

Supplementary Information

Substituent effect on the formation of rhenium carbyne and η^2 -vinyl complexes from the reactions of $\text{ReH}_5(\text{PMe}_2\text{Ph})_3$ with terminal alkynes

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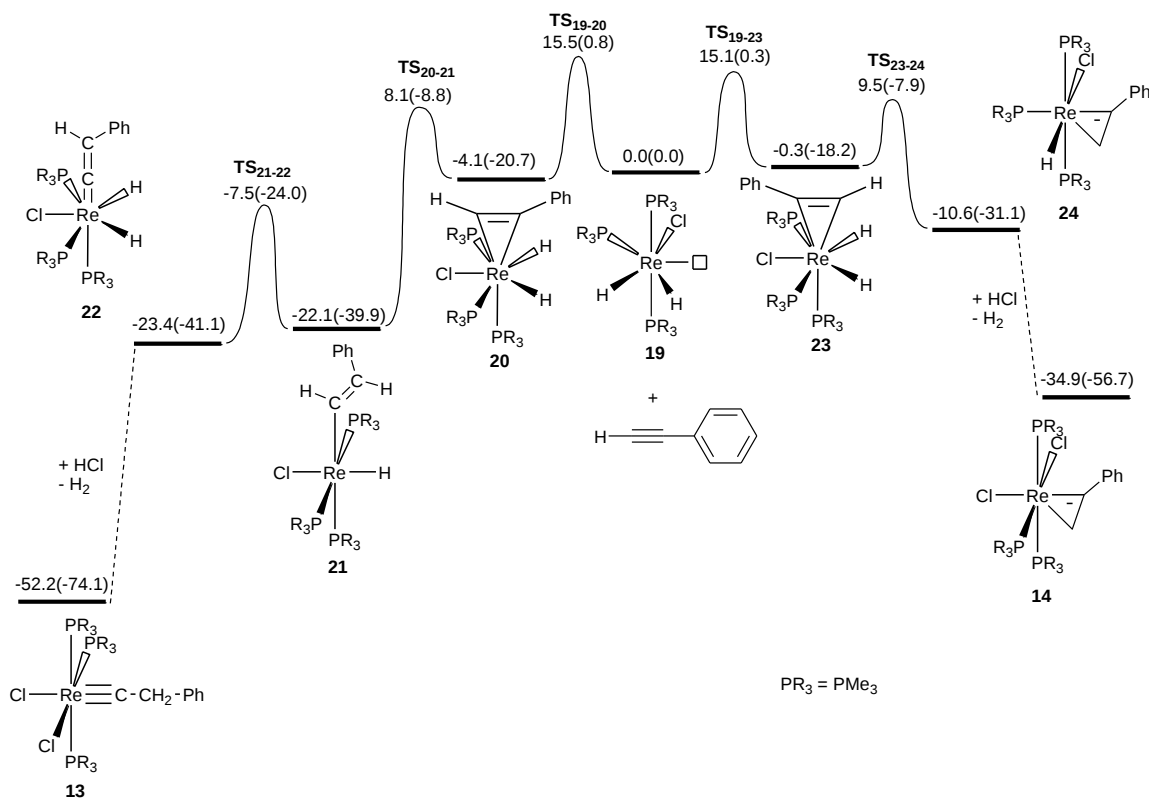


Fig. S1 The energy profile calculated for the reaction of *mer*- $\text{ReH}_2\text{Cl}(\text{PMe}_3)_3$ with $\text{HC}\equiv\text{CPh}$ in the presence of HCl with a better basis sets (6-31G** is used for those C and H atoms involved in the bond forming and breaking processes). The relative Gibbs free energies and electronic energies (in parentheses) at 298 K are given in kcal/mol

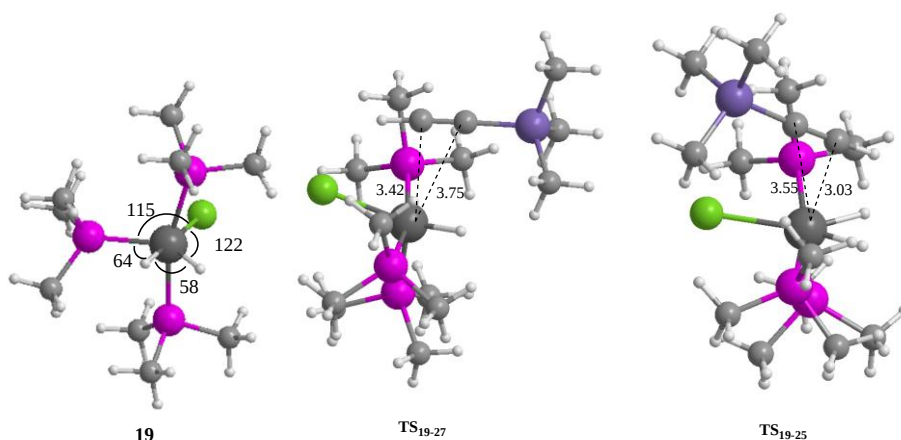


Fig. S2 Structural parameters (in Å and deg) calculated for 19, TS₁₉₋₂₅ and TS₁₉₋₂₇.

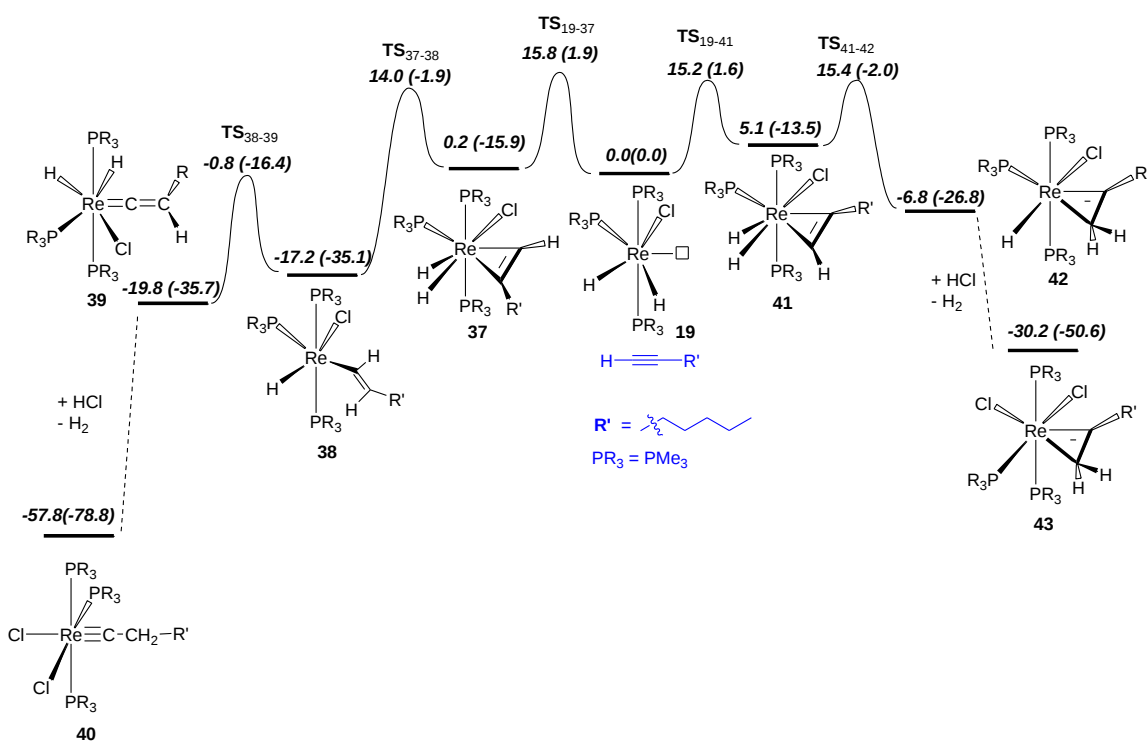


Fig. S3. The energy profile calculated for the reaction of *mer*-ReH₂Cl(PMe₃)₃ with HC≡C-*n*-penyl in the presence of HCl. The relative Gibbs free energies and electronic energies (in parentheses) at 298 K are given in kcal/mol.

Cartesian coordinates and electronic energies for all of the calculated structures

19				C	1.356122	-0.049926	0.000801
scf done: -474.074263				C	2.571517	-0.049907	0.001337
Re	-0.009106	-0.253854	-0.119106	H	3.635716	-0.049890	0.001805
Cl	-0.101970	-1.708297	1.870248	TS₁₉₋₂₀			
P	0.191690	2.012912	0.310056	scf done: -782.399659			
P	-2.395382	-0.390130	-0.203014	Re	0.589848	0.016162	-0.009902
C	-1.160505	3.185286	-0.197204	Cl	1.484234	0.053759	-2.391886
H	-0.933348	4.210928	0.116082	P	2.444678	0.124691	1.316161
H	-2.104820	2.876270	0.259122	P	0.831785	-2.398259	-0.314774
H	-1.272494	3.156736	-1.285364	C	-2.928647	-0.223987	-1.173623
C	-3.414358	0.062162	1.293674	C	-2.022630	-0.237984	-1.988413
H	-4.467026	-0.218266	1.169736	C	2.859529	-1.253760	-2.512748
H	-3.357696	1.140224	1.481506	H	3.747532	-1.001722	3.104415
H	-2.995990	-0.462278	2.158632	H	3.051698	-2.188614	1.979802
C	-3.347893	0.446662	-1.568519	H	2.009444	-1.403319	3.186129
H	-4.405723	0.158067	-1.551505	C	2.477208	-3.061662	-0.880072
H	-2.908697	0.158314	-2.528798	H	2.412349	-4.130437	-1.114703
H	-3.274586	1.534040	-1.473153	H	3.242089	-2.915051	-0.111728
C	1.663367	2.973994	-0.298057	H	2.769946	-2.505533	-1.775410
H	1.609614	4.020080	0.025241	C	0.398333	-3.543646	1.086245
H	2.584382	2.530994	0.090110	H	0.526120	-4.591723	0.791340
H	1.691161	2.935015	-1.391336	H	-0.646250	-3.371631	1.364218
P	2.325130	-0.748817	-0.244695	H	1.020424	-3.337673	1.960447
C	3.436194	-0.412080	1.216974	C	2.572074	1.535230	2.539122
H	4.432500	-0.848997	1.080703	H	3.512995	1.486628	3.099624
H	3.544940	0.667156	1.372544	H	2.523900	2.495368	2.017840
H	2.966756	-0.844696	2.106285	H	1.731855	1.478522	3.238536
C	3.356867	-0.096682	-1.653146	P	0.330719	2.429037	-0.402009
H	4.367450	-0.522341	-1.638387	C	1.861129	3.364345	-0.905860
H	2.866494	-0.359770	-2.595771	H	1.611279	4.387264	-1.210583
H	3.428628	0.993549	-1.600587	H	2.579830	3.408386	-0.081413
C	-2.940809	-2.155598	-0.447152	H	2.320720	2.832875	-1.744094
H	-2.550571	-2.758331	0.378314	C	-0.352418	3.501052	0.953513
H	-4.033692	-2.238435	-0.479196	H	-0.424572	4.547819	0.636208
H	-2.523233	-2.538986	-1.384029	H	-1.348408	3.135476	1.222791
C	0.277775	2.319903	2.147697	H	0.284449	3.435027	1.840167
H	1.160426	1.823575	2.560965	C	-0.255240	-3.106522	-1.649942
H	0.329058	3.393255	2.364482	H	0.009596	-2.639274	-2.602669
H	-0.606632	1.893275	2.629358	H	-0.117857	-4.191463	-1.726152
C	2.603969	-2.579908	-0.449967	H	-1.303448	-2.885347	-1.432302
H	3.672310	-2.820121	-0.506427	C	4.090333	0.309964	0.446627
H	2.154011	-3.098571	0.401622	H	4.067700	1.206362	-0.179984
H	2.109380	-2.922484	-1.364940	H	4.916954	0.387863	1.163173
H	0.021504	0.755133	-1.485627	H	4.259011	-0.547475	-0.210963
H	-0.047874	-0.853811	-1.662243	C	-0.790053	2.885158	-1.813797
HCl				H	-0.819133	3.972519	-1.949120
scf done: -15.556545				H	-0.407720	2.413389	-2.723616
Cl	0.634815	0.254777	0.000000	H	-1.799445	2.511320	-1.626252
H	-0.650929	0.254777	0.000000	H	-0.509465	-0.754075	0.961883
H₂				H	0.053831	0.666584	1.423494
scf done: -1.175482				C	-3.998250	-0.201443	-0.223081
H	0.000000	0.000000	-0.071394	C	-5.339557	-0.286616	-0.655591
H	0.000000	0.000000	0.671394	C	-3.726669	-0.089392	1.158423
1. HC≡CPh + mer-ReH₂Cl(PMe)₃				C	-6.381768	-0.260102	0.273028
HC≡CPh				H	-5.550576	-0.372601	-1.716195
scf done: -308.327518				C	-4.777201	-0.063876	2.078441
C	-2.188606	-1.261343	0.000038	H	-2.694381	-0.026820	1.485863
C	-0.792437	-1.265746	0.000661	C	-6.105157	-0.148699	1.641480
C	-0.075044	-0.049912	0.000173	H	-7.409241	-0.326171	-0.070611
C	-0.792347	1.166022	-0.000906	H	-4.558764	0.021622	3.138276
C	-2.188484	1.161737	-0.001506	H	-6.917824	-0.128603	2.360721
C	-2.890941	-0.049788	-0.001054	H	-1.209010	-0.235964	-2.680570
H	-2.728812	-2.202679	0.000402	20			
H	-0.245761	-2.202492	0.001496	scf done: -782.431811			
H	-0.245535	2.102689	-0.001269	Re	-0.325306	-0.003738	-0.065880
H	-2.728652	2.103094	-0.002343	Cl	-2.060615	0.083185	-1.946760
H	-3.976251	-0.049718	-0.001526	P	-2.160525	0.095042	1.538528
				P	-0.286072	2.425801	-0.569484

C	1.833031	-0.088170	-0.582658	H	-0.667531	-3.499349	1.162979
C	1.163905	-0.098279	-1.677752	H	0.853244	-3.212955	2.023865
C	-2.134584	1.503561	2.767575	C	2.255719	1.967794	2.376270
H	-2.953898	1.416211	3.490773	H	3.128971	2.017628	3.036897
H	-2.219676	2.464454	2.254024	H	2.249873	2.853481	1.735669
H	-1.179907	1.484455	3.303646	H	1.346295	1.971366	2.985267
C	-1.891565	3.361945	-0.599494	P	-0.209119	2.355485	-0.488712
H	-1.739425	4.376686	-0.984244	C	1.145692	3.492784	-1.064187
H	-2.326984	3.429061	0.400617	H	0.748335	4.481671	-1.320084
H	-2.582418	2.821162	-1.252237	H	1.907103	3.607224	-0.286758
C	0.779662	3.492168	0.513229	H	1.621088	3.039280	-1.938097
H	0.800418	4.530053	0.162154	C	-0.951586	3.321793	0.919615
H	1.796600	3.087555	0.513800	H	-1.198957	4.346087	0.617170
H	0.403410	3.465855	1.540631	H	-1.862819	2.813641	1.252045
C	-2.265680	-1.290236	2.790508	H	-0.254099	3.356625	1.761150
H	-3.074148	-1.115025	3.509921	C	0.221673	-3.248209	-1.769696
H	-2.437465	-2.248846	2.294181	H	0.575552	-2.743056	-2.673649
H	-1.313621	-1.349440	3.328444	H	0.516601	-4.303197	-1.798476
P	-0.555051	-2.428299	-0.531033	H	-0.868826	-3.175904	-1.737582
C	-2.260202	-3.164970	-0.593660	C	4.002148	0.550137	0.618077
H	-2.218819	-4.206212	-0.933350	H	4.013747	1.344325	-0.132494
H	-2.739243	-3.134336	0.388932	H	4.736117	0.763667	1.403287
H	-2.854105	-2.571867	-1.294676	H	4.268407	-0.377869	0.107691
C	0.344300	-3.593761	0.599822	C	-1.479297	2.681203	-1.811413
H	0.242818	-4.633863	0.270244	H	-1.669976	3.755861	-1.907150
H	1.403869	-3.319555	0.616499	H	-1.107458	2.294385	-2.765198
H	-0.047547	-3.497142	1.617066	H	-2.414366	2.169179	-1.569267
C	0.353028	2.852979	-2.259515	H	-0.921122	-0.898682	0.580062
H	-0.259200	2.329611	-2.999478	H	-0.114047	0.456156	1.402136
H	0.297163	3.933793	-2.430668	H	-1.255041	-0.426250	-2.670223
H	1.388857	2.520395	-2.360987	C	-3.173894	-0.478739	0.076150
C	-3.917823	0.174580	0.940242	C	-4.309985	-0.611826	-0.757472
H	-4.138337	-0.700029	0.323359	C	-3.377194	-0.327662	1.464683
H	-4.614402	0.215883	1.785312	C	-5.595479	-0.591700	-0.216488
H	-4.050500	1.056828	0.309038	H	-4.168192	-0.732010	-1.826855
C	0.077221	-2.966195	-2.191931	C	-4.667843	-0.305819	1.999932
H	-0.083270	-4.040259	-2.337485	H	-2.512632	-0.223151	2.112664
H	-0.459222	-2.405982	-2.963144	C	-5.783495	-0.437979	1.164778
H	1.143788	-2.742766	-2.272883	H	-6.454492	-0.695672	-0.872599
H	0.369852	0.796333	1.213900	H	-4.802401	-0.186000	3.070817
H	0.315344	-0.887119	1.186527	H	-6.785347	-0.422205	1.581776
C	3.137517	-0.101695	0.047452	21			
C	4.308165	-0.130611	-0.749887	scf done: -782.463292			
C	3.292213	-0.082977	1.449874	Re	0.667304	0.000067	-0.161823
C	5.574471	-0.139453	-0.165676	Cl	1.853871	0.000032	-2.348855
H	4.205263	-0.144865	-1.830645	P	2.517843	-0.000440	1.300175
C	4.563403	-0.092407	2.032000	P	0.506557	-2.403034	-0.362362
H	2.401972	-0.061120	2.067793	C	-2.380537	0.000000	0.935516
C	5.710259	-0.120156	1.230163	C	-1.326149	0.000185	0.080397
H	6.458059	-0.160885	-0.796964	C	2.692105	-1.415509	2.491717
H	4.658501	-0.077572	3.113890	H	3.563372	-1.270522	3.140516
H	6.696578	-0.126443	1.683631	H	2.810275	-2.356138	1.947589
H	1.158846	-0.124893	-2.753646	H	1.789226	-1.477812	3.106381
TS₂₀₋₂₁				C	2.003167	-3.392389	-0.863935
scf done: -782.410245				H	1.737847	-4.435926	-1.068862
Re	0.366109	0.004784	-0.132944	H	2.767311	-3.372954	-0.079580
Cl	2.001321	0.265087	-2.055953	H	2.421699	-2.936413	-1.766436
P	2.293884	0.417138	1.335765	C	-0.185045	-3.396228	1.048435
P	0.952989	-2.385646	-0.292860	H	-0.357278	-4.439593	0.759976
C	-1.843916	-0.489930	-0.503630	H	-1.132523	-2.940582	1.352962
C	-1.145488	-0.417721	-1.598899	H	0.498614	-3.370227	1.902112
C	2.569603	-0.798337	2.729067	C	2.692840	1.414529	2.491728
H	3.365517	-0.457066	3.401486	H	3.564217	1.269255	3.140317
H	2.841971	-1.782130	2.337772	H	2.811159	2.355129	1.947576
H	1.638098	-0.899133	3.295464	H	1.790133	1.477102	3.106620
C	2.739316	-2.854661	-0.518671	P	0.507126	2.403229	-0.362015
H	2.833135	-3.920063	-0.757448	C	2.004115	3.392286	-0.863029
H	3.318083	-2.646525	0.385826	H	1.739202	4.436017	-1.067498
H	3.142485	-2.253894	-1.338863	H	2.768167	3.372178	-0.078598
C	0.423292	-3.537008	1.071769	H	2.422589	2.936573	-1.765688
H	0.730163	-4.570113	0.870507	C	-0.184411	3.396142	1.049010

H	-0.356245	4.439683	0.760948	H	-1.312078	2.772982	-2.098577
H	-1.132099	2.940681	1.353166	Cl	2.106939	0.070006	-2.036124
H	0.499064	3.369567	1.902816	P	2.691550	0.003819	1.164818
C	-0.663589	-2.877398	-1.731283	C	2.529112	-0.132454	3.012349
H	-0.323744	-2.412618	-2.662301	H	3.507511	-0.146663	3.505709
H	-0.704025	-3.964726	-1.862657	H	1.947902	0.715896	3.387128
H	-1.666771	-2.507423	-1.496923	H	1.983057	-1.047029	3.262803
C	4.176015	-0.000806	0.459424	C	3.804799	1.488857	1.009562
H	4.258406	0.881119	-0.181136	H	4.724709	1.353175	1.589719
H	4.989266	-0.001209	1.194327	H	4.058101	1.617577	-0.046588
H	4.257857	-0.882507	-0.181507	C	3.295663	2.389731	1.363159
C	-0.662687	2.878378	-1.730944	H	3.954184	-1.316504	0.801183
H	-0.702977	3.965780	-1.861747	H	4.166683	-1.298809	-0.271574
H	-0.322714	2.414068	-2.662149	H	4.879207	-1.135157	1.360173
H	-1.665962	2.508397	-1.496993	H	3.571724	-2.305054	1.070012
H	0.316302	0.000236	1.477073	H	-1.042541	-0.559951	0.505198
H	-2.159979	-0.000263	2.003122	H	0.173111	0.408677	1.444527
C	-3.812246	0.000087	0.602891	22			
C	-4.312534	0.000478	-0.721105	scf done:	-782.466404		
C	-4.761596	-0.000247	1.651451	Re	-0.478019	0.027150	-0.033024
C	-5.684333	0.000519	-0.977224	P	-0.407349	2.453315	-0.487153
H	-3.620409	0.000757	-1.558472	P	-0.403352	-2.358555	-0.648914
C	-6.134318	-0.000206	1.394845	C	1.272096	0.059336	-0.676350
H	-4.405828	-0.000545	2.678691	H	2.800130	0.107283	-2.098361
C	-6.607984	0.000176	0.077349	C	2.571665	0.060597	-1.030319
H	-6.036253	0.000823	-2.005144	C	3.734650	0.001865	-0.134338
H	-6.835754	-0.000472	2.224452	C	3.609857	-0.070624	1.274126
H	-7.674298	0.000208	-0.125257	H	2.617643	-0.080211	1.713685
H	-1.561237	0.000504	-1.018918	C	4.739451	-0.129228	2.092059
TS₂₁₋₂₂				H	4.615723	-0.184441	3.170346
scf done:	-782.432536			C	6.027177	-0.117606	1.537457
Re	0.458217	0.016583	-0.143536	H	6.902733	-0.163761	2.177516
P	0.510178	-2.444307	-0.307981	C	6.167689	-0.045633	0.146033
P	0.315194	2.455538	-0.294398	H	7.158285	-0.035605	-0.300215
C	-1.346426	0.016455	-0.767162	C	5.040383	0.013178	-0.676513
H	-2.846634	0.077261	-2.181427	H	5.162208	0.068191	-1.755375
C	-2.648205	0.024053	-1.109772	C	-1.942325	3.494258	-0.395263
C	-3.830731	-0.029460	-0.243503	H	-1.762005	4.488918	-0.818497
C	-3.758769	0.035908	1.168657	H	-2.732160	2.996382	-0.965516
H	-2.792814	0.146767	1.651947	H	-2.264005	3.607267	0.643524
C	-4.913913	-0.025344	1.950740	C	0.805074	3.411693	0.532092
H	-4.829328	0.027579	3.032586	H	1.778316	2.915904	0.467688
C	-6.175947	-0.145993	1.353927	H	0.896678	4.444868	0.178991
H	-7.071423	-0.191219	1.965528	H	0.489327	3.413439	1.580021
C	-6.266225	-0.202630	-0.042602	C	0.166205	2.805438	-2.211113
H	-7.237227	-0.292719	-0.521064	H	-0.517538	2.322452	-2.913373
C	-5.113542	-0.145054	-0.827956	H	0.197546	3.884488	-2.399418
H	-5.195401	-0.192732	-1.910572	H	1.164176	2.379250	-2.341297
C	1.759065	-3.258602	-1.417056	C	0.172780	-2.606601	-2.389515
H	1.566401	-4.335530	-1.479358	H	1.177550	-2.187398	-2.487590
H	1.690059	-2.807729	-2.410186	H	0.189830	-3.670933	-2.649358
H	2.774211	-3.093592	-1.050785	H	-0.500411	-2.067490	-3.060597
C	0.676849	-3.434894	1.261930	C	-1.954498	-3.377957	-0.626213
H	-0.128191	-3.147984	1.946218	H	-2.698500	-2.874537	-1.250328
H	0.613072	-4.510883	1.061365	H	-1.770522	-4.384092	-1.019702
H	1.632053	-3.223019	1.751788	H	-2.342596	-3.462509	0.393507
C	-1.051291	-3.192292	-0.988484	C	0.793211	-3.390134	0.315348
H	-1.223069	-2.812518	-1.999461	H	0.461237	-3.469582	1.355194
H	-0.972355	-4.284734	-1.018183	H	0.890825	-4.394406	-0.111656
H	-1.910257	-2.907423	-0.374566	H	1.766993	-2.891257	0.303546
C	1.596919	3.363016	-1.288475	Cl	-2.066980	0.100810	-2.003945
H	1.624438	2.937068	-2.294643	P	-2.593077	-0.110351	1.451897
H	1.355510	4.430836	-1.339259	C	-2.428215	-1.326127	2.853774
H	2.588572	3.238110	-0.849357	H	-3.317380	-1.326060	3.494697
C	0.315177	3.419607	1.300798	H	-2.274771	-2.334824	2.458085
H	1.234951	3.230846	1.862827	H	-1.551040	-1.060870	3.452667
H	0.226222	4.496117	1.114463	C	-4.224451	-0.600594	0.708662
H	-0.530302	3.089630	1.913119	H	-5.028209	-0.559785	1.452531
C	-1.225221	3.143534	-1.073221	H	-4.451316	0.070378	-0.124049
H	-2.108579	2.813236	-0.521727	H	-4.157824	-1.614594	0.305027
H	-1.186018	4.238500	-1.083672	C	-3.102882	1.396540	2.425350

	-3.487771	2.162265	1.746301	C	-3.113790	-0.167485	-1.512584
H	-3.882655	1.150603	3.155626	C	4.031780	1.619774	-0.704225
H	-2.232698	1.800649	2.952655	H	5.105130	1.557829	-0.489426
H	0.005312	0.811967	1.353583	H	3.644745	2.552393	-0.281731
H	0.056460	-0.848507	1.274914	H	3.880277	1.639944	-1.788112
13							
scf done: -796.904134							
Re	-0.556511	0.024295	-0.178514	H	0.977202	3.239848	1.519702
Cl	-2.813913	-0.452076	-1.373538	C	0.559342	4.248076	1.622064
Cl	0.311146	0.823148	-2.409115	H	2.069538	3.309386	1.490516
P	-1.252533	2.418066	-0.092448	H	0.687584	2.631284	2.380683
P	0.274074	-2.191807	-0.900915	C	0.835552	3.610371	-1.343840
P	-1.912347	-0.850449	1.626511	H	0.520731	4.628601	-1.088208
C	0.844268	0.295174	0.844752	H	0.364301	3.312848	-2.285710
C	1.993998	0.529498	1.749664	H	1.919378	3.593026	-1.486054
H	1.962997	-0.189845	2.582552	C	4.246841	-1.191566	-0.609991
H	1.865657	1.521032	2.218351	H	5.297771	-0.946813	-0.414281
C	3.373123	0.468199	1.090282	H	4.014026	-2.142096	-0.120191
C	3.555072	0.788443	-0.265825	H	4.098795	-1.308721	-1.688401
H	2.697168	1.036444	-0.884266	P	0.788872	-2.415688	-0.028793
C	4.838686	0.768572	-0.826812	C	1.514583	-3.176506	1.505441
H	4.965634	1.016615	-1.876004	H	1.276256	-4.244614	1.566079
C	5.950025	0.430052	-0.046438	H	2.602589	-3.055189	1.512468
H	6.942692	0.416306	-0.485470	H	1.099007	-2.656612	2.372972
C	5.773220	0.104550	1.303628	C	1.473657	-3.507979	-1.368390
H	6.627997	-0.165339	1.916407	H	1.325119	-4.566599	-1.125712
C	4.492241	0.121307	1.865646	H	0.958950	-3.277803	-2.306369
H	4.360876	-0.134023	2.914424	C	2.539900	-3.316946	-1.511019
C	0.215355	3.537185	-0.266907	H	-1.476411	2.756833	0.120910
H	-0.098671	4.582871	-0.359697	H	-1.873054	2.202852	0.975614
H	0.769899	3.234073	-1.157796	H	-1.658738	3.828985	0.259122
H	0.867291	3.435018	0.606834	H	-1.988022	2.411237	-0.781575
C	-2.347970	2.959909	-1.478429	C	3.696555	0.266880	1.790973
H	-2.531319	4.039203	-1.428421	H	3.365556	-0.619975	2.339455
H	-3.291057	2.410315	-1.430856	H	4.788840	0.346267	1.853108
H	-1.857329	2.702210	-2.419942	H	3.241938	1.140606	2.268261
C	-0.897882	-3.309362	-1.799297	C	-0.956904	-3.049917	0.059727
H	-0.377913	-4.206185	-2.154403	H	-0.976471	-4.142840	0.142473
H	-1.317365	-2.759672	-2.645797	H	-1.444482	-2.604725	0.930868
H	-1.727498	-3.598453	-1.150338	H	-1.504341	-2.740872	-0.835757
C	1.709748	-2.142635	-2.071049	H	1.316388	0.826061	-1.676868
H	2.040680	-3.161130	-2.304368	H	0.944608	-0.716511	-1.781359
H	2.532042	-1.582973	-1.616695	C	-4.268898	-0.147744	-0.667423
H	1.414235	-1.621477	-2.983280	C	-4.122889	-0.221904	0.735669
C	-1.055407	-1.035196	3.266566	C	-5.563487	-0.046746	-1.220769
H	-1.733129	-1.447034	4.022714	C	-5.251590	-0.195714	1.557957
H	-0.695596	-0.057715	3.603246	H	-3.128106	-0.292090	1.165059
H	-0.192680	-1.700317	3.160253	C	-6.684624	-0.020819	-0.389067
C	-3.443641	0.075792	2.130497	H	-5.676636	0.011455	-2.298158
H	-4.053552	-0.531486	2.808602	C	-6.532925	-0.095534	1.001299
H	-4.018787	0.301996	1.228556	H	-5.129383	-0.251850	2.634966
H	-3.174891	1.005474	2.636727	H	-7.675697	0.058251	-0.824715
C	-2.659707	-2.541760	1.417482	H	-7.406390	-0.074722	1.645428
H	-3.266731	-2.800866	2.292151	H	-1.222201	-0.179144	-2.791162
H	-3.289058	-2.523827	0.524222	23			
H	-1.883805	-3.300490	1.290372	scf done: -782.427960			
C	-2.093743	3.203638	1.374623	Re	0.518473	-0.000037	-0.400677
H	-2.113095	4.293199	1.256088	Cl	0.084868	-0.035259	2.121898
H	-3.122469	2.844778	1.457293	P	2.901465	-0.017381	0.151314
H	-1.557135	2.958589	2.297169	P	0.238644	2.454213	-0.094542
C	0.993936	-3.294862	0.416061	C	-1.023665	-0.000987	-1.912350
H	0.259643	-3.532768	1.190414	C	-1.709427	0.004320	-0.822675
H	1.359322	-4.230345	-0.022846	C	3.935904	1.444909	-0.384534
H	1.835486	-2.772716	0.883559	H	4.997548	1.278512	-0.167147
TS₁₉₋₂₃							
scf done: -782.400797							
Re	0.866134	0.019131	-0.293148	H	3.611655	2.352218	0.132338
Cl	-0.272873	-0.106355	1.957907	H	3.811735	1.595790	-1.461901
P	3.110093	0.158871	0.016190	C	0.975820	3.244086	1.417672
P	0.342141	2.406405	-0.017996	H	0.685683	4.298866	1.481554
C	-2.117160	-0.177061	-2.212669	H	2.067331	3.179322	1.398990
				H	0.613224	2.704178	2.295863
				C	0.882114	3.545393	-1.454885
				H	0.678199	4.601924	-1.246905
				H	0.393536	3.262359	-2.392907

H	1.959846	3.404062	-1.575383	H	-0.578321	3.238418	-2.450416
C	3.924476	-1.344666	-0.673271	H	-2.031231	3.419445	-1.452747
H	4.984080	-1.256819	-0.406322	C	1.328845	-3.120514	0.123326
H	3.568073	-2.336621	-0.383673	H	1.734133	-2.673762	1.035136
H	3.818781	-1.247213	-1.758790	H	1.293131	-4.210747	0.229764
P	0.197289	-2.442455	-0.088912	H	1.991174	-2.858280	-0.705409
C	1.163267	-3.304584	1.245494	C	-3.437038	-0.270187	1.939555
H	0.839186	-4.347082	1.341281	H	-3.007039	0.498278	2.586583
H	2.235423	-3.290138	1.030660	H	-4.531056	-0.238788	1.996201
H	0.983167	-2.776834	2.186202	H	-3.077615	-1.234666	2.303134
C	0.532686	-3.511620	-1.569820	C	1.591663	3.095979	-0.262874
H	0.303707	-4.563517	-1.365740	H	1.602286	4.189648	-0.195008
H	-0.087669	-3.160992	-2.401039	H	2.180050	2.675111	0.556415
H	1.582161	-3.420419	-1.865945	H	2.053064	2.787110	-1.204438
C	-1.505920	3.077099	0.034850	H	-0.231037	-0.615978	-1.915716
H	-1.992224	2.621362	0.900325	H	-1.413366	0.634552	-1.585949
H	-1.512133	4.167798	0.141209	C	3.055478	-0.089280	-0.254814
H	-2.069091	2.793326	-0.857247	C	3.307764	0.010846	1.131825
C	3.440477	-0.181491	1.920717	C	4.164385	-0.221751	-1.126556
H	3.078611	-1.126383	2.332351	C	4.617779	-0.008757	1.621303
H	4.532945	-0.139992	1.996870	H	2.463164	0.097135	1.806571
H	2.993198	0.620148	2.513110	C	5.468330	-0.245685	-0.632631
C	-1.516294	-2.988465	0.365471	H	3.986478	-0.310299	-2.194301
H	-1.543816	-4.074516	0.510680	C	5.702712	-0.136605	0.745952
H	-1.814992	-2.485510	1.288086	H	4.790865	0.071463	2.690470
H	-2.221458	-2.707812	-0.419636	H	6.303436	-0.348913	-1.319530
H	1.185196	0.818826	-1.682855	H	6.718111	-0.155027	1.129907
H	1.170653	-0.835278	-1.676386	H	1.235810	0.307862	-2.968976
C	-3.063022	0.010799	-0.298233	24			
C	-3.330539	0.079102	1.087332	scf done: -782.447824			
C	-4.166601	-0.049018	-1.185531	Re	0.343624	0.000397	-0.314901
C	-4.646428	0.089896	1.561362	Cl	0.057475	0.001227	2.258485
H	-2.492918	0.118537	1.774900	P	2.884930	-0.001130	0.327685
C	-5.476715	-0.039074	-0.707199	P	0.323054	2.445812	-0.313454
H	-3.977833	-0.103291	-2.253619	C	-1.063699	0.000265	-1.959480
C	-5.725307	0.031084	0.671356	C	-1.580623	0.000017	-0.603614
H	-4.829039	0.142911	2.630855	C	3.927399	1.400902	-0.326697
H	-6.305981	-0.085793	-1.407470	H	4.979704	1.251045	-0.059084
H	-6.745344	0.038482	1.043220	H	3.598228	2.357824	0.084637
H	-1.035549	0.005390	-2.989473	H	3.836724	1.437708	-1.416502
TS₂₃₋₂₄				C	0.962384	3.335746	1.192032
scf done: -782.409414				H	0.686991	4.396385	1.173079
Re	-0.471174	0.039862	-0.348798	H	2.051253	3.257911	1.264074
Cl	-0.122741	-0.047369	2.163848	H	0.528541	2.846867	2.069822
P	-2.866283	0.017878	0.193633	C	1.144344	3.363818	-1.712067
P	-0.369633	-2.429435	-0.177686	H	1.006173	4.447422	-1.617398
C	1.098603	0.051986	-1.930144	H	0.702396	3.023266	-2.654370
C	1.701983	-0.057743	-0.779636	H	2.213209	3.139922	-1.742062
C	-3.914945	-1.206980	-0.750342	C	3.928186	-1.398897	-0.334530
H	-4.982446	-1.055462	-0.551642	H	4.980540	-1.249360	-0.066935
H	-3.651234	-2.232429	-0.477997	H	3.600336	-2.358284	0.072116
H	-3.724382	-1.075624	-1.820442	H	3.836741	-1.430225	-1.424453
C	-1.290413	-3.270322	1.202758	P	0.323543	-2.444739	-0.313992
H	-1.038646	-4.336146	1.239851	C	0.966399	-3.334295	1.190276
H	-2.371846	-3.169857	1.073363	H	0.689529	-4.394586	1.173084
H	-1.003026	-2.789995	2.142334	H	2.055630	-3.258081	1.258641
C	-0.889841	-3.440689	-1.652464	H	0.535763	-2.844102	2.068917
H	-0.779421	-4.514524	-1.460992	C	1.142335	-3.362033	-1.714528
H	-0.263150	-3.164870	-2.507454	H	1.007784	-4.445952	-1.618210
H	-1.930717	-3.225989	-1.911275	H	0.695626	-3.023949	-2.655503
C	-3.865905	1.545089	-0.208380	H	2.210306	-3.134651	-1.749118
H	-4.928314	1.380829	0.005811	C	-1.379100	3.188807	-0.406799
H	-3.517567	2.394727	0.385221	H	-1.959617	2.864333	0.460944
H	-3.751028	1.787927	-1.269243	H	-1.327116	4.283436	-0.423443
P	-0.156223	2.462889	-0.169185	H	-1.890436	2.841165	-1.309476
C	-0.706626	3.292205	1.401612	C	3.374266	-0.006002	2.117393
H	-0.413252	4.348178	1.408195	H	2.949848	-0.886140	2.606894
H	-1.792706	3.223656	1.513517	H	4.464864	-0.002891	2.226598
H	-0.248267	2.769561	2.244905	H	2.943702	0.867511	2.613298
C	-0.945364	3.544343	-1.464960	C	-1.378508	-3.188298	-0.404036
H	-0.703767	4.601508	-1.304007	H	-1.326245	-4.282915	-0.420955

H	-1.957348	-2.864103	0.464959	H	0.151170	-4.571733	0.918197
H	-1.891816	-2.840592	-1.305560	H	1.252839	-3.408786	1.692245
H	-1.153758	0.900646	-2.574193	H	-0.503197	-3.203494	1.848069
H	1.283145	0.000828	-1.703982	2. HC≡CSiMe₃ + mer-ReH₂Cl (PMe)₃			
C	-2.941936	-0.000580	-0.103109	HC≡CSiMe₃			
C	-4.024503	-0.000298	-1.018914	scf done: -200.392629			
C	-3.237666	-0.001587	1.283252	Si	1.355638	-0.749756	-0.008101
C	-5.345899	-0.000822	-0.571445	C	2.017446	0.170112	1.494808
H	-3.804281	0.000384	-2.081766	H	3.113584	0.193353	1.490701
C	-4.561775	-0.002157	1.725257	H	1.659431	1.206247	1.511215
H	-2.410556	-0.001878	1.984337	H	1.692571	-0.315267	2.424084
C	-5.618687	-0.001761	0.803557	C	-0.526794	-0.751557	-0.005015
H	-6.162072	-0.000532	-1.287653	H	-0.921050	0.271460	0.004832
H	-4.772841	-0.002959	2.790349	H	-0.921242	-1.254985	-0.895532
H	-6.646638	-0.002223	1.153799	H	-0.915869	-1.272936	0.879009
H	-1.153581	-0.899996	-2.574410	C	2.017369	-2.511496	-0.048191
14				H	1.665617	-3.043407	-0.940035
scf done: -796.873507				H	3.113626	-2.519804	-0.062542
Re	0.363536	0.000134	-0.138468	H	1.685929	-3.073793	0.834252
Cl	2.352974	0.002075	-1.724488	C	1.932593	0.121777	-1.523647
Cl	-0.805688	-0.001005	-2.400272	C	2.315387	0.699971	-2.529521
P	2.366366	0.000715	1.314277	H	2.649253	1.204300	-3.407105
P	0.247231	2.464381	-0.369513	TS₁₉₋₂₇			
C	-0.518207	-0.000490	1.852985	scf done: -674.463872			
H	-0.444764	0.903348	2.463641	Re	-0.485269	0.025711	0.010489
C	-1.385614	-0.000746	0.701942	Cl	-1.195637	0.073350	2.458865
C	-2.838606	-0.001140	0.655531	P	-2.444246	0.025600	-1.161744
C	-3.555474	-0.001401	1.880976	P	-0.611192	-2.387836	0.389038
H	-2.995828	-0.001290	2.810470	C	3.076441	-0.092406	0.844479
C	-4.950142	-0.001795	1.902888	C	2.304622	-0.067220	1.796689
H	-5.477195	-0.001988	2.852074	C	-2.875780	-1.389619	-2.308655
C	-5.668684	-0.001941	0.699849	H	-3.816671	-1.192464	-2.835491
H	-6.754383	-0.002248	0.714061	H	-2.981560	-2.324815	-1.751013
C	-4.980226	-0.001694	-0.521058	H	-2.070102	-1.508224	-3.039510
H	-5.534146	-0.001816	-1.454733	C	-2.188999	-3.091655	1.087029
C	-3.584653	-0.001294	-0.549280	H	-2.064150	-4.147158	1.356498
H	-3.045477	-0.001128	-1.488265	H	-3.007374	-3.005255	0.363854
C	3.556137	1.419843	1.112130	H	-2.446527	-2.511597	1.976797
H	4.456943	1.248607	1.712079	C	-0.238855	-3.563541	-1.004346
H	3.096329	2.357901	1.435059	H	-0.322082	-4.605861	-0.674968
H	3.825662	1.492024	0.056800	H	0.780539	-3.375679	-1.356244
C	1.498899	3.287039	-1.458912	H	-0.922368	-3.395561	-1.842600
H	1.265739	4.351591	-1.573250	C	-2.739694	1.410826	-2.385359
H	1.480258	2.792050	-2.433204	H	-3.722372	1.313502	-2.861668
H	2.504490	3.174630	-1.047802	H	-2.689177	2.379494	-1.880462
C	-1.337108	3.073395	-1.114115	H	-1.961612	1.381183	-3.152260
H	-1.320717	4.165075	-1.208341	P	-0.317006	2.455922	0.348604
H	-2.180227	2.774697	-0.484558	C	-1.846522	3.318224	0.965845
H	-1.464771	2.610645	-2.094843	H	-1.631952	4.361719	1.222804
C	3.559196	-1.415514	1.109418	H	-2.635899	3.295441	0.208399
H	4.459631	-1.243315	1.709653	H	-2.198620	2.786291	1.854788
H	3.101478	-2.355140	1.430785	C	0.189759	3.539240	-1.073311
H	3.828835	-1.485313	0.053964	H	0.218264	4.597021	-0.775382
H	-0.443997	-0.904394	2.463438	H	1.185321	3.234711	-1.413367
P	0.250698	-2.464199	-0.369748	H	-0.506541	3.417956	-1.906302
C	1.502112	-3.284282	-1.461348	C	0.589190	-3.015682	1.665162
H	1.270386	-4.349101	-1.576112	H	0.371540	-2.521290	2.615133
H	1.481420	-2.788636	-2.435265	H	0.498624	-4.101534	1.787315
H	2.508087	-3.170646	-1.051501	H	1.612232	-2.763376	1.368874
C	-1.333866	-3.075175	-1.112254	C	-4.023417	0.131627	-0.166220
H	-1.316022	-4.166769	-1.207221	H	-4.003847	1.036665	0.450813
H	-2.176424	-2.778121	-0.481157	H	-4.910227	0.153890	-0.813820
H	-1.463722	-2.611962	-2.092476	H	-4.087065	-0.724962	0.508637
C	0.290914	3.514751	1.170707	C	0.893095	2.998317	1.650961
H	1.244804	3.409493	1.694487	H	0.894733	4.090765	1.746897
H	0.142768	4.571213	0.919172	H	0.598465	2.549070	2.605835
H	-0.511159	3.201682	1.847469	H	1.897849	2.648979	1.399108
C	2.200867	-0.001517	3.169011	H	0.556702	-0.720896	-1.047103
H	1.655702	-0.888448	3.503798	H	-0.078088	0.682124	-1.462619
H	3.195603	-0.000903	3.627728	H	1.604586	-0.043520	2.601986
H	1.653612	0.883321	3.505886				
C	0.298256	-3.515170	1.169935				

C	3.960253	-1.772802	-1.498691	H	-6.028491	-0.003407	0.001990
C	3.826385	1.304025	-1.724974	H	-5.090426	0.882854	-1.216572
C	5.990810	-0.022384	0.053209	TS₂₇₋₂₈			
H	4.165509	-2.628307	-0.845966	scf done: -674.468373			
H	2.920677	-1.843816	-1.845706	Re	0.277680	0.027817	-0.092906
H	4.618703	-1.851222	-2.376252	Cl	1.697653	0.139960	-2.212640
H	3.986105	2.262242	-1.214744	P	2.400085	0.168569	1.127403
H	4.457683	1.291543	-2.621204	P	0.541201	-2.404828	-0.336184
H	2.778888	1.254881	-2.039365	C	-2.076905	-0.242019	-0.337697
H	6.709882	-0.045637	-0.773256	C	-1.388901	-0.157852	-1.430805
H	6.142280	0.913218	0.605628	C	2.685955	-1.114614	2.456328
H	6.222633	-0.854641	0.730766	H	3.599252	-0.900270	3.023894
Si	4.225150	-0.145073	-0.596820	H	2.773185	-2.112304	2.018718
27				H	1.828848	-1.110296	3.137571
scf done: -674.490563				C	2.208352	-3.081408	-0.813124
Re	0.221310	0.000039	-0.041730	H	2.135350	-4.144117	-1.070662
Cl	1.713800	0.000551	-2.145687	H	2.930957	-2.968304	-0.000087
P	2.204148	0.001269	1.343043	H	2.561975	-2.513080	-1.678234
P	0.321223	-2.434036	-0.518620	C	0.069143	-3.525583	1.076877
C	-2.061511	-0.000981	-0.430985	H	0.226878	-4.580582	0.821221
C	-1.398083	-0.001525	-1.523126	H	-0.988004	-3.369850	1.315561
C	2.383841	-1.397175	2.571997	H	0.656448	-3.280549	1.966121
H	3.267402	-1.259109	3.206261	C	2.683251	1.673728	2.199369
H	2.469533	-2.356112	2.053820	H	3.621048	1.581397	2.759509
H	1.489861	-1.426693	3.203684	H	2.729781	2.578046	1.587368
C	1.986639	-3.197000	-0.839768	H	1.853492	1.772033	2.906326
H	1.875799	-4.231439	-1.184362	P	-0.026912	2.433114	-0.341044
H	2.595804	-3.194012	0.068485	C	1.400347	3.415002	-1.022548
H	2.491358	-2.602178	-1.605022	H	1.101858	4.449477	-1.227745
C	-0.380338	-3.604322	0.742066	H	2.236372	3.423361	-0.317168
H	-0.299623	-4.644451	0.406101	H	1.736884	2.930258	-1.942915
H	-1.432228	-3.360206	0.914333	C	-0.498105	3.456006	1.144768
H	0.154212	-3.489972	1.689981	H	-0.609657	4.515165	0.883698
C	2.385996	1.403122	2.567856	H	-1.444534	3.083636	1.548782
H	3.269184	1.265274	3.202680	C	0.264168	3.358182	1.922811
H	2.473611	2.360377	2.046910	C	-0.472590	-3.155978	-1.705389
H	1.491979	1.436146	3.199308	H	-0.174495	-2.686539	-2.648139
P	0.318206	2.434197	-0.519087	H	-0.311234	-4.238101	-1.767980
C	1.982170	3.199052	-0.843257	H	-1.534019	-2.954382	-1.539772
H	1.869592	4.234121	-1.185395	C	4.016124	0.112562	0.213002
H	2.593833	3.194580	0.063306	H	4.045664	0.926690	-0.515102
H	2.485465	2.606249	-1.610989	H	4.857152	0.201089	0.910067
C	-0.382232	3.603838	0.742851	H	4.097586	-0.821699	-0.346543
H	-0.303587	4.643998	0.406490	C	-1.348145	2.973816	-1.539814
H	-1.433443	3.358391	0.917394	H	-1.408595	4.067090	-1.583293
H	0.154509	3.490450	1.689646	H	-1.100273	2.585581	-2.532860
C	-0.578207	-2.971848	-2.053169	H	-2.318913	2.568017	-1.244481
H	-0.150346	-2.438995	-2.907521	H	-0.985960	-0.717161	0.785424
H	-0.476434	-4.052127	-2.205213	H	0.007086	0.455388	1.500964
H	-1.636670	-2.711333	-1.974106	H	-1.511991	-0.137003	-2.500645
C	3.886778	-0.001223	0.554671	Si	-3.707456	-0.270425	0.536144
H	3.989040	0.874817	-0.090657	C	-3.882634	1.240200	1.650330
H	4.676816	0.003473	1.314302	H	-3.067056	1.276412	2.382692
H	3.990867	-0.884154	-0.080944	H	-3.859427	2.169843	1.069011
C	-0.584783	2.970843	-2.051935	H	-4.831459	1.211383	2.201597
H	-0.485277	4.051323	-2.203977	C	-3.837301	-1.820668	1.602347
H	-0.157530	2.438964	-2.907211	H	-4.789975	-1.845308	2.145985
H	-1.642592	2.708273	-1.971050	H	-3.775558	-2.730129	0.992159
H	-0.373555	-0.829468	1.272676	H	-3.027878	-1.852268	2.342604
H	-0.374104	0.828852	1.272920	C	-5.051826	-0.271894	-0.786900
H	-1.418262	-0.001951	-2.599851	H	-4.952285	-1.142215	-1.446448
Si	-3.593030	-0.001443	0.583319	H	-6.049912	-0.304871	-0.330528
C	-3.656394	-1.531780	1.684445	H	-4.993988	0.629474	-1.408764
H	-2.770973	-1.581338	2.328790	28			
H	-4.546324	-1.512044	2.326994	scf done: -674.505204			
H	-3.697567	-2.450413	1.086014	Re	0.584349	0.000057	-0.164462
C	-3.658485	1.529923	1.682897	Cl	1.798958	-0.000069	-2.336045
H	-3.699486	2.447932	1.083457	P	2.415924	-0.000400	1.321226
H	-4.549187	1.510325	2.324353	P	0.426185	-2.403051	-0.366958
H	-2.773901	1.580673	2.328298	C	-2.477359	0.000045	0.893571
C	-5.091019	-0.002922	-0.569461	C	-1.412056	0.000193	0.052089
H	-5.089155	-0.889203	-1.215889	C	2.574834	-1.415423	2.514967

H	3.437681	-1.270414	3.174917	C	-1.117296	-3.337889	-1.468754
H	2.699991	-2.356073	1.972441	H	-0.824186	-2.905612	-2.429257
H	1.664120	-1.477698	3.117965	H	-0.879608	-4.407631	-1.449466
C	1.929120	-3.392432	-0.849194	H	-2.196750	-3.207024	-1.367449
H	1.666454	-4.435976	-1.057477	C	-0.747679	-3.394503	1.397861
H	2.683109	-3.372969	-0.055073	H	-1.796261	-3.198538	1.639278
H	2.359232	-2.936493	-1.746253	H	-0.616068	-4.472630	1.248136
C	-0.283517	-3.396187	1.034863	H	-0.138032	-3.072776	2.248601
H	-0.452029	-4.439563	0.744252	C	1.478897	-3.171378	-0.319241
H	-1.234833	-2.940525	1.327156	H	2.120008	-2.858167	0.509651
H	0.389102	-3.370155	1.897264	H	1.416324	-4.265176	-0.335227
C	2.575581	1.414615	2.514876	H	1.933103	-2.816034	-1.246818
H	3.438540	1.269363	3.174629	Cl	-1.600629	0.017157	-2.255441
H	2.700896	2.355194	1.972255	P	-2.840118	-0.063499	0.728210
H	1.665037	1.477216	3.118100	C	-3.116014	-0.120142	2.567166
P	0.426771	2.403212	-0.366792	H	-4.182627	-0.141794	2.817613
C	1.930087	3.392243	-0.848542	H	-2.629292	-1.009830	2.978524
H	1.667831	4.435967	-1.056444	H	-2.651852	0.756647	3.029059
H	2.683982	3.372163	-0.054344	C	-3.899451	-1.479709	0.146264
H	2.360138	2.936493	-1.745724	H	-4.934091	-1.355983	0.485779
C	-0.282860	3.396183	1.035179	H	-3.872473	-1.491853	-0.947097
H	-0.450968	4.439713	0.744889	H	-3.519278	-2.433653	0.520144
H	-1.234385	2.940738	1.327134	C	-3.971692	1.325158	0.220201
H	0.389573	3.369639	1.897710	H	-3.955770	1.390592	-0.871454
C	-0.726253	-2.877464	-1.750803	H	-4.996606	1.134561	0.558419
H	-0.374455	-2.412722	-2.677389	H	-3.635528	2.277533	0.637860
H	-0.765000	-3.964797	-1.882644	H	1.062398	0.485649	0.784123
H	-1.732366	-2.507476	-1.529385	H	-0.329196	-0.317860	1.600465
C	4.084776	-0.000805	0.501880	Si	4.251474	0.056836	0.251086
H	4.175406	0.881094	-0.137602	C	5.284723	1.588565	-0.148263
H	4.888504	-0.001183	1.247186	H	4.715000	2.508592	0.031258
H	4.174854	-0.882532	-0.137911	H	6.192886	1.626207	0.467824
C	-0.725330	2.878312	-1.750678	H	5.595015	1.589896	-1.200987
H	-0.763928	3.965709	-1.882032	C	3.704162	0.116430	2.055544
H	-0.373405	2.413964	-2.677414	C	3.116873	1.016747	2.274820
H	-1.731533	2.508344	-1.529641	H	3.086624	-0.751508	2.316765
H	0.212289	0.000292	1.469783	H	4.578740	0.119750	2.718696
H	-2.270556	-0.000177	1.963926	C	5.336113	-1.466721	-0.025853
H	-1.632980	0.000469	-1.050160	H	5.649964	-1.542395	-1.074817
Si	-4.361226	0.000151	0.430271	H	6.243025	-1.421071	0.591463
C	-5.207542	1.584085	1.164097	H	4.799447	-2.388936	0.228224
H	-5.032357	2.415712	0.514015	29			
H	-6.260610	1.416864	1.253450	scf done:	-674.522502		
H	-4.796441	1.793291	2.129565	Re	-0.380539	0.011989	-0.001525
C	-4.552378	0.000394	-1.500289	P	-0.254294	2.423081	-0.518475
H	-4.083007	0.872603	-1.905063	P	-0.374111	-2.388385	-0.560981
H	-4.088143	-0.874692	-1.904775	C	1.426686	-0.028515	-0.500643
H	-5.591414	0.003407	-1.755820	H	3.067409	-0.066504	-1.788731
C	-5.207622	-1.583923	1.163705	C	2.743065	-0.062435	-0.740766
H	-4.861208	-1.742906	2.163515	C	-1.803609	3.416765	-0.765805
H	-6.269194	-1.450092	1.171093	H	-1.570381	4.390873	-1.210761
H	-4.959292	-2.432459	0.561028	H	-2.465479	2.860407	-1.435296
TS₂₈₋₂₉				H	-2.310054	3.580068	0.189313
scf done:	-674.488490			C	0.710483	3.474284	0.664406
Re	-0.366515	-0.002238	-0.039163	H	1.704377	3.034470	0.789923
P	-0.388646	2.444960	-0.090746	H	0.811553	4.501501	0.296461
P	-0.217297	-2.435514	-0.113391	H	0.214264	3.485711	1.639856
C	1.476276	-0.007417	-0.567843	C	0.624658	2.733220	-2.118898
H	2.984834	-0.068471	-1.956850	H	0.083527	2.213877	-2.914185
C	2.772690	-0.010754	-0.883571	H	0.675435	3.805423	-2.339573
C	-1.372613	3.335473	-1.393261	H	1.634574	2.320028	-2.053239
H	-1.177320	4.413087	-1.353730	C	0.428852	-2.729922	-2.193706
H	-1.091330	2.937769	-2.371786	H	1.463784	-2.379864	-2.156146
H	-2.441615	3.157520	-1.262087	H	0.409164	-3.800507	-2.426616
C	-0.880726	3.358704	1.459855	H	-0.103695	-2.169717	-2.966346
H	-0.239089	3.022262	2.280849	C	-1.981787	-3.299500	-0.750695
H	-0.769310	4.442470	1.334680	H	-2.587167	-2.769576	-1.491749
H	-1.918022	3.140850	1.729865	H	-1.812085	-4.328582	-1.087393
C	1.274298	3.236120	-0.370486	H	-2.523290	-3.323562	0.199883
H	1.692794	2.890202	-1.319093	C	0.585971	-3.488046	0.579539
H	1.180547	4.327617	-0.387136	H	0.116293	-3.500401	1.567919
H	1.966188	2.948685	0.426891	H	0.647669	-4.511579	0.193259

H	1.594316	-3.076504	0.684206	H	-2.488758	3.324898	1.319426
Cl	-1.730699	0.081116	-2.159649	H	-0.857556	3.292671	2.030662
P	-2.616848	0.006273	1.263231	C	0.604153	-3.463849	0.550098
C	-2.706115	-1.263738	2.624691	H	-0.058420	-3.510614	1.418791
H	-3.658489	-1.210552	3.164847	H	0.756804	-4.479776	0.168002
H	-2.586733	-2.269401	2.211177	H	1.567778	-3.058437	0.874072
H	-1.883240	-1.086555	3.324805	Si	3.946208	0.228451	0.552171
C	-4.209941	-0.297100	0.352766	C	4.332693	-1.603878	0.336943
H	-5.074369	-0.214889	1.021590	H	4.342358	-2.126268	1.302370
H	-4.298437	0.426310	-0.462355	H	3.602569	-2.100669	-0.311365
H	-4.193579	-1.293967	-0.096513	H	5.321961	-1.734911	-0.119957
C	-3.071442	1.517144	2.259594	C	3.899668	1.109943	-1.103246
H	-3.326497	2.343187	1.589868	H	3.048291	0.772238	-1.706845
H	-3.929545	1.318949	2.912616	H	3.801863	2.194775	-0.971654
H	-2.215410	1.816010	2.873065	H	4.822172	0.927305	-1.669145
H	0.044884	0.811093	1.396684	C	5.252312	0.992716	1.681885
H	0.025152	-0.845221	1.364452	H	5.270747	0.506031	2.665457
Si	4.096010	-0.068260	0.540561	H	6.252869	0.891225	1.242498
C	5.062834	1.559576	0.477211	H	5.067497	2.062927	1.839777
H	4.415266	2.410788	0.723925	TS₁₉₋₂₅			
H	5.899273	1.554138	1.188962	scf done: -674.459146			
H	5.476038	1.735660	-0.524358	Re	-0.657226	0.026287	-0.347941
C	3.394135	-0.295857	2.275446	Cl	0.442663	0.161807	1.938174
H	4.192197	-0.251250	3.027773	P	-2.866731	-0.152850	0.184601
H	2.657760	0.482213	2.507732	P	-0.327630	-2.403117	-0.147684
H	2.886839	-1.263067	2.374045	C	1.918237	0.157076	-1.931676
C	5.314376	-1.467245	0.164017	C	2.809517	0.090358	-1.091283
H	5.721829	-1.374450	-0.851169	C	-3.344560	-1.258862	1.619719
H	6.159502	-1.456681	0.865044	H	-4.416098	-1.185116	1.840008
H	4.825307	-2.446714	0.238025	H	-2.768161	-0.947697	2.496963
17				H	-3.105489	-2.304092	1.460663
scf done: -688.963420				C	-0.094967	-3.166001	1.531905
Re	-0.475591	0.016756	-0.182218	H	0.142513	-4.231884	1.439495
Cl	-2.906236	-0.202742	-1.095440	H	-1.001458	-3.047269	2.130766
Cl	0.261880	0.477674	-2.559490	H	0.711735	-2.642984	2.049711
P	-0.835221	2.482139	-0.301549	C	-1.601592	-3.545673	-0.887556
P	-0.106813	-2.358622	-0.770687	H	-1.274643	-4.588189	-0.800126
P	-1.722433	-0.463906	1.834726	H	-1.731918	-3.297576	-1.945473
C	1.049119	0.197101	0.681179	H	-2.566747	-3.439729	-0.386200
C	2.268607	0.430631	1.472457	C	-4.041992	-0.759701	-1.139767
H	2.297126	-0.228351	2.355812	H	-5.066912	-0.860707	-0.761911
H	2.253759	1.461551	1.865037	H	-4.029435	-0.040299	-1.965556
C	0.739568	3.369924	-0.713402	H	-3.703351	-1.722448	-1.530105
H	0.547441	4.429261	-0.918078	P	-0.490994	2.495972	-0.165184
H	1.177529	2.892659	-1.592681	C	-1.438802	3.523256	-1.393609
H	1.442352	3.289428	0.122245	H	-1.281807	4.593432	-1.216656
C	-1.970211	3.034183	-1.651251	H	-1.100116	3.270160	-2.403178
H	-1.994307	4.128225	-1.712034	H	-2.507980	3.303511	-1.332167
H	-2.972121	2.639772	-1.467344	C	1.215186	3.190045	-0.420920
H	-1.610066	2.608998	-2.590867	H	1.197455	4.282720	-0.332673
C	-1.554876	-3.339235	-1.384510	H	1.880815	2.774272	0.338071
H	-1.229876	-4.332949	-1.712909	H	1.600688	2.909213	-1.403856
H	-2.010069	-2.797627	-2.217320	C	1.171766	-3.072946	-1.026363
H	-2.312438	-3.441067	-0.604646	H	2.074848	-2.619479	-0.615983
C	1.109172	-2.654449	-2.139731	H	1.225098	-4.162105	-0.913124
H	1.268379	-3.729428	-2.281309	H	1.118365	-2.820467	-2.089506
H	2.059344	-2.166141	-1.910230	C	-3.847260	1.347863	0.733092
H	0.725909	-2.204012	-3.057225	H	-3.777807	2.148829	-0.008349
C	-0.725730	-0.626671	3.396312	H	-4.903490	1.086604	0.867589
H	-1.368543	-0.856287	4.253347	H	-3.451067	1.708733	1.686701
H	-0.192122	0.309168	3.589788	C	-0.916855	3.328863	1.442577
H	0.014732	-1.424208	3.280513	H	-0.606405	4.379722	1.423059
C	-3.042178	0.726274	2.382084	H	-1.992094	3.280562	1.626605
H	-3.646189	0.287711	3.184263	H	-0.398980	2.801007	2.247287
H	-3.681270	0.942183	1.521646	H	-0.891215	-0.801195	-1.781538
H	-2.593606	1.652742	2.746238	H	-1.213828	0.754488	-1.740482
C	-2.726818	-2.030444	1.886899	H	1.173183	0.211775	-2.692357
H	-3.280419	-2.099525	2.830013	C	4.003683	-1.508582	1.215214
H	-3.428056	-2.005697	1.048885	H	4.809848	-1.544852	1.959350
H	-2.086300	-2.910698	1.791132	H	3.049200	-1.429447	1.748067
C	-1.431534	3.521814	1.126772	H	4.021998	-2.452050	0.657466
H	-1.311539	4.585545	0.891091	C	4.288119	1.542907	1.144753

H	5.153525	1.510971	1.819302	Cl	0.146608	-0.060909	2.122130
H	4.371057	2.447769	0.532153	P	-2.675306	0.231128	0.413501
H	3.381940	1.613433	1.757173	P	-0.581835	-2.397443	-0.405106
C	5.785474	-0.184046	-0.947187	C	1.401609	-0.101319	-1.845832
H	6.673440	-0.250190	-0.305257	C	1.874260	-0.216214	-0.650593
H	5.749167	-1.087052	-1.568076	C	-3.968840	-0.775429	-0.482688
H	5.912638	0.677781	-1.612896	H	-4.976727	-0.482522	-0.166457
Si	4.225196	-0.014988	0.096921	H	-3.836585	-1.839866	-0.271369
25							
scf done: -674.480981							
Re	0.416617	0.002495	-0.384531	C	-1.280263	-3.267217	1.086061
Cl	0.068586	-0.020787	2.155870	H	-1.095826	-4.346003	1.032543
P	2.812472	-0.022416	-0.042062	H	-2.359560	-3.101724	1.159644
P	0.233175	2.445816	0.000992	H	-0.803164	-2.850627	1.978075
C	-1.255987	0.018736	-1.763984	C	-1.580132	-3.154802	-1.789924
C	-1.944557	0.012108	-0.679987	H	-1.624687	-4.245861	-1.688657
C	3.806758	1.419872	-0.699066	H	-1.095046	-2.906450	-2.740461
H	4.881465	1.245136	-0.571825	H	-2.595885	-2.756895	-1.817655
H	3.540755	2.345808	-0.183439	C	-3.557247	1.876854	0.318083
H	3.589023	1.542503	-1.765158	H	-4.563796	1.788933	0.742914
C	1.168783	3.171552	1.435483	H	-3.006414	2.637399	0.878372
H	0.959791	4.243507	1.526688	H	-3.641887	2.194166	-0.725191
H	2.246152	3.028715	1.318011	P	0.096568	2.456091	-0.376663
H	0.850619	2.651482	2.342345	C	0.073142	3.353962	1.253246
C	0.731105	3.566622	-1.396041	H	0.396433	4.394863	1.139228
H	0.587624	4.620704	-1.132674	H	-0.936599	3.337148	1.675075
H	0.120216	3.327600	-2.272615	H	0.728146	2.829536	1.953388
H	1.780032	3.400740	-1.656695	C	-0.986371	3.565293	-1.418126
C	3.766533	-1.359232	-0.934981	H	-0.620208	4.598318	-1.391806
H	4.844057	-1.263083	-0.758099	H	-0.966227	3.203961	-2.451739
H	3.444431	-2.351928	-0.611511	H	-2.019812	3.550941	-1.070532
H	3.570371	-1.269360	-2.008618	C	0.973175	-3.393835	-0.645343
P	0.185674	-2.436911	-0.008724	H	1.605535	-3.300378	0.238367
C	1.284004	-3.222060	1.270424	H	0.728862	-4.450020	-0.804980
H	0.995012	-4.265817	1.437669	H	1.528853	-3.014118	-1.506753
H	2.333236	-3.193838	0.965647	C	-3.082045	-0.191897	2.178865
H	1.169949	-2.654154	2.197826	H	-2.560607	0.499286	2.844058
C	0.432155	-3.546954	-1.477742	H	-4.164392	-0.123031	2.337526
H	0.267371	-4.599026	-1.219174	H	-2.735213	-1.196801	2.424398
H	-0.274870	-3.252282	-2.260159	C	1.731110	3.036001	-1.065893
H	1.445268	-3.425729	-1.872707	H	1.801011	4.126698	-0.986970
C	-1.458374	3.102107	0.374547	H	2.562876	2.581780	-0.528507
H	-1.862901	2.559035	1.232490	H	1.807667	2.748049	-2.118710
H	-1.417404	4.173281	0.602378	H	-0.054059	-0.540044	-1.959702
H	-2.111749	2.936727	-0.483495	H	-1.311886	0.590840	-1.636556
C	3.504052	-0.161120	1.678230	H	1.628117	0.055381	-2.887172
H	3.220463	-1.120780	2.117093	C	3.629679	1.117087	1.542470
H	4.596459	-0.074408	1.665591	H	4.488850	0.922341	2.198516
H	3.073701	0.621355	2.307501	H	3.808217	2.079036	1.049975
C	-1.459663	-3.025161	0.604391	H	2.733113	1.194819	2.166194
H	-1.434530	-4.101337	0.809807	C	3.511212	-1.891508	1.393719
H	-1.702526	-2.478637	1.518565	H	2.604929	-1.970363	2.004158
H	-2.222892	-2.817148	-0.146516	H	3.623913	-2.800811	0.793377
H	0.960786	0.823306	-1.723983	H	4.373225	-1.833647	2.071460
H	0.937133	-0.826438	-1.726036	C	4.897187	-0.331897	-0.866449
H	-1.296273	0.027318	-2.841281	H	4.838405	-1.185886	-1.552863
Si	-3.668061	0.013343	-0.002134	H	4.913930	0.584182	-1.470234
C	-3.725536	-0.103208	1.876189	H	5.851988	-0.397689	-0.328205
H	-4.741972	0.096759	2.240221	Si	3.443049	-0.327285	0.344423
H	-3.432298	-1.098795	2.226602	26			
H	-3.039291	0.612345	2.340969	scf done: -674.499664			
C	-4.654079	-1.423624	-0.749570	Re	-0.197086	0.000013	-0.378721
H	-5.712980	-1.332086	-0.471740	Cl	0.108925	0.000042	2.223609
H	-4.591935	-1.412518	-1.844893	P	-2.608286	0.000124	0.612686
H	-4.306239	-2.402040	-0.400199	P	-0.316918	-2.426723	-0.585175
C	-4.594448	1.579458	-0.536189	C	1.378045	-0.000109	-1.865570
H	-5.668700	1.450201	-0.346641	C	1.732199	-0.000126	-0.460925
H	-4.266859	2.468327	0.013051	C	-4.033630	0.000236	-0.589263
H	-4.464150	1.772072	-1.608375	H	-4.999294	0.000372	-0.070565
TS₂₅₋₂₆							
scf done: -674.461952							
Re	-0.350563	0.047507	-0.379220	H	-3.970472	-0.882599	-1.232488
				H	-3.970238	0.883005	-1.232550
				C	-0.158407	-3.474423	0.945676
				H	-0.242184	-4.541050	0.705783

H	-0.918979	-3.201540	1.679119	H	3.809595	-1.338323	-0.082104
H	0.816939	-3.275838	1.398583	H	-0.476238	-0.917354	2.472379
C	-1.824115	-3.155154	-1.406823	P	0.253451	-2.466234	-0.398303
H	-1.719906	-4.241039	-1.514419	C	1.539054	-3.224949	-1.495026
H	-1.932666	-2.701346	-2.396789	H	1.351986	-4.298526	-1.609040
H	-2.730902	-2.948195	-0.833048	H	1.491876	-2.730351	-2.468381
C	-3.081918	1.402712	1.741030	H	2.541297	-3.070205	-1.091671
H	-4.082591	1.236188	2.155325	C	-1.290564	-3.158862	-1.155027
H	-2.347908	1.434791	2.550276	H	-1.194179	-4.241642	-1.293213
H	-3.076789	2.360043	1.215038	H	-2.146133	-2.951910	-0.506769
P	-0.316563	2.426754	-0.585183	H	-1.461563	-2.664402	-2.113159
C	-0.157909	3.474484	0.945635	C	0.077651	3.507602	1.169171
H	-0.241201	4.541125	0.705626	H	0.981594	3.365105	1.767693
H	-0.918722	3.201953	1.678967	H	-0.018805	4.571318	0.923429
H	0.817280	3.275539	1.398722	H	-0.784752	3.208838	1.774123
C	-1.823704	3.155314	-1.406817	C	2.179840	-0.041906	3.113397
H	-1.719377	4.241182	-1.514502	H	1.674070	-0.959539	3.427087
H	-1.932340	2.701440	-2.396740	H	3.184256	-0.021744	3.550074
H	-2.730477	2.948520	-0.832961	H	1.608523	0.809121	3.494270
C	0.987160	-3.243899	-1.637858	C	0.350912	-3.514607	1.139950
H	1.984420	-2.962419	-1.288454	H	0.276937	-4.578330	0.886472
H	0.878817	-4.332273	-1.575388	H	1.288983	-3.344904	1.675895
H	0.883926	-2.937926	-2.682556	H	-0.478165	-3.255561	1.806700
C	-3.082143	-1.402413	1.741003	Si	-3.329920	-0.064651	0.733011
H	-2.348158	-1.434641	2.550265	C	-3.826898	-1.578506	1.757765
H	-4.082784	-1.235718	2.155304	H	-4.909967	-1.569624	1.937519
H	-3.077187	-2.359740	1.214998	H	-3.585733	-2.518986	1.247425
C	0.987581	3.243788	-1.637895	H	-3.322329	-1.579605	2.731404
H	0.879293	4.332171	-1.575484	C	-3.879951	1.471415	1.695841
H	1.984813	2.962273	-1.288434	H	-3.680611	2.397017	1.142471
H	0.884375	2.937771	-2.682583	H	-4.960339	1.427159	1.886096
H	1.540896	-0.894657	-2.464897	H	-3.368844	1.534881	2.664083
H	-1.071927	0.000131	-1.814895	C	-4.212524	-0.115450	-0.922353
H	1.541072	0.894392	-2.464918	H	-3.934518	-1.004969	-1.495632
Si	3.314706	-0.000184	0.537137	H	-5.299737	-0.125744	-0.764234
C	4.773424	-0.000265	-0.669141	H	-3.955927	0.750516	-1.539705
H	4.751748	0.885081	-1.317458	3. HC≡C(O,O'-C₆H₄Br₂) + mer-ReH₂Cl(PMe)₃			
H	5.730850	-0.000254	-0.131491	HC≡C(O,O'-C₆H₄Br₂)			
H	4.751716	-0.885683	-1.317360	scf done: -333.453480			
C	3.417148	1.542082	1.618235	C	-0.062905	0.263768	0.000095
H	2.572545	1.554389	2.314950	C	1.333141	0.267600	0.000769
H	4.351564	1.546756	2.194949	C	2.078793	1.475504	0.000270
H	3.393798	2.460456	1.017441	C	1.333249	2.683527	-0.000832
C	3.416865	-1.542457	1.618244	C	-0.062766	2.687484	-0.001461
H	4.351153	-1.547232	2.195164	C	-0.758365	1.475647	-0.001043
H	2.572095	-1.554686	2.314761	H	-0.596777	-0.677868	0.000431
H	3.393549	-2.460833	1.017448	H	-0.596591	3.629146	-0.002337
18				H	-1.842864	1.475728	-0.001557
scf done: -688.920657				C	3.502426	1.475454	0.000877
Re	0.262003	0.005705	-0.145376	C	4.716404	1.475389	0.001397
Cl	2.175871	0.074505	-1.823270	H	5.780810	1.475340	0.001853
Cl	-1.065230	-0.031082	-2.305127	Br	2.241060	4.378533	-0.001582
P	2.299320	0.030913	1.256810	Br	2.240731	-1.427535	0.002165
P	0.125277	2.478531	-0.384855	TS₁₉₋₃₀			
C	-0.576919	-0.015176	1.863870	scf done: -807.526858			
H	-0.513864	0.888933	2.475172	Re	1.841892	0.018874	0.054466
C	-1.459042	-0.032859	0.715530	Cl	1.310566	-0.044793	-2.408660
C	3.438472	1.493138	1.072625	P	4.091746	0.014742	0.382508
H	4.348477	1.343439	1.664247	P	1.699083	-2.412004	-0.241444
H	2.950301	2.411184	1.410828	C	-3.147899	-0.062088	-0.952262
H	3.700230	1.589446	0.016937	C	-2.445280	-0.094725	-1.942648
C	1.418966	3.330550	-1.401174	C	4.912825	-1.349146	1.366596
H	1.174488	4.393198	-1.509135	H	5.987481	-1.164046	1.481310
H	1.452140	2.851359	-2.382795	H	4.778121	-2.311815	0.864469
H	2.406038	3.228410	-0.947207	H	4.447929	-1.403567	2.356289
C	-1.412270	3.093089	-1.218191	C	2.787510	-3.216672	-1.517772
H	-1.380103	4.183907	-1.317286	H	2.505488	-4.264720	-1.671518
H	-2.290974	2.807673	-0.634359	H	3.836501	-3.174663	-1.207159
H	-1.491690	2.621911	-2.199655	H	2.676734	-2.664183	-2.455073
C	3.545757	-1.326587	0.977314	C	1.916184	-3.531871	1.225968
H	4.443583	-1.143163	1.578066				
H	3.132222	-2.298974	1.258827				

H	1.771884	-4.580579	0.941643	H	-0.394982	1.412210	4.386048
H	1.176713	-3.259441	1.985269	H	0.659532	1.593487	2.953527
H	2.911041	-3.410844	1.661290	H	-0.934815	2.361286	2.971286
C	4.872094	1.471984	1.258313	C	0.138034	-2.852913	-2.218138
H	5.959533	1.355425	1.336627	H	-0.306558	-3.544674	-1.496970
H	4.656997	2.393479	0.708458	H	0.128024	-3.303012	-3.217077
H	4.444881	1.558326	2.262497	H	1.169766	-2.651245	-1.920174
P	1.541732	2.428516	-0.320327	C	-4.727936	-0.003154	-0.150839
C	2.597347	3.222214	-1.630165	H	-4.793560	-0.385762	0.870796
H	2.288538	4.258540	-1.809945	H	-5.587851	0.643089	-0.360222
H	3.649153	3.212358	-1.326885	H	-4.742206	-0.866060	-0.820854
H	2.492810	2.641000	-2.550268	C	-0.171757	-1.388660	3.395032
C	1.731888	3.604720	1.104254	H	-0.290561	-1.287680	4.479487
H	1.530611	4.636043	0.792411	H	-0.572935	-2.352469	3.068793
H	1.025675	3.320502	1.890503	H	0.890221	-1.345581	3.140863
H	2.742890	3.543413	1.515759	H	-0.598558	0.948522	-1.107572
C	0.021085	-2.957747	-0.826730	H	-0.668371	1.355726	0.517976
H	-0.184692	-2.485550	-1.790263	C	2.531729	0.462422	-0.039362
H	-0.021172	-4.048217	-0.931796	C	3.768518	-0.261782	0.066288
H	-0.741199	-2.630460	-0.113748	C	2.714996	1.852777	-0.318781
C	5.152671	-0.023482	-1.159717	C	5.026524	0.319680	-0.086305
H	4.917759	0.843011	-1.785914	C	3.973738	2.444098	-0.472381
H	6.221138	-0.010810	-0.911248	C	5.135504	1.683860	-0.358438
H	4.927495	-0.923105	-1.740149	H	5.912418	-0.295953	0.007509
C	-0.156746	2.881940	-0.922030	H	4.033840	3.504844	-0.680946
H	-0.229573	3.961191	-1.100070	H	6.109191	2.145531	-0.478752
H	-0.356939	2.340093	-1.849577	H	0.965352	-2.376374	0.736041
H	-0.903793	2.584076	-0.181259	Br	1.259269	3.117491	-0.508554
H	1.505896	-0.715421	1.506049	Br	3.817347	-2.163154	0.433746
H	1.960416	0.804837	1.514407	TS₃₀₋₃₁			
C	-3.927557	-0.022357	0.237865	scf done: -807.527779			
C	-5.345263	-0.019322	0.213890	Re	0.989302	-0.250689	0.078990
C	-3.310170	0.016632	1.516568	Cl	2.291521	-2.192620	1.076806
C	-6.102291	0.019907	1.386243	P	3.171004	0.540365	-0.774350
C	-4.060324	0.056255	2.692900	P	1.409740	0.848476	2.255118
C	-5.456737	0.057658	2.625315	C	-1.284838	-0.064050	0.386634
H	-7.183327	0.020735	1.327483	C	-0.716190	-1.082716	0.981097
H	-3.555670	0.085413	3.650763	C	3.654469	2.304469	-0.391150
H	-6.042373	0.088189	3.537860	H	4.566021	2.587008	-0.930803
H	-1.774094	-0.119889	-2.770520	H	3.829897	2.437358	0.679516
Br	-6.278645	-0.070401	-1.468120	H	2.838230	2.967790	-0.695037
Br	-1.380465	0.015383	1.649663	C	3.078118	0.609731	3.040828
30				H	3.068862	0.950715	4.082133
scf done: -807.548339				H	3.848534	1.165411	2.498488
Re	-0.979926	-0.188189	0.030007	H	3.319225	-0.456052	2.997583
Cl	-2.299503	-2.327921	0.518002	C	1.163503	2.685583	2.420591
P	-3.135973	0.926618	-0.367524	H	1.361783	3.022675	3.444844
P	-0.844983	-1.279265	-2.198999	H	0.131265	2.933122	2.152829
C	1.263055	-0.213974	0.127807	H	1.825247	3.219774	1.733117
C	0.754710	-1.365138	0.436525	C	3.357173	0.649019	-2.630523
C	-3.390148	1.706989	-2.045765	H	4.329510	1.076994	-2.900566
H	-4.324452	2.279640	-2.077343	H	3.272951	-0.340760	-3.085880
H	-3.420243	0.944251	-2.828265	H	2.562168	1.285041	-3.032522
H	-2.550162	2.378545	-2.250860	P	0.531786	-1.770317	-1.788318
C	-2.419123	-1.868462	-2.990717	C	1.902587	-2.902373	-2.337124
H	-2.204672	-2.487228	-3.869174	H	1.548228	-3.601589	-3.102982
H	-3.040429	-1.024383	-3.300744	H	2.742986	-2.330866	-2.740758
H	-2.965021	-2.457284	-2.248422	H	2.255977	-3.453868	-1.461629
C	-0.038231	-0.311719	-3.560700	C	-0.040605	-1.032282	-3.396944
H	0.050792	-0.904242	-4.478153	H	-0.263495	-1.807127	-4.139684
H	0.958118	-0.002838	-3.229531	H	-0.942594	-0.440817	-3.208952
H	-0.620745	0.591343	-3.767344	H	0.725449	-0.361133	-3.795924
C	-3.456826	2.459454	0.650561	C	0.322414	0.232893	3.632153
H	-4.412348	2.924590	0.381674	H	0.501693	-0.838740	3.763121
H	-3.466852	2.217876	1.716083	H	0.538896	0.756883	4.569793
H	-2.646236	3.173107	0.470102	H	-0.728875	0.377224	3.368865
P	-1.090604	-0.042077	2.507253	C	4.727709	-0.368351	-0.326784
C	-2.747493	-0.190339	3.337275	H	4.627417	-1.416501	-0.618329
H	-2.627736	-0.279787	4.422950	H	5.595344	0.080087	-0.823535
H	-3.376110	0.679040	3.125727	H	4.872974	-0.349288	0.755905
H	-3.237800	-1.086674	2.946972	C	-0.802076	-3.033376	-1.498279
C	-0.374663	1.477870	3.292492	H	-0.920540	-3.677312	-2.377032

H	-0.526627	-3.647110	-0.635132	H	-0.585898	-1.352081	0.190137
H	-1.753528	-2.542529	-1.281121	Br	-2.611751	-2.829471	0.220322
H	-0.161244	1.005601	0.294696	Br	-3.583855	3.008761	-0.290001
H	0.809223	0.828805	-1.170484	TS₃₁₋₃₂			
C	-2.558499	0.479540	-0.030466	scf done: -807.556213			
C	-3.775595	-0.248517	0.185855	Re	1.273107	0.093783	0.149380
C	-2.751938	1.741800	-0.673299	P	0.924021	2.187329	-1.158768
C	-5.027106	0.205385	-0.230129	P	1.409392	-1.582309	1.921105
C	-4.002407	2.199018	-1.097770	C	-0.593606	0.010074	0.447930
C	-5.146073	1.430488	-0.887399	H	-2.166269	0.568985	1.587400
H	-5.902039	-0.402577	-0.036980	C	-1.929077	0.031793	0.669346
H	-4.073405	3.164035	-1.583596	C	-3.109386	-0.346801	-0.100613
H	-6.115581	1.785034	-1.218517	C	-3.194235	-1.360200	-1.098012
H	-0.963003	-1.942195	1.577934	C	-4.365258	-1.644776	-1.805616
Br	-1.315138	3.005305	-0.980119	H	-4.355171	-2.429931	-2.551591
Br	-3.806756	-1.950283	1.106411	C	-5.538653	-0.939301	-1.537988
31				H	-6.449575	-1.161772	-2.082273
scf done: -807.588680				C	-5.527245	0.050095	-0.551805
Re	1.457097	-0.147393	0.027870	H	-6.426537	0.607613	-0.321376
Cl	3.006336	-2.075245	0.311609	C	-4.347782	0.330761	0.135475
P	3.000609	1.622340	-0.209932	C	1.785152	3.718388	-0.559679
P	1.349693	-0.049639	2.446806	H	1.529490	4.574601	-1.193955
C	-1.688567	0.466316	-0.087844	H	1.478943	3.914280	0.470971
C	-0.531018	-0.250491	0.024866	H	2.867295	3.572339	-0.553885
C	2.937627	3.004094	1.030147	C	1.299207	2.222981	-2.983992
H	3.678505	3.774435	0.787973	H	0.764771	1.402150	-3.472522
H	3.140770	2.622841	2.033872	H	0.977998	3.173877	-3.425165
H	1.937673	3.447861	1.020167	H	2.369812	2.099096	-3.168425
C	2.925601	-0.084222	3.438222	C	-0.834406	2.786387	-1.202727
H	2.714431	-0.201051	4.507286	H	-1.204147	2.930666	-0.184374
H	3.503629	0.834489	3.294571	H	-0.899105	3.731999	-1.752381
H	3.525232	-0.930521	3.089149	H	-1.475499	2.044658	-1.687529
C	0.379856	1.310283	3.260916	C	3.023009	-1.982560	2.751667
H	0.268638	1.136165	4.337369	H	3.516982	-1.045425	3.022036
H	-0.609313	1.353562	2.794064	H	2.844741	-2.575198	3.656174
H	0.873268	2.274186	3.104364	H	3.672761	-2.550261	2.081693
C	2.945226	2.625999	-1.772263	C	0.745105	-3.274096	1.554675
H	3.675695	3.442002	-1.731926	H	1.364015	-3.753858	0.789250
H	3.166616	1.999218	-2.639821	H	0.734564	-3.900056	2.454190
H	1.941318	3.044574	-1.890026	H	-0.271000	-3.181627	1.161099
P	1.400333	-0.720943	-2.326699	C	0.402331	-1.076475	3.393133
C	3.004600	-0.993392	-3.231440	H	-0.642921	-0.965303	3.093450
H	2.828994	-1.372390	-4.244620	H	0.475673	-1.816978	4.197618
H	3.577383	-0.062989	-3.298708	H	0.771385	-0.109527	3.747212
H	3.593004	-1.722073	-2.665419	Cl	2.581163	1.457520	1.810389
C	0.439546	0.351848	-3.500494	P	3.606950	-0.143069	-0.933401
H	0.358403	-0.108494	-4.491891	C	3.578737	-0.850305	-2.654175
H	-0.561758	0.502602	-3.084921	H	4.588391	-0.937193	-3.071894
H	0.918453	1.330587	-3.599026	H	3.116547	-1.842009	-2.619080
C	0.509092	-1.558532	3.137166	H	2.969507	-0.222203	-3.309268
H	1.056549	-2.446309	2.805401	C	4.840026	-1.293810	-0.142544
H	0.486463	-1.533401	4.232705	H	5.765807	-1.336432	-0.728110
H	-0.515932	-1.618145	2.758481	H	5.069240	-0.941351	0.866495
C	4.789979	1.120328	-0.133564	H	4.415585	-2.300168	-0.076550
H	4.994325	0.381175	-0.912608	H	4.699833	1.350968	-1.142017
H	5.447135	1.987519	-0.266098	H	4.810998	1.835622	-0.167603
H	4.995278	0.648621	0.831347	H	5.686295	1.066015	-1.524797
C	0.592564	-2.374070	-2.598672	H	4.249897	2.066672	-1.835736
H	0.592332	-2.645969	-3.660437	H	-0.091727	-0.223703	-0.891402
H	1.144570	-3.128950	-2.030023	H	1.371190	-1.291469	-0.742652
H	-0.439121	-2.347889	-2.235104	Br	-1.688064	-2.499344	-1.518674
H	0.824251	1.386156	-0.188367	Br	-4.469098	1.752381	1.455258
H	-1.540845	1.529717	-0.237820	32			
C	-3.100401	0.097678	-0.033221	scf done: -807.589056			
C	-3.675812	-1.203684	0.093655	Re	-1.301207	-0.068887	-0.012243
C	-4.090787	1.134815	-0.117845	P	-1.047604	-0.975744	-2.299870
C	-5.051513	-1.445297	0.132737	P	-1.161992	-0.114596	2.456357
C	-5.464861	0.911521	-0.081652	C	0.549471	-0.194128	0.049064
C	-5.957404	-0.389212	0.045144	H	2.088324	-1.491933	0.294845
H	-5.406280	-2.464105	0.229930	C	1.882294	-0.437682	0.102254
H	-6.144426	1.751835	-0.151190	C	3.094415	0.355352	-0.034459
H	-7.025019	-0.574918	0.074603	C	3.177704	1.758920	-0.271613

C	4.385670	2.449445	-0.391999	H	-1.973550	1.847287	3.504471
H	4.367401	3.517249	-0.573144	C	0.758299	-0.834753	3.125516
C	5.600278	1.772007	-0.278973	H	1.162049	-0.507153	4.090385
H	6.539467	2.305827	-0.371084	H	1.580740	-1.099275	2.455305
C	5.587538	0.394830	-0.044881	H	0.132500	-1.719410	3.254402
H	6.515657	-0.155472	0.047896	C	-0.448978	3.159018	-1.360539
C	4.373891	-0.279783	0.070957	H	-0.779028	4.178914	-1.588409
C	-2.518556	-1.586259	-3.253505	H	-0.214767	2.644829	-2.298210
H	-2.196192	-2.106550	-4.162586	H	0.463096	3.200698	-0.759322
H	-3.081736	-2.280169	-2.622563	C	-3.234720	2.538207	-1.549454
H	-3.162934	-0.750163	-3.536574	H	-3.460939	3.609732	-1.588090
C	-0.212283	0.145442	-3.512885	H	-4.093485	1.998501	-1.141911
H	0.721128	0.505946	-3.071056	H	-3.027118	2.186921	-2.562505
H	0.003486	-0.375291	-4.452362	C	-2.176628	3.426948	0.915827
H	-0.849445	1.011706	-3.716214	H	-2.412642	4.411261	0.495925
C	0.040068	-2.473305	-2.329296	H	-3.041422	3.040425	1.460232
H	-0.394233	-3.232370	-1.674034	H	-1.337763	3.532475	1.607439
H	0.132199	-2.865878	-3.348082	C	-2.839910	-0.453104	-3.314089
H	1.029491	-2.206598	-1.949828	H	-3.128085	-1.216854	-4.045585
C	-0.120925	-1.512576	3.076506	H	-3.675227	0.239729	-3.187958
H	0.886628	-1.416120	2.663808	H	-1.975818	0.098924	-3.698552
H	-0.070876	-1.503956	4.171054	C	0.988521	1.904310	2.423188
H	-0.553867	-2.454000	2.729303	H	0.552018	2.849239	2.090608
C	-2.694363	-0.322272	3.484029	H	1.370678	2.032305	3.442670
H	-3.207800	-1.232376	3.160378	H	1.823542	1.660835	1.759269
H	-2.438051	-0.410209	4.545925	C	2.848426	-0.273597	-0.623266
H	-3.364196	0.532998	3.354519	C	3.740881	0.804113	-0.435424
C	-0.348801	1.358137	3.227238	C	3.238779	-1.504020	-0.044933
H	-0.968183	2.247390	3.074582	C	4.927386	0.684858	0.297159
H	-0.186126	1.208014	4.300224	C	4.420431	-1.644570	0.691301
H	0.611215	1.524176	2.730053	C	5.262176	-0.544648	0.866158
Cl	-2.218337	-2.399398	0.369867	H	5.578391	1.542214	0.411683
P	-3.793656	0.687540	-0.132715	H	4.675586	-2.607539	1.115397
C	-4.110482	2.270451	0.796781	H	6.179303	-0.646970	1.435819
H	-5.156013	2.587667	0.710399	Br	3.404393	2.546517	-1.219013
H	-3.863776	2.141620	1.854858	Br	2.148296	-3.075044	-0.256734
H	-3.461138	3.053564	0.392219	TS₁₉₋₃₄			
C	-5.140933	-0.419231	0.510245	scf done: -807.518309			
H	-6.130949	0.013683	0.327592	Re	1.403882	-0.146559	-0.194937
H	-5.062912	-1.394333	0.021830	Cl	1.139936	1.156352	1.968443
H	-5.010599	-0.578403	1.583985	P	3.559737	-0.934334	-0.084228
C	-4.509746	1.168302	-1.786629	P	2.054218	2.120280	-0.930052
H	-4.662945	0.275460	-2.398694	C	-0.752467	0.334780	-1.572228
H	-5.472387	1.678446	-1.665386	C	-1.836728	0.322616	-0.963857
H	-3.814630	1.834960	-2.306917	C	4.751259	-0.447955	-1.442598
H	-1.216667	1.205336	-1.076397	H	5.720091	-0.946226	-1.306743
H	-1.221018	1.491590	0.548339	H	4.912295	0.633845	-1.446129
Br	4.520394	-2.192872	0.397982	H	4.329244	-0.740152	-2.408230
Br	1.587929	2.839460	-0.449124	C	3.444948	2.958829	-0.021361
33				H	3.533688	4.006034	-0.333363
scf done: -822.027672				H	4.394973	2.452226	-0.211602
Re	-1.259598	-0.062415	0.178046	H	3.225895	2.912255	1.048021
Cl	-3.631329	0.316737	1.188156	C	2.551869	2.379288	-2.702998
Cl	-1.429600	-2.375546	1.155328	H	2.800249	3.430356	-2.892238
P	-2.418457	-1.254851	-1.684356	H	1.725261	2.086551	-3.357465
P	-0.252902	0.517697	2.363084	H	3.417275	1.757497	-2.947125
P	-1.769874	2.226589	-0.446911	C	3.854162	-2.779558	-0.169586
C	0.298256	-0.113308	-0.636417	H	4.925607	-3.011952	-0.156241
C	1.561505	-0.147451	-1.430872	H	3.377267	-3.285910	0.675259
H	1.625045	0.749758	-2.056905	H	3.413059	-3.166156	-1.095164
H	1.503680	-1.006408	-2.115557	P	0.529391	-1.906154	1.303276
C	-1.417592	-2.698133	-2.278206	C	1.500639	-2.254683	2.854607
H	-1.982386	-3.286549	-3.010161	H	0.954724	-2.949208	3.502207
H	-1.167153	-3.316406	-1.413484	H	2.478407	-2.687457	2.622320
H	-0.489796	-2.347323	-2.740824	H	1.650140	-1.304386	3.375243
C	-4.025385	-2.046536	-1.231897	C	0.252939	-3.610103	0.618960
H	-4.412704	-2.637814	-2.069440	H	-0.112967	-4.292682	1.393076
H	-4.744248	-1.276264	-0.943600	H	-0.487957	-3.544722	-0.185970
H	-3.854195	-2.686364	-0.363039	H	1.181696	-4.004315	0.195872
C	-1.416365	0.937801	3.739716	C	0.721949	3.399553	-0.744116
H	-0.866798	1.072241	4.678189	H	0.424783	3.421358	0.305117
H	-2.140001	0.125064	3.840396	H	1.079375	4.388366	-1.057687

H	-0.151651	3.116410	-1.337139	C	3.692774	-0.549304	0.490156
C	4.592483	-0.502396	1.415253	C	4.261452	1.618957	-1.139385
H	4.112947	-0.885680	2.317573	C	5.013646	-0.281958	0.126450
H	5.603429	-0.920252	1.335291	C	5.305357	0.809064	-0.693625
H	4.653068	0.585404	1.510931	H	4.461197	2.474031	-1.773225
C	-1.129967	-1.559041	2.056800	H	5.806114	-0.926192	0.486534
H	-1.377989	-2.308693	2.817170	H	6.329314	1.022695	-0.979619
H	-1.102571	-0.565354	2.511049	H	0.782771	-1.284134	2.302481
H	-1.895800	-1.573460	1.279455	Br	1.613846	2.535892	-1.478295
H	1.760875	-0.225340	-1.815935	Br	3.483206	-2.103576	1.633361
H	1.023225	-1.477645	-1.118347	TS₃₄₋₃₅			
C	-3.102543	0.214747	-0.336875	scf done: -807.518852			
C	-3.681763	1.257119	0.448693	Re	-1.074461	-0.255521	0.243934
C	-3.917497	-0.951278	-0.495055	Cl	-1.457348	0.977552	-1.907966
C	-4.925612	1.128232	1.062443	P	-3.516303	-0.598047	0.093228
C	-5.165720	-1.083626	0.112401	P	-1.309757	1.866405	1.522342
C	-5.666118	-0.047894	0.905078	C	0.697334	-0.796625	1.424414
H	-5.315262	1.944916	1.656081	C	1.200526	-0.013064	0.493585
H	-5.739209	-1.990200	-0.037233	C	-4.701927	0.275329	1.247518
H	-6.635014	-0.151416	1.387540	H	-5.731012	-0.045892	1.048919
H	-0.290103	0.483724	-2.550261	H	-4.640971	1.358765	1.107450
Br	-2.762319	2.926709	0.667270	H	-4.451787	0.035758	2.284732
Br	-3.324240	-2.405826	-1.606848	C	-2.064297	3.312634	0.634882
34				H	-1.964396	4.229679	1.226131
scf done: -807.541497				H	-3.125068	3.124567	0.441408
Re	-1.120212	-0.277495	0.258802	H	-1.566781	3.429830	-0.330619
Cl	-1.506036	1.209943	-1.756661	C	-2.243084	1.892522	3.138656
P	-3.541015	-0.641593	0.078397	H	-2.140682	2.873132	3.617978
P	-1.238652	1.829176	1.609569	H	-1.827863	1.127654	3.803431
C	0.605474	-0.752543	1.382716	H	-3.303056	1.684300	2.992593
C	1.210708	-0.081028	0.450455	C	-4.076533	-2.341178	0.454588
C	-4.685169	0.256298	1.250138	H	-5.158888	-2.445372	0.318224
H	-5.728875	-0.019592	1.060373	H	-3.564182	-3.049131	-0.202018
H	-4.578071	1.337642	1.124478	H	-3.818342	-2.591125	1.488763
H	-4.433971	-0.006619	2.281912	P	-0.467121	-2.060535	-1.308707
C	-2.077196	3.302076	0.856495	C	-1.673909	-2.570951	-2.628081
H	-1.994056	4.174204	1.514576	H	-1.223228	-3.316210	-3.293131
H	-3.133793	3.083934	0.676381	H	-2.582682	-2.995011	-2.191486
H	-1.613757	3.512481	-0.109823	H	-1.937142	-1.679944	-3.204767
C	-2.053783	1.728409	3.279464	C	-0.015331	-3.696628	-0.553356
H	-1.975738	2.687199	3.804391	H	0.298435	-4.418567	-1.315914
H	-1.553078	0.955587	3.871700	H	0.804397	-3.544555	0.155377
H	-3.108098	1.461928	3.184990	H	-0.873669	-4.099382	-0.005853
C	-4.075284	-2.383098	0.468596	C	0.281814	2.609201	2.140269
H	-5.165336	-2.487708	0.424743	H	0.925274	2.867096	1.297618
H	-3.620638	-3.084177	-0.236859	H	0.073791	3.509368	2.729379
H	-3.727142	-2.642194	1.473669	H	0.808812	1.881875	2.764606
P	-0.442313	-1.853443	-1.526895	C	-4.403814	-0.267404	-1.508933
C	-1.713189	-2.478427	-2.730667	H	-3.977593	-0.873223	-2.310535
H	-1.248208	-3.156806	-3.455078	H	-5.469496	-0.499698	-1.400678
H	-2.514672	-3.012763	-2.212647	H	-4.273133	0.780162	-1.787389
H	-2.137425	-1.622495	-3.262826	C	1.010990	-1.708913	-2.373507
C	0.327534	-3.433229	-0.936807	H	1.165011	-2.508893	-3.106732
H	0.717348	-4.018978	-1.776591	H	0.840123	-0.760015	-2.889677
H	1.144167	-3.195384	-0.249411	H	1.905965	-1.612350	-1.755479
H	-0.416126	-4.027231	-0.395897	H	-0.547929	-0.439083	1.887658
C	0.386234	2.566077	2.129401	H	-1.597517	-1.605003	1.041171
H	0.958969	2.863294	1.248684	C	2.556046	0.305793	0.060668
H	0.212006	3.442008	2.764678	C	2.869419	1.414777	-0.785911
H	0.967868	1.823405	2.681400	C	3.710143	-0.456576	0.440069
C	-4.436687	-0.314069	-1.515305	C	4.167219	1.728263	-1.200392
H	-4.050196	-0.955459	-2.309128	C	5.010623	-0.156006	0.029632
H	-5.509148	-0.501024	-1.389240	C	5.245276	0.943877	-0.795185
H	-4.264139	0.722099	-1.813549	H	4.323638	2.588874	-1.838493
C	0.830942	-1.214749	-2.709576	H	5.830641	-0.783318	0.355724
H	0.987008	-1.930117	-3.525257	H	6.252787	1.183754	-1.116605
H	0.485726	-0.258253	-3.108344	H	1.016352	-1.519386	2.157100
H	1.774853	-1.051746	-2.185811	Br	1.506204	2.600746	-1.440825
H	-1.680580	-0.623118	1.783863	Br	3.604208	-2.038191	1.562397
H	-1.276781	-1.857467	0.727233	35			
C	2.573313	0.238359	0.061881	scf done: -807.545719			
C	2.942854	1.335981	-0.773557	Re	-0.887196	-0.185614	0.266005

C1	-1.070578	0.735950	-2.134197	H	-4.084724	2.042371	-0.283472
P	-3.489491	-0.596287	-0.169309	H	-3.700501	2.199534	-2.022041
P	-1.388574	1.906786	1.442778	C	-1.451979	3.627006	0.665438
C	0.604291	-0.571361	1.759598	H	-1.771875	4.595381	0.264411
C	1.041445	0.030904	0.503039	H	-0.413706	3.670936	0.993472
C	-4.779305	0.431994	0.709005	H	-2.060432	3.360347	1.533419
H	-5.776651	0.126037	0.373646	C	-3.939749	-1.937478	-0.471561
H	-4.652837	1.496109	0.495354	H	-4.515340	-2.500944	-1.214675
H	-4.714216	0.273221	1.788118	H	-3.682858	-2.596706	0.362035
C	-2.170721	3.295407	0.484003	H	-4.537953	-1.119422	-0.067909
H	-2.252154	4.207102	1.086778	H	0.232660	-1.221511	-2.239671
H	-3.165128	3.005886	0.133373	P	-0.432689	-1.882107	1.729511
H	-1.554989	3.483576	-0.399661	C	-1.396309	-1.780473	3.306851
C	-2.439468	1.829564	2.982553	H	-1.056485	-2.565190	3.992392
H	-2.487575	2.809682	3.471235	H	-1.232113	-0.794825	3.746309
H	-1.984670	1.106387	3.667420	H	-2.464557	-1.889156	3.112339
H	-3.453892	1.498638	2.760940	C	1.298146	-1.990305	2.383205
C	-4.086600	-2.261923	0.423509	H	1.326189	-2.688352	3.227395
H	-5.153588	-2.397887	0.212754	H	1.979923	-2.341797	1.607630
H	-3.527703	-3.075994	-0.042852	H	1.602951	-0.995257	2.711981
H	-3.920330	-2.318677	1.503866	C	-0.894336	3.044063	-2.129582
P	-0.437248	-2.306714	-0.927059	H	-1.169328	2.459170	-3.013324
C	-1.575719	-2.910880	-2.273004	H	-1.250544	4.070897	-2.268527
H	-1.137495	-3.787627	-2.762811	H	0.193920	3.052098	-2.037183
H	-2.562426	-3.185343	-1.894165	C	-1.701712	-2.807492	-2.035148
H	-1.680992	-2.102245	-3.001885	H	-0.905432	-3.231116	-1.422789
C	-0.214169	-3.847828	0.091149	H	-2.498723	-3.548664	-2.157055
H	0.068403	-4.703885	-0.532565	H	-1.290245	-2.580835	-3.022557
H	0.567206	-3.676181	0.837410	C	-0.726031	-3.667285	1.270366
H	-1.144759	-4.076378	0.620678	H	-0.529953	-4.303737	2.140908
C	0.069699	2.793837	2.187838	H	-1.760231	-3.825179	0.950739
H	0.755538	3.104336	1.398342	H	-0.052846	-3.966785	0.462571
H	-0.275146	3.675853	2.739588	C	2.342262	0.112792	-0.361214
H	0.601229	2.133541	2.878306	C	3.150166	-1.045829	-0.528011
C	-4.179646	-0.492945	-1.891698	C	3.065343	1.284082	-0.015834
H	-3.697763	-1.218688	-2.546926	C	4.520435	-1.074957	-0.262295
H	-5.261271	-0.669656	-1.882827	C	4.438418	1.275002	0.252072
H	-3.959035	0.498721	-2.294134	C	5.166052	0.090264	0.152444
C	1.123528	-2.264473	-1.930011	H	5.071917	-1.998091	-0.389275
H	1.222366	-3.172527	-2.535579	H	4.030127	2.200855	0.522706
H	1.077212	-1.386960	-2.581462	H	6.228563	0.080059	0.368376
H	1.993020	-2.175622	-1.276732	Br	2.251577	3.027305	-0.032964
H	0.626756	0.039660	2.666028	Br	2.402196	-2.718252	-1.170676
H	-1.610194	-0.970246	1.544264	4. 1,2-hydrogen shift			
C	2.390714	0.359882	0.020646	TS _{20-21'}			
C	2.707386	1.518180	-0.756253	scf done: -782.376088			
C	3.531862	-0.451906	0.324178	Re	-0.611709	0.000103	-0.171596
C	4.004622	1.817481	-1.190115	Cl	-1.109060	0.000281	2.363442
C	4.825227	-0.169995	-0.119795	P	-2.923865	-0.000923	-0.884482
C	5.066729	0.972812	-0.880745	P	-0.555205	-2.413661	0.319150
H	4.170785	2.717644	-1.768030	C	2.691018	0.000799	-0.123231
H	5.634075	-0.842786	0.135199	C	1.409918	0.000634	-0.035205
H	6.069946	1.202702	-1.222432	C	-3.458811	-1.406141	-1.996071
H	0.832155	-1.606947	1.994675	H	-4.492906	-1.276580	-2.336962
Br	1.410749	2.848077	-1.250679	H	-3.380087	-2.362399	-1.470715
Br	3.426511	-2.108959	1.333693	H	-2.793569	-1.436139	-2.865101
36				C	-2.019406	-3.182062	1.169912
scf done: -821.976022				H	-1.811260	-4.221747	1.447955
Re	-0.885200	0.054168	0.155228	H	-2.899506	-3.159479	0.520450
Cl	-2.978515	0.391410	1.563606	H	-2.228086	-2.592934	2.066993
Cl	0.172191	1.183157	2.150867	C	-0.265334	-3.582933	-1.094034
P	-2.395644	-1.251635	-1.253514	H	-0.207638	-4.621442	-0.748371
P	-1.673279	2.305015	-0.609157	H	0.671506	-3.311095	-1.590286
C	0.138871	-0.238218	-1.786733	H	-1.074326	-3.489074	-1.824361
H	0.023757	0.552568	-2.531135	C	-3.460006	1.403670	-1.996308
C	0.889194	0.054063	-0.587963	H	-4.494082	1.273324	-2.336963
C	-3.142483	-0.498019	-2.786171	H	-3.381806	2.360123	-1.471227
H	-3.591465	-1.283041	-3.405593	H	-2.794961	1.433886	-2.865484
H	-2.371604	0.015395	-3.368144	P	-0.556808	2.413984	0.318409
H	-3.922018	0.215455	-2.513059	C	-2.021517	3.181665	1.168939
C	-3.471087	2.566408	-1.019077				
H	-3.698647	3.637659	-0.984349				

H	-1.814324	4.221801	1.446005	H	-4.610727	0.214538	1.793044
H	-2.901788	3.157608	0.519771	H	-4.053399	1.018481	0.293182
H	-2.229366	2.593116	2.066592	C	0.060151	-2.959661	-2.202269
C	-0.267770	3.582980	-1.095175	H	-0.101575	-4.033228	-2.349942
H	-0.210669	4.621636	-0.749857	H	-0.484936	-2.396399	-2.965144
H	0.669186	3.311539	-1.591424	H	1.125775	-2.735925	-2.294141
H	-1.076776	3.488384	-1.825394	H	0.372195	0.798218	1.212085
C	0.797932	-2.916848	1.488321	H	0.317591	-0.886190	1.185704
H	0.663015	-2.361779	2.421117	C	3.137777	-0.098676	0.046655
H	0.767605	-3.993308	1.691043	C	4.308368	-0.119852	-0.751021
H	1.769629	-2.656655	1.058445	C	3.292713	-0.085966	1.449135
C	-4.320260	-0.001421	0.354879	C	5.574821	-0.127483	-0.167071
H	-4.237463	0.880072	0.996875	H	4.205332	-0.129151	-1.831830
H	-5.298475	-0.001999	-0.141664	C	4.564015	-0.094317	2.030983
H	-4.236574	-0.882612	0.997169	H	2.402537	-0.069555	2.067335
C	0.795991	2.918495	1.487403	C	5.710809	-0.114643	1.228845
H	0.764590	3.994914	1.690189	H	6.458364	-0.142941	-0.798607
H	0.661779	2.363233	2.420183	H	4.659251	-0.084409	3.112936
H	1.767883	2.659338	1.057342	H	6.697233	-0.120044	1.682111
H	-0.354606	-0.811472	-1.601649	H	1.159922	-0.130468	-2.753943
H	-0.355046	0.811457	-1.601850	TS_{21'-22}			
C	4.103791	0.000536	-0.247374	scf done: -782.399600			
C	4.829482	1.218929	-0.317068	Re	0.575985	0.000002	0.004440
C	4.828848	-1.218127	-0.318907	Cl	1.681089	0.000100	-2.330006
C	6.217090	1.212960	-0.453229	P	2.380932	0.000090	1.403985
H	4.285319	2.155039	-0.267604	P	0.670953	-2.425446	-0.439262
C	6.216456	-1.212669	-0.455114	C	-2.820755	-0.000137	-0.801390
H	4.284209	-2.154031	-0.270836	C	-1.702622	-0.000122	-1.294355
C	6.916678	0.000014	-0.521508	C	2.557917	-1.403945	2.632074
H	6.755996	2.153633	-0.507476	H	3.418938	-1.244673	3.291999
H	6.754870	-2.153538	-0.510819	H	2.690946	-2.357017	2.111996
H	7.996809	-0.000187	-0.626731	H	1.646190	-1.461561	3.235298
H	1.739176	0.000956	1.102290	C	2.321957	-3.173820	-0.856742
21'				H	2.212374	-4.225285	-1.146234
scf done: -782.431798				H	2.999778	-3.110982	-0.000449
Re	-0.325008	-0.003203	-0.065829	H	2.751400	-2.605287	-1.686078
Cl	-2.060415	0.076684	-1.946779	C	0.029638	-3.590525	0.858123
P	-2.157546	0.092394	1.540775	H	0.116144	-4.633373	0.531969
P	-0.293611	2.425787	-0.569878	H	-1.022172	-3.357838	1.051254
C	1.833108	-0.087195	-0.583301	H	0.583566	-3.456250	1.790978
C	1.163679	-0.099935	-1.678182	C	2.557645	1.404028	2.632222
C	-2.140245	1.509584	2.760292	H	3.418683	1.244846	3.292148
H	-2.953554	1.417790	3.489730	H	2.690512	2.357174	2.112242
H	-2.239860	2.465987	2.240923	H	1.645896	1.461420	3.235434
H	-1.181736	1.505030	3.289813	P	0.670614	2.425474	-0.439184
C	-1.903453	3.354194	-0.612494	C	2.321529	3.174076	-0.856606
H	-1.751998	4.371421	-0.990931	H	2.211803	4.225513	-1.146143
H	-2.349884	3.414277	0.383204	H	2.999313	3.111377	-0.000273
H	-2.584904	2.813023	-1.274722	H	2.751102	2.605571	-1.685901
C	0.758679	3.498599	0.519656	C	0.029119	3.590426	0.858226
H	0.775307	4.536572	0.168609	H	0.115516	4.633298	0.532120
H	1.778089	3.100262	0.526904	H	-1.022670	3.357609	1.051311
H	0.375799	3.470141	1.544557	H	0.583031	3.456174	1.791093
C	-2.247235	-1.285120	2.802367	C	-0.317164	-2.979583	-1.915462
H	-3.061752	-1.117369	3.516705	H	0.053631	-2.451707	-2.798966
H	-2.400792	-2.250064	2.312421	H	-0.219799	-4.060491	-2.067537
H	-1.296888	-1.325008	3.345061	H	-1.371322	-2.727171	-1.769430
P	-0.552546	-2.428257	-0.531950	C	4.106250	0.000297	0.677277
C	-2.254752	-3.173131	-0.572207	H	4.232877	0.882218	0.042329
H	-2.213893	-4.211680	-0.920087	H	4.876582	0.000273	1.458149
H	-2.718308	-3.152130	0.418091	H	4.233011	-0.881465	0.042136
H	-2.862356	-2.578271	-1.259916	C	-0.317545	2.979528	-1.915386
C	0.370417	-3.589465	0.584189	H	-0.220297	4.060451	-2.067436
H	0.276446	-4.629269	0.251476	H	0.053320	2.451711	-2.798896
H	1.427094	-3.303888	0.590908	H	-1.371675	2.726995	-1.769373
H	-0.011541	-3.501140	1.606022	H	-0.266066	-0.798137	1.195561
C	0.355464	2.854457	-2.255700	H	-0.266111	0.797977	1.195636
H	-0.250814	2.329239	-2.999307	C	-4.075984	-0.000141	-0.121826
H	0.298086	3.935032	-2.427820	C	-5.290367	0.000162	-0.841613
H	1.392648	2.524062	-2.350496	C	-4.112322	-0.000454	1.291066
C	-3.917026	0.153357	0.946824	C	-6.509815	0.000149	-0.161827
H	-4.138259	-0.737671	0.354075	H	-5.265814	0.000402	-1.926087

C	-5.337767	-0.000459	1.959490	C	0.094076	3.365430	-1.312028
H	-3.177522	-0.000684	1.841098	H	0.331858	4.435366	-1.290304
C	-6.538768	-0.000160	1.238320	H	0.324657	2.961942	-2.302328
H	-7.437734	0.000383	-0.724813	H	-0.971683	3.220811	-1.121533
H	-5.355990	-0.000697	3.044720	H	-0.584062	-0.355227	0.865091
H	-7.488862	-0.000167	1.762844	H	0.527915	0.504864	1.593265
H	-0.819095	-0.000137	-1.918194	H	-1.022921	0.567185	-2.721604
5. HC≡CC₅H₁₁ + mer-ReH₂Cl (PMe)₃							
HC≡CC₅H₁₁							
scf done: -273.845515							
C	-1.772536	-0.236880	-2.409569	C	-6.000587	0.353049	0.723202
C	-2.571937	-0.484494	-1.530858	H	-5.324277	0.630885	-1.321014
H	-1.067987	-0.023415	-3.177882	H	-4.762324	-0.864850	-0.581260
C	-3.556109	-0.766301	-0.482772	C	-7.340295	-0.323652	0.379445
C	-4.929393	-0.092957	-0.731105	H	-5.610972	-0.069985	1.662025
H	-3.164518	-0.433638	0.489972	H	-6.174767	1.422998	0.916244
H	-3.700648	-1.853333	-0.394966	H	-7.724805	0.095185	-0.562159
C	-5.944917	-0.402110	0.381707	H	-7.166480	-1.393289	0.191153
H	-4.784902	0.992726	-0.813373	C	-8.397503	-0.161126	1.483139
H	-5.322579	-0.430605	-1.699485	H	-8.611046	0.898635	1.671343
C	-7.316426	0.259029	0.152318	H	-9.339977	-0.648463	1.208139
H	-6.077863	-1.492154	0.463044	H	-8.054625	-0.603870	2.426779
H	-5.539788	-0.068296	1.349657	37			
H	-7.183049	1.347757	0.070507	scf done: -747.945170			
H	-7.720433	-0.074243	-0.814904	Re	0.516857	0.002820	0.017201
C	-8.328785	-0.051960	1.266212	Cl	2.039470	0.000142	-2.058981
H	-7.965039	0.300146	2.239748	P	2.487979	-0.017028	1.429463
H	-9.293646	0.431675	1.075068	P	0.571142	-2.420767	-0.492227
H	-8.506142	-1.131722	1.348203	C	-1.695053	0.014042	-0.274811
TS₁₉₋₃₇							
scf done: -747.916721							
Re	0.787924	0.028290	0.018726	C	-1.178205	0.013035	-1.438539
Cl	1.703009	0.062624	-2.346262	C	2.609627	-1.402059	2.680852
P	2.633937	-0.505315	1.282489	H	3.501764	-1.295659	3.309250
P	0.359353	-2.316809	-0.457690	H	2.644643	-2.372687	2.178849
C	-2.592327	0.771922	-1.076244	H	1.718110	-1.377925	3.316397
C	-1.770932	0.662990	-1.967052	C	2.223903	-3.244634	-0.704889
C	2.640211	-2.023573	2.373004	H	2.102559	-4.269093	-1.074743
H	3.574982	-2.089721	2.942147	H	2.770898	-3.275843	0.241149
H	2.530908	-2.932588	1.776699	H	2.796802	-2.656499	-1.426900
H	1.798166	-1.959228	3.069557	C	-0.284453	-3.565025	0.695459
C	1.751061	-3.375331	-1.106029	H	-0.241445	-4.605787	0.354776
H	1.388624	-4.365663	-1.405048	H	-1.331356	-3.259027	0.788726
H	2.536428	-3.499824	-0.354949	H	0.181334	-3.487459	1.682572
H	2.178007	-2.863715	-1.973974	C	2.695833	1.393795	2.640349
C	-0.386444	-3.409250	0.853976	H	3.557498	1.229783	3.298232
H	-0.568192	-4.420988	0.472225	H	2.834944	2.339306	2.109592
H	-1.335594	-2.967240	1.173252	H	1.789137	1.470732	3.249520
H	0.269874	-3.466661	1.725816	P	0.594742	2.429187	-0.479015
C	3.209821	0.710433	2.581472	C	2.254083	3.233263	-0.715125
H	4.107213	0.340417	3.091055	H	2.139333	4.257931	-1.086509
H	3.439540	1.679353	2.129604	H	2.812193	3.261211	0.224351
H	2.411342	0.850231	3.317217	H	2.812320	2.636454	-1.441322
P	1.106232	2.444170	-0.050762	C	-0.225283	3.579448	0.727991
C	2.800951	3.044038	-0.544642	H	-0.170882	4.621252	0.392070
H	2.822984	4.135371	-0.646829	H	-1.275425	3.289664	0.835493
H	3.548345	2.742186	0.194989	H	0.254280	3.489412	1.707394
C	3.054455	2.578681	-1.501770	C	-0.226839	-2.898691	-2.099530
C	0.766418	3.457554	1.472261	H	0.271539	-2.349486	-2.903369
H	0.940911	4.524592	1.290743	H	-0.134009	-3.976494	-2.273867
H	-0.276318	3.306176	1.769147	H	-1.282919	-2.618475	-2.086977
H	1.404094	3.123032	2.295446	C	4.180335	-0.076131	0.663832
C	-0.866309	-2.592646	-1.832949	H	4.306279	0.774781	-0.010306
H	-0.473913	-2.132570	-2.744587	H	4.960166	-0.059264	1.433830
H	-1.025167	-3.663789	-2.003919	H	4.277689	-0.982972	0.061665
H	-1.817880	-2.114441	-1.588311	C	-0.223927	2.926293	-2.070268
C	4.222369	-0.750693	0.332361	H	-0.125703	4.004841	-2.236971
H	4.458619	0.164336	-0.218514	H	0.258221	2.380639	-2.886420
H	5.054827	-0.999707	1.001256	H	-1.281666	2.653346	-2.044562
H	4.089401	-1.549545	-0.401715	H	-0.061806	-0.834609	1.333349
				H	-0.049828	0.836732	1.341351
				H	-1.277019	0.014930	-2.508684
				C	-2.882002	0.016801	0.616197

C	-4.227915	0.009624	-0.141221	H	5.528277	-0.640073	1.395971
H	-2.837713	0.894161	1.280220	H	6.825168	-0.578275	-0.760488
H	-2.834106	-0.852871	1.289858	H	6.849565	1.179593	-0.697500
C	-5.446531	0.008326	0.798181	C	8.110497	0.228459	0.788832
H	-4.271433	0.886897	-0.802513	H	8.137310	-0.679842	1.404022
H	-4.265150	-0.872679	-0.796194	H	9.012504	0.237435	0.166116
C	-6.793684	-0.001186	0.052135	H	8.162617	1.090133	1.466274
H	-5.395222	-0.868973	1.461929	38			
H	-5.403219	0.891640	1.454448	scf done: -747.975692			
H	-6.844970	0.875536	-0.610277	Re	0.829119	-0.004642	-0.176108
H	-6.836072	-0.883372	-0.603630	Cl	2.080421	-0.261380	-2.317394
C	-8.006612	-0.003807	0.996252	P	2.481608	-0.562128	1.398512
H	-8.949730	-0.010766	0.437440	P	0.007961	-2.247259	-0.503913
H	-7.996905	-0.886841	1.647799	C	-2.167280	0.849586	0.745396
H	-8.005957	0.884156	1.641119	C	-1.109854	0.575298	-0.046636
TS₃₇₋₃₈				C	2.196377	-2.028770	2.505893
scf done: -747.922755				H	3.025457	-2.149139	3.212584
Re	-0.555660	-0.002853	-0.022676	H	2.104408	-2.941243	1.910898
Cl	-1.871073	-0.165319	-2.197231	H	1.266309	-1.878688	3.062279
P	-2.704369	-0.282158	1.116361	C	1.193685	-3.606883	-0.969571
P	-0.949286	2.417499	-0.243402	H	0.660586	-4.524675	-1.243444
C	1.741721	0.360069	-0.071327	H	1.875395	-3.830502	-0.142243
C	1.219861	0.324821	-1.244554	H	1.785800	-3.257778	-1.821280
C	-3.146762	0.971942	2.430298	C	-1.026507	-3.043383	0.820943
H	-4.069787	0.691419	2.951280	H	-1.477997	-3.980850	0.475883
H	-3.280162	1.962845	1.988887	H	-1.814749	-2.337343	1.101145
H	-2.326194	1.024230	3.153405	H	-0.416987	-3.245928	1.706679
C	-2.628370	2.997141	-0.797907	C	2.926608	0.694923	2.694117
H	-2.610800	4.067464	-1.033098	H	3.685696	0.296208	3.376760
H	-3.382539	2.821141	-0.025659	H	3.315461	1.602980	2.226030
H	-2.900314	2.424482	-1.689163	H	2.027550	0.952585	3.262014
C	-0.627505	3.529400	1.218267	P	1.389207	2.340313	-0.267023
H	-0.848487	4.577818	0.983034	C	3.154607	2.850078	-0.579026
H	0.426160	3.442006	1.504324	H	3.232824	3.926550	-0.770345
H	-1.235722	3.215240	2.071268	H	3.790976	2.599411	0.276274
C	-2.904547	-1.806802	2.178714	H	3.512325	2.295515	-1.452289
H	-3.876181	-1.807603	2.686370	C	0.879375	3.472508	1.118083
H	-2.826445	-2.709721	1.567827	H	1.051936	4.524942	0.864175
H	-2.108380	-1.826168	2.929780	H	-0.185980	3.311700	1.311120
P	-0.105655	-2.376026	-0.335524	H	1.433058	3.229500	2.030038
C	-1.464217	-3.437614	-1.038121	C	-1.155860	-2.338283	-1.955643
H	-1.097618	-4.445852	-1.262975	H	-0.631994	-1.981688	-2.848240
H	-2.299626	-3.515027	-0.336007	H	-1.504763	-3.363668	-2.124009
H	-1.827970	-2.958379	-1.951029	H	-2.018751	-1.691180	-1.770485
C	0.437346	-3.395636	1.128204	C	4.145931	-0.957372	0.665276
H	0.618179	-4.440108	0.847826	H	4.509367	-0.092270	0.104204
H	1.358871	-2.968746	1.538917	H	4.867861	-1.217997	1.447844
H	-0.327617	-3.360958	1.909291	H	4.047237	-1.789322	-0.036939
C	0.092617	3.256933	-1.536399	C	0.562703	3.167730	-1.716585
H	-0.125036	2.795690	-2.504571	H	0.844632	4.224305	-1.790602
H	-0.126170	4.329719	-1.583716	H	0.860754	2.645340	-2.631046
H	1.152819	3.108844	-1.315496	H	-0.523435	3.093538	-1.605778
C	-4.283550	-0.352969	0.138332	H	0.360614	0.026924	1.436592
H	-4.216293	-1.159125	-0.596286	H	-2.050753	0.750430	1.826618
H	-5.140956	-0.518535	0.800608	H	-1.278717	0.691235	-1.152430
H	-4.421912	0.577121	-0.417575	C	-3.539644	1.277535	0.269615
C	1.247925	-2.792477	-1.546915	C	-4.656602	0.261283	0.607294
H	1.387795	-3.876913	-1.617877	H	-3.520519	1.440603	-0.818638
H	0.970966	-2.397593	-2.529432	H	-3.812941	2.246195	0.721901
H	2.187302	-2.324875	-1.240690	C	-6.060815	0.733312	0.190059
H	0.590767	0.821350	0.933558	H	-4.426754	-0.695456	0.115170
H	-0.340713	-0.486404	1.560993	H	-4.645644	0.061142	1.689830
H	1.458724	0.333227	-2.294780	C	-7.173500	-0.278366	0.521444
C	2.974738	0.300141	0.767832	H	-6.283849	1.691511	0.684939
C	4.264763	0.319315	-0.084287	H	-6.069475	0.938265	-0.891916
H	2.954521	-0.612984	1.383129	H	-6.950279	-1.234980	0.026049
H	2.998404	1.135833	1.483404	H	-7.164039	-0.483598	1.602266
C	5.544223	0.265144	0.769285	C	-8.572276	0.202220	0.102436
H	4.247555	-0.530805	-0.779855	H	-9.342504	-0.536851	0.352665
H	4.270766	1.227110	-0.703753	H	-8.833208	1.141482	0.606426
C	6.836009	0.277021	-0.068997	H	-8.619355	0.382007	-0.979116
H	5.556241	1.119464	1.463693	TS₃₈₋₃₉			

scf done: -747.945934				H	0.791877	-4.434390	-1.459864
Re	0.672565	0.091444	-0.069223	H	2.084516	-3.200319	-1.415775
P	0.107780	-2.238209	-0.662415	H	1.490414	-3.933170	0.097655
P	1.085772	2.488820	-0.087543	C	-1.437436	-3.013798	0.145855
C	-1.068306	0.661769	-0.648127	H	-2.277416	-2.313228	0.174074
H	-2.532462	1.409535	-1.904476	H	-1.754284	-3.943855	-0.339319
C	-2.316466	1.088206	-0.881043	H	-1.131905	-3.226696	1.175005
C	1.163896	-3.106959	-1.920009	C	-0.695221	-2.161445	-2.502795
H	0.743895	-4.090751	-2.160119	H	0.090258	-1.777110	-3.158544
H	1.210356	-2.492327	-2.822602	H	-1.007692	-3.157473	-2.836479
H	2.185451	-3.224973	-1.553665	H	-1.545794	-1.475746	-2.533116
C	-0.038585	-3.535009	0.670262	C	0.852608	2.996998	-1.996425
H	-0.746912	-3.185898	1.428563	H	-0.225267	2.885886	-2.140296
H	-0.394119	-4.485616	0.253575	H	1.136976	4.048599	-2.115813
H	0.927341	-3.705271	1.154629	H	1.370647	2.383041	-2.737427
C	-1.558285	-2.443956	-1.463887	C	3.070216	2.889759	-0.188510
H	-1.598647	-1.839608	-2.374153	H	3.655414	2.236564	-0.842284
H	-1.737346	-3.495714	-1.713755	H	3.199383	3.931143	-0.505264
H	-2.345950	-2.089518	-0.794551	H	3.435356	2.787758	0.787907
C	2.770035	3.225996	0.197854	C	0.434850	3.604571	0.786226
H	3.491404	2.727161	-0.455604	H	0.725857	3.439674	1.828204
H	2.757368	4.297913	-0.030657	H	0.675905	4.634349	0.499708
H	3.079356	3.091697	1.237441	H	-0.644217	3.444673	0.701745
C	0.042599	3.507423	1.061265	Cl	2.236828	-0.252787	-1.950552
H	0.284485	3.254077	2.098613	P	2.607099	-0.634168	1.519995
H	0.200644	4.580673	0.903868	C	2.833047	0.474199	3.002224
H	-1.009301	3.264361	0.882751	H	3.647205	0.123799	3.647232
C	0.688105	3.236986	-1.736975	H	3.050886	1.496088	2.678477
H	-0.364476	3.053258	-1.966985	H	1.900368	0.491544	3.575344
H	0.883584	4.315467	-1.744311	C	4.332450	-0.700830	0.831552
H	1.303252	2.742532	-2.494087	H	5.049173	-1.047716	1.584620
Cl	2.423109	0.063381	-1.879974	H	4.346290	-1.368502	-0.033837
P	2.664915	-0.760576	1.304188	H	4.626247	0.292639	0.481958
C	2.223614	-1.367485	3.007527	C	2.527462	-2.272548	2.411113
H	3.104802	-1.733721	3.546934	H	2.635923	-3.092021	1.695613
H	1.771689	-0.544886	3.570895	H	3.321842	-2.355104	3.162231
H	1.483564	-2.169389	2.935522	H	1.554903	-2.367104	2.904857
C	4.054129	0.405342	1.734888	H	-0.141144	-0.751819	1.260303
H	4.827896	-0.109393	2.316652	H	0.291346	0.847953	1.412686
H	4.495483	0.795403	0.813896	C	-3.397813	1.236309	-0.041885
H	3.667404	1.242971	2.322233	C	-4.611633	0.301444	-0.247675
C	3.683300	-2.177300	0.650170	H	-3.744548	2.278115	-0.148524
H	4.019461	-1.918731	-0.358091	H	-3.031816	1.132403	0.988378
H	4.551343	-2.366717	1.291677	C	-5.794169	0.627303	0.682142
H	3.082857	-3.089754	0.595079	H	-4.942696	0.363563	-1.295807
H	-0.880075	-0.258906	0.589362	H	-4.291255	-0.738773	-0.087503
H	0.452140	0.469993	1.529129	C	-7.002961	-0.307764	0.492817
C	-3.473015	1.154742	0.098999	H	-5.458382	0.575889	1.729710
C	-4.691780	0.299093	-0.318195	H	-6.112583	1.667966	0.513392
H	-3.810082	2.198873	0.210682	H	-7.335542	-0.259661	-0.554756
H	-3.128111	0.833988	1.091981	H	-6.685740	-1.346854	0.666081
C	-5.872756	0.405498	0.664988	C	-8.180525	0.030750	1.421141
H	-5.022574	0.605710	-1.322066	H	-8.539670	1.052680	1.244989
H	-4.380021	-0.751888	-0.405694	H	-9.024183	-0.651866	1.264890
C	-7.088368	-0.448378	0.259661	H	-7.883867	-0.039335	2.475425
H	-5.537299	0.102906	1.669371	40			
H	-6.182382	1.458831	0.750004	scf done: -762.426368			
H	-7.426656	-0.142327	-0.741365	Re	-0.768822	0.024973	-0.189928
H	-6.776648	-1.499600	0.169559	Cl	-3.243753	-0.039734	-1.002757
C	-8.258218	-0.343756	1.251343	Cl	-0.147471	0.378511	-2.608566
H	-9.107109	-0.961992	0.936635	P	-0.913025	2.507157	-0.335940
H	-7.956127	-0.674546	2.253169	P	-0.536844	-2.375092	-0.728915
H	-8.611505	0.691695	1.336391	P	-1.984376	-0.334225	1.872267
39				C	0.802067	0.066080	0.594507
scf done: -747.976714				C	2.115727	0.109615	1.274371
Re	0.642757	0.021601	0.011338	H	2.187705	-0.713752	2.003926
P	-0.040627	-2.213209	-0.771074	H	2.189358	1.038564	1.863533
P	1.288279	2.376728	-0.307291	C	0.714072	3.224262	-0.862361
C	-1.026197	0.571757	-0.662802	H	0.620450	4.295165	-1.075490
H	-2.474499	1.127308	-2.068789	H	1.044413	2.692317	-1.757507
C	-2.253642	0.973134	-1.008210	H	1.454874	3.079652	-0.068872
C	1.201899	-3.587145	-0.898517	C	-2.080020	3.150099	-1.615429

H	-2.024469	4.242774	-1.678536	C	-1.992739	3.118001	1.526854
H	-3.096273	2.832685	-1.370123	H	-1.760990	4.178028	1.681839
H	-1.811585	2.700032	-2.573989	H	-3.066627	3.012406	1.337957
C	-2.022651	-3.267933	-1.379104	H	-1.735573	2.547618	2.423081
H	-1.758165	-4.287012	-1.682950	C	-1.499859	3.559247	-1.287082
H	-2.414042	-2.711064	-2.234233	H	-1.405521	4.609769	-0.989429
H	-2.808712	-3.302664	-0.621270	H	-0.848374	3.366152	-2.144368
C	0.723141	-2.745824	-2.037443	H	-2.530903	3.363123	-1.593678
H	0.793018	-3.826433	-2.205531	C	1.257679	-2.666152	0.488779
H	1.697619	-2.357579	-1.726426	H	1.504217	-2.102508	1.393014
H	0.441787	-2.233528	-2.959043	H	1.469500	-3.730599	0.644251
C	-0.953103	-0.539736	3.406486	H	1.868520	-2.286228	-0.335126
H	-1.583400	-0.710216	4.286487	C	-4.139880	-0.274560	1.433883
H	-0.353610	0.362281	3.565645	H	-3.915608	0.648044	1.977268
H	-0.270674	-1.386703	3.286009	H	-5.227099	-0.391506	1.344370
C	-3.195579	0.958198	2.438030	H	-3.730427	-1.106694	2.014061
H	-3.781604	0.587137	3.286337	C	0.683586	3.060121	0.499340
H	-3.864680	1.187357	1.604436	H	0.675875	4.147018	0.644555
H	-2.668624	1.864593	2.743087	H	1.028449	2.566198	1.411913
C	-3.093765	-1.824996	1.971518	H	1.366430	2.801135	-0.315821
H	-3.643048	-1.832887	2.919636	H	-1.075927	-0.821111	-1.716977
H	-3.796668	-1.769946	1.136500	H	-1.204632	0.775882	-1.721641
H	-2.516939	-2.749771	1.891986	C	1.136541	0.160084	-2.390344
C	-1.303190	3.609118	1.116131	H	4.100977	0.596194	-0.140154
H	-1.090215	4.654205	0.863257	C	5.427683	0.062072	-0.735794
H	-2.359693	3.523624	1.382279	H	3.899665	0.084004	0.811888
H	-0.694774	3.322685	1.980415	H	4.222739	1.660776	0.109123
C	0.076854	-3.510164	0.616394	C	6.615787	0.252859	0.221417
H	-0.605810	-3.524141	1.469821	H	5.309869	-1.003443	-0.976425
H	0.188512	-4.533128	0.238834	H	5.627311	0.577807	-1.685379
H	1.053126	-3.153908	0.961758	C	7.947393	-0.266469	-0.350929
C	3.318265	0.033105	0.298016	H	6.720395	1.321558	0.466580
C	4.673842	0.113994	1.021107	H	6.406209	-0.262064	1.171989
H	3.233957	0.844412	-0.436085	H	7.843241	-1.333533	-0.597579
H	3.255988	-0.903653	-0.271909	H	8.157962	0.249273	-1.299907
C	5.875765	0.036017	0.062280	C	9.131308	-0.073604	0.611015
H	4.726979	1.053526	1.593045	H	8.962708	-0.608281	1.554721
H	4.744851	-0.699885	1.759612	H	10.064264	-0.449535	0.176294
C	7.236255	0.118800	0.778776	H	9.276211	0.986408	0.850102
H	5.824076	-0.902906	-0.509949	41			
H	5.804615	0.849145	-0.675948	scf done: -747.941296			
H	7.286348	1.056902	1.351279	Re	0.674511	0.006818	-0.375115
H	7.306709	-0.694804	1.515970	Cl	0.232415	0.014265	2.152211
C	8.430108	0.042518	-0.186341	P	3.042750	-0.230569	0.081145
H	9.383590	0.104679	0.350768	P	0.683203	2.465481	-0.043505
H	8.423114	-0.899755	-0.748556	C	-1.048397	0.169486	-1.745742
H	8.401272	0.863259	-0.913937	C	-1.576548	0.221766	-0.586734
TS₁₉₋₄₁				C	4.200235	1.087595	-0.571748
scf done: -747.917162				H	5.246795	0.828643	-0.372247
Re	-1.052355	-0.010287	-0.260013	H	3.985176	2.054961	-0.110087
Cl	-0.311271	0.063560	2.158447	H	4.056147	1.181420	-1.653317
P	-3.302635	-0.223598	-0.239601	C	1.600150	3.149593	1.422578
P	-0.539501	-2.387746	0.105982	H	1.430452	4.228210	1.517340
C	1.996154	0.283900	-1.772881	H	2.674518	2.967505	1.331954
C	2.949287	0.430730	-1.029702	H	1.236020	2.635095	2.315748
C	-4.086639	-1.731361	-1.027302	C	1.349735	3.494897	-1.441024
H	-5.181417	-1.682232	-0.978213	H	1.309112	4.564657	-1.206208
H	-3.755364	-2.639627	-0.513942	H	0.750054	3.298904	-2.336004
H	-3.774615	-1.789095	-2.075107	H	2.383217	3.211444	-1.657465
C	-1.346274	-3.258670	1.537432	C	3.914031	-1.689007	-0.703179
H	-0.930335	-4.263069	1.670772	H	4.992442	-1.660361	-0.508063
H	-2.425645	-3.340251	1.369876	H	3.513550	-2.631561	-0.320306
H	-1.175353	-2.663736	2.437882	H	3.745018	-1.658180	-1.784756
C	-0.794799	-3.602322	-1.276135	P	0.193420	-2.407633	-0.058344
H	-0.481498	-4.609959	-0.976948	C	1.062120	-3.312233	1.315790
H	-0.208071	-3.283204	-2.142251	H	0.662206	-4.326970	1.423513
H	-1.848148	-3.626104	-1.569458	H	2.136830	-3.378299	1.125867
C	-4.355772	1.079022	-1.078388	H	0.902296	-2.751713	2.240988
H	-5.420569	0.824509	-1.026588	C	0.508781	-3.517899	-1.515258
H	-4.205078	2.050891	-0.598270	H	0.244024	-4.557835	-1.292931
H	-4.052520	1.158635	-2.127231	H	-0.090640	-3.164896	-2.360823
P	-1.017126	2.424852	0.102733	H	1.562975	-3.466332	-1.802546

C	-0.959668	3.297314	0.214527	C	1.641718	2.926957	-0.316170
H	-1.389563	2.952373	1.158423	H	1.722846	4.019568	-0.298088
H	-0.834499	4.385306	0.251605	H	2.187181	2.514961	0.537331
H	-1.638019	3.034690	-0.601063	H	2.095677	2.545399	-1.234307
C	3.632076	-0.364830	1.838320	H	-0.137779	-0.581010	-1.931242
H	3.154570	-1.221699	2.318560	H	-1.540974	0.548216	-1.644041
H	4.721658	-0.475628	1.877648	H	1.419558	0.025293	-2.816606
H	3.329548	0.525187	2.395253	C	2.740796	-0.369523	0.287839
C	-1.560227	-2.870573	0.344882	C	4.083733	-0.179191	-0.445628
H	-1.665594	-3.959951	0.398086	H	2.731390	-1.352514	0.779949
H	-1.825801	-2.434261	1.311173	H	2.650059	0.343725	1.116211
H	-2.233524	-2.476851	-0.420008	C	5.298085	-0.297826	0.492395
H	1.302194	0.771119	-1.712219	H	4.165051	-0.923289	-1.251523
H	1.147397	-0.858984	-1.710054	H	4.094348	0.806754	-0.932433
H	-1.146109	0.174904	-2.816304	C	6.647333	-0.099694	-0.222525
C	-2.791593	0.326376	0.260950	H	5.205382	0.442888	1.301721
C	-4.109880	0.094231	-0.511385	H	5.288021	-1.285322	0.979460
H	-2.826058	1.318783	0.732180	H	6.743613	-0.845128	-1.025804
H	-2.720312	-0.374511	1.102303	H	6.653527	0.884145	-0.714861
C	-5.357767	0.220331	0.380186	C	7.853062	-0.206065	0.725111
H	-4.172568	0.814730	-1.339823	H	8.798473	-0.061906	0.189080
H	-4.088483	-0.903461	-0.973900	H	7.798267	0.550935	1.517597
C	-6.677254	-0.017300	-0.377352	H	7.888873	-1.190488	1.208691
H	-5.284390	-0.496073	1.213069	42			
H	-5.379236	1.221270	0.838725	scf done: -747.962470			
H	-6.751150	0.700639	-1.207624	Re	-0.497321	-0.055682	-0.347972
H	-6.653829	-1.016333	-0.837510	Cl	-0.076713	-0.064644	2.229789
C	-7.919522	0.105117	0.519723	P	-2.755500	0.663155	0.727382
H	-7.984085	1.104143	0.969242	P	-1.270327	-2.359351	-0.408552
H	-8.842105	-0.066993	-0.047057	C	0.979482	-0.559828	-1.886058
H	-7.887795	-0.625299	1.338033	C	1.333644	-0.623404	-0.491468
TS₄₁₋₄₂				C	-4.173342	1.056109	-0.417727
scf done: -747.922901				H	-5.070150	1.355413	0.137168
Re	-0.635038	0.014325	-0.336771	H	-4.403706	0.176935	-1.027403
Cl	-0.199355	-0.040904	2.168710	H	-3.884111	1.862644	-1.098092
P	-3.001691	0.245341	0.270849	C	-1.334016	-3.331576	1.180250
P	-0.818524	-2.429663	-0.209930	H	-1.635525	-4.370298	0.999933
C	1.113348	-0.175918	-1.798327	H	-2.026452	-2.867906	1.885244
C	1.527203	-0.265138	-0.567422	H	-0.341721	-3.308139	1.640285
C	-4.234824	-0.940112	-0.486580	C	-2.948503	-2.694011	-1.148506
H	-5.260188	-0.664612	-0.213279	H	-3.167336	-3.767985	-1.156157
H	-4.047114	-1.961983	-0.147344	H	-2.951634	-2.315387	-2.175450
H	-4.134753	-0.911886	-1.576548	H	-3.737353	-2.179916	-0.594155
C	-1.636408	-3.175853	1.288114	C	-2.745078	2.157938	1.836011
H	-1.483269	-4.260497	1.318716	H	-3.718102	2.275317	2.326065
H	-2.711421	-2.974091	1.288343	H	-1.968018	1.997862	2.588029
H	-1.197593	-2.710061	2.175227	H	-2.523991	3.070969	1.278423
C	-1.659886	-3.335292	-1.604916	P	0.079655	2.290580	-0.636841
H	-1.704751	-4.414434	-1.417631	C	0.627798	3.268438	0.851394
H	-1.093123	-3.155569	-2.525491	H	0.913026	4.290051	0.573965
H	-2.672407	-2.952722	-1.753991	H	-0.166666	3.301485	1.599788
C	-3.872860	1.820968	-0.233357	H	1.480178	2.756488	1.307713
H	-4.930163	1.788774	0.054485	C	-1.201761	3.416587	-1.391911
H	-3.407147	2.687923	0.242376	H	-0.803958	4.430028	-1.519613
H	-3.802366	1.939498	-1.319209	H	-1.483442	3.012157	-2.369255
P	-0.147399	2.409078	-0.223311	H	-2.099676	3.470275	-0.771996
C	-0.639820	3.316308	1.325782	C	-0.281541	-3.556221	-1.442936
H	-0.314575	4.362462	1.292185	H	0.763810	-3.566489	-1.120949
H	-1.724499	3.284176	1.464001	H	-0.696967	-4.564111	-1.334444
H	-0.181193	2.806331	2.177294	H	-0.319579	-3.270796	-2.497733
C	-0.841780	3.514304	-1.554117	C	-3.564591	-0.525000	1.909906
H	-0.543395	4.558685	-1.404582	H	-2.839663	-0.753043	2.695770
H	-0.469114	3.169285	-2.524584	H	-4.459279	-0.072385	2.351921
H	-1.932642	3.451908	-1.570055	H	-3.852841	-1.451822	1.408604
C	0.790578	-3.368285	-0.164907	C	1.486324	2.694224	-1.794365
H	1.311015	-3.132644	0.767620	H	1.666505	3.774935	-1.785279
H	0.613816	-4.448448	-0.215368	H	2.399246	2.178880	-1.484627
H	1.421800	-3.061383	-1.003310	H	1.239734	2.386003	-2.814344
C	-3.497387	0.158289	2.059974	H	0.855789	-1.479738	-2.456415
H	-2.930425	0.898684	2.629187	H	-1.388679	0.148297	-1.763813
H	-4.573039	0.337943	2.169287	H	1.363400	0.241820	-2.514021
H	-3.243726	-0.822203	2.470027	C	2.549353	-1.016816	0.272266

C	3.814646	-0.214932	-0.125975	H	-5.128143	0.881425	1.570948
H	2.749578	-2.083867	0.063747	H	-5.957528	0.877341	-0.806637
H	2.364533	-0.921520	1.347163	H	-5.957503	-0.879992	-0.804854
C	5.078766	-0.697921	0.606828	C	-7.513250	-0.000099	0.423862
H	3.965208	-0.286429	-1.212616	H	-8.270180	-0.000849	-0.369164
H	3.649843	0.847834	0.104103	H	-7.684020	-0.885141	1.050169
C	6.336682	0.115251	0.249192	H	-7.683995	0.886150	1.048469
H	4.910901	-0.648136	1.693128				
H	5.253369	-1.758904	0.369652				
H	6.500657	0.068246	-0.837690				
H	6.160432	1.174679	0.487696				
C	7.597880	-0.371623	0.980704				
H	7.816624	-1.418532	0.734943				
H	8.475300	0.226460	0.707989				
H	7.472023	-0.305318	2.068721				
43							
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Re	0.473319	-0.000008	-0.050752				
Cl	2.065721	0.000145	-2.046224				
Cl	-1.185888	-0.000039	-1.959799				
P	2.748158	-0.000093	0.919524				
P	0.332939	2.466390	-0.248500				
C	0.040418	0.000100	2.087743				
H	0.234969	0.905010	2.670185				
C	-1.041510	0.000106	1.134774				
C	3.872013	1.414071	0.460952				
H	4.869805	1.257403	0.885909				
H	3.476121	2.360298	0.838714				
H	3.939970	1.460676	-0.627800				
C	1.318182	3.282711	-1.587540				
H	1.072266	4.348969	-1.646427				
H	1.080628	2.788746	-2.533115				
H	2.389105	3.163103	-1.410560				
C	-1.368599	3.101409	-0.623386				
H	-1.351337	4.187870	-0.765011				
H	-2.044303	2.855682	0.201312				
H	-1.733968	2.606213	-1.525650				
C	3.872167	-1.413946	0.460337				
H	4.870075	-1.257104	0.884963				
H	3.476637	-2.360321	0.838116				
H	3.939761	-1.460359	-0.628443				
H	0.234875	-0.904760	2.670290				
P	0.332996	-2.466314	-0.248497				
C	1.318098	-3.282555	-1.587691				
H	1.072012	-4.348764	-1.646741				
H	1.080611	-2.788392	-2.533178				
H	2.389044	-3.163156	-1.410689				
C	-1.368559	-3.101438	-0.623131				
H	-1.351268	-4.187910	-0.764667				
H	-2.044169	-2.855666	0.201627				
H	-1.734050	-2.606331	-1.525395				
C	0.731030	3.506852	1.248394				
H	1.770104	3.369877	1.560131				
H	0.564145	4.568803	1.035040				
H	0.082661	3.211160	2.080315				
C	2.988696	-0.000512	2.765809				
H	2.526267	-0.885987	3.210365				
H	4.058515	-0.000596	3.000801				
H	2.526312	0.884779	3.210779				
C	0.731345	-3.506777	1.248329				
H	0.564463	-4.568737	1.035011				
H	1.770454	-3.369761	1.559918				
H	0.083077	-3.211103	2.080337				
C	-2.504027	0.000362	1.447946				
C	-3.568181	-0.000132	0.339096				
H	-2.675106	0.869230	2.112095				
H	-2.675264	-0.867775	2.112998				
C	-4.993829	0.000424	0.922298				
H	-3.430273	0.869948	-0.310855				
H	-3.430542	-0.871088	-0.309749				
C	-6.090596	-0.000671	-0.158016				
H	-5.128135	-0.879284	1.572707				