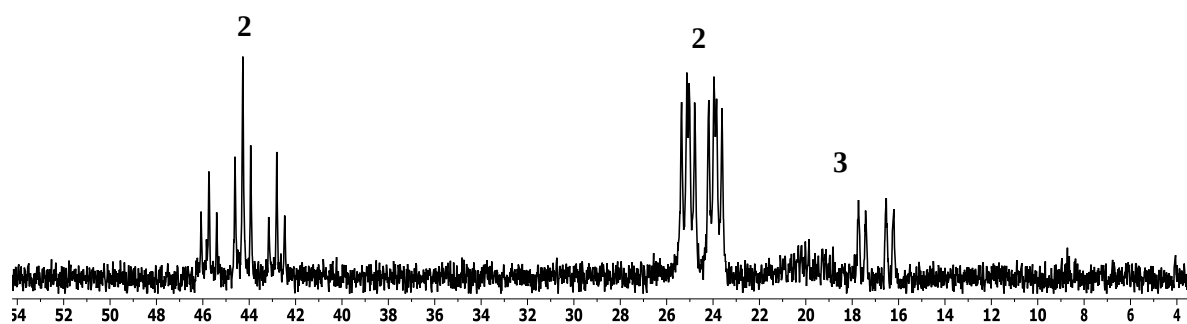
Activation of tetrafluoropropenes by rhodium(I) germyl and silyl complexes

Maria Talavera,^a Robert Müller,^b Theresia Ahrens,^a Cortney N. von Hahmann,^a Beatrice Braun-Cula,^a Martin Kaupp^{b,*} and Thomas Braun^{a,*}

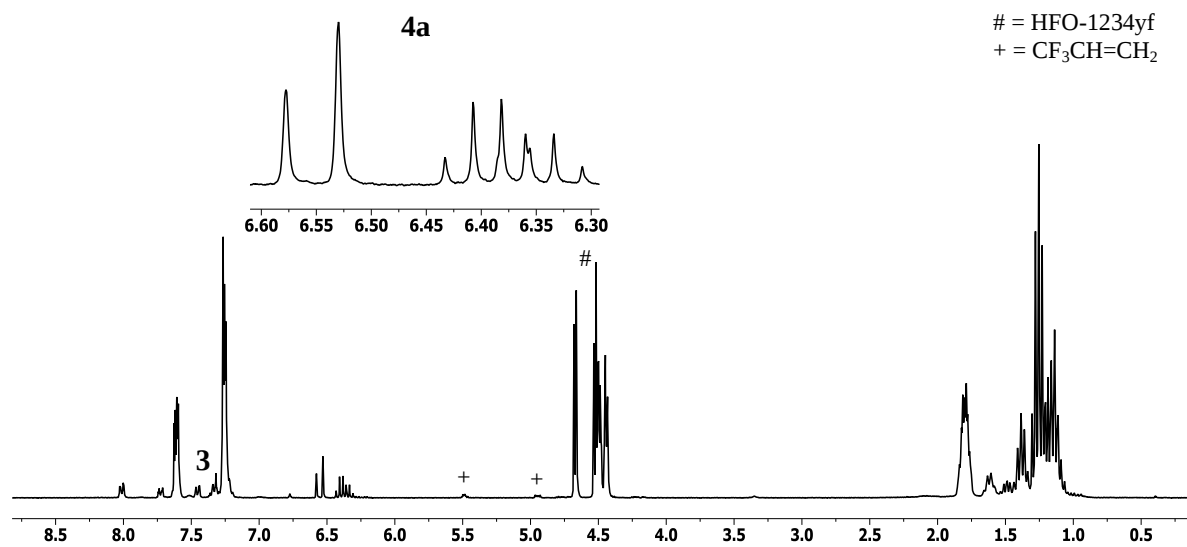
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^b *Institut für Chemie, Theoretische Chemie/Quantenchemie, Sekr. C7 Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany.*

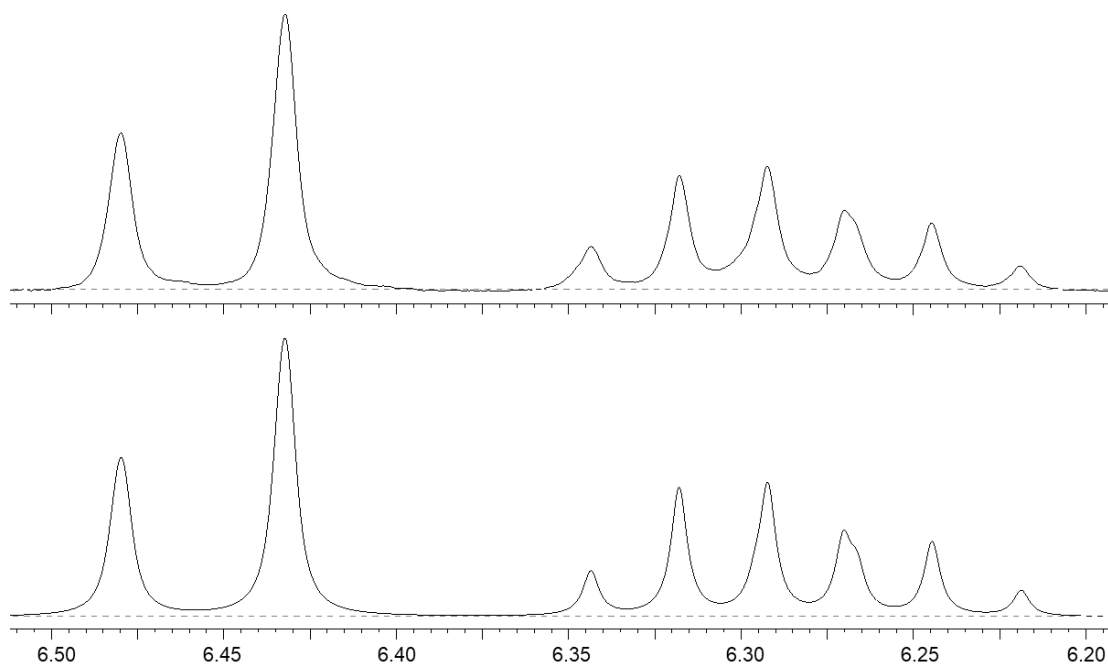
NMR Spectra of Stoichiometric reactions



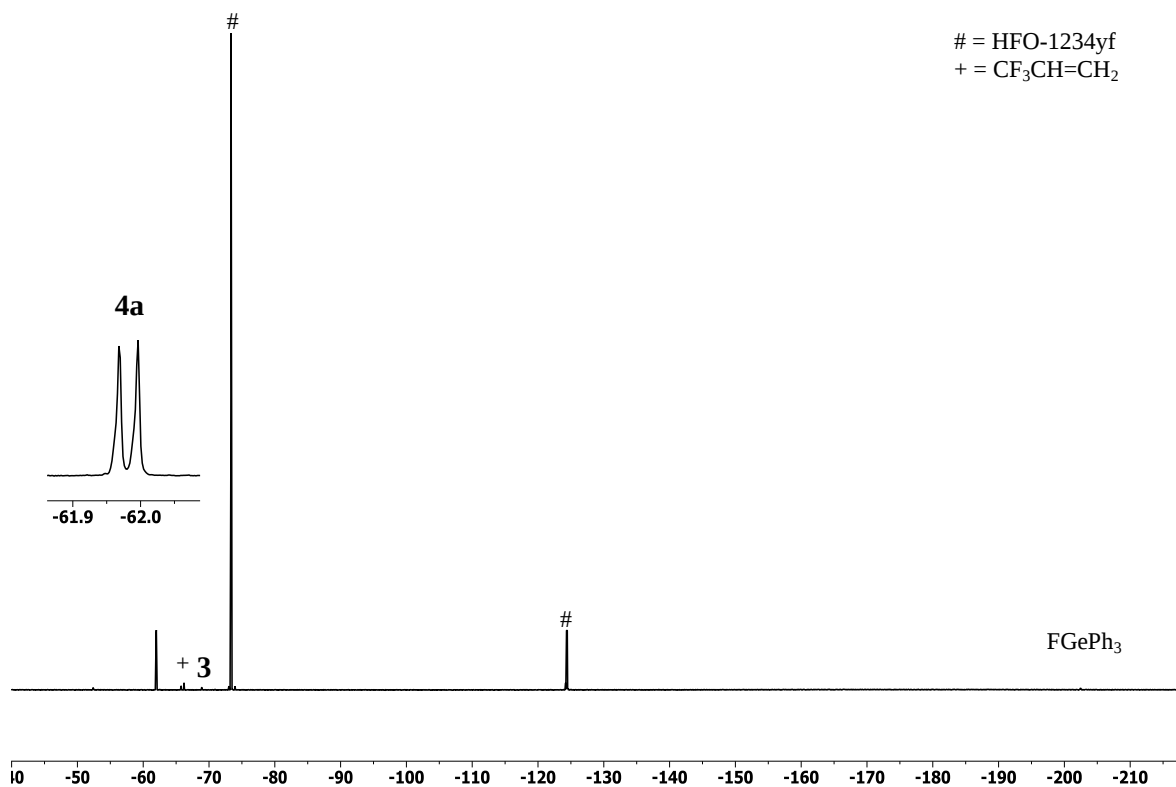
S1. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction of $[\text{Rh}(\text{GePh}_3)(\text{PEt}_3)_3]$ (**1**) with HFO-1234yf.



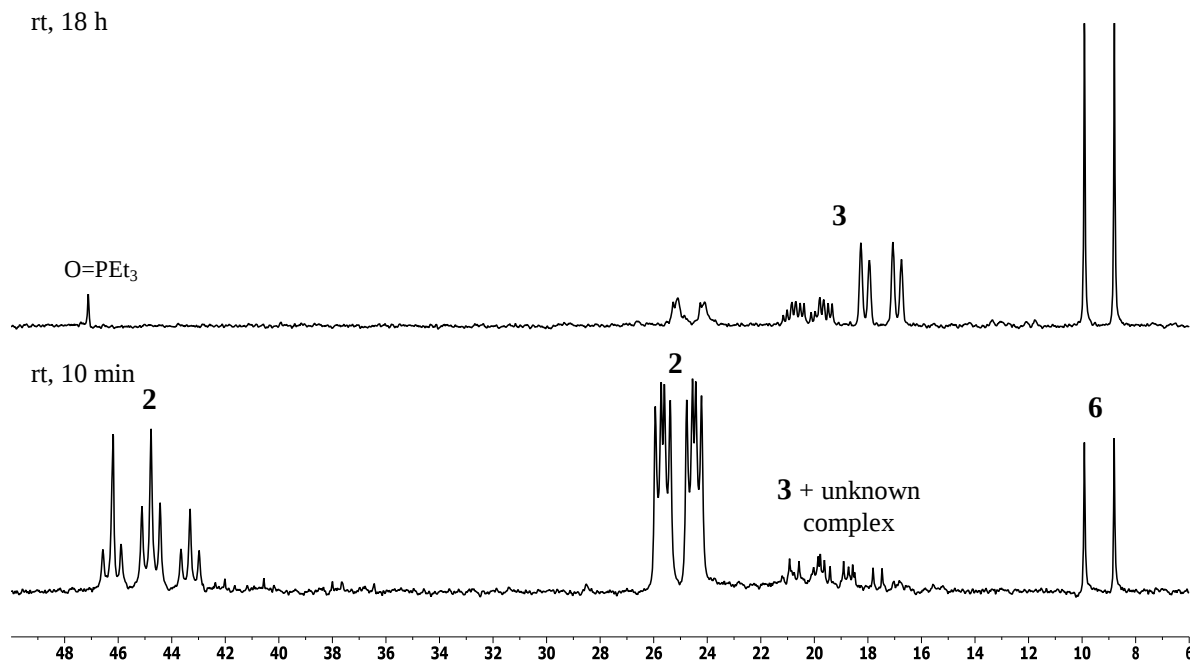
S2. ^1H NMR spectrum of the reaction of $[\text{Rh}(\text{GePh}_3)(\text{PEt}_3)_3]$ (**1**) with HFO-1234yf.



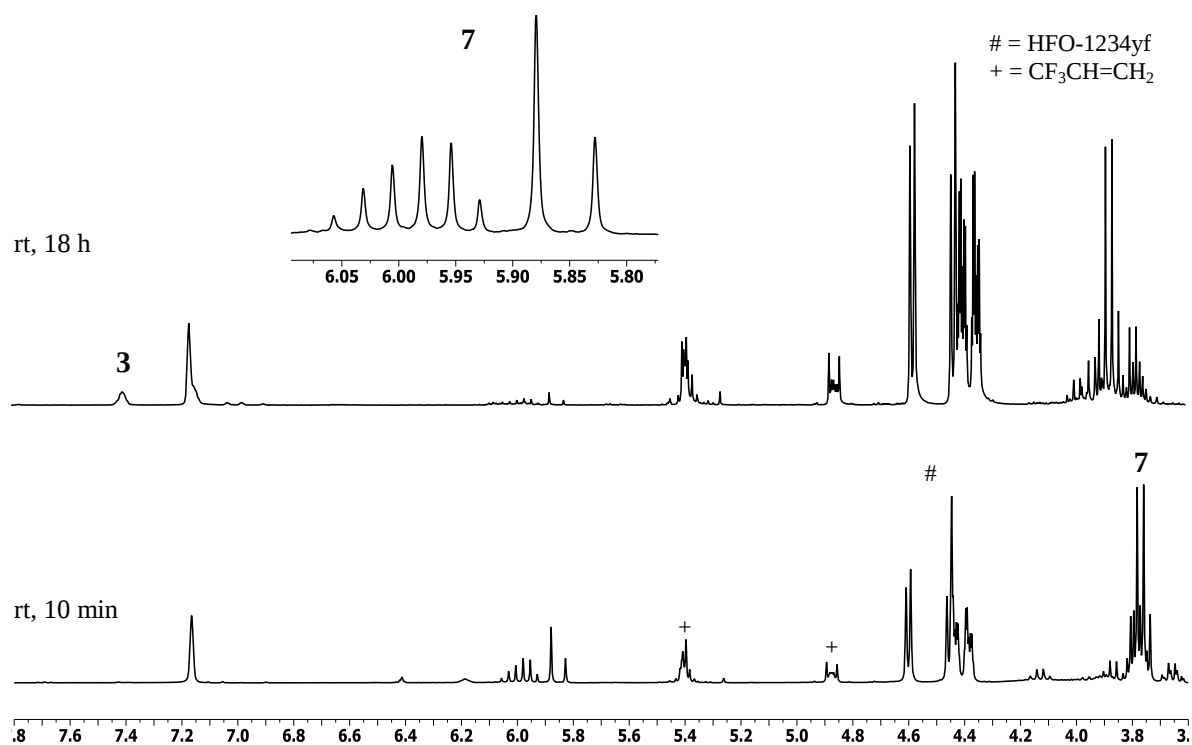
S3. Section ^1H NMR spectrum corresponding to the olefinic protons of $\text{Z-CF}_3\text{CH=CH(GePh}_3\text{)}$ (**4a**). Experimental (top) and simulated (bottom).^[1]



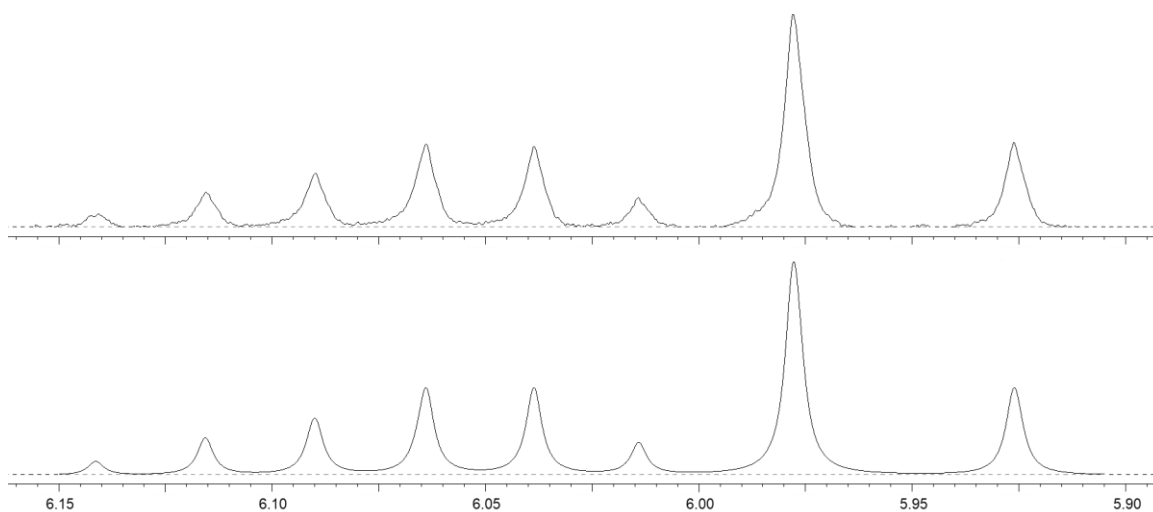
S4. Section of the ^{19}F NMR spectrum of the reaction of $[\text{Rh(GePh}_3\text{)(PEt}_3\text{)}_3]$ (**1**) with HFO-1234yf.



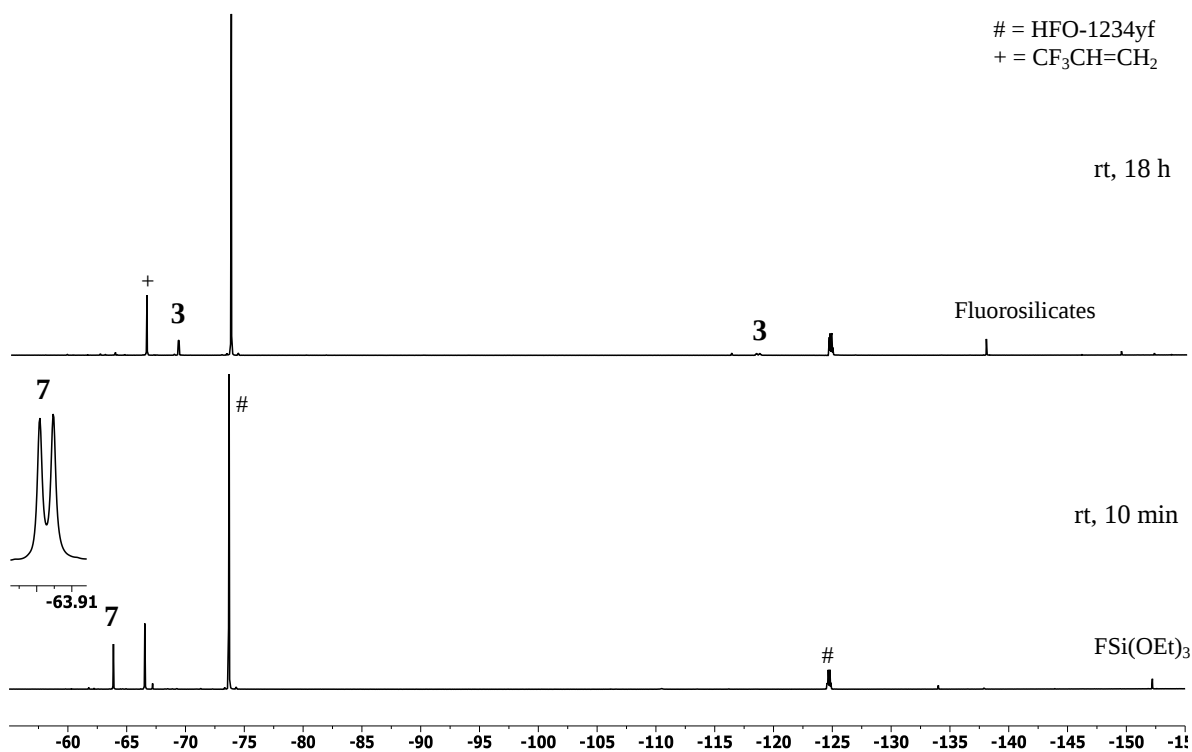
S5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of the reaction of $[\text{Rh}(\text{Si}(\text{OEt})_3)(\text{PEt}_3)_3]$ (**5**) with HFO-1234yf.



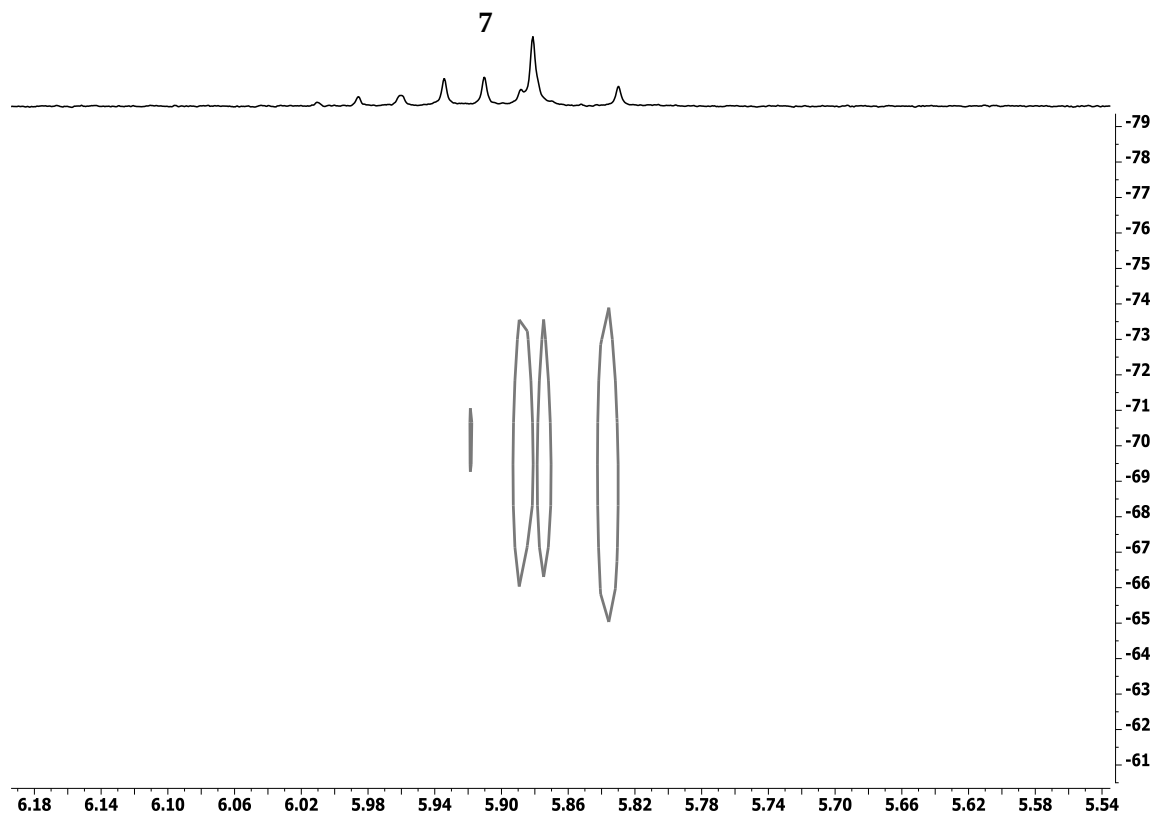
S6. ^1H NMR spectra of the reaction of $[\text{Rh}(\text{Si}(\text{OEt})_3)(\text{PEt}_3)_3]$ (**5**) with HFO-1234yf.



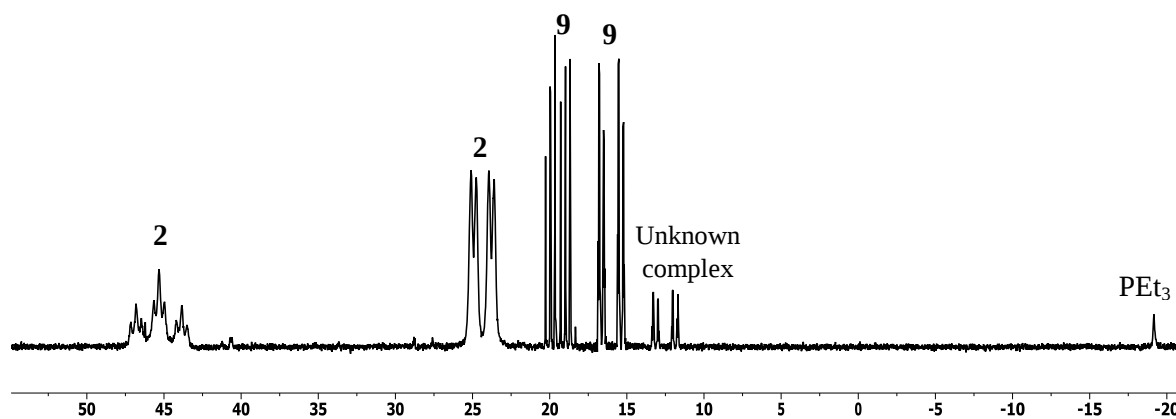
S7. Section ^1H NMR spectrum corresponding to the olefinic protons of $\text{Z-CF}_3\text{CH=CH(Si(OEt)}_3\text{)}$ (7). Experimental (top) and simulated (bottom).^[1]



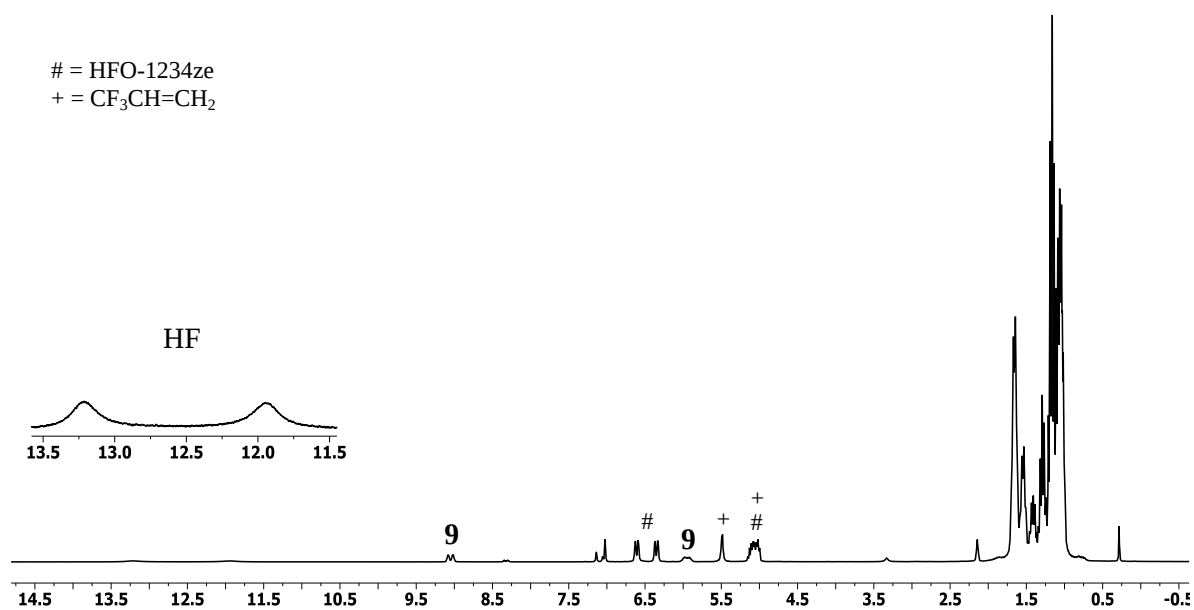
S8. Section of the ^{19}F NMR spectra of the reaction of $[\text{Rh(Si(OEt)}_3\text{)(PEt}_3\text{)}_3]$ (5) with HFO-1234yf.



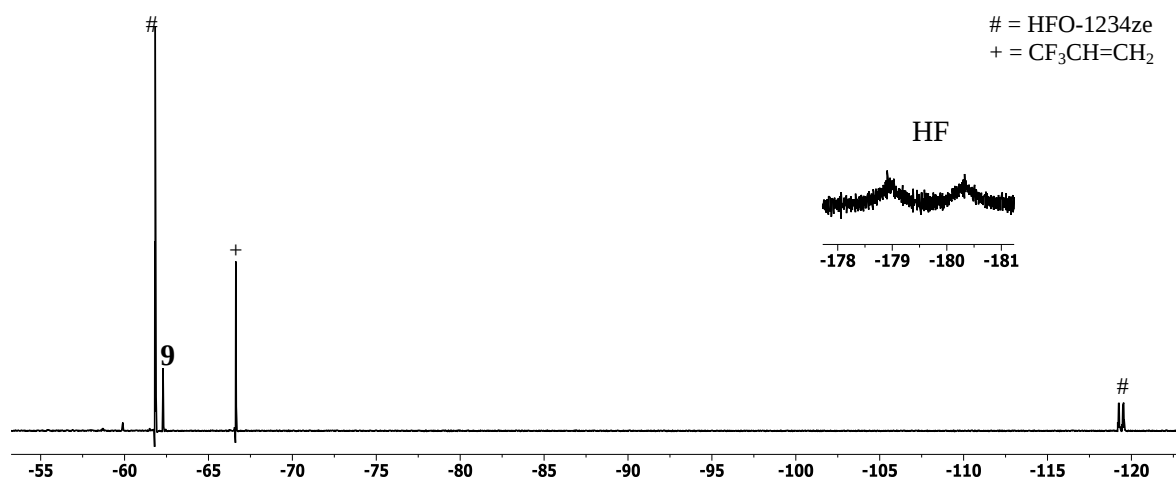
S9. Section of the ^1H , ^{29}Si HMBC spectrum of the reaction of $[\text{Rh}(\text{Si}(\text{OEt})_3)(\text{PEt}_3)_3]$ (**5**) with HFO-1234yf.



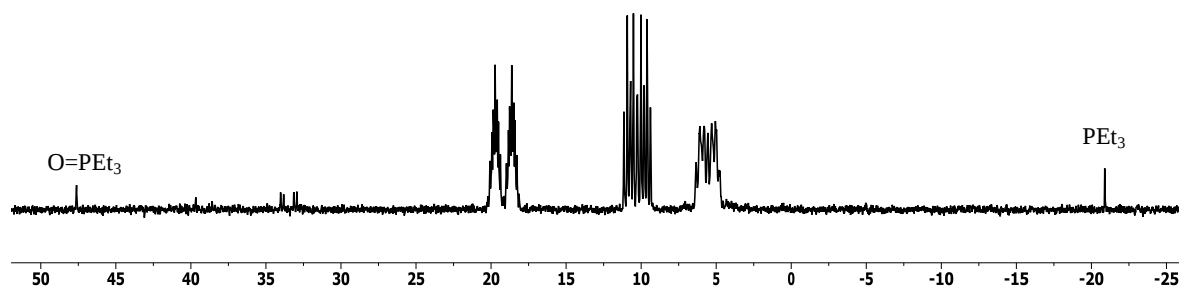
S10. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction of $[\text{RhH}(\text{PEt}_3)_3]$ (**8**) with HFO-1234ze.



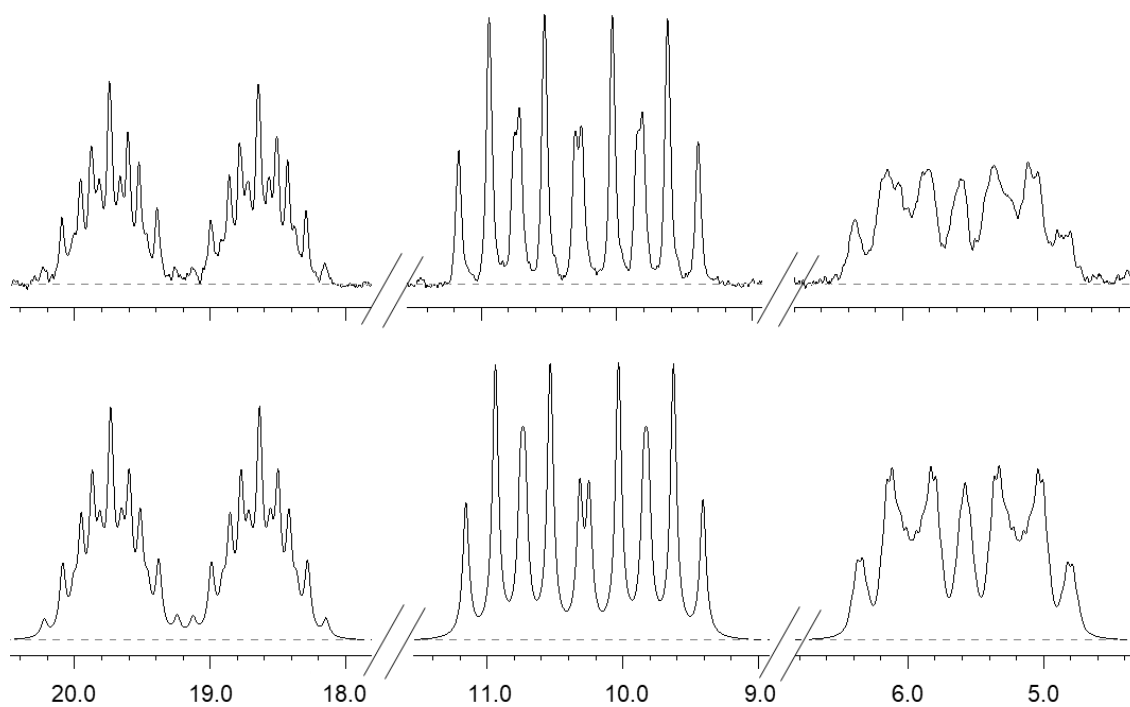
S11. ¹H NMR spectrum of the reaction of [Rh(H)(PEt₃)₃] (**8**) with HFO-1234ze.



S12. Section of the ¹⁹F NMR spectrum of the reaction of [RhH(PEt₃)₃] (**8**) with HFO-1234ze.

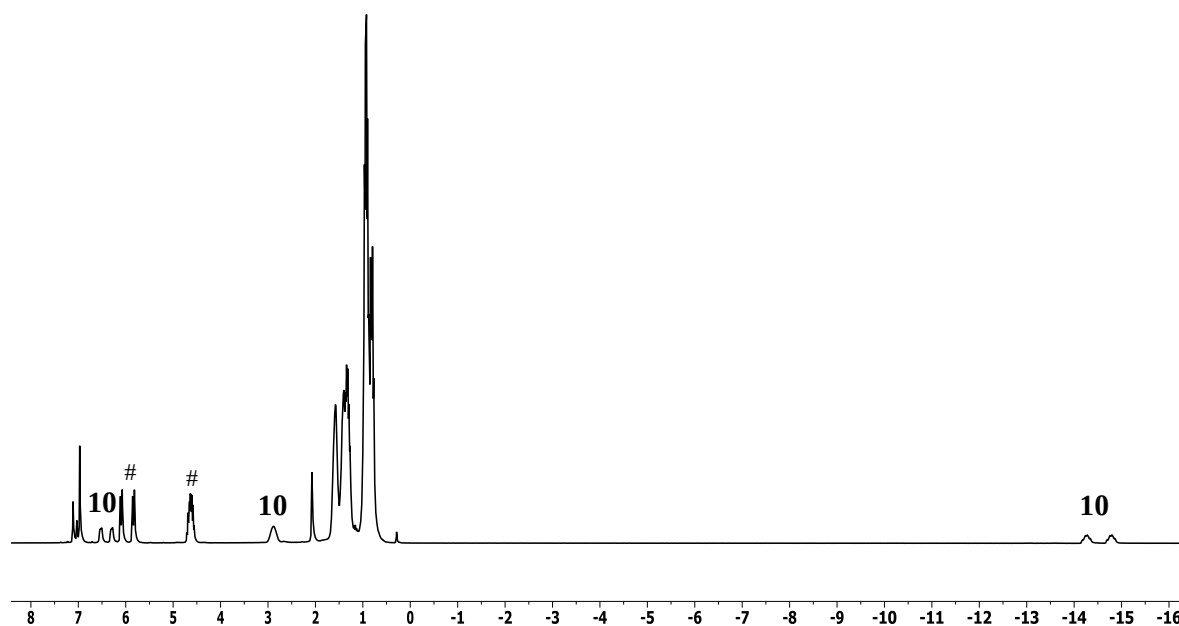


S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *fac*-[Rh(H)(η^2 -CHF=CHCF₃)(PEt₃)₃] (**10**) at 243 K.

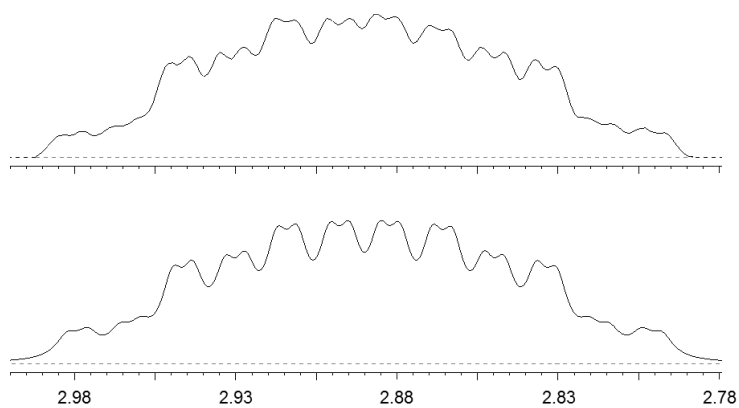


S14. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *fac*-[RhH(η^2 -CHF=CHCF₃)(PEt₃)₃] (**10**) at 243 K. Experimental (top) and simulated (bottom).^[1]

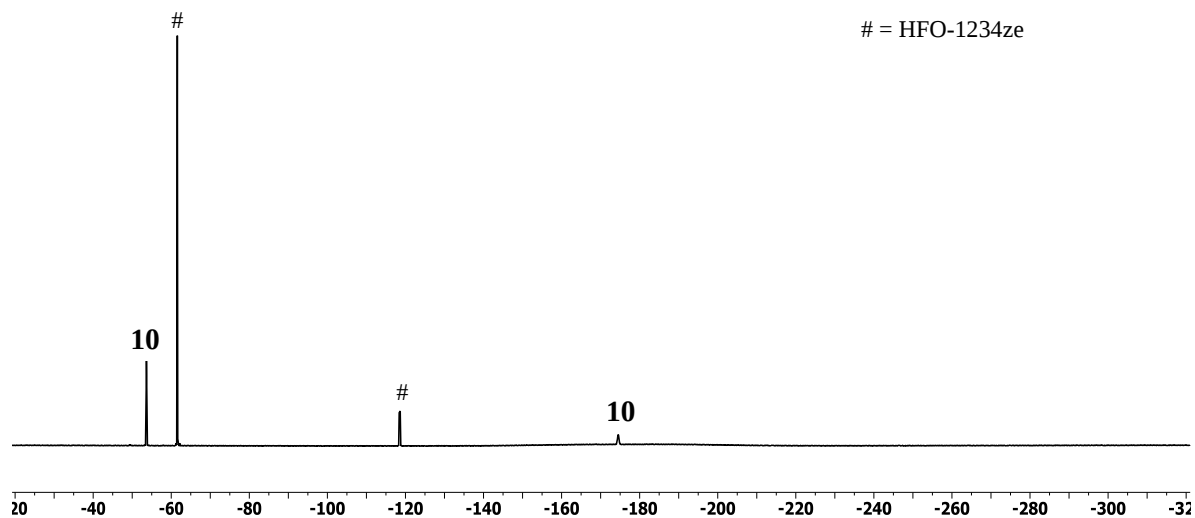
= HFO-1234ze



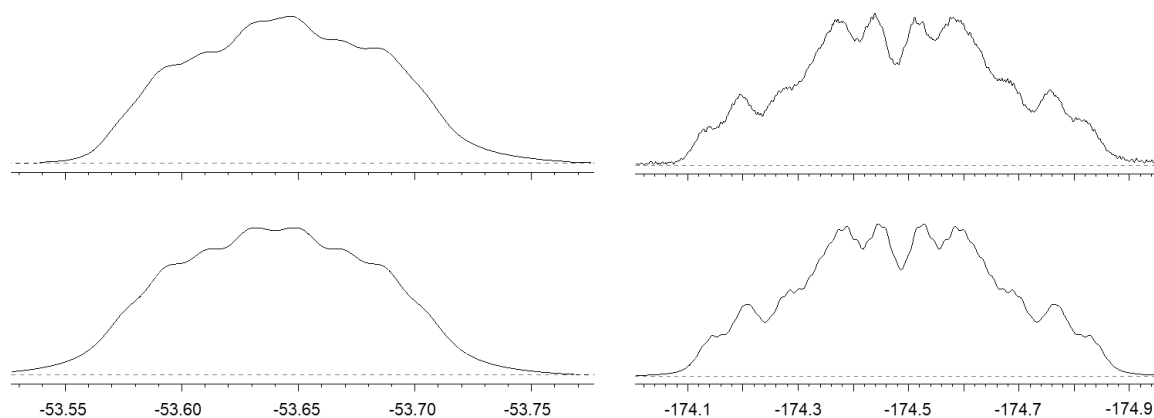
S15. ^1H NMR spectrum of *fac*-[RhH(η^2 -CHF=CHCF₃)(PEt₃)₃] (**10**) at 243 K.



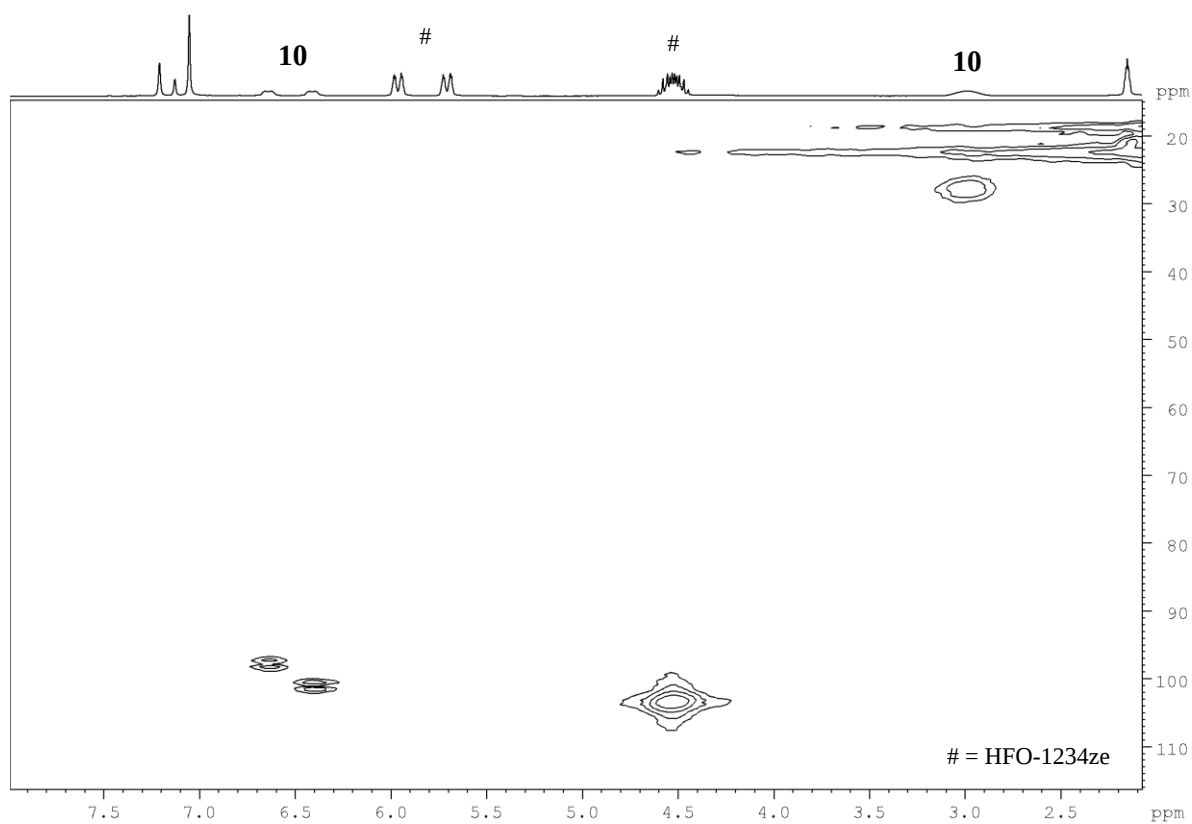
S16. Section of the $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum of *fac*-[RhH(η^2 -CHF=CHCF₃)(PEt₃)₃] (**10**) at 273 K. Experimental (top) and simulated (bottom).^[1]



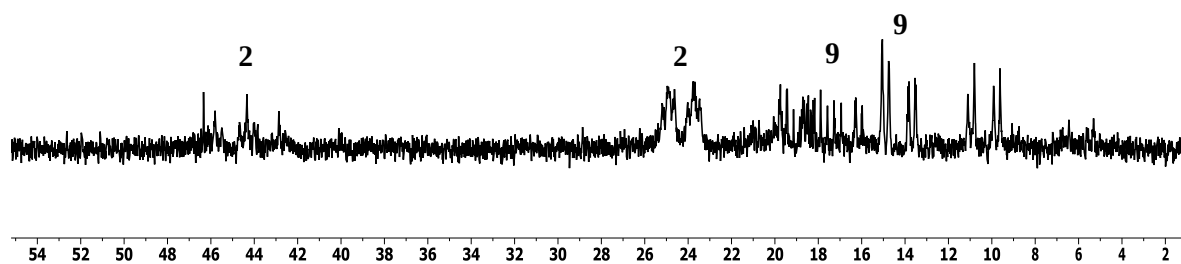
S17. ^{19}F NMR spectrum of *fac*-[RhH(η^2 -CHF=CHCF₃)(PEt₃)₃] (**10**) at 243 K.



S18. ^{19}F NMR spectrum of *fac*-[RhH(η^2 -CHF=CHCF₃)(PEt₃)₃] (**10**) at 243 K. Experimental (top) and simulated (bottom).^[1]

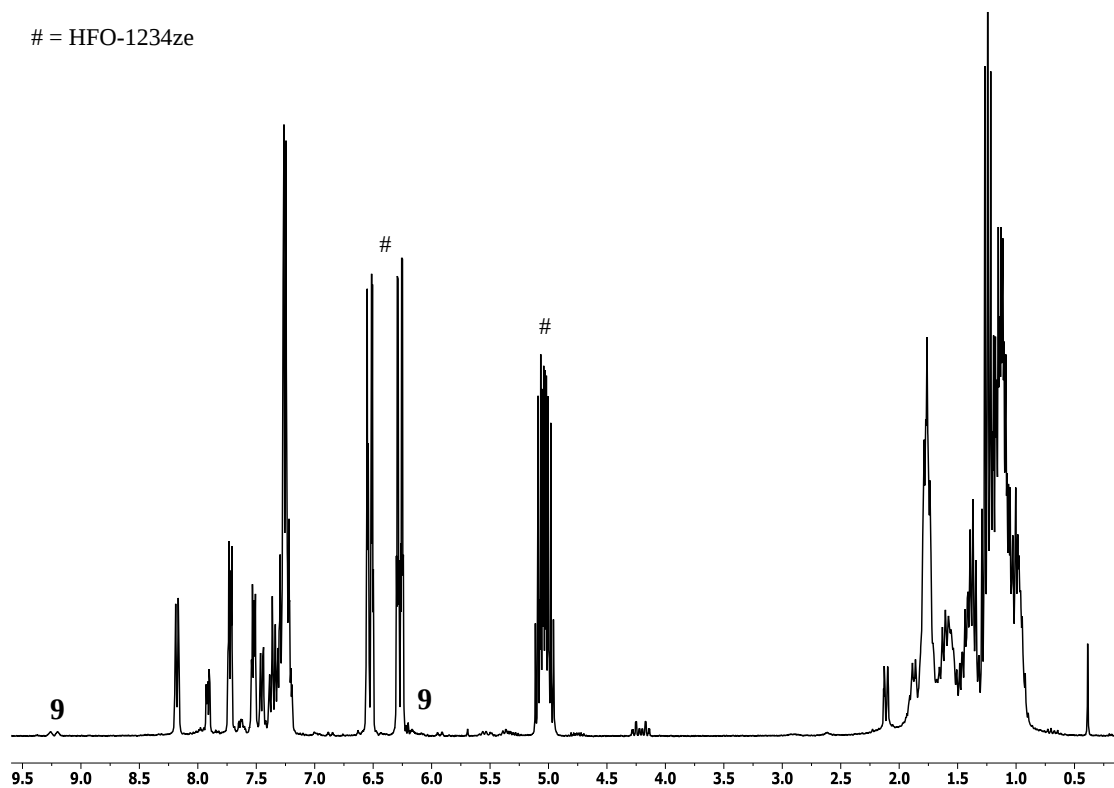


S19. Section of the ^1H - ^{13}C HMQC NMR spectrum of *fac*- $[\text{RhH}(\eta^2\text{-CHF=CHCF}_3)(\text{PEt}_3)_3]$ (**10**) at 213 K.

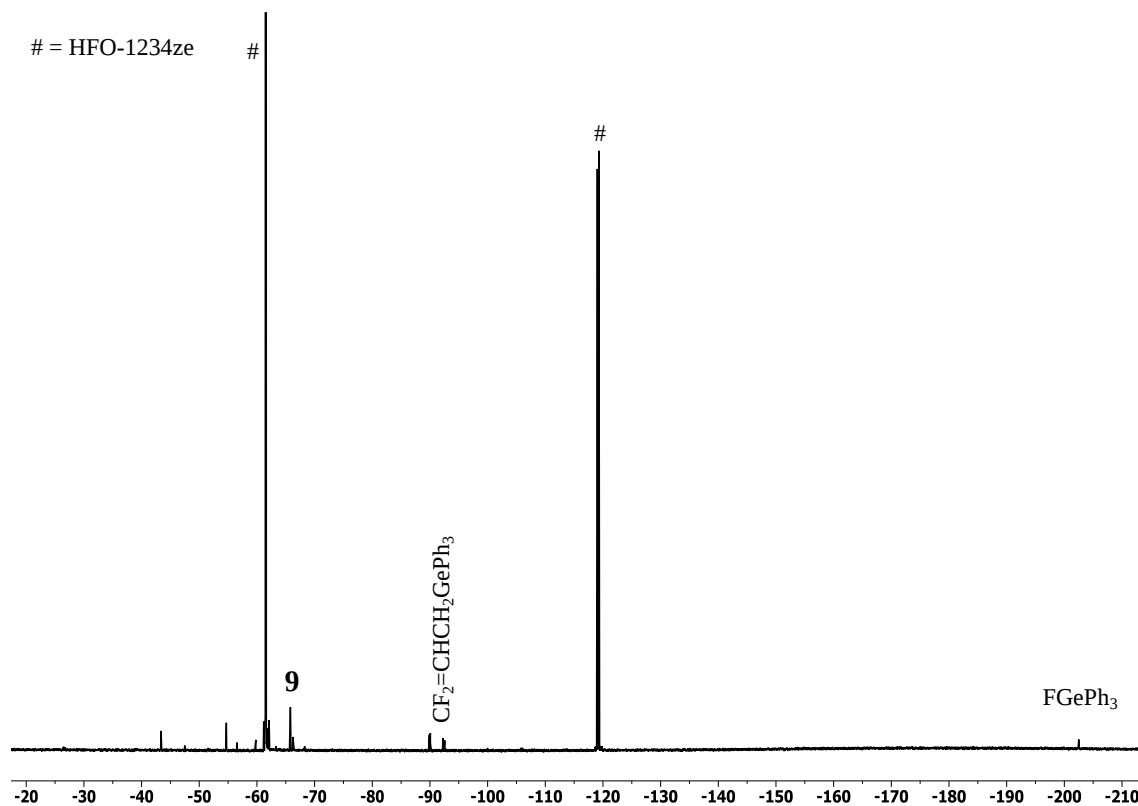


S20. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction of $[\text{Rh}(\text{GePh}_3)(\text{PEt}_3)_3]$ (**1**) with HFO-1234ze.

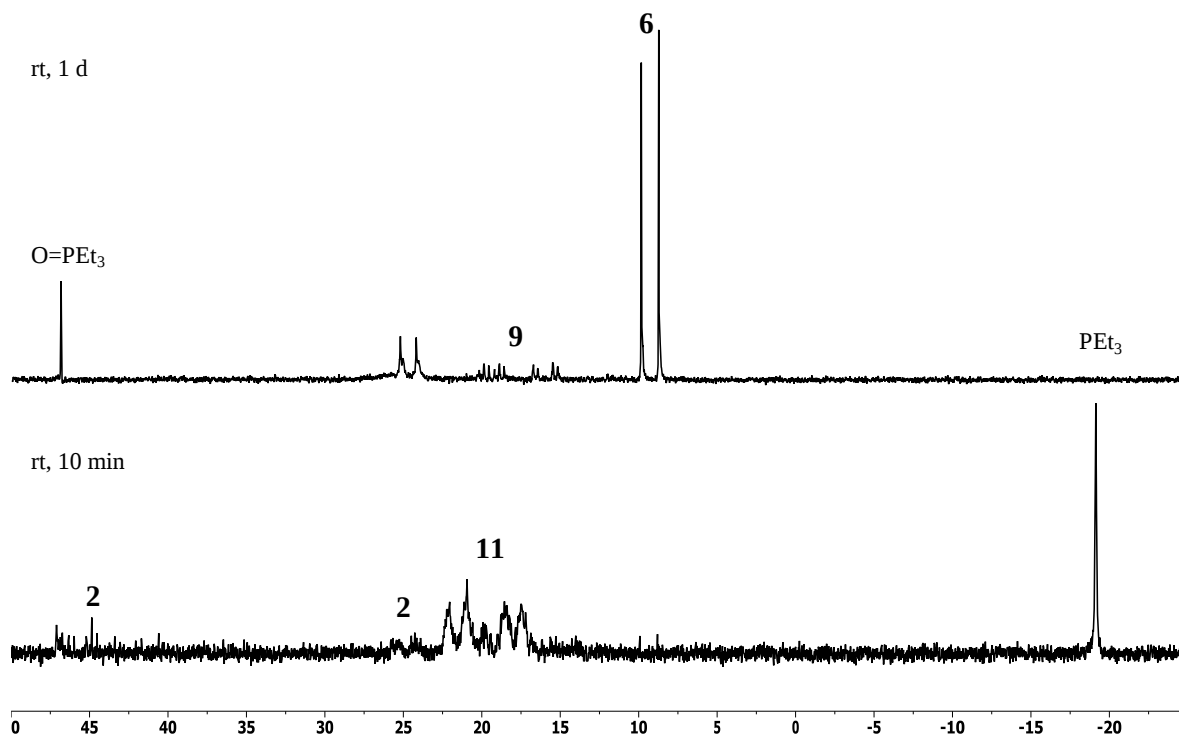
= HFO-1234ze



S21. ^1H NMR spectrum of the reaction of $[\text{Rh}(\text{GePh}_3)(\text{PEt}_3)_3]$ (**1**) with HFO-1234ze.

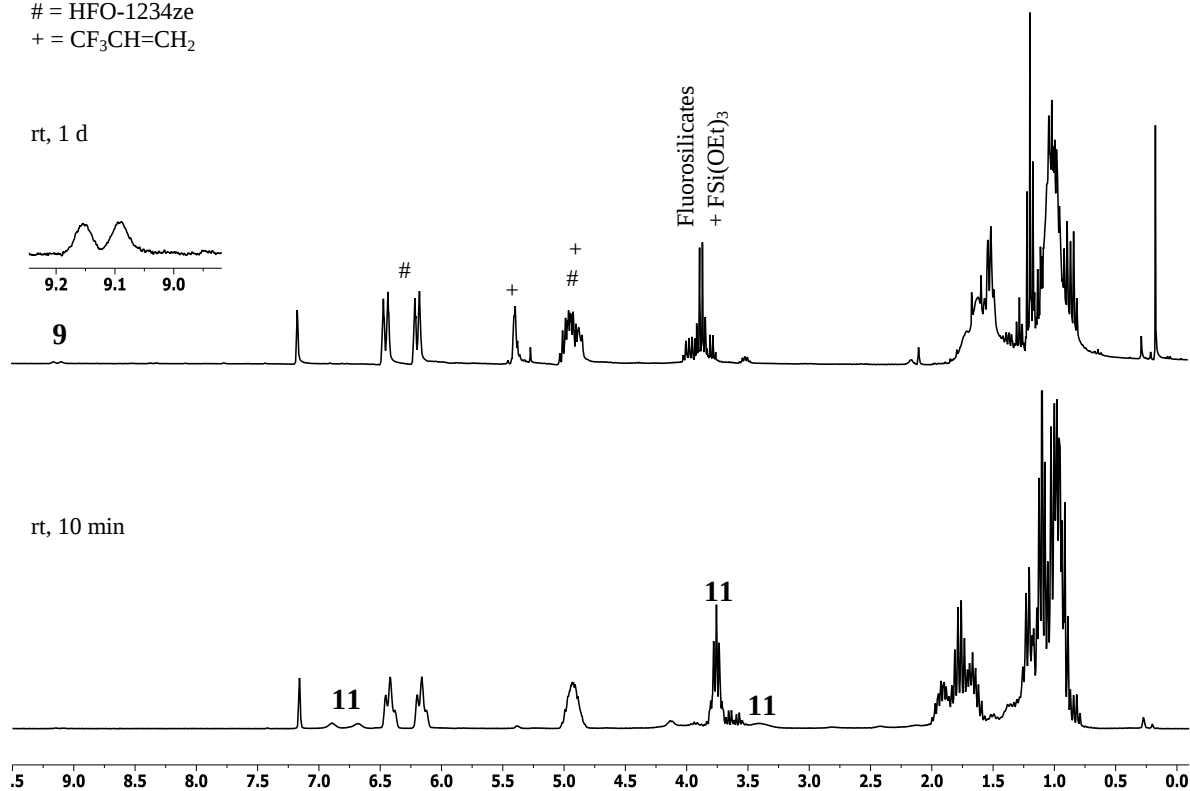


S22. Section of the ^{19}F NMR spectrum of the reaction of $[\text{Rh}(\text{GePh}_3)(\text{PEt}_3)_3]$ (**1**) with HFO-1234ze.

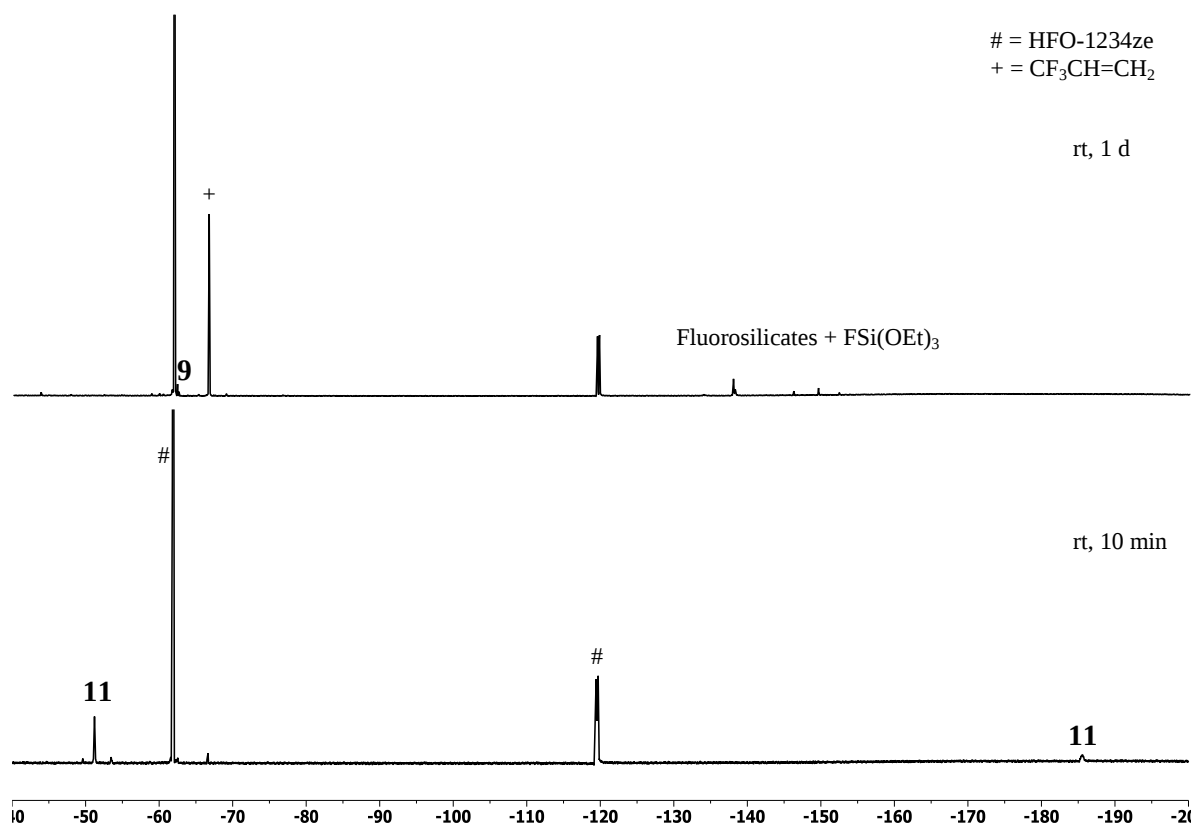


S23. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of the reaction of $[\text{Rh}(\text{Si}(\text{OEt})_3)(\text{PEt}_3)_3]$ (**5**) with HFO-1234ze.

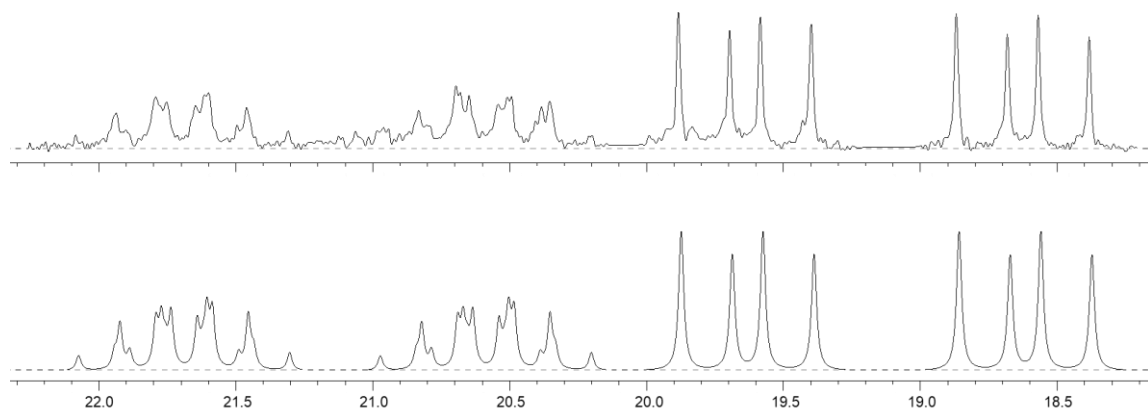
= HFO-1234ze
+ = $\text{CF}_3\text{CH}=\text{CH}_2$



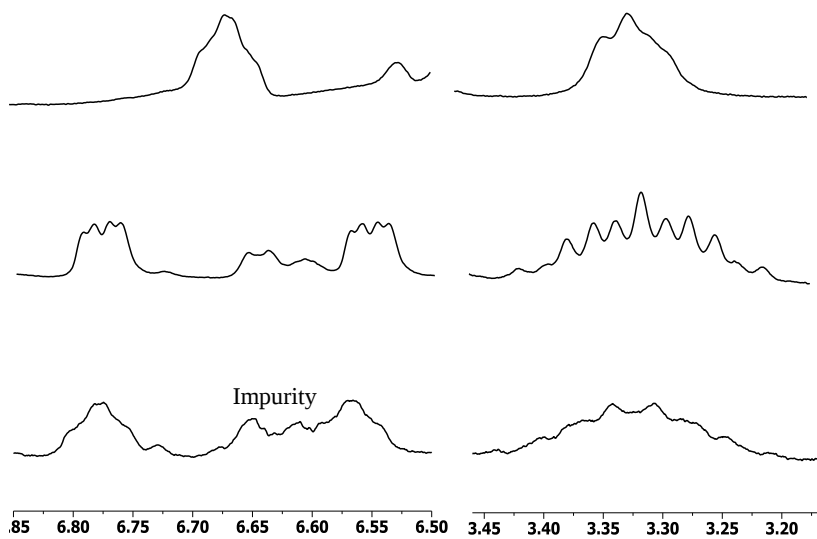
S24. ^1H NMR spectra of the reaction of $[\text{Rh}(\text{Si}(\text{OEt})_3)(\text{PEt}_3)_3]$ (**5**) with HFO-1234ze.



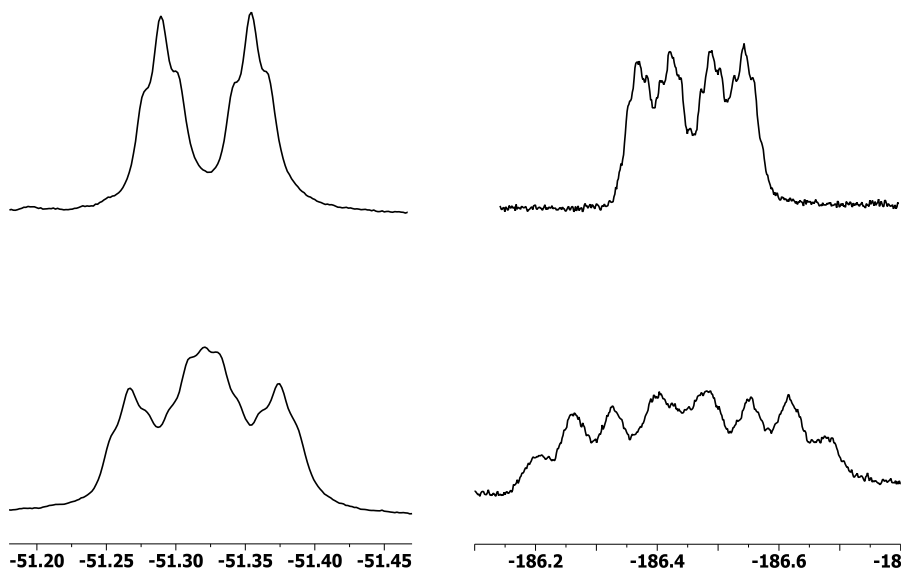
S25. Section of the ¹⁹F NMR spectra of the reaction of [Rh(Si(OEt)₃)(PEt₃)₃] (**5**) with HFO-1234ze.



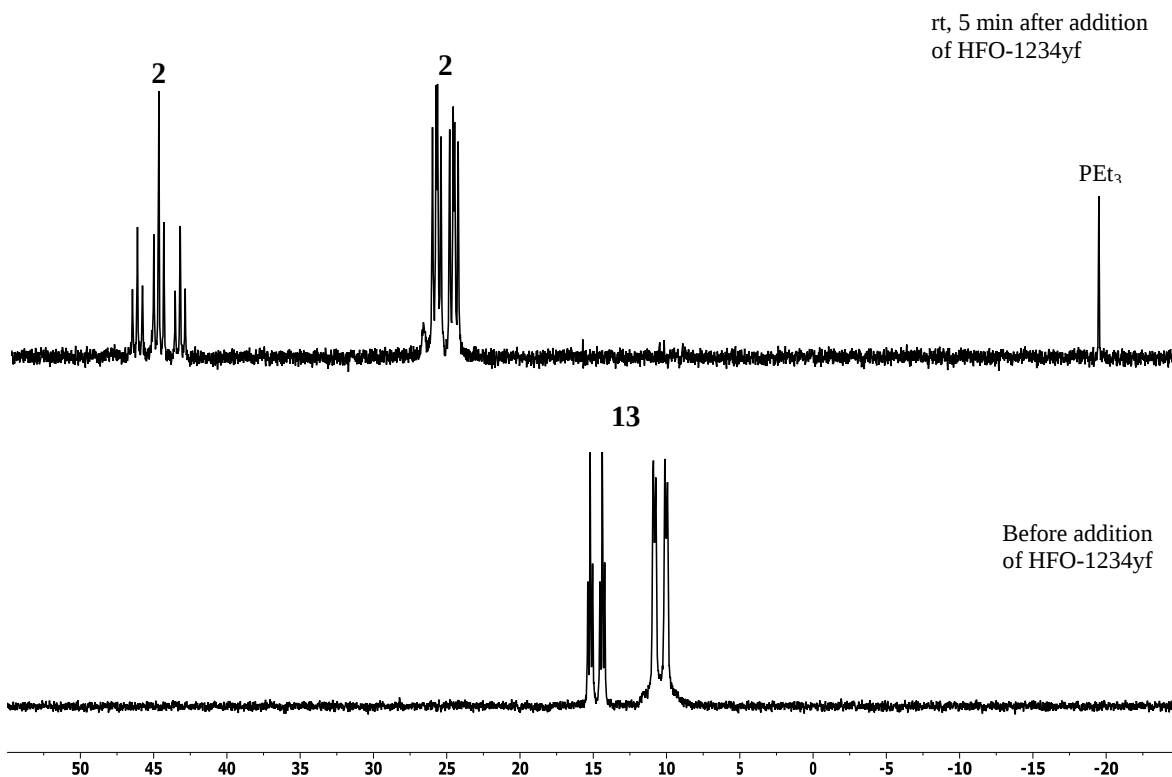
S26. ³¹P{¹H} NMR spectrum of Rh(Si(OEt)₃(η²-CHF=CHCF₃)(PEt₃)₃] (**11**) at 233 K. Experimental (top) and simulated (bottom).^[1]



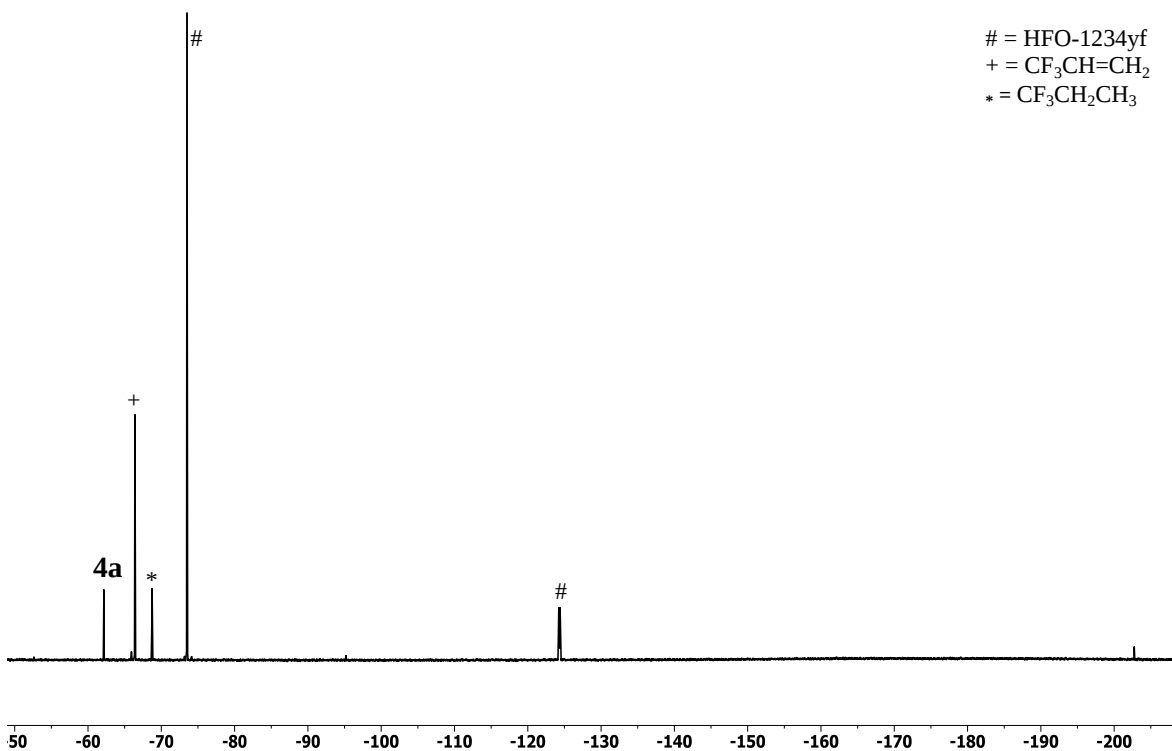
S27. ^1H NMR (bottom), $^1\text{H}\{^{31}\text{P}\}$ NMR (middle) and $^1\text{H}\{^{19}\text{F}\}$ NMR (top) spectra of $[\text{Rh}(\text{Si}(\text{OEt})_3(\eta^2\text{-CHF=CHCF}_3)(\text{PEt}_3)_3]$ (**11**) at 233 K.



S28. ^{19}F NMR (bottom) and $^{19}\text{F}\{^1\text{H}\}$ NMR (top) spectra of $[\text{Rh}(\text{Si}(\text{OEt})_3(\eta^2\text{-CHF=CHCF}_3)(\text{PEt}_3)_3]$ (**11**) at 233 K.



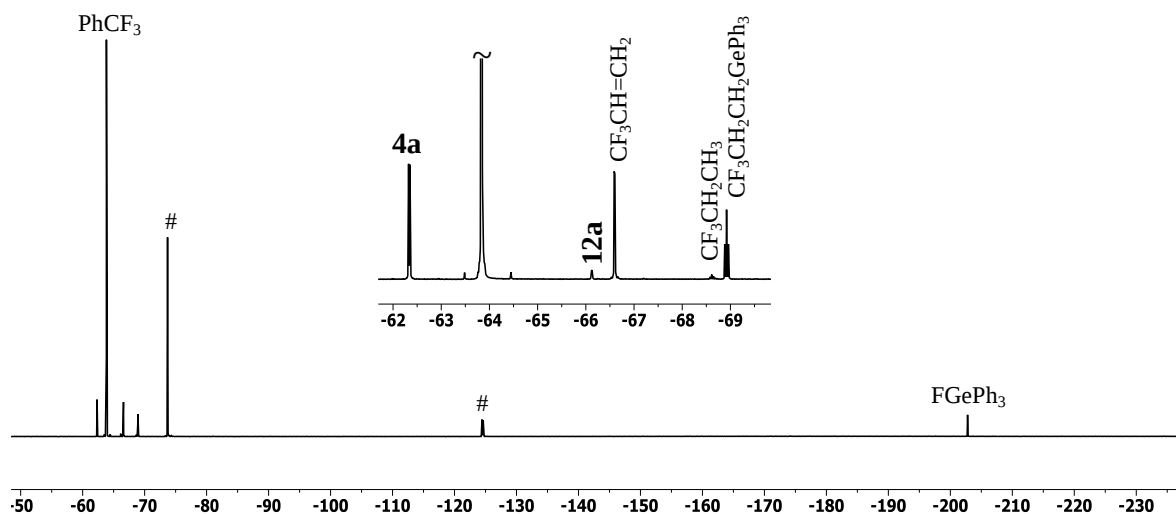
S29. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of the reaction of $[\text{Rh}(\text{H})_2(\text{GePh}_3)(\text{PEt}_3)_3]$ (**13**) with HFO-1234yf.



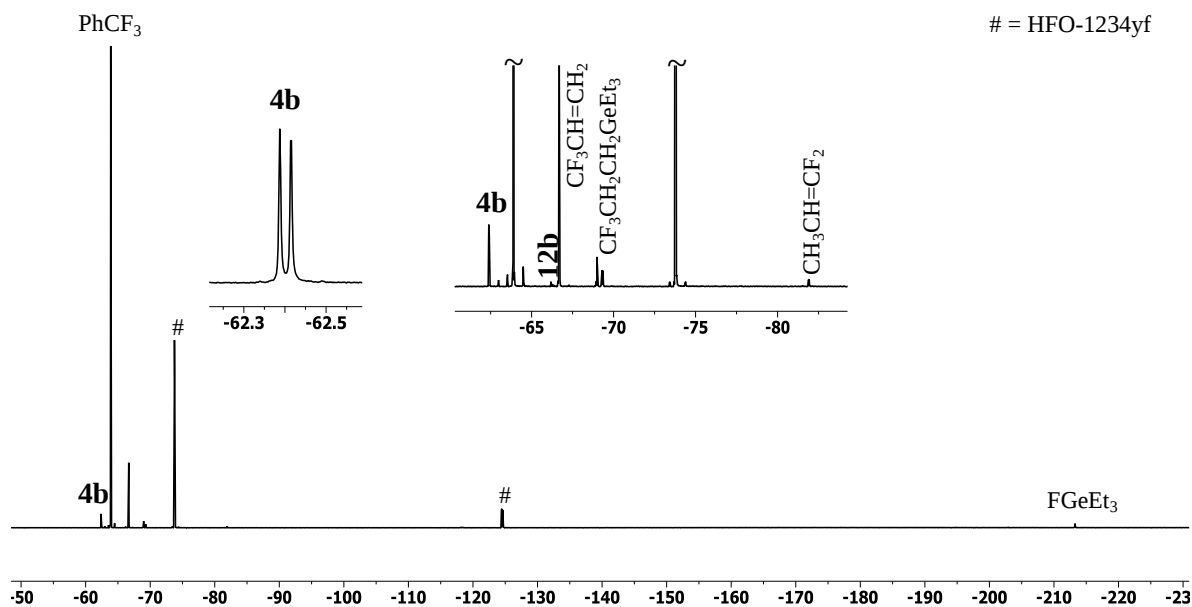
S30. Section of the ^{19}F NMR spectrum of the reaction of $[\text{Rh}(\text{H})_2(\text{GePh}_3)(\text{PEt}_3)_3]$ (**13**) with HFO-1234yf.

NMR Spectra of Catalytic reactions

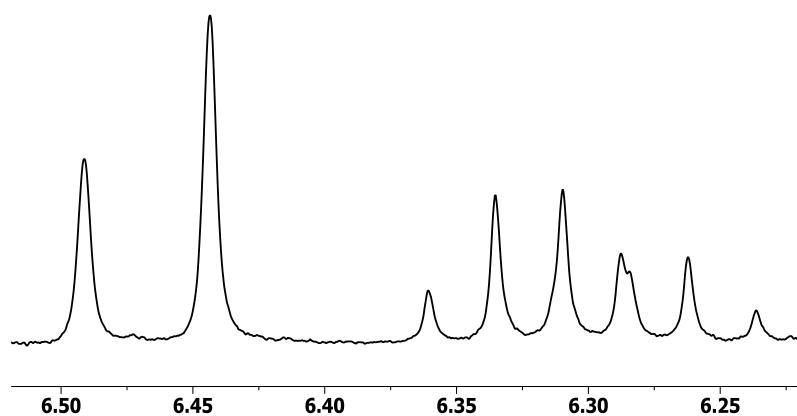
= HFO-1234yf



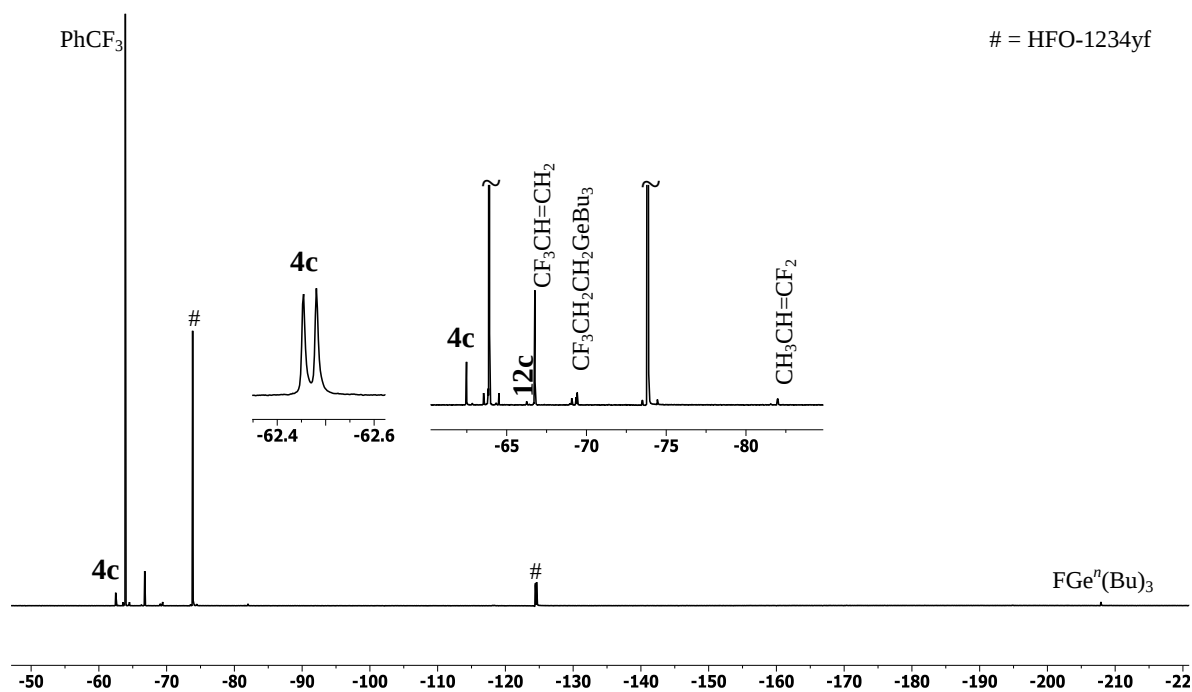
S31. ^{19}F NMR spectrum of the catalytic conversion of HFO-1234yf with HGePh_3 .



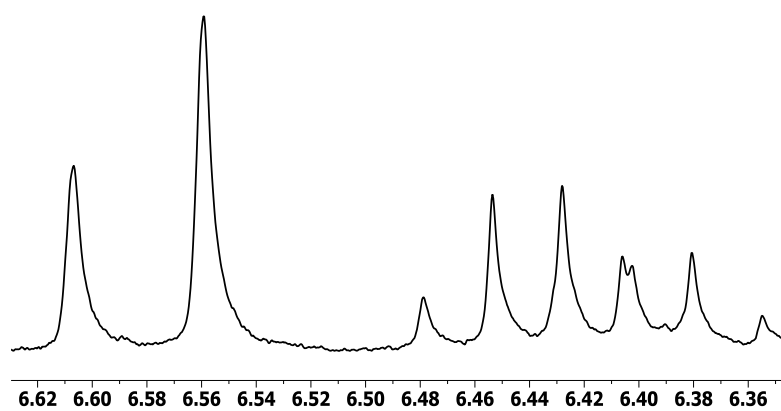
S32. ^{19}F NMR spectrum of the catalytic conversion of HFO-1234yf with HGeEt_3 .



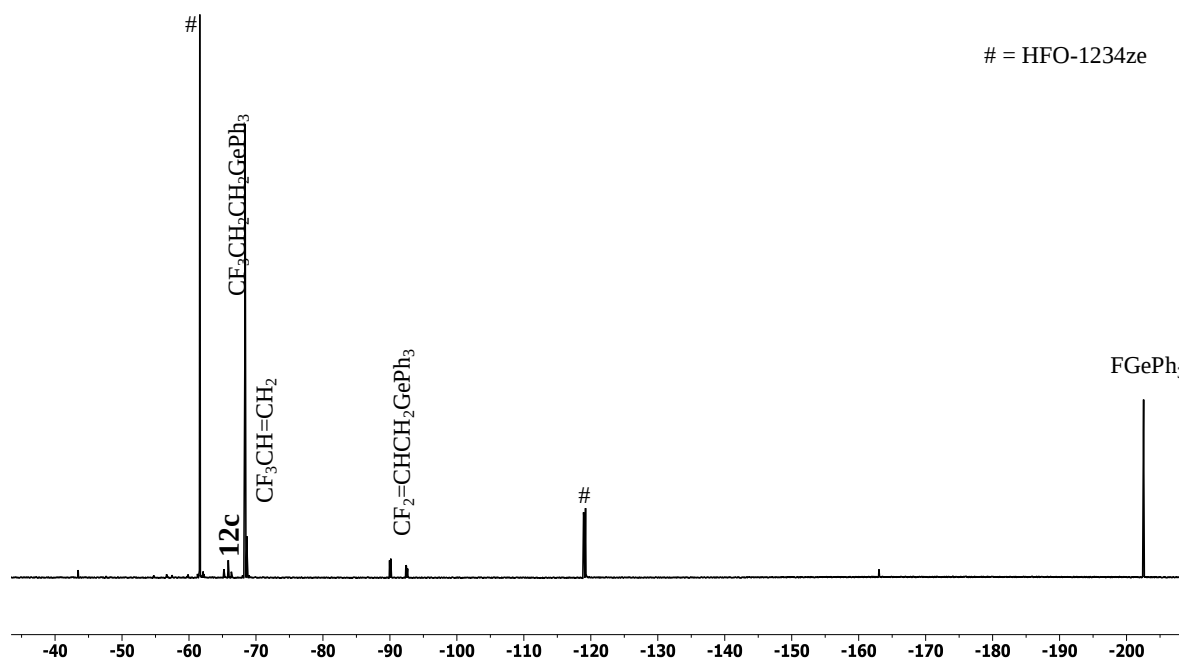
S33. ^1H NMR spectrum of the olefinic protons of $Z\text{-(CF}_3\text{)CH=CH(GeEt}_3\text{)}$ (**4b**).



S34. ^{19}F NMR spectrum of the catalytic conversion of HFO-1234yf with $\text{HGe}(\text{}^n\text{Bu})_3$.

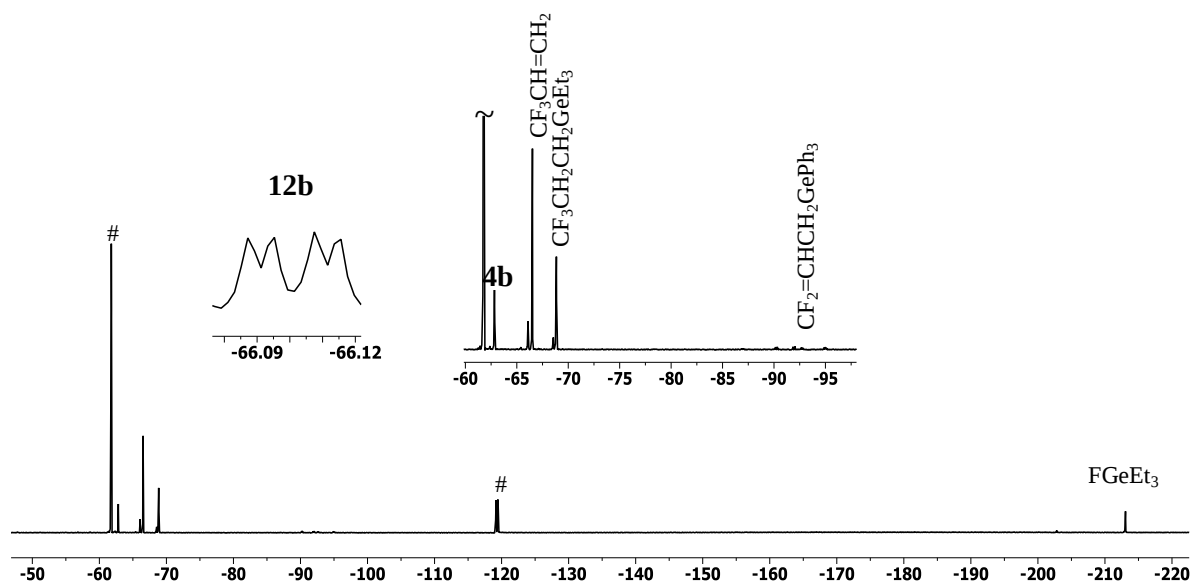


S35. ^1H NMR spectrum of the olefinic protons of $Z\text{-(CF}_3\text{)CH=CH(Ge}^n\text{Bu)}_3$ (**4c**).

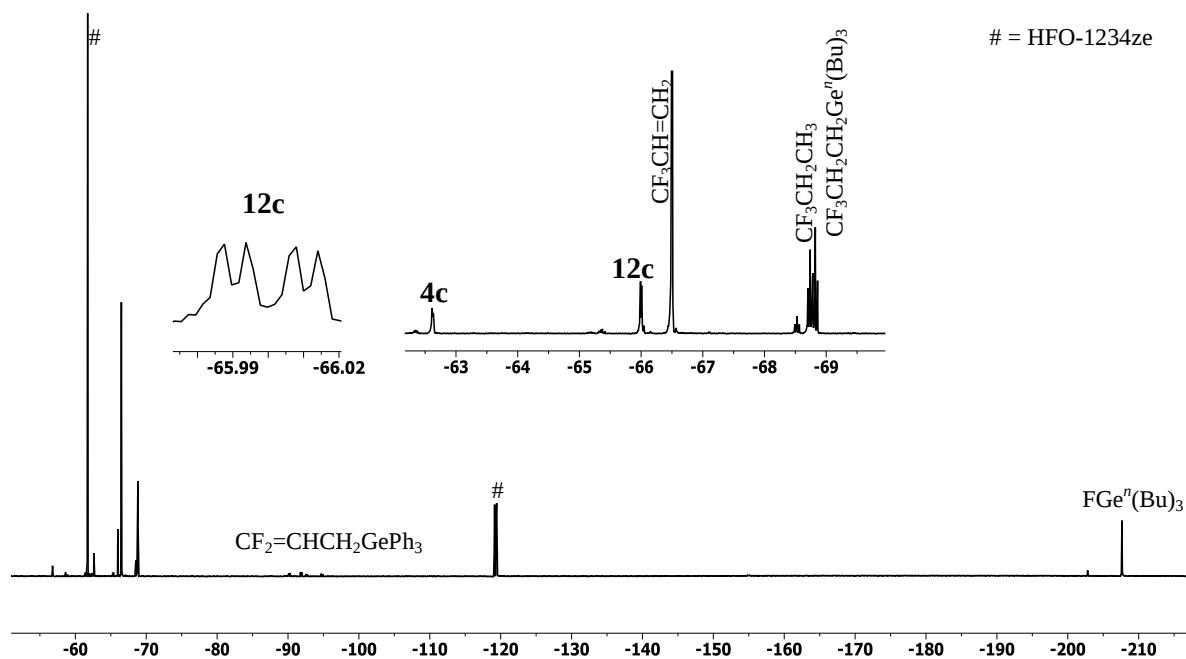


S36. ^{19}F NMR spectrum of the catalytic conversion of HFO-1234ze with HGePh_3 .

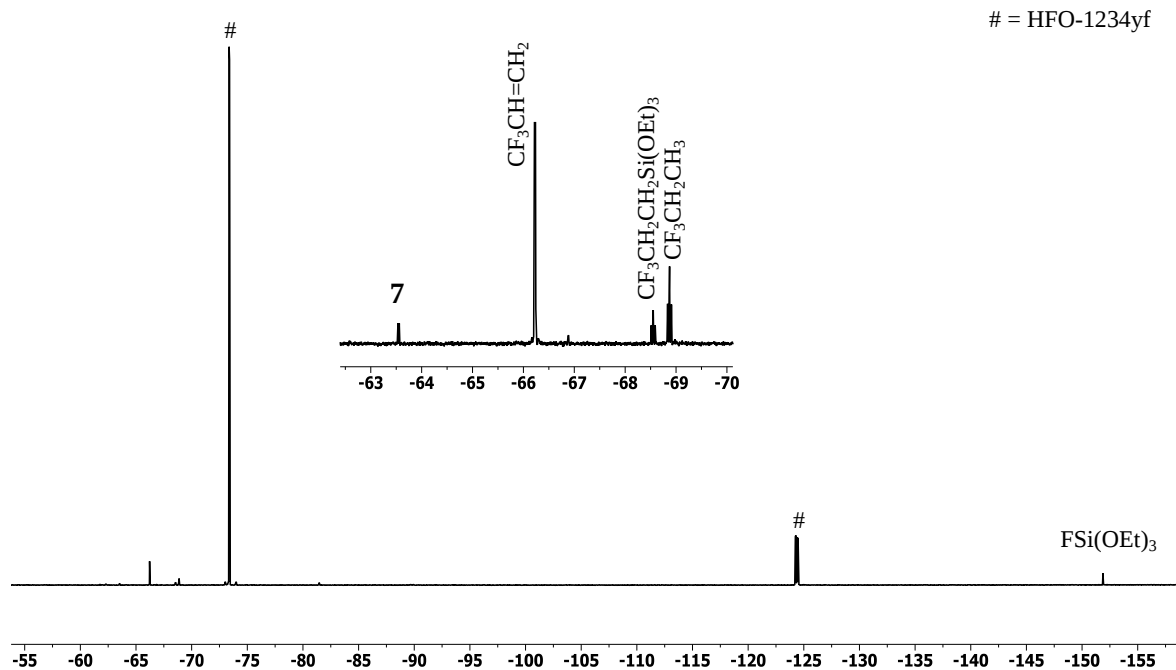
= HFO-1234ze



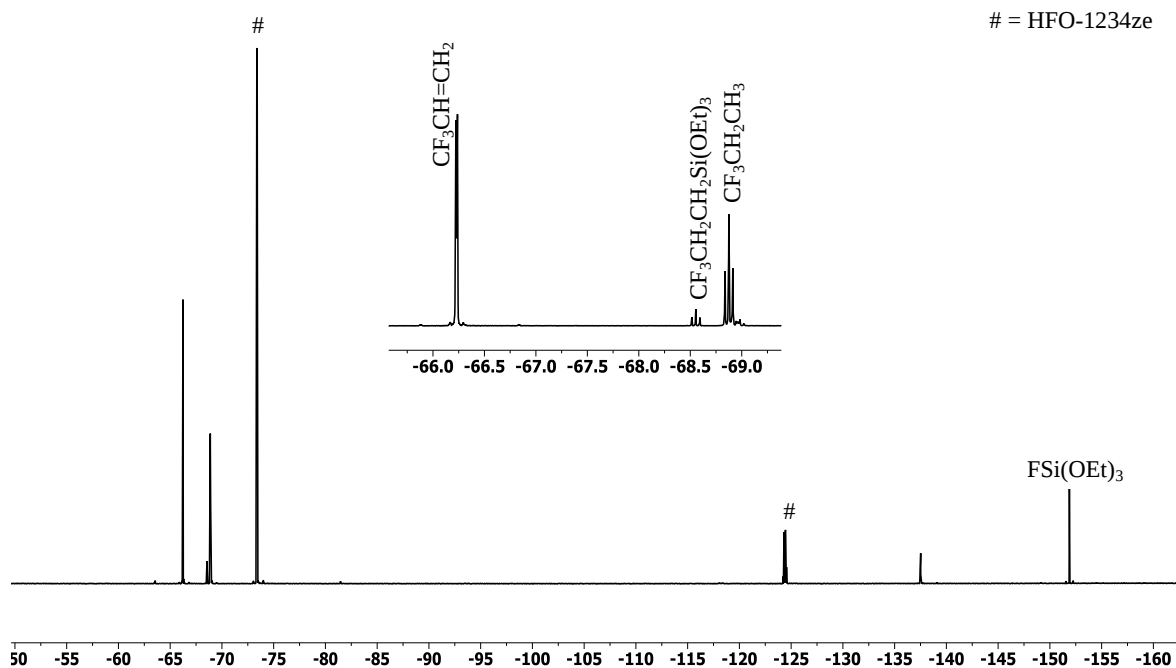
S37. ¹⁹F NMR spectrum of the catalytic conversion of HFO-1234ze with HGeEt₃.



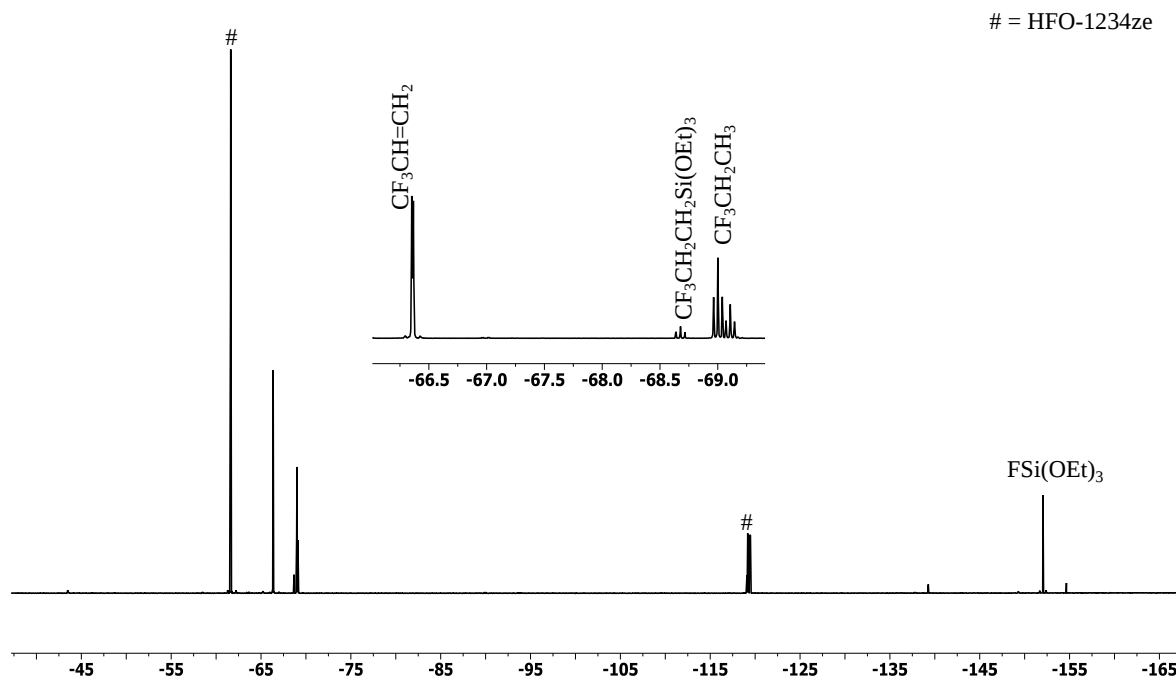
S38. ¹⁹F NMR spectrum of the catalytic conversion of HFO-1234ze with HGe(ⁿBu)₃.



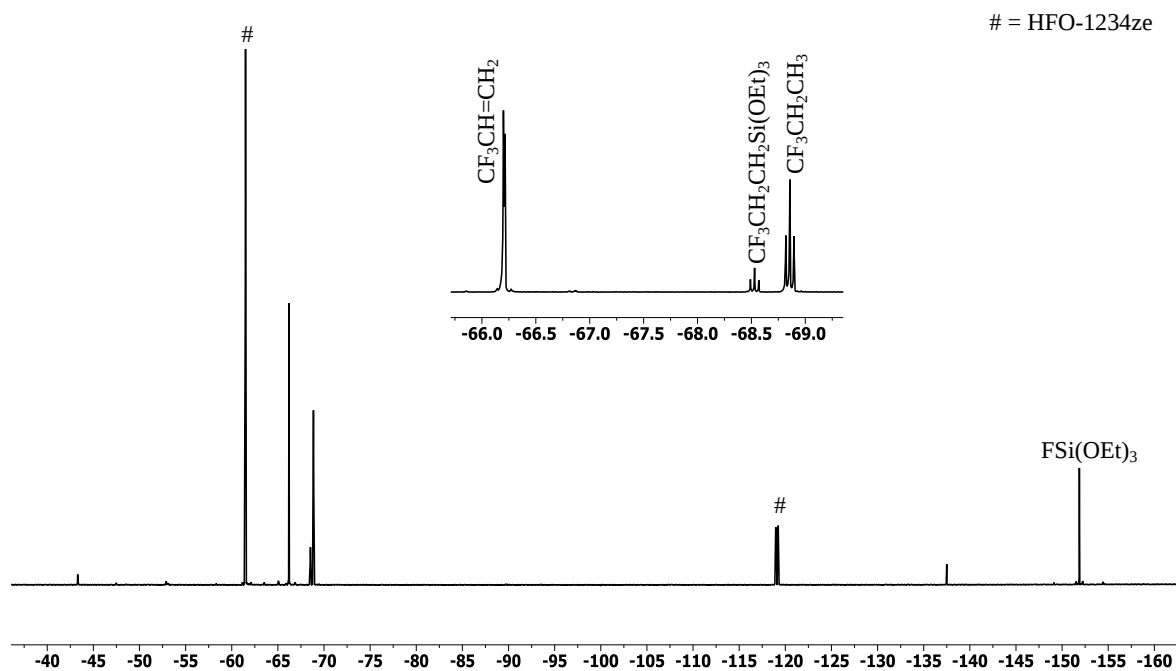
S39. ^{19}F NMR spectrum of the catalytic conversion of HFO-1234yf with $\text{HSi}(\text{OEt})_3$ and complex **5** as catalyst.



S40. ^{19}F NMR spectrum of the catalytic conversion of HFO-1234yf with $\text{HSi}(\text{OEt})_3$ and complex **1** as catalyst.



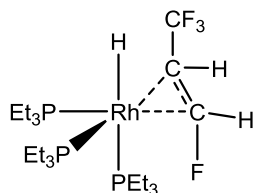
S41. ¹⁹F NMR spectrum of the catalytic conversion of HFO-1234ze with HSi(OEt)₃ and complex **5** as catalyst.



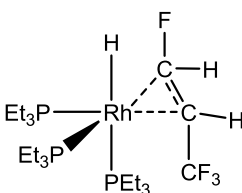
S42. ¹⁹F NMR spectrum of the catalytic conversion of HFO-1234ze with HSi(OEt)₃ and complex **1** as catalyst.

Structure, energy and xyz coordinates of the possible isomers of complex **10**

Complex **10**



Complex **10a**

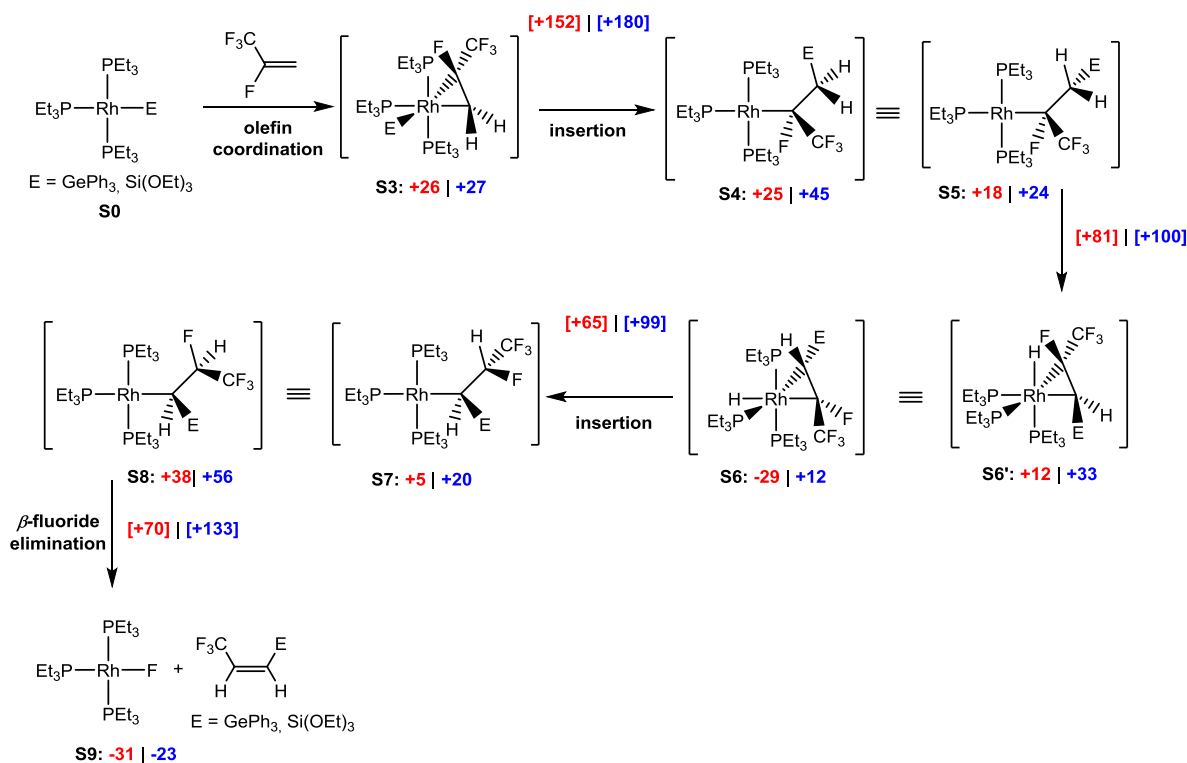


Energy in Hartree (corrected for zero-point energy): -2362.531409 for complex **10** and -2362.525054 for complex **10a**. Hence, structure **10** is favored by 16.7 kJ/mol.

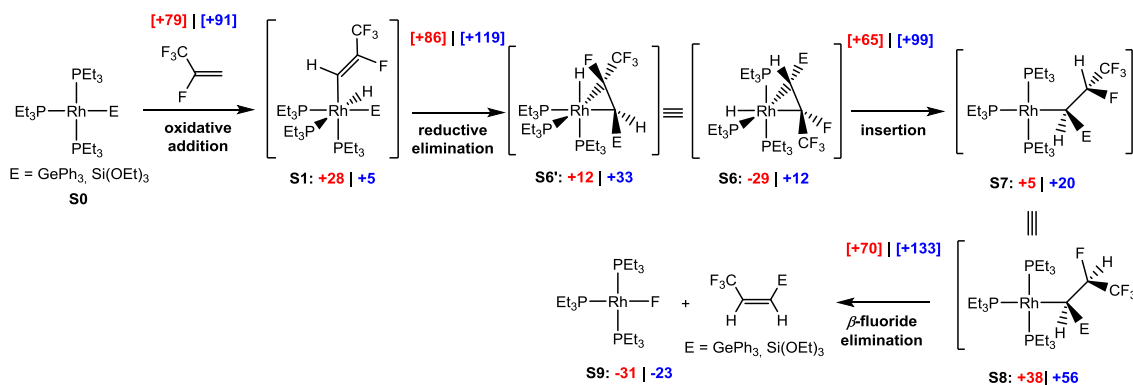
Table S1: Cartesian Coordinates of possible isomers of **10**.

Complex 10				Complex 10a			
Rh	-0.05068	0.11269	0.46169	Rh	-0.04350	-0.03081	-0.58553
H	0.33404	-1.05584	1.44270	H	-0.22370	0.93938	-1.81168
P	-0.59752	1.98191	-0.96980	P	0.34227	-1.55235	1.29146
P	-1.99218	-1.21404	0.47861	P	-2.34272	0.41421	-0.41043
P	1.56427	-1.01673	-0.89580	P	1.04424	1.94294	0.15544
C	-3.64097	-0.53253	-0.08471	C	-3.41976	-1.10596	-0.18416
C	-2.35493	-1.64193	2.27511	C	-2.91879	1.04922	-2.07043
C	-1.96870	-2.88842	-0.35801	C	-3.08697	1.73901	0.69109
C	3.11101	0.01801	-1.10662	C	2.74953	2.06006	-0.61462
C	2.13203	-2.55604	0.00752	C	0.16836	3.45747	-0.52074
C	1.20152	-1.63597	-2.63312	C	1.24567	2.35997	1.97645
C	-0.43739	1.75786	-2.81717	C	-0.39220	-1.14259	2.97046
C	-2.34113	2.62410	-0.80918	C	-0.28592	-3.29171	1.00685
C	0.38640	3.54492	-0.71166	C	2.09816	-1.92708	1.82518
C	1.05848	1.31202	1.82338	C	1.18514	-0.99665	-2.05242
C	-0.34592	1.24267	2.16977	C	-0.15976	-1.53062	-2.01337
H	1.43456	2.27850	1.47947	C	2.36093	-1.85622	-1.77363
C	2.05676	0.67132	2.72256	H	1.41139	-0.33427	-2.89193
F	-1.05873	2.45683	2.06579	H	-0.33138	-2.56641	-1.70537
H	-0.66857	0.73789	3.08543	F	-0.96972	-1.28781	-3.13596
H	2.69464	-2.17388	0.87459	H	0.38594	3.45407	-1.60174
C	2.90351	-3.64737	-0.73513	C	0.42973	4.83252	0.09653
H	1.20527	-2.97470	0.42923	H	-0.90154	3.21794	-0.43861
H	0.46967	-0.92878	-3.04777	H	1.23344	1.39212	2.49392
H	0.65585	-2.58349	-2.49785	H	0.30790	2.86370	2.26316
C	2.34954	-1.81598	-3.62984	C	2.45729	3.16810	2.44307
H	3.10001	0.66705	-0.22333	H	2.62176	1.52971	-1.57005
H	2.91768	0.66983	-1.97494	H	3.40387	1.40846	-0.01547
C	4.48297	-0.64976	-1.21660	C	3.41047	3.41737	-0.86054
C	-1.49966	0.81458	-3.38283	C	-1.86940	-1.49344	3.13927
H	0.57109	1.35200	-2.99417	H	-0.24429	-0.06228	3.12009
H	-0.47802	2.74005	-3.31704	H	0.20635	-1.65539	3.74171
C	1.87141	3.42026	-1.04699	C	2.94025	-0.71139	2.19696
H	0.24039	3.81058	0.34686	H	2.56643	-2.46264	0.99117
H	-0.06961	4.34579	-1.31402	H	2.04353	-2.62327	2.67751
H	-2.96536	1.78886	-1.11272	H	-1.36708	-3.19902	0.81822
C	-2.72084	3.88802	-1.58159	C	-0.00738	-4.34670	2.07935
H	-2.48698	2.75252	0.27333	H	0.16393	-3.60214	0.05398
H	-2.97083	-0.80550	2.64817	H	-2.48409	0.34496	-2.79398
H	-1.38673	-1.55667	2.78671	H	-2.37537	1.99847	-2.20767
C	-2.99608	-2.98755	2.61908	C	-4.41601	1.23805	-2.31220
C	-2.17294	-2.82194	-1.87181	C	-2.62044	1.74101	2.14393
H	-2.72907	-3.54546	0.09024	H	-4.18586	1.70686	0.63045
H	-0.98651	-3.32633	-0.11757	H	-2.78122	2.67903	0.20266
H	-3.73170	0.43759	0.42738	H	-3.48573	-1.54139	-1.19557
C	-4.89797	-1.37357	0.14313	C	-4.80187	-0.94236	0.44754
H	-3.52058	-0.30070	-1.15526	H	-2.82199	-1.81740	0.40066
H	4.70136	-1.25149	-0.32166	H	2.80770	4.04575	-1.53362
H	5.26906	0.12034	-1.28767	H	4.39010	3.27252	-1.34575
H	4.57492	-1.29970	-2.09751	H	3.58217	3.98120	0.06657
H	2.34501	2.61769	-0.46730	H	2.98729	-0.00571	1.35806
H	2.40132	4.36052	-0.82563	H	3.97142	-1.01657	2.43695
H	2.02936	3.19617	-2.11431	H	2.54028	-0.18297	3.07679
H	-2.51698	3.79100	-2.66075	H	-0.36093	-4.04005	3.07640
H	-2.17935	4.77379	-1.21728	H	1.06733	-4.56649	2.16058
H	-3.79753	4.09628	-1.46955	H	-0.51483	-5.29224	1.82688
H	-1.57125	-0.09648	-2.76987	H	-2.47862	-1.06047	2.33710
H	-1.26566	0.51487	-4.41677	H	-2.25576	-1.10621	4.09597
H	-2.49425	1.28655	-3.39102	H	-2.03402	-2.58085	3.13133
H	-5.10891	-1.50298	1.21498	H	-5.44201	-0.24978	-0.11748
H	-4.81437	-2.37601	-0.30516	H	-4.73063	-0.56131	1.47904
H	-5.77753	-0.88360	-0.30634	H	-5.32228	-1.91329	0.49351
H	-3.19750	-2.50980	-2.12724	H	-3.10269	0.94591	2.72965
H	-2.00445	-3.80769	-2.33505	H	-2.85548	2.69980	2.63413
H	-1.48214	-2.11088	-2.34323	H	-1.53338	1.58216	2.20033
H	-3.96486	-3.14319	2.12254	H	-4.95959	0.28139	-2.27637
H	-3.16729	-3.05505	3.70611	H	-4.58818	1.66822	-3.31267
H	-2.33967	-3.82719	2.34213	H	-4.87938	1.91823	-1.57994
H	3.86118	-3.28944	-1.13614	H	1.47725	5.14778	-0.00063
H	2.31873	-4.05696	-1.57366	H	0.17216	4.85088	1.16713
H	3.12269	-4.48542	-0.05279	H	-0.19313	5.59621	-0.39888
H	2.88894	-0.87129	-3.79814	H	3.39972	2.67311	2.16269
H	1.95829	-2.14792	-4.60613	H	2.45246	3.26541	3.54177
H	3.08108	-2.56347	-3.29394	H	2.47033	4.18267	2.02073
F	1.56269	-0.34686	3.47252	F	2.05153	-3.01039	-1.09982
F	2.59399	1.56070	3.60748	F	3.32853	-1.24347	-1.02184
F	3.13761	0.15129	2.05187	F	2.99960	-2.25832	-2.90651

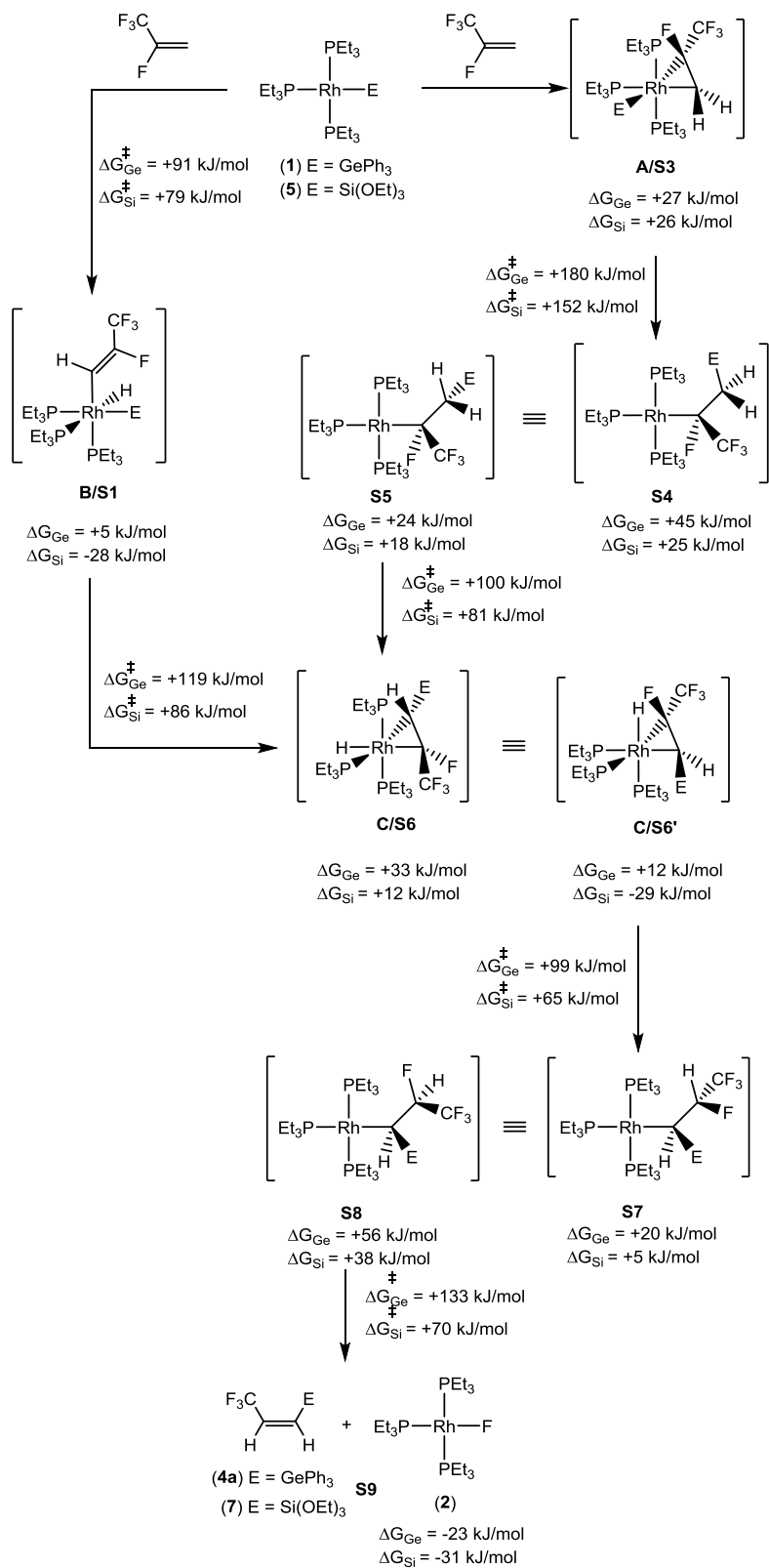
Mechanistic computational details



Scheme S1. Calculated reaction and activation free energies (298.15 K, 0.1 MPa; $\Delta G^\ddagger$ in square brackets) for the reaction of $[\text{Rh}(\text{E})(\text{PEt}_3)_3]$ ($\text{E} = \text{GePh}_3$ (**1**, blue), $\text{Si}(\text{OEt})_3$ (**5**, red)) with HFO-1234yf via intramolecular C–H activation (RI-BP86-D3(BJ)/def2-SVP/COSMO(toluene)).



Scheme S2. Calculated reaction and activation free energies (298.15 K, 0.1 MPa; $\Delta G^\ddagger$ in square brackets) for the reaction of $[\text{Rh}(\text{E})(\text{PEt}_3)_3]$ ($\text{E} = \text{GePh}_3$ (**1**, blue), $\text{Si}(\text{OEt})_3$ (**5**, red)) with HFO-1234yf via initial intermolecular C–H activation (RI-BP86-D3(BJ)/def2-SVP/COSMO(toluene)).



Scheme S3. Possible mechanisms for the activation of HFO-1234yf with complexes **1** and **5**. All calculated reaction and activation free energies (298.15 K, 0.1 MPa) are given relative to the separate reactants **1/5** and HFO-1234yf (RI-BP86-D3(BJ)/def2-SVP/COSMO(toluene)).

Table S1: Cartesian Coordinates of all optimized structures.

SO	Si	Ge	SO-Ge	Si	Si	Si	Ge				
C	-3.431962	0.446397	1.909904	C	0.582343	-2.882322	2.588372	C	-2.582088	1.056642	2.354995
P	-2.226272	1.387109	0.823129	P	0.289226	-2.568766	0.769411	C	-3.169942	2.130786	3.046315
C	-3.474984	2.383727	-0.160123	C	-1.328949	-3.470644	0.567253	C	-3.736740	3.198017	2.330529
C	-1.963244	1.573297	-1.238464	C	-1.774262	-3.698357	-0.874720	C	-3.712314	3.175491	0.925669
H	-3.470420	1.050272	-1.893782	H	-2.773061	-4.178339	-0.903480	C	-3.132392	2.092460	0.245676
H	-4.861790	0.803166	-0.798293	H	-1.073509	-4.351404	-1.434526	C	-2.555598	1.009158	0.944726
H	-4.825658	2.224548	-1.878551	H	-1.854584	-2.736069	-1.412559	Ge	-1.639840	-0.436627	-0.080662
H	-1.199676	2.841645	0.548230	H	-2.079044	-2.856218	1.102103	C	-2.464093	-0.212157	-1.883025
H	-2.910955	3.219443	-0.620333	H	-1.248058	-4.431508	1.118783	C	-1.759144	-2.283620	-2.927723
C	-1.655886	2.720178	2.007987	C	1.500785	-3.743824	-0.037461	C	-3.378264	0.475655	-4.236082
C	-0.616746	2.237720	0.327043	C	1.405804	-5.232786	0.301977	C	-3.741459	0.174560	-4.389466
H	-1.068336	1.584696	3.794932	H	1.196893	-5.804832	-0.225234	C	-4.472281	-0.307035	-3.288460
H	-0.136469	3.088933	3.547790	H	0.340751	-5.664047	-0.000600	C	-3.836182	-0.493194	-2.050035
H	0.172139	1.647981	2.513143	H	1.536345	-5.421663	1.386829	H	-4.542585	-0.863059	-1.195524
H	-1.223668	3.520784	3.710991	H	1.378675	-5.842666	-1.129171	H	-5.544572	-0.535882	-3.395306
H	-2.545223	3.161537	2.508175	H	2.506467	-3.345935	0.209500	H	-4.293984	0.320976	-5.362041
Rh	-0.393053	0.236884	-0.053571	Rh	0.336442	-2.74585	0.110725	H	-1.769820	0.867799	-5.087469
P	-1.296177	-1.830989	-0.531444	P	2.473741	0.324690	0.901164	H	-0.686214	0.539975	-2.875291
C	-0.730902	-3.468112	0.169315	C	3.617182	1.282407	-0.244528	C	-2.562561	-2.113741	0.546784
C	-1.181601	-3.754672	1.600152	C	3.425623	2.502632	0.323082	C	-2.886099	-1.338145	-0.373486
H	-0.830770	-2.968288	2.293721	H	5.013987	2.253099	1.168470	C	-3.442363	-4.359321	0.041195
H	-0.764523	-4.719137	1.955659	H	3.614178	3.260185	0.668205	C	-3.704574	-4.589050	1.402360
H	-2.285414	-3.818434	1.689420	H	4.964474	2.973185	-0.466313	C	-3.435052	-3.570949	2.331657
H	0.372398	-3.438693	0.112064	H	4.342366	0.540938	-0.639237	C	-2.879667	-2.352489	1.903775
H	-1.076025	-4.265680	-0.522656	H	2.976011	1.610818	-0.080261	H	-2.708345	-1.571022	2.656256
C	-0.922068	-2.107100	-2.336197	C	2.367227	1.390359	2.426500	H	-3.665027	-3.721096	3.398379
H	-1.506074	-1.015796	-2.333658	C	1.783438	0.670209	3.640442	H	-4.133495	-5.547242	1.733786
H	-2.615223	-1.049433	-3.252808	H	1.644824	1.375128	2.448941	C	-2.836294	-0.787331	2.052839
H	-1.199841	-0.081787	-2.858064	H	0.796109	0.231237	3.399648	H	-2.713367	-2.979573	-1.448248
H	-1.151059	-1.118437	-2.79664	H	2.441866	-1.049065	3.99571	Rh	0.213667	-0.219707	-0.114146
H	0.185596	-2.126362	-3.271774	H	3.373333	1.791916	2.657928	P	1.040569	-2.508465	-0.620356
H	-1.280841	-3.116151	-2.632321	H	1.735162	2.252095	2.131587	C	-0.401122	-3.743377	0.621443
C	-3.157467	-2.043978	-0.482990	C	3.636647	-1.034037	1.454193	C	0.233394	-5.193905	0.168388
C	-3.743152	-2.383907	-1.161634	C	4.973312	-0.611664	2.067062	H	-0.040029	-5.834090	1.031777
H	-3.356909	-4.222707	-0.715869	H	5.569854	-1.501576	2.356006	H	1.157614	-5.614609	-0.278641
H	-3.513913	-3.310060	-2.245760	H	4.833516	0.001315	2.979948	H	-0.581793	-5.292501	-0.574470
H	-4.848144	-3.302550	-0.058661	H	5.585940	-0.022154	1.356474	H	-0.559911	-3.342436	0.989945
H	-3.569049	-1.116576	-0.927854	H	3.801845	-1.685881	0.550872	H	1.108780	-3.672502	1.472383
C	-3.440151	-2.018086	0.588149	H	3.071428	-1.673533	2.159983	C	0.101497	-2.936386	-2.175105
Si	1.628894	-0.873401	0.163286	Si	-0.181623	1.994541	-0.099456	C	0.674001	-2.357482	-3.467315
O	0.263630	-2.046774	-0.107963	O	-0.926180	2.773026	1.217540	H	1.697489	-2.727394	-3.681020
C	2.936387	-1.152573	-0.822817	C	-1.359254	2.279238	2.468579	H	0.702865	-2.51785	-3.421408
C	2.617874	-4.231337	-1.850912	C	-2.975884	-0.163936	3.918633	H	0.033245	-2.633834	-4.327995
C	3.301160	-5.092569	-1.749925	C	-4.372876	-1.74614	3.760770	H	0.032342	-0.401339	-2.240277
H	1.580179	-4.600901	-1.723731	C	-4.925672	-0.132809	2.468813	H	-0.924176	-2.549666	-2.029021
H	2.710621	-3.826861	-2.879493	C	-0.083481	-0.946781	1.343146	C	2.689993	-3.287291	-1.037827
H	3.998816	-8.29655	-0.933617	H	-1.614767	-4.669482	2.448941	H	1.120396	-1.94278	2.583636
H	2.830964	-3.555320	0.216007	H	-0.619528	-0.131611	3.37829	H	-0.791238	2.804313	1.272465
O	1.727668	-1.852804	1.589895	H	-5.030537	-0.208608	6.443365	O	-1.197424	2.445086	-1.025222
C	1.196164	-1.325070	2.816679	H	-2.533983	-0.185909	4.927550	C	-2.571664	2.786207	-1.267969
C	2.118905	-0.325482	3.511253	H	-1.050321	-0.103311	2.910443	C	-2.769720	4.293722	-1.155759
H	1.680266	0.009859	4.474060	C	-2.217758	1.569466	-1.082054	H	-3.849000	5.456768	-1.094334
C	1.310423	-0.777844	3.717847	C	-1.894155	1.779119	-2.440890	H	-2.340281	4.616535	-0.253032
C	2.277413	0.564890	2.871475	C	-2.308442	2.933527	-3.124740	H	-2.268866	4.671166	-0.242234
H	1.013687	-2.194756	3.788391	C	-3.061697	3.915747	-2.457099	H	-3.106389	2.388391	-2.159477
H	0.206373	-0.842042	2.627668	C	-3.413036	3.718022	-1.110619	H	-3.071782	2.86519	-0.380468
O	3.003135	0.159345	0.303920	C	-2.999153	2.554465	-0.437533	O	1.203179	2.941347	-0.423529
C	4.305979	-0.304413	0.622043	H	-3.289242	2.417340	0.616228	C	1.147107	4.331397	-0.772728
C	5.116336	0.822272	1.251243	H	-4.013306	4.474276	-0.580162	C	1.147559	5.195296	0.531183
H	6.154263	0.494205	1.466409	H	-3.379313	3.027260	-2.986348	H	2.055061	5.003881	1.141032
H	4.652253	1.155042	2.201681	H	-2.035325	4.072764	-1.827443	H	0.261635	4.957328	1.151456
H	5.162473	1.697275	0.570923	H	-1.294785	1.030176	-2.980804	H	1.128774	6.274059	0.269999
H	4.249553	-1.172052	1.319514	C	-2.067284	-1.482126	-1.312405	H	2.035012	4.567464	-1.356936
H	4.817506	-0.665369	-0.302577	C	-3.120964	-2.370068	-1.002850	H	0.244702	4.548113	-1.341991
P	0.795118	2.085100	-0.715005	C	-3.499071	-3.393736	-1.890373	C	-1.660726	-0.302986	-0.352117
H	3.998816	-8.29655	-0.933617	H	-1.537893	-3.504447	-3.121627	H	-2.738640	-0.479777	0.425876
C	-1.064549	0.304114	-2.667723	C	-1.788663	-2.666560	-3.449937	F	6.683284	-0.725767	1.781239
H	-0.425227	2.802094	-3.544701	H	-1.405286	-1.661389	-2.546613	C	-1.168577	-0.553618	-0.018413
H	-1.784926	3.811192	-2.971642	H	-0.549700	-1.016339	-2.796804	F	-4.966092	0.362639	0.606572
H	-1.637647	2.104465	-2.434404	H	-1.254153	-2.779057	-4.406654	F	-4.178829	-1.773946	0.255676
H	-0.882540	3.842602	-0.650383	H	-3.135442	-4.339766	-3.820073	F	-4.297832	-0.347471	-1.352485
H	0.449993	4.294842	-1.737239	H	-3.418884	-0.078155	-1.619461	H	-1.954966	-0.901286	-1.390346
C	2.049107	1.812513	-2.080987	H	-3.655089	-2.270497	-0.044637	P	1.005423	-0.570428	-2.167352
C	1.700404	0.732403	-3.105710	P	0.854383	2.263680	0.548852	C	0.036663	-1.703903	-3.299695
H	2.510672	0.644306	-3.859483	C	0.435972	3.570829	-0.721506	C	-3.351778	-1.222658	-3.720081
H	1.589408	-0.253436	-2.613638	C	1.137394	3.401634	-2.066511	H	-1.331800	-0.194432	-4.132502
H	0.760194	0.948433	-3.648166	H	0.370728	4.113354	-2.813087	H	-0.276040	-1.224254	-2.882626
H	2.972450	1.524185	-1.542133	H	2.229261	3.584186	-1.994834	H	-1.766800	-1.887088	-0.507362
H	2.223884	2.793858	-2571265	H	0.987863	3.277850	-2.459161	H	-0.027949	-2.685445	-2.788349
C	1.798307	3.044389	0.536612	H	0.663924	4.561701	-0.276122	H	0.654608	-1.865048	-4.205009
C	2.757545	4.115766	0.013563	H	-0.659901	3.524155	-0.885869	C	2.752484	-1.254806	-2.350498
C	3.259328	4.631596	0.858577	C	-0.359509	2.681220	1.914393	C	3.076565	-2.231632	-3.490221
H	2.241574	4.894860	-1.058494	C	-0.620175	4.140974	2.232976	H	4.149925	-2.502949	-3.456813
H	3.553102	3.676937	-0.620276	H	-1.296887	4.229182	3.107966	H	2.881543	-1.787374	-4.489807
H	2.351681	2.257712	1.085299	H	-1.11627	4.657039	1.384779	H	2.491694	-3.161753	-3.417377
H	1.061189	3.482791	1.238093	H	0.307236	4.697635	2.479489	H	2.982162	-1.732079	-1.378986
C	-2.798752	-0.578036	2.850649	H	-1.306689	2.165573	1.646949	C	3.403982	-0.360075	-2.408349
H	-2.056099	-1.195809	2.308613	H	0.017088	2.123288	2.804949	C	1.060684	0.994455	-3.171176
H	-3.562152	-1.255572	3.284875	C	2.440448	3.205098	1.275234	H	1.577674	0.911326	-4.606917
H	-2.264014	-0.095007	3.690951	C	3.020500	2.027216	2.404165	H	1.539315	1.909050	-0.910666
H	-4.129222	-0.059109	1.211669	H	2.360325	2.172538	3.294652	H			

		H	-0.712416	0.818012	-2.789407			H	-2.846333	1.774604	2.530770
S5-Si			S5-Ge			S6-Si			S6-Ge		
C	-2.403031	-3.282557	-0.626274	C	4.148168	-1.625257	-2.072443	C	4.929969	1.349975	-0.193458
P	-1.872000	-1.936564	0.586182	P	4.205276	-0.442094	-0.622806	C	3.657290	1.191703	-0.782590
C	-0.667234	-2.805739	1.723131	C	5.663240	-1.252658	0.256441	C	3.364246	1.920272	-1.955210
C	-0.313125	-1.954236	2.944858	C	6.304295	-0.485062	1.411100	C	4.317758	2.778743	-2.528386
H	-0.081502	-0.913910	2.646032	H	6.659991	-0.517804	1.098017	C	5.581537	2.925323	-1.931488
H	-1.151372	-1.955299	3.668770	H	5.598116	-0.341810	2.250500	C	5.886120	2.209503	-0.760662
H	0.566972	-2.365226	3.479707	H	7.182214	-1.037113	1.805172	Ge	2.357174	-0.073769	-0.000800
H	-1.085406	-1.785102	2.031128	H	5.290015	-2.235389	0.610293	C	2.651185	-1.773488	-0.966993
H	0.229869	-3.023489	1.116233	H	6.420963	-1.477259	-0.524480	C	3.176692	-1.714980	-2.277016
C	-3.346770	-1.823154	1.737000	C	5.018175	1.048272	-1.412772	C	3.266137	-2.867249	-3.075996
C	-3.868232	-3.117486	2.363865	C	6.317537	0.843597	-2.192726	C	2.841273	-4.108373	-2.572380
H	-4.222637	-3.833020	1.594742	H	7.130949	0.445421	-1.552862	C	2.342041	-4.190557	-1.261733
H	-4.725907	-2.907650	3.036300	H	6.187433	0.145640	-0.043942	C	2.249744	-3.033336	-0.470117
C	-3.094923	-3.630703	2.970901	H	6.673211	1.807063	-2.612879	C	0.586828	0.560053	-0.537088
H	-3.047201	-1.093272	2.516707	H	5.165514	1.787953	-0.600522	C	-0.076278	1.742425	-0.020922
H	-4.148344	-1.317993	1.165888	H	4.225659	1.481124	-2.056320	F	0.353542	2.194559	1.252783
Rh	-1.189287	0.130851	-0.095516	Rh	1.983158	0.015161	-0.087378	Rh	-1.487033	0.196351	-0.159172
P	-3.268545	0.880049	-0.771904	P	2.317599	1.972945	1.066695	P	-1.282409	-0.632377	2.076156
C	-4.478470	2.017094	0.060554	C	1.093662	2.163977	2.469425	C	-0.690730	0.476279	3.452558
C	-5.030644	1.451647	1.404540	C	0.985359	0.918524	3.347607	C	-1.510258	1.750153	3.640960
H	-4.210499	1.159893	2.089983	H	0.861052	0.017854	2.712126	P	-1.720616	-1.762198	-1.428941
H	-5.651476	0.549244	1.228736	H	1.902075	0.759598	3.951271	C	-0.391650	-1.826463	-2.738669
H	-5.667743	2.193420	1.928104	H	0.126156	0.984612	0.404593	C	-0.436604	-0.707947	-3.778207
H	-5.297199	2.282821	-0.606017	H	1.375160	3.058715	3.063245	C	-3.252091	-1.906637	-2.492442
H	-3.916372	2.956841	0.281932	H	0.119347	2.398288	2.000802	C	-3.329081	-3.078373	-3.472545
C	-4.403036	-0.440951	-1.474205	C	2.279059	3.741051	-0.441669	C	-1.520441	-3.502693	-0.776771
C	-5.639108	0.002379	-2.258474	C	3.083130	3.983975	-0.834314	C	-2.638690	-3.982680	0.145742
H	-5.374366	0.609808	-1.346868	H	4.168830	3.826577	-0.674825	P	-3.626972	1.106036	0.017132
H	-6.205547	-0.879507	-2.622850	H	2.949921	5.024329	-1.195844	C	-5.088798	0.252384	0.827076
H	-6.333806	0.602173	-1.636052	H	2.757602	3.298118	-1.640810	C	-5.428255	-1.140861	0.304746
H	-4.701180	-1.089293	-0.626234	H	1.209357	3.967297	0.270207	C	-4.421371	1.528292	-1.621097
H	-3.735210	-1.066104	-2.102337	H	2.615730	4.408175	1.264552	C	-3.619863	2.475021	-2.511959
C	-2.961572	1.905682	-2.305878	C	3.922545	1.944797	2.032097	C	-3.716540	2.726425	0.946806
C	-2.035519	1.220959	-3.311307	C	4.154446	2.998552	3.115208	C	-4.956841	3.603645	0.760206
H	-1.082439	0.933735	-2.823511	H	5.154347	2.863762	3.577338	C	-0.073189	-2.051999	2.196861
H	-2.486217	0.294553	-3.721650	H	4.118711	4.030586	2.711005	C	0.636503	-2.353745	3.517518
H	-1.809184	1.890639	-1.166200	H	3.406284	2.931097	3.930140	C	-2.848068	-1.295860	2.856760
H	-3.939100	2.711795	-2.760808	H	3.964996	0.923826	2.460262	C	-2.739580	-2.298812	4.062332
H	-2.512978	2.854977	-1.954329	H	4.732556	1.980086	1.277447	C	-0.114021	2.996434	-0.872054
P	-0.475757	2.122400	0.642673	P	1.442816	-2.214719	0.249383	F	-1.112731	3.865834	-0.530480
C	1.260905	2.337947	1.324376	C	-0.153521	-2.426875	1.196267	C	2.922505	-0.262650	1.869290
C	1.705915	3.673337	1.921401	C	-0.525031	-3.825357	1.686931	C	2.736741	0.794074	2.786889
H	1.061225	4.003237	2.761660	H	0.239997	-4.256123	2.364245	C	3.242092	0.706606	4.094747
H	1.717727	4.484830	1.166304	H	-1.480566	-3.790962	2.500007	C	3.954952	-0.435114	4.501189
H	2.738959	3.582070	2.314566	H	-0.674036	-4.529813	0.844851	C	4.171395	-1.481113	3.589009
H	1.346211	1.535798	2.085089	H	-0.936837	-3.038211	1.387967	C	3.659387	-1.392813	2.282865
H	1.935858	2.043954	0.497679	H	-0.088161	-1.715922	2.045784	F	-0.267244	2.730482	-2.197560
C	-1.493091	2.737466	2.119684	C	2.675703	-3.038211	1.387967	F	1.041046	3.713401	-0.755722
C	-1.564582	1.664871	3.205383	C	3.010745	-2.210312	2.627058	H	-2.424440	-4.995588	0.543907
H	-2.253071	1.957621	0.424335	H	3.278555	-1.176140	2.327145	H	-2.768152	-3.305472	1.011476
H	-0.570114	1.470155	3.656299	H	1.142255	-2.138121	3.312567	H	-3.613122	-4.033548	-0.381294
H	-1.917036	0.711132	2.761831	H	3.854102	-2.650405	3.197537	H	-1.406423	-4.186231	-1.644505
H	-1.086680	3.692326	2.515580	H	3.582336	-3.212932	0.771814	H	-0.540740	-3.530816	-0.257394
H	-2.506453	2.963753	1.732755	H	2.295769	-4.044860	1.662301	H	-1.322667	-0.788783	-4.440796
C	-0.573484	3.786762	-0.362687	C	1.299061	-3.606603	-1.006756	H	-0.476942	0.290710	-3.299171
C	0.283374	3.752966	-1.628985	C	1.022884	-3.538798	-1.979543	H	0.465934	-0.742255	-4.422214
C	0.152292	4.677747	-2.227324	C	0.169632	-2.637436	-2.616189	H	0.563718	-1.801760	-2.183995
H	1.360079	3.657661	-1.383456	H	-0.850701	-3.508163	-1.453062	H	-0.436419	2.819794	-3.230223
H	0.023368	2.884158	-2.262994	H	0.116691	-4.431603	-6.238445	H	-1.160535	2.677661	-3.459100
H	-1.646270	3.929213	-0.610814	H	2.261446	-3.621990	-1.557560	H	-2.632626	2.039417	-2.760683
H	-0.295651	4.642421	0.288586	H	1.265723	-4.552287	-0.423649	H	-3.425671	3.446478	-2.015264
C	0.768042	-0.434288	-0.585226	C	0.005892	0.414055	-0.664958	H	-5.429118	1.941728	-1.405050
C	1.812109	-0.764409	0.486369	C	-1.067705	0.709759	0.375061	H	-4.582871	0.559255	-2.135613
H	1.521587	-0.337211	1.461242	H	-0.820338	0.227177	1.335194	H	-5.047717	3.975825	-0.279794
H	1.825390	-1.859634	0.659128	H	-1.087737	1.796508	0.586777	H	-5.897638	3.072101	1.010678
Si	3.608380	-0.241510	0.274038	Ge	-2.960939	0.200343	0.042619	H	-4.901074	4.493797	1.420462
O	4.112809	-0.102669	1.667581	C	-3.746597	0.119420	1.849098	H	-2.796891	3.275387	0.676810
C	5.425228	0.356119	2.205324	C	-3.082805	-0.563326	2.893241	C	-5.944700	2.438409	2.010131
C	5.430362	1.855375	2.479469	C	-3.641129	-0.636883	4.180872	H	-5.812060	-1.106227	-0.734662
H	5.119697	2.402711	1.568155	C	-4.877132	-0.022059	4.445652	H	-4.536728	-1.798010	0.309469
H	4.721736	2.102701	3.295999	C	-5.548520	0.663194	3.418289	H	-6.208669	-1.623001	0.928153
H	6.442025	2.199332	2.778789	C	-4.986298	0.731582	2.131670	H	-4.855330	0.215346	1.909121
H	5.750111	-0.208300	3.106786	H	-5.519421	1.273916	1.334276	H	-5.964391	0.926994	0.721486
H	6.147927	0.109632	1.393814	H	-6.515852	1.148997	3.620855	O	4.133678	1.138569	-1.114287
O	4.536964	-1.347368	-0.585192	H	-5.316425	-0.075879	5.453750	C	4.102640	0.588539	-2.468314
C	4.400931	-2.764190	-0.492949	H	-3.108864	-1.175022	4.980722	C	3.822633	-0.540353	-3.455680
C	4.864894	-3.313730	0.852680	H	-2.112561	-1.049742	2.705748	H	3.862430	-0.166276	-4.499344
H	5.915718	-3.021421	1.052534	C	-3.967340	1.540383	-0.974660	H	4.569223	-1.352848	-3.346907
H	4.243328	-2.921752	1.683546	C	-5.171931	1.174582	-1.613754	H	2.816897	-0.978737	-3.291362
H	4.802051	-4.412342	0.864089	C	-5.945530	2.130409	-2.294711	H	5.096143	1.039350	-2.679028
H	5.010433	-3.196876	-1.314714	C	-5.521657	3.469278	-2.346031	H	3.349269	1.399629	-2.585003
H	3.347713	-3.065337	-0.692558	C	-4.323092	3.846344	-1.715498	O	2.594301	-1.983261	-0.316363
O	3.955251	1.229952	-0.436922	C	-3.554102	2.887687	-1.035588	C	3.713697	-2.870484	-0.225536
H	-4.118705	1.433514	-1.845802	H	-2.611030	3.198538	-0.560183	C	3.946078	-3.347222	1.202950
C	5.583815	1.319936	-2.425204	H	-3.983196	4.892936	-1.757925	C	3.058598	-3.887456	1.589908
H	6.205053	2.039122	-1.673225	H	-6.124017	4.219573	-2.881211	H	4.815700	-0.403988	1.246298
H	5.712007	1.532272	-3.326982	H	-6.881880	1.828236	-2.789270	H	4.1415		

S7-Si	C	4.013221	-1.447148	-0.697143
C	3.309832	-1.965015	-1.950223	
H	2.237948	-2.152309	-1.741856	
H	3.347816	-1.227803	-2.776744	
H	3.767494	-2.907997	-2.313045	
P	3.172413	0.047629	0.050083	
C	4.376216	0.410526	1.447848	
C	4.275902	-0.532006	2.646812	
H	3.231006	-0.600889	3.011680	
H	4.905754	-0.177341	3.487991	
H	4.613952	-1.557539	2.395275	
H	5.406723	0.408740	1.032512	
H	4.166148	1.451175	1.765348	
C	3.718828	1.364956	-1.175129	
C	5.127852	1.287073	-1.767389	
H	5.912640	1.237831	-0.984990	
H	5.253890	0.406688	-2.427980	
H	5.335772	2.187306	-2.382046	
H	2.951812	1.356939	-1.975195	
H	3.591513	2.326114	-0.638063	
Rh	0.887472	0.022168	0.123707	
P	0.762330	2.323787	0.391941	
C	1.026232	3.583573	-0.974199	
C	0.034680	3.486296	-2.132207	
H	0.096963	2.507908	-2.640520	
H	-1.012857	3.618256	-1.792492	
H	0.233073	4.272797	-2.888661	
H	2.061158	3.540293	-1.343134	
H	0.988331	4.589723	-0.504681	
C	1.917442	3.041590	1.671983	
C	1.807608	2.343128	3.026081	
H	1.924865	1.248260	2.904487	
H	2.578688	2.706610	3.735777	
H	0.815186	2.514475	3.489801	
H	2.944165	2.953200	1.261554	
H	1.176283	4.129930	1.758190	
C	-0.886531	2.883320	1.060190	
C	-1.049957	4.353303	1.446444	
H	-0.353696	4.659439	2.251457	
H	-2.079376	4.531665	1.818569	
H	-0.892464	5.038469	0.586977	
H	-1.100094	2.207546	1.909061	
H	-1.644771	2.606360	3.01825	
P	0.607785	-2.169280	0.877502	
C	-0.424508	-3.481791	0.015094	
C	0.202135	-4.123606	-1.224287	
H	1.143905	-4.657963	-0.986819	
H	-0.491621	-4.860119	-1.678142	
H	0.443468	-3.378722	-2.010379	
H	-1.396625	-2.997261	-0.206065	
H	-0.654182	-4.260121	0.773058	
C	2.094950	-3.216225	1.339878	
C	1.859899	-4.740300	2.175845	
H	1.481585	-4.238866	3.189824	
H	1.135964	-5.168312	1.700279	
H	2.810176	-5.034726	2.304246	
H	2.577011	-3.485280	0.379717	
H	2.795339	-2.535220	1.857592	
C	-0.325129	-2.133110	2.493302	
C	0.212183	-1.114550	3.493055	
H	1.267946	-1.318287	3.768603	
H	0.161191	-0.102701	3.048191	
H	-0.383489	-1.122534	4.429574	
H	-0.321480	-3.162542	2.907648	
C	-1.172414	-1.899818	2.225511	
C	-1.106573	0.125266	-0.759295	
C	-1.117746	-0.810020	-1.927411	
F	-2.457338	-1.088124	-2.429172	
C	-0.415492	-0.315042	-3.197517	
F	0.874452	0.048405	-2.992285	
F	-0.400752	-1.283751	-4.148650	
F	-1.051115	0.760672	-3.733088	
H	-0.698513	-1.800981	-1.689611	
Si	-2.550063	-0.112600	0.377658	
C	-3.869069	0.870020	-0.013142	
C	-4.259184	1.306809	-1.313626	
C	-4.170064	2.823733	-1.420586	
H	-4.545959	3.171261	-2.404748	
H	-3.119460	3.164800	-1.317187	
H	-4.767259	3.311824	-0.624052	
H	-3.633714	0.825585	-2.094967	
H	-5.307159	0.973115	-1.489376	
O	-3.082883	-1.713075	0.485576	
C	-4.237560	-2.248280	-0.161230	
C	-5.506262	-1.994625	0.644177	
H	-5.682865	-0.904821	0.742844	
H	-5.419883	-2.428907	1.661272	
H	-6.386134	-2.451336	0.145193	
H	-4.063191	-3.340933	-0.275654	
H	-4.333425	-1.834779	-1.188186	
O	-2.195170	0.290438	1.967944	
C	-3.180715	0.256744	2.998469	
C	-3.841981	1.617198	3.193201	
H	-4.340332	1.929450	2.254947	
H	-3.090836	2.387299	3.463052	
H	-4.597165	1.572440	4.005146	
H	-3.948647	-0.518190	2.774829	
H	-2.664998	-0.063528	3.930580	
H	-1.242511	1.159054	-1.151984	
H	4.052758	-2.226366	0.085204	
H	5.066717	-1.170921	-0.907934	
TS_S3-S4-Si				
S7-Ge	C	-4.562348	-1.161797	0.654920
C	-6.074793	-1.079948	0.866465	
H	-6.445938	-2.003301	1.357177	
H	-6.360709	-0.228858	1.516303	
H	-6.626040	-0.973265	-0.089351	
P	-3.689744	0.303831	-0.126623	
C	-4.312784	1.670036	0.955774	
C	-3.765811	1.603702	2.420360	
H	-2.660478	1.547287	2.417578	
H	-4.074298	2.491658	0.009506	
H	-4.132678	0.705347	2.955554	
H	-4.029147	2.624657	0.507430	
H	-5.422749	1.649149	0.990942	
C	-4.835666	0.671035	-1.576098	
C	-4.895710	-0.391180	-2.670344	
H	-3.899389	-0.567962	-3.116189	
H	-5.577547	-0.078600	-3.487488	
H	-5.270127	-1.362076	-2.285608	
H	-5.847181	0.860163	-1.158309	
H	-4.492692	1.535772	-1.998658	
Rh	-1.395719	0.156575	-0.039924	
P	-1.140897	2.445149	-0.407564	
C	0.594939	2.948848	-1.003061	
C	0.779741	4.408296	-1.393357	
H	0.163680	4.717018	-2.262135	
H	1.843586	4.551181	-1.673643	
H	0.567952	5.108510	-0.560547	
H	1.247161	2.666531	-0.193733	
H	0.795227	2.277609	-1.846952	
C	-1.409863	3.740346	0.375651	
C	-0.393264	3.680102	2.060776	
H	-0.607438	4.460869	2.818895	
H	-0.418527	2.699971	2.570966	
H	0.644134	3.840812	1.703606	
H	-2.437150	3.606932	1.308012	
H	-1.389704	4.733553	0.422297	
C	-2.217797	3.138260	-1.764582	
C	-2.080075	2.363328	-3.075265	
H	-1.063582	2.471206	-3.503305	
H	-2.247614	1.280341	-2.901516	
H	-2.806457	2.716223	-3.835398	
H	-3.262913	3.113171	-1.394136	
H	-1.966859	4.210808	-1.901241	
P	-1.372878	-2.142193	-0.322078	
C	0.299425	-2.856947	-0.725281	
C	0.400447	-4.355736	-1.006502	
H	-0.201142	-4.661639	-1.885816	
H	1.454761	-4.631060	-1.213816	
H	0.072762	-4.963835	-0.140034	
H	0.958233	-2.591789	0.123327	
H	0.675193	-2.265858	-1.583189	
C	-1.921726	-3.283564	1.080195	
C	-2.738837	-4.531612	0.736914	
H	-2.972251	-5.101953	1.659854	
H	-3.705800	-4.271979	0.260944	
H	-2.203561	-5.216434	0.050939	
H	-0.984873	-3.567659	1.605662	
H	-2.477841	-2.651212	1.793775	
C	-2.344555	-2.765227	-1.793596	
C	-1.849004	-2.185298	-3.116755	
H	-1.859410	-1.078369	-3.080950	
H	-2.490321	-2.513683	-3.959701	
H	-0.809917	-2.493953	-3.345148	
H	-3.404157	-2.490131	-1.631044	
C	-2.303901	-3.872443	0.811598	
C	0.543490	0.147963	0.931507	
C	0.605967	-0.750934	2.129597	
C	-0.401444	-0.508073	3.267970	
F	-0.361139	0.770774	3.723411	
F	-1.684439	-0.768756	2.916749	
F	-0.127401	-1.312640	4.325202	
H	0.544517	-1.831490	1.882920	
F	1.857418	-0.594726	2.840680	
H	0.655610	1.176455	1.331323	
Ge	2.225263	-0.016105	-0.129436	
C	3.428479	-1.554097	0.241617	
C	4.216194	-1.595192	1.412664	
C	5.096376	-2.662548	1.656473	
C	5.211594	-3.711824	0.728081	
C	4.448640	-3.678175	-0.451042	
C	3.570898	-2.606592	-0.689329	
H	2.995191	-2.587831	-1.626862	
H	4.539646	-4.487167	-1.192903	
H	5.900332	-4.549223	0.919864	
H	5.699376	-2.673512	2.577993	
H	4.141660	-0.783488	2.149734	
C	2.018746	-0.046955	-2.091875	
C	0.764486	0.052877	-2.724629	
C	0.660165	0.063774	-4.124992	
C	1.815701	-0.026413	-4.919679	
C	3.074737	-0.138064	-3.405440	
C	3.172154	-0.151329	-2.902329	
H	4.165259	-0.255875	-2.436385	
H	3.984902	-0.218131	-4.919240	
H	1.735651	-0.016023	-6.017904	
H	-0.329549	0.140475	-4.601205	
H	-0.149474	0.117460	-2.085297	
C	3.289783	1.596367	0.320392	
C	3.957366	2.363934	-0.657910	
C	4.637216	3.544001	-0.311647	
C	4.662675	3.976785	1.025644	
C	4.007715	3.220204	2.012185	
C	3.326579	2.041616	1.661157	
H	2.800975	1.465079	2.437699	
H	4.021662	3.552042	3.062273	
H	5.190155	4.904227	1.297652	
H	5.144632	4.133473	-1.091554	
H	3.925867	2.053365	-1.713868	
H	-4.039613	-1.313388	1.620532	
H	-4.311214	-2.048270	0.040394	
TS_S3-S4-Ge				
S8-Si	C	3.239905	-1.927849	-0.930762
P	3.121665	-0.254300	-0.104228	
C	4.511420	-0.395628	1.164834	
C	4.580518	0.716243	2.207636	
C	4.691700	-2.361088	-1.395410	
C	3.969728	0.837867	-1.370113	
C	3.316501	0.745800	-2.750827	
Rh	0.871308	1.039617	0.002916	
P	1.008932	2.430237	-0.164458	
C	1.422827	3.444063	-1.692263	
C	0.389320	3.339688	-2.815627	
P	0.438429	-1.612791	1.480637	
C	-0.319020	-3.282672	1.082552	
C	0.619352	-4.297847	0.429746	
C	-1.083886	0.217682	0.940993	
Si	-2.674231	-0.040137	-0.040727	
O	-4.032314	0.251156	-0.107680	
C	-4.186795	1.400395	-1.842876	
C	-4.525534	2.659899	-1.049921	
C	1.879933	-1.232536	2.544833	
C	1.638653	-3.052840	3.732148	
C	-0.761783	-1.078578	2.809491	
C	-0.432693	0.266431	3.445949	
C	-1.050870	-0.387972	-2.329141	
C	-0.619590	-1.903666	-2.482153	
F	-1.902853	-2.559734	-1.816944	
F	0.024657	0.121282	-1.307116	
C	2.019346	3.204052	1.030711	
C	1.903364	2.880694	2.489020	
C	-0.584548	3.260345	0.357565	
C	-0.556526	4.769163	0.601211	
O	-3.031827	-1.538510	0.618888	
C	-1.117772	-2.395477	0.272266	
C	-5.388299	-2.028678	1.028596	
O	-2.646050			

Si	-2.245390	-0.257015	0.803477	Ge	1.769473	0.018743	-0.077498	C	2.444209	-2.294280	2.323025	C	3.147439	-3.229155	0.280487
O	-3.175693	-1.341301	1.729034	C	1.916650	0.304703	1.911220	C	3.964190	-2.203669	2.486258	P	3.290977	-1.382088	0.004880
C	-3.483425	-1.248306	3.110810	C	0.844341	0.475661	2.795616	P	1.434414	-0.703766	2.110160	C	4.615931	-1.089840	1.310149
C	-2.818987	-2.367659	3.905148	C	1.055642	0.749044	4.158820	Rh	-0.205051	-0.590380	0.366517	C	5.177877	0.325724	1.341103
H	-3.092590	-3.354149	3.477992	C	2.363260	0.840521	4.661740	C	1.142404	0.220755	-1.159523	H	5.727053	0.572843	0.410171
H	-3.140271	-2.341955	4.966474	C	3.452738	0.655965	3.919129	Si	0.968952	1.605320	-2.394912	H	4.361758	1.063300	1.451492
H	-1.714197	-2.278571	3.879291	C	3.229613	0.394856	2.429754	O	-0.454184	1.773556	-3.246375	H	5.882906	0.455159	2.187551
H	-3.191249	-0.254504	3.527448	H	4.096634	0.268133	1.762580	C	-0.740757	1.104576	-4.484020	H	4.148022	-1.354158	2.271376
H	-4.590146	-1.314121	3.220910	H	4.483452	0.721885	4.174461	C	-0.343016	1.965074	-5.674817	H	5.421737	-1.836213	1.173846
O	-2.606944	-0.908886	0.706610	H	2.535184	1.055450	5.277842	C	2.787655	0.565054	1.823586	C	4.300218	-1.278357	-1.563034
C	-3.788551	-1.668717	-0.991905	H	0.196304	0.895781	4.831240	C	2.308582	2.018459	1.819391	C	5.554933	-2.145981	-1.673105
C	-4.58675	-1.264802	-2.342980	H	-0.175722	0.397360	2.375746	C	1.030705	-0.346838	3.912654	H	6.300733	-1.908352	-0.887718
H	-3.608846	-1.390220	-3.148589	C	2.954054	1.521081	-0.676978	C	2.172544	-0.233525	4.925064	H	5.320296	-3.226751	-1.598196
H	-4.682189	-0.204650	-2.340545	C	3.194601	2.638547	0.154857	P	-1.396319	-2.515292	0.809267	H	6.050219	-1.986109	-2.653097
H	-5.237968	-1.894713	-2.588738	C	3.950744	3.736167	-0.286905	C	-2.458604	-3.286894	-0.524674	H	4.546872	-0.203277	-1.673490
H	-4.542451	-1.538332	-0.188279	C	4.495437	3.741894	-1.582339	C	-1.717508	-3.930853	-1.694834	H	5.583263	-1.504824	-2.374703
H	-3.520320	-2.750311	-0.993106	C	4.284952	2.634898	-2.421170	P	-2.110268	0.760955	0.410077	Rh	1.411908	-0.038176	0.123150
O	-2.934420	1.275692	0.960889	C	3.526333	1.541029	-1.970109	C	-3.624799	0.188587	-0.530845	P	2.126083	1.984721	-0.964448
C	-4.311223	1.536258	0.705322	H	3.386318	0.690737	-2.654282	C	-3.320989	-0.044849	-2.012106	C	0.867249	3.346630	-0.671830
C	-4.564064	0.302943	0.794596	H	4.715817	2.620046	-3.434560	C	0.739803	-1.142415	-1.437064	C	0.693540	3.796122	0.774293
H	-5.636496	3.260324	0.629127	H	5.085291	4.602025	-1.934656	F	-0.079533	-1.311445	-2.591050	H	0.425441	2.937414	1.419454
H	-3.967806	3.574151	0.033842	H	4.113428	4.593839	0.384654	C	-2.711427	-2.382075	2.131481	H	1.619679	4.249124	1.183080
H	-4.271824	3.415587	1.793259	H	2.780167	2.655843	1.174272	C	-2.87137	-1.940006	3.493775	H	-0.120570	4.542805	0.857241
H	-4.599078	1.163949	-0.306808	C	2.956689	-1.582856	-0.278285	C	-0.415046	-3.976663	1.429509	H	1.117623	4.208629	-1.326050
H	-4.946099	0.985289	1.437146	C	3.471396	-1.967691	-1.539477	C	-1.172663	-5.277694	1.702126	H	-0.094874	2.943976	-1.053477
Rh	0.530785	0.063991	-0.052515	C	4.268013	-3.115529	-1.688773	C	-1.848253	2.439491	-0.363064	C	3.112612	2.168102	-2.837628
P	-0.558065	1.833882	-1.298931	C	4.576844	-3.911251	-0.572409	C	-3.008420	3.433686	-0.318494	C	2.127029	1.313882	-3.607162
C	-0.802927	3.450615	-0.390821	C	4.081893	-3.545139	0.690105	C	-2.905902	1.258782	2.034596	H	4.166462	1.525530	-3.302596
C	0.504779	4.152333	-0.023558	C	3.281695	-2.398561	0.828924	C	-1.943513	2.056897	2.913415	H	3.050005	1.508590	-4.697367
H	1.049320	4.514321	-0.919659	H	2.909003	-2.129839	1.829347	C	1.814403	-2.197440	-1.548831	H	2.930686	0.237338	-3.447074
H	1.166878	3.468625	0.538321	H	4.316140	-4.158356	1.574547	F	2.849036	-1.966827	-0.694633	H	1.084327	1.915972	-3.148115
H	0.312047	5.033301	0.622766	H	5.201168	-4.810706	-0.686648	O	1.201499	2.986592	-1.481735	H	2.257394	3.244816	-3.072702
H	-1.440008	4.118650	-1.007832	H	4.652989	-3.387499	-2.684105	C	1.361370	4.278698	-2.076987	C	3.733385	2.862774	-0.549550
H	-1.375977	3.178138	0.515693	H	3.249513	-1.370820	-2.436798	C	0.036410	5.023598	-2.179196	C	3.995721	2.239776	-1.161265
C	-2.207152	1.665116	-2.191011	Rh	-1.109409	0.055823	-0.207194	O	2.151366	1.449132	-3.576163	H	4.965088	4.647346	-0.807497
C	-2.737538	2.847551	-3.002621	P	-0.982189	-2.331859	0.130182	C	3.482430	0.976205	-3.353399	H	4.041692	4.202735	-2.268242
C	-3.700894	2.580603	-3.486335	C	-0.328332	-2.641799	1.855302	C	4.283747	1.857079	-2.399692	H	3.211673	4.972937	-0.883400
H	-2.046053	3.164658	-3.809160	C	-0.781570	-3.876552	0.358429	F	2.365573	-2.246204	-2.805024	H	7.756963	2.916223	0.558316
H	-2.931912	3.735154	-2.367261	H	-1.883315	-3.912586	2.757180	F	1.376313	-3.465049	-1.305202	H	4.540022	2.151218	-0.821929
H	-2.935422	1.370272	-1.420564	H	-0.344694	-3.858968	3.655720	H	1.618378	2.228513	0.978195	P	1.305342	-0.248967	2.442287
H	-2.092980	0.764657	-2.827129	H	-0.469341	-4.822670	2.156827	H	1.780312	2.278403	2.759575	C	-0.351752	0.333396	3.068538
C	0.428406	2.452288	-2.776613	H	-0.544931	-1.723233	2.423301	H	3.168959	2.711963	1.718144	C	-7.000259	0.158805	4.544495
C	0.367084	1.526877	-3.994188	H	0.773554	-2.634440	1.731089	H	3.573332	0.422822	2.591070	H	0.000795	0.700452	5.211794
H	1.144193	1.787456	-4.741919	C	0.202442	-3.397142	-0.868051	H	3.268473	0.310541	0.855307	H	-1.719507	0.548488	4.748703
H	-0.614783	1.587291	-4.503434	C	0.765612	-4.677167	-0.245008	H	2.759722	-1.171377	4.991835	H	-0.700088	-0.908130	4.844916
H	0.520194	0.470414	-3.701567	H	1.326754	-4.473581	0.685722	H	1.776635	-0.023703	5.941134	H	-1.093573	-0.196587	2.439759
H	0.057881	3.466271	-0.303790	H	-0.008664	-5.436812	-0.030608	H	2.875314	0.586207	4.673565	H	-0.409409	1.398156	2.765004
H	1.472886	2.591586	-2.437229	H	1.491805	-5.126948	-0.952667	H	0.416744	0.577045	3.906533	C	2.460577	0.653526	3.618852
P	2.737443	0.258329	-0.552574	H	-0.290492	-3.613808	-1.830813	H	0.334325	-1.157100	4.207809	C	2.525920	2.159396	3.386696
C	4.171665	-0.837977	0.014136	H	1.055853	-2.737598	-1.098715	H	-1.630539	-0.988173	3.401655	H	2.734528	2.376041	2.319893
C	4.070780	-1.471596	1.396025	C	-2.611761	-3.251805	-0.007854	H	-1.496119	-2.691536	3.927917	H	1.566384	2.655876	3.635834
H	3.122765	-0.033813	1.500407	C	-2.619302	-4.765131	-0.235159	H	-3.015012	-1.793494	4.217167	H	3.318639	2.633300	4.000683
H	4.911830	-2.177149	1.558929	H	-2.167706	-5.322979	0.606779	H	-3.234689	-3.358844	2.199567	H	3.460984	0.196343	3.482155
H	4.092106	-0.720965	2.205466	H	-3.663985	-5.122005	-0.348067	H	-3.460454	-1.659621	1.747388	H	2.153633	0.420899	4.661182
H	4.237915	-1.639553	-0.747057	H	-2.078042	-5.042938	-1.160307	H	-1.651228	-5.681037	0.787522	C	1.424305	-1.941942	3.235164
H	5.101332	-0.238757	-0.087641	H	-3.126268	-2.744717	-0.847222	H	-0.478935	-6.057260	2.079341	C	0.388802	-0.252303	2.691677
C	3.500830	1.972827	-0.423032	H	-3.191305	-2.995555	0.902334	H	-1.965307	-5.148708	2.466793	O	0.368475	-2.901711	1.538393
C	3.848719	2.571133	0.932988	P	-2.678950	0.148136	1.514001	H	0.087877	-3.616363	2.348695	H	0.630910	2.659149	3.033086
H	2.948355	2.716607	1.554634	C	-3.081118	1.743162	2.423607	H	0.390070	-4.127687	0.685220	H	-0.947499	-3.961341	3.024525
H	4.331637	3.560584	0.793513	C	-4.448660	1.854991	3.100756	H	-1.088809	-3.192418	-2.221889	H	2.546451	-2.302882	3.041494
H	4.551909	1.932933	1.503619	H	-4.525859	2.816881	3.648604	H	-1.061531	-4.760539	-1.364289	H	1.342722	-1.833210	4.337784
H	2.776057	2.629823	-0.945108	H	-5.276488	1.830142	3.364115	H	-2.442389	-4.349498	-2.423099	C	0.097128	-1.165994	-1.123136
H	4.408816	1.931444	-1.063588	H	-4.627492	1.054266	2.863744	H	-3.121786	-4.024198	-0.023160	C	-0.603349	0.023475	-0.715130
C	2.986178	0.146929	-2.424693	H	-2.957976	2.568727	1.701752	H	-3.114480	-2.472448	-0.888730	H	0.155464	0.936422	0.429604
C	4.371169	-0.200019	-2.974038	H	-2.267302	1.877079	3.165772	H	-3.276928	3.729460	0.716003	H	-0.607763	0.805468	-1.498035
H	5.162404	0.462849	-2.568004	C	-4.311232	-0.227339	0.652199	H	-3.923276	3.029207	-0.797929	Ge	-2.457667	0.107958	-0.030218
H	4.667115	-1.244001	-2.749005	C	-4.623941	0.603815	-0.586201	H	-2.741243	4.361501	-0.865416	C	-2.709428	2.020694	0.377720
H	4.483236	-0.007281	-4.077998	H	-5.524886	2.15791	-1.103718	H	-0.936824	2.859057	0.107021	C	-2.685394	2	

P	-0.923030	0.341455	-2.229775	C	-4.499612	-3.603908	1.002553	C	4.467123	-1.760556	-0.143715	P	2.964195	-0.295216	1.650348
C	-2.544930	0.626616	-3.126965	C	-5.567532	-3.145650	1.794660	P	2.150912	-0.066135	-0.448220	P	0.965019	2.139648	0.540661
C	-2.473507	0.957773	-4.619348	C	-5.693271	-1.773394	2.067142	Rh	-0.093158	-0.344584	-0.883049	P	0.903341	-2.507638	0.381773
H	-1.985634	1.934957	-4.860691	C	-4.753338	-0.863752	1.550090	F	0.252065	-2.854453	-0.582787	C	3.147129	-1.646327	2.927111
H	-1.913499	0.190214	-5.191204	C	-3.675880	-1.310176	0.757324	C	2.881728	0.915516	0.974740	C	2.210978	-1.472959	4.129928
H	-3.493014	1.012642	-5.054529	Ge	-2.389446	-0.043726	-0.039506	C	4.068653	1.836496	0.694372	C	4.549107	-0.582005	0.700505
H	-3.127340	-0.304399	-2.970763	C	-0.603045	-0.845348	0.066342	C	3.044692	0.591632	-1.955118	C	4.796350	0.367661	-0.466104
H	-3.084796	1.415451	-2.570762	C	0.005249	-1.004687	1.389750	C	2.675130	-0.194930	-3.213642	C	3.346601	1.180500	2.722197
C	0.127712	1.717593	-2.938036	C	-0.404299	-0.061276	2.372566	P	-1.798673	-0.114177	-2.292250	C	4.626160	1.140023	3.557887
C	-0.298985	3.125815	-2.526646	C	-0.136563	-2.342117	1.217992	C	-3.622877	-1.053426	-1.849543	C	0.585194	3.013078	2.152300
H	0.402669	3.888444	-2.921833	F	-0.007464	-3.399734	1.288259	C	-3.967564	-1.928653	-0.643242	C	1.432122	-0.219028	2.556161
H	-0.340280	3.236755	-1.426356	F	0.809184	-2.492238	3.102678	P	-0.367964	1.777759	-1.383343	C	2.438496	3.029758	-0.199386
H	-1.309371	3.374698	-2.913829	F	-1.338398	-2.452119	2.736035	C	-2.149976	2.298972	-1.160525	C	2.585343	2.785044	-1.702559
H	1.162772	1.481347	-2.616518	Rh	1.452220	-0.165907	-0.001177	C	-2.704024	1.878046	0.201813	C	0.470559	-3.613893	1.824998
H	0.121295	1.611986	-0.4042547	P	1.079419	2.105502	-0.396545	C	-0.805816	-1.433127	1.209544	C	-0.684014	-3.051353	2.657174
Rh	-0.776236	0.011720	0.081328	C	2.540885	3.119305	-0.982277	C	-0.709042	-2.771875	0.723986	C	-0.374556	-3.052338	-0.878492
P	-3.004059	0.069397	0.643338	C	3.042952	2.686179	-2.359821	C	-0.081240	-3.902680	1.525022	C	-0.311817	-4.496441	-1.375917
C	-3.737606	1.774827	0.875455	H	4.025270	3.143318	-2.596780	F	-0.739381	-4.068126	2.711495	C	2.429226	-3.336855	-0.294437
C	-3.722526	2.661997	-0.365796	H	3.146268	1.583195	-2.410108	C	-1.523815	-2.766103	-2.864355	C	2.868130	-2.727369	-1.626518
H	-4.037407	3.696695	-0.120327	H	2.336997	2.981539	-3.161635	C	-0.192300	-2.950257	-3.594390	H	5.385926	-0.554205	1.430464
H	-4.407254	2.285088	-1.153184	H	3.337979	3.007644	-0.220498	C	-1.880213	-0.117631	-3.939716	H	4.490982	-1.628067	0.339420
H	-2.699021	2.705637	-0.788720	H	2.271028	4.194299	-0.986310	C	-2.773466	-0.692849	-5.041289	H	2.439918	1.271329	3.354548
H	-4.762173	1.676855	1.295157	C	-0.175185	2.562746	-1.695784	C	0.486992	2.923970	-0.190402	H	3.351774	2.070949	2.068273
C	-3.108601	2.232172	1.665337	C	-0.504203	0.039730	-1.902232	C	0.104869	4.044663	-0.203722	H	4.642369	0.285260	4.262445
C	-3.408725	-0.658096	2.322529	H	0.386556	0.634420	-2.190610	C	0.122835	2.529823	-3.046439	H	4.713953	2.064729	4.164573
C	-2.913201	0.142446	3.526094	H	-1.256327	4.159216	-2.709803	C	-0.807225	3.566260	-3.683713	H	5.535690	1.075471	2.926616
H	-1.846251	0.422088	3.423213	H	-0.935884	4.489902	-0.986673	Si	-0.046452	-0.646774	2.655880	H	4.215344	-1.683815	3.231302
H	-3.486064	1.080892	3.660971	H	-1.087002	2.000596	-1.426334	O	-0.162238	1.303531	2.446264	H	2.957081	-2.600903	2.401176
H	-3.013657	-0.448273	4.459087	H	0.178721	2.095533	-1.626657	C	-0.182011	1.943476	3.543228	H	2.662529	-0.797084	4.884482
H	-2.953532	-1.668742	3.218842	C	0.470736	3.077625	1.097010	C	1.183090	2.576130	3.793671	H	2.023687	-2.444015	4.632059
H	-4.508151	-0.800890	2.385148	C	0.970479	4.505164	1.326934	O	-0.839575	-0.990904	4.119077	H	1.243613	-1.012220	3.823982
C	-4.272772	-0.843949	-0.384425	H	0.730979	5.179926	0.481726	C	-2.198788	-1.408019	4.168328	H	5.679005	0.053772	-1.059210
C	-5.751287	-0.549556	-0.122009	H	0.493354	4.932161	2.236610	C	-3.178606	-0.270427	3.886631	H	4.979234	1.405130	-0.121416
H	-6.012538	0.496099	-0.381148	H	2.067969	4.546461	1.484414	O	1.553717	-1.031571	2.994865	H	3.916403	0.391873	-1.138659
H	-0.632720	-0.710770	0.938636	H	0.696836	2.441715	1.972454	C	1.994805	-1.835981	4.087676	H	0.587002	2.188368	2.896105
H	-6.397204	-1.211658	-0.735042	H	-0.632568	3.062631	0.012425	C	2.293897	-0.989377	5.318720	H	-0.479738	3.306285	2.069416
H	-0.421933	-0.646013	-1.441675	P	3.487215	0.282111	0.979863	F	-0.170407	-0.589429	0.870689	H	1.103378	4.598405	3.546000
H	-4.037357	-1.916332	-0.218087	C	3.437015	1.514742	2.384180	F	1.225088	-3.715343	1.830607	H	2.508680	3.970222	2.647141
P	-0.168521	-2.287986	0.412987	C	2.499882	1.080979	3.512493	H	4.865651	-1.119647	0.668859	H	1.345698	5.059862	1.837944
C	0.586433	-2.666003	2.081448	H	1.495276	0.821018	3.126748	H	4.825208	-2.792980	0.050492	H	3.346064	2.683553	0.329354
C	-0.281671	-2.294280	3.279140	H	2.888309	0.188941	4.044209	H	4.930578	-1.427212	-1.094824	H	2.346442	4.113535	0.015290
H	0.257213	-2.481994	0.230670	H	2.386277	1.890494	4.261702	H	3.824409	2.626851	-0.045185	H	1.803802	3.308817	-2.286599
H	-1.224261	-2.879132	3.313910	H	3.101368	2.477645	1.948123	H	4.951012	1.287618	0.309234	H	3.570150	3.140734	-2.067233
H	-0.548769	-1.221152	3.254551	H	4.463119	1.684995	2.678523	H	4.380681	2.351012	1.627363	H	2.503539	1.706835	-1.940515
H	1.522374	-2.076962	2.081785	C	4.177430	-1.225833	1.837900	H	2.039193	1.479647	1.409625	H	-1.301452	2.349807	-0.224123
H	0.872700	-3.736327	2.127133	C	5.475139	-1.064082	8.630034	H	3.120745	0.156523	1.744289	H	-0.172776	2.371839	-1.588690
C	-1.587698	-3.519799	3.397278	H	5.774385	-0.209027	3.088652	H	3.064968	0.294487	-4.129806	C	-0.361768	2.799362	-0.585907
C	-1.289243	-5.002706	0.606649	H	5.372071	-0.328075	3.452726	H	3.081519	-1.225735	-3.181416	C	-0.502193	4.320718	-0.642438
H	-0.787388	-5.179747	1.579563	H	6.314995	-0.734610	1.985509	H	1.569103	-0.281204	-3.286313	H	-0.693632	4.752469	0.359977
H	-2.224301	-5.601783	0.605405	H	4.293596	-1.981185	1.034258	H	2.747911	1.655487	-2.060287	H	0.398398	4.814637	-1.059306
H	-0.635158	-5.414034	-0.187949	H	3.355187	-1.605749	4.278679	H	4.139964	0.586828	-1.781249	H	-1.363043	4.599254	-1.283710
H	-2.087794	-3.366083	-0.599356	C	4.972922	-0.841197	0.036269	H	-0.032044	-4.015464	-3.858677	H	1.382592	-3.702786	2.447706
H	-2.311307	-3.147671	1.135026	C	5.903029	1.910395	0.542154	H	-0.145287	-2.361943	-4.533529	H	0.254466	-4.633913	1.445156
C	1.077093	-3.101272	-0.743758	H	6.367478	1.595637	1.497148	H	0.642402	-2.626860	-2.943307	H	-0.469725	-1.998924	2.938939
C	2.069652	-1.424900	-0.188676	H	5.371352	2.864859	0.730236	H	-2.386991	-3.058889	-3.499411	H	-0.835245	-3.645891	3.580719
H	2.750648	-3.648331	0.541533	H	6.724904	2.129374	-0.170657	H	-1.539986	-3.401617	-1.959704	H	-1.640271	-3.073821	2.093616
H	1.577183	-4.986462	0.303470	H	4.565850	1.176262	-1.007206	H	-2.465326	-1.717125	-5.331932	H	-1.365211	-2.871120	-0.418905
H	2.688891	-4.528454	-1.009896	H	5.541304	-0.085724	-0.257030	H	-8.839072	-0.734572	-4.738962	H	-0.309815	-2.344096	-1.727262
H	1.640015	-2.260186	-1.190148	P	2.146022	-1.574393	-1.751776	H	-2.717190	-0.062682	-5.952946	H	0.595279	-4.697827	-1.979552
H	0.473428	-3.541152	-1.563836	C	1.327825	-1.516227	-3.435384	H	-2.174871	0.926913	-3.713085	H	-0.337903	-5.230819	-0.545209
H	-0.607479	0.266224	1.681807	C	1.513693	-0.193103	-4.172866	H	-0.862671	-0.062741	-4.281074	H	-1.917192	-4.700462	-2.019849
C	0.461560	1.256876	1.399826	H	1.154926	0.654326	-3.556792	H	-3.707916	-2.991702	-0.821628	H	2.230947	-4.424810	-0.386222
H	0.17835	1.071469	0.123264	H	0.959601	-0.180818	-5.133599	H	-5.053790	-1.889198	-0.423297	H	3.225408	-3.233095	0.470290
Si	2.739115	0.273852	-0.146085	H	2.580871	0.001083	-4.404520	H	-3.433343	-1.599500	0.270303	H	3.842380	-3.138231	-1.960178
O	3.134497	-1.067672	0.772026	H	0.252807	-1.718370	-3.248995	H	-4.192279	-1.389099	-2.742146	H	2.961955	-1.626758	-1.531622
C	3.923157	-1.000108	1.965859	H	1.699197	-2.367036	-4.045388	H	-3.920358	-0.000658	-1.661669	H	2.127101	-2.920642	-2.427909
C	3.592867	-1.257210	1.665027	C	3.957449	-1.602377	-2.241097	H	0.289667	4.879693	-1.188557	H	-1.671219	-0.310674	0.647122
H	5.526132	-2.239322	1.167324	C	4.402440	-2.583542	-3.326507	H	-0.960834	4.564029	0.055197	H	-1.987326		

C	-1.396637	3.531242	-0.335536
C	-2.650917	3.698407	0.521400
H	-2.732506	2.893407	1.271911
H	-2.629267	4.664408	1.065930
H	-3.574166	3.686306	-0.093273
H	-0.483994	3.618186	0.285976
H	-1.330523	4.333567	-1.100278
C	-2.793458	1.973650	-2.323361
C	-3.037710	3.266653	-1.046255
H	-2.181696	3.511084	-3.770376
H	-3.197822	4.136559	-2.437969
H	-3.934336	3.170159	-3.745442
H	-2.696909	1.109539	-3.008190
H	-3.658128	1.737651	-1.669922
Rh	-0.769606	-0.140426	-0.242189
P	-2.860647	-0.976815	0.370503
C	-3.987882	0.324688	1.094528
C	-5.358432	-0.104158	1.619848
H	-5.274923	-0.846477	2.438870
H	-5.990611	-0.550173	0.825318
H	-5.910497	0.797223	0.204474
H	-0.088629	1.099346	0.307487
H	-3.379209	0.792370	1.894718
C	-2.949002	-2.330314	1.660339
C	-2.437571	-1.977865	3.053057
H	-1.400273	-1.598658	3.015278
H	-3.055209	-1.193674	3.533103
H	-2.457661	-2.870841	3.710912
H	-2.357974	-3.167927	1.236768
H	-4.001498	-2.684789	1.702693
C	-3.964463	-1.846052	-0.875631
C	-4.087276	-1.201051	-2.251317
H	-4.649104	-1.856724	-2.947740
H	-4.620688	-0.231573	-2.205219
H	-3.084352	-0.101129	-2.684992
H	-3.534140	-2.862965	-0.972003
H	-4.962365	-1.982894	-0.407396
P	0.272130	-2.164117	-0.744649
C	-0.891896	-3.426843	-1.476569
C	-0.288003	-4.708720	-2.052782
H	-1.089109	-5.388015	-2.411017
H	0.303893	-5.266990	-1.299734
H	0.374627	-4.499322	-2.915470
H	-1.617564	-3.671596	-0.674401
H	-1.464681	-2.973872	-2.248348
C	1.211310	-3.185572	0.495823
C	0.357940	-3.821915	1.589301
H	-0.197404	-3.051158	2.511899
H	-0.370210	-4.553947	1.182997
H	0.999183	-4.366600	3.212359
H	1.947244	-2.485488	0.925151
H	1.782191	-3.958008	-0.057691
C	1.505539	-1.921081	-2.133796
C	2.719862	-2.847785	-2.215570
H	3.382142	-2.686538	-1.343939
H	2.449235	-3.920842	-2.259855
H	3.310039	-2.618041	-3.126551
H	1.843073	-0.869162	-2.059282
H	0.886225	-1.973190	-3.055602
H	-1.005420	-0.423401	-1.826568
C	0.186679	0.312411	1.610813
C	0.982924	0.855017	0.518845
Si	2.774555	0.631908	0.183023
C	3.507854	-0.857372	0.618845
C	4.028416	-1.282584	1.683845
C	4.896755	-2.513059	1.479362
H	5.734988	-2.289772	0.788854
H	4.307616	-3.346966	1.047167
H	5.320677	-2.853166	2.446001
H	4.611649	-4.054858	2.141856
C	1.183653	-1.506418	2.374354
O	3.722064	1.671088	1.116398
C	3.285628	2.923684	1.640015
C	3.036832	3.970887	0.557637
H	3.943357	4.122025	-0.062452
H	2.759979	4.943332	1.014216
H	2.211438	3.668622	-0.119767
H	4.082546	3.277484	2.329008
H	2.370409	2.783081	2.257008
O	2.969714	1.029897	-1.438590
C	4.248245	1.327258	-2.006254
C	4.889466	0.096658	-2.634556
H	5.043495	-0.689670	-1.870133
H	4.242621	-0.320009	-3.432398
H	5.871138	0.355361	-3.082544
H	4.917752	1.759485	-1.228610
H	4.086741	2.116346	-2.727678
H	0.825042	1.945826	0.412268
C	-0.257792	1.236416	2.719150
H	0.720058	1.403692	3.667341
P	-1.353150	0.799141	3.405310
H	-0.561630	2.484257	2.275607
C	0.757588	-0.798867	2.294190
H	0.207625	1.421869	-3.653571
H	-0.675832	1.479607	-4.322582
H	0.316737	0.371631	-3.322176
H	1.102123	1.685885	-4.252334
H	1.024713	2.308243	-1.864553
H	-0.075421	3.399812	-2.765357
TS_S1-S6-Si			
C	0.027793	0.142893	0.022703
C	0.013576	0.159570	1.550815
P	1.730449	0.058294	-0.734364
C	4.439625	-0.668188	1.562775
C	5.714643	-0.337687	2.339742
H	5.523496	0.375650	3.166607
H	6.499514	0.101583	1.691337
H	6.141174	-1.256295	2.792976
H	3.685593	-1.154928	2.211455
H	4.647765	-1.396654	0.752970
C	4.888378	1.633206	-0.154914
C	5.494931	0.949298	-1.374359
H	5.961306	-0.022931	-1.117028
H	6.283080	1.585077	-1.827248
H	4.729014	0.759868	-2.149028
H	5.675151	1.853474	0.597211
H	4.463928	2.615035	-0.442872
Rh	1.491747	0.099761	-0.256760
P	2.097272	-1.867107	-1.352563
C	3.785004	-1.887572	-2.138818
C	4.156149	-3.106790	-2.984357
H	4.190111	-4.037928	-2.384670
H	3.441063	-3.270028	-3.815628
H	5.160127	-2.971643	-4.346804
H	3.827466	-0.958396	-2.739288
H	4.514000	-1.740375	-1.317411
C	0.993961	-2.167753	-2.831508
C	1.141215	-1.149704	-3.960212
H	2.134997	-1.214698	-4.448057
H	1.030439	-0.115796	-3.573783
H	0.374527	-1.317510	-4.742668
H	-0.042869	-2.166519	-2.437437
H	1.189764	-3.195244	-3.203838
C	2.023843	-3.581911	-0.610581
C	3.070606	-3.861731	0.466937
H	4.101813	-3.811816	0.060991
H	2.996896	-3.138071	1.298171
H	2.932382	-4.875911	0.893812
H	1.000376	-3.707811	-0.208421
H	1.212178	-4.301963	-1.450110
P	0.760659	2.293683	-0.477250
C	-0.572809	2.433705	-1.761890
C	-1.176150	3.807393	-2.046306
H	-1.690084	4.216764	-1.155122
H	-0.415714	5.426998	-2.378675
H	-1.935262	3.730508	-2.851983
H	-1.358205	1.727698	-1.438968
H	-0.134886	1.983763	-2.675921
C	0.077206	3.205184	1.006445
C	0.218286	4.273334	1.082965
H	-0.238808	5.245054	0.217579
H	1.277749	5.047961	1.146009
H	-0.291784	5.011680	1.994588
H	-0.986058	2.901913	1.057969
H	0.548059	2.728073	1.884785
C	2.012565	3.504857	-1.147511
C	2.609773	3.132679	-2.503111
H	3.027065	2.106775	-2.485612
H	1.843427	3.159983	-3.303875
H	3.416166	3.838672	-2.788615
H	2.803515	3.611436	-0.377728
H	1.514549	4.493372	-1.205299
H	1.895048	0.514764	-1.776219
C	0.286702	-0.520072	1.388656
C	-0.445099	-0.777275	0.155570
H	-0.413061	-1.843597	-0.140627
Ge	-2.351496	-0.338311	0.043245
C	-3.334177	-1.680293	1.108367
C	-2.831876	-2.986672	1.285590
C	-3.559520	-3.949057	2.004655
C	-4.807686	-3.618009	2.560167
C	-5.320843	-2.320419	2.394421
C	-4.586799	-1.360630	1.675756
H	-4.993456	-0.342700	1.563689
H	-6.296080	-0.052552	2.830540
H	-5.378261	-4.370627	2.136162
H	-3.148153	-4.961988	2.137065
H	-1.851519	-3.261252	0.867188
C	-3.034629	1.394673	0.683477
C	-2.969704	1.730601	2.054004
C	-3.477414	2.954596	2.517527
C	-0.063794	3.862328	1.617807
C	-4.157227	3.529623	0.255680
C	-3.652752	2.299786	-0.203262
H	-3.738607	2.045086	-1.271577
H	-4.626512	4.229114	-0.453546
H	-4.454503	4.842591	-1.979059
H	-3.410313	3.205271	3.587653
H	-2.492253	1.031779	2.781771
C	-2.981850	-0.543795	-1.809747
C	-2.105699	-0.405660	-2.905567
C	-2.576029	-0.520492	-4.225161
C	-3.936057	-0.779173	-4.465941
C	-4.820581	-0.926120	-3.382363
C	-4.344570	-1.080314	-2.065509
H	-5.044998	-0.936582	-1.223990
H	-5.886393	-1.134302	-3.565366
H	-4.307888	-0.868246	-5.498473
H	-1.878820	-0.403525	-5.069431
H	-1.042890	-0.200129	-2.717214
C	0.500608	-1.617699	2.404314
F	0.628306	-2.845279	1.833503
F	1.614851	-1.444062	3.184514
F	-0.539466	-1.714511	3.281723
F	-0.256011	0.547052	2.170055
C	2.597066	1.531439	3.380658
H	1.572063	1.211103	3.122467
H	3.091170	0.679514	3.887542
H	2.528385	2.262099	4.112900
H	2.892239	2.871196	1.690330
H	4.401363	2.292878	2.416771
TS_S1-S6-Ge			
C	3.958027	1.315973	-1.188976
C	5.202085	1.963106	-1.246557
C	6.092708	1.868486	-0.162469
C	-2.262117	-3.021355	0.180688
C	-2.791633	-2.743889	-1.221097
H	-3.877907	-2.958123	-1.278325
H	-2.289165	-3.370749	-1.986249
H	-2.645147	-1.683061	-1.493899
H	-2.819822	-2.423768	0.924979
H	-2.420809	-4.084112	0.460530
C	-0.767820	-4.055866	-0.426770
C	-0.040973	-5.486381	-0.070136
H	0.500580	-6.214858	-0.708173
H	-1.124930	-5.660416	-0.224086
H	0.193372	-5.733770	0.984204
H	0.183722	-3.852370	-1.501472
H	1.459355	-3.916185	-0.281028
Rh	0.297955	-0.406013	0.076998
P	2.324043	-0.490398	1.161234
C	3.723072	-0.290530	-0.085475
C	4.975900	0.484090	0.322688
H	5.494386	0.047224	1.198892
H	4.716886	1.533776	0.560287
H	5.702694	0.502858	-0.516438
H	3.972103	-1.323239	-0.410059
H	3.257274	-0.217772	-0.946186
C	2.785064	0.703612	2.531976
C	2.113728	0.390887	3.869944
H	2.287900	1.207863	4.599462
H	1.018082	0.275082	3.756774
H	2.502600	-0.544022	4.322138
H	3.886839	0.713256	2.651993
H	2.497009	1.707774	2.164182
C	2.815773	-2.114062	1.956487
C	4.257022	-2.260365	2.449408
H	4.408767	-3.249662	2.92

Rh	3.255874	1.640276	-0.087488	C	5.732172	1.122126	0.971781	C	1.232759	-2.914389	0.866333
P	4.450783	2.197164	-2.036760	C	4.484971	0.472846	1.020937	C	1.319265	-2.490415	2.333422
C	5.496749	3.755370	-2.023911	C	3.581966	0.564353	-0.055813	H	0.373181	-2.682605	2.875895
C	4.719607	5.068387	-2.149427	Ge	1.829538	-0.371097	-0.056208	H	1.510620	-1.401997	2.408083
C	1.281038	-0.346518	-2.507856	C	1.871130	-1.359379	1.640263	H	2.130133	-3.031210	2.864146
C	0.383510	0.690195	-3.184759	C	1.668225	-0.704594	2.873331	H	0.933402	-3.979804	0.764136
C	2.326062	-1.619013	-0.143541	C	1.799733	-1.400431	4.085097	H	2.225197	-2.823165	0.381363
C	1.369869	-2.810565	-0.236262	C	2.138297	-2.765681	4.081928	C	-1.502990	-2.906075	-0.006649
P	5.023715	1.353977	1.389573	C	2.366773	-3.423166	2.806042	C	-2.116264	-2.906383	1.394357
C	5.406142	-0.460151	1.625097	C	2.242260	-2.719784	1.648938	H	-1.505744	-3.494892	2.107604
C	5.972788	-1.159675	0.393007	H	2.442626	-3.239579	0.698565	H	-2.185709	-1.875126	1.794612
C	1.924137	3.479673	-0.401974	H	2.646459	-4.488108	2.850051	H	-3.134865	-3.346353	1.391148
C	0.553655	3.504573	-0.293365	H	2.233078	-3.314561	5.031466	H	-1.259623	-3.938755	-0.337918
C	-0.435012	3.845346	-1.357337	H	1.632694	-0.875926	5.038531	H	-2.219433	-2.497141	-0.744799
F	-1.388488	2.878160	-1.541913	H	1.411555	0.364618	2.881084	C	0.594597	-2.394533	-1.880006
C	6.722225	2.043087	1.007194	C	2.072147	-1.650876	-1.532107	C	-0.331680	-1.867377	-2.977314
C	7.882349	1.682954	1.936763	C	0.977162	-2.187312	-2.226510	H	0.079761	-2.065896	-3.988040
C	4.803242	1.837281	3.179854	C	1.150812	-3.128043	-3.253273	H	-0.474002	-0.773661	-2.866289
C	3.632129	1.140611	3.872520	C	2.446129	-3.550489	-3.596766	H	-1.334949	-2.337962	-2.928779
Si	2.914093	4.211366	1.044798	C	3.555576	-3.025621	-2.909540	H	0.686501	-3.502180	-1.919370
O	4.591312	4.359795	0.994397	C	3.370657	-2.079221	-1.887020	H	1.615958	-1.977767	-2.006366
C	5.341552	5.542744	1.285321	H	4.246721	-1.666289	-1.363137	P	2.271979	0.671376	0.202862
C	5.818562	5.565422	2.732092	H	4.572724	-3.353548	-3.175062	C	2.579029	1.791241	-1.248471
O	2.405610	3.655989	2.542419	H	2.593188	-4.287509	-4.401409	C	2.383487	1.093658	-2.595347
C	1.483565	4.306412	3.410246	H	0.277277	-3.536411	-3.786630	H	1.377922	0.627653	-2.637364
C	2.152820	5.376339	4.265116	H	-0.024922	-1.845646	-1.928996	H	2.469610	1.811590	-3.436553
O	2.514706	5.867635	0.985113	Rh	-1.199364	-0.082296	0.166526	H	3.132921	0.292580	-2.764948
C	1.306203	6.511751	0.623398	P	-1.613511	-2.278200	0.885308	H	1.820040	2.586362	-1.098078
C	1.394952	7.119488	-0.772038	C	-3.367689	-2.914690	0.684140	H	3.584310	2.256883	-1.164683
F	-0.099056	3.266300	0.888641	C	-4.401248	-2.313556	1.635775	C	3.653621	-0.579501	0.098393
C	1.068336	4.051375	-2.557002	H	-4.258698	-2.676386	2.672486	C	5.068663	-0.023026	-0.078058
F	-1.145909	4.981259	-1.069175	H	-5.431706	-2.586087	1.328774	H	5.172260	0.548668	-1.022036
C	3.468552	2.441799	-3.610584	H	-4.333417	-1.208267	1.657894	H	5.352773	0.651514	0.754548
C	4.238899	2.787226	-4.886656	H	-3.345491	-4.019819	0.794353	H	5.813726	-0.844698	-0.105769
C	5.726520	0.956485	-2.609719	H	-3.643246	-2.706922	-0.368840	H	3.393990	-1.261896	-0.737935
C	5.119075	-0.365301	-3.079952	C	-0.719056	-3.705840	0.057423	H	3.583983	-1.190754	1.021546
H	0.276719	0.476599	-2.468190	C	-0.742430	-5.074186	0.740461	C	2.763858	1.764905	1.620997
H	0.794055	1.711934	-3.084305	H	-1.771123	-5.429621	0.956886	C	2.593752	1.109790	2.992290
H	-0.632036	0.702232	-2.745779	H	-0.182814	-5.057714	1.696321	H	1.542910	0.783268	3.130555
H	0.800011	-1.347369	-2.535278	H	-0.262982	-5.835752	0.090905	H	2.841858	1.821882	3.806166
H	2.246769	-0.446435	-3.045152	H	-1.152523	-3.761791	-0.962912	H	3.246198	0.221324	3.120929
H	0.462569	-2.660738	0.382554	H	0.325067	-3.372075	-0.081226	H	3.797943	2.138837	1.464254
H	1.864734	-3.736167	0.124520	C	-1.291335	-2.675847	2.682589	H	2.062652	2.616530	1.512326
H	1.037174	-3.003520	-1.276266	C	-1.697010	-1.607926	3.693200	P	-2.218346	0.811614	-0.047025
H	3.260787	-1.815603	-0.708829	H	-1.220120	-0.645894	3.435631	C	-2.304907	2.209156	-1.269308
H	2.645478	-1.448936	0.904273	H	-1.367871	-1.893280	4.713313	C	-1.886931	1.807832	-2.683974
H	8.052382	0.588402	1.992203	H	-2.790781	-1.437823	3.720833	H	-2.541202	1.020996	-3.113967
H	7.714751	2.046523	2.970392	H	-0.200776	-2.854034	2.752239	H	-0.850347	1.414221	-2.670139
H	8.826639	2.143385	1.578580	H	-1.786705	-3.645192	2.902268	H	-1.917046	2.677819	-3.371917
H	6.944836	1.721961	-0.031169	P	-2.213894	1.849598	0.878109	H	-1.583437	2.934684	-0.842928
H	6.565910	3.136982	0.959375	C	-2.429416	3.220877	-0.389600	H	-3.318349	2.662807	-1.247095
H	3.491888	1.544510	4.896352	C	-2.614121	4.674027	0.060986	C	-2.826031	1.645233	1.498522
H	2.697730	1.317173	3.305966	H	-3.490449	4.808257	0.723376	C	-2.831795	0.725313	2.720666
H	3.788294	0.046322	3.964313	H	-1.720429	5.051409	0.589869	H	-1.825690	0.278289	2.862145
H	5.756213	1.626862	3.709521	H	-2.765447	5.324839	-0.825396	H	-3.561032	-0.104815	2.617120
H	4.643673	2.931082	3.180083	H	-1.527827	3.145551	-1.029215	H	-3.096971	1.284295	3.641657
H	6.971884	-0.765562	0.115273	H	-3.279067	2.911031	-1.030271	H	-2.084737	2.459854	1.630080
H	5.302900	-1.015381	-0.475298	C	-3.926347	1.535103	1.554351	H	-3.819399	2.110040	1.321672
H	6.082878	-2.250353	0.563040	C	-4.794078	2.708109	2.016091	C	-3.627536	-0.298318	-0.563250
H	4.446490	-0.926931	1.924388	H	-4.285292	3.331465	2.778654	C	-4.987790	0.372567	-0.771264
H	6.093761	-0.561240	2.492844	H	-5.074691	3.368203	1.171684	H	-4.958091	1.125701	-1.583767
H	2.566102	6.176782	3.619658	H	-5.736610	2.337710	2.470296	H	-5.339466	0.884350	0.147287
H	1.424380	5.831407	4.968007	H	-3.747254	0.820520	2.385316	H	-5.757332	-0.378436	-1.045074
H	2.981750	4.940162	4.859017	H	-4.445451	0.947347	0.772606	H	-3.291287	-0.802002	-1.493862
H	0.638546	4.743964	2.834707	C	-1.436914	2.824035	2.264924	H	-3.698789	-1.092454	0.206174
H	1.045786	3.514679	4.056625	H	-1.165071	2.062162	3.556551				
H	2.256678	7.814020	-0.839487	C	-0.719479	2.734262	4.317954				
H	0.469743	7.679554	-1.017476	H	-2.087991	1.627236	3.991140				
H	1.528870	6.330047	-1.538023	H	-0.456157	1.231535	3.379401				
H	0.441187	5.814712	0.672565	H	-0.498610	3.247228	1.861007				
H	1.110098	7.310018	1.375310	H	-2.104120	3.688235	2.458517				
H	6.434982	4.673642	2.964272	H	-0.632189	0.042417	1.638088				
H	4.958307	5.576308	3.429313	C	0.561661	1.180106	-0.459657				
H	6.432692	6.469312	2.925071	C	1.048519	2.342707	0.093935				
H	6.214812	5.542921	0.594410	F	1.555388	2.351369	1.374586				
H	4.732752	6.442186	1.058325	C	1.244036	3.670298	-0.543738				
H	2.215534	3.848462	-1.397413	F	0.724438	3.697749	-1.802128				
H	3.544062	2.912917	-5.742741	F	2.552648	4.040828	-0.641968				
H	4.957835	1.989717	-5.163240	F	0.646281	4.693372	0.159479				
H	4.812506	3.730364	-4.787859	H	0.373754	1.329056	-1.533654				
H	2.707911	3.217618	-3.384015	P	-2.254910	-0.166209	-1.976351				
H	2.892812	1.506026	-3.743550	C	-1.536375	0.959746	-3.298541				
H	4.560131	-0.245672	-0.430039	C	-0.242409	0.473838	-3.956664				
H	4.410269	-0.762560	-2.325836	H	0.559748	0.276817	-3.220056				
H	5.901419	-1.132740	-3.247729	H	-0.391265	-0.468445	-4.520292				
H	6.395248	0.786663	-1.741970	H	0.138442	1.232949	-4.669762				
H	6.350632	1.412890	-3.406976	H	-1.371163	1.935449	-2.796578				
H	4.161717	5.139409	-3.104437	H	-2.315726	1.137810	-4.069077				
H	3.998879	5.203519	-1.322408	C	-2.448555	-1.776666	-2.930514				
H	5.413148	5.933103	-2.110454	C	-3.209422	-1.733287	-4.257585				
H	6.249938	3.673511	-2.836648	H	-2.748370	-1.024925	-4.974954				
H	6.044668	3.733829	-1.062639	H	-4.268548	-1.435107	-4.128196				
H	2.500192	1.236069	1.256294	H	-3.208017	-2.733282	-4.738637				
H	0.592156	1.023471	1.932063	H	-1.428299	-2.167408	-3.096643				
H	-1.024522	0.242066	1.932754	H	-2.923422	-2.490080	-2.225460				
H	0.459766	-0.760287	1.981911	C	-4.039198	0.417415	-2.060711				
H	-0.440244	1.066281	-0.369352	C	-5.061774	-0					

