

Benchmarking Dual-level MS-T and DLPNO-CCSD(T) Methods for H-abstraction from Methyl Pentanoate by OH radical

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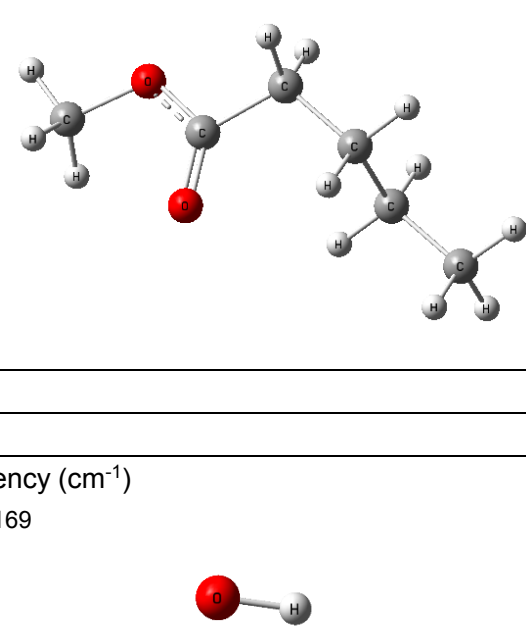
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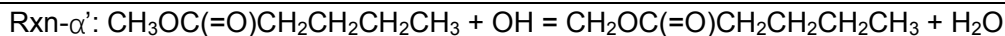
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Table S1: Optimized geometries and frequencies for involved species based on the ground structures captured by MS-T program at M06-2X/cc-pVTZ level.

Methyl Pentanoate								
Geometry				Frequency (cm ⁻¹)				
C	3.44090800	-0.64698100	-0.14916400	39.2436	72.0177	105.8732	164.9962	181.0096
H	3.87731100	-1.32818900	-0.87863700	223.4350	250.4534	263.2468	315.9504	377.7266
H	4.10651800	0.21231200	-0.05233100	530.5945	594.0244	663.7261	752.2912	853.0338
H	3.41654300	-1.15818100	0.81397800	859.7312	930.1622	956.4134	1028.3396	1067.9047
C	2.04148000	-0.20816800	-0.55920900	1083.6485	1129.4087	1149.0248	1191.6854	1219.4409
H	2.07771400	0.27525100	-1.53948300	1236.9729	1259.2313	1284.1796	1332.2579	1337.4559
H	1.39592300	-1.08232400	-0.65876700	1406.2787	1412.1784	1413.7750	1464.1740	1483.1322
C	1.42361100	0.75400000	0.44922600	1488.1478	1496.2654	1496.5642	1504.9256	1510.4822
H	1.38788600	0.27488600	1.42938000	1512.2731	1850.2143	3050.0003	3057.8964	3063.5918
H	2.06111600	1.63561800	0.54509800	3072.5976	3081.7620	3092.8864	3107.0269	3115.8407
C	0.02136400	1.19931500	0.06434800	3128.7604	3135.4647	3154.7377	3188.6622	
H	-0.01599300	1.57862300	-0.95847000					
H	-0.32804500	2.01490200	0.70188100					
C	-0.99847300	0.09598400	0.19149800					
O	-0.82641500	-0.95753100	0.74253000					
O	-2.16492700	0.44218700	-0.37431300					
C	-3.20387000	-0.52907700	-0.26608800					
H	-3.42521500	-0.73279600	0.77985300					
H	-4.06740300	-0.09991800	-0.76325100					
H	-2.90574200	-1.45787600	-0.74865300					

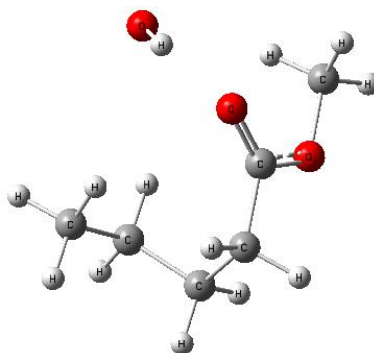
OH				
Geometry				Frequency (cm ⁻¹)
O	0.000000	0.000000	0.106747	3774.5169
H	0.000000	0.000000	-0.864787	





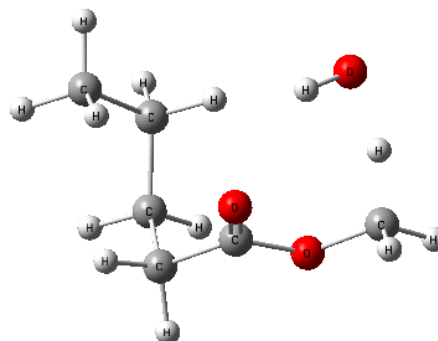
RC- α'

Geometry				Frequency (cm ⁻¹)				
C	-2.333786	1.284949	0.361229	22.5954	48.6842	63.2573	88.0163	128.8544
H	-2.408006	2.361399	0.214075	167.7881	169.0499	183.0520	217.0919	270.0832
H	-3.334755	0.903863	0.573768	315.8331	348.7694	373.9887	428.1419	438.9867
H	-1.714247	1.116682	1.242639	479.5215	635.3838	729.5122	773.9205	842.2096
C	-1.741982	0.609419	-0.870778	867.3011	916.7372	965.5103	986.7721	1054.1379
H	-2.312750	0.893871	-1.756042	1097.2889	1121.5704	1140.3271	1185.5082	1201.0064
H	-0.726774	0.984303	-1.031335	1226.0384	1256.8268	1310.6078	1330.5550	1357.4805
C	-1.720485	-0.915872	-0.781188	1381.9439	1397.0386	1419.1194	1479.5987	1483.5096
H	-2.741787	-1.297942	-0.727401	1494.4606	1496.3190	1499.7709	1506.4916	1510.8837
H	-1.269339	-1.327156	-1.684363	1520.1913	1814.1676	3052.6617	3059.6702	3068.3605
C	-0.951647	-1.446111	0.439361	3070.2545	3095.4267	3099.4974	3114.6790	3126.9960
H	-0.827412	-2.525710	0.358364	3140.0549	3150.2298	3160.0120	3191.7869	3658.0429
H	-1.472627	-1.220098	1.366302					
C	0.401781	-0.801916	0.519303					
O	0.745839	-0.017598	1.372657					
O	1.185994	-1.155618	-0.498728					
C	2.459796	-0.510199	-0.566993					
H	2.995227	-0.996512	-1.375147					
H	2.331932	0.550224	-0.785856					
H	2.993082	-0.623156	0.374054					
O	1.296175	2.449899	0.145145					
H	1.076723	1.801888	0.844153					

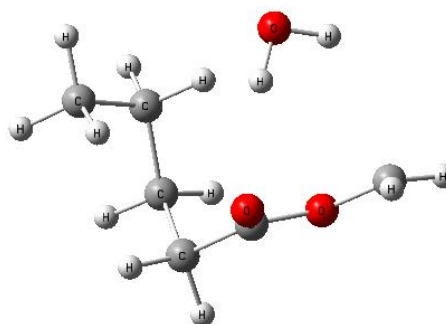


TS- α'

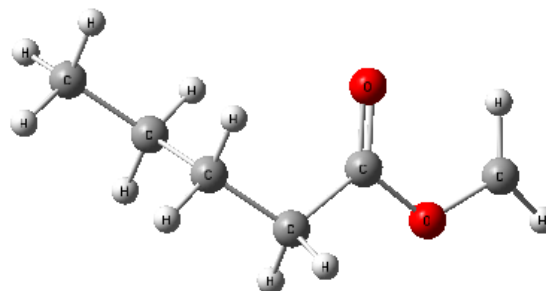
Geometry				Frequency (cm ⁻¹)				
C	-2.427482	1.204474	0.459671	-1156.0774				
H	-2.573922	2.280809	0.381526	37.1229	62.1053	100.0770	148.4333	151.8872
H	-3.405913	0.743432	0.609679	175.5849	216.8918	273.1895	307.8471	348.2526
H	-1.826004	1.019139	1.350029	350.5895	415.8842	435.4896	479.5419	628.5548
C	-1.751742	0.654460	-0.791961	725.3921	770.7031	797.8877	842.4628	876.7607
H	-2.304468	0.971180	-1.677694	913.1314	929.7739	965.5294	987.8531	1069.2873
H	-0.751182	1.086861	-0.887660	1103.4501	1128.6597	1150.6249	1163.7485	1206.3811
C	-1.653424	-0.870228	-0.806968	1252.4670	1258.5982	1303.1814	1323.7508	1355.0966
H	-2.654633	-1.305569	-0.816313	1370.9720	1382.6647	1398.6058	1419.7678	1472.0661
H	-1.151741	-1.194798	-1.718692	1478.9216	1492.9200	1501.0492	1511.7867	1521.1615
C	-0.900004	-1.444455	0.402818	1521.6112	1837.6794	3050.8511	3059.1529	3068.2190
H	-0.729701	-2.511638	0.260555	3094.9981	3097.8837	3112.2841	3115.0491	3127.0036
H	-1.456422	-1.297700	1.325087	3139.8303	3159.7251	3207.9961	3744.5431	
C	0.423953	-0.759370	0.568493					
O	0.732111	-0.028619	1.473744					
O	1.247701	-1.016084	-0.466546					
C	2.483117	-0.349136	-0.450860					
H	3.032837	-0.645595	-1.337396					
H	2.287781	0.820227	-0.528567					
H	3.026711	-0.507655	0.477464					
O	1.776078	2.054322	-0.295820					
H	1.413028	1.849885	0.583799					

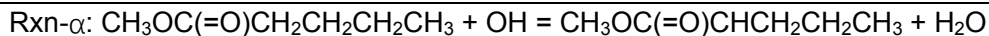


PC- α'				Frequency (cm ⁻¹)				
Geometry								
C	-2.342584	1.049725	0.395476	34.4972	71.0684	72.1088	97.5434	138.1688
H	-2.540971	2.102346	0.201267	162.2967	176.4005	192.8119	214.3319	233.0626
H	-3.282520	0.572572	0.681235	272.9649	309.8222	327.5310	357.5757	430.7046
H	-1.665394	.001891	1.249257	434.8301	487.7337	578.0668	629.2224	713.0092
C	-1.736299	0.381174	-0.833141	771.4404	841.6968	845.2178	907.9610	962.7068
H	-2.375129	0.555756	-1.700291	988.0944	1075.7619	1105.8259	1130.6111	1179.0593
H	-0.778763	0.858845	-1.055373	1205.1854	1238.6965	1259.4312	1294.9547	1320.3946
C	-1.540593	-1.125635	-0.675775	1355.5936	1382.0872	1393.9737	1421.6770	1465.0590
H	-2.509310	-1.618781	-0.573189	1476.2173	1493.8814	1499.1903	1510.6515	1518.3157
H	-1.068242	-1.529220	-1.571527	1637.0185	1843.7982	3054.9931	3066.4129	3068.4278
C	-0.693945	-1.504928	0.547522	3090.4112	3099.6201	3114.4906	3126.3493	3142.1226
H	-0.459614	-2.570080	0.520585	3158.5262	3188.7998	3336.4855	3831.3342	3925.4247
H	-1.215626	-1.289860	1.476619					
C	0.594302	-0.740426	0.586450					
O	0.950445	0.014960	1.449299					
O	1.347798	-0.983448	-0.520112					
C	2.547970	-0.349683	-0.629730					
H	3.105947	-0.648048	-1.499384					
H	1.650636	2.125835	-0.771839					
H	2.994154	0.041650	0.269462					
O	0.971932	2.492832	-0.199344					
H	1.010330	1.940988	0.589621					



MP- α'				Frequency (cm ⁻¹)				
Geometry								
C	3.403325	-0.601150	-0.181791	37.4651	71.9548	103.8816	163.5338	225.6197
H	3.848281	-1.250023	-0.935048	246.9817	259.9455	270.8871	317.9135	361.8669
H	4.052105	0.267959	-0.061797	395.5725	534.0469	583.8791	659.8429	749.9702
H	3.395365	-1.142899	0.764746	845.3057	849.8232	921.1882	952.7965	1036.6345
C	1.992949	-0.178119	-0.570262	1081.6880	1111.7455	1127.2686	1170.0441	1201.4728
H	2.013640	0.336656	-1.534816	1236.8855	1271.6701	1279.6766	1331.7318	1336.1849
H	1.364823	-1.061773	-0.694848	1401.3479	1410.3291	1413.7224	1460.0672	1463.5060
C	1.362733	0.739598	0.471539	1484.3060	1496.4817	1503.8731	1510.4776	1863.4850
H	1.342586	0.230717	1.437021	3050.2781	3058.6180	3064.9330	3070.7853	3092.5933
H	1.982497	1.630671	0.591236	3105.8972	3115.3022	3129.1186	3136.7546	3204.8852
C	-0.050062	1.169655	0.108020	3357.1458				
H	-0.101036	1.580034	-0.902268					
H	-0.412641	1.957865	0.772654					
C	-1.042700	0.043753	0.206050					
O	-0.861300	-1.023630	0.715940					
O	-2.231692	0.401291	-0.352285					
C	-3.261131	-0.488734	-0.289410					
H	-4.122043	-0.192908	-0.859820					
H	-3.050318	-1.487603	0.048828					





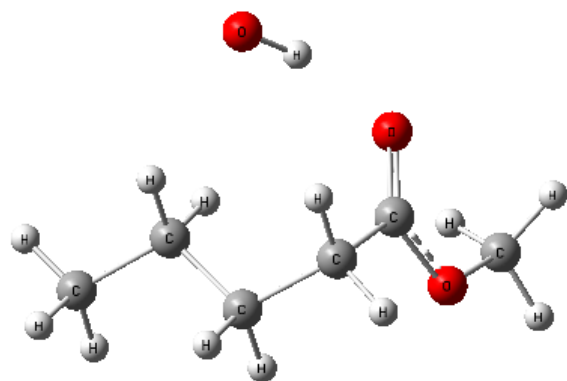
RC- α

Geometry

C	-3.091306	-1.235638	-0.558195
H	-3.562138	-1.060563	-1.524299
H	-2.788980	-2.283148	-0.515913
H	-3.843782	-1.076335	0.215403
C	-1.895666	-0.315827	-0.348297
H	-1.168926	-0.469258	-1.150263
H	-2.212403	0.728272	-0.419973
C	-1.231722	-0.544389	1.004865
H	-1.962015	-0.374424	1.798150
H	-0.909003	-1.584748	1.092195
C	-0.031653	0.379992	1.257830
H	0.355689	0.222625	2.263119
H	-0.329619	1.420523	1.138623
C	1.065466	0.097590	0.272826
O	1.272671	0.717450	-0.745663
O	1.790056	-0.967399	0.615685
C	2.818318	-1.339662	-0.304362
H	3.531079	-0.526110	-0.420687
H	3.297953	-2.212550	0.124736
H	2.387441	-1.574608	-1.275384
O	-0.850783	2.549145	-1.135303
H	-0.040021	1.994889	-1.137083

Frequency (cm^{-1})

29.7847	59.2398	84.3460	86.3341	107.8355
155.6493	160.5102	174.9668	219.7588	248.2622
277.9548	330.2002	444.3248	459.3203	491.6703
608.2469	642.9441	733.3198	784.8590	853.7582
870.7554	916.6293	965.9299	1021.9763	1058.7449
1086.2990	1129.5545	1142.1944	1191.7378	1221.9090
1229.9944	1262.6930	1314.5791	1334.1770	1352.8882
1373.6352	1412.2303	1414.8970	1484.3715	1489.4363
1496.0574	1497.8729	1501.7924	1504.8256	1509.5384
1513.6021	1810.8701	3046.8231	3058.4958	3063.1970
3076.7690	3085.7469	3094.8005	3107.5131	3125.9156
3139.9203	3153.4974	3160.8631	3195.6947	3568.3502



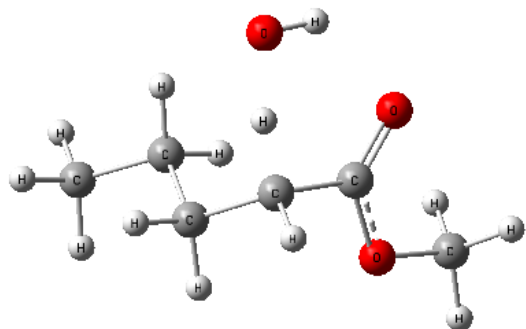
TS- α

Geometry

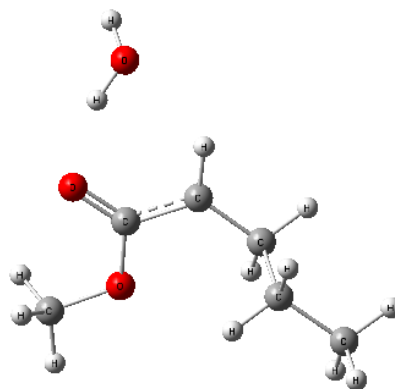
C	-2.954861	-1.419750	-0.497435
H	-3.301468	-1.590182	-1.515648
H	-2.730702	-2.390141	-0.051958
H	-3.777343	-0.977615	0.066273
C	-1.732736	-0.512472	-0.470649
H	-0.931383	-0.959269	-1.066572
H	-1.961423	0.450869	-0.930375
C	-1.231079	-0.270872	0.948762
H	-2.036520	0.137912	1.561568
H	-0.935211	-1.220950	1.404750
C	-0.050628	0.681682	1.001126
H	0.301394	0.877935	2.013480
H	-0.410375	1.743995	0.574429
C	1.093220	0.266186	0.118748
O	1.499879	0.878006	-0.835907
O	1.611100	-0.902683	0.508157
C	2.686870	-1.394075	-0.294523
H	3.514098	-0.687554	-0.288548
H	2.983146	-2.337288	0.151349
H	2.353101	-1.539811	-1.319930
O	-0.616496	2.758039	-0.245512
H	0.112614	2.525282	-0.847957

Frequency (cm^{-1})

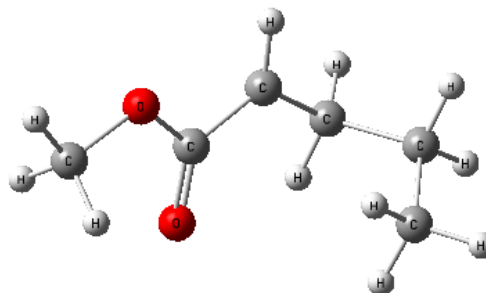
-1238.7492				
29.9537	70.5836	80.8715	95.2668	149.1382
162.3947	178.4794	207.9718	249.2102	274.6268
306.2823	396.5906	420.2997	477.5732	627.7462
691.0547	738.6128	781.7744	852.6565	867.5017
909.9529	937.5753	971.3542	1035.5404	1062.5854
1085.0902	1134.4737	1154.5771	1190.1427	1212.5500
1226.5808	1263.2753	1276.7927	1307.1191	1337.6633
1367.4804	1408.0312	1416.2924	1476.2915	1486.9160
1488.7920	1496.1920	1497.2783	1505.0282	1509.4129
1512.1351	1829.0291	3044.3217	3050.2363	3059.9996
3084.9938	3089.5641	3104.8537	3120.0066	3128.1896
3139.5142	3160.1354	3195.3550	3731.3616	

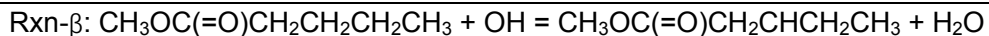


PC- α				Frequency (cm ⁻¹)				
Geometry								
C	-3.132998	-2.088074	-0.120202	29.4738	50.3408	79.3848	80.7495	97.7688
H	-3.611513	-2.475506	-1.018681	130.1185	156.6963	162.7414	183.4009	225.6486
H	-2.662057	-2.924250	0.398017	249.2116	285.2444	314.6268	337.4029	385.0028
H	-3.912491	-1.689344	0.530230	566.6862	620.1822	632.0030	651.6098	753.5301
C	-2.107313	-1.015596	-0.459535	780.9224	869.7855	896.6739	905.3883	1044.1292
H	-1.339868	-1.422041	-1.120025	1059.2431	1094.8150	1141.2795	1161.1997	1190.4969
H	-2.584390	-0.192184	-0.993883	1226.9975	1262.3662	1295.4830	1329.3592	1342.3187
C	-1.422678	-0.465558	0.806381	1366.4616	1412.3570	1426.4978	1485.0481	1492.3381
H	-2.186700	-0.064121	1.473836	1495.6165	1496.3883	1502.8404	1509.7192	1511.0252
H	-0.930226	-1.295563	1.316685	1649.2226	1734.5452	3060.4087	3062.0307	3073.5360
C	-0.435906	0.591717	0.484009	3080.7513	3098.6256	3117.5404	3134.4290	3138.7547
H	-0.697669	1.640889	0.495621	3153.5565	3188.3214	3217.4930	3736.3689	3939.8338
H	0.822404	4.179670	0.639232					
C	0.910026	0.306223	0.045667					
O	1.731707	1.152131	-0.265710					
O	1.194415	-1.008042	0.008173					
C	2.514499	-1.331913	-0.420040					
H	3.249817	-0.890589	0.250159					
H	2.577775	-2.414764	-0.397031					
H	2.689007	-0.958319	-1.427275					
O	0.397797	3.671384	-0.053639					
H	0.999916	2.932397	-0.225598					



MP- α				Frequency (cm ⁻¹)				
Geometry								
C	2.195061	-1.352047	0.352991	43.2784	58.5550	109.9455	153.8824	178.9668
H	2.986675	-1.960199	0.788872	212.7802	259.3145	314.7604	349.4122	402.3312
H	1.307144	-1.460760	0.977210	478.0693	586.7824	684.6796	758.4467	791.7762
H	1.951751	-1.755085	-0.630525	848.0584	888.5425	955.0298	1012.2602	1072.3919
C	2.617690	0.107667	0.248692	1086.9477	1102.9352	1176.5922	1190.5400	1217.5615
H	2.808725	0.514743	1.244098	1235.8284	1263.2789	1282.8965	1351.4508	1372.1735
H	3.551835	0.187552	-0.309162	1421.4793	1452.1116	1481.4132	1490.6333	1494.2374
C	1.560197	0.975538	-0.461318	1498.8885	1503.5823	1508.3784	1512.7331	1761.2861
H	1.944548	1.994238	-0.552350	3056.9966	3061.1848	3062.9716	3077.5756	3097.8793
H	1.390168	0.581503	-1.463745	3120.9179	3131.9934	3139.3542	3148.2175	3185.4685
C	0.272245	0.998608	0.267712	3215.4859				
H	0.160140	1.559898	1.184659					
C	-0.856413	0.212968	-0.184703					
O	-0.858459	-0.497303	-1.166601					
O	-1.930024	0.351652	0.621014					
C	-3.073229	-0.400221	0.228510					
H	-2.844085	-1.464574	0.217351					
H	-3.841350	-0.183079	0.963587					
H	-3.400994	-0.104097	-0.766595					





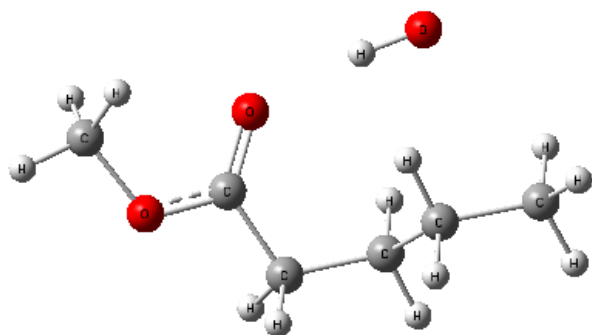
RC-β

Geometry

C	-3.299381	-0.514777	-0.544737
H	-3.708566	-0.761029	-1.523568
H	-3.896538	-1.029842	0.209630
H	-3.414564	0.558918	-0.393931
C	-1.833322	-0.914155	-0.439777
H	-1.724522	-1.986714	-0.624067
H	-1.260603	-0.402896	-1.216895
C	-1.248016	-0.585303	0.930312
H	-1.357291	0.482952	1.128599
H	-1.823965	-1.105810	1.698199
C	0.212830	-0.985439	1.071272
H	0.373140	-2.029897	0.798112
H	0.554431	-0.888814	2.104931
C	1.151275	-0.146531	0.246218
O	0.877765	0.898276	-0.295139
O	2.372817	-0.676168	0.193071
C	3.343585	0.076760	-0.537304
H	3.471411	1.060463	-0.090515
H	4.264341	-0.493311	-0.480302
H	3.027325	0.195420	-1.571390
O	-1.606386	2.202226	-0.781099
H	-0.716947	1.822755	-0.619488

Frequency (cm⁻¹)

39.6061	48.7521	95.8407	112.7883	128.7198
153.4229	166.8982	180.3367	229.0880	252.2562
267.7180	324.4699	382.5040	449.9824	531.7381
558.7880	593.6274	670.6792	759.8534	852.0261
865.5811	935.9487	956.1691	1025.7795	1065.4854
1084.8041	1130.6237	1147.7484	1190.8681	1221.2432
1241.1214	1266.9077	1290.8039	1330.2238	1335.9627
1405.8751	1415.7874	1416.1518	1459.9056	1490.9624
1492.6762	1495.3025	1496.9130	1501.5095	1509.5708
1512.6281	1818.9084	3047.6218	3058.3586	3065.0506
3071.4013	3083.3081	3085.6176	3105.7934	3115.3387
3129.4030	3138.9758	3160.8706	3195.6454	3606.1044



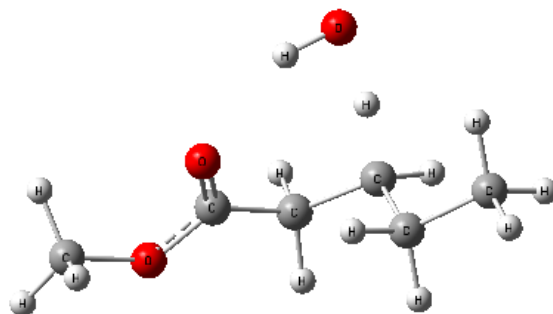
TS-β

Geometry

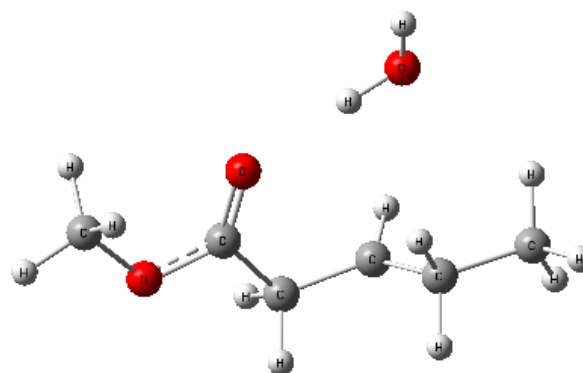
C	-3.213381	-0.620593	-0.757242
H	-3.552176	-1.070855	-1.689095
H	-3.858707	-0.981314	0.045087
H	-3.337248	0.459741	-0.829168
C	-1.755625	-0.959153	-0.474451
H	-1.626672	-2.044841	-0.404697
H	-1.129097	-0.619283	-1.301137
C	-1.267895	-0.326479	0.812758
H	-1.437065	0.836693	0.718694
H	-1.907093	-0.593643	1.656277
C	0.185091	-0.579077	1.153568
H	0.385478	-1.647976	1.256123
H	0.444745	-0.125822	2.113299
C	1.163574	-0.022616	0.149222
O	0.936750	0.847496	-0.654037
O	2.362528	-0.596715	0.267990
C	3.375782	-0.090790	-0.603205
H	3.531976	0.970758	-0.423018
H	4.272900	-0.655317	-0.373775
H	3.085265	-0.234501	-1.641717
O	-1.441976	2.155774	0.315883
H	-0.656004	2.046170	-0.249457

Frequency (cm⁻¹)

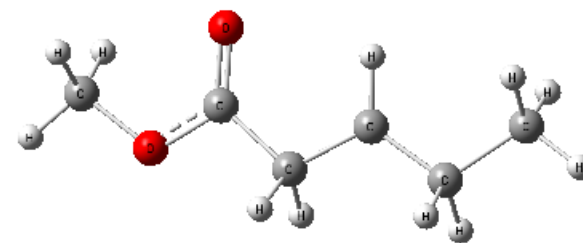
-918.6851				
31.6934	76.2116	92.3415	122.6832	159.6501
161.2607	181.1002	206.9419	255.8729	272.3068
315.4433	384.7896	461.4528	532.9190	591.6846
630.3649	734.7834	822.6475	854.7325	922.0452
940.9725	953.8116	1028.9837	1064.6087	1066.5781
1104.6766	1138.0160	1148.6321	1190.6058	1220.1200
1230.5908	1258.1401	1274.9105	1306.1696	1320.5961
1399.0776	1409.1729	1416.0634	1449.7115	1453.3780
1488.7108	1489.8232	1496.4493	1504.3704	1509.1803
1513.1452	1829.1102	3034.2815	3062.2976	3068.1181
3084.7146	3085.0890	3101.0090	3106.3647	3132.6586
3145.3936	3159.4547	3194.7754	3720.6612	

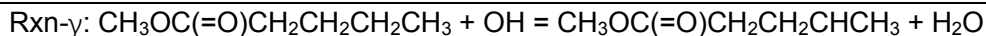


PC- β				Frequency (cm ⁻¹)				
Geometry								
C	-3.388604	-0.520158	-0.388987	33.1396	46.8650	81.4243	102.0194	119.1966
H	-3.942990	-0.503416	-1.326484	136.9058	151.4048	155.9504	174.0860	217.1665
H	-3.827653	-1.285255	0.252210	254.7040	260.3779	297.1380	315.5263	377.0631
H	-3.500708	0.449034	0.095019	450.8208	540.8200	548.7037	589.2364	705.8460
C	-1.909669	-0.798346	-0.626736	775.7207	859.2349	915.7470	961.5036	1043.5945
H	-1.775215	-1.740475	-1.171165	1059.2973	1074.4774	1122.4273	1170.2588	1190.5327
H	-1.501490	-0.014370	-1.279762	1217.5010	1234.2137	1262.4201	1278.1972	1326.4755
C	-1.123500	-0.842981	0.634624	1365.0598	1407.7022	1428.0531	1453.1291	1470.6079
H	-1.581567	3.057699	-0.097266	1486.7556	1496.8013	1499.6307	1509.7919	1514.5123
H	-1.506398	-0.329032	1.505478	1643.3679	1820.1455	2994.4707	3029.3886	3055.7722
C	0.302057	-1.261111	0.617563	3065.0778	3084.4505	3100.2282	3133.3765	3150.6692
H	0.461325	-2.125069	-0.034292	3159.4288	3193.7405	3205.0601	3763.7639	3939.9022
H	0.658392	-1.556192	1.607058					
C	1.249424	-0.180064	0.132654					
O	0.950601	0.961540	-0.116539					
O	2.496313	-0.639065	0.013859					
C	3.467111	0.315221	-0.419802					
H	3.520788	1.144027	0.283024					
H	4.410997	-0.217652	-0.457358					
H	3.203605	0.700483	-1.402581					
O	-1.627747	2.219468	0.365393					
H	-0.762126	1.809483	0.228905					



MP- β				Frequency (cm ⁻¹)				
Geometry								
C	-3.830774	0.421164	0.100608	23.1143	50.9010	84.9763	110.2738	154.7441
H	-4.792143	-0.089966	0.083491	175.4948	237.7946	261.6728	281.2641	323.9739
H	-3.751370	0.966424	1.041033	366.5060	499.6080	583.9958	711.9429	770.6234
H	-3.820762	1.150925	-0.709251	913.3900	923.9613	941.1857	1046.0200	1063.2219
C	-2.674120	-0.559885	-0.049377	1073.5907	1145.9305	1158.6971	1190.4921	1197.8974
H	-2.717954	-1.312564	0.747647	1215.8695	1235.2397	1274.3312	1297.3113	1384.9118
H	-2.796694	-1.130831	-0.981001	1416.0546	1443.0396	1447.4732	1477.3990	1488.1283
C	-1.345187	0.104254	-0.035837	1496.4553	1503.0993	1509.1736	1511.4250	1858.4755
H	-1.260201	1.176446	-0.137044	2983.9892	2999.9609	3016.3845	3033.5331	3065.3867
C	-0.105599	-0.707887	-0.044390	3081.4326	3133.3543	3142.3248	3154.4125	3188.9531
H	-0.045754	-1.358506	-0.928278	3220.7629				
H	-0.063752	-1.401708	0.803855					
C	1.157672	0.115904	-0.021753					
O	1.218180	1.313282	-0.061856					
O	2.241696	-0.672178	0.043242					
C	3.491027	0.016021	0.057860					
H	3.548758	0.677782	0.919888					
H	4.254802	-0.752410	0.113675					
H	3.607956	0.608147	-0.847768					





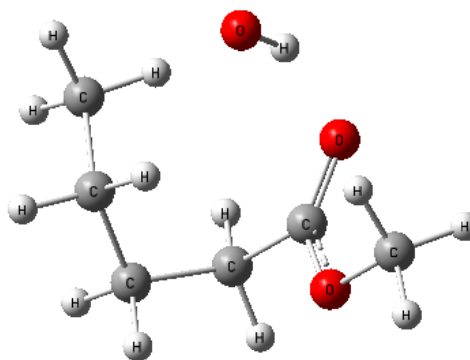
RC- γ

Geometry

C	2.447654	0.699731	0.397933
H	2.751435	1.735207	0.254058
H	1.816052	0.668563	1.286149
H	3.341372	0.104563	0.596000
C	1.710363	0.177326	-0.830143
H	0.812919	0.781383	-1.003167
H	2.331874	0.313019	-1.716543
C	1.322113	-1.297406	-0.733213
H	0.789789	-1.593927	-1.637135
H	2.222298	-1.912043	-0.671815
C	0.443098	-1.621280	0.485728
H	1.001029	-1.527205	1.413880
H	0.059046	-2.637798	0.405150
C	-0.710633	-0.663767	0.559104
O	-0.844986	0.194558	1.400581
O	-1.562131	-0.823814	-0.452554
C	-2.631597	0.124590	-0.522879
H	-2.229821	1.127820	-0.655432
H	-3.227836	-0.166249	-1.380788
H	-3.225216	0.089193	0.388083
O	-0.175109	2.666025	0.166676
H	-0.445845	1.996679	0.827289

Frequency (cm^{-1})

44.1119	66.3588	79.9187	93.6835	132.5167
168.0629	174.8782	197.1146	218.9185	273.1300
315.4564	348.2022	420.6259	436.0761	464.5099
482.9386	636.5746	730.4255	770.9505	842.2506
866.2613	916.1455	964.3265	986.4639	1051.4330
1096.7660	1119.1591	1139.9289	1192.8969	1201.4660
1228.0373	1253.8813	1309.6165	1330.5916	1355.6360
1381.3224	1395.7604	1417.6451	1476.1084	1485.7020
1494.0065	1497.8138	1500.1931	1506.6765	1509.6126
1516.7272	1812.4008	3017.3377	3058.5061	3069.2068
3081.6549	3091.2134	3100.2981	3114.8989	3127.5695
3143.2168	3159.5074	3160.9260	3193.9368	3648.2953



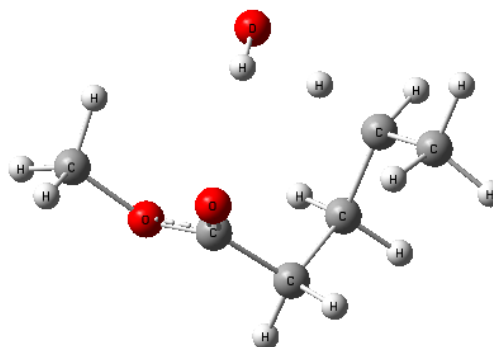
TS- γ

Geometry

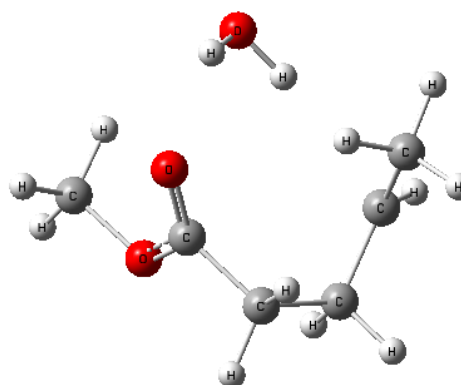
C	2.571330	0.386313	0.675869
H	3.064466	1.353131	0.757811
H	1.888434	0.285523	1.519473
H	3.334143	-0.392156	0.762065
C	1.837808	0.269223	-0.645071
H	1.022800	1.101228	-0.676111
H	2.477829	0.550363	-1.482481
C	1.188606	-1.078131	-0.919709
H	0.611342	-1.025210	-1.843164
H	1.977301	-1.819015	-1.078534
C	0.282154	-1.593717	0.207856
H	0.846421	-1.748085	1.124369
H	-0.169423	-2.536900	-0.095700
C	-0.806020	-0.599340	0.501118
O	-0.814571	0.157817	1.441673
O	-1.751134	-0.612255	-0.438121
C	-2.771432	0.381658	-0.313270
H	-2.337567	1.368515	-0.461660
H	-3.494167	0.162278	-1.091807
H	-3.234039	0.325444	0.669536
O	0.106897	2.188108	-0.452524
H	-0.137493	1.911579	0.448879

Frequency (cm^{-1})

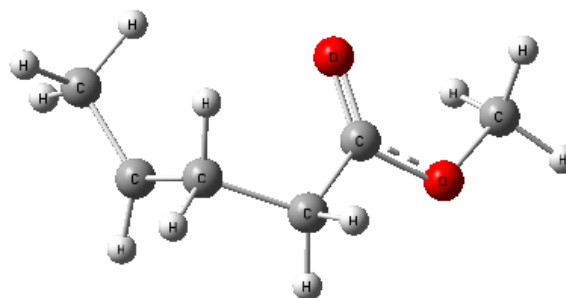
-721.1528				
59.6879	83.2170	104.4979	135.3020	165.5266
181.2050	194.3068	210.6916	260.1261	321.0122
335.1580	430.5408	448.7917	474.1634	634.2819
692.3229	747.7521	837.0286	842.7716	898.4730
922.8444	963.2685	989.8393	1056.2037	1058.4277
1101.1366	1129.6022	1166.0353	1191.1283	1203.6880
1227.2693	1258.1406	1319.7033	1345.4346	1363.2731
1388.8123	1401.7780	1422.5433	1461.4440	1477.7132
1480.1225	1491.5659	1495.0208	1497.9235	1514.2897
1516.0060	1821.3559	3050.2188	3053.0764	3084.2867
3093.7375	3103.4074	3110.9083	3121.4575	3147.9011
3161.6182	3164.0063	3192.3116	3731.6416	

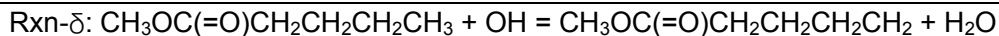


PC- γ				Frequency (cm ⁻¹)				
Geometry								
C	2.556179	0.409328	0.517868	45.6717	76.6771	89.9527	103.3853	139.2869
H	2.952763	1.421024	0.461372	145.6299	154.8037	187.5570	195.3990	210.6239
H	1.851997	0.372501	1.352415	246.4766	305.0116	312.6944	325.4111	430.2711
H	3.387795	-0.260437	0.774504	445.5352	453.6098	557.1403	633.0652	723.0752
C	1.915528	0.001915	-0.764131	853.2942	864.6773	921.9688	970.0797	997.9180
H	0.539499	2.022099	-0.510753	1002.5797	1068.5495	1127.5824	1153.0454	1196.3387
H	2.221603	0.499818	-1.674922	1202.5395	1219.1374	1229.5242	1322.1720	1361.4793
C	1.252121	-1.328268	-0.906522	1379.9058	1393.2228	1424.2183	1469.2679	1479.3492
H	0.671451	-1.358608	-1.828305	1483.3841	1491.8394	1499.5842	1502.7579	1519.6722
H	2.011141	-2.117993	-0.990838	1641.2725	1824.8911	2996.1963	3000.6753	3082.8887
C	0.337841	-1.691391	0.274420	3083.4757	3101.5268	3107.6655	3143.4237	3160.4861
H	0.902171	-1.778400	1.199598	3164.8289	3188.3910	3191.8603	3822.1680	3902.2823
H	-0.155942	-2.641173	0.071951					
C	-0.708757	-0.629228	0.478854					
O	-0.762606	0.113472	1.428623					
O	-1.565350	-0.579433	-0.540597					
C	-2.575621	0.434148	-0.464805					
H	-2.115529	1.419159	-0.509425					
H	-3.220095	0.269180	-1.321586					
H	-3.136120	0.332312	0.462053					
O	-0.016715	2.599787	0.020595					
H	-0.255248	2.049878	0.775781					



MP- γ				Frequency (cm ⁻¹)				
Geometry								
C	-2.722225	1.220839	-0.146357	38.2262	69.5602	94.8825	108.4192	168.3076
H	-2.992245	1.861981	-0.983457	183.2661	201.5637	277.3907	330.5400	372.4944
H	-3.629390	1.058384	0.449551	401.6579	506.9812	599.6119	666.0174	840.9179
H	-2.019330	1.761421	0.493800	864.9525	943.4020	971.8728	990.2135	1019.9721
C	-2.124227	-0.060926	-0.598249	1076.3602	1130.9126	1153.9443	1191.6396	1216.1440
H	-2.197451	-0.358189	-1.636287	1227.3660	1231.6219	1273.8808	1330.0807	1399.0241
C	-1.528732	-1.027141	0.368117	1404.1525	1432.1346	1463.4258	1475.1297	1479.4847
H	-1.564306	-0.607604	1.374530	1487.9714	1492.2194	1496.8392	1511.8944	1847.9591
H	-2.098507	-1.962568	0.388281	3003.7067	3025.2960	3065.6075	3071.0411	3081.8343
C	-0.078619	-1.366676	0.026155	3100.0801	3119.9979	3136.2211	3154.9610	3186.7262
H	0.015404	-1.728556	-0.998408	3188.9709				
H	0.312738	-2.157461	0.671172					
C	0.826991	-0.172762	0.190029					
O	0.544879	0.843235	0.766117					
O	2.026466	-0.385932	-0.370827					
C	2.961393	0.681955	-0.227917					
H	3.154942	0.878175	0.824965					
H	3.866730	0.355835	-0.728930					
H	2.573168	1.588423	-0.688203					





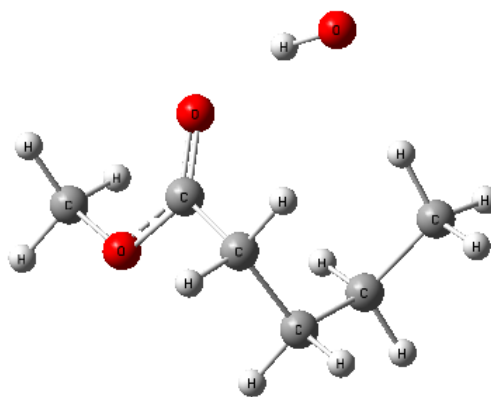
RC- δ

Geometry

C	2.509179	-0.413555	-0.769512
H	2.186817	0.564315	-0.409505
H	3.264265	-0.786925	-0.075650
H	2.986976	-0.261605	-1.736197
C	1.344906	-1.391040	-0.881105
H	0.576782	-0.973456	-1.539609
H	1.684279	-2.311198	-1.359522
C	0.718857	-1.750667	0.464783
H	-0.082541	-2.474464	0.315113
H	1.468298	-2.225461	1.100789
C	0.156154	-0.539014	1.220589
H	0.943173	0.149395	1.520551
H	-0.370460	-0.877213	2.113418
C	-0.815075	0.222484	0.364511
O	-0.664722	1.353883	-0.037327
O	-1.887916	-0.503827	0.051317
C	-2.840667	0.133361	-0.802044
H	-2.376532	0.399361	-1.749633
H	-3.634317	-0.590205	-0.952631
H	-3.225069	1.035086	-0.330341
O	1.764845	2.469059	0.870598
H	0.871595	2.253243	0.523798

Frequency (cm⁻¹)

41.2720	59.0235	95.7006	101.8957	120.1855
158.8702	166.9292	176.4579	203.8904	262.2923
329.3568	359.0322	440.2458	476.8757	507.4603
626.7883	655.1343	725.9089	768.2091	844.4523
869.5344	916.9236	965.3290	991.3818	1056.9592
1098.0082	1120.8547	1143.5946	1189.4779	1206.4667
1226.7562	1253.6688	1311.1888	1339.1604	1363.4438
1384.8684	1396.7560	1421.1068	1482.5533	1485.7793
1493.4994	1496.9663	1501.5483	1506.9978	1508.5667
1552.8247	1812.1642	3044.7170	3063.7109	3069.8255
3084.8223	3092.0486	3095.2904	3115.5167	3130.5890
3141.4127	3158.1740	3160.0497	3195.0500	3566.6065



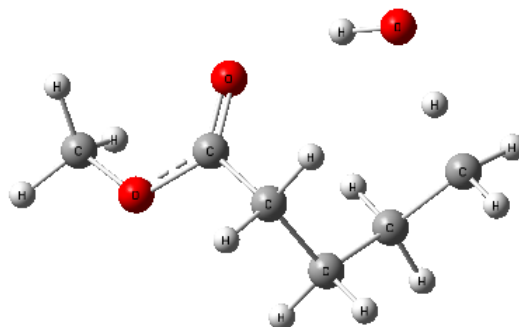
TS- δ

Geometry

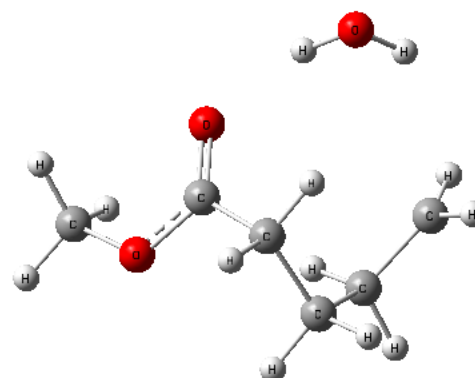
C	2.680480	-0.218761	-0.491238
H	2.353022	0.837566	-0.054966
H	3.301751	-0.645982	0.296662
H	3.289215	0.043032	-1.353676
C	1.491140	-1.085944	-0.845535
H	0.829221	-0.543357	-1.524996
H	1.851965	-1.953588	-1.405322
C	0.707726	-1.596066	0.362520
H	-0.042382	-2.318024	0.035599
H	1.387354	-2.125955	1.032592
C	0.007633	-0.493883	1.174740
H	0.726323	0.241738	1.529986
H	-0.508401	-0.939563	2.023011
C	-0.997082	0.216385	0.314421
O	-0.793601	1.234302	-0.304736
O	-2.160287	-0.435931	0.252232
C	-3.148742	0.145894	-0.599649
H	-2.782161	0.196334	-1.622876
H	-4.016098	-0.501867	-0.533717
H	-3.391741	1.151015	-0.261736
O	1.900764	2.052873	0.346719
H	0.990637	1.951177	0.004373

Frequency (cm⁻¹)

-1065.0487				
32.1076	81.5233	118.9282	133.2493	168.1725
174.9243	177.4256	227.1636	325.3664	356.3243
365.0755	454.3618	466.5727	567.4712	636.9790
719.3732	755.1613	834.2221	844.1705	886.5764
915.1553	940.5530	975.3830	1019.6551	1067.0542
1102.6330	1130.9748	1138.2069	1190.0632	1197.8842
1225.8767	1248.1276	1298.1531	1325.9114	1332.7945
1368.5833	1384.8348	1406.7586	1427.8481	1467.9320
1485.3043	1486.0257	1495.8962	1496.9813	1505.5075
1509.8362	1817.4191	3048.1383	3064.6970	3080.0814
3085.2198	3091.8231	3101.7773	3111.7465	3160.2354
3161.3774	3161.8318	3193.9750	3649.1017	



PC- δ				Frequency (cm ⁻¹)				
Geometry								
C	2.455593	-0.474251	-0.832253	33.0116	53.7490	94.0765	99.2710	122.4904
H	2.481836	1.985563	0.240564	147.3417	163.9906	168.8887	203.5436	218.0249
H	3.166298	-0.560711	-0.021577	241.8261	289.6083	323.4092	352.3832	445.0651
H	2.737802	0.121882	-1.686846	466.0680	532.7165	590.4804	637.4059	733.2695
C	1.307680	-1.415784	-0.909799	800.6044	853.6161	889.5261	915.3143	979.4637
H	0.534842	-1.004902	-1.566525	1034.9387	1066.0831	1114.3267	1136.6802	1177.8685
H	1.624413	-2.353741	-1.385236	1191.5231	1217.1935	1227.5870	1281.2394	1332.8610
C	0.704785	-1.753506	0.455394	1364.8688	1383.3018	1396.1808	1466.6848	1475.7910
H	-0.093639	-2.484331	0.328217	1485.9204	1488.5801	1495.9598	1499.7369	1510.6736
H	1.467977	-2.212823	1.085979	1647.8356	1823.4338	2996.5453	3056.0062	3076.3947
C	0.153023	-0.522078	1.185861	3083.1356	3095.5600	3119.7207	3156.6240	3157.3100
H	0.946264	0.175325	1.446606	3159.9363	3192.4758	3264.8809	3767.1569	3929.7116
H	-0.362654	-0.834460	2.093825					
C	-0.823529	0.213476	0.312388					
O	-0.651441	1.305823	-0.172080					
O	-1.927482	-0.504003	0.080485					
C	-2.889203	0.106718	-0.780652					
H	-2.450957	0.299587	-1.758020					
H	-3.708543	-0.599533	-0.860135					
H	-3.231643	1.048050	-0.356077					
O	1.846284	2.387677	0.836137					
H	0.991286	2.199063	0.424722					



MP- δ				Frequency (cm ⁻¹)				
Geometry								
C	1.238252	1.660986	0.269890	33.7944	87.9677	121.3065	172.6814	190.1462
H	1.060796	2.582658	-0.262454	197.6330	248.6413	310.4179	325.4953	416.2790
H	0.863222	1.577587	1.279975	467.4741	533.5523	614.9846	718.1998	814.8204
C	2.207379	0.655470	-0.242783	845.3040	885.5997	944.6083	963.4087	1021.5955
H	2.312149	0.757553	-1.325814	1080.3030	1106.4370	1135.9552	1181.6997	1189.5572
H	3.204208	0.853126	0.174609	1221.1270	1238.9437	1265.3435	1296.0578	1368.9632
C	1.830178	-0.789658	0.096367	1384.5677	1399.4461	1464.6717	1473.3922	1478.8270
H	2.627252	-1.455760	-0.234176	1488.0589	1494.9102	1495.7281	1507.5363	1843.5555
H	1.735502	-0.905678	1.177512	2992.5363	3068.3773	3077.5223	3078.2914	3082.5000
C	0.517578	-1.223114	-0.556749	3119.6083	3138.0044	3150.3981	3169.0223	3188.1112
H	0.390729	-2.301844	-0.450066	3274.4789				
H	0.507430	-0.983475	-1.619011					
C	-0.672185	-0.586960	0.115662					
O	-0.873516	-0.605068	1.300949					
O	-1.503325	-0.004459	-0.759667					
C	-2.620609	0.660699	-0.174977					
H	-2.275216	1.456141	0.484200					
H	-3.192263	1.069789	-1.001387					
H	-3.222637	-0.038424	0.401905					

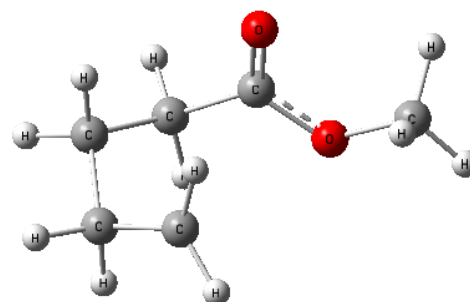


Table S2: Enthalpies of reaction and Gibbs free energies of reaction ($\Delta H_{r,298.15\text{ K}}$, $\Delta G_{r,298.15\text{ K}}$ in kcal mol⁻¹ at 298.15 K) at the M06-2X/cc-pVTZ and DLPNO-CCSD(T)/CBS(T-Q) levels.

Reaction channel	M06-2X/cc-pVTZ		DLPNO-CCSD(T)/CBS(T-Q)	
	$\Delta H_{r,298.15\text{ K}}$	$\Delta G_{r,298.15\text{ K}}$	$\Delta H_{r,298.15\text{ K}}$	$\Delta G_{r,298.15\text{ K}}$
Rxn- α'	-18.1	-19.3	-19.1	-20.3
Rxn- α	-24.0	-25.1	-24.1	-25.2
Rxn- β	-18.4	-21.1	-19.3	-21.9
Rxn- γ	-19.2	-21.1	-19.7	-21.6
Rxn- δ	-16.5	-17.4	-16.8	-17.7

Table S3: Calculated MS-T factors for MP and each TS by using the full high-level MS-T (M06-2X) and dual-level MS-T (M06-2X/AM1) methods.

T(K)	MP	TS- α'	TS- α	TS- β	TS- γ	TS- δ	
	M06-2X	M06-2X/AM1	M06-2X	M06-2X	M06-2X	M06-2X	M06-2X/AM1
200	5.146	11.846	4.346	2.493	6.793	2.399	2.44
250	6.963	14.661	6.199	2.965	8.518	2.805	2.693
298	8.793	17.274	8.144	3.485	12.326	3.748	3.327
350	10.746	20.060	10.31	4.168	19.837	5.918	4.836
400	12.516	22.777	12.359	4.992	30.963	9.646	7.449
500	15.563	28.575	16.123	7.267	64.433	23.102	16.823
600	17.864	34.977	19.25	10.355	108.742	44.341	31.428
700	19.454	41.811	21.691	13.993	157.228	71.08	49.622
800	20.439	48.747	23.493	17.827	204.161	100.289	69.387
900	20.938	55.453	24.743	21.548	245.859	129.306	89.018
1000	21.063	61.671	25.534	24.94	280.518	156.232	107.325
1200	20.554	72.028	26.071	30.313	327.6	199.853	137.499
1400	19.461	79.279	25.656	33.691	349.012	228.226	158.027
1600	18.115	83.607	24.672	35.341	351.854	243.047	169.826
1800	16.701	85.500	23.37	35.678	342.637	247.429	174.71
2000	15.318	85.508	21.915	35.093	326.275	244.43	174.52

Table S4: Calculated rate constants ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$) for each reaction channel after compensating the uncertainty of energy barriers.

T (K)	Rxn- α'	Rxn- α	Rxn- β	Rxn- γ	Rxn- δ
200	6.05072E10	1.88455E12	3.85457E13	3.47084E11	3.16479E11
250	3.11766E10	7.35666E11	8.43879E12	1.7405E11	9.29623E10
298	2.39942E10	4.93534E11	3.27659E12	1.44425E11	5.49718E10
350	2.19762E10	4.13221E11	1.72681E12	1.56768E11	4.89967E10
400	2.24248E10	3.96521E11	1.19541E12	1.90966E11	5.55716E10
500	2.74714E10	4.35581E11	8.90056E11	3.06136E11	8.90006E10
600	3.74133E10	5.29024E11	9.01065E11	4.78487E11	1.4593E11
700	5.30049E10	6.65479E11	1.03926E12	7.10193E11	2.28393E11
800	7.55933E10	8.45E11	1.26054E12	1.00564E12	3.40001E11
900	1.06803E11	1.07089E12	1.55445E12	1.3696E12	4.84663E11
1000	1.48417E11	1.34741E12	1.91568E12	1.80647E12	6.66185E11
1200	2.70352E11	2.07107E12	2.85208E12	2.91399E12	1.15342E12
1400	4.5673E11	3.05273E12	4.08699E12	4.35272E12	1.82577E12
1600	7.22616E11	4.32558E12	5.63709E12	6.13853E12	2.70177E12
1800	1.08231E12	5.9174E12	7.51756E12	8.28064E12	3.79504E12
2000	1.54897E12	7.85044E12	9.73746E12	1.07822E13	5.11502E12

An example of input file for MESS code

```
! MP + OH => RC_delta => TS_delta => MP_delta + H2O
! Reactants  W1      B      Products
!
! Frequencies calculated at M06-2X/cc-pVTZ (scaled by 0.985), energies at DLPNO-CCSD(T)/CBS
! Reactants set to zero of energy
!
TemperatureList[K]  200 250 298 350 400 500 600 700 800 900 1000 1200 1400 1600 1800 2000
PressureList[atm]  1
EnergyStepOverTemperature  0.2
ExcessEnergyOverTemperature  30
ModelEnergyLimit[kcal/mol]  250
!
WellCutoff  10
ChemicalEigenvalueMax  0.2
ChemicalEigenvalueMin  1.e-6
CalculationMethod  direct
EigenvalueOutput  eigenvalue.out
! End of global input
!
Model
EnergyRelaxation
  Exponential
    Factor[1/cm]  200  ! Delta E down
    Power  0.85  ! Exponent normally 0.85
    ExponentCutoff  15
  End
CollisionFrequency
  LennardJones
    Epsilons[K]  362  143.78
    Sigmas[angstrom]  7.34  3.3237
    Masses[amu]  133  40
  End
! %%%%%%%%%%%
%%%%%%%%%%
Well  W1  #RC_delta
Species
RRHO
Geometry[angstrom]  22
C  2.509179  -0.413555  -0.769512
H  2.186817  0.564315  -0.409505
H  3.264265  -0.786925  -0.075650
H  2.986976  -0.261605  -1.736197
C  1.344906  -1.391040  -0.881105
H  0.576782  -0.973456  -1.539609
H  1.684279  -2.311198  -1.359522
C  0.718857  -1.750667  0.464783
H  -0.082541  -2.474464  0.315113
```

H	1.468298	-2.225461	1.100789
C	0.156154	-0.539014	1.220589
H	0.943173	0.149395	1.520551
H	-0.370460	-0.877213	2.113418
C	-0.815075	0.222484	0.364511
O	-0.664722	1.353883	-0.037327
O	-1.887916	-0.503827	0.051317
C	-2.840667	0.133361	-0.802044
H	-2.376532	0.399361	-1.749633
H	-3.634317	-0.590205	-0.952631
H	-3.225069	1.035086	-0.330341
O	1.764845	2.469059	0.870598
H	0.871595	2.253243	0.523798

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 60

40.6529
58.1381
94.2650
100.3672
118.3827
156.4871
164.4252
173.8110
200.8320
258.3579
324.4164
353.6467
433.6421
469.7225
499.8484
617.3864
645.3072
715.0202
756.6859
831.7855
856.4913
903.1697
950.8490
976.5110
1041.1048
1081.5380
1104.0418
1126.4406
1171.6357
1188.3697
1208.3548
1234.8637

1291.5209
1319.0729
1342.9921
1364.0953
1375.8046
1399.7902
1460.3150
1463.4926
1471.0969
1474.5118
1479.0250
1484.3928
1485.9382
1529.5323
1784.9817
2999.0462
3017.7552
3023.7781
3038.5499
3045.6678
3048.8610
3068.7839
3083.6301
3094.2915
3110.8013
3112.6489
3147.1242
3513.1074

ZeroEnergy[kcal/mol] -3.5

ElectronicLevels[1/cm] 1

0.0 2

End

End

! %%%%%%%%%%
%%%%%%%%%

Bimolecular R !MP + OH

Fragment !MP

RRHO

Geometry[angstrom] 20

C	3.440908	-0.646981	-0.149164
H	3.877311	-1.328189	-0.878637
H	4.106518	0.212312	-0.052331
H	3.416543	-1.158181	0.813978
C	2.041480	-0.208168	-0.559209
H	2.077714	0.275251	-1.539483
H	1.395923	-1.082324	-0.658767
C	1.423611	0.754000	0.449226
H	1.387886	0.274886	1.429380
H	2.061116	1.635618	0.545098

C	0.021364	1.199315	0.064348
H	-0.015993	1.578623	-0.958470
H	-0.328045	2.014902	0.701881
C	-0.998473	0.095984	0.191498
O	-0.826415	-0.957531	0.742530
O	-2.164927	0.442187	-0.374313
C	-3.203870	-0.529077	-0.266088
H	-3.425215	-0.732796	0.779853
H	-4.067403	-0.099918	-0.763251
H	-2.905742	-1.457876	-0.748653

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 54

38.6549

70.9374

104.2851

162.5212

178.2944

220.0834

246.6966

259.2981

311.2111

372.0607

522.6355

585.1140

653.7702

741.0068

840.2382

846.8352

916.2097

942.0672

1012.9145

1051.8861

1067.3937

1112.4675

1131.7894

1173.8101

1201.1492

1218.4183

1240.3428

1264.9169

1312.2740

1317.3940

1385.1845

1390.9957

1392.5683

1442.2113

1460.8852

1465.8255
1473.8214
1474.1157
1482.3517
1487.8249
1489.589
1822.4610
3004.2503
3012.0279
3017.6379
3026.5086
3035.5355
3046.4931
3060.4215
3069.1030
3081.8289
3088.4327
3107.4166
3140.8322

ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0.0 1

End

!

Fragment !OH

RRHO

Geometry[angstrom] 2 !

O 0.000000 0.000000 0.106747
H 0.000000 0.000000 -0.864787

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 1

3717.8991

ZeroEnergy[kcal/mol] 0.0 !

ElectronicLevels[1/cm] 1

0.0 2

End

GroundEnergy[kcal/mol] 0.0 ! Reactants: 0.0

End

! %%%%%%%%%%

Bimolecular P ! MP_delta + H2O

Fragment ! MP_delta

RRHO

Geometry[angstrom] 19

C 1.238252 1.660986 0.269890
H 1.060796 2.582658 -0.262454
H 0.863222 1.577587 1.279975
C 2.207379 0.655470 -0.242783

H	2.312149	0.757553	-1.325814
H	3.204208	0.853126	0.174609
C	1.830178	-0.789658	0.096367
H	2.627252	-1.455760	-0.234176
H	1.735502	-0.905678	1.177512
C	0.517578	-1.223114	-0.556749
H	0.390729	-2.301844	-0.450066
H	0.507430	-0.983475	-1.619011
C	-0.672185	-0.586960	0.115662
O	-0.873516	-0.605068	1.300949
O	-1.503325	-0.004459	-0.759667
C	-2.620609	0.660699	-0.174977
H	-2.275216	1.456141	0.484200
H	-3.192263	1.069789	-1.001387
H	-3.222637	-0.038424	0.401905

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 51

33.2874

86.6481

119.4869

170.0911

187.2940

194.6685

244.9116

305.7616

320.6128

410.0348

460.4619

525.5490

605.7598

707.4268

802.5980

832.6244

872.3157

930.4391

948.9575

1006.2715

1064.0984

1089.8404

1118.9158

1163.9742

1171.7138

1202.8101

1220.3595

1246.3633

1276.6169

1348.4287

1363.7991
1378.4544
1442.7016
1451.2913
1456.6446
1465.7380
1472.4865
1473.2921
1484.9232
1815.9021
2947.6482
3022.3516
3031.3594
3032.1170
3036.2625
3072.8141
3090.9343
3103.1421
3121.4869
3140.2895
3225.3617

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0.0 2

End

!

Fragment ! H2O

RRHO

Geometry[angstrom] 3

O 0.000000 0.115777 -0.000000

H 0.759563 -0.469814 0.000000

H -0.759563 -0.469814 -0.000000

Core RigidRotor

SymmetryFactor 2

End

Frequencies[1/cm] 3

1604.7215

3813.7819

3913.8209

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0.0 1

End

GroundEnergy[kcal/mol] -17.0

End

! %%%%%%%%%%%

Barrier B1 W1 P !RC_delta => TS_delta => MP_delta + H2O

RRHO

Geometry[angstrom] 22 ! TS_delta

C	2.680480	-0.218761	-0.491238
H	2.353022	0.837566	-0.054966
H	3.301751	-0.645982	0.296662
H	3.289215	0.043032	-1.353676
C	1.491140	-1.085944	-0.845535
H	0.829221	-0.543357	-1.524996
H	1.851965	-1.953588	-1.405322
C	0.707726	-1.596066	0.362520
H	-0.042382	-2.318024	0.035599
H	1.387354	-2.125955	1.032592
C	0.007633	-0.493883	1.174740
H	0.726323	0.241738	1.529986
H	-0.508401	-0.939563	2.023011
C	-0.997082	0.216385	0.314421
O	-0.793601	1.234302	-0.304736
O	-2.160287	-0.435931	0.252232
C	-3.148742	0.145894	-0.599649
H	-2.782161	0.196334	-1.622876
H	-4.016098	-0.501867	-0.533717
H	-3.391741	1.151015	-0.261736
O	1.900764	2.052873	0.346719
H	0.990637	1.951177	0.004373

Core RigidRotor

SymmetryFactor 1

End

Tunneling

Eckart

ImaginaryFrequency[1/cm] 1065.05

WellDepth[kcal/mol] 3.1 ! TSa - RCa

WellDepth[kcal/mol] 16.6 ! TSa - Products-a

End

Frequencies[1/cm] 59

31.6259

80.3004

117.1442

131.2505

165.6499

172.3004

174.7642

223.7561

320.4859

350.9794

359.5993

447.5463

459.5741

558.9591

627.4243

708.5826

743.8338

821.7087

831.5079
873.2777
901.4279
926.4447
960.7522
1004.3602
1051.0483
1086.0935
1114.0101
1121.1338
1172.2122
1179.9159
1207.4885
1229.4056
1278.6808
1306.0227
1312.8025
1348.0545
1364.0622
1385.6572
1406.4303
1445.9130
1463.0247
1463.7353
1473.4577
1474.5265
1482.9248
1487.1886
1790.1578
3002.4162
3018.7265
3033.8801
3038.9415
3045.4457
3055.2506
3065.0703
3112.8318
3113.9567
3114.4043
3146.0653
3594.3651

ZeroEnergy[kcal/mol] -0.4
ElectronicLevels[1/cm] 1
0.0 2

End

! %%%%%%%%%%

! %%%%%%%%%%

Barrier B2 W1 R! MP + OH => RC_delta

RRHO

Stoichiometry C6H13O3

Core PhaseSpaceTheory ! V(R) = -C/(R)^6 R=3.517

FragmentGeometry[angstrom] 20 ! MP

C	3.440908	-0.646981	-0.149164
H	3.877311	-1.328189	-0.878637
H	4.106518	0.212312	-0.052331
H	3.416543	-1.158181	0.813978
C	2.041480	-0.208168	-0.559209
H	2.077714	0.275251	-1.539483
H	1.395923	-1.082324	-0.658767
C	1.423611	0.754000	0.449226
H	1.387886	0.274886	1.429380
H	2.061116	1.635618	0.545098
C	0.021364	1.199315	0.064348
H	-0.015993	1.578623	-0.958470
H	-0.328045	2.014902	0.701881
C	-0.998473	0.095984	0.191498
O	-0.826415	-0.957531	0.742530
O	-2.164927	0.442187	-0.374313
C	-3.203870	-0.529077	-0.266088
H	-3.425215	-0.732796	0.779853
H	-4.067403	-0.099918	-0.763251
H	-2.905742	-1.457876	-0.748653

FragmentGeometry[angstrom] 2 ! OH

O	0.000000	0.000000	0.106747
H	0.000000	0.000000	-0.864787

SymmetryFactor 1

PotentialPrefactor[au] 480.7 ! C

PotentialPowerExponent 6 ! n

End

Frequencies[1/cm] 55

38.6549
70.9374
104.2851
162.5212
178.2944
220.0834
246.6966
259.2981
311.2111
372.0607
522.6355
585.1140
653.7702
741.0068
840.2382
846.8352
916.2097
942.0672

1012.9145
1051.8861
1067.3937
1112.4675
1131.7894
1173.8101
1201.1492
1218.4183
1240.3428
1264.9169
1312.2740
1317.3940
1385.1845
1390.9957
1392.5683
1442.2113
1460.8852
1465.8255
1473.8214
1474.1157
1482.3517
1487.8249
1489.589
1822.4610
3004.2503
3012.0279
3017.6379
3026.5086
3035.5355
3046.4931
3060.4215
3069.1030
3081.8289
3088.4327
3107.4166
3140.8322
3717.8991

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0.0 2

End

End

!