

Supporting Information

Probing Mechanism of Conversion Methyl Levulinate into γ - valerolactone Catalyzed by $\text{Al}(\text{O}i\text{Pr})_3$ in Alcohol Solvent: A DFT Study

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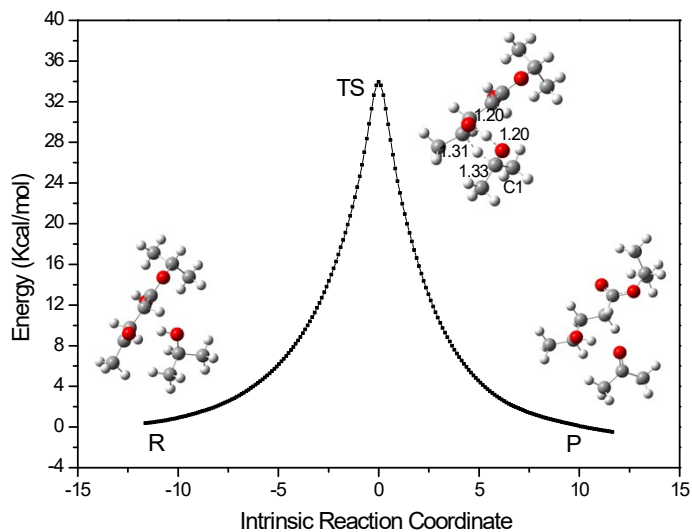


Figure S1 IRC of inter-molecular hydrogen transfer between IPL and *i*-PrOH to form 2HIPL (maxpoint=100, stepsize=10).

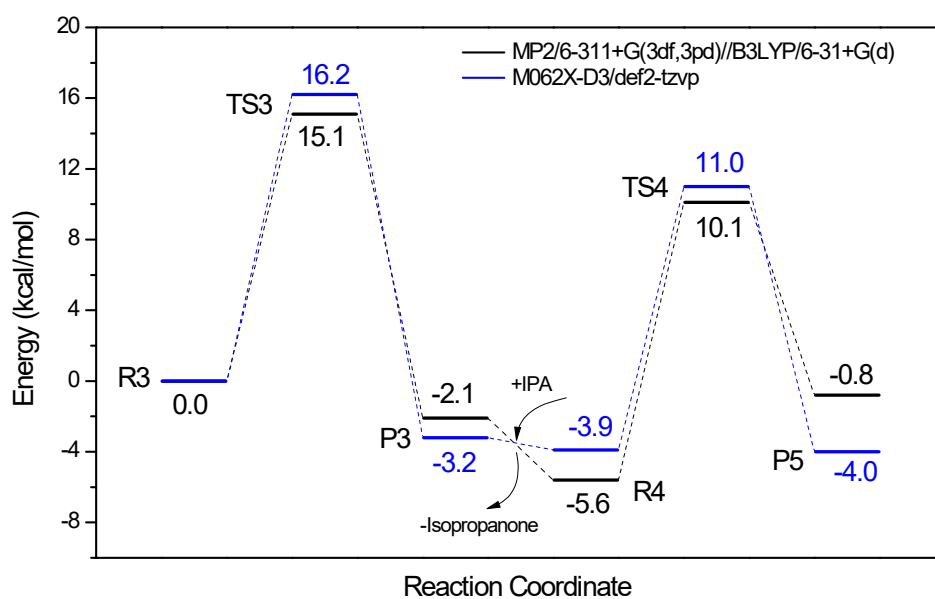
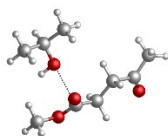
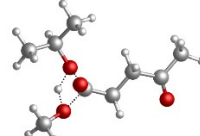


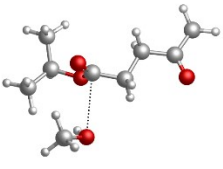
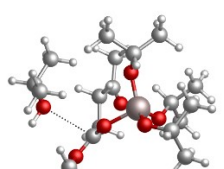
Figure S2 Compared the free energy (kcal/mol) for the MPV hydrogenation of IPL to 2HIPL catalyzed by $\text{Al}(\text{O}i\text{Pr})_3$ in *i*-PrOH medium at MP2/6-311+G(3df, 3pd)//B3LYP/6-31+G(d) and M06-2X-D3/def2-tzvp level.

Coordinates and snapshots of optimized structures

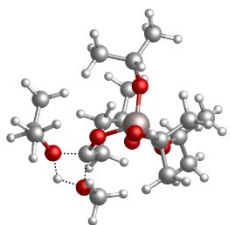
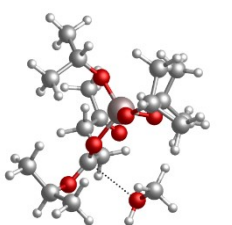
1. The structures of reactants, TS and products in the ester change

Table S 1 The snapshots and coordinates of of reactants, TS and products optimized at M06-2X-D3/def2-tzvp SMD=2-propanol level in the ester change.

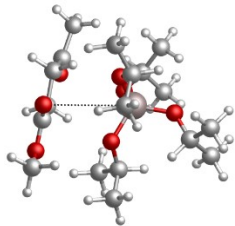
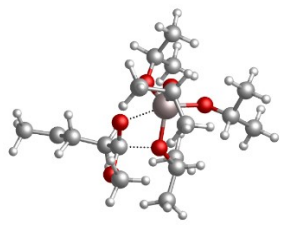
Ra				TSa			
							
C	3.832323	1.366956	0.393825	C	4.198885	1.038696	0.139926
H	4.895783	1.327567	0.165631	H	5.227943	0.685124	0.118207
H	3.673160	1.511774	1.463448	H	3.996363	1.567615	1.072611
H	3.386215	2.224489	-0.119009	H	4.046242	1.750341	-0.676476
C	3.138395	0.125316	-0.084540	C	3.242759	-0.103979	-0.041857
C	1.757768	-0.116934	0.467504	C	1.796901	0.179363	0.278150
H	1.200960	0.823229	0.422443	H	1.516283	1.103994	-0.235489
H	1.876907	-0.342156	1.532503	H	1.740505	0.398979	1.349800
C	1.012555	-1.226429	-0.245038	C	0.865354	-0.958735	-0.096253
H	1.562585	-2.170077	-0.181904	H	1.130441	-1.869641	0.444817
H	0.885902	-1.003654	-1.304765	H	0.918348	-1.170456	-1.163189
C	-0.341736	-1.468677	0.356134	C	-0.551223	-0.628389	0.292870
O	3.656240	-0.634155	-0.879519	O	3.611666	-1.191218	-0.438873
O	-0.685590	-1.140052	1.468189	O	-0.932963	-0.392937	1.419357
O	-1.134289	-2.150746	-0.473633	O	-1.458837	-1.734467	-0.538646
C	-2.453217	-2.441192	0.004180	C	-2.528519	-2.299532	0.213124
H	-2.407420	-3.064377	0.896958	H	-2.121081	-3.008810	0.933862
H	-2.948870	-2.975141	-0.801863	H	-3.178228	-2.825240	-0.485652
H	-2.985729	-1.516420	0.227801	H	-3.097633	-1.532383	0.738893
C	-3.256253	1.506118	0.192023	C	-3.203743	1.226353	0.020904
H	-3.822154	2.378056	0.526651	H	-3.819757	2.127364	0.045472
H	-2.988792	0.907853	1.066911	H	-3.093121	0.852132	1.038061
H	-3.906130	0.909966	-0.453630	H	-3.728911	0.477620	-0.577353
C	-2.005683	1.938585	-0.551843	C	-1.859130	1.559470	-0.603893
H	-2.292618	2.556762	-1.409922	H	-2.036116	1.998041	-1.589025
C	-1.057822	2.721256	0.332124	C	-1.036636	2.535139	0.216245
H	-0.772537	2.123190	1.201576	H	-0.804185	2.130247	1.201305

H	-0.156012	2.999056	-0.216820	H	-0.106349	2.780783	-0.298087
H	-1.538944	3.634930	0.685187	H	-1.603257	3.459024	0.346892
O	-1.279519	0.798659	-1.030638	O	-1.081024	0.377178	-0.902044
H	-1.875023	0.255305	-1.562599	H	-1.646121	-0.683497	-1.098294
Pa				Rb			
							
C	-4.564142	-0.833814	-0.082179	C	-1.643896	3.383409	2.014390
H	-5.515437	-0.313072	0.009645	H	-1.588250	4.449390	2.225116
H	-4.458588	-1.579373	0.707181	H	-0.806990	2.865084	2.490521
H	-4.536831	-1.365141	-1.037910	H	-2.561413	2.965061	2.435274
C	-3.423932	0.141176	-0.053107	C	-1.604584	3.133487	0.535247
C	-2.052661	-0.444833	0.176860	C	-1.745711	1.693857	0.111540
H	-1.918092	-1.272270	-0.526974	H	-2.730693	1.348049	0.434361
H	-2.055891	-0.891484	1.177138	H	-1.025026	1.105934	0.689629
C	-0.935306	0.586369	0.044689	C	-1.579055	1.500744	-1.388037
H	-1.076194	1.393581	0.761641	H	-0.684196	2.030520	-1.731821
H	-0.920663	1.002626	-0.961726	H	-2.433584	1.883114	-1.942319
C	0.379913	-0.079070	0.343342	C	-1.356843	0.075972	-1.760065
O	-3.591422	1.331633	-0.221580	O	-1.467692	4.031279	-0.271120
O	0.876090	-0.135227	1.445610	O	-0.541541	-0.673617	-1.199581
O	1.533797	2.432662	-0.623937	O	-2.030196	-0.344917	-2.783513
C	2.506106	2.673193	0.386938	C	-1.812680	-1.707371	-3.212505
H	2.207025	3.582813	0.906757	H	-0.779348	-1.829851	-3.531861
H	3.500773	2.826728	-0.039645	H	-2.495146	-1.856008	-4.042919
H	2.546168	1.855023	1.110516	H	-2.041820	-2.386392	-2.392677
C	3.317932	-0.769533	-0.261025	C	-3.009155	-2.969676	0.349357
H	4.179305	-1.423618	-0.410928	H	-3.119522	-3.675628	1.175104
H	3.300594	-0.454423	0.781076	H	-1.949100	-2.726905	0.236165
H	3.450261	0.105322	-0.901297	H	-3.354466	-3.462342	-0.562952
C	2.063737	-1.533000	-0.640465	C	-3.808778	-1.706525	0.613171
H	2.159496	-1.877801	-1.669766	H	-4.868732	-1.962307	0.719795
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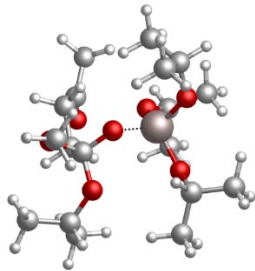
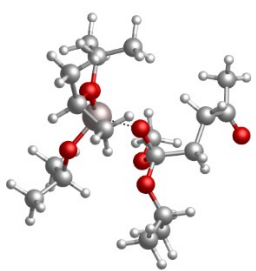
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H	2.554716	-3.478621	0.085103	H	-3.434886	-1.624215	2.730313
O	0.899867	-0.656970	-0.740984	O	-3.667035	-0.788480	-0.481466
H	1.814674	1.674787	-1.150837	H	-4.024083	-1.205996	-1.275804
				C	2.116488	-0.966402	3.296745
				H	2.438155	-1.698771	4.040966
				H	1.687543	-0.106145	3.818607
				H	2.997959	-0.631487	2.746625
				C	1.083706	-1.567526	2.355644
				H	1.548041	-2.406356	1.820099
				C	-0.113671	-2.100810	3.125337
				H	-0.608329	-1.286575	3.662671
				H	-0.836190	-2.556466	2.446188
				H	0.200585	-2.853973	3.851709
				O	0.654014	-0.589933	1.422535
				C	3.010645	2.170990	0.891768
				H	3.154986	3.078495	1.482829
				H	3.900028	2.013521	0.274897
				H	2.908509	1.327906	1.578209
				C	1.779675	2.290831	0.005727
				H	0.908978	2.449249	0.658075
				C	1.898718	3.476512	-0.936802
				H	2.789160	3.364480	-1.561875
				H	1.026887	3.543620	-1.589924
				H	1.981194	4.412007	-0.378988
				O	1.594221	1.114319	-0.756438
				C	3.803324	-1.212628	-2.334807
				H	4.852639	-1.435581	-2.541975
				H	3.707464	-0.138539	-2.154251
				H	3.216244	-1.468079	-3.219430
				C	3.310104	-1.996808	-1.126652
				H	3.472673	-3.063633	-1.320167
				C	4.080830	-1.616635	0.129752
				H	3.934732	-0.554311	0.354808

				H	3.740219	-2.203659	0.985056
				H	5.151947	-1.788189	0.000242
				O	1.918887	-1.812542	-0.947232
				Al	1.066118	-0.465198	-0.261354
TSb				Pb			
							
C	-2.807778	3.331339	1.436559	C	4.666821	0.254341	0.708493
H	-3.240351	4.318092	1.283219	H	5.657552	0.147410	0.271303
H	-1.787221	3.437191	1.817633	H	4.284367	-0.732836	0.987083
H	-3.374683	2.776443	2.186159	H	4.710559	0.852357	1.620429
C	-2.749397	2.569255	0.145941	C	3.713380	0.860682	-0.277282
C	-2.433030	1.098474	0.259590	C	2.391563	1.324529	0.285556
H	-3.277591	0.623974	0.770361	H	2.592094	2.170918	0.950902
H	-1.576888	0.996136	0.936177	H	1.999997	0.519588	0.917645
C	-2.163140	0.451036	-1.086877	C	1.399849	1.702610	-0.814299
H	-1.430258	1.037043	-1.644297	H	1.285552	0.874292	-1.512023
H	-3.069882	0.383251	-1.687192	H	1.726783	2.586481	-1.356737
C	-1.562208	-0.922170	-0.937610	C	0.065293	1.959859	-0.200073
O	-2.926747	3.106240	-0.929332	O	3.972329	0.951569	-1.459631
O	-0.503195	-1.074305	-0.226014	O	-0.665800	1.050246	0.232075
O	-1.452865	-1.518489	-2.336034	O	-0.932982	1.875022	-2.700893
C	-0.146791	-1.957547	-2.750205	C	-1.954989	0.883326	-2.744601
H	0.501504	-1.084343	-2.818849	H	-1.464052	-0.082610	-2.639282
H	-0.278061	-2.401956	-3.733780	H	-2.492235	0.907696	-3.696691
H	0.259484	-2.684047	-2.049131	H	-2.671049	1.010554	-1.928238
C	-1.394002	-3.802412	0.417614	C	-2.724034	3.177486	-0.050114
H	-1.573022	-4.626162	1.111290	H	-3.564651	3.727233	0.377844
H	-0.459918	-3.313816	0.686524	H	-2.895297	2.113533	0.106178
H	-1.301607	-4.225241	-0.585345	H	-2.693665	3.390244	-1.119399
C	-2.576588	-2.856369	0.493568	C	-1.464814	3.656700	0.639977
H	-3.495519	-3.424088	0.345416	H	-1.371814	4.734172	0.518295

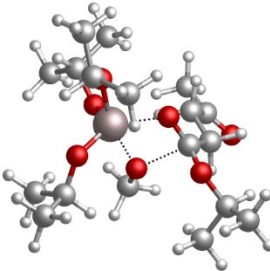
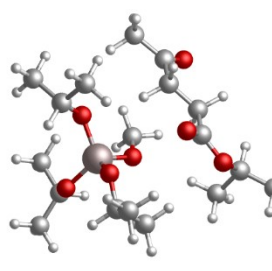
C	-2.669584	-2.070298	1.782282	C	-1.391276	3.304821	2.109923
H	-1.822695	-1.394383	1.891626	H	-1.583666	2.247361	2.279484
H	-3.596520	-1.497118	1.822464	H	-0.416393	3.569648	2.522609
H	-2.661177	-2.769561	2.620307	H	-2.152049	3.881606	2.638408
O	-2.633645	-1.931423	-0.648787	O	-0.243523	3.205945	-0.057408
H	-2.248696	-2.262532	-1.767213	H	-1.329528	2.735101	-2.881340
C	1.920755	0.939952	3.809598	C	1.360635	-1.781322	3.662941
H	2.373829	0.497365	4.699479	H	1.151304	-1.951156	4.721215
H	1.015527	1.474855	4.110876	H	2.085452	-0.966037	3.579023
H	2.623589	1.663403	3.390455	H	1.812557	-2.686248	3.251562
C	1.576981	-0.125522	2.781948	C	0.091658	-1.430855	2.904136
H	2.504264	-0.641923	2.497282	H	-0.624264	-2.255099	3.026152
C	0.620718	-1.162431	3.352862	C	-0.548471	-0.160846	3.445695
H	-0.319775	-0.685256	3.642609	H	0.129230	0.687073	3.308886
H	0.402604	-1.934262	2.609531	H	-1.484837	0.052343	2.923060
H	1.049369	-1.648358	4.232711	H	-0.772434	-0.257009	4.510562
O	1.014416	0.497947	1.643161	O	0.408176	-1.292730	1.533425
C	1.957470	3.210046	-0.261135	C	1.492998	-3.304804	-1.130679
H	1.722480	4.252337	-0.031697	H	2.497642	-3.711734	-1.268020
H	2.812645	3.191089	-0.942257	H	0.807074	-3.848932	-1.786054
H	2.239119	2.707326	0.665929	H	1.193707	-3.476097	-0.094630
C	0.766279	2.514979	-0.906634	C	1.456641	-1.820256	-1.463104
H	-0.085938	2.584439	-0.212594	H	2.152447	-1.302154	-0.786020
C	0.383138	3.200919	-2.208631	C	1.897038	-1.569534	-2.896396
H	1.229156	3.176819	-2.901585	H	1.242221	-2.112967	-3.583587
H	-0.461829	2.702006	-2.686802	H	1.843453	-0.507180	-3.143680
H	0.110034	4.243882	-2.032623	H	2.923481	-1.907855	-3.054735
O	1.058785	1.153678	-1.163890	O	0.149695	-1.304483	-1.289716
C	3.644173	-1.267769	-2.181281	C	-3.277203	-2.316762	-1.527861
H	4.682231	-1.256851	-2.522298	H	-3.912775	-3.166353	-1.788390
H	3.143771	-0.375556	-2.568452	H	-2.325529	-2.422899	-2.055735
H	3.154379	-2.150033	-2.599419	H	-3.764920	-1.403070	-1.874573
C	3.567493	-1.286546	-0.660657	C	-3.040974	-2.258258	-0.025036
H	4.095001	-2.178711	-0.300850	H	-4.015459	-2.191657	0.473109
C	4.246926	-0.060653	-0.062977	C	-2.334597	-3.512806	0.470156

H	3.788240	0.855237	-0.447605	H	-1.366274	-3.628011	-0.029358
H	4.161256	-0.062476	1.026431	H	-2.166377	-3.462972	1.548200
H	5.308485	-0.040671	-0.320590	H	-2.927468	-4.405189	0.256866
O	2.222171	-1.396037	-0.243506	O	-2.316333	-1.091353	0.318702
Al	1.043446	-0.137702	0.015197	Al	-0.605412	-0.822827	0.200975
R1				TS1			
							
C	-3.213658	3.031080	0.784756	C	-5.991405	-0.385719	-1.198869
H	-3.469450	3.944608	0.251120	H	-6.628565	-1.268275	-1.204120
H	-2.219809	3.124261	1.229509	H	-5.727510	-0.098831	-2.217720
H	-3.916941	2.865657	1.604389	H	-6.540112	0.450140	-0.755205
C	-3.225949	1.849939	-0.141252	C	-4.758349	-0.629314	-0.376209
C	-2.999957	0.507994	0.501423	C	-3.635636	0.361418	-0.544748
H	-3.859144	0.305723	1.150316	H	-4.058203	1.365349	-0.431334
H	-2.130911	0.592853	1.159564	H	-3.299164	0.291752	-1.584827
C	-2.796055	-0.598666	-0.510306	C	-2.476442	0.122404	0.411536
H	-1.998138	-0.328838	-1.204066	H	-2.045756	-0.861341	0.235712
H	-3.692673	-0.780468	-1.107230	H	-2.817789	0.182276	1.444931
C	-2.391514	-1.890348	0.135204	C	-1.396270	1.155209	0.170122
O	-3.423441	1.974114	-1.334916	O	-4.681388	-1.566599	0.393751
O	-2.223637	-2.063420	1.320688	O	-0.767171	1.193305	-0.928071
O	-2.253204	-2.871182	-0.761695	O	-1.745371	2.317009	0.792550
C	-1.804480	-4.132028	-0.252303	C	-0.901924	3.441869	0.579953
H	-1.741429	-4.794850	-1.111017	H	-1.400421	4.285494	1.053611
H	-2.518368	-4.526816	0.470705	H	-0.766948	3.641918	-0.483220
H	-0.826250	-4.022853	0.216666	H	0.067292	3.282497	1.054025
C	4.309259	0.372426	-1.435113	C	3.611392	-1.326328	2.402349
H	5.145435	-0.291238	-1.669117	H	4.474056	-0.885973	2.909318
H	4.705699	1.373858	-1.243123	H	3.857376	-2.359295	2.138050
H	3.658668	0.426568	-2.310632	H	2.773296	-1.348629	3.102807
C	3.537574	-0.116750	-0.215588	C	3.246114	-0.548762	1.141411

H	3.163408	-1.130495	-0.427108	H	3.040937	0.494833	1.438949
C	4.452677	-0.196302	0.999764	C	4.430616	-0.531264	0.176145
H	4.840986	0.798668	1.236432	H	4.708267	-1.557968	-0.082633
H	3.908743	-0.566884	1.871166	H	4.162051	-0.006618	-0.741878
H	5.298977	-0.862372	0.813763	H	5.301405	-0.042209	0.622108
O	2.460881	0.751760	0.043966	O	2.112536	-1.121309	0.549063
C	0.197684	-0.184403	4.134983	C	1.541096	2.629157	-2.889292
H	0.770867	-0.580584	4.976555	H	2.027337	3.537268	-3.255599
H	-0.743530	-0.737355	4.063797	H	0.597448	2.905566	-2.413994
H	-0.035784	0.862779	4.339703	H	1.317722	1.989175	-3.746001
C	0.970023	-0.309659	2.830528	C	2.438565	1.889512	-1.900639
H	1.910689	0.253232	2.935670	H	3.405066	1.721154	-2.401670
C	1.324915	-1.764153	2.541704	C	2.708170	2.744514	-0.668779
H	0.411949	-2.356918	2.435826	H	1.775329	2.905465	-0.123224
H	1.894079	-1.849510	1.612021	H	3.417864	2.250062	-0.001994
H	1.927088	-2.189161	3.349062	H	3.118733	3.719630	-0.943878
O	0.202342	0.249812	1.790381	O	1.912175	0.641980	-1.562481
C	0.619777	3.568715	0.534359	C	1.559419	-2.717488	-2.453910
H	0.704366	4.657335	0.485110	H	1.762830	-3.695705	-2.897804
H	1.620477	3.153334	0.685155	H	2.406232	-2.440336	-1.820749
H	0.010604	3.311759	1.403695	H	1.480470	-1.984706	-3.259891
C	0.004191	3.012122	-0.745624	C	0.270855	-2.750004	-1.638016
H	-0.968792	3.502013	-0.895414	H	-0.534841	-3.073869	-2.313414
C	0.876846	3.337560	-1.952520	C	0.354373	-3.779928	-0.516251
H	1.864671	2.882391	-1.835549	H	1.169581	-3.531026	0.166224
H	0.423559	2.944427	-2.865195	H	-0.579891	-3.797674	0.050402
H	1.005201	4.416675	-2.070205	H	0.526575	-4.781966	-0.918740
O	-0.227746	1.626914	-0.663203	O	-0.080913	-1.480540	-1.151260
Al	0.733761	0.368172	0.112176	Al	0.877276	-0.190861	-0.399098
C	1.299681	-2.885427	-2.122316	C	-0.578916	1.128561	3.373998
H	0.436069	-3.532931	-1.945222	H	-1.661973	1.125016	3.238510
H	2.060214	-3.116424	-1.372437	H	-0.209405	2.137569	3.181228
H	1.706418	-3.112987	-3.110644	H	-0.365255	0.877529	4.415390
C	0.877258	-1.427470	-2.018158	C	0.096953	0.116529	2.461614
H	1.755757	-0.802524	-2.242281	H	1.165775	0.110476	2.692207

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H	-1.076156	-1.724700	-2.894069	H	-1.533453	-1.315332	2.581168
H	-0.491710	-0.052342	-2.984445	H	-0.009417	-1.982617	1.963642
H	0.181171	-1.282694	-4.064667	H	-0.193590	-1.628811	3.688997
O	0.423863	-1.168363	-0.706580	O	-0.002197	0.525141	1.098221
P1				R2			
							
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H	2.059572	4.721992	-0.222651	H	-5.531646	2.536506	-0.180732
H	2.288549	3.166446	0.627382	H	-4.132462	3.004508	-1.199593
H	1.387080	4.458309	1.414173	H	-3.893980	2.652631	0.508225
C	0.340309	3.438587	-0.147384	C	-4.197479	0.926091	-0.666607
C	-0.497948	2.579331	0.762020	C	-2.861054	0.626059	-1.297646
H	-1.063465	3.266784	1.401474	H	-2.134788	1.365389	-0.958518
H	0.176872	2.031430	1.419682	H	-3.010643	0.845743	-2.361573
C	-1.424766	1.626060	0.015919	C	-2.339932	-0.799550	-1.114073
H	-0.997601	1.389816	-0.959307	H	-2.148193	-1.240060	-2.092622
H	-2.397080	2.086413	-0.147070	H	-3.095146	-1.417648	-0.624482
C	-1.596129	0.306495	0.768814	C	-1.005165	-0.895072	-0.346478
O	0.004258	3.697921	-1.288194	O	-5.011246	0.059038	-0.412822
O	-0.411803	-0.292915	1.062100	O	-0.163581	0.088462	-0.734546
O	-2.280943	0.632334	1.964607	O	-1.171860	-0.886549	1.073024
C	-2.417012	-0.434979	2.887967	C	-1.964486	0.156078	1.609220
H	-3.169294	-0.128034	3.614172	H	-3.028696	-0.013762	1.417761
H	-1.477219	-0.629868	3.409301	H	-1.657945	1.132248	1.226494
H	-2.747611	-1.351732	2.394833	H	-1.808797	0.146440	2.688013
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H	-1.623110	-4.168739	-1.993238	H	3.286498	-0.929951	-3.400112
H	-0.856761	-3.085699	-3.170656	H	1.792993	0.030038	-3.410931
H	-1.963761	-2.428960	-1.952521	H	2.091478	-1.135669	-2.111562
C	-0.010782	-2.951591	-1.195034	C	3.247528	0.693718	-1.958411

H	-0.372605	-3.061046	-0.160196	H	3.995968	0.216168	-1.308569
C	1.076535	-3.992780	-1.430152	C	3.967106	1.679190	-2.866180
H	1.446265	-3.915253	-2.456690	H	3.254919	2.141653	-3.555700
H	1.915253	-3.832593	-0.750271	H	4.435010	2.469460	-2.275412
H	0.694914	-5.005166	-1.275570	H	4.743693	1.182582	-3.452702
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C	2.726572	0.155078	2.552651	C	3.293367	-2.426159	1.981216
H	3.159517	0.305883	3.544484	H	3.148069	-3.198084	2.740768
H	1.735729	0.619533	2.538262	H	4.159632	-1.820637	2.263068
H	3.356840	0.665605	1.821592	H	3.512844	-2.917189	1.030490
C	2.620457	-1.330849	2.226483	C	2.060435	-1.544773	1.846998
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C	1.757986	-2.057139	3.251600	C	1.729868	-0.857228	3.165488
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H	2.170884	-1.958249	4.258602	H	1.572008	-1.590393	3.960669
O	2.129305	-1.553079	0.925720	O	2.286601	-0.604770	0.825098
C	3.661090	0.377612	-1.671674	C	-0.317914	3.514401	-0.135828
H	4.331563	0.658491	-2.487662	H	-0.391723	4.572280	-0.400776
H	3.411715	-0.682439	-1.784512	H	-1.291417	3.186312	0.240513
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C	2.389921	1.219558	-1.690511	C	0.760415	3.295179	0.921085
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H	0.721828	1.638255	-2.999237	H	1.213241	3.916708	2.940696
H	2.258573	1.405413	-3.849579	H	0.345464	5.137134	1.993015
O	1.555927	0.916862	-0.599814	O	0.908411	1.930283	1.242405
Al	0.962200	-0.635297	-0.023563	Al	1.319995	0.657905	0.091436
C	-4.625361	0.308232	0.253540	C	-0.091551	-4.398943	-1.098883
H	-4.369965	1.352027	0.435975	H	0.721430	-4.496481	-0.374872
H	-4.745503	-0.192457	1.215166	H	0.333916	-4.111950	-2.061849
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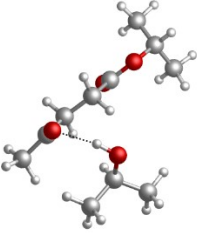
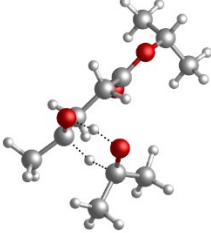
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H	-2.584261	-0.177413	-2.513073	H	-2.458626	-3.043833	1.041887
H	-4.333984	0.071750	-2.567639	H	-2.129235	-4.735662	0.640900
O	-2.334496	-0.662502	0.033731	O	-0.358379	-2.126711	-0.613078
TS2				P2			
							
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H	-2.730456	4.185012	-0.864667	H	0.093294	4.811772	0.533744
H	-2.428402	3.856326	0.837213	H	-0.961598	3.767999	-0.410805
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C	-2.585101	-0.021269	-0.730075	C	2.464335	1.403790	-0.194245
H	-3.222407	-0.223281	-1.598038	H	3.415642	1.933513	-0.306194
H	-3.140268	-0.352818	0.147107	H	2.229580	0.970812	-1.165995
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H	3.206747	-2.278303	-2.983805	H	0.810509	-4.148333	0.798835
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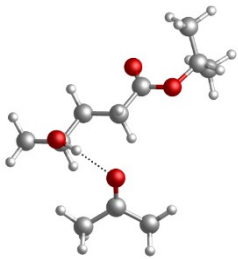
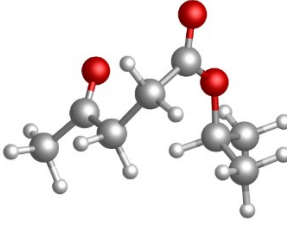
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O	2.191205	0.464530	-1.308226	O	-0.750794	-1.265295	1.555650
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H	2.736873	-3.291317	3.275731	H	-4.134283	-2.994206	-3.164434
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C	1.920976	-1.639807	2.117354	C	-3.025690	-1.649096	-1.870627
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H	1.432096	4.492172	-1.177515	H	-2.083154	2.214972	3.634554
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C	1.559338	2.899408	0.302239	C	-2.599531	1.408977	1.682445
H	2.581942	2.636034	-0.001104	H	-3.032171	0.499630	2.127355
C	1.643959	3.839619	1.498829	C	-3.734695	2.382498	1.402269
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O	0.846742	1.749108	0.671362	O	-1.942557	1.092565	0.474389
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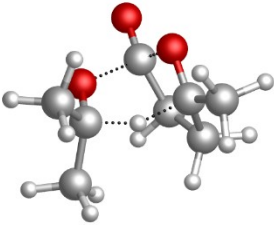
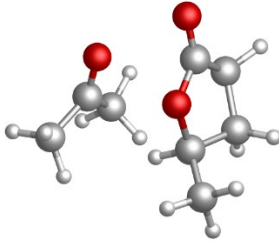
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H	-2.681792	-2.064341	1.527679	H	2.156378	-1.205352	-1.783278
H	-3.499188	-3.620924	1.331722	H	3.562571	-1.783435	-2.697788
O	-1.463971	-2.175174	-0.932153	O	3.485661	-0.714703	0.494267

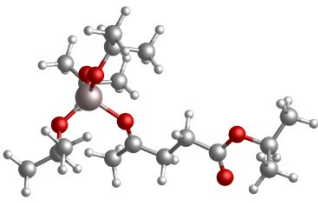
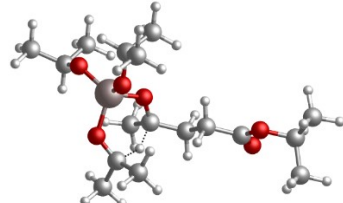
2. The structures of reactants, TS and products in Meerwein-Ponndorf-Verley (MPV) Hydrogenation

Table S 2 The snapshots and coordinates of of reactants, TS and products optimized at M06-2X-D3/def2-tzvp SMD=2-propanol level in the MPV hydrogenation.

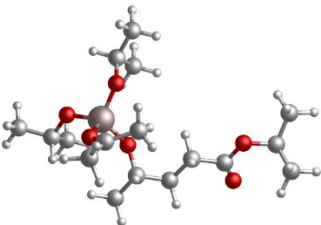
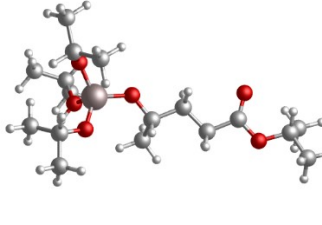
Rc				TSc			
							
H	3.698279	-2.861400	-0.278073	H	-4.017878	1.760665	-0.568006
C	2.812525	-2.525424	-0.813702	C	-2.989326	1.994392	-0.842152
C	1.862085	-1.834553	0.116278	C	-2.015063	1.204698	0.000700
H	2.325944	-3.360684	-1.319348	H	-2.814424	3.056574	-0.650557
H	3.109977	-1.807912	-1.585403	H	-2.837992	1.804846	-1.905273
C	0.460364	-1.621278	-0.390354	C	-0.567764	1.254175	-0.472190
C	-0.379125	-0.747746	0.518657	C	0.395802	0.638276	0.527069
H	0.010130	-2.611780	-0.514255	H	-0.315460	2.306292	-0.640838
H	0.528722	-1.202758	-1.398850	H	-0.490825	0.757782	-1.441446
C	-1.749579	-0.487793	-0.047286	C	1.758939	0.395649	-0.064544
H	0.095931	0.222975	0.684985	H	0.028183	-0.320416	0.901646
H	-0.501403	-1.200805	1.504654	H	0.518163	1.273984	1.405958
O	-2.144686	-0.900291	-1.113871	O	2.061849	0.619479	-1.214437
O	-2.471434	0.265184	0.778928	O	2.592128	-0.108194	0.843536
O	2.216292	-1.447303	1.215810	O	-2.225054	1.202288	1.297999
C	2.619319	1.466498	-0.122144	C	-2.766442	-1.194063	0.057863
O	2.288918	1.455332	1.270074	O	-2.643704	-1.110196	1.362588
H	1.954827	0.770529	-0.651816	H	-2.323458	-0.015822	-0.374264
H	2.299952	0.533331	1.567970	H	-2.457436	0.054428	1.562702

C	2.353997	2.868935	-0.627972	C	-1.804139	-2.108549	-0.664486
H	2.985436	3.584755	-0.095755	H	-2.112911	-3.139499	-0.467702
H	2.573581	2.939601	-1.694387	H	-1.830479	-1.943210	-1.741326
H	1.309168	3.143043	-0.470309	H	-0.787078	-1.979462	-0.296261
C	4.061563	1.039459	-0.335836	C	-4.176468	-1.153435	-0.484705
H	4.300819	1.008774	-1.401089	H	-4.192748	-0.955441	-1.556705
H	4.736968	1.747773	0.150931	H	-4.633982	-2.130932	-0.305429
H	4.240316	0.047210	0.085276	H	-4.762497	-0.399083	0.041188
C	-3.823688	0.682051	0.422379	C	3.962503	-0.462967	0.487757
H	-4.107803	1.257718	1.302913	H	4.341402	-0.831584	1.440672
C	-3.815648	1.603111	-0.782258	C	3.997055	-1.594403	-0.521700
H	-3.604017	1.063367	-1.704030	H	3.695759	-1.263168	-1.514222
H	-4.798547	2.069292	-0.873555	H	5.017006	-1.978749	-0.580745
H	-3.076021	2.395517	-0.653702	H	3.346535	-2.411311	-0.204140
C	-4.762388	-0.502249	0.287493	C	4.769931	0.754580	0.079456
H	-4.642452	-1.186967	1.128893	H	4.631941	1.564092	0.798447
H	-5.790073	-0.134331	0.296987	H	5.827749	0.484717	0.074166
H	-4.598999	-1.046688	-0.641101	H	4.498501	1.108160	-0.913749
Pc				Rd			
							
H	-3.560349	3.002532	-0.489526	C	-2.961955	-1.481156	-0.137185
C	-2.472766	3.051174	-0.567142	H	-3.831243	-1.177365	0.451749
C	-1.852538	1.725214	-0.176363	H	-2.515424	-2.341524	0.366045
H	-2.112622	3.841393	0.096534	H	-3.276584	-1.755132	-1.142052
H	-2.209554	3.314569	-1.593038	C	-1.978968	-0.350400	-0.183531
C	-0.334285	1.752954	-0.316800	C	-1.348529	0.053377	1.126854
C	0.303244	0.426839	0.058865	H	-0.839370	-0.817028	1.546715
H	0.061118	2.551662	0.317887	H	-2.161016	0.268763	1.826892
H	-0.082695	2.002569	-1.350713	C	-0.456421	1.284676	1.029275
C	1.799367	0.419314	-0.106895	H	0.140649	1.376142	1.940162
H	-0.096056	-0.389427	-0.551783	H	-1.080901	2.175156	0.978497

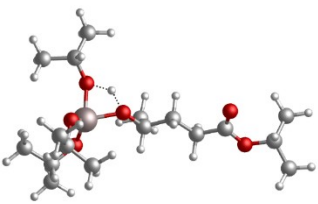
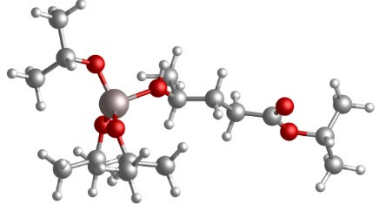
H	0.089404	0.161289	1.097361	C	0.497338	1.443173	-0.139817
O	2.454371	1.343185	-0.532589	O	-1.694522	0.219822	-1.217897
O	2.316248	-0.747672	0.276662	O	0.602804	2.515361	-0.695360
O	-2.238577	1.453498	1.172605	O	1.311318	0.471100	-0.562489
C	-2.989031	-1.805082	0.141169	C	1.431192	-0.863904	-0.003167
O	-2.255666	-1.374212	1.015612	H	0.443992	-1.322482	0.026279
H	-2.249864	0.933531	-0.825365	C	2.283540	-1.620734	-0.999694
H	-2.231646	0.490191	1.302675	H	2.397651	-2.654886	-0.672176
C	-2.667728	-3.077305	-0.581731	H	1.816118	-1.617147	-1.984948
H	-3.551440	-3.714875	-0.642832	H	3.273466	-1.166814	-1.076568
H	-2.380169	-2.825636	-1.606993	C	2.063584	-0.822666	1.372869
H	-1.849035	-3.602232	-0.093597	H	3.031920	-0.320091	1.319988
C	-4.239822	-1.085843	-0.265492	H	1.443535	-0.308703	2.106564
H	-4.275664	-0.981018	-1.351806	H	2.221728	-1.843341	1.725196
H	-5.100868	-1.694243	0.025445				
H	-4.305130	-0.110889	0.214520				
C	3.752742	-0.990030	0.216673				
H	3.813872	-2.002834	0.614117				
C	4.259158	-0.995307	-1.213279				
H	4.294296	0.008303	-1.634580				
H	5.269472	-1.408808	-1.223474				
H	3.628694	-1.626281	-1.842309				
C	4.519902	-0.059714	1.137656				
H	4.039330	-0.005808	2.116176				
H	5.525696	-0.460588	1.277014				
H	4.602737	0.944944	0.726000				
TSd				Pd			
							
C	0.001529	2.597177	-0.530639	C	1.892612	2.251777	-0.429977
H	0.916536	3.175709	-0.685823	H	2.947193	1.978402	-0.498288
H	-0.593587	3.086017	0.239191	H	1.789094	3.060804	0.295673

H	-0.553367	2.554663	-1.467025	H	1.552632	2.613403	-1.401129
C	0.401947	1.232192	-0.084297	C	1.077359	1.070672	0.025801
C	0.986366	0.952041	1.282474	C	1.498495	0.455222	1.359434
H	0.250498	1.089669	2.072918	H	0.989397	0.927347	2.197411
H	1.789863	1.674733	1.441880	H	2.576113	0.574889	1.489384
C	1.515592	-0.479287	1.135382	C	1.144325	-1.015871	1.175419
H	1.059368	-1.190633	1.819037	H	0.110380	-1.231995	1.457100
H	2.596610	-0.525132	1.257735	H	1.797322	-1.718646	1.688173
C	1.212227	-0.879103	-0.311651	C	1.242893	-1.203736	-0.317692
O	0.943190	0.439254	-0.981849	O	1.237641	-0.012544	-0.934852
O	1.843334	-1.696466	-0.963147	O	1.328732	-2.232123	-0.939299
O	-0.422675	-1.333218	-0.332328	O	-1.684423	-1.120290	-0.520793
C	-1.368339	-0.471237	0.044928	C	-2.216857	-0.112477	-0.096032
H	-0.835979	0.666809	0.089094	H	0.013469	1.319856	0.035258
C	-2.419549	-0.221015	-1.014522	C	-2.594632	1.018369	-1.009289
H	-3.114439	0.562108	-0.710454	H	-2.423821	1.983824	-0.530581
H	-1.943334	0.050196	-1.957745	H	-2.047882	0.951729	-1.948620
H	-2.977730	-1.148786	-1.164774	H	-3.667199	0.944159	-1.214501
C	-1.894122	-0.610175	1.458102	C	-2.527652	0.059764	1.362563
H	-2.555240	-1.481104	1.476878	H	-3.535056	0.460073	1.492315
H	-1.092490	-0.780537	2.174742	H	-2.421431	-0.883625	1.894894
H	-2.471406	0.266174	1.754289	H	-1.835071	0.797116	1.781091
R3				TS3			
							
C	-1.049832	-2.321235	-1.459005	C	-1.101171	-2.696884	-1.045402
H	-1.091953	-2.044944	-2.519442	H	-1.140322	-2.628336	-2.135888
H	-2.050178	-2.257165	-1.034594	H	-2.118910	-2.615193	-0.659318
H	-0.659004	-3.336991	-1.402050	H	-0.675115	-3.661595	-0.769846
C	-0.116528	-1.371313	-0.805716	C	-0.250597	-1.558107	-0.546307
C	1.345085	-1.608448	-0.938959	C	1.231735	-1.682881	-0.835995
H	1.547085	-1.827484	-1.991991	H	1.316828	-1.805137	-1.921579

H	1.549910	-2.544861	-0.406714	H	1.607543	-2.603098	-0.385770
C	2.198849	-0.473126	-0.415081	C	2.038921	-0.480433	-0.386648
H	1.986598	-0.272281	0.637537	H	1.958935	-0.321211	0.691157
H	2.000572	0.455140	-0.955225	H	1.682316	0.435113	-0.862089
C	3.667155	-0.779492	-0.531336	C	3.500574	-0.630025	-0.706323
O	-0.513212	-0.380077	-0.178396	O	-0.761813	-0.351099	-0.665609
O	4.125894	-1.824077	-0.933758	O	4.003311	-1.603710	-1.219478
O	4.408247	0.250967	-0.133238	O	4.188733	0.454774	-0.353119
C	5.856892	0.103260	-0.143445	C	5.628047	0.458071	-0.567469
H	6.122265	-0.463214	-1.036506	H	5.819159	-0.032474	-1.522675
C	6.414988	1.506033	-0.222020	C	6.032842	1.913096	-0.631712
H	7.504635	1.462810	-0.254617	H	7.106332	1.985313	-0.812491
H	6.062677	2.015098	-1.119857	H	5.511575	2.426722	-1.440460
H	6.118320	2.086672	0.653941	H	5.806603	2.416606	0.310504
C	6.291777	-0.637754	1.104534	C	6.302351	-0.295955	0.560724
H	6.010524	-0.071999	1.995367	H	6.095971	0.191704	1.515954
H	5.840749	-1.629154	1.157065	H	5.957941	-1.329537	0.607324
H	7.376565	-0.756882	1.098850	H	7.381933	-0.301708	0.401891
C	-1.099915	3.547939	2.587183	C	-1.126217	4.229432	1.406264
H	-0.807695	4.588838	2.433217	H	-1.305000	5.233863	1.016882
H	-0.301879	3.040407	3.136220	H	-0.047664	4.086520	1.515728
H	-2.003748	3.530991	3.199248	H	-1.585586	4.153770	2.393754
C	-1.341540	2.848890	1.260491	C	-1.695749	3.174621	0.473592
H	-2.133720	3.385620	0.721741	H	-2.775988	3.344556	0.371306
C	-0.086581	2.855262	0.397657	C	-1.063363	3.254910	-0.909158
H	0.718546	2.314678	0.902928	H	0.012615	3.073180	-0.839526
H	-0.273750	2.379650	-0.569121	H	-1.496738	2.508730	-1.582418
H	0.248186	3.877600	0.207788	H	-1.220740	4.238577	-1.357350
O	-1.772483	1.523471	1.520520	O	-1.476799	1.896297	1.046737
C	-4.424599	1.037368	-2.904237	C	-5.793961	-0.139813	-0.935122
H	-4.650038	0.597310	-3.878133	H	-6.384020	-0.899879	-1.451603
H	-4.353176	2.122087	-3.021566	H	-6.003262	0.832076	-1.390260
H	-5.250750	0.817337	-2.225458	H	-6.110201	-0.107317	0.109191
C	-3.120121	0.489251	-2.350520	C	-4.309245	-0.445316	-1.031750
H	-3.228777	-0.598735	-2.240370	H	-4.128393	-1.425484	-0.567520

C	-1.958547	0.770911	-3.292834	C	-3.844575	-0.501876	-2.479615
H	-1.857788	1.848961	-3.445932	H	-4.033163	0.457740	-2.969046
H	-1.017565	0.399131	-2.880209	H	-2.773205	-0.706826	-2.533213
H	-2.115447	0.296525	-4.264400	H	-4.371776	-1.284091	-3.030927
O	-2.866114	1.077772	-1.087923	O	-3.590699	0.552492	-0.326883
C	-2.086437	-1.528074	3.068204	C	0.170139	-0.941654	2.678647
H	-1.771913	-2.339868	3.727957	H	1.089131	-1.525408	2.722255
H	-2.859709	-0.945722	3.576065	H	-0.214370	-0.809692	3.694339
H	-1.224340	-0.878407	2.896106	H	0.369269	0.046189	2.260642
C	-2.623916	-2.079213	1.755438	C	-0.900362	-1.650881	1.884948
H	-1.809375	-2.628992	1.259558	H	-0.254869	-1.822082	0.747212
C	-3.774657	-3.044038	1.982819	C	-1.173841	-3.084187	2.254249
H	-4.593830	-2.533343	2.496055	H	-1.600478	-3.089031	3.261539
H	-4.149047	-3.421854	1.029076	H	-1.898043	-3.527164	1.571345
H	-3.459534	-3.894277	2.591153	H	-0.256690	-3.672319	2.263327
O	-3.067553	-1.037478	0.905446	O	-1.971127	-0.934169	1.598204
Al	-2.191853	0.341952	0.325083	Al	-2.025203	0.391350	0.387791
P3				R4			
							
C	-0.913485	-3.073435	-0.655874	C	0.703482	1.233657	-1.548378
H	-0.982005	-3.045630	-1.746368	H	1.512189	1.148427	-2.276743
H	-1.925319	-3.041473	-0.244986	H	0.742283	2.229257	-1.097628
H	-0.454668	-4.019593	-0.359994	H	-0.238170	1.136472	-2.094672
C	-0.099750	-1.893189	-0.149845	C	0.804773	0.164345	-0.468955
C	1.323037	-1.923844	-0.697437	C	2.086027	0.279401	0.350195
H	1.277818	-1.844123	-1.787838	H	2.054601	-0.483938	1.130944
H	1.780804	-2.886551	-0.456828	H	2.097980	1.252817	0.849049
C	2.163485	-0.795460	-0.127588	C	3.343606	0.099432	-0.484514
H	2.225837	-0.865780	0.963148	H	3.486257	0.924959	-1.187014
H	1.713556	0.176351	-0.347445	H	3.292015	-0.811815	-1.087177
C	3.572455	-0.772870	-0.648375	C	4.594220	0.026069	0.347418

O	-0.706494	-0.675729	-0.515762	O	-0.288703	0.247828	0.424859
O	4.037903	-1.559991	-1.441432	O	4.649390	0.213690	1.541397
O	4.269427	0.238902	-0.125655	O	5.661139	-0.273276	-0.397274
C	5.666420	0.382490	-0.500701	C	6.957829	-0.351508	0.256407
H	5.747004	0.157970	-1.564921	H	6.807413	-0.816913	1.230858
C	6.016774	1.829646	-0.237367	C	7.811255	-1.236889	-0.623498
H	7.059386	2.008954	-0.503839	H	8.796178	-1.361967	-0.171557
H	5.388678	2.495232	-0.830823	H	7.357194	-2.221771	-0.739061
H	5.883854	2.067404	0.820243	H	7.938125	-0.788572	-1.611005
C	6.503872	-0.585095	0.310761	C	7.523645	1.044910	0.418828
H	6.393117	-0.374681	1.376856	H	7.644036	1.518920	-0.557748
H	6.211894	-1.618285	0.120363	H	6.875254	1.666882	1.036650
H	7.556205	-0.472315	0.044602	H	8.502326	0.989371	0.898246
C	-1.224328	4.303091	0.125702	H	0.800712	-0.820265	-0.958245
H	-1.419473	5.146809	-0.539509	C	-2.252749	-2.597941	1.910990
H	-0.144912	4.226766	0.283733	H	-2.600080	-3.569673	2.268998
H	-1.699383	4.505813	1.087607	H	-1.448016	-2.253474	2.566043
C	-1.755171	3.008708	-0.465397	H	-1.843126	-2.741790	0.906058
H	-2.836430	3.115683	-0.626890	C	-3.388836	-1.583764	1.900084
C	-1.100383	2.698621	-1.805279	H	-4.179801	-1.957319	1.233894
H	-0.022269	2.568919	-1.675657	C	-3.980418	-1.396225	3.286376
H	-1.508004	1.779107	-2.237753	H	-3.210282	-1.041896	3.976610
H	-1.271188	3.505299	-2.521630	H	-4.784380	-0.657993	3.259856
O	-1.525073	1.958041	0.459177	H	-4.385689	-2.334910	3.669683
C	-5.643935	-0.743899	-1.155233	O	-2.945624	-0.326909	1.420465
H	-6.139482	-1.597682	-1.622461	C	-4.536688	-1.005687	-1.710651
H	-5.919683	0.159987	-1.705183	H	-5.410976	-1.616523	-1.946015
H	-6.011651	-0.649123	-0.131731	H	-4.447811	-0.224402	-2.471808
C	-4.134727	-0.915924	-1.167325	H	-4.711581	-0.528922	-0.741642
H	-3.888811	-1.830624	-0.609854	C	-3.272839	-1.855269	-1.682401
C	-3.602834	-1.057939	-2.585978	H	-3.396063	-2.630929	-0.913372
H	-3.863366	-0.171642	-3.171435	C	-3.034029	-2.539163	-3.016728
H	-2.515554	-1.159044	-2.579254	H	-2.922887	-1.791111	-3.806280
H	-4.027264	-1.935934	-3.078808	H	-2.122122	-3.138000	-2.979456
O	-3.542905	0.203284	-0.531466	H	-3.867960	-3.195234	-3.274463

C	-0.074646	0.285016	2.839752	O	-2.137011	-1.067900	-1.365587
H	0.645924	-0.254071	3.454421	Al	-1.951699	-0.044873	0.026380
H	-0.209727	1.278212	3.284060	C	-2.722900	4.001652	-0.305836
H	0.287096	0.406004	1.819828	H	-3.044540	4.812505	0.348907
C	-1.395557	-0.387220	2.885666	H	-3.190354	4.143905	-1.283332
H	-0.036198	-1.966142	0.947933	H	-1.639810	4.053184	-0.418016
C	-1.819483	-1.059127	4.133723	C	-3.139449	2.677369	0.290024
H	-1.543390	-0.453102	4.997843	H	-2.630142	2.506228	1.238801
H	-2.884148	-1.278112	4.121629	C	-4.634181	2.523308	0.451920
H	-1.251966	-1.994016	4.204070	H	-5.134561	2.625328	-0.514564
O	-2.157891	-0.395649	1.906326	H	-4.877878	1.551980	0.882317
Al	-1.962038	0.300856	0.170164	H	-5.010315	3.302897	1.116136
				O	-2.635169	1.602920	-0.573947
				H	-3.046607	1.634634	-1.453167
TS4				P4			
							
C	0.675844	0.631874	-2.100205	C	0.529750	1.646124	-1.906064
H	1.452759	0.200557	-2.732891	H	1.298844	1.338782	-2.615687
H	0.827997	1.713757	-2.050716	H	0.703441	2.690747	-1.635793
H	-0.287781	0.434385	-2.574484	H	-0.439119	1.559719	-2.399462
C	0.715177	0.030024	-0.707438	C	0.571056	0.764642	-0.679291
C	1.975002	0.380116	0.069755	C	1.825265	0.895322	0.164817
H	1.882295	-0.036390	1.075295	H	1.709255	0.271934	1.053545
H	2.032694	1.467666	0.170286	H	1.929092	1.931869	0.498275
C	3.236254	-0.153206	-0.589178	C	3.065411	0.465884	-0.603173
H	3.417142	0.321940	-1.557568	H	3.285194	1.146685	-1.429859
H	3.163819	-1.227358	-0.780072	H	2.937616	-0.527281	-1.041618
C	4.467044	0.089873	0.240944	C	4.291558	0.434946	0.268043
O	-0.405031	0.497557	0.056478	O	-0.572915	1.081605	0.177491
O	4.506107	0.769057	1.241578	O	4.344039	0.844905	1.404841
O	5.532099	-0.531145	-0.268235	O	5.331349	-0.099434	-0.371636

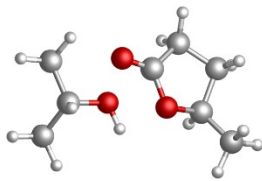
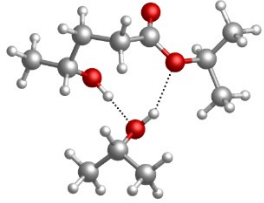
C	6.817198	-0.341315	0.386743	C	6.610660	-0.153348	0.320526
H	6.638427	-0.321951	1.462075	H	6.409722	-0.405313	1.362089
C	7.657168	-1.541944	0.013888	C	7.397179	-1.257894	-0.348184
H	8.632834	-1.466911	0.496542	H	8.365601	-1.364521	0.142490
H	7.180497	-2.467033	0.340361	H	6.867762	-2.208745	-0.277776
H	7.808375	-1.583334	-1.066700	H	7.566847	-1.024315	-1.401195
C	7.421301	0.969352	-0.074613	C	7.288032	1.198304	0.222865
H	7.575119	0.952513	-1.155800	H	7.478720	1.448972	-0.822882
H	6.779171	1.813502	0.178755	H	6.676256	1.982332	0.669903
H	8.388289	1.118471	0.408770	H	8.242803	1.167610	0.750180
H	0.622299	-1.058809	-0.776621	H	0.408556	-0.277491	-0.954853
C	-1.880079	-2.392889	1.970847	C	-0.515700	-1.922781	1.778991
H	-2.024590	-3.377131	2.421431	H	-0.107260	-2.888686	2.084232
H	-1.054972	-1.892933	2.485855	H	-0.104160	-1.149278	2.432861
H	-1.594643	-2.549628	0.924657	H	-0.179803	-1.728471	0.755746
C	-3.145352	-1.552896	2.076163	C	-2.036101	-1.925506	1.863598
H	-3.954048	-2.069515	1.541484	H	-2.418051	-2.701857	1.186505
C	-3.567060	-1.357589	3.520951	C	-2.511286	-2.246192	3.270760
H	-2.776301	-0.842632	4.072880	H	-2.131998	-1.499861	3.973919
H	-4.475724	-0.754823	3.574984	H	-3.602019	-2.237011	3.314150
H	-3.759944	-2.317807	4.003530	H	-2.161914	-3.231067	3.587735
O	-2.949132	-0.275347	1.486102	O	-2.568208	-0.672264	1.480750
C	-4.858050	-1.319071	-1.314180	C	-3.654935	-2.437102	-1.492799
H	-5.662027	-2.050482	-1.422503	H	-3.717471	-3.514663	-1.661067
H	-4.994053	-0.539499	-2.068852	H	-4.327384	-1.935714	-2.194242
H	-4.950700	-0.864249	-0.323635	H	-4.000078	-2.229205	-0.476785
C	-3.498547	-1.979673	-1.486538	C	-2.232221	-1.935340	-1.690523
H	-3.380684	-2.745543	-0.707881	H	-1.576637	-2.466444	-0.985907
C	-3.369969	-2.647209	-2.843565	C	-1.736548	-2.209879	-3.100376
H	-3.494923	-1.906156	-3.637450	H	-2.376096	-1.700118	-3.825799
H	-2.385639	-3.106685	-2.952262	H	-0.715507	-1.842751	-3.225392
H	-4.128271	-3.422628	-2.969323	H	-1.747749	-3.279811	-3.318242
O	-2.454617	-1.024894	-1.353879	O	-2.158244	-0.541993	-1.447550
Al	-2.179091	0.032766	-0.024339	Al	-2.280830	0.292406	0.068182
C	-2.298501	4.209663	-0.099681	C	-4.972411	3.329272	0.457778

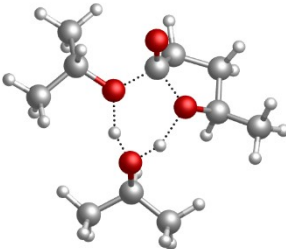
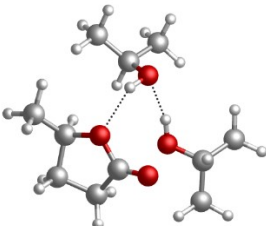
H	-2.776872	5.026752	0.443207	H	-5.993467	3.464282	0.820473
H	-2.473558	4.352115	-1.168766	H	-4.925901	3.667892	-0.580699
H	-1.224118	4.254627	0.088392	H	-4.309656	3.957669	1.055915
C	-2.864965	2.878281	0.348436	C	-4.550917	1.873141	0.548889
H	-2.678805	2.739669	1.418578	H	-4.619153	1.555415	1.598025
C	-4.350042	2.751500	0.074774	C	-5.459921	0.977943	-0.281974
H	-4.546017	2.852759	-0.995425	H	-5.402484	1.258710	-1.337138
H	-4.724336	1.781560	0.411048	H	-5.165781	-0.071463	-0.187611
H	-4.900731	3.530244	0.605272	H	-6.498459	1.062995	0.045472
O	-2.183156	1.831570	-0.362684	O	-3.205292	1.761483	0.117773
H	-0.989501	1.551293	-0.183549	H	-0.527834	1.997544	0.497489

3. The structures of reactants, TS and products in Ring-closure step

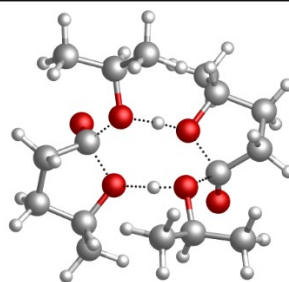
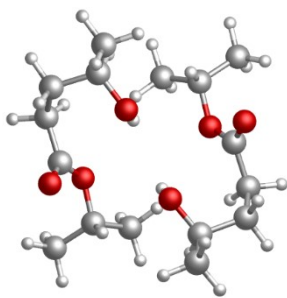
Table S 3 The snapshots and coordinates of of reactants, TS and products optimized at M06-2X-D3/def2-tzvp SMD=2-propanol level in the ring-closure.

Re				TSe			
C	3.897402	0.646184	-0.378694	C	-3.295539	1.301899	0.307860
H	3.861001	0.276302	-1.405952	H	-3.477605	0.876550	1.297152
H	4.674895	0.102012	0.161678	H	-4.199680	1.184810	-0.293420
H	4.175095	1.702493	-0.398849	H	-3.089811	2.367723	0.416420
C	2.549089	0.460592	0.291446	C	-2.136485	0.591384	-0.352882
C	2.123654	-0.996739	0.330673	C	-2.347082	-0.911926	-0.528322
H	2.850314	-1.552024	0.925952	H	-3.002954	-1.134193	-1.369399
H	2.143138	-1.409637	-0.681989	H	-2.792621	-1.322264	0.382279
C	0.733244	-1.179140	0.934639	C	-0.942786	-1.475285	-0.720298
H	0.632350	-0.617648	1.863669	H	-0.564121	-1.238317	-1.714218
H	0.561241	-2.235197	1.160638	H	-0.882755	-2.549585	-0.555605
C	-0.362186	-0.781544	-0.018760	C	-0.092222	-0.790640	0.331014
O	-0.427455	-1.154916	-1.168987	O	0.285811	-1.240760	1.382183
O	-1.287701	-0.011575	0.554267	O	0.973904	0.175450	-0.443554

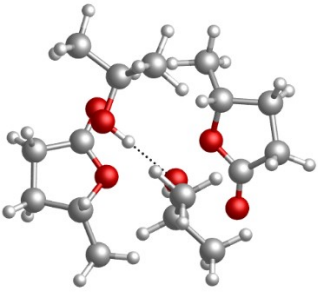
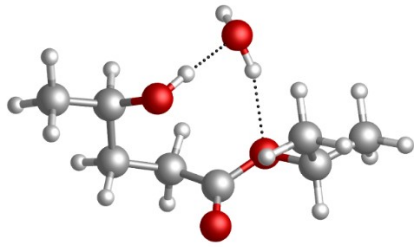
C	-2.424399	0.404900	-0.250307	C	2.258845	0.353597	0.195295
H	-2.056344	0.610902	-1.256142	H	2.095039	0.361172	1.275209
C	-3.452041	-0.708221	-0.277482	C	3.145515	-0.811344	-0.190776
H	-4.311420	-0.401742	-0.876302	H	4.112457	-0.721657	0.307309
H	-3.038969	-1.618832	-0.712327	H	2.694582	-1.759708	0.104745
H	-3.797177	-0.924574	0.736041	H	3.310195	-0.818828	-1.270605
C	-2.943143	1.671753	0.391269	C	2.807609	1.691198	-0.255783
H	-3.270892	1.476108	1.414452	H	2.941363	1.704431	-1.339460
H	-2.170059	2.441297	0.408984	H	2.137747	2.504809	0.027917
H	-3.793855	2.048633	-0.178489	H	3.776891	1.865480	0.214241
O	1.526021	1.171652	-0.414891	O	-0.965653	0.694688	0.468663
H	1.728844	2.114213	-0.380908	H	0.121314	0.908259	-0.129655
H	2.595202	0.839700	1.319730	H	-1.919664	1.042985	-1.327898
Pe				Rf			
							
C	3.126374	1.608411	-0.341029	C	3.052973	-2.531857	-0.615166
H	3.744888	1.016413	-1.018322	H	2.578988	-3.350076	-1.163295
H	3.755519	1.976777	0.471434	H	3.626525	-2.956779	0.210669
H	2.724434	2.466322	-0.881303	H	3.741295	-2.017751	-1.288097
C	2.021726	0.761552	0.232951	C	1.996727	-1.574663	-0.101302
C	2.472178	-0.497400	0.970292	C	1.065513	-2.252445	0.899579
H	2.667696	-0.297131	2.021573	H	1.656004	-2.563260	1.764087
H	3.383001	-0.884049	0.508153	H	0.640730	-3.155190	0.451326
C	1.307835	-1.452161	0.734115	C	-0.057662	-1.334305	1.371493
H	0.520618	-1.332320	1.482598	H	0.318814	-0.335986	1.600350
H	1.573925	-2.505084	0.672042	H	-0.503606	-1.730619	2.288827
C	0.746645	-0.975810	-0.582011	C	-1.198885	-1.237277	0.394217
O	0.016506	-1.562432	-1.341175	O	-1.693458	-2.180645	-0.176751
O	-1.360386	0.598942	0.825308	O	-1.657855	0.015085	0.266807
C	-2.409542	0.304672	-0.108123	C	-2.847496	0.235606	-0.545790
H	-1.967211	0.178638	-1.102323	H	-2.778479	-0.422402	-1.412046

C	-3.026657	-1.004952	0.333911	C	-4.074200	-0.094611	0.279384
H	-3.806619	-1.313329	-0.364200	H	-4.972568	0.072298	-0.317284
H	-2.271747	-1.792195	0.375267	H	-4.066112	-1.136582	0.601056
H	-3.472921	-0.895882	1.325771	H	-4.119611	0.548529	1.161094
C	-3.419983	1.436853	-0.146061	C	-2.794792	1.684123	-0.975410
H	-3.876225	1.570642	0.838043	H	-2.788847	2.343295	-0.104072
H	-2.939751	2.374172	-0.437077	H	-1.906361	1.882662	-1.576582
H	-4.209915	1.223840	-0.869127	H	-3.674546	1.917488	-1.576810
O	1.199484	0.255870	-0.860465	O	1.265609	-1.074612	-1.222485
H	-0.944245	1.427811	0.557398	H	1.034025	-0.143785	-1.041714
H	1.362263	1.359340	0.866455	H	2.485162	-0.730057	0.401907
				C	2.935450	2.254092	-0.391699
				H	3.734000	2.671776	0.223146
				H	2.771924	2.915388	-1.246200
				H	3.259022	1.279401	-0.763517
				C	1.661927	2.124232	0.414807
				H	1.833201	1.445800	1.258790
				C	1.157559	3.456589	0.936020
				H	0.988498	4.148301	0.107356
				H	0.217364	3.326892	1.477636
				H	1.884526	3.899596	1.619512
				O	0.685321	1.531435	-0.455676
				H	-0.139557	1.384053	0.031906
TSf				Pf			
							
C	3.056291	-1.855381	-0.449599	C	-3.719541	-0.208205	0.116095
H	2.829497	-2.592247	-1.222899	H	-4.130754	-0.999723	0.745352
H	3.764404	-2.293972	0.256951	H	-4.366516	-0.084074	-0.754597
H	3.532827	-0.992409	-0.918383	H	-3.717315	0.725060	0.679531
C	1.791738	-1.456135	0.273047	C	-2.335887	-0.580885	-0.347152
C	1.019816	-2.603834	0.909153	C	-2.238419	-1.923353	-1.070124

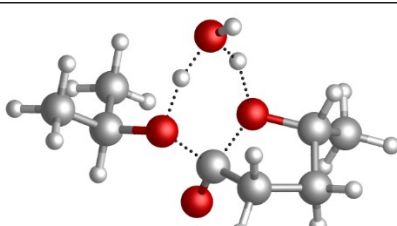
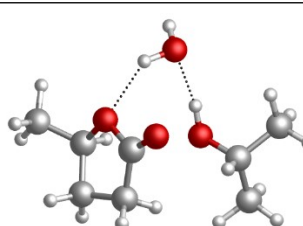
H	1.445641	-2.896845	1.868240	H	-2.385425	-1.811311	-2.142172
H	1.032056	-3.468535	0.239998	H	-2.998267	-2.601994	-0.677346
C	-0.386057	-2.029973	1.017445	C	-0.844803	-2.410221	-0.691391
H	-0.439438	-1.315166	1.840323	H	-0.076631	-2.011692	-1.359199
H	-1.159428	-2.785341	1.144467	H	-0.728464	-3.489640	-0.625336
C	-0.587096	-1.312262	-0.327523	C	-0.619449	-1.772560	0.654676
O	-1.144095	-1.902530	-1.284268	O	0.161800	-2.077748	1.517103
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C	-2.593615	0.221455	-0.305649	C	2.746519	-0.690804	0.132730
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C	-2.892684	1.708275	-0.308284	C	3.884951	0.315697	0.158697
H	-2.682501	2.144641	0.671472	H	4.159953	0.599816	-0.860509
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H	0.977126	0.549013	-0.841020	H	-0.605177	1.121491	1.072658
H	2.013231	-0.698363	1.035640	H	-1.888126	0.216949	-0.945889
C	2.741610	2.207713	0.105916	C	-1.577516	3.219159	-0.062868
H	3.264832	2.684415	0.935752	H	-1.840530	3.800482	-0.948705
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H	1.031791	1.615848	1.273396	H	-0.272595	1.889189	-1.124118
C	0.654856	3.585200	0.492578	C	0.897429	3.541880	-0.436584
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H	-0.423041	3.530657	0.653170	H	1.849336	3.022220	-0.564832
H	1.101205	4.107790	1.339765	H	0.718353	4.154971	-1.321155
O	0.598785	1.529106	-0.743682	O	0.106569	1.758864	0.903613
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Rg				TSg			

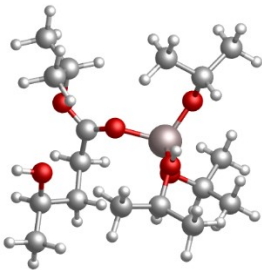
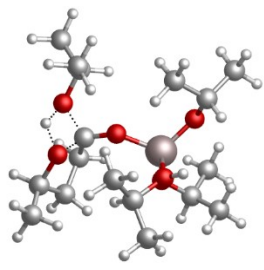


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H	2.195049	-4.175976	2.282921	H	2.333436	3.698941	-2.003501
H	0.483329	-3.734095	2.410402	H	0.644378	3.160568	-1.997103
C	1.615509	-2.515237	1.039410	C	1.957509	2.042777	-0.706089
C	3.035178	-2.003339	0.827563	C	3.372984	1.477310	-0.592648
H	3.693917	-2.862459	0.684713	H	4.035495	2.179489	-0.090266
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C	3.147826	-1.082307	-0.383514	C	3.201199	0.175355	0.184921
H	2.601774	-1.484514	-1.238332	H	2.976734	0.372320	1.232920
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O	2.989630	0.968432	0.868660	O	2.034087	-1.152941	-1.483896
O	1.964472	0.824793	-1.120256	O	0.993911	-1.090173	0.689359
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H	2.605151	4.105946	-1.528924	H	2.757488	-3.775487	1.694981
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H	-0.382874	1.787307	-1.739240	H	-0.760807	-2.543021	1.909719
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O	0.697323	-1.421397	1.161217	O	1.094294	0.865054	-0.673875
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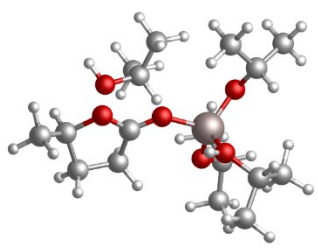
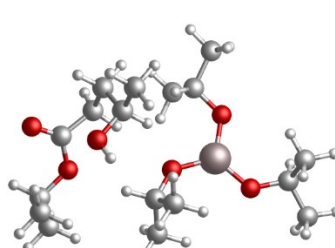
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C	-3.158552	1.118426	-0.298561	C	-3.146386	-0.184554	0.343628
H	-2.640480	1.515148	-1.172837	H	-2.883458	-0.475859	1.362366
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O	-3.010823	-0.952549	0.921445	O	-2.104651	1.169993	-1.371551
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H	-1.411465	-2.494983	-0.078367	H	-0.849098	3.036784	0.247189
C	-2.936137	-3.003941	-1.513114	C	-2.586618	2.671674	1.452082
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C	-0.553886	-2.377957	-2.053016	C	-0.220770	2.578979	2.262359
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Pg				Rh			
							
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H	-2.346382	-3.836865	-0.274515	H	-4.562499	0.181001	0.150881

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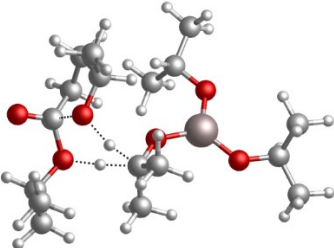
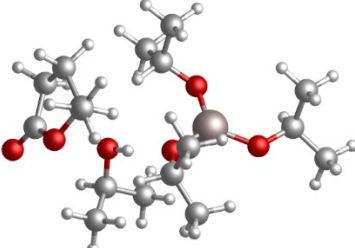
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O	1.743330	0.308786	-1.574984				
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C	-2.281882	0.505730	-0.128808	C	-2.097492	-0.160415	-0.729227
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H	0.233171	1.858083	-2.222468	H	0.314169	3.311848	-0.862339
R5				TS5			
							
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H	-3.476555	-4.178331	-0.425875	H	-3.551324	-3.894677	0.203633
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C	-3.224623	-2.039220	-0.364762	C	-3.028377	-1.941186	-0.451856
C	-1.962035	-1.948302	-1.200628	C	-1.951229	-2.224628	-1.489975
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C	-1.852841	-0.601447	-1.919384	C	-1.615037	-0.838572	-2.036813
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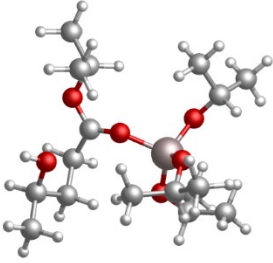
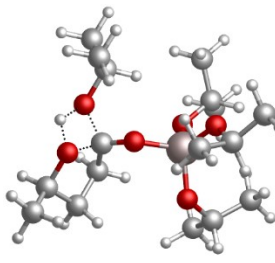
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H	-2.882099	4.707566	-0.249319	H	-2.758555	4.486069	-1.129053
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C	-2.679673	2.364543	1.257060	C	-2.427738	2.698572	0.964413
H	-3.749465	2.148784	1.280712	H	-3.491289	2.612430	1.201290
H	-2.134079	1.516320	1.670991	H	-1.872506	1.956551	1.539481
H	-2.487635	3.236695	1.884349	H	-2.089572	3.691440	1.264528
O	-3.134995	-0.976838	0.592442	O	-2.575494	-0.669230	0.142103
H	-3.983036	-0.886157	1.044148	H	-3.167290	0.380062	-0.140356
H	-4.090348	-1.858271	-1.012057	H	-3.981818	-1.729848	-0.940166
C	2.072546	-2.742823	2.506731	C	0.921708	-2.960615	2.543870
H	1.846195	-3.794740	2.685944	H	0.163025	-3.673254	2.870929
H	2.189636	-2.249211	3.474694	H	1.534446	-2.692216	3.407919
H	3.010432	-2.676399	1.955506	H	1.550653	-3.440795	1.793974
C	0.939604	-2.117410	1.731173	C	0.244571	-1.737307	1.975965
H	0.840296	-2.576840	0.747325	H	-0.306162	-1.993972	1.069076
C	-0.377220	-2.105828	2.467417	C	-0.649163	-1.013506	2.954347
H	-0.269264	-1.590619	3.425359	H	-0.084317	-0.724210	3.844220
H	-1.154307	-1.613822	1.880717	H	-1.083503	-0.122297	2.499836
H	-0.685602	-3.133217	2.667469	H	-1.461807	-1.673191	3.263590
O	1.313019	-0.720812	1.414964	O	1.277335	-0.806938	1.493339
C	3.205670	-0.487555	-2.929245	C	3.353444	-0.622218	-2.866540
H	4.065712	-0.914537	-3.449456	H	4.280856	-0.998756	-3.303534
H	3.555356	0.342213	-2.308444	H	3.566056	0.329121	-2.370911
H	2.512309	-0.093638	-3.674650	H	2.640154	-0.441579	-3.672918
C	2.524245	-1.538589	-2.069364	C	2.783968	-1.616148	-1.867487
H	2.208473	-2.367356	-2.711186	H	2.598720	-2.564073	-2.383968
C	3.455564	-2.081337	-0.997890	C	3.751729	-1.872980	-0.721716
H	3.789793	-1.272656	-0.338180	H	3.977308	-0.939784	-0.194274
H	2.949445	-2.839558	-0.397113	H	3.331758	-2.585842	-0.009161

H	4.342061	-2.534901	-1.445983	H	4.693084	-2.280144	-1.096526
O	1.343387	-1.006397	-1.481896	O	1.528058	-1.157434	-1.387189
C	3.450413	3.387220	0.602022	C	3.291966	3.414887	0.616532
H	3.744969	4.006528	1.451639	H	3.508310	4.086929	1.449254
H	3.025548	4.035052	-0.169060	H	2.791058	3.984520	-0.170641
H	4.343353	2.907337	0.197734	H	4.237763	3.038907	0.221857
C	2.430057	2.346769	1.023867	C	2.408897	2.264720	1.062960
H	2.880431	1.710441	1.797895	H	2.926614	1.715383	1.861912
C	1.175439	2.991490	1.594377	C	1.074294	2.756218	1.603505
H	0.732218	3.666388	0.857739	H	0.521560	3.276476	0.816263
H	0.430787	2.237091	1.866690	H	0.464270	1.920987	1.960061
H	1.412530	3.568317	2.490834	H	1.222071	3.444337	2.438719
O	2.113436	1.539719	-0.102840	O	2.216172	1.390980	-0.040191
Al	1.153955	0.126816	-0.216629	Al	1.198408	0.014732	-0.174992
H	1.497612	-0.216841	2.226358	H	1.854973	-0.494208	2.208789
P5				R5'			
							
C	4.809357	-2.284063	-1.351500	C	-1.164266	2.434390	2.884199
H	4.243602	-3.192724	-1.562928	H	-2.083301	2.918469	3.223275
H	5.713980	-2.557191	-0.805619	H	-0.424361	3.206785	2.662086
H	5.101718	-1.812023	-2.289536	H	-0.776562	1.817489	3.698190
C	4.002552	-1.344439	-0.501928	C	-1.434106	1.588826	1.654665
C	3.482000	-1.905301	0.819301	C	-2.008074	2.399510	0.506403
H	4.162800	-1.680232	1.636349	H	-1.313680	3.208826	0.270911
H	3.367001	-2.987072	0.738676	H	-2.951069	2.857617	0.818929
C	2.116851	-1.236801	0.981687	C	-2.221819	1.547093	-0.743041
H	2.146604	-0.317368	1.570999	H	-1.327010	0.963779	-0.966501
H	1.336635	-1.876962	1.391322	H	-2.434774	2.189322	-1.602147
C	1.783511	-0.856158	-0.421714	C	-3.404182	0.623363	-0.615195
O	0.683451	-0.464565	-0.865650	O	-4.512892	0.978392	-0.281079
O	2.906522	1.602556	0.148867	O	-3.113709	-0.627504	-0.974200

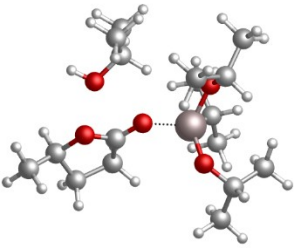
C	1.739426	2.401724	0.384453	C	-4.157344	-1.633342	-0.876620
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C	2.027851	3.487727	1.403625	C	-3.742873	-2.749324	-1.808379
H	1.120188	4.046937	1.639209	H	-4.503972	-3.531019	-1.805037
H	2.418981	3.057848	2.327526	H	-3.627836	-2.381075	-2.828670
H	2.766513	4.190498	1.007156	H	-2.796599	-3.185023	-1.480622
C	1.207039	2.959932	-0.922479	C	-4.281242	-2.085712	0.564725
H	1.925852	3.667396	-1.346981	H	-3.333839	-2.510003	0.907485
H	1.041923	2.157937	-1.644185	H	-4.556004	-1.257243	1.217685
H	0.263017	3.485914	-0.765142	H	-5.051841	-2.854755	0.641547
O	2.763805	-0.997830	-1.240616	O	-2.384165	0.554439	1.941667
H	3.561158	2.151236	-0.303864	H	-1.979119	-0.076588	2.549955
H	4.508069	-0.390310	-0.358491	H	-0.501706	1.122180	1.315372
C	-3.336109	2.410686	-2.147411	C	5.289797	-0.228850	1.143539
H	-3.904108	2.464394	-3.078213	H	6.359468	-0.009903	1.147771
H	-2.705635	3.300783	-2.072794	H	5.045249	-0.789356	2.049377
H	-4.039340	2.413340	-1.312321	H	4.750191	0.721796	1.164889
C	-2.475400	1.162254	-2.112714	C	4.911340	-1.036512	-0.086113
H	-3.129442	0.282287	-2.186819	H	5.156385	-0.455304	-0.982523
C	-1.484851	1.125058	-3.264788	C	5.644694	-2.362624	-0.140865
H	-0.823202	1.993685	-3.222157	H	5.403921	-2.958450	0.743312
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O	-1.792044	1.123053	-0.866052	O	3.507748	-1.304150	-0.076584
C	-2.586608	-3.749532	0.245549	C	2.175461	3.734934	-0.906223
H	-3.506591	-4.288039	0.477898	H	1.426002	4.517925	-1.039643
H	-2.056886	-3.540835	1.177624	H	2.973415	3.889644	-1.636952
H	-1.966247	-4.389234	-0.384565	H	2.598943	3.830223	0.095293
C	-2.929226	-2.459777	-0.458970	C	1.554225	2.364989	-1.096117
H	-3.424262	-2.644473	-1.411801	H	0.752231	2.234147	-0.358671
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H	-3.272777	-1.369370	1.366212	H	1.753036	2.313798	-3.239980
H	-3.876672	-0.543469	-0.100469	H	0.527545	1.200421	-2.604010
H	-4.726244	-1.945630	0.547767	H	0.192283	2.937277	-2.673511
O	-1.665208	-1.775373	-0.810976	O	2.560783	1.375107	-0.867300

C	-1.598907	-0.280220	3.817690	C	0.069437	-2.959176	-0.184200
H	-2.184987	0.233573	4.582198	H	-0.521430	-3.746601	0.288965
H	-0.579406	-0.408394	4.191194	H	1.120109	-3.265418	-0.171665
H	-2.034129	-1.268716	3.655450	H	-0.251221	-2.860642	-1.222852
C	-1.582090	0.515419	2.525671	C	-0.099628	-1.642008	0.551753
H	-2.614529	0.638585	2.173859	H	-1.154822	-1.353401	0.534644
C	-0.975030	1.895010	2.716838	C	0.362308	-1.734522	1.996262
H	0.063509	1.807443	3.048411	H	1.413666	-2.036745	2.041760
H	-0.997350	2.459765	1.781361	H	0.257715	-0.768966	2.497973
H	-1.532265	2.458046	3.468835	H	-0.226861	-2.473686	2.543719
O	-0.837188	-0.218118	1.558521	O	0.601687	-0.609469	-0.128663
Al	-0.970194	-0.190964	-0.145597	Al	2.233706	-0.212668	-0.341849
H	-1.131290	-2.317162	-1.414242				
TS5'				P5'			
							
C	-2.089608	1.935181	3.026486	C	-2.768161	0.348793	2.990100
H	-3.169684	2.096993	3.013210	H	-3.823068	0.425172	3.261725
H	-1.601872	2.858340	3.348529	H	-2.218134	1.131800	3.515944
H	-1.859380	1.153303	3.752634	H	-2.386241	-0.620301	3.316042
C	-1.608009	1.552545	1.645631	C	-2.602347	0.531969	1.504160
C	-1.913488	2.594813	0.560211	C	-3.118839	1.857613	0.946161
H	-1.100013	3.312655	0.458434	H	-2.343378	2.622295	0.958515
H	-2.824505	3.142398	0.813569	H	-3.964765	2.200471	1.545709
C	-2.138769	1.750690	-0.686897	C	-3.577253	1.475644	-0.456907
H	-1.192924	1.347882	-1.054011	H	-2.771631	1.547896	-1.191243
H	-2.655457	2.274564	-1.489547	H	-4.440451	2.025462	-0.826125
C	-3.024313	0.630859	-0.149208	C	-3.912740	0.011954	-0.319340
O	-4.246836	0.821730	0.011711	O	-4.567493	-0.677898	-1.061156
O	-2.663877	-0.652174	-0.870433	O	-1.373650	-0.554040	-1.487719
C	-3.726832	-1.633274	-0.969296	C	-1.346686	-1.779919	-2.222600
H	-4.632715	-1.071150	-1.190281	H	-2.075907	-1.648310	-3.025755

C	-3.406632	-2.549719	-2.132791	C	0.031136	-2.004976	-2.825950
H	-4.267504	-3.190672	-2.332170	H	0.036979	-2.887530	-3.469215
H	-3.195735	-1.970122	-3.032891	H	0.334699	-1.141449	-3.420989
H	-2.551276	-3.190515	-1.915690	H	0.770508	-2.165298	-2.033561
C	-3.895095	-2.377881	0.343059	C	-1.775203	-2.937800	-1.337656
H	-2.976640	-2.909120	0.607947	H	-1.069028	-3.054742	-0.509760
H	-4.148677	-1.692324	1.152258	H	-2.769373	-2.761503	-0.923704
H	-4.696293	-3.113731	0.250321	H	-1.794771	-3.871770	-1.903269
O	-2.259128	0.338323	1.214464	O	-3.398257	-0.478028	0.817813
H	-1.355903	-0.661345	0.767288	H	-0.748988	-1.861150	1.727982
H	-0.532106	1.351607	1.662101	H	-1.564931	0.366833	1.201181
C	5.201904	-0.486440	1.306730	C	4.896996	1.293137	0.660441
H	6.292383	-0.437276	1.332028	H	5.820089	1.816692	0.403640
H	4.854133	-0.969812	2.223049	H	4.993935	0.893104	1.672907
H	4.819329	0.537227	1.283432	H	4.082742	2.023348	0.648404
C	4.730174	-1.267026	0.092705	C	4.627057	0.165634	-0.321302
H	5.070885	-0.754431	-0.814024	H	4.512701	0.588490	-1.325685
C	5.260365	-2.687011	0.087606	C	5.749259	-0.853921	-0.338241
H	4.926369	-3.214655	0.984605	H	5.880749	-1.283274	0.658309
H	4.900741	-3.228436	-0.789021	H	5.524922	-1.661749	-1.036722
H	6.351804	-2.688661	0.070373	H	6.687420	-0.385377	-0.641535
O	3.301183	-1.326940	0.079108	O	3.417394	-0.508942	0.035873
C	2.417713	3.850192	-0.799552	C	0.502276	3.398406	0.240693
H	1.724840	4.673853	-0.982721	H	-0.373833	4.047563	0.298784
H	3.259202	3.944278	-1.490616	H	1.369909	4.010273	-0.018966
H	2.795037	3.936107	0.220836	H	0.670649	2.958132	1.227736
C	1.724069	2.518126	-1.002547	C	0.301273	2.311564	-0.800590
H	0.878939	2.447881	-0.306568	H	-0.530739	1.669817	-0.485432
C	1.202692	2.355492	-2.419348	C	-0.015252	2.873891	-2.171596
H	2.025046	2.433394	-3.135159	H	0.805905	3.508162	-2.515773
H	0.723055	1.381464	-2.548202	H	-0.157920	2.065733	-2.891651
H	0.465852	3.128626	-2.648842	H	-0.927057	3.473987	-2.140896
O	2.655419	1.471318	-0.704514	O	1.492749	1.527865	-0.894255
C	-0.218182	-2.586560	-0.529050	C	1.146033	-2.858799	1.586524
H	-0.905285	-3.374031	-0.218869	H	0.941506	-3.535066	2.418977

H	0.803219	-2.967523	-0.444420	H	2.211780	-2.613561	1.596116
H	-0.411609	-2.326148	-1.570276	H	0.918301	-3.380685	0.655441
C	-0.331654	-1.361300	0.374218	C	0.314436	-1.596019	1.717614
H	-1.542422	-1.086234	-0.186390	H	-0.814934	-0.672927	-0.696485
C	-0.038448	-1.743116	1.823614	C	0.652613	-0.820474	2.977972
H	0.949266	-2.209360	1.871974	H	1.719348	-0.570775	2.987078
H	-0.048913	-0.865688	2.472483	H	0.076548	0.105607	3.026874
H	-0.779536	-2.456626	2.187930	H	0.434765	-1.412196	3.869401
O	0.506612	-0.331071	-0.081651	O	0.496610	-0.753588	0.580445
Al	2.183542	-0.091203	-0.226323	Al	1.831945	0.084899	-0.064531
R5''				TS5''			
							
C	-3.860059	-2.930499	0.193144	C	-4.349472	-2.441398	0.946649
H	-2.999079	-3.239727	0.790192	H	-3.568260	-2.794544	1.621565
H	-4.054852	-3.694876	-0.561899	H	-4.820767	-3.304894	0.473578
H	-4.732514	-2.868176	0.847002	H	-5.108066	-1.910054	1.522216
C	-3.587705	-1.591086	-0.463380	C	-3.759896	-1.557436	-0.119030
C	-2.362350	-1.632726	-1.358333	C	-2.631929	-2.166000	-0.942315
H	-2.540813	-2.336801	-2.172334	H	-3.018707	-2.777568	-1.755386
H	-1.501076	-1.998077	-0.794840	H	-1.999214	-2.784791	-0.300947
C	-2.040467	-0.266005	-1.962112	C	-1.856447	-0.945877	-1.431323
H	-2.906398	0.157060	-2.470318	H	-2.393033	-0.436874	-2.231838
H	-1.227411	-0.365971	-2.687541	H	-0.845188	-1.172736	-1.762846
C	-1.558973	0.717070	-0.946649	C	-1.833972	-0.058062	-0.196858
O	-0.587689	0.514689	-0.199399	O	-0.815690	-0.038618	0.593236
O	-2.184815	1.848963	-0.921020	O	-2.403602	1.303726	-0.495091
C	-1.722321	2.908422	-0.009476	C	-1.704079	2.495297	-0.011464
H	-0.633337	2.893030	-0.040929	H	-0.642206	2.258161	-0.082777
C	-2.259425	4.193514	-0.590361	C	-2.056275	3.611475	-0.967919
H	-1.928796	5.029819	0.026884	H	-1.510113	4.513044	-0.685662
H	-1.890759	4.346161	-1.605048	H	-1.785513	3.346331	-1.990485

H	-3.350857	4.182312	-0.603358	H	-3.125751	3.829863	-0.928893
C	-2.227424	2.616788	1.386266	C	-2.094363	2.784810	1.421204
H	-3.319062	2.598078	1.399640	H	-3.165827	2.988991	1.489937
H	-1.847790	1.666058	1.760455	H	-1.846793	1.947671	2.074448
H	-1.887186	3.408791	2.055561	H	-1.553360	3.666080	1.769833
O	-3.335197	-0.578764	0.517835	O	-3.103286	-0.408283	0.527776
H	-4.139038	-0.434000	1.031609	H	-3.303533	0.740492	0.143237
H	-4.454712	-1.291934	-1.064117	H	-4.532633	-1.146445	-0.771569
C	1.507470	-1.716823	3.721168	C	3.238855	0.702057	3.399188
H	1.254900	-2.616975	4.285756	H	3.570457	0.229986	4.326558
H	1.107308	-0.849376	4.253387	H	2.783533	1.665873	3.643316
H	2.594984	-1.625780	3.684395	H	4.114149	0.884761	2.772196
C	0.929844	-1.773119	2.317104	C	2.236835	-0.174212	2.666591
H	1.337032	-2.659467	1.809836	H	2.712105	-1.143787	2.458840
C	-0.586620	-1.895399	2.343820	C	0.996551	-0.427108	3.512742
H	-1.026625	-1.017282	2.825052	H	0.479363	0.516779	3.706684
H	-0.985082	-1.965153	1.329552	H	0.303576	-1.098453	2.998613
H	-0.899620	-2.787460	2.891945	H	1.260726	-0.882737	4.469876
O	1.324794	-0.609940	1.616190	O	1.890915	0.450664	1.446013
C	2.533474	-1.495635	-3.075634	C	1.589691	-2.945759	-2.119224
H	3.336420	-2.027888	-3.591042	H	2.307053	-3.548863	-2.681117
H	2.878541	-0.482828	-2.850775	H	1.473424	-1.983471	-2.626406
H	1.677109	-1.427657	-3.750042	H	0.626674	-3.461191	-2.129361
C	2.140053	-2.209821	-1.791046	C	2.059514	-2.723674	-0.688317
H	1.818425	-3.226482	-2.046581	H	2.171488	-3.702924	-0.206848
C	3.318198	-2.310552	-0.830149	C	3.411104	-2.021021	-0.658138
H	3.696161	-1.312871	-0.581445	H	3.357343	-1.070031	-1.199198
H	3.021571	-2.811052	0.094503	H	3.718264	-1.819026	0.370828
H	4.137956	-2.876620	-1.277922	H	4.182205	-2.631799	-1.132857
O	1.034427	-1.557932	-1.190227	O	1.083493	-2.002305	0.036965
C	4.069725	2.494847	-0.386121	C	2.560303	1.369215	-3.092708
H	4.713516	3.071024	0.282187	H	3.400104	2.011493	-3.366954
H	3.660636	3.172580	-1.140635	H	1.696937	1.644966	-3.705071
H	4.680667	1.744892	-0.893056	H	2.826744	0.335371	-3.324169
C	2.941185	1.827593	0.381539	C	2.217087	1.511192	-1.618750

H	3.381275	1.157764	1.132723	H	3.102118	1.231255	-1.029999
C	2.076910	2.850101	1.106764	C	1.855986	2.947128	-1.266355
H	1.653316	3.559862	0.390449	H	0.972551	3.260962	-1.830137
H	1.255912	2.355077	1.633598	H	1.637563	3.037037	-0.199535
H	2.662321	3.409426	1.840585	H	2.678025	3.626288	-1.505009
O	2.158886	1.069978	-0.523897	O	1.141393	0.645506	-1.309693
Al	1.100356	-0.234727	-0.065273	Al	0.940140	-0.264192	0.169835
P5''							
							
C	-4.902935	-1.941405	1.328477				
H	-4.382123	-2.711682	1.899765				
H	-5.724558	-2.408775	0.783043				
H	-5.318897	-1.202885	2.014068				
C	-3.967797	-1.300986	0.340901				
C	-3.263114	-2.248249	-0.627257				
H	-3.825473	-2.362139	-1.550866				
H	-3.142764	-3.226303	-0.159050				
C	-1.901064	-1.587556	-0.832698				
H	-1.878213	-0.892361	-1.674614				
H	-1.064008	-2.277778	-0.934316				
C	-1.754124	-0.771489	0.410608				
O	-0.731631	-0.229966	0.850634				
O	-2.588744	1.503633	-0.942717				
C	-1.573867	2.470587	-0.635519				
H	-0.635842	1.921233	-0.737491				
C	-1.602032	3.608844	-1.639520				
H	-0.782386	4.306046	-1.454104				
H	-1.509767	3.228768	-2.658262				
H	-2.543966	4.159432	-1.558147				
C	-1.717808	2.963643	0.792501				
H	-2.652447	3.521825	0.905849				

H	-1.724233	2.125772	1.490894
H	-0.890540	3.627434	1.052319
O	-2.855808	-0.682356	1.088037
H	-3.449713	1.916650	-0.792453
H	-4.445125	-0.475716	-0.188959
C	2.967277	2.747977	2.207228
H	3.438203	2.915450	3.178278
H	2.210483	3.521711	2.049857
H	3.729436	2.849891	1.432150
C	2.323955	1.373715	2.144718
H	3.103149	0.617163	2.314304
C	1.259377	1.208642	3.220327
H	0.460326	1.940660	3.073484
H	0.822507	0.207157	3.184235
H	1.686111	1.353457	4.215555
O	1.768996	1.189400	0.853864
C	2.138852	-3.734806	-0.163230
H	2.946476	-4.441274	-0.368922
H	1.775360	-3.338679	-1.116328
H	1.322332	-4.275734	0.319668
C	2.617732	-2.595637	0.724484
H	2.991148	-3.021072	1.663738
C	3.754732	-1.826373	0.064078
H	3.445368	-1.462022	-0.921063
H	4.054399	-0.972253	0.677128
H	4.628440	-2.466107	-0.078391
O	1.531694	-1.747728	1.046301
C	2.019607	-0.608154	-3.557362
H	2.731514	-0.198280	-4.277271
H	1.065692	-0.772018	-4.066613
H	2.394665	-1.574328	-3.212283
C	1.820388	0.335446	-2.382700
H	2.793661	0.498886	-1.899054
C	1.289552	1.686374	-2.836373
H	0.295558	1.566103	-3.276597

H	1.216749	2.375275	-1.992149	
H	1.950052	2.131403	-3.584393	
O	0.919549	-0.261618	-1.466517	
Al	1.038738	-0.273789	0.266015	