

Supplementary Material for:

Kinetic modeling of methyl pentanoate pyrolysis based on *ab initio* calculations

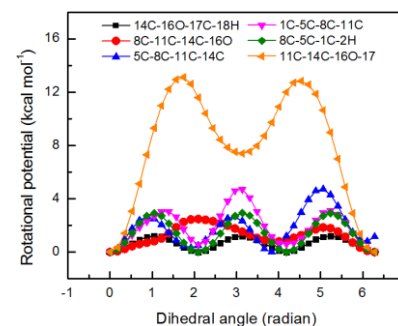
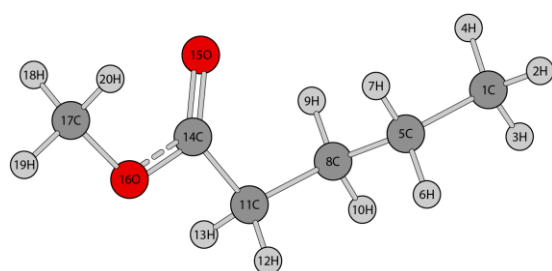
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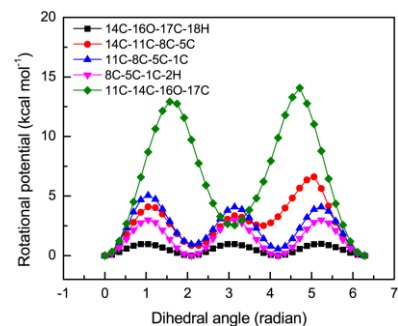
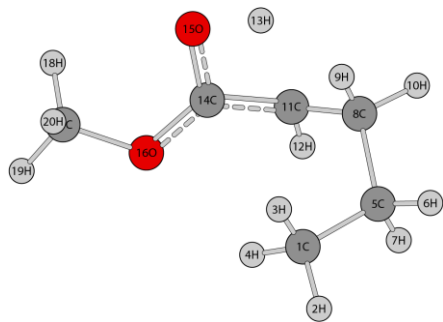
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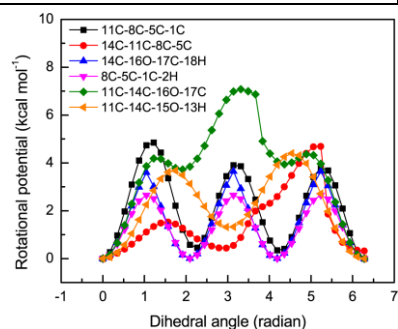
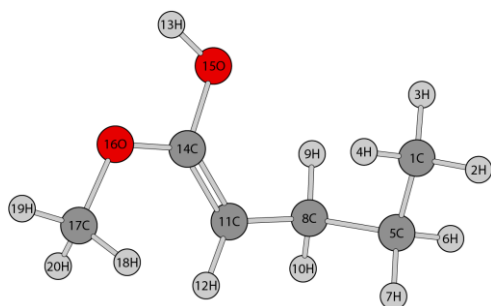
Table S1. Optimized geometries, frequencies, and rotational constants of involved species with the lowest energies for MP decomposition at the M06-2X/cc-pVTZ level of theory.



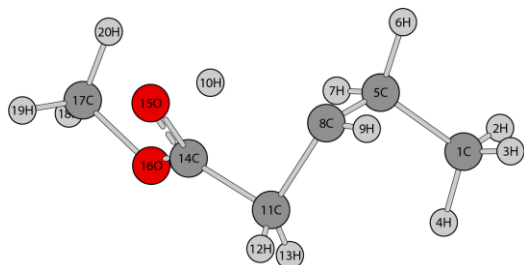
Geometry – Methyl Pentanoate – C ₁				Frequency (cm ⁻¹)				
C	3.440908	-0.646981	-0.149164	39.2436	72.0177	105.8732	164.9962	181.0096
H	3.877311	-1.328189	-0.878637	223.4350	250.4534	263.2468	315.9504	377.7266
H	4.106518	0.212312	-0.052331	530.5945	594.0244	663.7261	752.2912	853.0338
H	3.416543	-1.158181	0.813978	859.7312	930.1622	956.4134	1028.3396	1067.9047
C	2.041480	-0.208168	-0.559209	1083.6485	1129.4087	1149.0248	1191.6854	1219.4409
H	2.077714	0.275251	-1.539483	1236.9729	1259.2313	1284.1796	1332.2579	1337.4559
H	1.395923	-1.082324	-0.658767	1406.2787	1412.1784	1413.7750	1464.1740	1483.1322
C	1.423611	0.754000	0.449226	1488.1478	1496.2654	1496.5642	1504.9256	1510.4822
H	1.387886	0.274886	1.429380	1512.2731	1850.2143	3050.0003	3057.8964	3063.5918
H	2.061116	1.635618	0.545098	3072.5976	3081.7620	3092.8864	3107.0269	3115.8407
C	0.021364	1.199315	0.064348	3128.7604	3135.4647	3154.7377	3188.6622	
H	-0.015993	1.578623	-0.958470					
H	-0.328045	2.014902	0.701881	Rotational constants (cm ⁻¹)				
C	-0.998473	0.095984	0.191498	0.1755	0.0301	0.0282		
O	-0.826415	-0.957531	0.742530					
O	-2.164927	0.442187	-0.374313	T ₁ value: 0.011				
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					



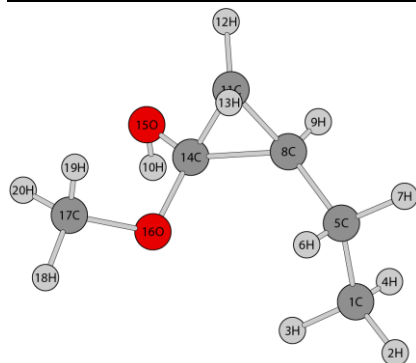
Geometry – TS1 – C ₁				Frequency (cm ⁻¹)				
C	-1.770518	-1.541666	-0.386948	-2089.2276				
H	-2.415070	-2.418930	-0.340912	61.3421	72.6386	127.1259	133.6857	165.9341
H	-1.446712	-1.418090	-1.423070	246.9192	287.9880	302.9375	340.8344	438.0311
H	-0.886240	-1.746693	0.216538	490.3380	711.6598	756.7105	796.9367	826.8699
C	-2.492348	-0.293153	0.102746	856.4309	900.3091	967.8709	997.6773	1071.5823
H	-3.431402	-0.171851	-0.442950	1087.9216	1110.0993	1127.3631	1160.1411	1188.6662
H	-2.756973	-0.410638	1.156657	1220.1734	1249.9406	1296.8420	1317.0518	1370.0534
C	-1.659367	0.980994	-0.064678	1374.6532	1414.7708	1447.4833	1479.6290	1491.1131
H	-1.436114	1.121269	-1.125998	1495.5144	1502.6846	1509.3712	1513.8323	1547.4670
H	-2.259252	1.839984	0.239275	1561.1349	2036.2838	3048.5368	3052.1452	3054.2648
C	-0.360023	0.982686	0.739902	3084.7417	3089.3333	3097.4956	3122.7060	3137.3856
H	-0.494809	0.764834	1.795199	3155.9376	3170.5057	3196.2527		
H	0.416323	1.872390	-0.213955					
C	0.798976	0.434100	0.136786	Rotational constants (cm ⁻¹)				
O	1.220436	1.163968	-0.837474	0.1135	0.0415	0.0347		
O	1.489326	-0.594908	0.556521					
C	2.777951	-0.798798	-0.039456	T ₁ value: 0.012				
H	3.344120	0.129587	-0.025579					
H	3.263237	-1.561210	0.560155					
H	2.661163	-1.136757	-1.065968					



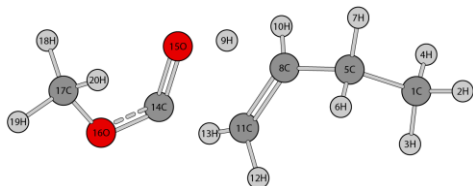
Geometry – CH ₃ OC(OH)=CHCH ₂ CH ₂ CH ₃ – C ₁ (P1)				Frequency (cm ⁻¹)				
C	2.308889	0.591938	1.088973	38.2150	77.7211	119.8305	166.8679	223.7647
H	3.055587	0.568832	1.882389	243.5346	285.0549	300.4115	318.1022	353.1893
H	2.473062	1.490070	0.491723	481.5490	535.1514	588.4713	665.0811	769.4717
H	1.325092	0.681512	1.550265	797.5741	835.9703	895.1474	933.6486	1014.3739
C	2.383778	-0.653399	0.215473	1087.9877	1099.1781	1110.0532	1167.9844	1192.6919
H	3.378660	-0.732851	-0.228185	1215.6218	1251.9549	1256.2871	1292.7659	1335.2553
H	2.243177	-1.545974	0.830739	1366.3144	1373.3768	1411.0006	1420.6734	1486.5266
C	1.338236	-0.645718	-0.906725	1489.7424	1492.2921	1500.6191	1502.7363	1509.5033
H	1.462282	0.261925	-1.499654	1522.7814	1797.7812	3049.4782	3052.0450	3059.9708
H	1.526293	-1.488705	-1.574909	3060.2172	3086.2682	3108.0739	3116.9885	3129.7232
C	-0.073557	-0.724742	-0.403192	3133.7724	3175.9008	3241.3662	3868.3542	
H	-0.445301	-1.678508	-0.061923					
H	-1.232193	2.163286	-0.609649	Rotational constants (cm ⁻¹)				
C	-0.872968	0.336703	-0.327471	0.1153	0.0375	0.0344		
O	-0.477250	1.573429	-0.703605					
O	-2.151821	0.381152	0.113689	T ₁ value: 0.010				
C	-2.725634	-0.837899	0.537191					
H	-2.171812	-1.250561	1.382363					
H	-3.742727	-0.609002	0.839468					
H	-2.734027	-1.562735	-0.278757					



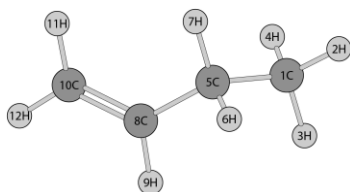
Geometry – TS2 – C ₁				Frequency (cm ⁻¹)				
C	3.420828	0.915738	-0.268971	-962.1432				
H	4.341447	0.330925	-0.208964	58.7810	94.8974	140.1988	147.7681	187.6052
H	3.631074	1.820681	-0.840982	236.5854	294.5400	302.9493	355.0727	453.1338
H	3.155663	1.223932	0.744598	466.0137	611.7830	713.3260	755.8408	827.7772
C	2.275321	0.133417	-0.922516	830.1839	887.3072	939.8482	949.2657	1024.3879
H	2.589512	-0.175433	-1.922505	1066.6521	1083.9605	1103.7986	1121.0298	1184.7698
H	2.131531	-0.801977	-0.367140	1188.1221	1216.1238	1242.2600	1285.5249	1320.3974
C	0.967088	0.889139	-1.010654	1373.0716	1396.7379	1426.3558	1445.0256	1478.3718
H	1.051672	1.845649	-1.521808	1494.9657	1497.2265	1499.8313	1504.1156	1527.0684
H	-0.832593	0.352245	-1.562471	1567.0131	2696.4561	3007.4552	3038.5915	3043.8948
C	0.252155	1.046483	0.331468	3063.4103	3097.5569	3107.4714	3109.2180	3118.1220
H	-0.366696	1.943545	0.369152	3124.5704	3184.7389	3208.8888		
H	0.825570	0.938433	1.256133					
C	-0.600168	-0.118902	0.091676	Rotational constants (cm ⁻¹)				
O	-1.425658	-0.184512	-0.920105	0.1229	0.0378	0.0341		
O	-0.540385	-1.139268	0.883020					
C	-1.165376	-2.369070	0.466023	T ₁ value: 0.014				
H	-0.867225	-3.105293	1.203307					
H	-2.244461	-2.248507	0.452341					
H	-0.807745	-2.637245	-0.524605					



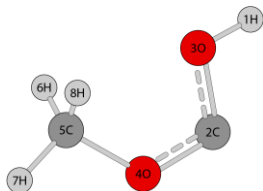
Geometry – c-C(CH ₃ O,OH)CH ₂ CH-CH ₂ CH ₃ – C ₁ (P ₂)				Frequency (cm ⁻¹)				
C	-2.475934	0.855397	-0.613800	77.7833	112.7375	147.3722	168.6443	198.5625
H	-3.267999	1.521711	-0.273462	258.4568	307.5711	350.0240	369.7139	444.4734
H	-1.709235	1.457627	-1.101770	477.0181	509.9292	602.6079	753.4533	788.9807
H	-2.902768	0.180024	-1.357034	823.4209	924.5307	946.5446	986.3536	1015.7743
C	-1.865664	0.074765	0.545355	1036.0432	1042.8507	1103.1195	1129.3068	1148.0095
H	-1.433140	0.770536	1.264981	1190.9185	1198.6522	1219.9692	1263.8802	1293.6781
H	-2.638005	-0.491255	1.070596	1310.3303	1340.3073	1372.9090	1408.4914	1431.3713
C	-0.790422	-0.870019	0.074525	1479.9870	1489.0943	1495.3165	1501.9530	1510.6341
H	-1.113575	-1.652859	-0.601436	1521.9731	1528.5613	3045.1859	3057.6159	3064.5536
H	1.020675	-0.567037	-2.038379	3105.0227	3111.5869	3129.5992	3137.5481	3162.5167
C	0.359424	-1.254418	0.998051	3164.5785	3170.4120	3262.1064	3843.5174	
H	0.739151	-2.263629	0.953769					
H	0.369098	-0.780893	1.970213	Rotational constants (cm ⁻¹)				
C	0.588624	-0.379965	-0.182167	0.0976	0.0500	0.0441		
O	1.336234	-0.941901	-1.209416					
O	0.805959	0.972860	0.001251	T ₁ value: 0.009				
C	2.110199	1.266165	0.470401					
H	2.174617	2.345857	0.574694					
H	2.285828	0.794432	1.440865					
H	2.865716	0.918592	-0.235297					



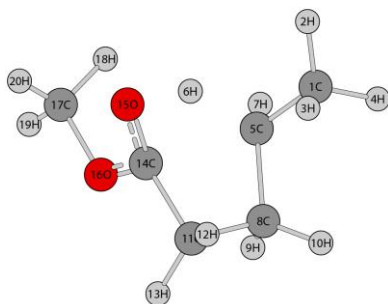
Geometry – TS3 – C ₁				Frequency (cm ⁻¹)				
C	3.690372	-0.161133	-0.393432	-906.4237				
H	4.292783	-0.823299	-1.016728	48.4431	74.2404	127.1184	144.6678	190.6623
H	3.677202	0.827557	-0.853530	225.3853	253.0905	304.3642	341.6001	434.1102
H	4.182724	-0.066889	0.575262	455.6302	544.1035	616.3385	765.7991	782.4136
C	2.264935	-0.686614	-0.220870	845.9323	905.1178	962.9318	974.1017	1030.2460
H	1.790767	-0.776103	-1.202879	1041.7400	1086.1122	1103.6164	1173.3815	1189.3792
H	2.306499	-1.698864	0.188541	1209.9879	1249.2115	1276.5288	1298.7220	1311.5487
C	1.409731	0.202299	0.654238	1367.3558	1404.7394	1434.9050	1470.2305	1487.5382
H	0.078834	-0.587212	0.735760	1499.0485	1499.8957	1500.9819	1507.1542	1532.4906
H	1.654627	0.238393	1.711440	1577.1753	1890.8974	3041.5537	3053.7703	3075.0093
C	0.705216	1.262625	0.121403	3088.6338	3125.2657	3128.8868	3154.0294	3166.1225
H	0.750953	1.485918	-0.937320	3170.0095	3197.7042	3243.4961		
H	0.381917	2.091874	0.734596					
C	-1.267967	0.368610	-0.007875	Rotational constants (cm ⁻¹)				
O	-1.009271	-0.743698	0.520843	0.2010	0.0254	0.0242		
O	-2.497028	0.563948	-0.403128					
C	-3.458466	-0.493399	-0.209855	T ₁ value: 0.014				
H	-3.548799	-0.721565	0.849469					
H	-4.395712	-0.117682	-0.605326					
H	-3.140914	-1.384222	-0.746538					



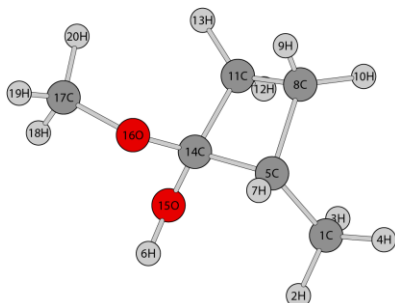
Geometry – CH ₂ =CHCH ₂ CH ₃ – C ₁ (P ₃)				Frequency (cm ⁻¹)				
C	-2.702593	1.423739	-0.070739	107.1192	232.5970	318.8282	439.3194	662.4470
H	-3.157989	2.104138	-0.789312	797.4147	871.4182	969.2932	991.0802	1036.0775
H	-3.186935	1.579700	0.893925	1049.7237	1101.7385	1204.8869	1293.0646	1322.5602
H	-1.651740	1.691153	0.037242	1349.1035	1409.6907	1457.8636	1487.3523	1502.1005
C	-2.844048	-0.030943	-0.519766	1510.4530	1740.7405	3052.5573	3062.8799	3096.4892
H	-3.904438	-0.260129	-0.655324	3133.4376	3140.4594	3148.9036	3161.4366	3246.7495
H	-2.360231	-0.175989	-1.486975					
C	-2.258044	-0.981736	0.477716	Rotational constants (cm ⁻¹)				
H	-2.687587	-0.944823	1.475643	0.7557	0.1401	0.1367		
C	-1.264224	-1.821867	0.234739	T ₁ value: 0.010				
H	-0.808569	-1.882148	-0.746711					
H	-0.872925	-2.476544	1.001390					



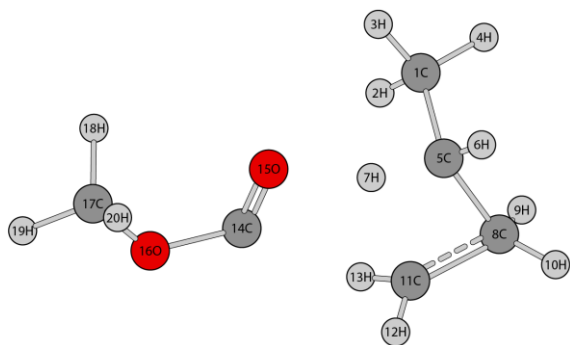
Geometry – CH ₃ OCO – C _s (P ₃)				Frequency (cm ⁻¹)				
H	0.007153	-0.003941	0.504889	192.3314	356.5974	365.7846	706.8750	728.7688
C	1.633823	-0.575488	-0.174097	953.3006	1137.2179	1164.5447	1207.8410	1253.9568
O	0.880662	0.377112	0.380120	1398.7937	1490.8838	1499.9182	1507.0058	3093.0098
O	2.834207	-0.106491	-0.364787	3173.1517	3200.6054	3892.5020		
C	3.189636	1.242862	0.001648	Rotational constants (cm ⁻¹)				
H	3.051786	1.391806	1.069501	0.6363	0.2449	0.1829		
H	4.234176	1.349125	-0.268183	T ₁ value: 0.014				
H	2.577346	1.955133	-0.545444					



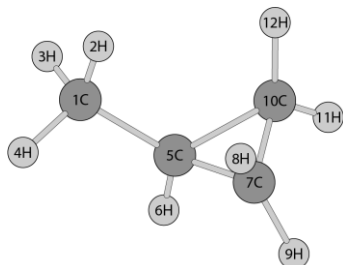
Geometry – TS4 – C ₁				Frequency (cm ⁻¹)				
C	2.394662	-1.050331	-0.502384	-2104.4766				
H	2.346258	-2.134514	-0.610881	90.5237	128.2519	158.6857	185.4855	202.3594
H	2.085817	-0.611783	-1.454413	237.3555	300.9924	365.8764	390.1922	470.2922
H	3.441758	-0.778081	-0.341609	543.1804	616.5468	715.4522	779.8384	842.8126
C	1.522114	-0.538564	0.643730	848.9947	943.3821	954.1605	985.4962	1021.1568
H	0.357459	-1.177872	-0.088470	1034.8257	1073.6369	1122.4727	1129.0214	1180.9457
H	1.765031	-1.027515	1.584904	1187.0575	1216.1110	1233.0776	1283.3426	1301.3175
C	1.500481	0.998911	0.726622	1332.1379	1359.7276	1399.5688	1431.0018	1480.4272
H	1.443398	1.327752	1.762198	1490.5793	1494.4001	1498.8260	1499.9614	1504.6808
H	2.357317	1.481886	0.255823	1514.5456	2085.8924	3032.9916	3066.3573	3076.8608
C	0.161545	1.261822	0.023236	3090.9299	3103.9239	3112.1719	3122.1146	3135.6140
H	0.261084	1.313993	-1.058362	3156.4833	3167.3758	3196.0953		
H	-0.428855	2.100099	0.387540					
C	-0.426271	-0.084348	0.383371	Rotational constants (cm ⁻¹)				
O	-0.777663	-1.004235	-0.496802	0.1018	0.0527	0.0474		
O	-1.011506	-0.067600	1.578178					
C	-1.500089	-1.323997	2.045819	T ₁ value: 0.011				
H	-0.673545	-2.034536	2.109021					
H	-1.909193	-1.134901	3.032574					
H	-2.259965	-1.712650	1.374601					



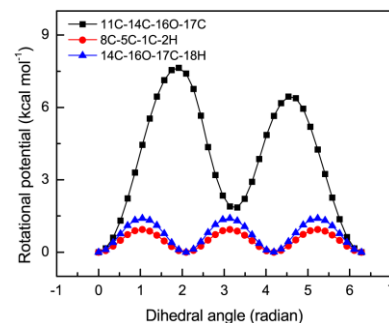
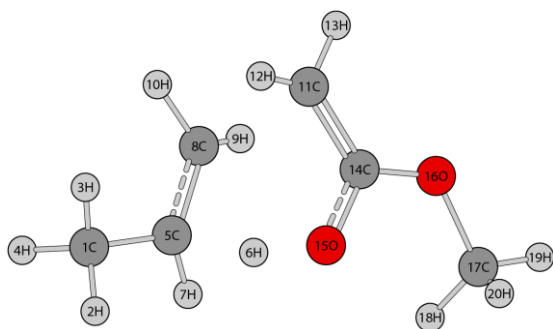
Geometry – c-C(CH ₃ O,OH)CH ₂ CH ₂ CHCH ₃ – C ₁ (P4)				Frequency (cm ⁻¹)				
C	-2.254867	-0.821185	-0.236175	47.9718	109.9199	187.2020	228.5170	251.2204
H	-2.109296	-1.858396	-0.539185	290.7857	337.6790	347.0733	391.3566	452.8551
H	-2.366134	-0.808256	0.848786	477.9130	567.1608	679.7436	744.6617	823.2325
H	-3.185922	-0.466764	-0.678888	890.8174	914.4574	962.6021	973.5143	1011.4724
C	-1.098292	0.056188	-0.673983	1069.2042	1086.8795	1121.4804	1178.9144	1190.7446
H	0.454790	-2.117457	0.112351	1202.6275	1204.0842	1218.7475	1238.9195	1266.5045
H	-0.965021	0.032711	-1.754518	1274.2382	1309.5409	1361.9866	1384.0380	1416.0103
C	-1.115273	1.464936	-0.029332	1471.3111	1483.7818	1495.3746	1497.7694	1502.9232
H	-0.690407	2.222037	-0.683376	1504.0721	1522.2666	3050.2116	3060.6742	3098.0741
H	-2.079433	1.805018	0.343194	3106.3836	3111.0800	3115.7514	3130.1361	3135.4699
C	-0.098423	0.973534	1.027287	3153.0408	3158.9278	3171.5731	3840.0643	
H	-0.579125	0.621560	1.937051					
H	0.725440	1.633606	1.285131	Rotational constants (cm ⁻¹)				
C	0.213788	-0.209196	0.098421	0.1117	0.0560	0.0481		
O	0.365513	-1.422094	0.773492					
O	1.275953	0.016219	-0.788336	T ₁ value: 0.009				
C	2.549808	0.103011	-0.180733					
H	2.767868	-0.785293	0.413295					
H	3.274593	0.188474	-0.986126					
H	2.629505	0.984216	0.460225					



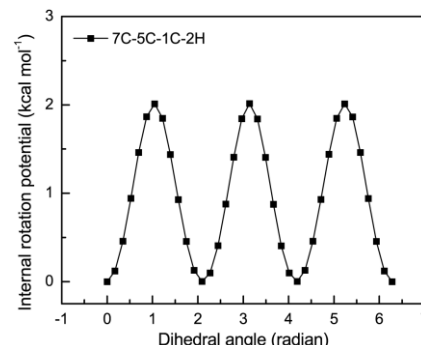
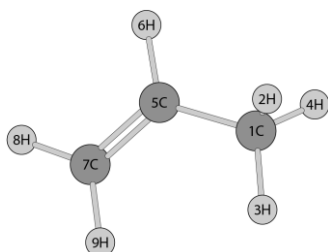
Geometry – TS5 – C ₁				Frequency (cm ⁻¹)				
C	0.970379	-1.354909	1.279499	-633.2918				
H	0.067063	-1.038893	1.803779	42.3678	68.6715	128.3465	170.3745	188.3861
H	0.713245	-2.239849	0.701138	196.3343	206.1943	216.5031	363.9873	385.1656
H	1.730216	-1.610296	2.018314	402.5453	412.5727	679.6356	733.2958	800.5562
C	1.444878	-0.253356	0.354492	814.5732	827.3158	918.0262	977.7731	987.6079
H	2.315295	-0.492934	-0.255621	1001.7445	1059.5630	1116.7980	1150.1981	1164.7330
H	0.640831	-0.268603	-0.499243	1168.9450	1192.4217	1218.8716	1229.3649	1237.7097
C	1.749899	1.084755	1.095539	1310.2353	1414.0779	1434.9807	1458.0724	1471.4848
H	1.713093	0.978524	2.173210	1487.6900	1491.5891	1500.1034	1506.7540	1525.5237
H	2.657392	1.560747	0.748257	1564.0186	2114.3103	3062.0335	3071.5164	3099.8191
C	0.528304	1.468443	0.440824	3129.8072	3141.0400	3141.1372	3154.6398	3171.5469
H	0.537814	2.003955	-0.495077	3216.6679	3226.3193	3335.4341		
H	-0.422591	1.414731	0.938581					
C	-1.258268	0.124292	-1.034002	Rotational constants (cm ⁻¹)				
O	-0.498147	-0.756052	-1.442997	0.1374	0.0306	0.0272		
O	-2.491291	0.178996	-1.579549					
C	-2.800932	-0.793797	-2.583203	T ₁ value: 0.020				
H	-2.722908	-1.801535	-2.177633					
H	-3.819807	-0.590489	-2.899783					
H	-2.116234	-0.706839	-3.425669					



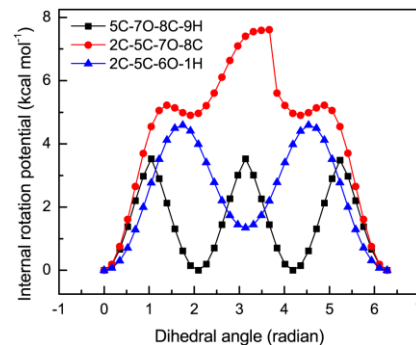
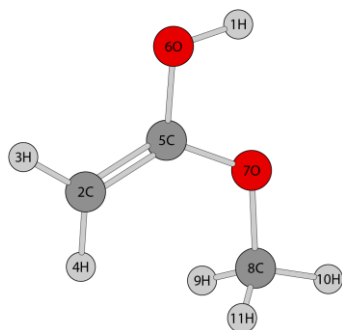
Geometry – c-CH ₂ CH ₂ CH-CH ₃ – C _s (P5)				Frequency (cm ⁻¹)				
C	1.956544	-1.433847	0.553579	230.7734	347.7364	368.1169	783.4867	813.5882
H	2.090486	-1.096041	1.582622	824.7991	904.8126	947.4191	1015.7575	1060.3421
H	0.963469	-1.877615	0.474902	1072.7381	1114.2009	1148.5608	1197.2445	1215.3203
H	2.693389	-2.214210	0.360164	1247.5114	1396.8372	1431.7453	1468.8402	496.8743
C	2.118295	-0.278408	-0.398723	1504.6205	1524.8510	3054.7043	3121.8126	123.9706
H	2.000528	-0.525059	-1.445706	3162.0937	3166.5338	3181.9053	3243.4325	256.3292
C	3.115259	0.796418	-0.092573					
H	3.670221	0.706803	0.830746	Rotational constants (cm ⁻¹)				
H	3.664960	1.240782	-0.908590	0.5243	0.2142	0.1883		
C	1.643575	1.083489	0.005202	T ₁ value: 0.007				
H	1.201416	1.720796	-0.745702					
H	1.217571	1.185668	0.993382					



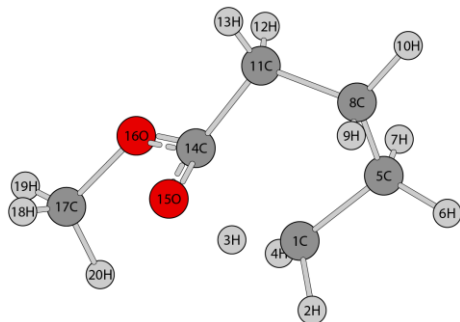
Geometry – TS6 – C ₁				Frequency (cm ⁻¹)				
C	3.055524	-1.076381	0.039634	-1183.3762				
H	2.912717	-2.100703	-0.303753	69.1932	94.2173	117.2191	127.4065	162.4261
H	3.003409	-0.427920	-0.836774	191.7266	310.5372	372.6454	406.7141	453.5940
H	4.067297	-1.003441	0.444079	487.1294	533.9089	656.7050	740.8066	779.9768
C	2.009996	-0.672958	1.055025	827.3536	883.4963	896.8605	928.9928	973.1577
H	0.754092	-1.100159	0.438248	1001.8618	1047.1413	1072.4040	1104.0606	1147.7015
H	1.885822	-1.321610	1.916854	1150.3074	1188.1611	1189.5537	1226.0796	1281.0606
C	1.662433	0.660719	1.223109	1384.6367	1409.9674	1426.8828	1454.6051	1489.6937
H	1.196768	0.988352	2.142990	1495.4047	1499.7365	1508.5676	1513.8907	1547.7341
H	2.195745	1.433435	0.685018	1616.6335	1779.8472	3048.7193	3072.3569	3106.2260
C	-0.069316	1.181146	-0.022799	3124.6537	3141.3086	3152.9845	3162.5151	3179.1748
H	0.502043	1.118529	-0.933880	3198.9577	3242.2885	3298.8574		
H	-0.399139	2.152108	0.313679					
C	-0.755910	0.059136	0.363460	Rotational constants (cm ⁻¹)				
O	-0.330223	-1.114962	0.052131	0.1210	0.0389	0.0354		
O	-1.724730	0.176464	1.293163					
C	-2.280330	-1.035330	1.787270	T ₁ value: 0.013				
H	-1.531242	-1.626810	2.311733					
H	-3.067515	-0.739434	2.473660					
H	-2.694066	-1.631707	0.975315					



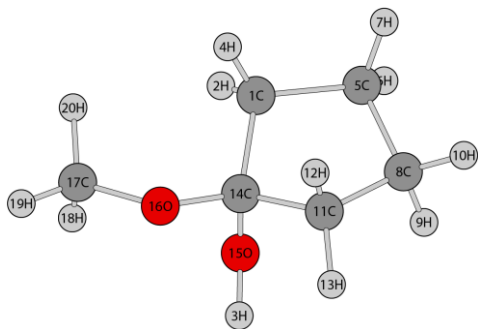
Geometry – CH ₂ =CHCH ₃ – C _s (P6)				Frequency (cm ⁻¹)				
C	-3.068791	-0.741600	0.251885	206.0517	430.4660	596.0016	938.4166	947.4326
H	-2.660519	-1.394126	1.025676	967.2257	1036.3298	1079.5133	1195.4866	330.5968
H	-3.370970	0.196152	0.715963	1407.1364	1454.2341	1484.5453	1497.2064	742.3533
H	-3.959356	-1.235146	-0.141203	3056.6034	3111.8852	3138.6438	3159.0501	3168.5654
C	-2.065704	-0.507832	-0.832739	3248.8397				
H	-1.706219	-1.390043	-1.353457	Rotational constants (cm ⁻¹)				
C	-1.600498	0.679185	-1.188206	1.5672	0.3132	0.2742		
H	-0.874088	0.789240	-1.981618					
H	-1.933759	1.583996	-0.693639	T ₁ value: 0.010				



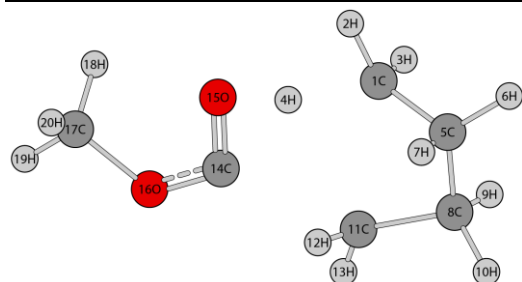
Geometry – CH ₂ =C(OH)OCH ₃ – C _S (P6)				Frequency (cm ⁻¹)				
H	1.356028	-1.604111	0.000750	135.4297	247.1750	271.6922	337.8554	479.8859
C	0.557716	1.408011	0.000101	568.2954	677.1430	705.5150	780.5417	907.7006
H	1.519033	1.892728	0.000234	986.3220	1145.1128	1191.9086	1226.9182	1258.3057
H	-0.337044	2.003787	-0.000104	1393.2542	1431.4130	1494.2764	1500.2658	1521.3493
C	0.516873	0.078864	0.000085	1774.9025	3055.1302	3121.3195	3177.8338	3231.5445
O	1.629321	-0.681049	0.000115	3328.9588	3871.5179			
O	-0.579521	-0.708487	-0.000012					
C	-1.832521	-0.053591	-0.000029					
H	-1.938961	0.567526	-0.890796					
H	-2.586670	-0.834076	-0.000064					
H	-1.939001	0.567500	0.890753					
				Rotational constants (cm ⁻¹)				
				0.3211	0.1464	0.1025		
				T ₁ value: 0.011				



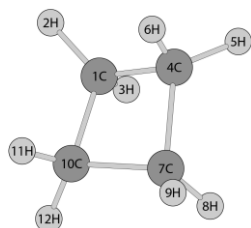
Geometry – TS7 – C ₁				Frequency (cm ⁻¹)				
C	0.189800	-0.813032	-1.694779	-2102.5040				
H	0.557648	-1.850062	-1.722029	81.4439	131.7310	172.7108	233.6976	252.6352
H	-0.162291	-1.263647	-0.379719	323.6788	380.3030	413.4198	488.1113	547.8148
H	-0.554667	-0.717968	-2.479531	586.9896	608.4529	695.2700	839.3723	844.8080
C	1.337309	0.187550	-1.762298	886.1780	923.3748	962.8901	991.8624	1026.9552
H	2.268275	-0.261581	-2.108260	1059.4879	1075.3999	1107.0134	1140.6794	1185.1013
H	1.091851	0.987955	-2.463109	1205.0791	1215.0078	1230.9274	1272.7279	1295.2042
C	1.506884	0.795440	-0.365804	1349.5605	1357.5768	1387.3156	1424.4987	1437.2674
H	1.896588	0.046018	0.325945	1471.5918	1494.0009	1494.7939	1495.6411	1506.5905
H	2.188390	1.644721	-0.359448	1512.5068	1942.6532	3001.6242	3064.4325	3066.7769
C	0.109052	1.199349	0.074993	3074.7466	3080.0759	3109.2555	3127.7087	3139.0610
H	-0.276085	2.013751	-0.538474	3154.1534	3155.9625	3195.3766		
H	0.066047	1.490824	1.125806					
C	-0.803947	0.008375	-0.058011					
O	-0.656373	-1.037566	0.733745					
O	-2.027758	0.345373	-0.459590					
C	-2.986198	-0.709944	-0.484327					
H	-3.116008	-1.135431	0.506052					
H	-3.908110	-0.264802	-0.843593					
H	-2.651288	-1.489615	-1.171445					
				Rotational constants (cm ⁻¹)				
				0.1207	0.0499	0.0460		
				T ₁ value: 0.012				



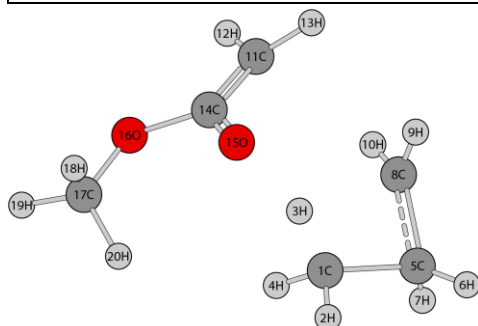
Geometry – <i>c</i> -CH ₂ CH ₂ CH ₂ CH ₂ C(OH,OCH ₃) – C ₁ (P7)				Frequency (cm ⁻¹)				
C	-0.290528	1.200305	0.078924	28.6847	123.4130	173.0398	213.7694	244.5591
H	0.104483	1.736889	0.938977	358.5670	383.8681	419.4926	470.7163	506.5532
H	0.614212	-1.604474	1.322242	621.5737	657.4645	769.4770	807.5375	852.0698
H	0.012123	1.727166	-0.826101	905.8574	942.1518	981.0820	1027.3159	1045.4482
C	-1.823624	1.018788	0.129883	1053.3241	1081.5506	1121.8647	1188.1909	1193.9857
H	-2.229648	1.320522	1.092739	1207.6607	1223.8307	1242.0832	1259.3625	1291.8696
H	-2.303024	1.638453	-0.626301	1311.1644	1323.4515	1347.8025	1369.7683	1404.2702
C	-2.090175	-0.482473	-0.137832	1479.0739	1481.4102	1493.3595	1495.5498	1504.7254
H	-2.278812	-0.997576	0.802803	1521.2531	1523.1952	3044.5633	3077.6223	3086.3648
H	-2.950963	-0.645142	-0.782982	3091.8381	3098.0527	3109.2691	3122.9211	3128.2029
C	-0.789206	-1.000313	-0.747481	3141.9360	3152.0843	3156.0624	3851.0554	
H	-0.711182	-0.738448	-1.803552	Rotational constants (cm ⁻¹) 0.1268 0.0522 0.0486				
H	-0.645846	-2.077146	-0.652408					
C	0.274885	-0.219749	0.013008	T ₁ value: 0.009				
O	0.379472	-0.671001	1.348274					
O	1.500466	-0.351337	-0.650772					
C	2.544177	0.441532	-0.122129					
H	2.664204	0.273730	0.949284					
H	3.454911	0.149674	-0.638707					
H	2.362718	1.505066	-0.298837					



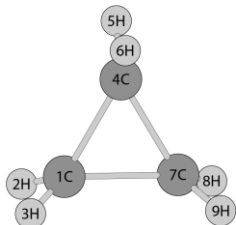
Geometry – TS8 – C ₁				Frequency (cm ⁻¹)				
C	1.533242	1.130567	-0.260885	-1242.2175				
H	1.320027	2.150080	0.081705	65.1645	87.6399	105.3752	150.3155	185.0679
H	1.457204	1.092733	-1.347691	251.1975	322.3603	332.4941	427.8022	444.6831
H	0.166297	0.883896	0.105146	503.4602	518.9571	684.8271	704.6565	850.1007
C	2.839053	0.551966	0.227282	900.9900	912.9472	953.9095	960.6124	977.5104
H	3.729473	1.030168	-0.185534	991.9058	1024.6224	1050.2491	1127.7998	1169.7303
H	2.901818	0.610236	1.316168	1191.6389	1201.9494	1241.5351	1252.7575	1269.3096
C	2.616345	-0.879577	-0.197249	1319.0396	1338.6134	1352.3637	1462.7042	1463.4485
H	2.700130	-0.965523	-1.282021	1478.2763	1489.4836	1497.3829	1501.4440	1508.2075
H	3.266112	-1.644371	0.243862	1514.6620	1746.3875	3028.2268	3029.8536	3058.1835
C	1.190108	-1.081376	0.230121	3084.1376	3085.3365	3102.0752	3127.1056	3162.5419
H	1.006633	-0.937508	1.288903	3165.4760	3191.3320	3278.5488		
H	0.667860	-1.928916	-0.180330	Rotational constants (cm ⁻¹) 0.1765 0.0283 0.0253				
C	-1.170546	-0.348656	-0.097784					
O	-0.992359	0.870713	0.129814	T ₁ value: 0.019				
O	-2.420571	-0.759601	-0.144016					
C	-3.464986	0.210442	0.061334					
H	-3.405940	0.988750	-0.696214					
H	-4.398497	-0.335870	-0.020908					
H	-3.367829	0.661259	1.046540					



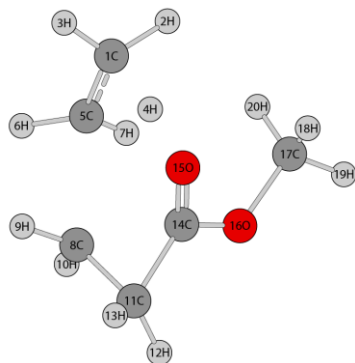
Geometry – $c\text{-CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 - D_{2d}$ (P8)				Frequency (cm^{-1})				
C	1.884389	0.796962	-0.108380	225.0324	623.4911	762.4013	762.4472	902.0575
H	1.349660	1.520253	0.503492	932.5616	932.6624	959.5168	965.7170	1042.5273
H	1.686800	1.006469	-1.159171	1171.0398	1179.0381	1254.4157	1254.4986	1255.6820
C	3.395852	0.603531	0.140888	1259.0070	1291.1667	1291.2612	1485.5018	1485.5548
H	4.095256	1.145047	-0.492368	1492.5987	1527.3563	3086.0840	3086.3081	3086.5210
H	3.646055	0.788749	1.184969	3088.7386	3129.0250	3140.7181	3140.8799	3154.9611
C	3.192052	-0.904986	-0.118785	Rotational constants (cm^{-1}) 0.3600 0.3599 0.2148				
H	3.337390	-1.142086	-1.172187					
H	3.756894	-1.612191	0.484739					
C	1.694624	-0.703881	0.200408	T ₁ value: 0.008				
H	1.497447	-0.861577	1.260218					
H	0.964779	-1.261376	-0.382669					



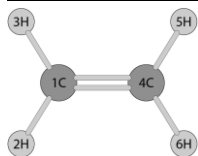
Geometry – TS9 – C ₁				Frequency (cm^{-1})				
C	-0.986334	1.066865	0.025808	-676.6307				
H	-0.899307	1.867562	0.761038	52.0732	61.1797	105.7654	133.6463	185.2740
H	-0.356359	0.256630	0.568808	197.4467	222.4628	284.5605	330.8331	457.0109
H	-0.474105	1.279032	-0.904433	503.9698	660.3771	665.3417	686.7450	703.8792
C	-2.509526	0.809214	-0.222183	743.8416	800.5586	831.0566	867.3687	914.8579
H	-3.093912	1.107612	0.639135	941.8602	966.7475	1040.7457	1145.3157	1156.2884
H	-2.877179	1.227419	-1.149956	1175.0041	1188.2284	1217.7496	1231.5421	1246.1633
C	-2.095719	-0.563364	-0.246432	1285.4142	1330.2370	1409.7723	1452.8163	1477.9401
H	-2.070407	-1.146956	0.661388	1492.7766	1501.9728	1510.8207	1515.7743	1536.8122
H	-1.887106	-1.080082	-1.167445	1604.4140	2178.3818	3050.7326	3075.2817	3117.2795
C	0.239664	-2.169180	-0.575430	3146.9027	3159.4419	3196.7964	3205.9753	3210.8234
H	0.472807	-2.579803	-1.545540	3224.3108	3295.6261	3326.4636		
H	-0.424502	-2.708681	0.079606	Rotational constants (cm^{-1}) 0.1081 0.0384 0.0330				
C	1.054057	-1.206201	-0.018265					
O	0.867083	-0.633499	1.083979					
O	2.076175	-0.766200	-0.823321	T ₁ value: 0.021				
C	2.861149	0.282038	-0.291836					
H	3.301636	0.002655	0.664539					
H	3.642758	0.473386	-1.022626					
H	2.270418	1.188131	-0.139972					



Geometry – $c\text{-CH}_2\text{CH}_2\text{CH}_2$ – D_{3h} (P9)				Frequency (cm^{-1})				
C	1.654193	-0.992484	-0.100433	744.6462	745.5660	861.6976	924.2315	924.8003
H	1.387591	-1.471345	0.829565	1055.5647	1058.2367	1090.6760	1158.2501	1211.4156
H	1.056083	-1.290046	-0.948353	1212.1620	1241.4271	1473.5281	1474.6716	1530.3813
C	3.100815	-0.682684	-0.338191	3170.1147	3171.8375	3178.2354	3250.0079	3251.5885
H	3.807334	-0.952639	0.432022	3269.5861				
H	3.477249	-0.771597	-1.345960	Rotational constants (cm^{-1})				
C	2.135327	0.425533	-0.045372	0.6794	0.6791	0.4252		
H	2.192542	0.901816	0.921640					
H	1.861439	1.083377	-0.856234	T ₁ value: 0.007				

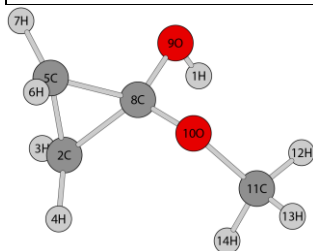


Geometry – TS10 – C ₁				Frequency (cm^{-1})				
C	1.442193	-1.798657	0.082299	-1308.8518				
H	0.679300	-2.545205	-0.111529	74.7783	137.6300	193.8502	215.1150	223.2511
H	2.317600	-2.156531	0.609107	316.0263	370.5094	389.7368	431.9257	442.8541
H	0.660148	-1.111975	1.029881	532.1996	551.5632	653.1155	698.0674	745.2988
C	1.599003	-0.753898	-0.824872	803.2256	823.9072	895.7797	939.8321	979.8462
H	2.583831	-0.362743	-1.031415	1013.9078	1033.2998	1063.6261	1110.7580	1137.7570
H	0.891662	-0.619594	-1.632628	1174.7772	1187.9637	1204.8906	1223.9833	1248.1706
C	1.307534	1.301369	-0.046554	1271.8290	1294.6000	1349.0098	1435.1077	1461.8818
H	2.245492	1.198265	0.476841	1464.7014	1488.9918	1502.0155	1513.4731	1521.9953
H	1.375991	1.652572	-1.065084	1566.4467	1683.0266	3067.3884	3136.3813	3140.3250
C	0.222035	1.964366	0.774590	3149.3862	3160.9320	3172.5242	3173.0142	3220.3542
H	-0.378705	2.694998	0.249659	3232.6878	3255.6356	3270.7058		
H	0.489191	2.250078	1.783120					
C	-0.259581	0.591923	0.644232	Rotational constants (cm^{-1})				
O	-0.055713	-0.312721	1.525923	0.0750	0.0692	0.0496		
O	-1.202449	0.416338	-0.325084					
C	-1.732816	-0.888850	-0.502478	T ₁ value: 0.014				
H	-1.906062	-1.371570	0.457154					
H	-2.673629	-0.758750	-1.029498					
H	-1.069368	-1.510628	-1.105554					



Geometry – C ₂ H ₄ – D _{2h} (P10)				Frequency (cm^{-1})				
C	2.919262	0.178710	0.247074	829.1750	990.3555	1002.9377	1071.0185	1243.1145
H	2.864454	-0.901105	0.290289	1388.3429	1473.7893	1719.2741	3159.8639	
H	3.417229	0.675843	1.069222	3176.0230				
C	2.402881	0.858469	-0.761418	3235.6677	3262.0974			
H	2.458324	1.938387	-0.804593	Rotational constants (cm^{-1})				
H	1.904957	0.362524	-1.584362	4.9215	1.0180	0.8435		

T₁ value: 0.010



Geometry – *c*-CH₂CH₂C(OH,OCH₃) – C₁ (P10)

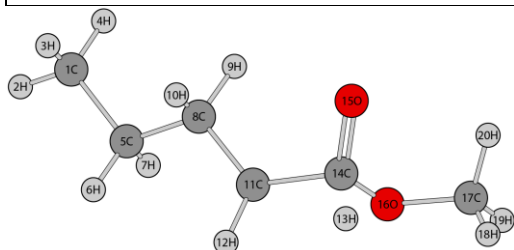
Frequency (cm⁻¹)

H	0.601279	0.014808	1.416731	120.4600	203.1678	267.4330	308.1201	372.4214
C	-0.756161	1.188302	-0.589599	385.7331	500.0654	582.2686	752.6054	787.4668
H	-0.094493	1.978351	-0.266242	914.9317	938.8639	989.0429	1005.1788	1040.9818
H	-0.769204	0.981598	-1.649514	1081.4285	1143.1386	1186.2966	1188.6165	1222.3995
C	-2.073043	1.029557	0.162147	1289.1025	1316.1729	1392.4801	1444.5265	1479.8081
H	-2.933637	0.718958	-0.409601	1502.2301	1523.5599	1530.7057	3026.3510	3086.2571
H	-2.256219	1.700083	0.987181	3158.6425	3165.7750	3181.2652	3258.3896	3279.2098
C	-0.995633	0.041489	0.338232	3868.6200				
O	-0.348039	0.027799	1.565714					
O	-1.226588	-1.204064	-0.215801					
C	-0.042160	-1.875353	-0.585755					
H	0.553258	-2.141106	0.291546					
H	-0.335948	-2.787320	-1.098199					
H	0.561721	-1.260478	-1.261452					

Rotational constants (cm⁻¹)

0.1942 0.1055 0.0889

T₁ value: 0.009



Geometry – TS11 – C₁

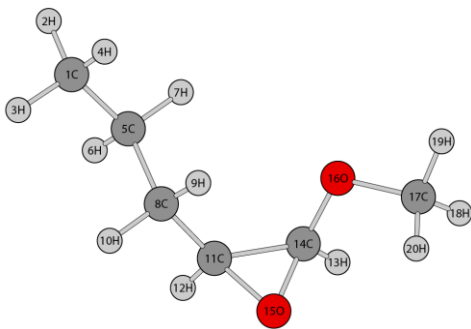
Frequency (cm⁻¹)

C	3.287010	-0.231614	-1.992841	-454.8710				
H	3.776600	-0.094054	-2.955487	61.0225	83.7174	100.9925	160.4644	163.8424
H	3.942741	0.165945	-1.217688	198.9328	255.3845	299.0097	340.7327	394.5935
H	3.176252	-1.301942	-1.819864	510.1312	601.5380	751.8958	803.1865	821.5868
C	1.931995	0.463649	-1.963318	878.3491	913.7070	997.9349	1057.0774	1073.6072
H	2.054720	1.532846	-2.148909	1085.1997	1143.4529	1169.5857	1187.7223	1210.8925
H	1.298554	0.073282	-2.760951	1226.8415	1242.8425	1269.0740	1293.4687	1320.0270
C	1.237058	0.254143	-0.611178	1372.4652	1388.0397	1411.5879	1417.5410	1454.7643
H	1.109035	-0.793469	-0.321366	1477.2304	1492.8442	1497.9176	1503.7111	1511.7884
H	1.865881	0.690525	0.176868	1522.1584	2534.3011	3011.7225	3025.7089	3062.2464
C	-0.072670	0.892977	-0.586585	3066.3334	3074.0159	3104.2545	3112.7205	3135.2034
H	-0.144021	1.908109	-0.977570	3137.7570	3145.9945	3160.3298		
H	-1.524820	1.406151	0.639753					
C	-1.191800	0.378350	0.257241					
O	-0.669198	-0.320744	1.196313					
O	-2.244102	-0.141353	-0.523360					
C	-3.330007	-0.550274	0.286523					
H	-3.761896	0.303899	0.819548					
H	-4.078303	-0.972951	-0.378716					
H	-3.015172	-1.298871	1.013109					

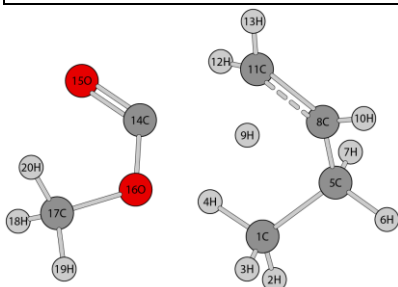
Rotational constants (cm⁻¹)

0.1852 0.0267 0.0256

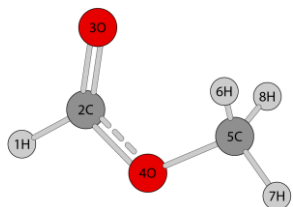
T₁ value: 0.033



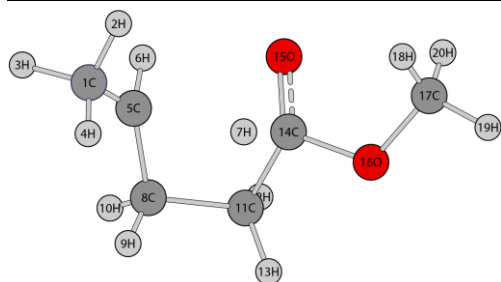
Geometry– <i>c</i> -CH(CH ₂ CH ₂ CH ₃)OCH(OCH ₃)– C ₁ (P11)				Frequency (cm ⁻¹)				
C	-3.286653	0.524736	0.760652	45.8716	79.5100	98.4835	155.1455	184.8171
H	-3.953567	1.359859	0.550093	208.5473	253.0820	303.9149	396.5582	435.7254
H	-3.877499	-0.391984	0.735259	588.9009	600.6498	752.7029	850.3697	865.8551
H	-2.906393	0.645714	1.775672	913.1673	921.2545	1024.1100	1048.8080	1077.9683
C	-2.139732	0.458540	-0.238897	1114.6711	1127.3064	1158.4457	1185.0760	1186.6776
H	-2.538725	0.359135	-1.251858	1203.1521	1260.0860	1262.2612	1298.135	1322.7608
H	-1.570060	1.390119	-0.216434	1333.9256	1383.3395	1406.5592	1415.8320	1476.0034
C	-1.190657	-0.700057	0.053020	1489.9908	1497.9067	1499.1352	1504.8243	1512.2438
H	-0.738429	-0.574268	1.036271	1517.3627	1537.2566	3036.1674	3050.0273	3058.9433
H	-1.742821	-1.643354	0.061648	3062.9192	3087.4730	3104.8135	3115.2439	3122.4385
C	-0.097399	-0.779862	-0.972446	3128.7571	3135.5693	3141.0046	3166.7435	
H	-0.415642	-0.999394	-1.988040					
H	1.754473	0.263356	-1.653152					
C	1.152115	-0.048133	-0.801730					
O	1.117411	-1.440353	-0.598515					
O	1.304778	0.739136	0.309404					
C	2.634677	0.723453	0.796793					
H	3.332435	1.076088	0.031248					
H	2.671401	1.392989	1.651277					
H	2.918280	-0.284183	1.105666					
				Rotational constants (cm ⁻¹)				
				0.1236 0.0368 0.0312				
				T ₁ value: 0.009				



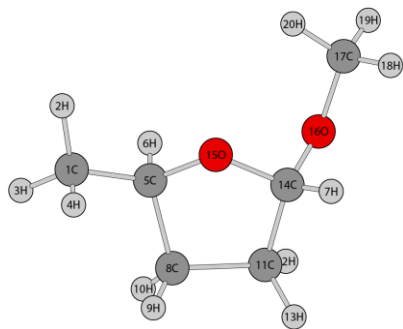
Geometry –TS12 – C ₁				Frequency (cm ⁻¹)				
C	2.741557	0.220661	-0.651644	27.1281	48.7367	52.2407	75.9928	133.1686
H	3.718996	0.122813	-1.120549	155.0460	242.7144	256.2977	311.7453	336.8124
H	2.614212	-0.596473	0.059666	391.6643	415.4555	500.6983	670.4653	780.3264
H	1.986755	0.095889	-1.429658	784.6870	832.8140	896.2464	980.4042	1005.3315
C	2.609685	1.577155	0.046478	1034.0936	1084.4611	1088.0755	1115.2641	1169.9702
H	3.397243	1.677400	0.791857	1173.7683	1201.9444	1251.0297	1279.8485	1304.4355
H	2.770781	2.373964	-0.686424	1359.7372	1405.7276	1428.0425	1461.0507	1488.5211
C	1.278379	1.769058	0.722585	1491.1406	1499.6890	1507.5052	1508.7201	1512.7895
H	0.541977	0.581647	0.586292	1790.2734	2249.4253	3036.7687	3061.0675	3076.7292
H	1.226946	2.017750	1.771950	3109.2982	3130.7771	3145.1588	3149.4444	3177.7928
C	0.064677	1.599236	0.026852	3181.2835	3226.8222	3275.7911		
H	0.044007	1.541855	-1.052500					
H	-0.870828	1.862615	0.495486					
C	-0.681697	-0.554507	-0.156438					
O	-1.557766	-0.705904	-0.962557					
O	-0.172776	-1.588512	0.565813					
C	-0.746893	-2.876222	0.303145					
H	-0.606928	-3.144134	-0.742683					
H	-0.232845	-3.579135	0.951182					
H	-1.813557	-2.863254	0.519928					
				Rotational constants (cm ⁻¹)				
				0.1025 0.0341 0.0294				
				T ₁ value: 0.016				



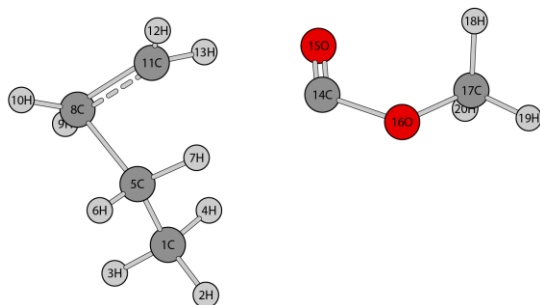
Geometry –CH ₃ OCHO – C _s (P12)				Frequency (cm ⁻¹)				
H	-0.304077	0.650194	0.237985	155.7110	319.7363	343.5383	792.4406	984.7244
C	-1.320767	0.390196	-0.076765	1065.0876	1192.3570	1207.3276	1272.9758	1410.5754
O	-1.953367	0.978754	-0.902001	1481.8137	1497.5270	1509.5465	1856.6623	3083.1415
O	-1.740503	-0.678266	0.598840	3087.6514	3158.4391	3194.6393		
C	-3.061492	-1.117118	0.273939	Rotational constants (cm ⁻¹)				
H	-3.120623	-1.384575	-0.779190	0.6749	0.2336	0.1794		
H	-3.251652	-1.981408	0.900727					
H	-3.781390	-0.327140	0.478347	T ₁ value: 0.014				



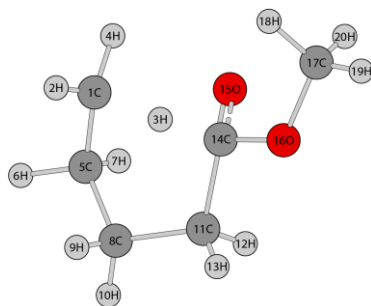
Geometry –TS13 – C ₁				Frequency (cm ⁻¹)				
C	2.385546	-0.744148	2.006780	-854.6119				
H	1.881952	-1.669861	2.290283	69.8675	101.9965	123.3460	168.0537	220.3824
H	3.419517	-1.028113	1.765304	244.3906	286.5658	357.5242	395.2215	468.2391
H	2.385984	-0.036882	2.831765	515.6546	665.5761	777.5200	799.0396	820.3547
C	1.770458	-0.207060	0.786410	849.4599	910.7471	956.5528	997.3431	1018.1227
H	1.643715	-0.900977	-0.032769	1027.4381	1104.4540	1141.4635	1178.1715	1190.1432
H	0.033320	0.120999	1.734857	1199.4388	1220.1144	1223.4790	1291.0303	1299.4573
C	1.609140	1.214732	0.463960	1319.3487	1362.3062	1377.6699	1415.1796	1460.2381
H	1.905284	1.832528	1.310162	1468.6913	1476.4538	1484.4628	1487.5753	1514.0401
H	2.249989	1.440595	-0.396984	1518.3898	2099.0738	3009.4766	3033.6516	3037.9915
C	0.130761	1.458726	0.086448	3095.5444	3096.5070	3120.3443	3122.1507	3157.5843
H	-0.045813	1.402397	-0.986530	3158.7601	3167.1812	3236.1234		
H	-0.209401	2.422454	0.461406					
C	-0.610831	0.243790	0.737730	Rotational constants (cm ⁻¹)				
O	-0.550069	-0.860602	0.078824	0.1180	0.0418	0.0363		
O	-1.884046	0.716667	1.093203					
C	-2.832530	-0.306547	1.316202	T ₁ value: 0.026				
H	-2.480871	-0.999311	2.086965					
H	-3.743460	0.181168	1.655685					
H	-3.025078	-0.874111	0.408074					



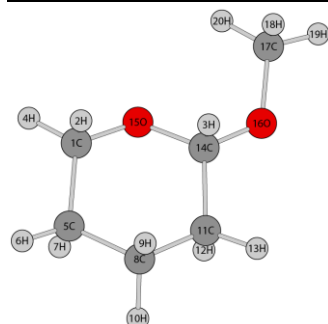
Geometry– <i>c</i> -OCH(CH ₃)CH ₂ CH ₂ CH(OCH ₃)– C ₁ (P13)				Frequency (cm ⁻¹)				
C	2.370491	-1.402693	-0.110710	52.2731	115.3389	134.2633	203.8811	236.6528
H	2.041367	-2.421361	-0.309531	265.3975	329.0037	421.8613	463.5650	573.0411
H	3.177730	-1.158044	-0.800948	619.7245	759.9682	827.8398	876.5627	898.6859
H	2.753259	-1.354040	0.908834	924.4451	970.5967	1018.7763	1051.5252	1086.1160
C	1.228801	-0.430079	-0.275185	1127.3962	1144.3454	1172.6844	1179.9145	1190.6905
H	0.810152	-0.500779	-1.285632	1214.2002	1235.8636	1261.6126	1310.1973	1320.5897
H	-1.119874	0.323701	1.732057	1367.3743	1385.0656	1396.5953	1408.6568	1427.2610
C	1.552298	1.026699	0.046438	1481.0605	1485.0629	1488.7820	1495.9904	1504.0224
H	2.252376	1.056975	0.882555	1506.6954	1523.1045	3027.2711	3028.4500	3057.1633
H	2.000628	1.550756	-0.795087	3067.1268	3079.8574	3101.6906	3109.7800	3137.4297
C	0.186888	1.597310	0.454157	3143.3343	3148.1697	3157.7622	3160.0833	
H	-0.284261	2.156185	-0.351212	Rotational constants (cm ⁻¹) 0.1190 0.0518 0.0404				
H	0.250407	2.242724	1.326641					
C	-0.662761	0.350131	0.738423	T ₁ value: 0.010				
O	0.206393	-0.751206	0.669281					
O	-1.665536	0.282077	-0.237534					
C	-2.537414	-0.812266	-0.053911					
H	-3.029466	-0.756468	0.923133					
H	-3.290770	-0.759089	-0.835608					
H	-2.002027	-1.760351	-0.124479					



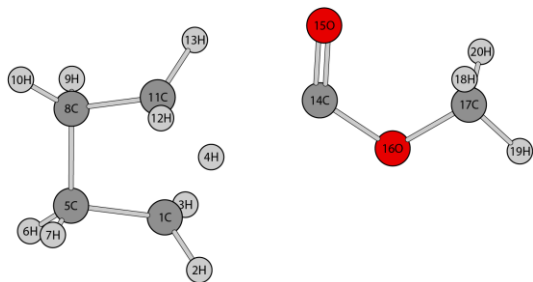
Geometry – TS14 – C ₁				Frequency (cm ⁻¹)				
C	1.878416	-1.175649	0.089511	-604.7666				
H	2.171405	-1.864315	-0.699992	37.4639	52.7117	79.3540	109.1690	180.0798
H	2.415971	-1.425717	1.002153	190.4335	207.8717	218.9834	291.0992	371.1168
H	0.805551	-1.302313	0.243467	378.3374	397.6753	532.7174	756.1977	773.4635
C	2.153495	0.245907	-0.351799	823.1036	832.8481	972.9823	992.7413	1014.9235
H	3.174149	0.503624	-0.623200	1041.9726	1076.1272	1138.9132	1161.3300	1169.2180
H	1.531917	0.392816	-1.266364	1175.9740	1201.6934	1222.7723	1255.2089	1304.4771
C	1.768801	1.305543	0.822708	1366.2139	1418.3449	1429.0024	1452.9883	1485.7151
H	1.518608	0.762301	1.724225	1488.9467	1492.4156	1503.2665	1509.4680	1554.9811
H	2.547992	2.045802	0.941453	1591.0510	2713.5205	2919.7241	3062.0698	3068.4628
C	0.732652	1.548916	-0.102674	3125.8926	3132.2441	3146.9442	3155.6314	3158.6358
H	0.843992	2.323861	-0.851117	3160.7810	3224.8231	3245.5313		
H	-0.243660	1.046434	-0.082620	Rotational constants (cm ⁻¹) 0.1269 0.0294 0.0264				
C	-0.719074	0.035458	-1.845086					
O	-1.600550	0.270050	-1.014650	T ₁ value: 0.014				
O	-1.106316	-0.670674	-2.955538					
C	-2.479861	-1.045885	-3.029913					
H	-3.125821	-0.168168	-3.014322					
H	-2.601903	-1.585460	-3.965934					
H	-2.757864	-1.682204	-2.189560					



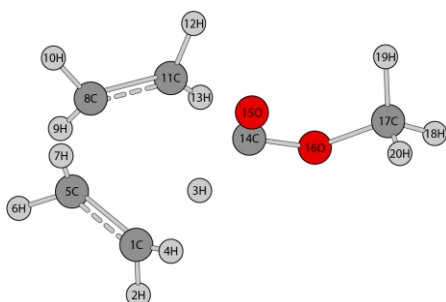
Geometry – TS15 – C ₁				Frequency (cm ⁻¹)				
C	0.746291	-1.522014	0.864739	-1524.4705				
H	0.657813	-1.452500	1.944869	97.6079	135.0559	144.7060	221.8983	270.6968
H	-0.661361	-0.402544	1.151555	306.9299	367.3399	426.2020	491.1378	523.8645
H	0.420679	-2.445782	0.421638	591.8434	693.8318	819.3430	826.8948	846.3290
C	1.788283	-0.697154	0.244721	897.1754	936.5723	986.2372	1014.2067	1035.2347
H	2.723074	-0.883168	0.788603	1093.6485	1121.9204	1156.6863	1177.9807	1186.6149
H	1.901598	-0.959100	-0.803238	1203.3165	1214.1097	1230.1910	1256.5838	1278.2048
C	1.441619	0.799555	0.409620	1331.0036	1345.1457	1354.6232	1376.7153	1452.0333
H	1.439777	1.033129	1.477050	1474.3999	1480.1882	1490.1860	1492.9722	1516.7793
H	2.229804	1.392688	-0.049909	1517.9299	2040.7381	3020.5698	3030.1057	3063.4333
C	0.082057	1.108086	-0.190676	3082.7815	3126.4998	3129.2228	3142.5895	3146.7069
H	0.144836	1.235309	-1.272226	3161.5185	3166.6319	3306.0646		
H	-0.336658	2.010980	0.248963					
C	-0.906309	-0.056570	0.022849	Rotational constants (cm ⁻¹)				
O	-0.758012	-1.103443	-0.749569	0.1321	0.0470	0.0393		
O	-2.179757	0.506614	0.040433					
C	-3.227960	-0.443265	0.012437	T ₁ value: 0.023				
H	-3.138858	-1.136393	0.855779					
H	-4.155793	0.115953	0.102548					
H	-3.219883	-1.015418	-0.912015					



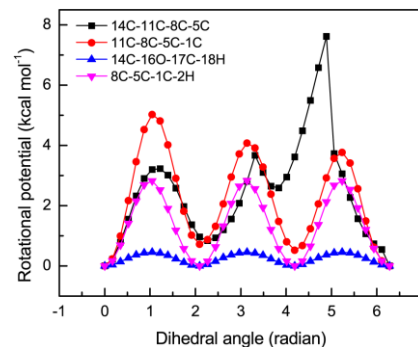
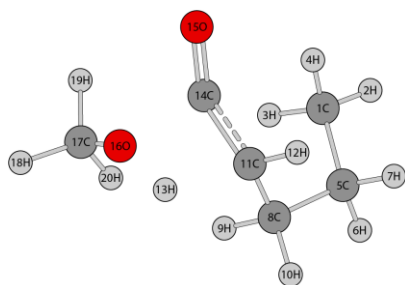
Geometry – c-OCH ₂ CH ₂ CH ₂ CH ₂ CH-OCH ₃ – C ₁ (P15)				Frequency (cm ⁻¹)				
C	1.107277	1.434061	-0.057250	100.4881	134.2005	192.4014	249.5807	262.4795
H	1.107070	1.598070	-1.144327	364.4341	393.9748	463.1873	501.7844	546.5648
H	-0.512397	-0.080940	-1.366412	594.8655	833.6222	861.1523	881.4623	938.1444
H	1.250383	2.396813	0.429499	959.4036	991.2014	1068.1013	1076.2954	1108.6442
C	2.202310	0.446298	0.314930	1146.8065	1162.7469	1189.6959	1190.8408	1218.4428
H	3.167545	0.817833	-0.032269	1248.0669	1266.4974	1285.8565	1317.4897	1346.6055
H	2.246575	0.368613	1.403443	1369.3761	1384.5209	1397.2833	1424.2292	1434.0930
C	1.889733	-0.920686	-0.289430	1477.3711	1485.3747	1491.0238	1496.3530	1500.5527
H	1.971547	-0.858252	-1.378938	1514.2545	1521.8988	2923.5864	2996.3476	3031.1516
H	2.612683	-1.666725	0.039120	3047.6418	3064.9859	3075.9340	3109.7701	3112.3608
C	0.472510	-1.347936	0.087112	3114.7057	3125.8342	3130.0941	3161.2789	
H	0.391287	-1.511343	1.163542					
H	0.181858	-2.268331	-0.418638	Rotational constants (cm ⁻¹)				
C	-0.510349	-0.253468	-0.273073	0.1401	0.0495	0.0393		
O	-0.162164	0.964868	0.353472					
O	-1.772174	-0.622663	0.151064	T ₁ value: 0.009				
C	-2.785460	0.286763	-0.226305					
H	-2.779321	0.443397	-1.310301					
H	-3.734077	-0.156217	0.065028					
H	-2.659341	1.247547	0.272412					



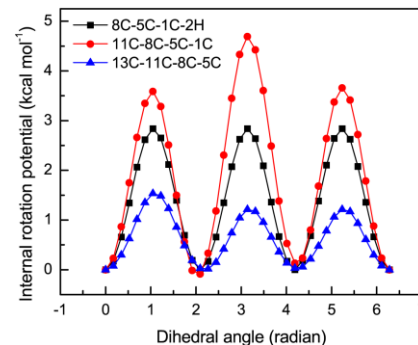
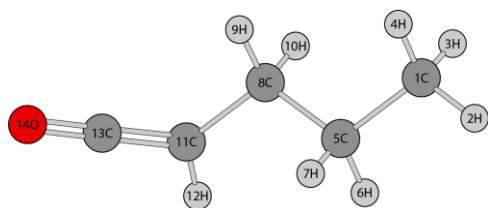
Geometry – TS16 – C ₁				Frequency (cm ⁻¹)				
C	1.700166	1.093844	-0.207851	-1158.4105				
H	1.185295	1.840535	0.392074	53.2944	57.7911	67.8639	109.7338	174.7916
H	1.547741	1.229964	-1.276312	200.8561	251.3042	274.1521	353.1538	394.3085
H	0.779017	0.165166	-0.064298	468.8345	588.5679	683.0202	765.4112	778.4714
C	3.076360	0.608123	0.190322	857.0934	919.1274	947.1657	957.3056	986.2860
H	3.887984	1.094178	-0.346459	1006.7003	1024.7262	1049.1788	1087.0590	1152.6274
H	3.235876	0.745014	1.258865	1169.8735	1201.0950	1201.6541	1230.9471	1261.2101
C	2.870190	-0.863665	-0.141761	1290.7770	1328.3583	1348.0617	1454.5154	1455.3863
H	2.992710	-1.039269	-1.210091	1459.8208	1488.7021	1495.2881	1509.0488	1515.5218
H	3.491175	-1.579723	0.396559	1688.0300	1788.1345	3067.1036	3085.4299	3095.9649
C	1.405787	-0.989282	0.241499	3101.9561	3126.3548	3132.1242	3134.2933	3148.7857
H	1.205470	-0.949589	1.307372	3165.4749	3195.7238	3220.9506		
H	0.761415	-1.704721	-0.258745					
C	-1.100692	-0.567470	0.018589	Rotational constants (cm ⁻¹)				
O	-1.359194	-1.753310	-0.037500	0.1581	0.0263	0.0232		
O	-2.128802	0.335153	0.060950					
C	-3.447426	-0.216036	0.029049	T ₁ value: 0.017				
H	-3.608743	-0.877957	0.879239					
H	-4.133933	0.625357	0.068592					
H	-3.602647	-0.790103	-0.883814					



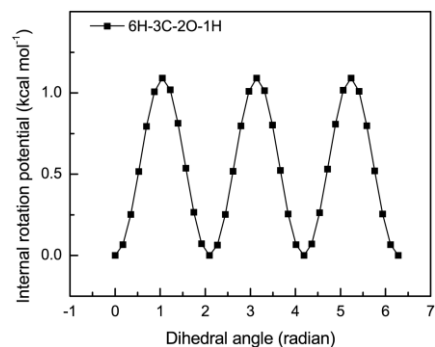
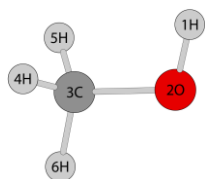
Geometry – TS17 – C ₁				Frequency (cm ⁻¹)				
C	0.017373	-1.032235	2.052397	-1177.6865				
H	0.070423	-0.733610	3.092338	47.1311	98.5837	104.5279	145.0569	182.2097
H	-0.821084	0.064878	1.470432	224.3741	256.3323	282.1615	345.1039	415.7299
H	-0.748253	-1.750820	1.796024	478.9225	546.8730	645.0894	681.7134	768.2028
C	1.134615	-0.897857	1.236387	789.6660	856.6141	912.3199	978.8585	990.8997
H	2.094666	-0.720157	1.696396	1006.8592	1025.9739	1049.7677	1093.4290	1157.7823
H	1.163397	-1.495973	0.336597	1184.3464	1204.1401	1221.0419	1246.2475	1265.2376
C	1.227168	0.940247	0.353675	1277.0338	1302.1722	1354.3240	1458.6440	1470.3846
H	1.857763	1.353574	1.127167	1473.3888	1493.1089	1510.9969	1544.8920	1559.3956
H	1.761593	0.556402	-0.503617	1732.3280	1785.4184	3075.5055	3146.3237	3155.6238
C	-0.003028	1.554046	0.144459	3164.6228	3174.1801	3180.3476	3183.2725	3239.4521
H	-0.405582	1.595415	-0.857871	3247.5010	3265.2262	3272.4331		
H	-0.316668	2.345368	0.809244					
C	-1.617403	0.365133	0.596616	Rotational constants (cm ⁻¹)				
O	-1.870694	-0.455464	-0.249363	0.1096	0.0402	0.0350		
O	-2.525525	1.250005	1.065766					
C	-3.809574	1.175786	0.449084	T ₁ value: 0.012				
H	-4.423696	1.920736	0.944921					
H	-3.734170	1.392521	-0.615656					
H	-4.236984	0.182337	0.572960					



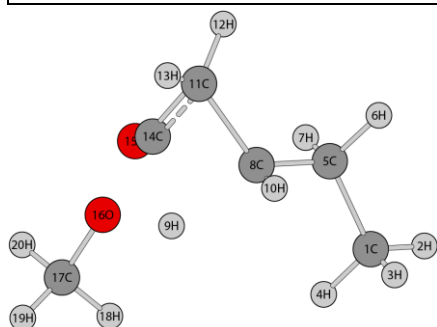
Geometry – TS18 – C ₁				Frequency (cm ⁻¹)				
C	-1.943972	-0.170392	-1.316499	-1585.9005				
H	-2.830732	-0.342720	-1.925255	40.3949	83.1122	101.9074	124.4109	146.4501
H	-1.309809	0.543217	-1.848932	190.9606	249.0472	270.7639	321.9316	393.5462
H	-1.401079	-1.112798	-1.250153	454.7820	533.9753	612.8059	715.4235	793.6302
C	-2.313308	0.360887	0.062101	822.2448	856.9231	900.0557	975.5438	1044.5962
H	-2.962874	1.233501	-0.040900	1078.9941	1095.6683	1135.6201	1144.6301	1168.9902
H	-2.886729	-0.392577	0.607129	1181.5279	1252.0637	1286.9609	1316.6379	1351.4119
C	-1.092275	0.758574	0.896402	1375.7838	1391.8333	1416.7212	1473.3505	1481.1994
H	-0.547285	1.540062	0.359619	1490.6792	1498.8488	1502.1449	1511.1332	1514.1622
H	-1.427698	1.210331	1.830721	1912.5385	2017.8535	3050.5042	3053.6190	3054.1555
C	-0.162645	-0.401573	1.247978	3058.2081	3088.5070	3100.9298	3122.8382	3131.1111
H	-0.648407	-1.193974	1.810343	3141.6005	3144.4692	3153.9757		
H	1.062326	0.469324	1.266635					
C	0.725991	-0.911179	0.279429	Rotational constants (cm ⁻¹)				
O	1.114227	-1.827170	-0.333363	0.0875	0.0442	0.0412		
O	1.783753	0.398938	0.357100					
C	2.031368	1.221870	-0.771816	T ₁ value: 0.013				
H	2.946638	1.787461	-0.607319					
H	2.163205	0.570073	-1.636218					
H	1.202517	1.906219	-0.955499					



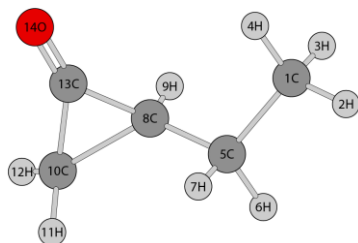
Geometry – CH ₃ CH ₂ CH ₂ CH=C=O – C ₁ (P18)				Frequency (cm ⁻¹)				
C	-3.331822	-0.805826	0.308452	60.2720	93.9569	197.2999	239.0064	266.8547
H	-4.208230	-0.601574	0.921925	388.5208	545.6122	596.0477	655.6223	745.0754
H	-3.675115	-1.026549	-0.703273	865.5471	907.4400	994.7546	1068.9567	1114.1135
H	-2.852086	-1.704626	0.698641	1122.4837	1161.2731	1260.3077	1301.9802	1327.5032
C	-2.363862	0.369777	0.309920	1384.3935	1414.9205	1447.3125	1486.1722	1496.9820
H	-2.864382	1.266412	-0.063019	1503.8795	1512.3432	2248.8065	3049.9703	3058.2485
H	-2.042231	0.596086	1.327995	3063.1476	3087.2912	3106.8450	3128.4886	3137.7172
C	-1.131037	0.094775	-0.549030	3218.5616				
H	-0.608561	-0.782616	-0.164011					
H	-1.449675	-0.158232	-1.563702	Rotational constants (cm ⁻¹)				
C	-0.181914	1.267876	-0.603283	0.4618	0.0453	0.0443		
H	-0.495112	2.217081	-1.014964					
C	1.039685	1.215875	-0.140594	T ₁ value: 0.012				
O	2.122206	1.157964	0.268434					



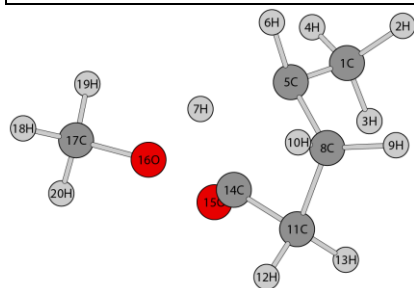
Geometry – CH ₃ OH – C _S (P18)				Frequency (cm ⁻¹)				
H	1.665267	-1.369695	-1.401207	311.5542	1074.1440	1116.9564	1182.1481	1377.6544
O	1.987730	-0.986590	-0.583886	1489.2446	1509.5844	1521.8500	3031.8488	3083.6256
C	1.948303	-1.974209	0.425372	3144.5881	3904.2618			
H	0.932872	-2.333761	0.612211	Rotational constants (cm ⁻¹)				
H	2.587598	-2.829749	0.191549	4.3057	0.8334	0.8044		
H	2.318784	-1.512206	1.337710	T ₁ value: 0.008				



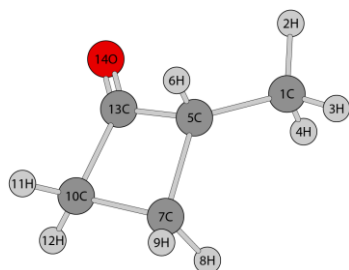
Geometry – TS19 – C ₁				Frequency (cm ⁻¹)				
C	0.118049	1.929180	-3.370857	- 960.5221				
H	-0.398051	2.630064	-4.026499	59.4252	96.4329	109.7262	153.1576	182.4733
H	1.187090	2.000460	-3.578107	246.5013	252.7060	338.4528	360.9432	393.4182
H	-0.203555	0.919060	-3.628058	418.8419	466.4310	543.7459	753.0211	765.8767
C	-0.168533	2.217819	-1.901676	802.0483	830.4184	960.7576	971.0749	1048.7611
H	0.090231	3.259789	-1.678136	1067.0145	1078.6374	1091.2664	1119.4859	1181.9041
H	-1.244362	2.124917	-1.724394	1187.6201	1195.0553	1200.8713	1278.8291	1314.7425
C	0.566672	1.268716	-0.991582	1378.3302	1409.0408	1449.9430	1457.7372	1484.0451
H	0.713121	-0.359519	-0.928114	1494.6805	1499.7957	1501.9333	1506.8945	1509.8167
H	1.650858	1.285027	-1.102555	1959.9512	2100.5197	3010.8616	3054.5688	3058.6532
C	0.148173	1.286419	0.502748	3063.0832	3096.7656	3111.0387	3121.5059	3132.6757
H	-0.427263	2.134622	0.865778	3143.8695	3170.0236	3208.4598		
H	0.927225	0.972107	1.186028	Rotational constants (cm ⁻¹)				
C	-0.658924	0.213484	-0.027447	0.0945	0.0442	0.0393		
O	-1.773454	-0.055800	-0.302377	T ₁ value: 0.013				
O	0.451541	-1.126089	-0.204944					
C	-0.184896	-2.217913	-0.860707					
H	-0.380894	-1.972489	-1.905896					
H	0.475092	-3.079045	-0.794904					
H	-1.130230	-2.427027	-0.365470					



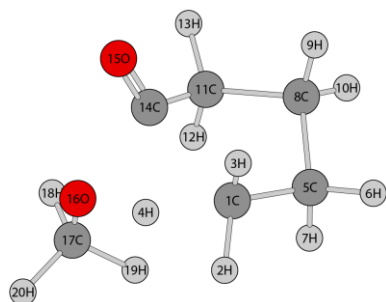
Geometry – <i>c</i> -CH(CH ₃)CH ₂ C=O – C ₁ (P19)				Frequency (cm ⁻¹)				
C	2.561884	-1.266749	-0.228977	82.4199	130.4767	230.3103	282.7483	348.7983
H	3.565124	-1.409509	-0.628118	448.0413	538.9810	725.8917	774.8638	820.8324
H	2.482204	-1.840044	0.695149	838.2069	965.1365	973.5685	1017.1861	1058.8350
H	1.846385	-1.678291	-0.940786	1097.6466	1112.6773	1152.0931	1183.1115	1279.9534
C	2.272692	0.208632	0.021466	1336.4245	1378.6258	1416.5382	1427.2544	1493.6011
H	2.993951	0.628474	0.725584	1502.3558	1510.8243	1988.7285	3056.5386	3064.5946
H	2.379356	0.769039	-0.910306	3092.0289	3134.8894	3143.5039	3143.8731	3157.8909
C	0.873100	0.416988	0.555916	3234.3565				
H	0.651962	-0.068825	1.500398					
C	0.148942	1.784463	0.335686	Rotational constants (cm ⁻¹)				
H	0.690857	2.551858	-0.203644	0.2054	0.0872	0.0672		
H	-0.490760	2.144104	1.130360					
C	-0.232641	0.566564	-0.385852	T ₁ value: 0.012				
O	-0.913243	0.068924	-1.228157					



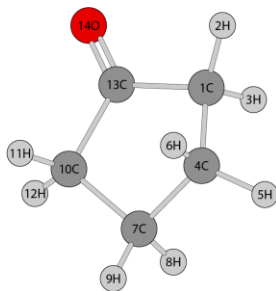
Geometry – TS20 – C ₁				Frequency (cm ⁻¹)				
C	-1.837041	1.422955	-0.146576	-1469.7469				
H	-2.829988	1.510966	-0.594771	99.1293	110.9466	138.8598	154.9765	216.6994
H	-1.972752	1.201276	0.913827	231.0040	287.4535	307.4632	395.5040	410.5192
H	-1.352145	2.397684	-0.205962	459.8745	522.8228	609.5919	698.6703	802.2357
C	-1.004939	0.360898	-0.838935	893.8470	902.9587	962.2262	983.6376	992.5794
H	-0.929374	0.595865	-1.906953	1066.9512	1077.0532	1128.4660	1136.1305	1182.6483
H	0.453270	0.052784	-0.904857	1184.2758	1202.2309	1253.3171	1287.7582	1310.5191
C	-1.438975	-1.081745	-0.551187	1325.5475	1413.1385	1463.0499	1466.4387	1483.8152
H	-2.516410	-1.219031	-0.450323	1492.7947	1498.0616	1501.8902	1506.3059	1510.6412
H	-1.081276	-1.762043	-1.322070	1788.5973	1934.3387	3032.0536	3043.0639	3048.2789
C	-0.677724	-1.301298	0.762380	3077.3960	3099.1168	3103.8196	3124.6469	3125.6455
H	-0.110854	-2.226853	0.846624	3128.1299	3153.8453	3156.4247		
H	-1.290840	-1.177826	1.653817					
C	0.249110	-0.108755	0.695416	Rotational constants (cm ⁻¹)				
O	0.667525	0.659850	1.480824	0.0944	0.0514	0.0492		
O	1.393315	-0.529498	-0.570441					
C	2.509651	0.344322	-0.534242	T ₁ value: 0.013				
H	3.240203	-0.009296	-1.258690					
H	2.213350	1.366424	-0.783514					
H	2.947060	0.344587	0.462791					



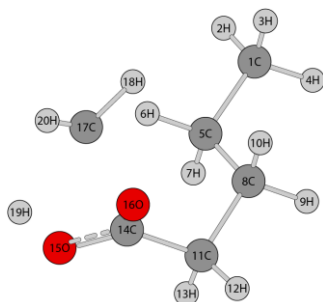
Geometry – <i>c</i> -CH(CH ₃)CH ₂ CH ₂ C=O – C ₁ (P20)				Frequency (cm ⁻¹)				
C	-1.529037	-1.834854	-0.300651	94.3660	186.0774	198.4146	330.8847	439.2622
H	-0.687772	-2.496930	-0.501896	543.9457	678.0437	744.2170	757.0696	880.3289
H	-2.229410	-2.354271	0.352667	923.5745	945.8446	972.9791	1058.8722	1116.4496
H	-2.028760	-1.633747	-1.248817	1142.0154	1168.5035	1202.5565	1231.9917	1247.5265
C	-1.045750	-0.544599	0.324996	1269.1988	1352.2465	1408.0644	1447.1519	1495.3028
H	-0.542024	-0.727676	1.277697	1496.7831	1500.2453	1917.6056	3064.6935	3070.5624
C	-1.995624	0.679529	0.458036	3093.7276	3102.6207	3135.4707	3144.1014	3156.1018
H	-2.823142	0.611734	-0.246021	3168.7326				
H	-2.382344	0.888190	1.450930					
C	-0.874918	1.619138	-0.062549	Rotational constants (cm ⁻¹)				
H	-0.327299	2.102572	0.746721	0.1591	0.1330	0.0795		
H	-1.113000	2.353042	-0.828433					
C	-0.157228	0.356429	-0.528096	T ₁ value: 0.012				
O	0.658058	0.128916	-1.369269					



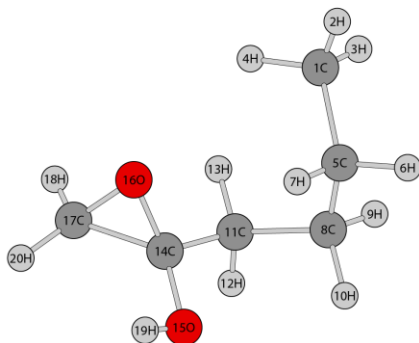
Geometry – TS21 – C ₁				Frequency (cm ⁻¹)				
C	-2.478846	1.633004	-1.381112	-1566.0433				
H	-3.569520	1.622036	-1.498521	72.5311	114.9780	207.4822	230.2052	264.3687
H	-2.049533	1.741994	-2.374513	297.8717	346.7611	385.6985	418.8677	481.6094
H	-2.691153	0.300614	-0.891118	523.4465	549.3912	683.2612	754.7835	849.7231
C	-2.035075	2.723162	-0.420335	875.9641	894.8401	948.4895	979.3588	1002.6272
H	-2.111062	3.720227	-0.857352	1067.7138	1095.5022	1109.1880	1139.5168	1178.8626
H	-2.673900	2.716903	0.467027	1187.6804	1204.2692	1240.4152	1290.7240	1342.6302
C	-0.595414	2.430743	0.004129	1350.0962	1365.1179	1421.0219	1446.6350	1475.8394
H	0.087434	2.620966	-0.826261	1478.7095	1492.9408	1504.4207	1506.8148	1516.0190
H	-0.276484	3.041919	0.847025	1723.6800	1937.1489	3016.1021	3031.9739	3052.1591
C	-0.546739	0.946241	0.360119	3072.6894	3087.4482	3094.9848	3110.8436	3117.4291
H	-1.155869	0.756383	1.240032	3130.1197	3139.6424	3171.0425		
H	0.463479	0.580794	0.534162					
C	-1.073290	0.206606	-0.838565	Rotational constants (cm ⁻¹)				
O	-0.502552	-0.263677	-1.750245	0.0867	0.0546	0.0487		
O	-2.494690	-0.783873	-0.428881					
C	-2.932940	-0.907859	0.903919	T ₁ value: 0.013				
H	-2.143209	-1.324711	1.532407					
H	-3.248841	0.054442	1.323048					
H	-3.786936	-1.585280	0.927160					



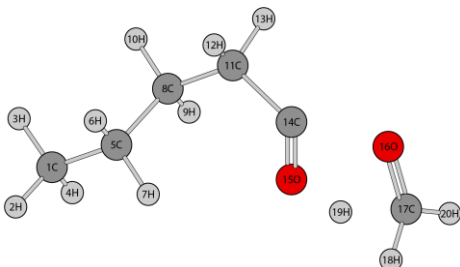
Geometry – c-CH ₂ CH ₂ CH ₂ CH ₂ C=O – C ₂ (P21)				Frequency (cm ⁻¹)				
C	-0.977171	-0.087695	-1.217074	99.5268	243.7572	451.8104	476.0283	565.3057
H	-0.297130	-0.485684	-1.966527	585.2925	718.1181	826.8350	853.8046	915.8333
H	-1.725095	0.516895	-1.738117	927.6477	964.0374	980.1003	1044.4089	1168.5202
C	-1.646732	-1.118125	-0.308264	1178.4559	1181.0717	1223.6555	1260.3665	1305.5717
H	-2.531396	-1.571271	-0.749729	1312.6209	1345.4904	1346.0970	1454.6435	1454.6690
H	-0.943750	-1.920631	-0.076387	1498.6486	1512.1304	1880.4054	3063.0415	3063.8106
C	-1.959007	-0.323890	0.971142	3071.3236	3078.0899	3135.1080	3138.7311	3145.7509
H	-2.840557	0.298971	0.807194	3146.5901				
H	-2.161702	-0.964635	1.826255					
C	-0.725815	0.559922	1.156087	Rotational constants (cm ⁻¹)				
H	0.076261	0.010153	1.656915	0.2227	0.1128	0.0811		
H	-0.882314	1.484968	1.705948					
C	-0.244702	0.846176	-0.261239	T ₁ value: 0.012				
O	0.572416	1.667615	-0.571973					



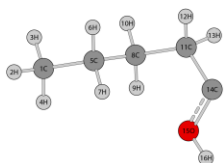
Geometry – TS22 – C ₁				Frequency (cm ⁻¹)				
C	-3.056488	0.720432	0.173798	-707.8963				
H	-3.520856	1.137310	1.066216	41.7784	77.3502	105.5550	175.2914	240.9205
H	-2.870672	1.541015	-0.520433	249.1422	302.2207	368.4394	400.3682	455.5824
H	-3.774044	0.044530	-0.294023	479.3284	644.3925	680.9936	746.9894	796.1459
C	-1.759972	-0.004404	0.509535	812.2065	853.6713	910.1755	961.0757	1016.7219
H	-1.062116	0.687430	0.986461	1055.4607	1080.5903	1121.0457	1130.3013	1188.8210
H	-1.954312	-0.803882	1.229256	1215.1565	1220.7968	1259.3402	1326.0304	1333.0488
C	-1.108366	-0.598307	-0.733419	1346.7194	1405.1872	1416.5017	1423.2674	1444.7900
H	-1.797636	-1.291638	-1.218430	1488.2068	1496.6914	1503.7799	1506.9133	1513.5414
H	-0.892452	0.192658	-1.455438	1619.0647	3050.6797	3058.4401	3066.2878	3082.8698
C	0.193818	-1.361017	-0.432852	3087.7750	3089.2543	3109.8504	3127.0463	3138.9389
H	0.573340	-1.810174	-1.351679	3152.9174	3178.2436	3563.0697		
H	0.027430	-2.128611	0.320125					
C	1.232004	-0.408824	0.042233	Rotational constants (cm ⁻¹)				
O	1.602661	-0.555005	1.294817	0.1059	0.0397	0.0367		
O	1.831845	0.308774	-0.831593	T ₁ value: 0.015				
C	1.575468	1.625733	-0.084218					
H	0.793838	2.093166	-0.676603					
H	2.030011	0.295764	1.522969					
H	2.512645	2.170593	-0.164671					



Geometry – <i>c</i> -CH ₂ OC(CH ₂ CH ₂ CH ₂ CH ₃ ,OH) – C ₁ (P22)				Frequency (cm ⁻¹)				
C	2.284735	-1.148971	-0.004380	62.1527	97.2572	150.1309	206.8053	258.9576
H	2.842262	-1.753596	-0.718974	271.7325	307.2872	380.6789	397.9571	438.7946
H	2.929217	-0.974464	0.860014	514.9980	568.3189	731.7969	773.1371	820.2485
H	1.425894	-1.735407	0.320020	865.3202	903.7530	932.5168	966.7365	996.5697
C	1.843857	0.169920	-0.629204	1040.6391	1083.5126	1112.4994	1130.3169	1138.3112
H	2.705968	0.666118	-1.079026	1153.8358	1188.0234	1239.1515	1268.3652	1321.5856
H	1.141141	-0.028196	-1.441064	1347.4473	1366.2110	1385.3020	1399.5306	1415.5546
C	1.204892	1.134266	0.369016	1468.2438	1482.1727	1493.6665	1495.9075	1504.1178
H	1.935928	1.393925	1.138797	1519.8401	1559.2009	3055.2817	3058.5010	3064.2229
H	0.939022	2.059359	-0.142870	3079.3415	3098.9253	3108.7741	3119.8570	3125.4947
C	-0.042711	0.586123	1.062166	3126.4026	3141.3934	3211.9207	3867.9854	
H	-0.463854	1.350217	1.717770					
H	0.199843	-0.277899	1.681623					
C	-1.113600	0.165431	0.094163	Rotational constants (cm ⁻¹)				
O	-1.423230	1.186308	-0.783923	0.1066	0.0498	0.0429		
O	-1.002878	-1.111078	-0.487914					
C	-2.095318	-0.872333	0.413185	T ₁ value: 0.009				
H	-2.042804	-1.412336	1.351495					
H	-1.958468	0.822817	-1.496116					
H	-3.071931	-0.833579	-0.056506					



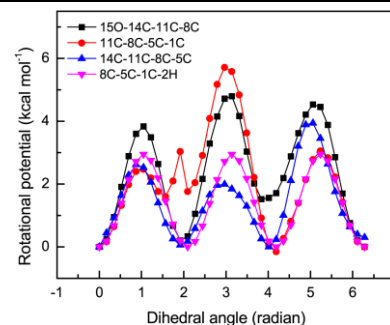
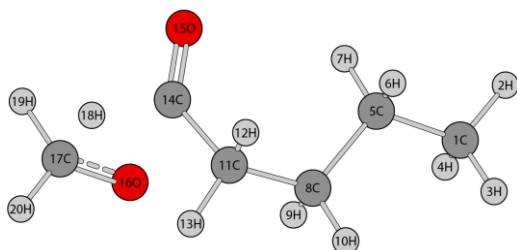
Geometry – TS23 – C ₁				Frequency (cm ⁻¹)				
C	3.495929	-0.745729	-0.053160	-966.9892				
H	3.918602	-1.451412	-0.767045	36.4117	71.6068	99.0584	179.2558	204.0683
H	4.179203	0.101022	0.026497	246.9294	253.3711	272.8467	284.8706	427.8815
H	3.459598	-1.235203	0.920912	518.6974	560.4327	605.5047	716.6593	766.5703
C	2.107882	-0.284737	-0.477585	792.8938	879.8427	920.9542	955.7730	1031.1188
H	2.157809	0.177668	-1.466802	1076.8727	1095.2917	1126.6271	1144.0282	1182.7302
H	1.445873	-1.147888	-0.569528	1229.1948	1237.8671	1267.6530	1325.6987	1331.6879
C	1.506790	0.712109	0.507432	1362.6698	1402.8824	1414.9280	1427.0604	1486.1796
H	1.456684	0.260850	1.500663	1493.6011	1497.5110	1504.1045	1512.3265	1545.9354
H	2.165542	1.580429	0.586964	1616.5638	1941.0114	2983.3170	3049.7520	3054.0846
C	0.115268	1.188320	0.097800	3058.6858	3062.4021	3069.4652	3084.3931	3093.4238
H	0.102689	1.591791	-0.917472	3108.0577	3129.0983	3137.5040		
H	-0.232878	2.018572	0.722654					
C	-1.002021	0.206048	0.184859	Rotational constants (cm ⁻¹)				
O	-0.804660	-0.854518	0.771413	0.1627	0.0265	0.0244		
O	-3.042721	-0.157509	-0.278540					
C	-3.224753	-1.291766	0.223284	T ₁ value: 0.016				
H	-3.183854	-2.187185	-0.409441					
H	-1.774177	-1.408561	0.739342					
H	-3.696113	-1.389061	1.209233					



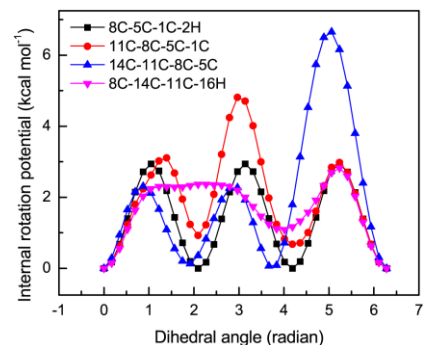
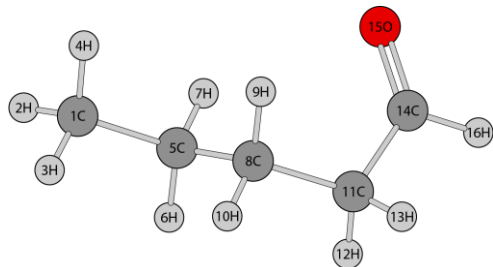
Geometry – CH ₃ CH ₂ CH ₂ CH ₂ COH – C ₁ (P23)				Frequency (cm ⁻¹)				
C	-3.570216	-0.912020	0.067296	80.3118	103.3380	138.8223	245.8679	254.2030
H	-3.964321	-1.632553	0.783210	295.2179	408.9562	638.0397	650.6316	750.4325
H	-4.328346	-0.142302	-0.085645	841.0071	867.0438	916.8366	929.1643	1026.0232
H	-3.426643	-1.427691	-0.883271	1075.8983	1092.2035	1127.7149	1215.0553	1252.1348
C	-2.263319	-0.296578	0.549400	1309.4542	1314.7804	335.3241	1348.3638	1389.5876
H	-2.418847	0.190135	1.515903	1402.1417	1413.0937	1435.8226	1488.5738	1496.7712
H	-1.523299	-1.082140	0.712292	1503.9402	1511.1794	3020.8596	3051.1285	3056.5888
C	-1.706262	0.725185	-0.437712	3060.5877	3070.5468	3087.9794	3105.7561	3126.5875
H	-1.559963	0.247396	-1.408466	3133.6597	3828.1945			
H	-2.446487	1.515127	-0.586083					
C	-0.395371	1.349566	0.031193	Rotational constants (cm ⁻¹)				
H	-0.480658	1.760208	1.041954	0.2327	0.0644	0.0560		
H	-0.123819	2.223440	-0.578115					
C	0.871577	0.550958	0.005841	T ₁ value: 0.012				
O	0.654957	-0.556476	-0.667188					
H	1.481502	-1.050332	-0.707107					



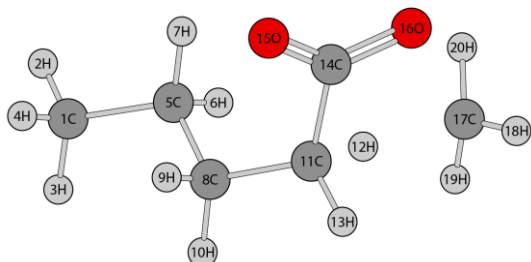
Geometry – CH ₂ O – C ₁ (P23)				Frequency (cm ⁻¹)				
O	-2.882376	-0.294323	-0.856713	1215.3662	1278.9914	1545.2799	1876.9085	2944.8415
C	-2.970105	-1.279730	-0.185829	3016.5670				
H	-3.101771	-1.228618	0.908303	Rotational constants (cm ⁻¹) T ₁ value: 0.015				
H	-2.923380	-2.289578	-0.627298	9.5148	1.3162	1.1562		



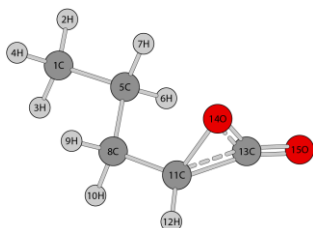
Geometry – TS24 – C ₁				Frequency (cm ⁻¹)				
C	-3.301628	0.047688	-0.589300	-1106.2678				
H	-3.997232	-0.786375	-0.670848	42.8169	75.3211	117.7026	193.2715	214.3710
H	-3.812613	0.862168	-0.073318	250.6062	268.3589	340.7681	371.1990	412.3235
H	-3.068450	0.389153	-1.598582	483.4636	551.4463	698.4971	742.6704	807.8798
C	-2.032011	-0.356624	0.148939	846.2951	912.9727	953.6022	971.3631	1043.1734
H	-2.284716	-0.713931	1.151133	1084.7485	1134.9524	1148.2143	1214.7006	1243.2057
H	-1.551268	-1.188197	-0.366081	1274.7554	1292.5139	1324.8235	1336.0927	1340.3344
C	-1.054858	0.808151	0.261394	1374.2798	1407.3442	1415.3854	1460.9071	1487.5073
H	-0.756417	1.151148	-0.730007	1499.3328	1504.7885	1514.7406	1515.4881	1553.7265
H	-1.552917	1.645981	0.756223	1693.5523	1946.2496	2978.6959	3052.0825	3054.9667
C	0.209106	0.499761	1.060147	3057.7501	3059.8480	3066.7295	3105.5639	3117.9162
H	-0.045639	0.070165	2.033079	3133.3729	3137.7412	3167.6945		
H	0.803488	1.394669	1.214984					
C	1.067889	-0.540137	0.388009	Rotational constants (cm ⁻¹)				
O	0.885579	-1.641952	0.019967	0.1340	0.0344	0.0325		
O	1.729380	0.625052	-0.954332					
C	2.787085	0.300360	-0.294392	T ₁ value: 0.016				
H	2.297060	-0.284249	0.876979					
H	3.355358	-0.592156	-0.587355					
H	3.389968	1.085968	0.183824					



Geometry – CH ₃ CH ₂ CH ₂ CH ₂ CHO – C ₁ (P24)				Frequency (cm ⁻¹)				
C	-2.581792	-0.392379	-0.074816	80.2686	111.1152	156.5855	242.7673	261.3594
H	-3.197247	-0.946848	0.632514	277.5800	415.2901	666.2760	708.3835	759.1046
H	-3.116693	0.520557	-0.341768	859.9542	896.3689	910.2405	1004.2378	1039.9697
H	-2.483254	-0.995743	-0.977998	1078.9658	1145.5851	1156.0294	1244.0356	1274.8534
C	-1.212093	-0.070101	0.507372	1330.6376	1334.9581	1384.7266	1405.5165	1413.7241
H	-1.329002	0.507413	1.428676	1428.1106	1449.5601	1485.9424	1497.1606	1503.7209
H	-0.697785	-0.994335	0.774252	1511.2221	1863.7598	2940.9494	3041.3988	3049.9163
C	-0.345914	0.719179	-0.469044	3057.8690	3062.0619	3073.3450	3094.2729	3110.6574
H	-0.232618	0.146371	-1.391729	3129.0683	3136.0699			
H	-0.852873	1.650606	-0.729924					
C	1.033850	1.036426	0.085771	Rotational constants (cm ⁻¹)				
H	0.975516	1.469094	1.090415	0.2308	0.0647	0.0558		
H	1.554706	1.786280	-0.519489					
C	1.954282	-0.151748	0.157389	T ₁ value: 0.011				
O	1.691756	-1.244870	-0.263266					
H	2.939750	0.042321	0.623859					



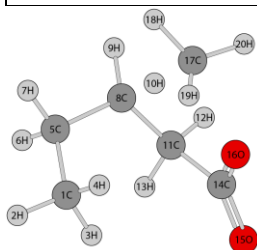
Geometry – TS25 – C ₁				Frequency (cm ⁻¹)				
C	3.050230	-0.429685	-1.458011	-855.1486				
H	3.215447	-0.946140	-2.402282	43.4187	74.0341	88.0967	115.9156	208.5540
H	3.742900	0.412014	-1.409454	243.2109	254.1588	274.0231	329.8192	428.8149
H	3.303753	-1.117367	-0.650786	524.3909	584.7902	626.1017	723.1109	747.8597
C	1.608129	0.039815	-1.326436	809.6613	835.5109	856.7409	930.0376	942.9216
H	1.356151	0.699666	-2.162437	978.0565	1060.4985	1089.7335	1135.8429	1145.6127
H	0.930679	-0.814295	-1.376342	1213.0232	1259.4198	1280.2455	1307.6950	1325.5307
C	1.361883	0.774368	-0.014475	1336.5522	1380.3895	1407.0705	1416.6768	1440.7916
H	1.578183	0.099610	0.823579	1444.7213	1449.9629	1493.8438	1505.6036	1509.5104
H	2.025790	1.635646	0.086933	1735.5454	2231.9647	3027.8510	3044.0534	3060.5505
C	-0.071574	1.160488	0.190000	3082.7064	3103.3328	3104.6104	3115.9221	3129.9185
H	-0.494592	1.716180	-0.747882	3140.9867	3265.8462	3333.2736		
H	-0.229268	1.830686	1.035996					
C	-1.122994	0.021808	0.208436	Rotational constants (cm ⁻¹)				
O	-0.795461	-1.000556	0.793877	0.0947	0.0391	0.0324		
O	-2.188025	0.346318	-0.380308					
C	-1.740402	2.300677	-1.323852	T ₁ value: 0.023				
H	-2.510965	2.528842	-0.608238					
H	-1.052444	3.112351	-1.546233					
H	-2.025815	1.680444	-2.156721					



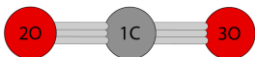
Geometry – $c\text{-CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{OC}=\text{O} - \text{C}_1$ (P25)				Frequency (cm^{-1})				
C	-3.202117	-0.486190	-0.457595	68.3547	98.3207	148.0340	245.8742	259.2185
H	-3.601128	-0.545659	-1.468728	327.6285	505.8549	551.0300	687.8625	751.4328
H	-3.330083	-1.462522	0.011634	760.3426	858.4897	884.1943	952.8703	1042.4788
H	-3.805425	0.232169	0.098947	1074.6609	1094.2737	1135.3735	1186.9330	1224.9727
C	-1.736815	-0.073031	-0.466212	1281.6718	1320.3830	1342.5645	1384.4231	1417.0155
H	-1.149602	-0.789468	-1.045466	1418.8968	1473.3074	1499.5646	1505.4843	1514.3895
H	-1.624529	0.893926	-0.958457	2055.3259	3049.1985	3060.4096	3067.1623	3083.8468
C	-1.168439	0.017050	0.944668	3107.4133	3131.1599	3143.6138	3170.4716	
H	-1.748312	0.726843	1.541322					
H	-1.252284	-0.950707	1.447387					
C	0.275588	0.417701	1.001485	Rotational constants (cm^{-1})				
H	0.732255	0.467928	1.983378	0.1854	0.0509	0.0457		
C	1.148741	0.409730	-0.152706	T ₁ value: 0.013				
O	0.669580	1.603688	0.154035					
O	1.849658	-0.075553	-0.971436					



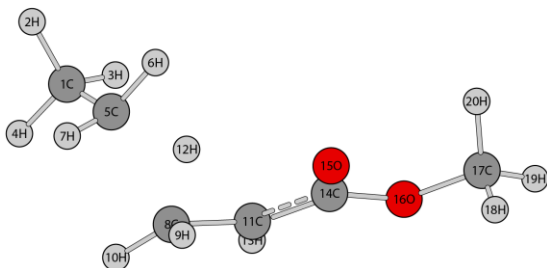
Geometry – $\text{CH}_4 - \text{T}_d$ (P25)				Frequency (cm^{-1})				
H	0.856014	-2.028771	0.195436	1339.6758	1340.1967	1341.0643	1564.7789	1564.9961
C	1.883110	-2.275179	-0.061619	3064.3306	3177.4176	3177.9990	3178.5775	
H	2.560972	-1.675868	0.540866	Rotational constants (cm^{-1})				
H	2.062086	-3.329758	0.131803	5.3081	5.3075	5.3072		
H	2.053051	-2.065941	-1.114725	T ₁ value: 0.007				



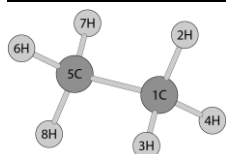
Geometry – $\text{TS26} - \text{C}_1$				Frequency (cm^{-1})				
C	1.467666	-0.986370	-1.212943	-784.2056				
H	2.262082	-1.443964	-1.799630	46.4506	72.3185	104.3621	122.1629	188.4747
H	0.651697	-1.704431	-1.132749	256.3198	289.9425	378.5129	419.4871	450.2434
H	1.086087	-0.126936	-1.765359	545.6504	573.1464	670.4559	695.8565	762.4528
C	1.985831	-0.569691	0.159226	810.4294	829.5237	858.5015	929.1507	961.6377
H	2.363331	-1.445594	0.695771	1007.2958	1044.5258	1094.0758	1118.6216	1163.2788
H	2.834540	0.110122	0.055396	1181.5428	1207.3996	1241.1309	1286.7684	1341.4499
C	0.931155	0.073798	1.034610	1350.8775	1367.1296	1398.7581	1430.0733	1449.1182
H	1.331430	0.474088	1.965073	1459.4010	1464.6700	1482.5872	1498.4924	1511.9361
H	0.597110	1.050315	0.465616	1764.3129	2090.6576	3046.6755	3070.6206	3082.0292
C	-0.381819	-0.611281	1.143083	3084.2265	3088.2041	3118.9816	3138.9453	3146.0833
H	-0.893808	-0.357604	2.070365	3148.7899	3248.1038	3321.4047		
H	-0.280476	-1.694638	1.084397					
C	-1.396470	-0.272262	-0.009734	Rotational constants (cm^{-1})				
O	-2.233076	-1.122718	-0.253259	0.0767	0.0540	0.0435		
O	-1.265116	0.864639	-0.555518	T ₁ value: 0.023				
C	0.257022	2.296699	-0.182488					
H	1.224013	2.597750	0.218275					
H	0.219519	2.225537	-1.256179					
H	-0.589133	2.771296	0.285087					



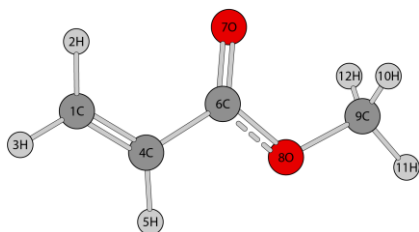
Geometry – CO ₂ – D _{∞h} (P26)				Frequency (cm ⁻¹)		
C	-2.021652	0.031747	-0.595342	688.7843	1416.4528	2465.0237
O	-2.653846	-0.922419	-0.444882	Rotational constants (cm ⁻¹) T ₁ value: 0.017		
O	-1.389164	0.985765	-0.745454	*****	0.3953	0.3953



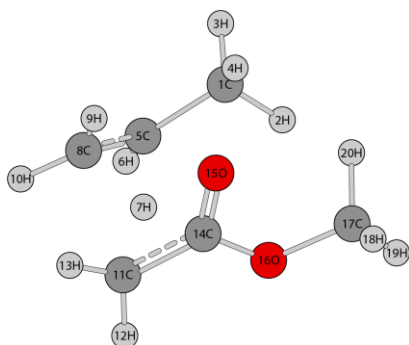
Geometry – TS27 – C ₁				Frequency (cm ⁻¹)				
C	2.989096	0.316398	-1.341767	-1565.6631				
H	3.594243	-0.163067	-2.110596	36.4937	73.2929	89.7063	139.5550	167.8784
H	2.289982	0.987333	-1.847261	189.5412	212.1292	250.8593	349.3573	408.4814
H	3.648348	0.922072	-0.720493	492.5749	574.8068	595.9298	659.4595	753.3449
C	2.249262	-0.706279	-0.512529	764.2866	799.1678	923.5864	971.8895	1011.9284
H	1.635812	-1.402284	-1.087456	1058.0999	1080.8491	1096.3893	1160.1464	1190.1053
H	2.862950	-1.261510	0.186293	1210.1924	1216.8630	1234.4580	1244.7173	1245.3313
C	1.196122	0.133161	0.886370	1306.5819	1407.7908	1419.5018	1424.5285	1473.4623
H	0.994063	-0.776785	1.437020	1492.4708	1493.3045	1495.6875	1501.6526	1516.1187
H	2.003494	0.755649	1.246394	1724.2716	2297.6314	3051.7738	3071.4804	3094.4091
C	-0.001199	0.847303	0.414670	3117.4881	3138.2891	3138.9669	3142.6616	3171.6192
H	1.076221	0.041801	-0.326555	3192.0959	3246.0373	3287.1317		
H	0.005932	1.911930	0.269007					
C	-1.147195	0.037649	0.193401	Rotational constants (cm ⁻¹)				
O	-1.161572	-1.185507	0.261888	0.1550	0.0289	0.0284		
O	-2.259559	0.747362	-0.123335					
C	-3.415797	-0.036999	-0.373350	T ₁ value: 0.013				
H	-3.685197	-0.622599	0.504387					
H	-4.207958	0.665609	-0.615320					
H	-3.249198	-0.720350	-1.205179					



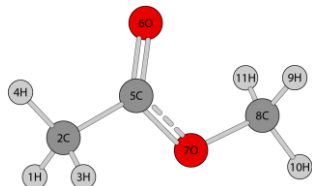
Geometry – C ₂ H ₆ – D _{3d} (P27)				Frequency (cm ⁻¹)				
C	3.337501	0.634188	-0.828520	307.1688	822.2673	824.2750	1020.2416	1221.2579
H	4.409353	0.687826	-1.016797	1221.9735	1407.0352	1425.2942	1507.8899	1508.3549
H	2.840559	1.262363	-1.567197	1510.1386	1510.7285	3066.4418	3068.5669	3121.9960
H	3.152335	1.068969	0.153259	3122.1777	3145.3801	3145.5549		
C	2.835939	-0.802946	-0.899104	Rotational constants (cm ⁻¹)				
H	3.022116	-1.238213	-1.880465	2.7025	0.6702	0.6702		
H	3.331990	-1.430853	-0.159594					
H	1.763869	-0.856335	-0.711974	T ₁ value: 0.007				



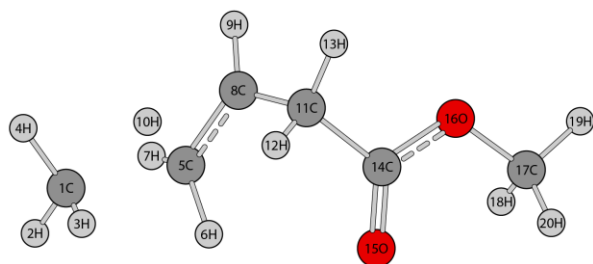
Geometry – CH ₂ CH=C(=O)OCH ₃ – C _s (P27)				Frequency (cm ⁻¹)				
C	1.088165	-0.010040	1.475952	90.8367	159.6773	200.4455	231.3484	357.8628
H	1.165469	-1.077324	1.312347	480.5163	536.5794	678.1218	847.4009	889.9616
H	1.897000	0.492858	1.986867	1033.6077	1036.7617	1072.8804	1085.6271	1190.4378
C	0.019949	0.645943	1.052786	1220.8824	1261.4937	1347.0675	1440.5532	1486.6779
H	-0.109649	1.710329	1.189149	1495.5824	1509.5335	1729.9010	1844.0512	3081.7426
C	-1.070427	-0.080595	0.355015	3154.3509	3175.2798	3190.8094	3225.5002	3271.1992
O	-1.087572	-1.259578	0.122432	Rotational constants (cm ⁻¹)				
O	-2.059131	0.755590	0.006038					
C	-3.154551	0.143900	-0.671739	0.3489	0.0783	0.0647	T ₁ value: 0.014	
H	-3.609106	-0.619154	-0.042843					
H	-3.860723	0.940852	-0.879043					
H	-2.815389	-0.319609	-1.596188					



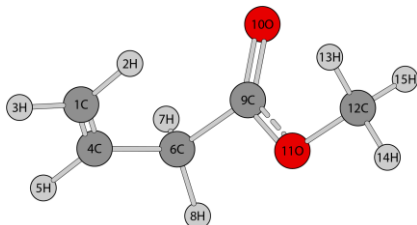
Geometry – TS28 – C ₁				Frequency (cm ⁻¹)				
C	1.418331	-1.121008	1.153415	-1312.3266				
H	0.914912	-1.853597	0.523449	60.0011	73.6897	112.6320	147.9367	161.2555
H	2.236519	-1.631151	1.666678	186.4982	208.0469	308.8702	311.3017	388.3952
H	0.707806	-0.761671	1.897441	434.2463	459.9224	619.1037	674.0742	700.4104
C	1.962184	0.022648	0.356059	746.4623	813.7761	852.1659	893.9518	939.7545
H	2.630160	-0.173138	-0.472058	1005.9391	1047.0136	1055.0114	1086.8055	1138.8910
H	0.958239	0.742935	-0.182846	1188.3782	1194.2177	1217.1094	1226.0249	1275.6945
C	1.688201	1.362433	0.673009	1307.1461	1406.6661	1433.9190	1452.5274	1474.2210
H	1.142616	1.596210	1.578055	1484.2584	1490.6094	1497.5933	1517.3543	1529.9854
H	2.223202	2.156480	0.176825	1739.1418	2167.6651	3053.3200	3069.9367	3117.5700
C	-0.405297	2.150783	-0.264409	3135.6336	3144.3283	3164.7647	3166.3924	3173.6596
H	-0.424498	2.100516	-1.344293	3208.6083	3273.2997	3286.0387	Rotational constants (cm ⁻¹)	
H	-0.340665	3.125517	0.195158					
C	-1.093941	1.153193	0.464097	0.0802	0.0542	0.0407	T ₁ value: 0.015	
O	-1.361283	1.134834	1.656968					
O	-1.269413	0.012016	-0.299152					
C	-1.979589	-1.034286	0.341960					
H	-2.964834	-0.692757	0.656715					
H	-2.075130	-1.830801	-0.391383					
H	-1.449575	-1.394839	1.223186					



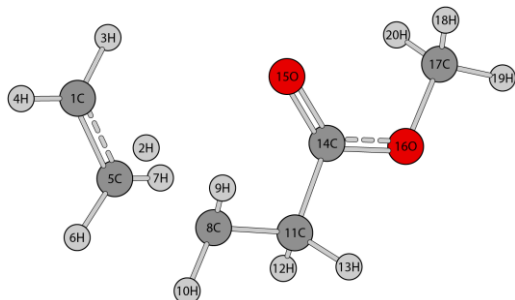
Geometry – CH ₃ C(=O)OCH ₃ – C _s (P28)				Frequency (cm ⁻¹)				
H	-0.399009	1.652135	1.240289	62.7159	163.1906	187.4101	298.3460	432.8317
C	0.461599	1.926124	0.632303	616.9572	657.1828	887.8004	1002.7883	1074.8859
H	1.223452	2.323693	1.300762	1115.0603	1190.7008	1225.1308	1308.6457	1405.8466
H	0.181065	2.670099	-0.104952	1474.5921	1481.4121	1487.9153	1496.9683	1510.5991
C	0.991446	0.707838	-0.066025	1862.0186	3082.0103	3088.8369	3154.9993	3156.7695
O	1.090752	0.570183	-1.253956	3189.0504	3201.1523			
O	1.352693	-0.238889	0.814729					
C	1.869938	-1.436094	0.236717	Rotational constants (cm ⁻¹)				
H	2.759360	-1.219047	-0.351628	0.3458	0.1403	0.1036		
H	2.110993	-2.089500	1.068548					
H	1.125710	-1.896552	-0.410200	T ₁ value: 0.013				



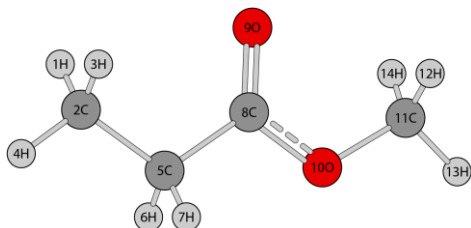
Geometry – TS29 – C ₁				Frequency (cm ⁻¹)				
C	3.604637	0.277292	-0.416008	-2031.0109				
H	4.086374	-0.674942	-0.613906	43.3347	47.3024	71.1067	122.2627	136.0937
H	3.447803	0.845807	-1.328707	166.9355	217.4403	300.8832	379.8289	404.8283
H	4.170167	0.847418	0.323874	419.4180	435.8561	476.0120	589.7724	646.9166
C	1.798418	-0.509571	0.232804	731.9674	802.1484	876.4839	908.5639	935.8776
H	1.545036	-0.808210	-0.776890	1014.1388	1081.6094	1111.7847	1120.0792	1190.7510
H	2.259558	-1.272645	0.842429	1201.1165	1216.7114	1228.5186	1234.7355	1283.7852
C	0.964438	0.458465	0.886354	1307.1560	1359.4531	1391.4545	1440.3567	1456.4136
H	0.937444	0.491076	1.961781	1458.3211	1471.9006	1486.3087	1494.1293	1510.5771
H	2.338762	0.619510	0.397578	1826.8757	2180.3639	3034.0563	3053.4187	3079.9009
C	0.025333	1.297968	0.060493	3147.0470	3150.4821	3152.1791	3170.0294	3187.1761
H	0.539341	1.778441	-0.778380	3203.8477	3245.5314	3263.0969		
H	-0.437102	2.068929	0.671099					
C	-1.030467	0.400122	-0.530820	Rotational constants (cm ⁻¹)				
O	-0.860443	-0.304782	-1.494081	0.1624	0.0300	0.0285		
O	-2.170426	0.407873	0.174827					
C	-3.166425	-0.508757	-0.272777	T ₁ value: 0.013				
H	-2.791536	-1.529377	-0.221113					
H	-4.013712	-0.378734	0.392460					
H	-3.448686	-0.290919	-1.301031					



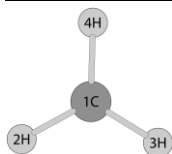
Geometry – CH ₂ =CHCH ₂ C(=O)OCH ₃ – C ₁ (P29)				Frequency (cm ⁻¹)				
C	-1.217064	0.014180	-1.366310	26.2555	102.5486	122.4150	168.7739	228.2530
H	-0.468793	-0.763832	-1.460519	300.1322	424.8964	477.8959	562.0326	646.8525
H	-1.989107	0.046109	-2.122099	810.1605	890.4007	937.6661	966.0732	981.4424
C	-1.205462	0.882161	-0.369135	1037.6598	1080.4034	1108.0747	1191.0289	1197.8993
H	-1.983296	1.635070	-0.308274	1224.4051	1307.7990	1327.1382	1381.2092	1458.5585
C	-0.190425	0.932872	0.742749	1472.3435	1490.2538	1496.1600	1509.7774	1738.8834
H	-0.672024	0.691893	1.690733	1858.3973	3080.2717	3084.0103	3130.1707	3152.6164
H	0.222371	1.939456	0.813464	3164.7243	3180.8245	3190.1805	3253.7759	
C	0.927162	-0.052778	0.528532	Rotational constants (cm ⁻¹)				
O	0.933260	-1.186550	0.922362					
O	1.919523	0.478176	-0.199743					
C	2.987843	-0.415280	-0.507727	0.1579	0.0595	0.0561	T ₁ value: 0.013	
H	2.617211	-1.263985	-1.080058					
H	3.698650	0.158826	-1.092429					
H	3.449290	-0.783725	0.406339					



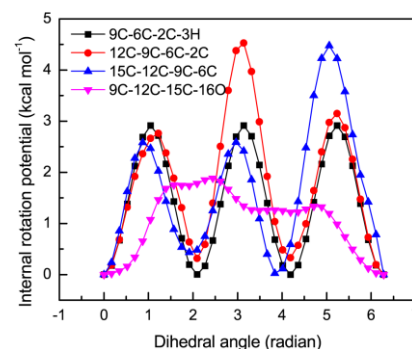
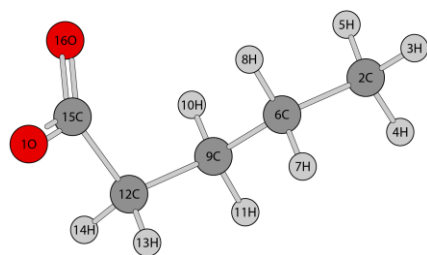
Geometry – TS30 – C ₁				Frequency (cm ⁻¹)				
C	2.632455	-1.355435	-0.401596	-1908.4333				
H	1.989298	-0.230940	0.259137	41.8372	74.7209	103.8724	153.5780	164.1631
H	1.950397	-2.174579	-0.253655	196.8877	221.0909	342.2158	350.5074	405.2657
H	3.649655	-1.425662	-0.055173	447.0982	520.5219	583.9728	615.6676	678.0378
C	2.166202	-0.144721	-0.985592	721.2495	772.3303	887.5413	896.3533	998.0517
H	2.895356	0.586881	-1.300654	1023.9821	1060.2681	1076.0301	1142.5411	1191.3706
H	1.243245	-0.160958	-1.549585	1195.5896	1198.7997	1212.2464	1226.5661	1259.4582
C	1.312600	1.235339	0.420201	1269.1405	1289.8073	1395.7244	1437.7187	1446.1563
H	1.376136	0.898409	1.461074	1464.1594	1484.5906	1488.1787	1495.8837	1510.6731
H	1.940823	2.110265	0.277010	1834.9457	2174.3429	3035.2610	3039.6444	3062.9241
C	-0.109625	1.436630	-0.024273	3082.2889	3149.0282	3155.0813	3157.4534	3191.3853
H	-0.157474	1.701452	-1.087032	3207.6396	3247.0657	3320.7674		
H	-0.639764	2.242928	0.491388	Rotational constants (cm ⁻¹)				
C	-0.927101	0.180325	0.141396					
O	-0.479738	-0.903743	0.413097					
O	-2.232447	0.399728	-0.063249	0.1235	0.0363	0.0304	T ₁ value: 0.013	
C	-3.068261	-0.751103	0.049588					
H	-2.991959	-1.177626	1.047778					
H	-4.078634	-0.406396	-0.143198					
H	-2.774773	-1.505571	-0.677908					



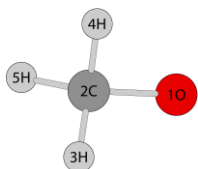
Geometry – CH ₃ CH ₂ C(=O)OCH ₃ – C _s (P30)				Frequency (cm ⁻¹)					
H	1.815739	0.662261	0.554036	56.4640	146.4414	168.1588	215.7131	223.7866	
C	1.213910	1.546229	0.755860	347.3789	455.2379	588.4075	669.8945	819.8014	
H	1.003852	1.560132	1.823571	883.8156	1012.1893	1059.5379	1116.3203	1127.7937	
H	1.797024	2.429999	0.503742	1191.1466	1219.8097	1258.6057	1286.1792	1400.4164	
C	-0.075728	1.511637	-0.044407	1423.8973	1467.8534	1486.2978	1496.0582	1497.8181	
H	0.112933	1.501723	-1.119307	1506.5031	1511.1890	1855.3680	3078.5642	3080.5925	
H	-0.692939	2.392478	0.140801	3081.6472	3111.3918	3153.2214	3155.6305	3156.7118	
C	-0.913572	0.301426	0.275395	3188.2961					
O	-0.627496	-0.556667	1.064873						
O	-2.048387	0.289180	-0.441554						
C	-2.904728	-0.825715	-0.201287						
H	-3.212207	-0.849554	0.842466						
H	-3.763688	-0.688615	-0.849710						
H	-2.391166	-1.755956	-0.436652						
				Rotational constants (cm ⁻¹)					
				0.3224	0.0723	0.0610			
				T ₁ value: 0.012					



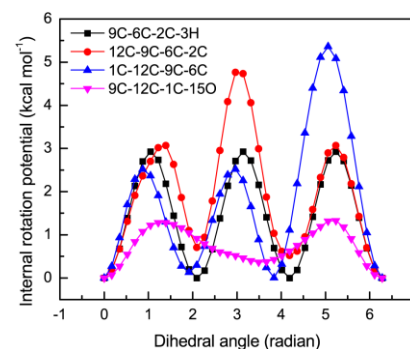
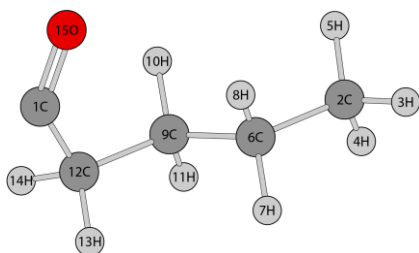
Geometry – CH ₃ – D _{3h} (P31)				Frequency (cm ⁻¹)				
C	3.711198	-0.730495	-0.066344	420.2100	1412.2100	1412.8182	3142.4431	3320.5271
H	3.792164	-1.333251	-0.954648	3321.9616				
H	4.034422	0.296275	-0.080941					
H	3.303496	-1.153567	0.835779	9.6218	9.6191	4.8102		
				Rotational constants (cm ⁻¹) T ₁ value: 0.014				



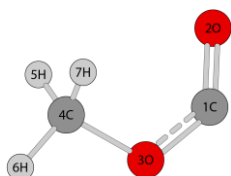
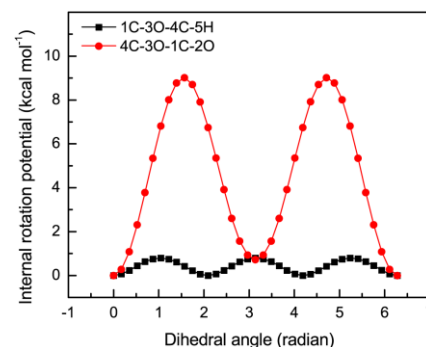
Geometry – O(C=O)CH ₂ CH ₂ CH ₂ CH ₃ – C ₁ (P31)				Frequency (cm ⁻¹)					
O	-0.871346	1.279073	-0.769697	27.0610	80.3769	107.9508	231.4413	245.8433	
C	3.652377	-1.727684	-0.128265	276.1774	307.9457	422.1605	536.9017	635.1809	
H	3.765733	-2.533069	-0.852417	743.1262	803.5576	848.7725	896.7518	951.5742	
H	4.616070	-1.225716	-0.030534	1028.6528	1058.6460	1083.7333	1126.7465	1193.6855	
H	3.410585	-2.175127	0.836334	1243.2057	1271.2180	1328.5258	1335.6330	1369.7015	
C	2.568435	-0.745673	-0.552147	1406.3712	1416.0389	1461.7076	1483.7411	1495.9922	
H	2.809859	-0.326495	-1.532568	1504.2353	1510.7993	1788.9598	3050.7296	3061.0610	
H	1.617809	-1.272913	-0.658745	3068.1079	3074.0202	3087.8111	3112.7713	3122.3007	
C	2.401117	0.388215	0.451825	3130.6316	3139.9746				
H	2.147210	-0.022430	1.429980						
H	3.344345	0.927599	0.560111						
C	1.321746	1.386146	0.044979						
H	1.490368	1.774669	-0.960820						
H	1.292084	2.241984	0.722313						
C	-0.052694	0.747864	0.122217						
O	-0.405520	-0.110988	0.882428						
				Rotational constants (cm ⁻¹)					
				0.1849	0.0451	0.0426			
				T ₁ value: 0.016					



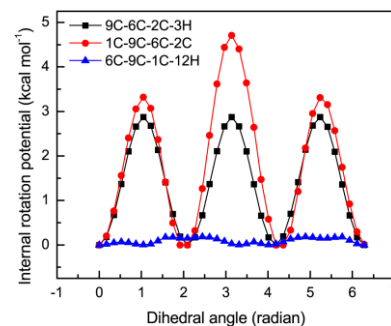
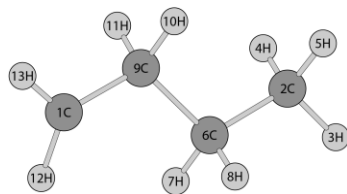
Geometry – CH ₃ O – C ₁ (P32)				Frequency (cm ⁻¹)				
O	-6.416266	0.814107	-0.026218	433.3159	973.5133	1140.5043	1386.3341	1387.9630
C	-7.172968	-0.270752	-0.371072	1522.7546	2962.0160	3034.1664	3076.8742	
H	-7.138689	-1.069432	0.376839	Rotational constants (cm ⁻¹)				
H	-8.212263	0.097112	-0.399670	5.2837	0.9338	0.9281		
H	-6.943427	-0.648246	-1.372828	T ₁ value: 0.018				



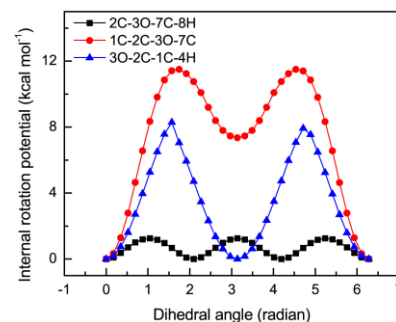
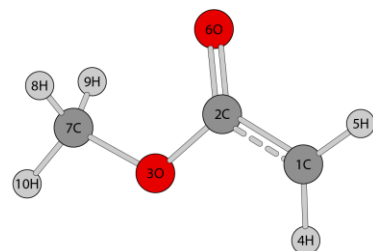
Geometry – (C=O)CH ₂ CH ₂ CH ₂ CH ₃ – C ₁ (P32)				Frequency (cm ⁻¹)				
C	0.632323	-0.632123	0.460291	80.4237	96.9686	155.1899	236.0297	251.1305
C	4.896139	0.220469	-0.863959	264.7861	411.3323	640.5620	750.0125	779.6154
H	5.206245	0.210571	-1.907942	821.0713	893.6929	919.8006	1017.9326	1076.4805
H	5.425382	1.033086	-0.364018	1096.4457	1133.3846	1221.2419	1259.7494	1319.5157
H	5.220419	-0.716429	-0.409410	1327.4779	1345.0753	1403.3787	1415.4593	1444.2493
C	3.388444	0.389891	-0.731252	1483.0100	1497.0912	1504.6249	1511.5566	1977.8921
H	3.076365	1.319378	-1.214898	3050.8045	3057.7765	3060.6958	3074.0849	3090.3859
H	2.879024	-0.423071	-1.251244	3106.2361	3113.7584	3129.2333	3137.8769	
C	2.941792	0.412239	0.725784	Rotational constants (cm ⁻¹)				
H	3.248927	-0.514104	1.215869					
H	3.443298	1.231062	1.247556	T ₁ value: 0.015				
C	1.433666	0.583329	0.887041					
H	1.052941	1.432432	0.316020					
H	1.145321	0.765453	1.924550					
O	1.037912	-1.684581	0.130391					



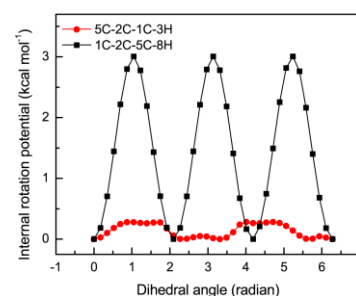
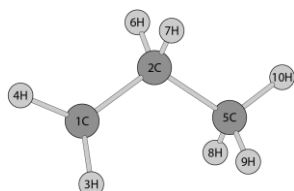
Geometry – CH ₃ OC(=O) – C _s (P33)				Frequency (cm ⁻¹)				
C	-3.619676	-0.243737	0.229056	118.0415	288.4408	382.1496	775.1564	953.9898
O	-3.903341	-1.227283	0.818076	1169.5573	1183.1459	1223.2486	1465.9607	1493.0554
O	-4.377491	0.598555	-0.426800	1502.0183	1903.6860	3089.5314	3171.9919	3208.5562
C	-5.788946	0.274626	-0.432188	Rotational constants (cm ⁻¹)				
H	-6.160156	0.254842	0.589653	0.7678	0.2306	0.1835		
H	-6.268636	1.058651	-1.006146	T ₁ value: 0.019				
H	-5.936027	-0.696898	-0.897880					



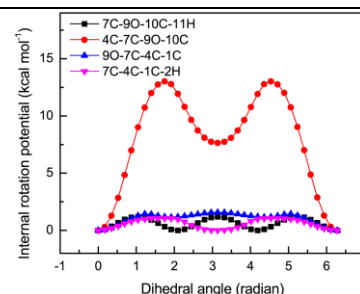
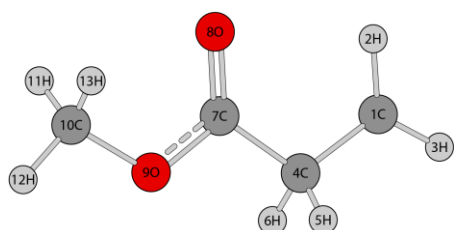
Geometry – CH ₂ CH ₂ CH ₂ CH ₃ – C ₁ (P33)				Frequency (cm ⁻¹)				
C	3.361944	1.886194	0.348534	115.3225	136.6855	240.3190	264.4115	428.7367
C	5.429571	-1.286745	-0.425083	465.0530	729.9505	830.3313	872.7348	966.2398
H	5.349564	-2.065187	-1.182888	1054.7773	1080.0011	1109.5984	1176.0461	1251.2755
H	6.411741	-0.821965	-0.523879	1313.0240	1325.1616	1396.0936	1414.6490	1468.4584
H	5.388508	-1.766899	0.553731	1473.7806	1495.9814	1503.1787	1510.9614	2971.1633
C	4.323322	-0.250374	-0.566524	3049.2419	3055.8035	3059.3379	3090.5986	3125.2229
H	4.364815	0.204954	-1.559118	3135.0604	3166.8491	3270.5305		
H	3.346305	-0.732090	-0.488559					
C	4.418349	0.851889	0.486371	Rotational constants (cm ⁻¹)				
H	4.380764	0.407873	1.485951	0.8429	0.1286	0.1194		
H	5.415110	1.313381	0.415030	T ₁ value: 0.011				
H	2.960116	2.124965	-0.625833					
H	3.094882	2.526703	1.174946					



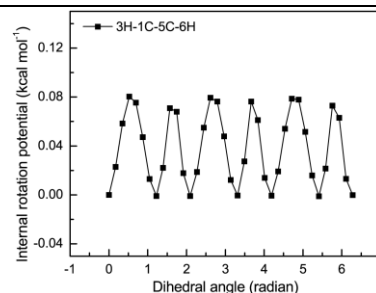
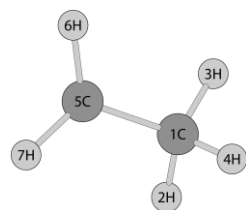
Geometry – CH ₃ OC(=O)CH ₂ – C _s (P34)				Frequency (cm ⁻¹)				
C	-2.751726	1.554766	-0.168094	158.1884	184.8101	301.0731	335.8625	430.5499
C	-3.448478	0.328995	0.151965	616.1947	668.3421	763.8566	885.2498	1018.2774
O	-4.644771	0.247987	-0.463884	1123.9140	1189.6951	1228.0374	1320.1979	1457.4339
H	-3.192207	2.280768	-0.831018	1490.9455	1495.2185	1510.4267	1769.9341	3078.4493
H	-1.782950	1.716635	0.272754	3149.3585	3188.2136	3202.0725	3325.5191	
O	-3.021749	-0.533250	0.884874					
C	-5.379024	-0.940392	-0.185719	Rotational constants (cm ⁻¹)				
H	-4.816508	-1.817344	-0.501473	0.3634	0.1481	0.1073		
H	-5.581774	-1.021049	0.880861	T ₁ value: 0.015				
H	-6.304699	-0.857999	-0.745636					



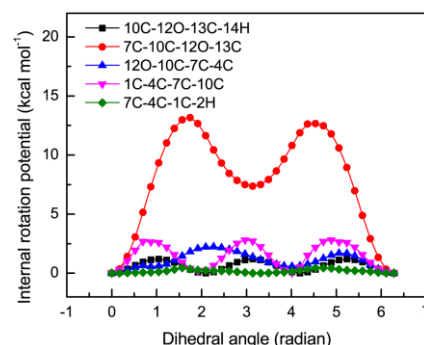
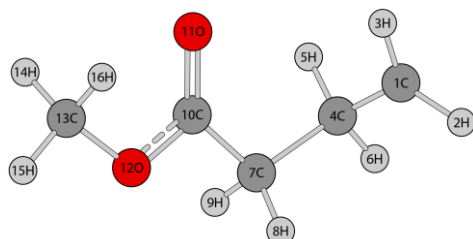
Geometry – CH ₂ CH ₂ CH ₃ – C _s (P34)				Frequency (cm ⁻¹)				
C	-1.290666	-0.297515	-0.031175	94.0966	253.6749	373.5946	453.8106	756.2158
C	-0.079327	0.559053	0.046265	896.1800	928.9401	1053.0293	1101.1568	1178.1973
H	-1.254807	-1.321921	0.311093	1271.2351	1363.5016	1410.5709	1469.6512	1474.7776
H	-2.256315	0.122079	-0.268560	1502.3998	1508.7504	2984.2988	3059.1143	3062.5712
C	1.216104	-0.243283	-0.035505	3130.3855	3139.1987	3166.9072	3270.3170	
H	-0.105600	1.309820	-0.748058					
H	-0.084343	1.132969	0.983581					
H	1.273527	-0.785658	-0.979229					
H	1.264541	-0.974635	0.772159					
H	2.090358	0.401812	0.041321					
				Rotational constants (cm ⁻¹)				
				1.0948 0.3035 0.2622				
				T ₁ value: 0.012				



Geometry – CH ₃ OC(=O)CH ₂ CH ₂ – C ₁ (P35)				Frequency (cm ⁻¹)				
C	-2.498419	0.120878	0.004001	57.0582	150.0977	172.9698	185.0380	226.9557
H	-2.415058	1.194876	-0.008028	357.5667	404.8868	463.6306	581.3400	660.6282
H	-3.470416	-0.344263	0.013214	876.0059	918.0197	1019.1237	1055.9351	1138.4605
C	-1.276725	-0.714746	-0.003271	1189.7311	1196.5378	1219.6725	1258.6524	1401.1385
H	-1.232350	-1.380020	-0.873879	1441.5558	1453.6614	1487.7903	1496.1860	1510.7880
H	-1.230371	-1.392095	0.857370	1860.5336	3025.5297	3042.0245	3081.7881	3154.8069
C	-0.003596	0.095942	-0.000786	3189.9581	3192.7233	3306.5391		
O	0.066923	1.293255	-0.001030					
O	1.072154	-0.704769	0.000717					
C	2.329421	-0.030374	0.001502					
H	2.422274	0.596056	0.886526					
H	3.085517	-0.808289	0.002296					
H	2.423700	0.595650	-0.883666					
				Rotational constants (cm ⁻¹)				
				0.3307 0.0753 0.0628				
				T ₁ value: 0.014				



Geometry – CH ₂ CH ₃ – C ₁ (P35)				Frequency (cm ⁻¹)				
C	3.085247	1.021540	-0.110663	122.1966	443.7284	810.7281	982.5242	1080.9499
H	3.266022	1.592923	0.800314	1195.4919	1403.6122	1471.2642	1487.0006	1489.2668
H	3.262669	1.675383	-0.964459	3004.6510	3085.2928	3129.2670	3174.8673	3276.5020
H	2.015630	0.775584	-0.118655					
C	3.931972	-0.196358	-0.168935					
H	4.201647	-0.637310	-1.115892					
H	4.153843	-0.756529	0.726122					
				Rotational constants (cm ⁻¹)				
				3.4783 0.7624 0.7069				
				T ₁ value: 0.013				



Geometry – CH ₃ OC(=O)CH ₂ CH ₂ CH ₂ – C ₁ (P36)				Frequency (cm ⁻¹)				
C	1.913871	-0.183720	-0.626134	44.9252	100.0120	116.8503	163.5693	182.7643
H	2.497647	0.167173	-1.463443	213.7092	303.2287	366.0248	439.5928	523.0411
H	1.615542	-1.219758	-0.600464	599.3564	662.0989	789.9372	899.5278	909.8217
C	1.388850	0.767902	0.389401	996.3804	1063.0843	1088.9014	1127.3858	1190.7786
H	1.375603	0.294011	1.372524	1211.8973	1220.0911	1253.1443	1298.8245	1347.2549
H	2.029528	1.647791	0.453641	1400.9680	1457.9337	1463.4314	1486.6095	1488.7312
C	-0.036961	1.237045	0.074747	1496.2833	1511.0298	1850.7031	3067.2816	3071.4259
H	-0.105253	1.669358	-0.923959	3081.8993	3111.5810	3122.5904	3155.0825	3177.4480
H	-0.359500	2.012840	0.773844	3188.9222	3285.8784			
C	-1.036320	0.113303	0.173365					
O	-0.825098	-0.967538	0.653030	Rotational constants (cm ⁻¹)				
O	-2.227404	0.472670	-0.326850	0.2147	0.0498	0.0456		
C	-3.246418	-0.522151	-0.241310					
H	-3.428227	-0.790044	0.797760	T ₁ value: 0.013				
H	-4.133232	-0.080340	-0.683241					
H	-2.949617	-1.415466	-0.787331					

Table S2 Scanned M06-2X/cc-pVTZ reaction energies (kcal mol⁻¹), DLPNO-CCSD(T)/CBS(T-Q) reaction enthalpies (kcal mol⁻¹), and the conversion factors between them for MP bond fission reactions

Reactions	Reaction energy	Reaction enthalpy	Conversion factor
R31	148.4	90.4	0.609
R32	164.9	99.5	0.603
R33	152.5	93.7	0.614
R34	142.3	85.6	0.602
R35	151.2	87.7	0.580
R36	154.6	88.4	0.572

Table S3 Standard enthalpy of formation ($\Delta_f H_{298}^\circ$, kcal mol⁻¹), standard molar entropy (S_{298}° , cal mol⁻¹ K⁻¹), heat capacity at constant pressure (C_p° , cal mol⁻¹ K⁻¹) for involved species studied in this work at the DLPNO-CCSD(T)/CBS(T-Q)//M06-2X/cc-pVTZ level.

Species	$\Delta_f H_{298}^\circ$ K	S_{298}° K	$C_p^\circ(T)$						
			298	300	500	800	1000	1200	1500
MP	-110.92 (-118.55) ^a	99.82 (90.95) ^a	36.67	36.85	54.44	72.85	81.03	87.11	93.45
CH ₃ CH ₂ CH ₂ CH=C(OH)OCH ₃	-85.31	98.00	38.53	38.73	57.40	75.02	82.44	87.89	93.64
CH ₃ CH=CH ₂	5.98 (4.77) ^b	63.63	15.25	15.32	22.49	30.40	34.12	36.99	40.09
CH ₂ =C(OH)OCH ₃	-70.89	74.23	22.57	22.68	32.60	41.53	45.23	47.94	50.79
CH ₃ CH ₂ CH ₂ CH=C=O	-22.57 (-33.32) ^a	83.70 (78.55) ^a	26.97	27.09	38.98	51.04	56.44	60.50	64.82
CH ₃ OH	-48.84 (-47.98) ^b (-48.70) ^c	57.32 (57.20) ^c	10.43	10.46	14.08	18.82	21.14	22.95	24.95
CH ₃ CH ₂ CH ₂ CH ₂ CHO	-52.99 (-59.09) ^a	84.33 (81.82) ^a	28.69	28.84	43.32	58.04	64.49	69.25	74.24
CH ₂ O	-25.70 (-26.08) ^b (-25.90) ^c	53.61 (53.60) ^c	8.41	8.43	10.31	13.16	14.59	15.68	16.84
CH ₃	35.02 (34.99) ^b (34.90) ^c	46.68 (46.60) ^c	9.61	9.62	10.97	12.89	14.03	15.03	16.20
CH ₃ CH ₂ CH ₂ CH ₂ C(=O)O	-53.90 (-65.02) ^a	92.35 (82.70) ^a	31.35	31.51	45.76	59.64	65.65	70.10	74.81
CH ₃ O	4.76 (5.17) ^b (4.80) ^c	57.23 (58.8) ^c	10.36	10.39	13.53	17.22	19.01	20.37	21.84
CH ₃ CH ₂ CH ₂ CH ₂ C(=O)	-15.03 (-21.80) ^a	87.25 (83.79) ^a	27.91	28.05	41.19	54.51	60.33	64.65	69.21
CH ₃ OC(=O)	-36.17 (-37.65) ^b (-37.70) ^c	69.74 (69.80) ^b	14.79	14.84	19.89	25.64	28.16	29.95	31.73
CH ₃ CH ₂ CH ₂ CH ₂	20.12 (15.18) ^a (19.33) ^b	78.32 (70.73) ^a	22.41	22.53	33.61	45.05	50.30	54.30	58.61
CH ₃ OC(=O)CH ₂	-49.06 (-50.7) ^c	76.17 (77.7) ^c	21.14	21.23	29.45	37.99	41.71	44.38	47.05
CH ₃ CH ₂ CH ₂	24.93 (21.11) ^a (24.10) ^b	70.96 (63.32) ^a	17.33	17.41	25.30	33.73	37.73	40.84	44.21
CH ₃ OC(=O)CH ₂ CH ₂	-49.62	87.50	26.64	26.74	36.62	47.51	52.52	56.27	60.20
CH ₃ CH ₂	29.35 (28.64) ^b (29.1) ^c	59.35 (59.4) ^c	12.33	12.38	17.22	22.81	25.56	27.71	30.07
CH ₃ OC(=O)CH ₂ CH ₂ CH ₂	-55.61	96.18	31.64	31.78	44.76	58.43	64.66	69.36	74.30

a: from Dévart *et al.*'s model ¹; b: from ATcT table ²; c: by Ning *et al.* at the CCSD(T)/CBS(T-Q) level of theory ³

Table S4 Fitted pre-exponential factors (A' , s^{-1}) and activation energies (E' , $cal\ mol^{-1}$) for the high-pressure limit rate constants of MP unimolecular decompositions using the standard Arrhenius equation.

Reaction	A' (s^{-1})	E' ($cal\ mol^{-1}$)
R1	2.408E+13	77767.4
R6	4.258E+12	72975.7
R18	3.262E+13	81647.4
R24	1.603E+13	80568.3
R31	3.669E+15	95634.4
R32	7.115E+15	101277.0
R33	2.280E+17	100066.4
R34	7.695E+15	81027.5
R35	5.252E+15	81690.2
R36	2.787E+16	94263.1

Table S5 Updated unimolecular decomposition and hydrogen abstraction reactions of MP as well as some key reactions from Aramco-3.0.

Reaction	A ($s^{-1}/cm^3\ mol^{-1}\ s^{-1}$)	n	E ($cal\ mol^{-1}$)	
MP \rightleftharpoons CH ₃ CH ₂ CH ₂ CH=C(OH)OCH ₃	1.161E+10	0.975	74099.7	this work
PLOG/ 0.01	1.735E+68	-16.524	98384.5/	
PLOG/ 0.1	2.980E+62	-14.624	96630.3/	
PLOG/ 1	2.418E+56	-12.647	94946.4/	
PLOG/ 10	1.083E+34	-6.062	84765.3/	
PLOG/ 100	6.410E+19	-1.942	77502.3/	
MP \rightleftharpoons CH ₃ CHCH ₂ +CH ₃ C(=O)OCH ₃	9.368E+08	1.068	68961.1	this work
PLOG/ 0.01	1.708E+69	-16.752	97025.3/	
PLOG/ 0.1	1.423E+63	-14.827	94975.6/	
PLOG/ 1	4.032E+51	-11.333	90644.9/	
PLOG/ 10	2.728E+31	-5.454	80516.7/	
PLOG/ 100	4.178E+21	-2.589	76161.6/	
MP \rightleftharpoons CH ₃ CH ₂ CH ₂ CHCO+CH ₃ OH	1.540E+11	0.708	78983.4	this work
PLOG/ 0.01	2.568E+81	-20.106	111581.2/	
PLOG/ 0.1	1.272E+75	-18.044	110387.8/	
PLOG/ 1	1.074E+59	-13.276	102141.9/	
PLOG/ 10	6.568E+35	-6.495	90770.1/	
PLOG/ 100	6.606E+23	-3.007	85050.3/	
MP \rightleftharpoons CH ₃ CH ₂ CH ₂ CH ₂ CHO+CH ₂ O	1.826E+10	0.874	77278.5	this work
PLOG/ 0.01	8.040E+79	-19.745	109942.4/	
PLOG/ 0.1	5.164E+72	-17.451	107772.9/	
PLOG/ 1	1.463E+59	-13.371	101991.1/	
PLOG/ 10	7.808E+35	-6.585	90324.5/	
PLOG/ 100	1.128E+24	-3.144	84662.4/	
MP \rightleftharpoons CH ₃ CH ₂ CH ₂ CH ₂ C(=O)O+CH ₃	2.908E+10	1.455	90153.7	this work
PLOG/ 0.01	2.426E+95	-23.858	128444.4/	
PLOG/ 0.1	1.315E+84	-20.343	123697.5/	
PLOG/ 1	2.012E+70	-16.088	118949.9/	
PLOG/ 10	9.954E+40	-7.512	104858.3/	
PLOG/ 100	7.506E+22	-2.324	94213.9/	
MP \rightleftharpoons CH ₃ CH ₂ CH ₂ CH ₂ C(=O)+CH ₃ O	6.864E+14	0.355	99940.9	this work
PLOG/ 0.01	6.518E104	-26.556	139456.3/	
PLOG/ 0.1	2.262E+97	-24.008	139327.5/	

PLOG/	1	6.050E+80	-18.972	132202.9/	
PLOG/	10	2.214E+46	-8.957	114206.5/	
PLOG/	100	1.614E+31	-4.556	106996.4/	
MP<=>CH ₃ CH ₂ CH ₂ CH ₂ +CH ₃ OC(=O)		1.305E+12	1.493	94441.6	this work
PLOG/	0.01	2.584E100	-24.901	133506.9/	
PLOG/	0.1	4.442E+92	-22.295	132580.3/	
PLOG/	1	7.392E+75	-17.211	125149.2/	
PLOG/	10	2.170E+44	-7.990	109831.3/	
PLOG/	100	2.036E+28	-3.352	101639.9/	
MP<=>CH ₃ CH ₂ CH ₂ +CH ₃ OC(=O)CH ₂		2.996E+21	-1.425	86390.6	this work
PLOG/	0.01	5.544E+93	-22.778	122221.4/	
PLOG/	0.1	3.316E+87	-20.702	121598.2/	
PLOG/	1	7.542E+72	-16.313	114703.7/	
PLOG/	10	4.130E+47	-8.967	101509.4/	
PLOG/	100	6.126E+35	-5.519	96087.7/	
MP<=>CH ₃ CH ₂ +CH ₃ OC(=O)CH ₂ CH ₂		4.866E+22	-1.796	88449.6	this work
PLOG/	0.01	8.264E+97	-23.986	126409.8/	
PLOG/	0.1	7.734E+88	-21.129	123516.5/	
PLOG/	1	1.325E+75	-16.981	117299.8/	
PLOG/	10	5.956E+53	-10.710	107516.8/	
PLOG/	100	5.446E+39	-6.674	99664.2/	
MP<=>CH ₃ +CH ₃ OC(=O)CH ₂ CH ₂ CH ₂		7.504E+11	1.312	89321.3	this work
PLOG/	0.01	6.872E+96	-23.960	128447.8/	
PLOG/	0.1	6.264E+86	-20.783	124909.9/	
PLOG/	1	1.745E+72	-16.339	119249.9/	
PLOG/	10	1.057E+42	-7.536	103820.6/	
PLOG/	100	7.352E+26	-3.152	96047.6/	
MP+OH<=>H ₂ O+CH ₂ CH ₂ CH ₂ CH ₂ C(=O)OCH ₃		2.220E+03	2.844	217.3	ref. 4
MP+OH<=>H ₂ O+CH ₃ CHCH ₂ CH ₂ C(=O)OCH ₃		2.919E+04	2.594	-63.2	
MP+OH<=>H ₂ O+CH ₃ CH ₂ CHCH ₂ C(=O)OCH ₃		1.862E+01	3.450	-3056.3	
MP+OH<=>H ₂ O+CH ₃ CH ₂ CH ₂ CHC(=O)OCH ₃		2.048E+01	3.428	-2463.4	
MP+OH<=>H ₂ O+CH ₃ CH ₂ CH ₂ CH ₂ C(=O)OCH ₂		3.242E-02	4.007	-2048.3	
MP+HO ₂ <=>H ₂ O ₂ +CH ₂ CH ₂ CH ₂ CH ₂ C(=O)OCH ₃		1.600E-01	4.110	12337.0	ref. 5
MP+HO ₂ <=>H ₂ O ₂ +CH ₃ CHCH ₂ CH ₂ C(=O)OCH ₃		9.100E-02	4.020	8193.0	
MP+HO ₂ <=>H ₂ O ₂ +CH ₃ CH ₂ CHCH ₂ C(=O)OCH ₃		4.880E-02	3.760	7806.0	
MP+HO ₂ <=>H ₂ O ₂ +CH ₃ CH ₂ CH ₂ CHC(=O)OCH ₃		7.670E-04	4.180	7005.0	
MP+HO ₂ <=>H ₂ O ₂ +CH ₃ CH ₂ CH ₂ CH ₂ C(=O)OCH ₂		3.650E-03	4.020	10081.0	
HO ₂ +OH<=>H ₂ O+O ₂		2.456E+13	0	-497.0	ref. 6
C ₂ H ₃ +O ₂ <=>CH ₂ CHO+O		1.760E+12	0.150	4205.0	ref. 6
DUP					
PLOG/	0.01	7.880E+20	-2.670	6742.0/	
PLOG/	0.1	7.720E+20	-2.670	6713.0/	
PLOG/	0.316	9.870E+20	-2.700	6724.0/	
PLOG/	1	7.100E+20	-2.650	6489.0/	
PLOG/	3.16	4.500E+20	-2.530	6406.0/	
PLOG/	10	1.760E+23	-3.220	8697.0/	
PLOG/	31.6	3.140E+25	-3.770	11530.0/	
PLOG/	100	1.020E+26	-3.800	13910.0/	
C ₂ H ₃ +O ₂ <=>CH ₂ CHO+O		1.760E+12	0.150	4205.0	
DUP					
PLOG/	0.01	1.360E+10	0.620	-277.6/	
PLOG/	0.1	1.420E+10	0.620	-247.7	
PLOG/	0.316	1.660E+10	0.600	-162.5	
PLOG/	1	2.020E+10	0.580	38.4	
PLOG/	3.16	9.750E+09	0.670	248.0	
PLOG/	10	7.340E+09	0.720	778.1	
PLOG/	31.6	1.570E+09	0.920	1219.0	
PLOG/	100	7.850E+07	1.280	1410.0	

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