

Electronic Supplementary Information (ESI)

Theoretical Kinetic Study for Methyl levulinate: Oxidation by OH and CH₃ radicals and further unimolecular decomposition pathways

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CH3

O 2

C	0.00000000	0.00000000	0.00000000
H	0.00000000	1.08779300	0.00000000
H	0.94205600	-0.54389600	0.00000000
H	-0.94205600	-0.54389600	0.00000000

Frequencies

494.7080 1424.5124 1424.5124
3165.0819 3364.4803 3364.4803

Methyl levulinate

O 1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51208600
O	1.03899900	0.00000000	2.17133400
C	-1.36534000	0.00494200	2.19565800
C	-1.28901200	-0.62022300	3.58510000
C	-0.88008800	-2.07481600	3.47595900
O	-0.78715000	-2.69978000	2.42704600
O	-0.63879000	-2.61447700	4.69653400
C	-0.23732400	-4.00667200	4.65362000
H	-2.09288900	-0.52540400	1.56182000
H	-1.69489400	1.05774100	2.26303200
H	-2.25960500	-0.57309200	4.10518000
H	-0.54967200	-0.10186300	4.21285800
H	-0.07822200	-4.29017000	5.69962600
H	0.68823900	-4.11270500	4.07157800
H	-1.02935700	-4.61582600	4.19673700
H	-0.70735300	0.75117000	-0.38773800
H	-0.34908100	-0.98988600	-0.33940800
H	1.01124300	0.18936800	-0.38209500

Frequencies

20.1571 49.0044 84.9870
155.5924 157.0663 176.8444
210.5847 261.3881 327.0225
359.8173 458.9715 477.9568
557.5031 619.0318 657.2946
777.1504 813.2206 898.3497
948.3197 986.7006 1015.2096
1027.1059 1083.4276 1168.6189
1177.9076 1198.3293 1203.2410
1223.2522 1251.7769 1356.0331
1378.1734 1398.7767 1435.5061
1443.8365 1455.6444 1458.7700
1469.1069 1480.3669 1487.7142
1735.9661 1754.4235 3060.2524
3067.3867 3090.1489 3094.5277
3134.7293 3147.3229 3159.3541
3189.9938 3196.3208 3223.8856

MLR1

0 2

C	3.00567600	-0.77459900	-0.35067600
C	1.83201500	-0.08812400	0.31186600
O	1.39530600	-0.43951100	1.40710800
C	1.20525200	1.07764400	-0.44858400
C	-0.21988700	1.34742600	0.02230000
C	-1.10093100	0.15626800	-0.27806500
O	-0.79803600	-0.79717700	-0.97350900
O	-2.32751000	0.29718100	0.33327200
C	-3.24923500	-0.71368300	0.11003800
H	1.23349400	0.86287900	-1.52853000
H	1.84309300	1.96370000	-0.27737700
H	-0.65292200	2.22660100	-0.48282300
H	-0.25373500	1.53614400	1.10509400
H	-2.88002400	-1.65308700	-0.29434100
H	-4.13078000	-0.61449100	0.73608200
H	3.71968000	-0.03279400	-0.74377700
H	2.62398100	-1.35309100	-1.20900900
H	3.50180200	-1.44939800	0.35845000

Frequencies

20.9838 49.7717 85.1630
147.7739 149.2608 212.9709
249.3968 269.1904 324.8808
377.9044 460.4137 477.3655
526.5102 552.5258 617.7188
651.0971 775.6685 797.8530

888.8169 943.5813 992.2448
1023.1689 1069.3197 1110.7834
1173.8023 1189.6220 1206.1681
1222.9598 1247.4809 1356.5799
1376.4355 1398.8890 1434.1006
1442.3836 1450.5581 1455.5109
1469.1093 1735.8848 1774.7334
3060.8267 3068.3588 3092.3730
3132.3949 3147.7728 3159.0543
3197.1722 3218.3458 3384.8532

MLR3

O 2

C	2.77663200	-1.04861200	-0.32910400
C	1.90965400	0.02256300	0.28883300
O	1.72289900	0.11980500	1.49856100
C	1.25536600	1.02582800	-0.68368000
C	-0.15063100	1.30661200	-0.26874800
C	-1.05713300	0.14967000	-0.24148600
O	-0.72430900	-0.98361000	-0.57596700
O	-2.29624400	0.48081400	0.19076800
C	-3.21220500	-0.64281000	0.24670100
H	1.27552800	0.60320400	-1.70325500
H	1.86593400	1.94349800	-0.67671700
H	-0.49441300	2.27570900	0.08982000
H	-4.15547500	-0.22193900	0.61084400
H	-2.82658800	-1.40611400	0.93583700
H	-3.33363500	-1.08001500	-0.75357200
H	3.49953100	-0.59827800	-1.02917400
H	2.12088400	-1.71872400	-0.90934900
H	3.29937800	-1.61291700	0.45357200

Frequencies

34.2342 58.4495 68.9996
148.8076 165.8259 174.9249
200.9263 252.3347 326.1439
346.7956 453.0747 466.5539
482.7421 626.1517 681.7433
751.0840 794.0491 849.8953
920.4957 979.4811 1010.1993
1045.1143 1101.0989 1168.4582
1170.6382 1200.1859 1225.9652
1250.9940 1298.0337 1370.6473
1422.7767 1438.0373 1455.1872
1467.9934 1478.5640 1480.7866
1486.5702 1736.7554 1809.2960
3060.7269 3065.7588 3092.9671
3135.1109 3149.5582 3193.7584

3198.2146 3226.9756 3279.0658

MLR4

O 2

C	-3.22310800	-0.52608300	0.41462000
C	-1.89478900	-0.21716900	-0.24459400
O	-1.33966200	-0.97760300	-1.00790000
C	-1.26957400	1.08778400	0.10208200
C	0.11262800	1.33036400	-0.41036000
C	1.07830100	0.33788200	0.22774300
O	0.90096800	-0.20899000	1.30617200
O	2.18112700	0.17171700	-0.53991200
C	3.14410300	-0.75909900	0.01749400
H	-1.76645100	1.78063600	0.78343200
H	0.46475500	2.34675900	-0.17598700
H	0.15320900	1.18557700	-1.50171000
H	3.96275700	-0.79070400	-0.70949100
H	2.68114800	-1.74819900	0.13393800
H	3.49683100	-0.39999100	0.99404800
H	-3.93177000	0.30072300	0.24686600
H	-3.06142400	-0.61140200	1.50206100
H	-3.62388400	-1.46646500	0.01806300

Frequencies

26.9115 33.6325 92.1490
103.8092 133.8445 157.6400
178.9967 230.7277 283.4674
352.9290 457.6637 482.2330
549.5146 593.8032 619.8258
697.9669 869.5095 900.5158
921.6834 967.8108 1014.6726
1031.0138 1133.4678 1165.8880
1169.6288 1171.5952 1198.5664
1220.1428 1332.1612 1375.2843
1403.2564 1447.5539 1453.9794
1466.8447 1469.9603 1481.2087
1488.1168 1759.9692 2090.0686
3056.0720 3067.7022 3091.8170
3091.9242 3155.5468 3192.1450
3210.7933 3226.7734 3252.3740

MLR6

O 2

C	-3.10040900	-0.72776800	0.44339000
C	-1.88197800	-0.24315700	-0.24623500
O	-1.36110500	-0.87316100	-1.13870000

C	-1.33898700	1.10761700	0.21212400
C	0.06463100	1.34019600	-0.33428900
C	1.01597900	0.30587400	0.23207700
O	0.80786400	-0.35409600	1.24186700
O	2.15193800	0.22343900	-0.50257500
C	3.10139800	-0.75168500	-0.00409700
H	-1.35193900	1.14424900	1.31269700
H	-2.04222200	1.87832900	-0.15178800
H	0.43847600	2.33751100	-0.04892700
H	0.08283800	1.27103700	-1.43041200
H	3.94829600	-0.70551100	-0.69733200
H	2.64574100	-1.75112300	-0.00476000
H	3.41325400	-0.49096000	1.01670400
H	-3.55696400	-0.16232800	1.25686700
H	-3.53086700	-1.67712400	0.12439500

Frequencies

23.5850 51.5567 89.1734
 158.1563 178.3223 211.8403
 258.3152 270.4305 318.4491
 369.9958 468.8749 496.7581
 571.8136 619.9943 649.3105
 698.8532 782.7698 853.2750
 928.5441 974.9665 997.9506
 1017.5947 1072.9661 1168.7238
 1174.1655 1198.6376 1199.6507
 1231.6147 1254.0268 1373.2356
 1400.1511 1427.0682 1441.3440
 1458.7312 1465.2328 1480.1863
 1487.6284 1756.5187 2085.4350
 3071.3098 3089.9445 3093.3020
 3137.9556 3169.6306 3190.0819
 3199.8453 3223.4605 3338.2719

OH

O 2

O	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	0.97518200

Frequencies

3767.6941

TS_CH3_MLR1a

O 2

C	0.24529600	-0.22962900	0.19165600
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C	0.08210200	-0.22638000	1.69569300
O	1.03666700	-0.37513000	2.45922400
C	-1.33432400	-0.04385900	2.22989200
C	-1.42875200	-0.43488200	3.70204100
C	-1.05349300	-1.89245900	3.86935500
O	-1.10227600	-2.73445400	2.98335700
O	-0.66904700	-2.16285800	5.14648700
C	-0.23814000	-3.50671500	5.35708500
H	-2.02401200	-0.64422200	1.61511700
H	-1.61307400	1.01577800	2.08604700
H	-2.45645500	-0.30049500	4.07890300
H	-0.75876300	0.17383900	4.32479100
H	-0.00383900	-3.61460600	6.42057700
H	0.88459300	-3.62754400	4.65713100
H	-0.93623300	-4.24873000	4.94989700
H	-0.32938600	0.59070100	-0.26740400
H	-0.16587600	-1.17763100	-0.19501900
H	1.30704300	-0.15400900	-0.07545800
C	1.95664600	-3.54193000	3.85801500
H	1.93465900	-2.50398300	3.50537400
H	2.81434200	-3.78297200	4.49646000
H	1.76270200	-4.28017300	3.07219200

Frequencies

1970.5563i 30.2105 41.5492
 68.4103 86.9649 101.6352
 111.7403 138.0816 196.3415
 208.5038 269.3865 316.8940
 332.4369 368.9344 456.0312
 465.5198 542.4585 556.3194
 612.0840 623.5847 654.1863
 692.3829 778.1709 812.8411
 898.8049 940.9366 991.8391
 1019.5829 1040.7258 1086.3037
 1143.1061 1158.6602 1177.0383
 1199.9521 1207.6200 1230.4509
 1249.3002 1357.9096 1362.8265
 1379.1861 1397.2667 1400.3418
 1431.4888 1443.8396 1446.5220
 1449.5071 1456.0455 1469.1940
 1473.2040 1731.3180 1756.1659
 3060.9024 3067.7685 3088.2937
 3090.4503 3123.4434 3129.5070
 3148.0452 3164.5927 3196.6159
 3245.8554 3248.5161 3249.6774

TS_CH3_MLR1b

0 2

C	0.01645400	-0.16388500	0.07986000
C	-0.02105300	-0.02153300	1.58474100
O	1.00051300	0.00703800	2.27006700
C	-1.40204200	0.09109100	2.22647900
C	-1.37869800	-0.39054900	3.67373900
C	-1.01465900	-1.85964900	3.72337600
O	-0.91898300	-2.59506800	2.75137400
O	-0.81723800	-2.27423000	5.00737000
C	-0.45863100	-3.65210100	5.14361400
H	-2.12962300	-0.48080200	1.62982300
H	-1.70126200	1.15391900	2.17746300
H	-2.35911900	-0.26273200	4.16079600
H	-0.63765700	0.16629400	4.26547700
H	-0.26555500	-3.75021900	6.47028400
H	0.49287400	-3.88571400	4.64987200
H	-1.28101400	-4.32801000	4.87617200
H	-0.65631100	0.56814800	-0.39596900
H	-0.35580100	-1.17047600	-0.17542900
H	1.04252000	-0.04182300	-0.28989400
C	-0.10321300	-3.70449800	7.77501500
H	0.18570600	-4.72059800	8.06764900
H	-1.07750100	-3.39472300	8.17011800
H	0.68663800	-2.96118800	7.93246400

Frequencies

1975.9794i 10.5834 21.5075
47.1835 50.8700 67.0675
85.8478 152.6924 155.9654
198.1487 253.1020 304.6240
312.0995 337.7176 448.4476
472.9254 534.7100 554.4863
581.2629 621.0673 669.1931
675.7868 776.5471 822.7770
908.1651 947.4770 990.8781
1021.4729 1037.4731 1085.1060
1147.2995 1167.6011 1174.1658
1179.7714 1202.1770 1213.7562
1247.8318 1355.7958 1365.2737
1376.5473 1393.5542 1399.6839
1435.2389 1443.7625 1452.4640
1455.6649 1461.8262 1469.0257
1475.8547 1735.9186 1755.8776
3060.2612 3067.1205 3093.3354
3094.1870 3109.2374 3134.3290
3147.3095 3159.3656 3196.5070
3220.8380 3245.6701 3248.1895

TS_CH3_MLR1c

0 2

C	-0.14870300	-0.03353300	0.00273400
C	-0.04668500	0.18330400	1.49565100
O	1.01878500	0.44415900	2.05301400
C	-1.34353800	0.06749700	2.29363900
C	-1.06696300	-0.33111700	3.73995400
C	-0.42763300	-1.70258300	3.78352800
O	-0.29253000	-2.44836300	2.82362800
O	-0.02203000	-2.01731700	5.04588500
C	0.57007000	-3.30783000	5.17308600
H	-2.01119900	-0.65784700	1.80316400
H	-1.84309800	1.05249100	2.25330200
H	-1.99296700	-0.36385100	4.33693700
H	-0.38409600	0.38223700	4.22414900
H	0.92965500	-3.40540700	6.20214900
H	1.31485900	-3.51130400	4.39355800
H	-0.40070100	-4.18657900	4.99050000
H	-0.99843700	0.53143600	-0.41400100
H	-0.34568700	-1.10476200	-0.17217300
H	0.78727000	0.25822200	-0.49047600
C	-1.48752200	-4.94596100	4.76445900
H	-1.52678100	-5.03265300	3.67355100
H	-1.29366000	-5.89073600	5.28464700
H	-2.31387100	-4.36806600	5.19497100

Frequencies

1964.8754i 15.8234 31.4450
43.9420 47.7990 68.3388
104.7281 156.4917 180.3560
212.6735 260.3897 323.3536
330.2814 361.2858 454.0512
475.4491 526.1065 549.8055
584.7196 629.9664 652.0298
693.1687 776.3334 812.8136
897.3160 947.4996 991.2700
1021.8173 1041.9100 1086.3033
1140.7883 1159.0514 1178.8711
1201.1957 1206.9694 1224.9547
1249.6659 1355.6962 1367.7786
1377.1052 1397.3977 1402.9214
1435.1754 1442.4843 1443.5889
1447.9354 1455.6311 1468.9156
1471.6742 1736.0943 1756.3270
3060.1947 3067.6256 3092.5829
3093.1697 3123.9503 3134.2450
3147.1090 3157.7607 3196.4986
3244.8182 3247.7262 3255.8866

TS_CH3_MLR3a

O 2

C	-0.01927000	-0.10712200	0.04764000
C	-0.01249500	-0.04759600	1.56059900
O	1.02301200	-0.13344800	2.21810600
C	-1.37385500	0.11988900	2.23709200
C	-1.32931900	-0.26673400	3.69826900
C	-1.03303500	-1.71175500	3.90586600
O	-1.14711300	-2.57942900	3.04525300
O	-0.67950700	-1.96970600	5.19283400
C	-0.41495300	-3.36966100	5.45532800
H	-2.11329100	-0.49310700	1.69556100
H	-1.67751100	1.17603900	2.11742600
H	-2.54394000	-0.14787100	4.14571900
H	-0.74337700	0.38982600	4.35164500
H	-0.14313500	-3.41473900	6.51567300
H	0.41106900	-3.72170800	4.82244600
H	-1.31217000	-3.97078700	5.25276200
H	-0.66611000	0.68019900	-0.37204100
H	-0.44275100	-1.07956400	-0.25575900
H	1.00326300	-0.01366400	-0.34009200
C	-3.84460100	-0.04816000	4.55444000
H	-3.78801100	-0.27093500	5.62479900
H	-4.35609100	-0.80994600	3.95615300
H	-4.12619400	0.98317300	4.31722900

Frequencies

1744.4873i 27.1821 44.9199
56.8295 64.4758 73.0584
76.4591 140.8550 157.7872
176.9438 211.4984 244.5665
315.3600 348.5973 443.7233
456.9302 471.2777 525.5692
560.9758 627.3528 674.6848
742.3958 807.4955 824.4740
910.6755 950.2937 1003.6125
1012.2290 1046.5335 1113.5613
1148.5525 1167.9588 1173.2666
1199.5580 1205.6766 1247.2256
1302.2896 1355.3608 1356.2476
1379.4123 1409.4116 1430.7760
1439.4040 1440.2053 1455.4569
1461.4741 1468.8964 1479.5063
1487.8263 1733.6618 1744.2983
3058.7503 3062.5150 3088.2705
3097.6418 3121.7643 3147.9614

3182.2037 3187.3527 3195.8495
3221.0810 3258.3927 3262.5188

TS_CH3_MLR4a

O 2

C	-0.03217400	-0.12912400	0.08026700
C	-0.10885300	-0.00128100	1.58600200
O	0.88822100	0.08168400	2.29468100
C	-1.48854700	0.06288600	2.18172900
C	-1.55417800	-0.41331900	3.61561900
C	-1.23610200	-1.89618900	3.68926200
O	-1.07729000	-2.62924300	2.72232000
O	-1.15836200	-2.31827100	4.97630500
C	-0.84543900	-3.72750700	5.11300900
H	-2.28367400	-0.31021500	1.52267800
H	-1.67770800	1.35821600	2.23705200
H	-2.54896400	-0.24742200	4.06039900
H	-0.81632000	0.12163700	4.23328100
H	-0.81487000	-3.90943600	6.19270100
H	0.12683900	-3.94283000	4.64938600
H	-1.62356300	-4.33664300	4.63284800
H	-0.70792600	0.59753700	-0.40012000
H	-0.38154400	-1.13861600	-0.19411600
H	1.00025900	0.01695800	-0.26134200
C	-1.79376700	2.69550300	2.42648500
H	-0.89134700	2.94356500	2.99527900
H	-2.73042700	2.80979800	2.98240100
H	-1.81775100	3.10898800	1.41259500

Frequencies

1686.3398i 27.2760 40.9924
56.2662 67.3715 69.2987
84.1000 144.3300 154.0217
176.4561 205.2157 253.8936
295.3882 357.5506 450.1860
459.6116 511.2815 539.3996
558.1004 627.0057 640.0868
708.7073 799.5811 874.4259
930.3796 951.3479 1003.6134
1017.7834 1050.7943 1102.3437
1153.8120 1168.3327 1175.1298
1197.7167 1219.2392 1238.2782
1302.6143 1354.3706 1361.1309
1367.8096 1417.1875 1432.0829
1440.1799 1442.2407 1453.6047
1456.3832 1468.1716 1480.3099
1487.6762 1751.6376 1985.0386
3059.7022 3086.7018 3090.4137

3097.0464 3145.6121 3146.8313
3160.1797 3190.3178 3198.5113
3223.7108 3257.2480 3259.9547

TS_CH3_MLR4b

0 2

C	0.33223600	0.23726200	0.15441400
C	0.02368400	-0.36991900	1.50932500
O	0.81066400	-1.09776400	2.09888200
C	-1.32911100	-0.05930200	2.08379000
C	-1.53795200	-0.57060400	3.49557800
C	-1.29864500	-2.06772200	3.57564200
O	-1.67852500	-2.87849700	2.74221700
O	-0.66054400	-2.40456500	4.72267700
C	-0.38512800	-3.82202200	4.83698000
H	-2.14445200	-0.71260000	1.27676300
H	-1.65098200	0.97829600	1.91153800
H	-2.57528800	-0.38091200	3.82014000
H	-0.86238900	-0.06464100	4.20362400
H	0.13192500	-3.93623800	5.79604500
H	0.25509000	-4.14248900	4.00370700
H	-1.32216500	-4.39573100	4.82374200
H	0.40549000	1.33268700	0.25734200
H	-0.49020600	0.02639300	-0.54836900
H	1.27850800	-0.16475700	-0.22846200
C	-3.01135400	-1.32881800	0.44944900
H	-3.26584000	-0.57877800	-0.30804500
H	-2.43152100	-2.18287600	0.08622300
H	-3.83556700	-1.60810300	1.11274200

Frequencies

1720.6025i 35.1693 54.4036
79.5473 95.1817 103.6316
112.4959 123.8038 165.0517
181.0563 204.2382 260.7386
303.7382 376.2484 430.9235
447.1651 492.2123 554.2517
592.8401 621.4353 642.1218
743.8411 805.7618 855.4884
910.3977 960.2965 997.7614
1011.4711 1040.3802 1092.7076
1158.1966 1168.3135 1178.5599
1194.2664 1203.6219 1244.0743
1303.5303 1340.2288 1364.2700
1372.0177 1407.0630 1434.1498
1435.4749 1442.3463 1453.7835
1457.1505 1468.3940 1479.7466

1487.1427 1761.2459 2055.4059
3062.6743 3074.0630 3088.2248
3097.4473 3135.2351 3141.7802
3149.8337 3188.2934 3200.9646
3221.4774 3255.7826 3266.3573

TS_CH3_MLR6a

O 2

C	-2.87979000	-0.26561100	0.29600800
C	-1.48334800	-0.76534400	0.44779200
O	-0.86347400	-0.67906700	1.50103200
C	-0.82827300	-1.32551100	-0.81200900
C	0.67695600	-1.48799200	-0.62722400
C	1.32499600	-0.14065800	-0.38682000
O	0.86123200	0.93373900	-0.75045800
O	2.51265600	-0.26663100	0.25158700
C	3.17908200	0.99505900	0.50424500
H	-1.05740200	-0.65185500	-1.65423400
H	-1.30763800	-2.29543000	-1.03530200
H	1.13707000	-1.92479500	-1.52960800
H	0.90674200	-2.14436100	0.22308600
H	4.10723700	0.72895400	1.02156500
H	2.54527500	1.63173500	1.13627300
H	3.38976800	1.51032600	-0.44302100
H	-3.45037200	-0.66005000	-0.55362300
H	-2.62720700	0.99124400	-0.03316000
H	-3.43364700	-0.18329900	1.23740600
C	-2.27102100	2.25776100	-0.30801100
H	-1.21717700	2.15217000	-0.58843800
H	-2.94326800	2.55418200	-1.12036300
H	-2.44429500	2.78063400	0.63824100

Frequencies

1694.7209i 28.4572 35.8373
69.1430 83.6412 88.7527
118.6320 160.1236 178.6294
213.1140 270.4521 315.6741
353.2506 370.6897 463.3598
464.5793 517.7381 575.5544
596.0389 627.0812 685.2059
730.1462 787.4197 846.5858
927.4496 954.4825 1000.4057
1009.9047 1026.8507 1078.0524
1161.5570 1168.4145 1173.2615
1199.9258 1204.5433 1234.6642
1249.4927 1329.6544 1332.7089
1371.6987 1395.4962 1427.1384
1432.6693 1441.5212 1443.4095

1450.6464 1459.6130 1480.4992
1486.9142 1752.3920 1999.7608
3067.1690 3088.4180 3089.6155
3092.9721 3124.8024 3135.5688
3167.3664 3188.9127 3223.1829
3245.7701 3258.6066 3262.3570

TS_CH3_MLR6b

O 2

C	-0.16420500	-0.09324600	-0.07099200
C	-0.21487400	-0.13466300	1.42276400
O	0.79818500	-0.16285900	2.10883600
C	-1.59946200	-0.03906100	2.05373900
C	-1.51849200	-0.06964900	3.57621400
C	-0.96750600	-1.40185700	4.04204000
O	-1.07155200	-2.45345600	3.42514500
O	-0.37749800	-1.29630500	5.25863200
C	0.16575500	-2.54503300	5.75299400
H	-2.20807500	-0.87616400	1.67376000
H	-2.07121100	0.89286600	1.69281300
H	-2.52094600	0.05065700	4.02055800
H	-0.87591900	0.73407300	3.96095000
H	0.60659200	-2.29978200	6.72548300
H	0.92920500	-2.92087900	5.05828100
H	-0.63274000	-3.29227800	5.85977900
H	0.75884900	-0.50384700	-0.49461500
H	-0.03582400	1.20292800	-0.26066900
H	-1.08493500	-0.36812800	-0.59968500
C	0.18368500	2.52851200	-0.37462600
H	0.46354500	2.66391100	-1.42425900
H	0.99437900	2.70524400	0.34003800
H	-0.77274100	2.98726800	-0.10071800

Frequencies

1722.8353i 19.8149 32.2385
44.0997 52.5312 80.2880
99.2318 159.5961 179.5984
213.8624 269.2342 308.0856
333.1958 372.5696 449.8563
462.6199 511.4967 579.8280
585.6495 625.2669 684.0190
725.0577 788.1560 844.1016
924.0400 956.2938 997.4667
1016.0419 1024.6670 1079.2067
1154.3274 1168.6799 1176.0023
1197.6951 1199.8177 1232.9598

1251.6958 1335.2760 1341.9877
1371.5850 1393.8906 1423.6507
1438.2059 1438.7154 1443.9259
1449.4918 1458.6373 1479.8209
1487.6450 1759.8764 2031.9199
3063.8982 3087.7516 3089.2606
3098.5484 3124.8644 3135.9401
3166.0228 3188.7671 3221.8598
3245.5640 3257.9740 3264.3325

TS_MLR1_isomerization_MLR3_and_reverse

O 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.50959300
O	1.02722100	0.00000000	2.18390500
C	-1.37125200	-0.01499300	2.21405500
C	-1.48274200	-1.26790500	3.06280500
C	-1.79333500	-2.52927600	2.29465100
O	-1.32702600	-2.87863600	1.22991600
O	-2.75568400	-3.27740000	2.95294200
C	-3.28412200	-2.55300200	4.06057500
H	-2.19225000	0.03612000	1.48243900
H	-1.41015100	0.87848500	2.85938600
H	-2.53683000	-1.43455300	3.85716700
H	-0.63592100	-1.40091100	3.75299000
H	-3.01097300	-3.00035600	5.02311600
H	-4.34731800	-2.32312300	3.92381300
H	-0.58129100	0.86008600	-0.37232200
H	-0.50264200	-0.91921100	-0.34304800
H	1.02863000	0.04082800	-0.38015100

Frequencies

1961.3797i 39.8648 50.7855
90.3963 154.6889 175.7435
222.3149 232.4610 352.3369
427.9947 489.3083 518.7763
553.9145 655.8194 676.0112
699.6649 777.7330 811.5178
900.2515 959.1847 985.5759
1030.6119 1042.7435 1081.0428
1115.0678 1159.9739 1161.7041
1205.2711 1218.7649 1279.7538
1351.0242 1374.5808 1408.2629
1451.3227 1459.7106 1467.8035
1480.5861 1739.9699 1754.0017
1829.5923 3059.8046 3075.8650
3125.4467 3137.0714 3148.7247

3149.4609 3198.1582 3243.1993

TS_MLR1_isomerization_MLR4_and_reverse

O 2

C	-0.00000100	0.00000700	0.00000000
C	0.00000100	-0.00001200	1.51526400
O	1.02951800	-0.00003300	2.17465600
C	-1.34743500	0.06604000	2.17623100
C	-1.41630700	-0.42653400	3.60843100
C	-2.45079500	0.32181100	4.43706000
O	-3.21496800	-0.18659000	5.22980200
O	-2.51702700	1.69448700	4.23154700
C	-1.53673900	2.27874300	3.40798300
H	-2.21212900	-0.15424100	1.53599600
H	-0.42068000	-0.27419500	4.06261300
H	-1.66917600	-1.49394600	3.68359200
H	-1.92096300	3.20656900	2.97321400
H	-1.39208500	1.35569800	2.42849800
H	-0.53725400	2.33779500	3.86094800
H	-0.65456800	0.80110500	-0.38032700
H	-0.41603000	-0.95791100	-0.35454800
H	1.02315900	0.12484300	-0.37525500

Frequencies

1624.4665i 60.6029 76.2192
107.8604 122.2382 172.1043
236.5908 306.9811 384.0195
462.0175 503.0354 546.8655
594.9482 605.2760 635.1215
691.2033 787.6363 831.1073
893.1018 947.4679 996.7512
1041.6454 1084.9368 1111.6380
1127.9622 1155.8528 1176.7076
1211.9256 1249.7563 1269.1836
1360.9305 1381.0698 1414.0394
1447.3699 1451.4525 1467.3789
1476.8307 1561.5393 1789.3879
2067.2514 3062.6632 3069.4690
3112.5453 3148.4982 3153.8511
3166.7131 3203.5095 3246.4401

TS_MLR1_to_ch2o

O 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51311900
O	1.03741700	0.00000000	2.17651200
C	-1.35832400	-0.02480500	2.21276300
C	-1.58549000	-1.41747600	2.83381600
C	-1.62679200	-2.45321100	1.73106200
O	-2.43554200	-2.55908600	0.82045600
O	-1.34075000	-3.90983300	2.53329100
C	-1.90685400	-4.87189600	1.99513900
H	-2.17381000	0.20754900	1.51029300
H	-1.34384000	0.72834200	3.01616600
H	-2.55034100	-1.43425300	3.37849400
H	-0.77322900	-1.65626900	3.53447500
H	-2.66891600	-4.68420700	1.21915800
H	-1.61092900	-5.88992100	2.28029100
H	1.02632400	-0.07731300	-0.38121900
H	-0.46750800	0.93245300	-0.36011800
H	-0.61916200	-0.83531300	-0.36592800

Frequencies

1512.0536i 46.7571 50.7847
 79.0704 154.6269 172.5304
 172.9880 272.1590 311.4886
 339.7283 375.8998 469.5388
 510.7862 534.6573 597.8243
 643.3135 781.3314 824.2729
 935.9105 963.8569 1012.6997
 1034.2965 1072.3608 1149.3852
 1166.6621 1176.2591 1229.8568
 1239.7003 1309.6386 1342.3358
 1378.8097 1434.1095 1451.3281
 1454.3977 1465.6503 1469.4586
 1697.8221 1730.8893 1813.0054
 3021.8613 3056.7687 3085.5443
 3087.8489 3142.6109 3149.2178
 3160.9700 3195.7576 3229.0600

TS_MLR3_isomerization_MLR6_and_reverse

O 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51711000
O	0.99675600	0.00000000	2.21725400
C	-1.45419900	-0.08383600	2.01579100
C	-2.21050200	-0.75727600	0.88244100
C	-3.31221200	0.01718900	0.24904500
O	-3.41338200	1.23914800	0.27652900

O	-4.16761000	-0.79642400	-0.42495000
C	-5.21967700	-0.08505600	-1.12557900
H	-1.82453200	0.94707200	2.15253600
H	-1.49478600	-0.61426800	2.97730000
H	-2.39015800	-1.83558800	0.96066800
H	-5.81385800	-0.86498400	-1.61391100
H	-4.78423000	0.60073000	-1.86511800
H	-5.82906500	0.48622900	-0.41217400
H	-0.27995100	0.96217200	-0.45169300
H	-1.23400200	-0.64172300	-0.00443700
H	0.81659200	-0.52880100	-0.50285700

Frequencies

1828.6189i 48.5549 56.6187
 86.2554 160.7846 185.9510
 216.3460 309.6799 365.5030
 405.1558 463.4526 494.1237
 587.9552 634.7266 698.0067
 737.8416 795.5336 813.2473
 891.2447 916.4322 962.0862
 1010.8309 1045.2869 1092.0755
 1167.1990 1167.6986 1192.3164
 1200.1555 1217.6836 1242.3827
 1351.6575 1398.7184 1415.6578
 1436.1457 1462.2832 1479.4840
 1487.1669 1647.6863 1749.8111
 1953.8539 3079.1719 3090.8539
 3128.2824 3165.0779 3190.9504
 3192.2320 3224.6870 3245.1625

TS_MLR3_to_2methylpropenoate

0 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51296000
O	0.91341200	0.00000000	2.28310200
C	-1.96016200	-0.75401000	2.26702600
C	-1.86666100	-2.07762700	2.02282500
C	-2.33451100	-2.61531900	0.73039200
O	-2.70455200	-1.95441100	-0.23950600
O	-2.30503500	-3.97532100	0.72965000
C	-2.76742000	-4.57047700	-0.50651900
H	-2.50942400	-0.11558700	1.56997300
H	-1.72319100	-0.34671500	3.25122500
H	-1.43100800	-2.77415700	2.74042900
H	-2.69097300	-5.65188900	-0.34836800
H	-2.13224600	-4.24927100	-1.34347100

H	-3.80642900	-4.27373000	-0.70455100
H	-0.29635800	1.01150900	-0.32042900
H	-0.76152700	-0.70352800	-0.36311700
H	1.00387000	-0.23770900	-0.38523600

Frequencies

503.2234i 41.5702 49.4467
105.2807 122.0521 149.5123
168.4716 183.3626 216.4305
268.6986 351.2849 411.6633
456.1191 495.1904 653.8380
686.9802 849.8611 867.8631
879.9976 963.2290 1020.4953
1039.3974 1050.9756 1076.4536
1102.2062 1167.7373 1198.2001
1231.4184 1318.9510 1347.6228
1426.4568 1447.0195 1454.4975
1461.3818 1478.6527 1486.6413
1648.1449 1741.3268 1918.6953
3057.6903 3089.4274 3164.0040
3187.9435 3190.1846 3190.9450
3221.5024 3258.2072 3305.1457

TS_MLR3_to_acetylradical

O 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51081500
O	1.03034200	0.00000000	2.18077900
C	-1.37435500	-0.03505400	2.19465100
C	-1.34966600	0.83136500	3.42436800
C	-2.06636500	1.97319000	3.56801300
O	-2.72701900	2.86547100	3.93278000
O	-0.94517500	2.52262600	1.98763200
C	0.13721700	3.29140000	2.45750700
H	-1.59079100	-1.08510400	2.46690200
H	-2.15426600	0.29966700	1.49657500
H	-0.65634800	0.61706300	4.24165700
H	0.37509600	4.02414800	1.66285100
H	1.03512000	2.67410300	2.63982800
H	-0.11560800	3.86739900	3.36901600
H	-0.62648700	-0.82589400	-0.37675600
H	1.02439800	-0.09463500	-0.38264000
H	-0.45284300	0.94517900	-0.34028600

Frequencies

716.8579i 56.2800 66.0820

81.9112 119.1268 169.8794
182.7647 204.6724 224.4398
242.0740 297.0294 354.2665
467.6740 489.6822 518.2365
619.6138 642.1103 800.2966
868.9332 953.2047 1007.1772
1037.5844 1071.8122 1124.7516
1155.0998 1170.5284 1194.0566
1227.5774 1317.8618 1370.9060
1404.6368 1437.1978 1454.2643
1455.7660 1460.4030 1468.7870
1492.8782 1739.7768 2085.1647
2995.4619 3054.0942 3060.5811
3077.5600 3098.5954 3149.6401
3153.2367 3195.2906 3234.4811

TS_MLR4_to_methylradical

O 2

C	-3.00362600	1.34569000	-0.21164300
H	-3.06126900	1.31470600	-1.30137600
H	-2.41198800	2.15499900	0.21698300
H	-3.90860100	1.05528500	0.33109800
C	-2.16905700	-0.47095800	-0.00752100
C	-1.16180300	-0.10542400	0.80511800
H	-1.25674000	0.72768400	1.49195700
C	0.15602100	-0.82967500	0.66451100
H	0.07684300	-1.68034800	-0.03060400
H	0.48153600	-1.24952400	1.63430400
C	1.27673300	0.08041000	0.18166600
C	3.53087800	0.14916300	-0.49908000
H	3.79587000	0.88002400	0.27729400
H	4.34309300	-0.56903800	-0.65555800
H	3.28897500	0.67849700	-1.43090000
O	2.39902200	-0.64747000	-0.06932500
O	1.21396200	1.29348900	0.05230600
O	-2.75330800	-1.18695900	-0.74941700

Frequencies

1029.4283i 16.7821 38.9363
66.5475 78.9943 154.8447
177.2686 209.2872 231.6257
306.7095 327.1171 411.9744
512.4330 563.5903 594.6407
638.0633 685.6298 717.7134
747.3213 889.6275 925.6563
1006.5708 1028.0817 1084.0527

1168.7175 1179.1758 1191.6671
1202.6994 1227.1247 1333.9689
1413.9178 1427.4523 1436.2569
1454.1631 1471.7906 1480.3003
1488.0873 1760.4372 2216.5372
3052.8038 3089.8723 3118.4990
3134.2655 3189.1234 3222.8528
3297.6846 3316.7383 3325.2493

TS_MLR4_to_MVK

O 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51391400
O	1.02410300	0.00000000	2.17063700
C	-1.35806300	0.02590600	2.16640500
C	-1.45055100	-0.24799900	3.48163600
C	-0.61433000	1.66664100	4.29784200
O	-0.74515200	2.72963900	3.74953100
O	0.33831200	1.23664700	5.12498800
C	1.47580100	2.15748100	5.24356900
H	-2.21760200	0.36412700	1.58225800
H	-0.59490400	-0.68830900	3.99865500
H	-2.41361600	-0.24385500	3.99665400
H	2.16047400	1.66836700	5.94383000
H	1.13029100	3.12493000	5.63101000
H	1.93553200	2.27444400	4.25344700
H	1.02603200	-0.08017700	-0.37882800
H	-0.46311200	0.93789500	-0.35101500
H	-0.62215300	-0.83044600	-0.37186000

Frequencies

516.6527i 28.3764 40.3242
45.6195 116.0961 128.1745
143.8994 161.8695 224.1903
283.7341 295.4255 404.9177
458.8402 547.1973 602.6433
721.8979 748.3402 797.3176
908.3486 958.4166 1008.0625
1037.3142 1067.8559 1097.2755
1099.3521 1151.3593 1186.9688
1212.0321 1307.9156 1366.2775
1432.2471 1437.0141 1450.0994
1465.2925 1478.0130 1482.6858
1617.8359 1800.3396 2178.5087
3062.1209 3095.4002 3148.8276
3191.3714 3205.3224 3207.8122
3235.8254 3235.9780 3305.3603

TS_MLR6_to_ketene

0 2

C	1.35831000	1.45954300	0.84165500
C	1.99041400	0.61098400	-0.01301300
O	2.70688000	0.39120700	-0.94885100
C	1.37792200	-1.14555300	0.40825600
C	0.15289000	-1.31300800	-0.44977800
C	-1.02277800	-0.53535700	0.11024400
O	-1.32129800	-0.50502300	1.29592000
O	-1.71220200	0.09017200	-0.86835800
C	-2.84712600	0.85675700	-0.38604800
H	1.21991000	-1.02038600	1.48491200
H	2.24838600	-1.74371700	0.12828000
H	-0.13158800	-2.38373700	-0.44223600
H	0.35656900	-1.03142200	-1.49228700
H	-3.29312800	1.29852000	-1.28333100
H	-2.50001400	1.63465800	0.30739600
H	-3.55888400	0.19548900	0.12627500
H	0.74406400	1.11905900	1.66628500
H	1.46984700	2.52048600	0.60713200

Frequencies

469.7929i 25.4202 56.4129
105.7072 158.9412 175.3359
177.7091 255.5666 289.4486
353.1639 424.7895 432.3608
501.6152 556.9990 593.7016
649.8065 682.0901 763.5692
857.8331 865.8125 952.9924
992.2594 1034.2060 1071.1866
1114.8084 1167.5361 1189.9820
1203.3741 1211.2504 1249.5934
1385.7489 1432.0131 1439.8142
1457.6348 1459.9006 1480.3457
1485.4356 1763.3717 2006.4932
3041.5308 3092.1525 3155.4406
3162.3359 3193.7879 3203.9627
3228.9514 3279.2293 3360.4305

TS_OH_MLR1a

0 2

C	-3.12602000	1.03092600	-0.55676900
C	-2.09979400	0.28212000	0.26426300
O	-1.55152900	0.77856700	1.24712500
C	-1.77066500	-1.13895500	-0.18595600
C	-0.41714500	-1.59402800	0.34943500
C	0.68672100	-0.72869500	-0.21469900

O	0.54381900	0.12496200	-1.08127000
O	1.88853000	-1.02379500	0.35087900
C	2.98542500	-0.26707800	-0.15865900
H	-1.80071800	-1.18712800	-1.28603700
H	-2.57439700	-1.79821800	0.18892700
H	-0.20433900	-2.64100800	0.07883200
H	-0.37753200	-1.51970700	1.44618300
H	3.88261400	-0.60065000	0.37253900
H	2.83318300	0.89565400	0.11215700
H	3.05931600	-0.32857900	-1.25181600
H	-4.00135000	0.39331900	-0.76151900
H	-2.66924900	1.28599500	-1.52802200
H	-3.43099400	1.94907800	-0.03879100
O	2.38916900	2.12735400	0.22956400
H	1.57242700	1.98878700	-0.28852300

Frequencies

2014.6255i 19.8481 39.9698
 41.1363 98.0716 120.6332
 148.0790 190.0709 208.4356
 260.4547 314.9648 321.2339
 357.4898 377.8236 459.8627
 476.3800 554.1190 619.6414
 652.6865 749.6805 777.7337
 819.8303 892.8669 911.6329
 944.0447 991.0377 1022.4496
 1049.5402 1089.8133 1120.8142
 1178.6746 1202.2385 1207.4334
 1228.3017 1254.1055 1329.3353
 1358.1301 1381.6147 1399.9434
 1434.2320 1442.4739 1455.3257
 1455.7140 1466.8612 1469.1642
 1736.7476 1754.9558 3060.5691
 3068.3648 3094.0046 3130.6052
 3131.5881 3147.0860 3157.7257
 3197.2879 3244.3611 3723.0167

TS_OH_MLR1b

0 2

C	0.00037900	-0.00076700	-0.00024100
C	0.00048300	-0.00051800	1.51275300
O	1.04048100	-0.00096600	2.17077600
C	-1.36324900	-0.00901700	2.19617700
C	-1.24384900	-0.37827200	3.67123400
C	-0.69172200	-1.77978400	3.81394200
O	-0.67118900	-2.62854600	2.93616200
O	-0.23213300	-2.00566800	5.08104700
C	0.29130600	-3.32444900	5.27730700

H	-2.02500300	-0.71020700	1.66279700
H	-1.80181000	0.99860900	2.08110600
H	-2.22768300	-0.35176500	4.16861200
H	-0.57837900	0.31418500	4.20556000
H	0.62740300	-3.33864100	6.43057000
H	1.18787200	-3.50329200	4.67036100
H	-0.47763300	-4.09816600	5.15573200
H	-0.72781000	0.72739800	-0.39220900
H	-0.31447900	-1.00063200	-0.34413800
H	1.00668600	0.21776300	-0.37957700
O	0.88253500	-3.00294500	7.67012500
H	0.66343800	-2.05707500	7.57981800

Frequencies

1976.0334i 13.7426 33.3988
 53.1217 75.0151 87.7390
 135.4987 141.4895 171.8946
 193.5870 254.8246 304.8874
 329.5405 347.7784 455.6093
 466.6404 561.4358 613.6001
 635.5503 723.7920 777.5251
 837.8212 880.4001 921.7722
 940.0781 991.7895 1021.9771
 1039.4876 1087.7395 1137.1546
 1172.9252 1198.3000 1215.7311
 1227.6035 1249.3280 1262.0858
 1358.3236 1380.2786 1400.2406
 1432.3002 1443.2499 1455.7077
 1469.1518 1471.4785 1498.3394
 1733.8007 1765.0848 3061.4676
 3068.9788 3091.8138 3119.2497
 3130.1503 3148.6847 3163.2898
 3197.4901 3221.3993 3757.4192

TS_OH_MLR1c

0 2

C	0.28309400	-0.09418700	0.18194500
C	0.05663600	-0.44924900	1.63395500
O	0.92075000	-1.01104100	2.31021300
C	-1.30313500	-0.10913400	2.22828800
C	-1.41083000	-0.55625800	3.68668400
C	-1.14666400	-2.04456200	3.77448200
O	-1.48947800	-2.86203900	2.93467100
O	-0.47341200	-2.36539800	4.91667800
C	-0.03449800	-3.72143200	4.98111100
H	-2.07168000	-0.60342700	1.60990700
H	-1.46689900	0.97831800	2.13227900

H	-2.42599200	-0.36170200	4.06997100
H	-0.69239100	-0.02528400	4.32583200
H	0.32550500	-3.89892600	5.99922900
H	0.91323400	-3.84518600	4.24883300
H	-0.79574500	-4.43095900	4.63432200
H	0.02257300	0.95993200	-0.00404600
H	-0.38412300	-0.71318000	-0.44107600
H	1.32744300	-0.28535200	-0.09454900
O	1.93948100	-3.66261600	3.43414200
H	1.66445300	-2.79511600	3.07374100

Frequencies

2023.6242i 29.1408 50.7390
 66.6251 98.1969 112.9789
 126.5695 198.0664 200.3387
 270.2742 312.0829 325.8635
 380.5589 385.6127 455.1469
 457.8805 591.6873 602.8313
 668.0823 746.2777 780.7288
 814.7281 897.2601 904.6274
 932.9191 993.6796 1018.9046
 1048.6412 1090.4375 1161.0499
 1176.4282 1199.6999 1215.9136
 1234.7437 1248.8201 1302.7575
 1362.4441 1380.3281 1397.2279
 1426.5862 1450.1667 1454.2406
 1456.5135 1468.4798 1476.4141
 1731.2588 1769.1715 3063.8891
 3071.9778 3093.4203 3124.8614
 3135.4541 3150.9716 3169.1253
 3200.0836 3248.6489 3692.6138

TS_OH_MLR3a

O 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51173000
O	1.03473800	0.00000000	2.17589800
C	-1.37147800	0.00627800	2.19219500
C	-1.28588700	-0.62880500	3.56688700
C	-0.96138200	-2.09750600	3.48815300
O	-0.79640200	-2.72263600	2.45077600
O	-0.89603200	-2.65390200	4.72795300
C	-0.58249400	-4.07157700	4.71752300
H	-2.10171900	-0.52274700	1.56100700
H	-1.69911600	1.05792700	2.27139300
H	-2.35946200	-0.56111700	4.09144300
H	-0.60394800	-0.11218500	4.25522400
H	-0.55561100	-4.36556200	5.77226600

H	0.39200500	-4.23516800	4.23835300
H	-1.35857500	-4.62569600	4.17225400
H	-0.70276000	0.75590900	-0.38657300
H	-0.35475800	-0.98735400	-0.34060200
H	1.01281800	0.18407300	-0.38040000
O	-3.44599700	-0.80864200	4.83164700
H	-3.02741700	-1.47984500	5.40375200

Frequencies

1710.1940i 27.0946 49.6886
 65.1805 78.8812 87.8141
 152.2751 157.5776 176.1345
 214.9993 239.5439 276.3000
 323.6196 345.7114 446.0914
 465.6371 552.6504 598.7850
 621.8454 659.2376 808.5843
 820.0769 878.6894 924.0400
 946.2244 984.6033 1011.9000
 1046.0001 1117.3767 1169.2049
 1174.0764 1198.6280 1203.9201
 1235.3286 1251.3642 1311.1692
 1366.0062 1392.9005 1429.6967
 1443.0367 1455.2182 1461.8167
 1468.4585 1480.6368 1488.8882
 1735.2532 1762.6132 3061.1777
 3075.2705 3092.2397 3142.3530
 3148.9100 3163.9570 3193.6072
 3197.6325 3225.7591 3740.1945

TS_OH_MLR3b

0 2

C	-0.03667300	-0.27541900	0.08736400
C	0.03424300	0.00113000	1.56807500
O	1.10775600	0.18526300	2.14542400
C	-1.29638100	0.09293500	2.31933000
C	-1.28089700	-0.65415500	3.64460100
C	-0.91892200	-2.10379200	3.47431800
O	-0.53408600	-2.59333800	2.41728500
O	-1.06301300	-2.79609100	4.62454400
C	-0.66573000	-4.18850700	4.52861800
H	-2.10555600	-0.29694900	1.68014900
H	-1.49729400	1.16361400	2.49993300
H	-2.19456100	-0.52869400	4.24311300
H	-0.44298000	-0.18786300	4.38481900
H	-0.82774700	-4.59886800	5.53078800
H	0.39204000	-4.25614500	4.24080500

H	-1.28487800	-4.70736900	3.78415500
H	-0.72574500	0.43810400	-0.39434100
H	-0.45081900	-1.28713000	-0.05086100
H	0.96160400	-0.20639100	-0.36245800
O	0.58815600	0.40390000	4.90958300
H	1.06966900	0.47046100	4.05467900

Frequencies

1960.7869i 44.7015 66.1872
 74.1825 93.0682 149.9170
 164.6186 170.7228 181.7025
 210.9709 245.5522 330.0610
 356.5164 452.4390 495.5380
 556.3104 570.8067 616.5031
 677.4070 725.8195 791.2607
 821.3886 910.5511 925.2333
 979.9522 995.9964 1017.5124
 1040.0128 1086.6769 1122.7613
 1168.0901 1197.0650 1204.5445
 1220.5889 1233.3908 1347.3662
 1373.2271 1386.7970 1420.1915
 1442.5514 1455.2251 1461.1372
 1468.7746 1481.0073 1486.6658
 1735.6509 1743.0212 3062.5915
 3068.5541 3091.8235 3128.9240
 3148.6506 3151.3471 3192.6968
 3200.0442 3228.3528 3592.9483

TS_OH_MLR4a

0 2

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.50780700
O	1.03203100	0.00000000	2.18061400
C	-1.34815700	0.04123400	2.20906100
C	-1.43531300	-0.93268100	3.37444100
C	-1.34242000	-2.35611200	2.86240200
O	-1.13992000	-2.66191800	1.69315100
O	-1.50302600	-3.25536400	3.86096400
C	-1.39301700	-4.63791100	3.43295200
H	-2.20144200	-0.01572100	1.51814300
H	-1.39345300	1.14576700	2.67195000
H	-2.36832900	-0.80993800	3.94509500
H	-0.59838200	-0.76602300	4.07072600
H	-1.54250900	-5.22949900	4.34228200
H	-0.39886900	-4.81964300	3.00271900
H	-2.16467900	-4.86327900	2.68442500
H	-0.58001600	0.86369100	-0.36590600

H	-0.50519600	-0.91567800	-0.34638500
H	1.02797100	0.04240400	-0.38134300
O	-0.98921400	2.24361000	3.32906500
H	-0.05310300	1.97587800	3.41386300

Frequencies

1684.6336i 37.1906 50.5138
62.3725 76.4837 100.9662
153.8582 164.1552 173.7526
195.4781 244.8026 301.0152
314.9807 348.2584 457.0745
487.3222 554.7975 613.5886
663.8573 737.8356 782.5062
871.9418 923.1057 961.5285
976.2295 980.5195 1017.3954
1031.5085 1100.2801 1139.0523
1168.3730 1183.7298 1198.0933
1218.1043 1241.8835 1350.1500
1368.4911 1397.1015 1436.9125
1455.1598 1458.3269 1467.3139
1481.0658 1487.2389 1490.6990
1747.1207 1759.2857 3062.7675
3092.0187 3096.8312 3143.1321
3152.5879 3159.3328 3193.0213
3199.8123 3227.2477 3722.5154

TS_OH_MLR4b

O 2

C	0.13559000	0.43993300	0.11449500
C	0.03497800	-0.27371400	1.44344200
O	0.93734800	-0.96216900	1.90578800
C	-1.26720500	-0.08887700	2.21101700
C	-1.39054200	-1.00416900	3.41452200
C	-1.49643600	-2.44430700	2.94898000
O	-1.79160100	-2.78946800	1.81258600
O	-1.24871400	-3.30826700	3.96220200
C	-1.34028600	-4.70397800	3.57786700
H	-2.13611000	-0.12525500	1.53738600
H	-1.19747100	1.03489700	2.59213700
H	-2.29049600	-0.76702300	4.00499000
H	-0.51726300	-0.90861500	4.07457000
H	-1.11360300	-5.26572500	4.49034200
H	-0.60904600	-4.92283100	2.78805800
H	-2.35215000	-4.93158500	3.21554200
H	-0.14921100	1.49744600	0.23364900
H	-0.57667800	-0.02363500	-0.58850700
H	1.15552500	0.35631300	-0.28105300
O	-1.28092300	2.34958900	2.93725800

H -2.23299400 2.47158800 2.76544300

Frequencies

1382.5972i 26.6206 44.4335
60.6122 67.7941 91.4110
123.1536 138.4948 156.1067
177.0560 229.2428 261.4965
306.9723 363.9688 456.3146
481.4660 552.6240 594.8912
628.8115 684.0152 785.8174
867.1842 891.8740 941.1829
956.8612 998.8595 1015.0302
1028.1241 1097.7358 1157.6052
1168.2149 1171.9969 1200.0680
1233.6117 1239.1511 1344.8361
1371.3211 1376.1465 1404.6096
1439.5120 1456.0482 1457.5490
1469.3957 1480.3174 1487.3362
1754.5865 1903.0892 3063.1628
3090.9049 3095.6363 3137.7403
3152.4976 3168.5752 3191.5480
3200.9475 3225.4494 3757.9469

TS_OH_MLR6a

O 2

C	-0.00005700	-0.00001000	-0.00004200
C	-0.00009800	-0.00015700	1.50953600
O	1.04991300	-0.00034800	2.14582400
C	-1.35785800	0.07128800	2.18909200
C	-1.22726300	0.03276700	3.70754200
C	-0.65116000	-1.29565200	4.15394500
O	-0.69583100	-2.33107800	3.50337800
O	-0.10590000	-1.20635000	5.39247700
C	0.45087800	-2.45350400	5.87722700
H	-1.96844900	-0.77201500	1.82627400
H	-1.84962700	0.99960100	1.84837700
H	-2.21496400	0.14618600	4.18487300
H	-0.58107700	0.84099500	4.07760300
H	0.84859700	-2.22139300	6.87117100
H	1.24883600	-2.79392600	5.20338500
H	-0.33216600	-3.22200600	5.93591500
H	-0.86353800	-0.49936100	-0.46057800
H	0.96374700	-0.30704400	-0.42214200
H	-0.16019500	1.15291000	-0.28691100
O	-0.15383600	2.49344000	-0.27697400
H	0.74774200	2.61586300	0.07613300

Frequencies

1646.9366i 14.5338 30.0374
43.2253 73.6471 92.1591
158.9889 178.5689 182.9935
214.6541 265.3338 307.5876
344.1511 372.6436 451.4544
468.3591 576.5053 611.4473
651.5905 731.2046 782.4466
848.3923 896.8640 929.1399
968.6421 988.8196 1009.1827
1053.9895 1099.1289 1168.6935
1175.8813 1197.9378 1200.0551
1230.0012 1254.0239 1262.8436
1373.2125 1394.5256 1409.5149
1428.6659 1444.0005 1447.9257
1458.6393 1480.0982 1487.6684
1759.5919 1869.5976 3070.6873
3089.4305 3090.7157 3124.8388
3129.4925 3163.1515 3189.5823
3223.2267 3229.7755 3746.8812

TS_OH_MLR6b

O 2

C	-0.09964300	-0.52318500	0.12664400
C	0.03837300	0.10472300	1.49002700
O	1.12891100	0.42653100	1.96354000
C	-1.25242200	0.34055200	2.26848500
C	-1.01327800	0.21110800	3.77108800
C	-0.54599800	-1.19410200	4.09235500
O	-0.43816300	-2.09556900	3.26966800
O	-0.26350000	-1.33650500	5.40864200
C	0.20455500	-2.66152000	5.77028100
H	-2.02261700	-0.36782100	1.92773300
H	-1.60138800	1.35849400	2.01762700
H	-1.92862300	0.41766000	4.34819000
H	-0.24054400	0.91674800	4.11057800
H	0.39099300	-2.61301000	6.84836100
H	1.12591900	-2.89657600	5.22050800
H	-0.56422100	-3.41047900	5.53631900
H	-0.32592500	-1.59633900	0.21813400
H	0.97055300	-0.44308500	-0.44476200
H	-0.84123100	-0.01509900	-0.50747700
O	2.21504100	-0.21447600	-0.65259700
H	2.40533600	0.08407600	0.26053800

Frequencies

2102.7726i 23.9686 32.5099
63.7479 90.7629 129.3976
163.3890 177.5636 207.1219
260.2281 287.8318 305.7845
349.3147 449.9504 454.3332
479.3346 555.7126 610.7653
662.0771 715.1088 800.7714
818.2599 896.4296 923.7246
984.9538 994.5647 1018.3028
1026.9811 1080.8767 1168.4809
1179.5078 1197.6338 1201.9584
1221.5406 1234.0587 1256.5660
1367.4251 1387.2616 1415.8973
1437.2704 1445.6321 1459.6530
1479.6717 1480.7573 1487.3426
1729.2519 1750.9585 3070.6171
3091.7556 3097.2959 3102.5363
3140.0233 3159.3583 3188.8609
3192.5103 3226.6690 3677.7389