Electronic supplementary information to the paper

New theoretical insight into the reaction kinetics of toluene and hydroxyl radicals

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1) Table S1. Structure and frequency of all stationary points shown on the toluene+OH PES optimized by the B2PLYPD3/6-311++G(d,p) method.

C6H5CH3

C	-0.00763900	-1.19953600	1.20517200
C	-0.00763900	0.19581200	1.20217500
C	-0.00388100	0.91356100	0.00000000
C	-0.00763900	0.19581200	-1.20217500
C	-0.00763900	-1.19953600	-1.20517200
C	-0.00648200	-1.90320000	0.00000000
H	-0.01220200	-1.73580100	2.14733200
H	-0.01234000	0.73486900	2.14413000
H	-0.01234000	0.73486900	-2.14413000
H	-0.01220200	-1.73580100	-2.14733200
H	-0.00930500	-2.98687900	0.00000000
C	0.02927600	2.42117200	0.00000000
H	1.05986700	2.78965500	0.00000000
H	-0.46581000	2.82728400	-0.88435100
H	-0.46581000	2.82728400	0.88435100

Frequencies[1/cm]

44.69 202.96 341.60 398.43 447.41
526.70 537.82 634.09 722.96 800.02
840.70 882.53 915.15 936.50 967.28
977.87 1010.97 1019.50 1070.19 1137.99
1159.51 1191.28 1296.73 1310.74 1369.93
1417.20 1442.75 1454.09 1472.11 1565.98
1586.86 2927.97 2986.81 3009.30 3052.75
3054.42 3067.12 3075.29 3087.53

OH

O	0.00000000	0.00000000	0.10800700
H	0.00000000	0.00000000	-0.86405300

Frequencies[1/cm]

3614.32

OH···C6H5CH3 #pre-reaction complex

C	0.98053000	-0.41677600	0.00000300
C	0.26374200	-0.47554900	1.20263700
C	-1.12900000	-0.58244200	1.20565300
C	-1.83124600	-0.63613400	0.00000700
C	-1.12900000	-0.58246600	-1.20564000
C	0.26374300	-0.47557500	-1.20262800
H	0.80056000	-0.43321500	2.14440900
H	-1.66337000	-0.62475800	2.14756700
H	-2.91142300	-0.71752500	0.00000700
H	-1.66337100	-0.62480100	-2.14755300
H	0.80056000	-0.43326100	-2.14440200
C	2.47848900	-0.24830700	0.00000100
H	2.92678100	-0.70407000	0.88472600
H	2.92677900	-0.70407500	-0.88472200
H	2.74571400	0.81268200	-0.00000200
O	-0.36116300	2.76685000	-0.00002400
H	-0.45646600	1.79772300	-0.00003400

Frequencies[1/cm]

20.81 35.62 60.98 102.21 114.15
175.36 219.13 342.17 399.15 460.29
527.08 631.74 646.79 735.07 800.12
853.75 897.15 955.48 962.99 969.50
978.45 1010.64 1024.39 1070.20 1138.41
1160.14 1192.36 1295.95 1308.98 1370.17
1414.50 1443.95 1453.14 1471.03 1559.81
1582.95 2930.84 2991.98 3013.05 3058.03
3059.31 3072.02 3079.39 3091.32 3594.43

m-CH3C6H4• # P1m

C	-0.25343300	-1.24974700	-0.00962600
C	1.12063000	-1.27682000	0.00330000
C	1.95220100	-0.18048800	0.00814000
C	1.31803200	1.07076900	0.00208400
C	-0.07510300	1.15684400	-0.00917700
C	-0.88065700	0.01164900	-0.01092400
H	3.03200900	-0.26461200	0.01382700
H	1.91641500	1.97551800	0.00091800
H	-0.54683600	2.13347500	-0.01759400
C	-2.38573500	0.11566100	0.00983300
H	-2.71946100	1.06725300	-0.40772900
H	-2.84460900	-0.69006400	-0.56654700
H	-2.76623800	0.04899600	1.03346600
H	-0.84688900	-2.15777400	-0.01812600

Frequencies[1/cm]

45.17 200.87 344.21 407.23 463.45
517.58 576.53 626.64 738.76 793.19

836.05 873.07 923.76 996.81 970.24
1017.51 1022.06 1060.18 1137.13 1173.96
1253.92 1276.21 1367.83 1384.65 1434.92
1441.41 1445.14 1513.69 1583.68 2929.90
2989.98 3012.02 3054.79 3060.06 3070.22
3083.44

H2O # P
O 0.00000000 0.00000000 0.11747400
H 0.00000000 0.75947900 -0.46989500
H 0.00000000 -0.75947900 -0.46989500
Frequencies[1/cm]
1553.79 3699.35 3805.91

o-CH3C6H4• #P1o
C 0.14867000 -1.19274800 -0.00000100
C -1.22413800 -1.23410100 -0.00000100
C -1.89314700 0.00117300 0.00000300
C -1.15453200 1.18376100 0.00000400
C 0.24221200 1.15341600 -0.00000100
C 0.94544000 -0.06409400 -0.00000200
H -1.77397100 -2.16810700 0.00000000
H -2.97702200 0.02887400 0.00000400
H -1.66697400 2.13864500 0.00000600
H 0.80285000 2.08338700 0.00000200
C 2.45142200 -0.12345000 -0.00000200
H 2.87884500 0.88047600 -0.00004600
H 2.82035800 -0.65347300 0.88114100
H 2.82035100 -0.65354600 -0.88110400
Frequencies[1/cm]
15.77 198.31 329.38 402.68 456.67
517.13 530.63 631.41 731.66 798.40
827.87 898.19 909.03 986.62 968.42
1008.80 1017.12 1093.50 1132.82 1184.06
1233.02 1288.52 1368.39 1391.00 1423.69
1436.09 1453.82 1524.91 1583.80 2936.16
2997.04 3014.24 3048.22 3061.97 3074.98
3085.53

p-CH3C6H4• #P1p
C -0.13092100 1.20604100 -0.00869100
C 1.27190700 1.22137000 0.00276700
C 1.90400500 -0.00017400 0.00939800
C 1.27149500 -1.22163000 0.00271600
C -0.13121100 -1.20591500 -0.00879500
C -0.84250300 0.00021200 -0.01101100

H	1.81628900	-2.15837200	0.00207300
H	-0.67249200	-2.14708300	-0.01797400
C	-2.35158600	0.00011300	0.00950600
H	-2.75315000	-0.87818200	-0.49955400
H	-2.72979200	-0.01103200	1.03624300
H	-2.75296000	0.88921700	-0.48047800
H	-0.67190900	2.14735800	-0.01781800
H	1.81690500	2.15799300	0.00217000

Frequencies[1/cm]

51.48 216.70 343.63 395.03 444.07
530.64 582.26 615.27 767.29 786.35
804.70 888.82 932.70 961.92 973.11
1016.78 1021.61 1072.79 1140.64 1185.65
1259.22 1285.76 1346.06 1371.89 1429.29
1443.45 1449.61 1546.28 1569.65 2929.45
2988.59 3010.86 3050.68 3050.92 3076.31
3078.08

TS_{abs-m}

C	-1.31246000	-0.41849100	0.01082200
C	-1.50905200	0.96848800	0.05567700
C	-0.43405900	1.85843300	0.02272800
C	0.87852100	1.37826800	-6.67E-021400
C	1.05248400	0.00411000	-0.09929300
C	0.00588600	-0.90158100	-0.06066200
H	-2.52260600	1.35769800	0.12012900
H	-0.61567500	2.92977900	0.06015900
H	1.72584700	2.05701400	-0.07575800
H	2.24578000	-0.46049100	-0.21722000
H	0.19667500	-1.97153300	-0.08975100
C	-2.48278000	-1.37496700	0.01371700
H	-3.35545700	-0.93687500	0.50923000
H	-2.78401000	-1.63537000	-1.00962900
H	-2.23537800	-2.31055900	0.52650800
O	3.34835000	-0.90256800	-0.01580800
H	3.36677500	-0.89466900	0.96054400

Frequencies[1/cm]

-1263.99 49.43 82.01 99.58 108.27
203.32 338.00 357.71 422.35 466.97
524.13 557.71 644.34 741.77 770.72
855.45 860.48 887.81 931.90 1004.59
1010.42 1055.49 1058.85 1099.01 1125.31
1188.74 1218.87 1270.90 1318.77 1345.62
1423.09 1450.60 1498.37 1501.90 1509.93
1600.91 1637.56 3045.41 3108.02 3130.74
3177.03 3189.49 3193.89 3211.51 3783.29

TS_{abs-o}

C	-1.31174500	-0.41955200	0.01115400
C	-1.50972600	0.96596000	0.06143600
C	-0.43532800	1.85575500	0.02418400
C	0.87573700	1.37555800	-0.05560000
C	1.05353000	0.00136800	-0.11185400
C	0.00384400	-0.90271700	-0.06541600
H	-2.52069400	1.35351600	0.13003400
H	-0.61578500	2.92400600	0.06578700
H	1.72072800	2.05212900	-0.08316800
H	2.18564500	-0.43628900	-0.22681400
H	0.19384500	-1.96974700	-0.10026500
C	-2.48037900	-1.37337400	0.01489300
H	-3.33475500	-0.94653200	0.54344200
H	-2.80044900	-1.59955200	-1.00658700
H	-2.21770900	-2.31753100	0.49565300
O	3.35745800	-0.89830100	-0.00666300
H	3.35391400	-0.89158700	0.96243200

Frequencies[1/cm]

-1208.58 60.53 93.95 97.86 127.03
199.18 327.13 372.60 431.70 483.99
532.09 581.53 646.78 740.84 774.59
829.68 846.16 921.85 935.38 970.04
986.81 1005.74 1020.96 1049.26 1114.64
1138.48 1178.42 1211.77 1255.92 1295.87
1371.38 1409.63 1439.97 1444.60 1457.77
1543.34 1573.66 2932.36 2993.19 3026.92
3053.22 3067.96 3079.73 3089.68 3639.32

TS_{abs-p}

C	-1.31174500	-0.41955200	0.01115400
C	-1.50972600	0.96596000	0.06143600
C	-0.43532800	1.85575500	0.02418400
C	0.87573700	1.37555800	-0.05560000
C	1.05353000	0.00136800	-0.11185400
C	0.00384400	-0.90271700	-0.06541600
H	-2.52069400	1.35351600	0.13003400
H	-0.61578500	2.92400600	0.06578700
H	1.72072800	2.05212900	-0.08316800
H	2.18564500	-0.43628900	-0.22681400
H	0.19384500	-1.96974700	-0.10026500
C	-2.48037900	-1.37337400	0.01489300
H	-3.33475500	-0.94653200	0.54344200
H	-2.80044900	-1.59955200	-1.00658700
H	-2.21770900	-2.31753100	0.49565300

O		3.35745800	-0.89830100	-0.00666300
H		3.35391400	-0.89158700	0.96243200

Frequencies[1/cm]

-1297.65 43.32 77.79 86.76 118.23
218.15 344.20 374.22 398.27 443.13
567.43 591.73 627.13 754.08 791.85
821.76 822.87 908.30 945.54 967.52
982.11 1020.75 1032.33 1032.39 1091.07
1149.62 1187.01 1219.70 1278.39 1295.49
1365.88 1370.45 1443.19 1447.81 1462.49
1556.50 1563.74 2930.76 2990.73 3012.90
3056.85 3057.02 3084.51 3085.59 3641.84

C6H5CH2• #P2

C	0.25231700	1.21362000	0.00000600
C	-1.13207900	1.20859100	0.00001700
C	-1.83606400	0.00000200	-0.00002900
C	-1.13208300	-1.20859000	-0.00002600
C	0.25231300	-1.21362000	-0.00003600
C	0.98817300	-0.00000100	0.00001100
H	0.79309900	2.15371800	0.00003900
H	-1.67301500	2.14795900	0.00001200
H	-2.91922800	0.00000200	-0.00001700
H	-1.67302000	-2.14795700	-0.00006000
H	0.79309500	-2.15371900	-0.00003600
C	2.40133200	-0.00000200	0.00004900
H	2.95780500	-0.92793000	0.00002300
H	2.95780600	0.92792800	0.00008600

Frequencies[1/cm]

192.09 355.22 374.93 431.25 456.03
472.36 533.82 623.48 630.07 719.79
829.95 838.15 876.01 914.62 940.52
976.50 963.58 1009.32 1080.72 1133.11
1141.75 1232.11 1280.82 1305.32 1429.06
1440.71 1448.76 1546.36 1558.84 3047.04
3059.70 3062.05 3074.18 3079.56 3092.51
3146.51

$TS_{abs\text{-}CH3}$

C	0.29824900	-0.00015600	0.55535900
C	-0.37095900	1.20508500	0.29753800
C	-1.67019700	1.20687600	-0.20752300
C	-2.32409400	0.00016400	-0.46262300
C	-1.67035300	-1.20670800	-0.20788200
C	-0.37111200	-1.20523400	0.29717300
H	0.13233500	2.14541000	0.49653000

H	-2.17336700	2.14781800	-0.39770300
H	-3.33502700	0.00028600	-0.85269400
H	-2.17364200	-2.14753100	-0.39834000
H	0.13206500	-2.14568200	0.49588200
C	1.70121700	-0.00031000	1.06308700
H	1.94873900	0.89581200	1.63325800
H	1.94867400	-0.89666300	1.63292200
H	2.44631700	-0.00016300	0.18343700
O	3.14858400	0.00025500	-1.14261400
H	2.32872700	0.00037400	-1.66315400

Frequencies[1/cm]

-1687.57 76.85 98.75 133.64 217.76
339.50 396.69 440.36 490.52 514.99
528.22 596.03 632.47 726.29 770.88
833.92 841.53 896.25 928.39 945.90
997.75 979.95 1012.40 1071.22 1072.80
1140.01 1160.47 1187.03 1200.93 1301.59
1309.49 1381.04 1423.02 1428.00 1468.18
1563.32 1580.02 2979.51 3056.35 3059.99
3062.63 3072.71 3081.15 3091.56 3633.74

C6H5OH

C	0.24040500	1.21022500	-0.01434700
C	-1.15490900	1.20699800	0.00591300
C	-1.85625000	0.00030700	0.01602100
C	-1.15540600	-1.20666300	0.00606000
C	0.23991700	-1.21049000	-0.01396500
C	0.93254700	-0.00029900	-0.00920900
H	0.79975300	2.13770300	-0.03780300
H	-1.69266800	2.14793200	0.00425000
H	-2.93948400	0.00053700	0.02829300
H	-1.69355000	-2.14737500	0.00464300
H	0.79899500	-2.13812800	-0.03685700
O	2.32049600	-0.00105500	-0.08827700
H	2.68515900	0.00729800	0.80085400

Frequencies[1/cm]

156.12 222.96 405.31 409.85 453.28
529.68 533.30 628.39 739.04 823.15
830.30 882.52 913.59 936.76 978.39
1004.00 1051.70 1133.65 1136.74 1148.69
1225.40 1275.53 1307.53 1425.90 1469.04
1570.30 1579.22 3063.25 3071.71 3082.77
3088.27 3093.65 3709.39

CH3

C	0.00000000	0.00000000	-0.00008100
H	0.00000000	1.07906800	0.00016200
H	-0.93450000	-0.53953400	0.00016200
H	0.93450000	-0.53953400	0.00016200

Frequencies[1/cm]

513.14 1369.86 1369.86 3012.76 3190.07 3190.09

ipso-HOC6H5CH3

C	0.03666100	-1.24694500	0.01494200
C	1.39748600	-1.22569600	-0.03284600
C	2.11019800	-0.00000300	-0.07136700
C	1.39748600	1.22569300	-0.03284100
C	0.03666200	1.24695000	0.01495800
C	-0.80174700	0.00000900	0.02675100
H	-0.50761800	-2.18452300	0.05611300
H	1.94977000	-2.15899900	-0.03381000
H	3.19194200	0.00000100	-0.10777300
H	1.94977800	2.15899100	-0.03380600
H	-0.50758400	2.18454700	0.05615000
C	-1.79326700	0.00000300	-1.14188200
H	-2.42709900	0.88757200	-1.08419800
H	-1.26004800	0.00001600	-2.09355000
H	-2.42708400	-0.88757500	-1.08420000
O	-1.64992300	0.00000200	1.21042100
H	-1.06355300	-0.00011200	1.97541100

Frequencies[1/cm]

82.89 228.40 256.73 339.32 342.33
386.17 393.06 454.57 536.45 582.65
586.16 692.09 733.83 772.25 819.87
898.42 961.48 966.98 970.32 980.93
994.23 1020.80 1056.54 1083.45 1099.19
1158.20 1250.17 1272.03 1278.69 1350.94
1351.56 1401.96 1436.99 1445.50 1497.81
1560.77 2935.53 3012.38 3022.72 3056.44
3057.95 3074.17 3075.36 3096.04 3673.71

$TS_{elim\text{-}ipso}$

C	1.39903800	1.21170600	-0.08840500
C	0.02710300	1.21406900	-0.26806800
C	-0.71588100	-0.00042000	-0.30898500
C	0.02735300	-1.21470400	-0.26617000
C	1.39926500	-1.21181400	-0.08659200
C	2.09366800	0.00009700	0.00260400
H	1.93789900	2.15004300	-0.03114500
H	-0.51321200	-2.15117500	-0.34037500
H	1.93833000	-2.14995300	-0.02800700

H	3.16876200	0.00030200	0.13786800
O	-1.34603100	0.00187400	1.59411600
H	-0.50542900	0.00251800	2.07618900
H	-0.51365500	2.15032200	-0.34361900
C	-2.11935100	-0.00111900	-0.85695500
H	-2.65971300	0.88340700	-0.52045800
H	-2.09198900	-0.00296700	-1.95048100
H	-2.65991400	-0.88438600	-0.51748300

Frequencies[1/cm]

-689.5 135.90 180.55 203.45 245.74
282.34 398.23 421.77 435.60 520.34
612.31 622.99 665.14 672.51 717.01
793.18 809.75 867.02 974.17 982.76
988.69 974.28 1000.99 1057.84 1125.85
1138.32 1146.64 1201.95 1286.75 1317.97
1382.98 1383.55 1436.12 1451.93 1536.98
1565.81 2963.06 3052.86 3067.37 3074.88
3089.86 3096.07 3107.00 3126.80 3704.19

$TS_{add\text{-}ipso}$

C	1.39903800	1.21170600	-0.08840500
C	0.02710300	1.21406900	-0.26806800
C	-0.71588100	-0.00042000	-0.30898500
C	0.02735300	-1.21470400	-0.26617000
C	1.39926500	-1.21181400	-0.08659200
C	2.09366800	0.00009700	0.00260400
H	1.93789900	2.15004300	-0.03114500
H	-0.51321200	-2.15117500	-0.34037500
H	1.93833000	-2.14995300	-0.02800700
H	3.16876200	0.00030200	0.13786800
O	-1.34603100	0.00187400	1.59411600
H	-0.50542900	0.00251800	2.07618900
H	-0.51365500	2.15032200	-0.34361900
C	-2.11935100	-0.00111900	-0.85695500
H	-2.65971300	0.88340700	-0.52045800
H	-2.09198900	-0.00296700	-1.95048100
H	-2.65991400	-0.88438600	-0.51748300

Frequencies[1/cm]

-411.6 106.81 146.65 171.39 218.37
265.42 338.04 407.51 408.71 529.67
622.56 646.63 739.16 785.77 805.41
839.48 920.97 973.90 979.14 968.14
971.61 1007.68 1016.53 1080.70 1129.01
1156.24 1192.19 1268.01 1299.69 1367.04
1407.06 1443.02 1447.98 1450.60 1539.91
1567.93 2938.29 3009.51 3036.00 3064.73

3070.54 3079.13 3085.37 3093.07 3634.88

m-HOC6CH4CH3

C	0.03828900	-0.98332300	-0.01103200
C	-1.21419400	-0.36747800	0.00155700
C	-1.31683100	1.02422600	0.00783400
C	-0.15108900	1.79118800	0.00251200
C	1.10089000	1.18051600	-0.00905900
C	1.20539600	-0.21732100	-0.01208300
H	-2.29153300	1.50193700	0.01367200
H	-0.22618900	2.87251300	0.00277400
H	1.99944500	1.78707000	-0.01692600
O	-2.31206400	-1.18783600	0.00152300
H	-3.10835700	-0.64861900	0.00128900
H	0.08363700	-2.06635100	-0.01979200
C	2.55658700	-0.88788300	0.01051600
H	2.91140200	-1.01152500	1.03818800
H	2.51470600	-1.87797900	-0.44695700
H	3.29911700	-0.29390900	-0.52590100

Frequencies[1/cm]

50.00 198.61 222.19 244.56 295.05
427.33 445.22 521.41 538.70 546.11
558.40 741.48 743.99 834.52 847.66
912.44 947.09 974.50 988.51 1018.59
1071.93 1134.08 1143.48 1165.80 1255.31
1287.04 1319.62 1369.79 1428.64 1443.52
1462.20 1467.25 1572.12 1598.85 2929.96
2989.47 3012.20 3051.32 3063.99 3075.65
3081.82 3706.83

o-HOC6CH4CH3

C	-0.58741200	-0.62124200	-0.00003100
C	-0.39709600	0.76973300	-0.00000600
C	0.88413500	1.32167300	0.00001700
C	1.99797900	0.48646800	0.00001400
C	1.83489000	-0.89976800	-0.00004700
C	0.54852700	-1.43744100	-0.00007500
H	0.98536700	2.40000700	0.00003400
H	2.99111300	0.91992900	0.00003400
H	2.69768500	-1.55439500	-0.00007200
H	0.41480900	-2.51417900	-0.00013200
O	-1.44958500	1.64859900	0.00011500
H	-2.27720700	1.15968200	-0.00069600
C	-1.97801700	-1.20387200	0.00007400
H	-2.54736500	-0.90051000	0.88608300
H	-2.54800600	-0.89932200	-0.88512400

H -1.93774900 -2.29330800 -0.00072200
Frequencies[1/cm]
94.00 149.91 186.29 259.01 301.30
424.19 434.14 512.90 529.95 581.51
591.00 746.70 758.39 835.09 850.50
903.58 918.78 963.53 1011.53 1018.60
1082.58 1134.16 1146.18 1191.56 1239.63
1281.99 1328.43 1368.32 1428.31 1438.52
1462.05 1470.31 1568.76 1599.29 2908.11
2955.21 3014.00 3057.11 3070.55 3085.32
3093.61 3713.37

p-HOC6CH4CH3
C 0.72793300 -1.21888100 -0.00140500
C 1.43852100 -0.01733900 0.00327400
C 0.74887800 1.19466900 -0.00111900
C -0.64762000 1.19870300 -0.00908100
C -1.37951600 0.00884900 -0.00977600
C -0.66342400 -1.19615200 -0.00894900
H 1.29558600 2.13295400 -0.00313800
H -1.17062800 2.14924600 -0.01586800
O 2.80767300 -0.09363200 0.00788400
H 3.17287700 0.79589800 0.00413700
H 1.27506500 -2.15356700 -0.00346800
H -1.20434700 -2.13691500 -0.01568900
C -2.88816700 0.01551700 0.01221100
H -3.27078800 -0.15261500 1.02360800
H -3.28284400 0.97204200 -0.33574400
H -3.29593400 -0.77018500 -0.62783500
Frequencies[1/cm]
44.94 139.99 242.46 305.27 317.85
405.67 425.02 465.80 492.40 539.38
655.70 747.07 781.78 814.56 851.84
874.72 927.98 1010.00 992.28 1019.39
1087.49 1151.12 1152.28 1192.89 1233.22
1291.99 1322.85 1371.40 1404.16 1441.86
1454.47 1491.65 1576.32 1598.79 2926.43
2983.71 3006.69 3045.99 3057.34 3065.82
3089.47 3708.61

m-HOC6CH5CH3
C 0.14099700 -0.97869900 -0.32239800
C 1.21099700 -0.18524500 -0.03819900
C 1.01290600 1.21583700 0.15518800
C -0.28100600 1.78068600 0.06851000
C -1.37041600 1.01057500 -0.21359600

C	-1.26403800	-0.46815400	-0.42165900
H	1.86322500	1.84760900	0.38399600
H	-0.40260700	2.84570600	0.23380800
H	-2.36371900	1.44077000	-0.26934000
C	2.60530400	-0.74771900	0.08222800
H	2.61160600	-1.82600200	-0.08195000
H	3.27417400	-0.28656500	-0.64966000
H	3.01997100	-0.54980900	1.07447700
O	-2.13809300	-1.18196200	0.49153600
H	-1.81337900	-0.99991100	1.38073800
H	-1.68362200	-0.73293100	-1.40072400
H	0.27063700	-2.04685600	-0.46407300

Frequencies[1/cm]

91.89 121.80 175.96 289.74 330.34
371.13 435.12 466.20 495.93 535.98
619.64 699.25 762.67 786.67 847.46
897.67 950.54 961.86 986.66 989.91
1024.75 1040.74 1084.71 1133.73 1161.11
1175.99 1272.16 1282.10 1324.70 1344.54
1369.46 1389.61 1437.26 1449.26 1515.76
1577.37 2898.68 2929.59 2986.09 3014.93
3058.36 3060.12 3075.37 3084.80 3670.76

TS_{elim-m}

C	-0.05072100	-0.97334300	-0.01973500
C	-1.22376700	-0.22700800	-0.01481400
C	-1.13291700	1.17672500	-0.00966100
C	0.11461100	1.81011600	-0.03017800
C	1.28954600	1.07397300	-0.02420500
C	1.22096500	-0.34003500	0.08041800
H	-2.04231800	1.77201500	-0.01640800
H	0.16514000	2.89520600	-0.06675600
H	2.26645400	1.54472200	-0.05273600
C	-2.57297900	-0.90803600	-0.01993900
H	-3.04075900	-0.86432200	0.97231300
H	-3.26148700	-0.42565600	-0.72290500
H	-2.49022500	-1.96356100	-0.29816800
O	2.38642900	-1.02527200	-0.17468600
H	2.24484800	-1.96376100	0.02515200
H	1.29299000	-0.40571800	1.82435600
H	-0.09450600	-2.06110000	-0.03868200

Frequencies[1/cm]

-1207.49 59.18 201.96 207.01 274.54
296.67 416.91 453.07 504.34 518.52
525.68 583.48 677.41 693.96 752.96
802.40 858.55 913.03 950.31 983.14
975.51 990.57 1025.98 1069.44 1130.44

1144.81 1161.71 1238.16 1287.10 1302.23
1370.47 1405.74 1442.05 1453.30 1475.50
1567.40 1585.66 2932.14 2992.28 3013.28
3051.30 3064.63 3080.30 3101.60 3703.68

$TS_{add\text{-}m}$

C	-1.19598000	-0.12495800	-0.06173800
C	-0.89788600	1.20197800	0.29864400
C	0.38518000	1.72980200	0.13073700
C	1.39686600	0.94537900	-0.39842100
C	1.14714500	-0.41725200	-0.70284300
C	-0.18186600	-0.90615000	-0.59157500
H	-1.68379700	1.82844800	0.70796000
H	0.58112700	2.76118300	0.39933800
H	2.39389000	1.34339000	-0.53688300
H	1.85243700	-0.95737100	-1.31838900
H	-0.38269200	-1.93058600	-0.88288200
C	-2.59072600	-0.66860500	0.12367400
H	-3.33791800	0.01944800	-0.27869300
H	-2.70732800	-1.63015500	-0.37820100
H	-2.81465900	-0.81493000	1.18419500
O	2.02555500	-1.28789100	0.84403100
H	1.51810300	-0.87746300	1.56044800

Frequencies[1/cm]

-449.63 52.35 103.68 133.30 184.01
220.51 340.88 393.34 463.09 519.31
622.62 655.47 773.11 786.64 836.42
885.99 912.04 984.81 997.30 966.60
991.57 1019.42 1028.26 1065.89 1137.22
1150.17 1189.10 1270.61 1303.34 1370.39
1404.16 1440.53 1450.88 1458.91 1543.19
1573.47 2931.63 2989.78 3014.34 3058.05
3074.73 3078.08 3093.80 3105.29 3632.07

o-HOC6CH5CH3

C	0.72707500	-0.56931700	0.11837200
C	-0.23304100	-1.49219200	-0.18886700
C	-1.60934300	-1.16231400	-0.22480300
C	-2.02716900	0.15946600	0.07390800
C	-1.11888800	1.12448100	0.38666100
C	0.35577700	0.86978400	0.37224100
H	0.06630600	-2.51384400	-0.40152900
H	-2.34081200	-1.91973100	-0.47590700
H	-3.08484700	0.39817000	0.05694200
H	-1.43232400	2.13779500	0.61109000
C	2.18409800	-0.90674900	0.19889500

H	2.56334100	-0.72514800	1.21144700
H	2.36617300	-1.95252200	-0.05359700
H	2.76721900	-0.27131000	-0.47271800
O	1.00495600	1.74222300	-0.59603100
H	0.57819900	1.57286500	-1.44396200
H	0.80604800	1.19698700	1.31803800

Frequencies[1/cm]

77.96 149.76 220.62 267.37 323.45
377.09 401.02 485.87 507.54 567.10
632.51 697.17 766.85 795.22 876.05
910.95 962.75 972.28 997.92 984.75
1010.78 1025.34 1085.97 1138.84 1162.89
1175.05 1263.16 1294.47 1342.65 1364.06
1374.74 1383.84 1426.23 1444.83 1504.05
1569.86 2902.16 2914.34 2972.35 3012.16
3051.22 3060.36 3078.53 3093.82 3667.04

TS_{elim-m}

C	0.57534600	-0.66804400	-0.02000100
C	-0.57107100	-1.45073500	-0.01224800
C	-1.84920600	-0.88642800	-0.00578300
C	-1.99427800	0.50136700	-0.03766100
C	-0.87381400	1.31428600	-0.05503100
C	0.41333500	0.74135900	0.08055000
H	-0.46295400	-2.52986600	-0.03341900
H	-2.72330900	-1.52576600	-0.00002100
H	-2.98130500	0.94627900	-0.07947800
H	-0.97040700	2.39450500	-0.08857200
C	1.95781800	-1.24791000	-0.02879400
H	2.53690000	-0.86961700	-0.87442800
H	2.49775400	-0.96016600	0.87872200
H	1.91960800	-2.33642500	-0.08480100
O	1.55225300	1.48958600	-0.13565200
H	1.36508400	2.41059200	0.06877600
H	0.45181400	0.73040100	1.77224700

Frequencies[1/cm]

-1156.69 152.38 163.32 249.66 274.75
290.19 408.53 445.67 495.21 536.66
565.02 582.06 673.28 717.45 756.64
806.77 848.00 880.92 950.43 981.69
973.56 1027.50 1033.31 1079.50 1136.20
1147.73 1194.93 1215.66 1280.65 1300.48
1368.76 1411.86 1429.87 1454.07 1474.94
1565.42 1588.92 2928.12 2985.80 3018.19
3057.53 3062.49 3077.57 3092.48 3706.17

$TS_{add\text{-}o}$

C	-0.15229700	-1.44479400	0.31625700
C	0.75283600	-0.53218700	-0.20946900
C	0.27056900	0.74043100	-0.63358700
C	-1.12431700	0.99162400	-0.64527000
C	-2.00612400	0.06602400	-0.11425200
C	-1.51962900	-1.15512900	0.36657900
H	0.20609500	-2.40216100	0.67823600
H	0.91769200	1.36492800	-1.23496500
H	-1.48198700	1.93856300	-1.03034800
H	-3.06882600	0.27498000	-0.08959600
H	-2.20740600	-1.88583400	0.77632500
C	2.22464800	-0.81304400	-0.27745300
H	2.76195900	-0.07939600	0.32911800
H	2.45820800	-1.81431400	0.08697500
H	2.59174700	-0.72543000	-1.30408100
O	0.86801000	1.83247500	0.92487500
H	0.20432300	1.55131100	1.57250600

Frequencies[1/cm]

-406.00 109.79 129.26 132.58 199.21
208.50 344.19 395.59 476.62 522.76
625.48 681.02 753.95 792.87 812.70
875.91 949.53 980.41 991.43 983.74
998.24 1013.24 1025.27 1062.32 1134.91
1153.94 1186.92 1277.38 1301.91 1361.15
1403.65 1433.81 1452.92 1469.41 1542.84
1572.15 2929.38 2989.36 3016.66 3061.40
3072.28 3 081.24 3087.44 3096.59 3633.95

p-HOC6CH5CH3

C	0.70827100	1.24600900	-0.30063200
C	-0.63855300	1.21997800	-0.10413700
C	-1.36430000	0.00032000	-0.00082100
C	-0.63866600	-1.21968600	-0.10425800
C	0.70800700	-1.24599300	-0.30064900
C	1.53505900	-0.00006800	-0.37954300
H	-1.18469100	-2.15502600	-0.02613300
H	1.24027100	-2.18763800	-0.37457500
O	2.56611500	-0.00021400	0.64458400
H	2.10928400	-0.00002200	1.49352900
H	2.12595000	-0.00014600	-1.30348800
H	1.24070600	2.18755300	-0.37455300
H	-1.18433700	2.15543700	-0.02593900
C	-2.84079900	-0.00008900	0.26276900
H	-3.32083100	-0.88095900	-0.16944000
H	-3.05106300	-0.01072200	1.33947900

H	-3.31831500	0.89040200	-0.15192000

Frequencies[1/cm]

15.74 72.37 214.82 268.57 330.97
361.72 395.45 453.35 492.38 600.78
626.33 748.09 762.53 766.19 871.29
953.40 960.88 968.20 986.61 971.90
996.28 1019.91 1127.94 1150.12 1177.04
1205.34 1223.74 1295.01 1344.94 1365.69
1366.55 1419.02 1434.20 1437.59 1485.01
1571.82 2905.71 2908.24 2968.89 3005.24
3047.94 3048.96 3076.11 3078.07 3669.76

$TS_{elim\text{-}p}$

C	0.69740100	-1.22292600	-0.03502200
C	-0.68505400	-1.19954000	-0.03932500
C	-1.40195500	0.00567400	-0.02000200
C	-0.67362900	1.20190200	-0.04259800
C	0.71062700	1.20612300	-0.05191700
C	1.41917400	-0.01294000	0.08290300
H	-1.20475800	2.14685600	-0.08732100
H	1.26080600	2.14042400	-0.08507200
O	2.77762500	-0.08966600	-0.14790800
H	3.19031600	0.73067600	0.13826000
H	1.46461900	0.00862900	1.77073400
H	1.25091600	-2.15301500	-0.05705100
H	-1.22766500	-2.13812000	-0.08112700
C	-2.90808000	0.01209500	0.01956800
H	-3.32062200	-0.84569100	-0.51582700
H	-3.27440100	-0.03614000	1.04992200
H	-3.31110500	0.92138900	-0.43089100

Frequencies[1/cm]

-1196.85 55.86 131.99 250.17 303.19
314.70 393.25 427.27 448.62 510.65
531.54 651.35 656.58 709.66 758.72
823.29 837.48 881.46 965.16 976.72
972.21 988.36 1024.64 1092.88 1142.86
1153.44 1198.79 1217.56 1268.16 1310.57
1370.56 1412.85 1441.40 1451.98 1473.50
1553.42 1597.62 2925.43 2983.17 3008.09
3055.98 3061.47 3072.62 3096.32 3705.05

$TS_{add\text{-}p}$

C	1.44477800	-0.00000400	-0.62586600
C	0.72190000	1.21567800	-0.51618000
C	-0.61750100	1.20791700	-0.17197100
C	-1.31141800	0.00000500	0.01072000

C	-0.61751200	-1.20791500	-0.17197300
C	0.72188700	-1.21568100	-0.51617400
H	2.41148300	-0.00001100	-1.10829300
H	1.24533900	2.15259400	-0.66021300
H	-1.14911000	2.14660700	-0.05798800
H	-1.14912800	-2.14660200	-0.05799100
H	1.24532200	-2.15260000	-0.66020500
C	-2.76125500	0.00000500	0.41397200
H	-2.85895300	-0.00020900	1.50451400
H	-3.27613900	0.88608800	0.03807300
H	-3.27622900	-0.88588100	0.03772500
O	2.45234200	-0.00000400	1.09048700
H	1.70341400	0.00001800	1.70530700

Frequencies[1/cm]

-427.07 48.02 102.89 124.64 179.49

225.81 342.81 406.48 439.23 525.75

625.89 679.96 778.49 800.74 819.32

841.16 956.33 981.58 994.36 966.87

991.07 1015.05 1020.70 1064.71 1135.84

1162.07 1200.68 1264.61 1310.03 1368.44

1421.19 1441.87 1449.57 1452.36 1530.58

1575.81 2926.50 2986.53 3014.14 3061.52

3061.82 3088.38 3091.44 3108.45 3633.94

2). Table S2. T1 diagnostic values of stationary points.

species	T1 value	species	T1 value
toluene	0.0100	Tsadd-p	0.0373
OH	0.0070	ipso-OHC6H5CH3	0.0293
TSabs-m	0.0202	m-OHC6H5CH3	0.0292
TSabs-o	0.0200	o-OHC6H5CH3	0.0293
TSabs-p	0.0200	p-OHC6H5CH3	0.0295
TSabs-CH3	0.0165	TSelimipso	0.0351
m-CH3C6H4	0.0427	C6H5OH	0.0106
o-CH3C6H4	0.0427	CH3	0.0079
p-CH3C6H4	0.0429	TSelimm	0.0350
C6H5CH2	0.0374	TSelimo	0.0351
H2O	0.0065	Tselimp	0.0352
Tsaddipso	0.0374	mOHC6H4CH3	0.0113
Tsadd-m	0.0370	oOHC6H4CH3	0.0110
Tsadd-o	0.0373	pOHC6H4CH3	0.0108

3). Detailed information(K(T), k_{diss}, f_i) by particle-in-the-box approximation from Multiwell Package

Table S3. Equilibrium constants K(T), for the association of the OH radical and toluene into the pre-reaction complex, unimolecular reaction rates for dissociation of the pre-reaction complex k_{diss}, and relative adduct populations f_i (summed for all adducts), calculated with harmonic oscillator and particle-in-the-box models applied to the relative translation of OH radical and toluene in the pre-reaction complex.

	$k_{diss}(s^{-1})$		K($cm^3molecule^{-1}$)		fi		ratio
T(K)	Particle in the box	Harmonic oscillator	Particle in the box	Harmonic oscillator	Particle in the box	Harmonic oscillator	k_total_box /harmo
210	2.26E+12	2.94E+12	1.84E-21	3.45E-21	7.08E-04	2.25E-04	1.29
230	2.30E+12	2.99E+12	8.67E-22	1.69E-21	7.78E-04	2.43E-04	1.26
250	2.33E+12	3.04E+12	4.66E-22	9.43E-22	8.46E-04	2.64E-04	1.21
277	2.36E+12	3.08E+12	2.36E-22	4.98E-22	9.32E-04	2.82E-04	1.20
300	2.40E+12	3.13E+12	1.47E-22	3.21E-22	1.06E-03	3.13E-04	1.19
350	2.46E+12	3.21E+12	6.70E-23	1.56E-22	1.29E-03	3.70E-04	1.15
400	2.51E+12	3.28E+12	3.83E-23	9.47E-23	1.54E-03	4.20E-04	1.14
450	2.55E+12	3.34E+12	2.54E-23	6.61E-23	1.81E-03	4.78E-04	1.11
500	2.59E+12	3.40E+12	1.86E-23	5.08E-23	2.08E-03	5.34E-04	1.08
550	2.63E+12	3.45E+12	1.47E-23	4.19E-23	2.36E-03	5.82E-04	1.08
600	2.66E+12	3.49E+12	1.22E-23	3.62E-23	2.64E-03	6.33E-04	1.07
650	2.69E+12	3.53E+12	1.06E-23	3.26E-23	2.90E-03	6.71E-04	1.07
700	2.72E+12	3.56E+12	9.46E-24	3.01E-23	3.15E-03	7.10E-04	1.07
750	2.74E+12	3.60E+12	8.65E-24	2.84E-23	3.42E-03	7.44E-04	1.07
800	2.76E+12	3.63E+12	8.07E-24	2.73E-23	3.67E-03	7.77E-04	1.06
850	2.78E+12	3.65E+12	7.64E-24	2.66E-23	3.91E-03	8.16E-04	1.05
900	2.80E+12	3.68E+12	7.32E-24	2.62E-23	4.16E-03	8.49E-04	1.04
950	2.82E+12	3.70E+12	7.09E-24	2.60E-23	4.39E-03	8.75E-04	1.04
1000	2.83E+12	3.72E+12	6.92E-24	2.60E-23	4.65E-03	9.02E-04	1.05

4). Table S4. The relative adduct population calculated from Multiwell package. The uncertainities come from noninfinite number of Monte-Carlo trials.

	fi(relative adduct populations) calculated by particle-in-the-box model				
T	ortho-adduct	ipso-adduct	para-adduct	meta-adduct	benzyl radical + H_2O
210	4.81E-04	6.69E-05	7.34E-05	7.75E-05	9.92E-06
230	5.08E-04	7.13E-05	8.68E-05	9.92E-05	1.26E-05
250	5.34E-04	7.85E-05	1.02E-04	1.16E-04	1.57E-05
277	5.72E-04	8.31E-05	1.17E-04	1.39E-04	2.03E-05
300	6.16E-04	9.43E-05	1.43E-04	1.77E-04	2.70E-05
350	6.95E-04	1.13E-04	1.92E-04	2.49E-04	4.17E-05

400	7.71E-04	1.32E-04	2.42E-04	3.37E-04	6.11E-05
450	8.43E-04	1.52E-04	2.95E-04	4.37E-04	8.23E-05
500	9.12E-04	1.68E-04	3.54E-04	5.36E-04	1.08E-04
550	9.74E-04	1.85E-04	4.14E-04	6.46E-04	1.38E-04
600	1.03E-03	2.02E-04	4.70E-04	7.56E-04	1.73E-04
650	1.08E-03	2.20E-04	5.27E-04	8.59E-04	2.09E-04
700	1.12E-03	2.34E-04	5.84E-04	9.69E-04	2.45E-04
750	1.18E-03	2.49E-04	6.39E-04	1.07E-03	2.83E-04
800	1.22E-03	2.61E-04	6.89E-04	1.17E-03	3.32E-04
850	1.25E-03	2.76E-04	7.40E-04	1.27E-03	3.75E-04
900	1.29E-03	2.83E-04	7.87E-04	1.37E-03	4.25E-04
950	1.31E-03	2.94E-04	8.36E-04	1.47E-03	4.75E-04
1000	1.33E-03	3.07E-04	8.92E-04	1.61E-03	5.16E-04
fi(relative adduct populations) calculated by harmonic oscillator model					
210	1.53E-04	2.05E-05	2.34E-05	2.50E-05	3.04E-06
230	1.60E-04	2.22E-05	2.70E-05	2.92E-05	3.96E-06
250	1.69E-04	2.39E-05	3.17E-05	3.46E-05	4.55E-06
277	1.76E-04	2.46E-05	3.42E-05	4.09E-05	5.85E-06
300	1.83E-04	2.84E-05	4.23E-05	5.13E-05	7.89E-06
350	2.03E-04	3.24E-05	5.33E-05	6.95E-05	1.17E-05
400	2.11E-04	3.57E-05	6.57E-05	9.16E-05	1.62E-05
450	2.25E-04	3.99E-05	7.82E-05	1.13E-04	2.13E-05
500	2.36E-04	4.26E-05	9.01E-05	1.37E-04	2.77E-05
550	2.41E-04	4.66E-05	1.03E-04	1.58E-04	3.38E-05
600	2.51E-04	4.89E-05	1.14E-04	1.79E-04	4.03E-05
650	2.57E-04	5.09E-05	1.22E-04	1.95E-04	4.73E-05
700	2.60E-04	5.27E-05	1.28E-04	2.16E-04	5.33E-05
750	2.58E-04	5.38E-05	1.39E-04	2.32E-04	6.22E-05
800	2.57E-04	5.53E-05	1.46E-04	2.49E-04	6.94E-05
850	2.62E-04	5.68E-05	1.51E-04	2.67E-04	7.91E-05
900	2.65E-04	5.85E-05	1.60E-04	2.78E-04	8.77E-05
950	2.64E-04	5.95E-05	1.66E-04	2.93E-04	9.30E-05
1000	2.69E-04	6.18E-05	1.67E-04	3.00E-04	1.04E-04

5). Table S5. The stochastic uncertainties resulting from noninfinite number of Monte-Carlo trials. The final uncertainties were calculated by $\sigma = \sqrt{\frac{f_i(1-f_i)}{N_{MC}}}$, where N_{MC} is number of Monte-Carlo trials (1E8). The ortho and meta adducts populations are counted in twice, as there are two ortho and meta positions on toluene.

σ (stochastic uncertainties)

calculated by particle-in-the-box model					
T	ortho-adduct	ipso-adduct	para-adduct	meta-adduct	benzyl radical + H_2O
210	2.19E-06	8.18E-07	8.57E-07	8.80E-07	3.15E-07
230	2.25E-06	8.44E-07	9.31E-07	9.96E-07	3.55E-07
250	2.31E-06	8.86E-07	1.01E-06	1.08E-06	3.96E-07
277	2.39E-06	9.12E-07	1.08E-06	1.18E-06	4.51E-07
300	2.48E-06	9.71E-07	1.20E-06	1.33E-06	5.20E-07
350	2.64E-06	1.06E-06	1.38E-06	1.58E-06	6.46E-07
400	2.78E-06	1.15E-06	1.55E-06	1.84E-06	7.82E-07
450	2.90E-06	1.23E-06	1.72E-06	2.09E-06	9.07E-07
500	3.02E-06	1.30E-06	1.88E-06	2.31E-06	1.04E-06
550	3.12E-06	1.36E-06	2.04E-06	2.54E-06	1.17E-06
600	3.21E-06	1.42E-06	2.17E-06	2.75E-06	1.32E-06
650	3.29E-06	1.48E-06	2.30E-06	2.93E-06	1.45E-06
700	3.35E-06	1.53E-06	2.41E-06	3.11E-06	1.57E-06
750	3.43E-06	1.58E-06	2.53E-06	3.28E-06	1.68E-06
800	3.49E-06	1.62E-06	2.62E-06	3.42E-06	1.82E-06
850	3.54E-06	1.66E-06	2.72E-06	3.56E-06	1.94E-06
900	3.59E-06	1.68E-06	2.80E-06	3.70E-06	2.06E-06
950	3.62E-06	1.72E-06	2.89E-06	3.84E-06	2.18E-06
1000	3.64E-06	1.75E-06	2.99E-06	4.00E-06	2.27E-06
			σ (stochastic uncertainties)		
			calculated by harmonic oscillator model		
210	1.24E-06	4.52E-07	4.83E-07	5.00E-07	1.74E-07
230	1.27E-06	4.72E-07	5.20E-07	5.40E-07	1.99E-07
250	1.30E-06	4.89E-07	5.63E-07	5.88E-07	2.13E-07
277	1.33E-06	4.96E-07	5.84E-07	6.39E-07	2.42E-07
300	1.35E-06	5.33E-07	6.51E-07	7.16E-07	2.81E-07
350	1.43E-06	5.69E-07	7.30E-07	8.34E-07	3.42E-07
400	1.45E-06	5.98E-07	8.10E-07	9.57E-07	4.03E-07
450	1.50E-06	6.32E-07	8.84E-07	1.06E-06	4.62E-07
500	1.54E-06	6.53E-07	9.49E-07	1.17E-06	5.26E-07
550	1.55E-06	6.83E-07	1.01E-06	1.26E-06	5.82E-07
600	1.58E-06	7.00E-07	1.07E-06	1.34E-06	6.34E-07
650	1.60E-06	7.14E-07	1.10E-06	1.39E-06	6.88E-07
700	1.61E-06	7.26E-07	1.13E-06	1.47E-06	7.30E-07
750	1.61E-06	7.33E-07	1.18E-06	1.52E-06	7.88E-07
800	1.60E-06	7.43E-07	1.21E-06	1.58E-06	8.33E-07
850	1.62E-06	7.54E-07	1.23E-06	1.64E-06	8.89E-07
900	1.63E-06	7.65E-07	1.26E-06	1.67E-06	9.36E-07
950	1.62E-06	7.71E-07	1.29E-06	1.71E-06	9.64E-07
1000	1.64E-06	7.86E-07	1.29E-06	1.73E-06	1.02E-06

6). Table S6. The correction ratios between particle-in-the-box approximation and harmonic

oscillator model calculated from Multiwell package

T	ortho-adduct	ipso-adduct	para-adduct	meta-adduct	benzyl radical + H_2O
210	1.28	1.34	1.28	1.27	1.33
230	1.25	1.26	1.26	1.34	1.25
250	1.20	1.25	1.22	1.27	1.31
277	1.18	1.23	1.25	1.23	1.26
300	1.18	1.17	1.19	1.21	1.20
350	1.12	1.15	1.18	1.18	1.17
400	1.13	1.14	1.14	1.14	1.16
450	1.10	1.11	1.11	1.13	1.13
500	1.08	1.10	1.10	1.09	1.09
550	1.08	1.06	1.08	1.10	1.09
600	1.06	1.06	1.06	1.09	1.10
650	1.05	1.07	1.07	1.09	1.10
700	1.04	1.07	1.09	1.08	1.10
750	1.06	1.07	1.07	1.08	1.06
800	1.06	1.06	1.06	1.06	1.07
850	1.05	1.06	1.07	1.04	1.04
900	1.04	1.03	1.05	1.05	1.03
950	1.03	1.03	1.05	1.05	1.06
1000	1.00	1.01	1.09	1.09	1.00

7). Table S7. Final rate coefficients(cm^3 $molecule^{-1}$ s^{-1}) for various channels at 1atm.

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.53E-13	9.43E-14	3.25E-12	1.26E-13	2.34E-15	4.47E-15
230	3.00E-13	1.13E-13	2.84E-12	1.31E-13	2.95E-15	5.67E-15
250	2.72E-13	1.21E-13	2.49E-12	1.34E-13	3.87E-15	7.45E-15
277	2.44E-13	1.38E-13	2.23E-12	1.49E-13	5.77E-15	1.10E-14
300	2.20E-13	1.54E-13	2.11E-12	1.53E-13	8.17E-15	1.54E-14
350	2.03E-13	1.92E-13	1.84E-12	1.78E-13	1.69E-14	3.08E-14
400	1.98E-13	2.31E-13	1.75E-12	1.98E-13	3.23E-14	5.70E-14
450	1.94E-13	2.72E-13	1.60E-12	2.15E-13	5.73E-14	9.80E-14
500	1.91E-13	2.92E-13	1.44E-12	2.27E-13	9.49E-14	1.58E-13
550	1.79E-13	3.04E-13	1.25E-12	2.22E-13	1.48E-13	2.42E-13
600	1.65E-13	2.91E-13	1.01E-12	2.05E-13	2.20E-13	3.55E-13
650	1.47E-13	2.64E-13	7.94E-13	1.81E-13	3.14E-13	4.99E-13
700	1.25E-13	2.26E-13	6.04E-13	1.53E-13	4.32E-13	6.79E-13
750	1.03E-13	1.87E-13	4.56E-13	1.23E-13	5.77E-13	9.00E-13
800	8.23E-14	1.50E-13	3.35E-13	9.65E-14	7.50E-13	1.16E-12

850	6.73E-14				9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.90E-16	4.82E-13	1.92E-22	2.86E-24	5.09E-23	2.01E-24
230	1.12E-15	4.10E-13	9.36E-22	1.95E-23	2.47E-22	1.35E-23
250	1.46E-15	4.02E-13	3.94E-21	1.00E-22	1.02E-21	7.41E-23
277	2.20E-15	3.75E-13	2.17E-20	7.46E-22	5.77E-21	6.05E-22
300	3.13E-15	3.58E-13	7.57E-20	3.42E-21	2.17E-20	2.77E-21
350	6.63E-15	3.73E-13	8.23E-19	5.63E-20	2.36E-19	4.83E-20
400	1.30E-14	4.20E-13	5.75E-18	5.24E-19	1.63E-18	4.57E-19
450	2.38E-14	4.72E-13	2.77E-17	3.20E-18	7.44E-18	2.79E-18
500	4.06E-14	5.32E-13	1.00E-16	1.36E-17	2.55E-17	1.21E-17
550	6.53E-14	6.29E-13	2.82E-16	4.48E-17	6.96E-17	4.00E-17
600	9.99E-14	7.50E-13	6.63E-16	1.19E-16	1.58E-16	1.07E-16
650	1.46E-13	8.70E-13	1.33E-15	2.70E-16	3.17E-16	2.45E-16
700	2.07E-13	1.01E-12	2.35E-15	5.39E-16	5.73E-16	4.98E-16
750	2.83E-13	1.11E-12	3.81E-15	9.85E-16	9.65E-16	9.19E-16
800	3.76E-13	1.27E-12	5.74E-15	1.67E-15	1.53E-15	1.58E-15
850	4.89E-13	1.38E-12	8.21E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.57E-13	1.74E-12	1.96E-14	8.73E-15	6.54E-15	8.52E-15

8). Table S8. Final rate coefficients(cm^3 $molecule^{-1}$ s^{-1}) for various channels at 0.1, 0.4, 0.6, 0.8, 1.2atm.

0.1atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.40E-13	9.46E-14	3.09E-12	1.26E-13	2.29E-15	4.39E-15
230	2.91E-13	1.13E-13	2.73E-12	1.31E-13	2.92E-15	5.63E-15
250	2.66E-13	1.21E-13	2.41E-12	1.34E-13	3.86E-15	7.43E-15
277	2.40E-13	1.36E-13	2.16E-12	1.48E-13	5.77E-15	1.10E-14
300	2.16E-13	1.51E-13	2.02E-12	1.50E-13	8.19E-15	1.55E-14
350	1.95E-13	1.81E-13	1.67E-12	1.67E-13	1.70E-14	3.10E-14
400	1.79E-13	1.99E-13	1.42E-12	1.70E-13	3.27E-14	5.76E-14
450	1.57E-13	2.02E-13	1.09E-12	1.60E-13	5.81E-14	9.95E-14
500	1.32E-13	1.80E-13	7.95E-13	1.39E-13	9.64E-14	1.61E-13

550	1.02E-13	1.51E-13	5.51E-13	1.10E-13	1.50E-13	2.46E-13
600	7.62E-14	1.17E-13	3.62E-13	8.21E-14	2.23E-13	3.59E-13
650	5.52E-14	8.66E-14	2.34E-13	5.92E-14	3.17E-13	5.04E-13
700	3.86E-14	6.15E-14	1.48E-13	4.14E-14	4.35E-13	6.84E-13
750	2.72E-14				5.80E-13	9.05E-13
800					7.53E-13	1.17E-12
850					9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.69E-16	4.33E-13	1.79E-21	2.56E-23	4.18E-22	1.73E-23
230	1.10E-15	3.84E-13	8.49E-21	1.61E-22	1.85E-21	1.08E-22
250	1.46E-15	3.86E-13	3.41E-20	7.67E-22	6.86E-21	5.37E-22
277	2.20E-15	3.67E-13	1.73E-19	4.97E-21	3.29E-20	3.72E-21
300	3.14E-15	3.54E-13	5.57E-19	1.98E-20	1.05E-19	1.48E-20
350	6.67E-15	3.73E-13	4.72E-18	2.34E-19	8.11E-19	1.83E-19
400	1.32E-14	4.22E-13	2.44E-17	1.56E-18	3.98E-18	1.25E-18
450	2.42E-14	4.77E-13	8.69E-17	7.02E-18	1.39E-17	5.70E-18
500	4.13E-14	5.39E-13	2.37E-16	2.35E-17	3.84E-17	1.96E-17
550	6.63E-14	6.38E-13	5.28E-16	6.38E-17	8.97E-17	5.44E-17
600	1.01E-13	7.60E-13	1.02E-15	1.49E-16	1.85E-16	1.30E-16
650	1.48E-13	8.80E-13	1.78E-15	3.08E-16	3.47E-16	2.75E-16
700	2.08E-13	1.02E-12	2.85E-15	5.85E-16	6.05E-16	5.31E-16
750	2.84E-13	1.12E-12	4.32E-15	1.04E-15	9.97E-16	9.58E-16
800	3.77E-13	1.28E-12	6.28E-15	1.73E-15	1.56E-15	1.62E-15
850	4.90E-13	1.38E-12	8.71E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.39E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.11E-15	4.77E-15	5.92E-15
1000	9.56E-13	1.74E-12	1.96E-14	8.72E-15	6.54E-15	8.51E-15

856

857 0.4atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.45E-13	9.45E-14	3.16E-12	1.26E-13	2.32E-15	4.43E-15
230	2.96E-13	1.13E-13	2.79E-12	1.31E-13	2.93E-15	5.65E-15
250	2.69E-13	1.21E-13	2.45E-12	1.34E-13	3.86E-15	7.44E-15
277	2.42E-13	1.37E-13	2.21E-12	1.49E-13	5.77E-15	1.10E-14
300	2.18E-13	1.53E-13	2.08E-12	1.52E-13	8.17E-15	1.54E-14
350	2.01E-13	1.90E-13	1.80E-12	1.76E-13	1.69E-14	3.08E-14
400	1.94E-13	2.23E-13	1.66E-12	1.91E-13	3.24E-14	5.72E-14

450	1.84E-13	2.52E-13	1.44E-12	1.99E-13	5.76E-14	9.86E-14
500	1.72E-13	2.54E-13	1.20E-12	1.97E-13	9.55E-14	1.59E-13
550	1.51E-13	2.44E-13	9.58E-13	1.78E-13	1.49E-13	2.44E-13
600	1.29E-13	2.15E-13	7.15E-13	1.51E-13	2.22E-13	3.57E-13
650	1.06E-13	1.80E-13	5.18E-13	1.23E-13	3.16E-13	5.02E-13
700	8.33E-14	1.43E-13	3.66E-13	9.66E-14	4.34E-13	6.82E-13
750	6.39E-14	1.10E-13	2.57E-13	7.22E-14	5.79E-13	9.02E-13
800	4.92E-14				7.52E-13	1.17E-12
850					9.56E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.79E-16	4.57E-13	4.74E-22	7.00E-24	1.22E-22	8.79E-16
230	1.11E-15	3.97E-13	2.30E-21	4.69E-23	5.80E-22	1.11E-15
250	1.46E-15	3.94E-13	9.58E-21	2.37E-22	2.32E-21	1.46E-15
277	2.19E-15	3.71E-13	5.18E-20	1.70E-21	1.26E-20	2.19E-15
300	3.14E-15	3.56E-13	1.77E-19	7.48E-21	4.49E-20	3.14E-15
350	6.64E-15	3.73E-13	1.79E-18	1.10E-19	4.31E-19	6.64E-15
400	1.31E-14	4.20E-13	1.13E-17	9.03E-19	2.59E-18	1.31E-14
450	2.40E-14	4.74E-13	4.85E-17	4.85E-18	1.05E-17	2.40E-14
500	4.09E-14	5.35E-13	1.56E-16	1.84E-17	3.23E-17	4.09E-14
550	6.58E-14	6.33E-13	3.96E-16	5.52E-17	8.13E-17	6.58E-14
600	1.01E-13	7.55E-13	8.47E-16	1.37E-16	1.75E-16	1.01E-13
650	1.47E-13	8.75E-13	1.58E-15	2.94E-16	3.36E-16	1.47E-13
700	2.07E-13	1.02E-12	2.65E-15	5.69E-16	5.95E-16	2.07E-13
750	2.83E-13	1.11E-12	4.13E-15	1.02E-15	9.87E-16	2.83E-13
800	3.77E-13	1.28E-12	6.06E-15	1.73E-15	1.56E-15	3.77E-13
850	4.90E-13	1.38E-12	8.72E-15	2.74E-15	2.34E-15	4.90E-13
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	6.23E-13
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	7.77E-13
1000	9.56E-13	1.74E-12	1.96E-14	8.72E-15	6.54E-15	9.56E-13

0.6atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.48E-13	9.44E-14	3.20E-12	1.26E-13	2.33E-15	4.45E-15
230	2.97E-13	1.13E-13	2.81E-12	1.31E-13	2.94E-15	5.66E-15
250	2.70E-13	1.21E-13	2.47E-12	1.34E-13	3.87E-15	7.45E-15
277	2.43E-13	1.38E-13	2.22E-12	1.49E-13	5.77E-15	1.10E-14
300	2.19E-13	1.53E-13	2.09E-12	1.53E-13	8.17E-15	1.54E-14

350	2.02E-13	1.91E-13	1.82E-12	1.77E-13	1.69E-14	3.08E-14
400	1.96E-13	2.27E-13	1.71E-12	1.95E-13	3.24E-14	5.71E-14
450	1.89E-13	2.62E-13	1.52E-12	2.07E-13	5.74E-14	9.83E-14
500	1.82E-13	2.72E-13	1.31E-12	2.11E-13	9.52E-14	1.59E-13
550	1.64E-13	2.72E-13	1.09E-12	1.99E-13	1.49E-13	2.43E-13
600	1.46E-13	2.49E-13	8.42E-13	1.75E-13	2.21E-13	3.56E-13
650	1.24E-13	2.16E-13	6.32E-13	1.48E-13	3.15E-13	5.01E-13
700	1.01E-13	1.77E-13	4.61E-13	1.20E-13	4.33E-13	6.81E-13
750	7.97E-14	1.41E-13	3.34E-13	9.22E-14	5.78E-13	9.01E-13
800	6.23E-14	1.11E-13		7.19E-14	7.52E-13	1.16E-12
850					9.56E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.83E-16	4.67E-13	3.18E-22	4.72E-24	8.33E-23	3.31E-24
230	1.11E-15	4.03E-13	1.55E-21	3.19E-23	4.00E-22	2.21E-23
250	1.46E-15	3.97E-13	6.49E-21	1.63E-22	1.62E-21	1.20E-22
277	2.20E-15	3.73E-13	3.54E-20	1.19E-21	9.01E-21	9.56E-22
300	3.13E-15	3.57E-13	1.22E-19	5.34E-21	3.30E-20	4.28E-21
350	6.63E-15	3.73E-13	1.28E-18	8.31E-20	3.36E-19	7.02E-20
400	1.31E-14	4.20E-13	8.51E-18	7.22E-19	2.15E-18	6.20E-19
450	2.39E-14	4.73E-13	3.85E-17	4.11E-18	9.17E-18	3.52E-18
500	4.08E-14	5.34E-13	1.31E-16	1.64E-17	2.95E-17	1.44E-17
550	6.56E-14	6.32E-13	3.47E-16	5.11E-17	7.68E-17	4.50E-17
600	1.00E-13	7.53E-13	7.71E-16	1.30E-16	1.69E-16	1.16E-16
650	1.47E-13	8.73E-13	1.48E-15	2.85E-16	3.30E-16	2.58E-16
700	2.07E-13	1.02E-12	2.54E-15	5.59E-16	5.88E-16	5.13E-16
750	2.83E-13	1.11E-12	4.01E-15	1.01E-15	9.80E-16	9.36E-16
800	3.77E-13	1.28E-12	5.94E-15	1.70E-15	1.56E-15	1.60E-15
850	4.90E-13	1.38E-12	8.72E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.56E-13	1.74E-12	1.96E-14	8.72E-15	6.54E-15	8.51E-15

860

861 0.8atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.51E-13	9.43E-14	3.23E-12	1.26E-13	2.34E-15	4.46E-15
230	2.99E-13	1.13E-13	2.83E-12	1.31E-13	2.94E-15	5.67E-15
250	2.71E-13	1.21E-13	2.48E-12	1.34E-13	3.87E-15	7.45E-15

277	2.44E-13	1.38E-13	2.22E-12	1.49E-13	5.77E-15	1.10E-14
300	2.19E-13	1.53E-13	2.10E-12	1.53E-13	8.17E-15	1.54E-14
350	2.02E-13	1.92E-13	1.83E-12	1.78E-13	1.69E-14	3.08E-14
400	1.97E-13	2.29E-13	1.74E-12	1.97E-13	3.23E-14	5.70E-14
450	1.92E-13	2.68E-13	1.57E-12	2.12E-13	5.73E-14	9.82E-14
500	1.87E-13	2.84E-13	1.38E-12	2.20E-13	9.50E-14	1.59E-13
550	1.73E-13	2.90E-13	1.18E-12	2.12E-13	1.48E-13	2.43E-13
600	1.57E-13	2.73E-13	9.37E-13	1.92E-13	2.21E-13	3.55E-13
650	1.37E-13	2.43E-13	7.21E-13	1.66E-13	3.15E-13	5.00E-13
700	1.14E-13	2.04E-13	5.39E-13	1.38E-13	4.33E-13	6.80E-13
750	9.24E-14	1.66E-13	3.99E-13	1.09E-13	5.78E-13	9.01E-13
800	7.38E-14	1.34E-13		8.68E-14	7.51E-13	1.16E-12
850	5.83E-14				9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.87E-16	4.76E-13	2.40E-22	3.56E-24	6.31E-23	2.50E-24
230	1.11E-15	4.07E-13	1.17E-21	2.42E-23	3.05E-22	1.68E-23
250	1.46E-15	4.00E-13	4.90E-21	1.24E-22	1.25E-21	9.15E-23
277	2.20E-15	3.74E-13	2.69E-20	9.17E-22	7.03E-21	7.41E-22
300	3.13E-15	3.57E-13	9.35E-20	4.17E-21	2.62E-20	3.36E-21
350	6.63E-15	3.73E-13	1.00E-18	6.70E-20	2.77E-19	5.72E-20
400	1.31E-14	4.20E-13	6.85E-18	6.06E-19	1.85E-18	5.25E-19
450	2.39E-14	4.73E-13	3.21E-17	3.59E-18	8.20E-18	3.11E-18
500	4.07E-14	5.33E-13	1.13E-16	1.48E-17	2.73E-17	1.31E-17
550	6.55E-14	6.30E-13	3.11E-16	4.77E-17	7.29E-17	4.23E-17
600	1.00E-13	7.51E-13	7.11E-16	1.24E-16	1.63E-16	1.11E-16
650	1.47E-13	8.71E-13	1.40E-15	2.77E-16	3.23E-16	2.51E-16
700	2.07E-13	1.02E-12	2.44E-15	5.49E-16	5.80E-16	5.05E-16
750	2.83E-13	1.11E-12	3.91E-15	9.96E-16	9.72E-16	9.27E-16
800	3.76E-13	1.28E-12	5.84E-15	1.68E-15	1.56E-15	1.59E-15
850	4.89E-13	1.38E-12	8.31E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.57E-13	1.74E-12	1.96E-14	8.73E-15	6.54E-15	8.52E-15

1.2atm

T(K)	R-> ipso-add	R-> meta-add	R-> ortho-add	R-> para-add	R-> meta-abs	R-> ortho-abs
210	3.55E-13	9.42E-14	3.27E-12	1.26E-13	2.35E-15	4.48E-15

230	3.01E-13	1.13E-13	2.85E-12	1.31E-13	2.95E-15	5.68E-15
250	2.73E-13	1.21E-13	2.50E-12	1.34E-13	3.87E-15	7.46E-15
277	2.45E-13	1.38E-13	2.24E-12	1.49E-13	5.77E-15	1.10E-14
300	2.20E-13	1.54E-13	2.11E-12	1.53E-13	8.17E-15	1.54E-14
350	2.03E-13	1.93E-13	1.84E-12	1.79E-13	1.69E-14	3.08E-14
400	1.99E-13	2.32E-13	1.77E-12	1.99E-13	3.23E-14	5.69E-14
450	1.95E-13	2.75E-13	1.63E-12	2.18E-13	5.72E-14	9.80E-14
500	1.94E-13	2.98E-13	1.48E-12	2.32E-13	9.47E-14	1.58E-13
550	1.83E-13	3.14E-13	1.30E-12	2.30E-13	1.48E-13	2.42E-13
600	1.72E-13	3.06E-13	1.07E-12	2.15E-13	2.20E-13	3.54E-13
650	1.55E-13	2.82E-13	8.55E-13	1.93E-13	3.14E-13	4.98E-13
700	1.34E-13	2.45E-13	6.61E-13	1.66E-13	4.32E-13	6.79E-13
750	1.12E-13	2.06E-13	5.06E-13	1.35E-13	5.77E-13	8.99E-13
800	9.08E-14	1.67E-13	3.77E-13	1.08E-13	7.49E-13	1.16E-12
850	7.54E-14				9.55E-13	1.47E-12
900					1.19E-12	1.83E-12
950					1.45E-12	2.23E-12
1000					1.75E-12	2.69E-12

T(K)	R-> para-abs	R-> methyl-abs	R-> ipso-subs	R-> meta-subs	R-> ortho-subs	R-> para-subs
210	8.92E-16	4.88E-13	1.60E-22	2.39E-24	4.26E-23	1.68E-24
230	1.12E-15	4.13E-13	7.82E-22	1.63E-23	2.07E-22	1.13E-23
250	1.47E-15	4.04E-13	3.29E-21	8.42E-23	8.56E-22	6.23E-23
277	2.20E-15	3.76E-13	1.82E-20	6.29E-22	4.90E-21	5.12E-22
300	3.13E-15	3.58E-13	6.36E-20	2.90E-21	1.86E-20	2.35E-21
350	6.63E-15	3.73E-13	6.98E-19	4.85E-20	2.06E-19	4.19E-20
400	1.30E-14	4.20E-13	4.96E-18	4.62E-19	1.46E-18	4.06E-19
450	2.38E-14	4.72E-13	2.43E-17	2.89E-18	6.83E-18	2.54E-18
500	4.06E-14	5.32E-13	9.03E-17	1.26E-17	2.39E-17	1.13E-17
550	6.52E-14	6.28E-13	2.60E-16	4.24E-17	6.66E-17	3.80E-17
600	9.98E-14	7.49E-13	6.22E-16	1.15E-16	1.54E-16	1.03E-16
650	1.46E-13	8.69E-13	1.27E-15	2.63E-16	3.11E-16	2.40E-16
700	2.06E-13	1.01E-12	2.28E-15	5.30E-16	5.66E-16	4.91E-16
750	2.82E-13	1.11E-12	3.72E-15	9.74E-16	9.58E-16	9.10E-16
800	3.76E-13	1.27E-12	5.64E-15	1.66E-15	1.52E-15	1.57E-15
850	4.89E-13	1.38E-12	8.12E-15	2.74E-15	2.34E-15	2.60E-15
900	6.23E-13	1.51E-12	1.17E-14	4.17E-15	3.40E-15	4.00E-15
950	7.77E-13	1.70E-12	1.53E-14	6.12E-15	4.77E-15	5.92E-15
1000	9.57E-13	1.74E-12	1.96E-14	8.73E-15	6.54E-15	8.52E-15

9) Table S9. The computed RRKM/ME rate coefficients (cm^3 $molecule^{-1}$ s^{-1}) in the format of $k=A\cdot T^n\cdot\exp(-E_a/RT)$ at 210-1000K, 1atm.

	A (cm^3 $molecule^{-1}$)	n	E_a (kcal mol^{-1})
R-> ipso-add	2.45E-09	-1.50	0.36
R-> meta-add	3.19E-11	-0.62	1.07
R-> ortho-add	2.45E-07	-1.88	0.51
R-> para-add	2.82E-09	-1.37	1.12
R-> meta-abs	1.16E-22	3.46	0.92
R-> ortho-abs	5.33E-12	3.29	0.80
R-> para -abs	1.40E-21	3.05	1.43
R-> methyl-abs	4.37E-14	0.53	0.35
R-> ipso-subs	8.42E-13	0.17	9.75
R-> meta-subs	5.94E-18	1.79	10.07
R-> ortho-subs	1.28E-17	1.53	8.64
R-> para-subs	4.45E-17	1.53	10.60

10) Table S10. The branching ratios from previous studies at ~300K, 1atm

Ref.	**Branching ratios**	**Method or technique**
this work	ipso-add (7.3%), meta-add (5.1%), ortho-add (69.8%), para-add (5.1%), methyl-abs (11.9%)	CCSD(T)-F12/ccpVQZ-F12//B2PLYP-D3/6-311++G(d,p) μVTST
Suh et al.[1]	ipso-add (3%), meta-add (11%), ortho-add (52%), para-add (34%)	B3LYP/6-31G(d,p); TST
Ji et al.[2]	meta-add (34%), ortho-add (75.8), para-add (20.8)	QCISD(T)/6-311+G(2d,p) //M06-2X/6-311G(d,p); CVTST
Uc et al.[3]	ipso-add (13%), meta-add (17%), ortho-add (42%), para-add (17%), methyl-abs (10%)	CBS-QB3; TST
Wu et al.[4]	ipso-add (15%), meta-add (59%), ortho-add (5%), para-add (14%)	ROCBS-QB3//M06-2X/6 311++G(2df,2p); TST
Zhang et al.[5]	ipso-add (4.2%), meta-add (3.4%), ortho-add (59.9%), para-add (3.6%), methyl-abs (30.2%)	M08-SO/MG3S; MSCVT/SCT
Knispel et al.[6]	$k_{methy\text{-}abs}/k_{add}$＜0.022	FP-RF
Smith et al.[7]	methy-abs（0.067±0.07）	a
Klotz et al.[8]	methy-abs（0.067±0.07）	b

a: Derived from the measured yield of benzaldehyde [C6H5CHO] plus an estimated benzyl nitrate [C6H5CH2ONO2] yield in irradiated CH3ONO-NO-toluene-air mixtures at 298 K and atmospheric pressure of air.

b: Derived from the measured yield of benzaldehyde [C6H5CHO] plus an estimated benzyl nitrate [C6H5CH2ONO2] yield in irradiated NOx-toluene-air mixtures at 298 K and atmospheric pressure of air.

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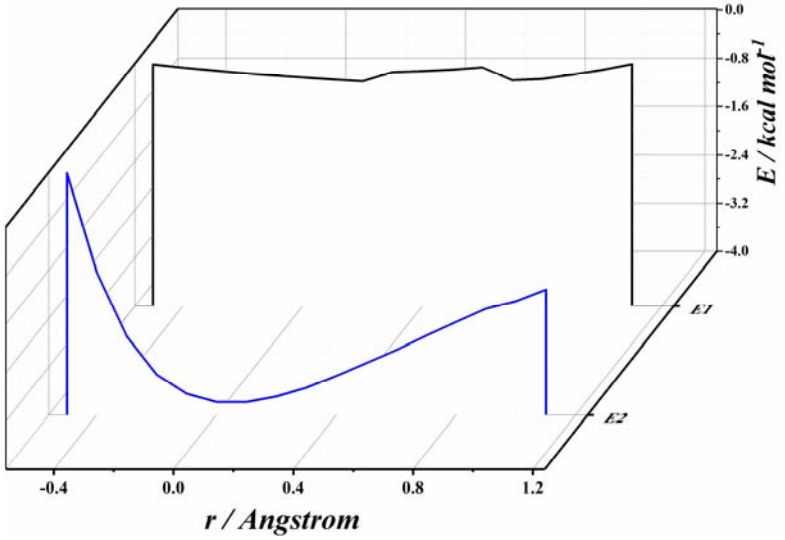
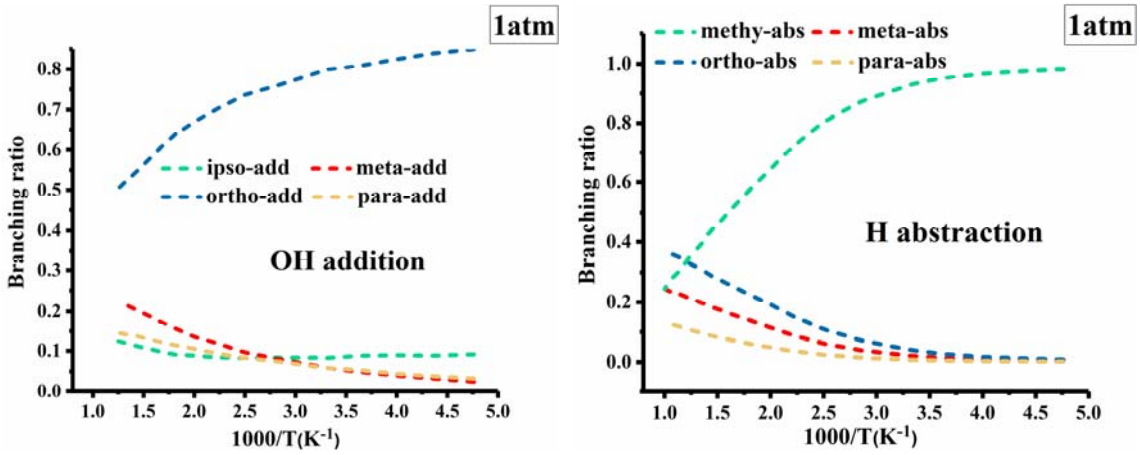
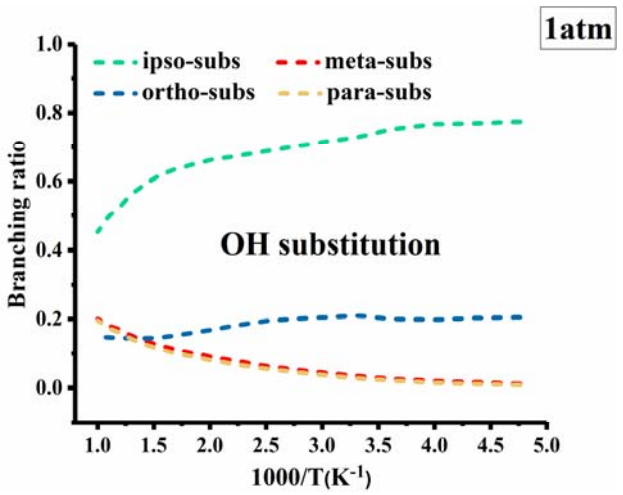
8. B. Klotz, S. Sørensen, I. Barnes and K. H. Becker, J. Phys. Chem. A, 1998, 102, 10289-10299.

11). Figure S1. Potential energy surface of the toluene-OH pre-reaction complex obtained at the B2PLYPD3/6-311++G(d,p) level. The OH radical was translated in both parallel (E1) and vertical direction (E2) on the benzene ring.



12). Figure S2. The detailed branching ratios for some stationary points in OH addition, H abstraction and OH substitution reaction





902
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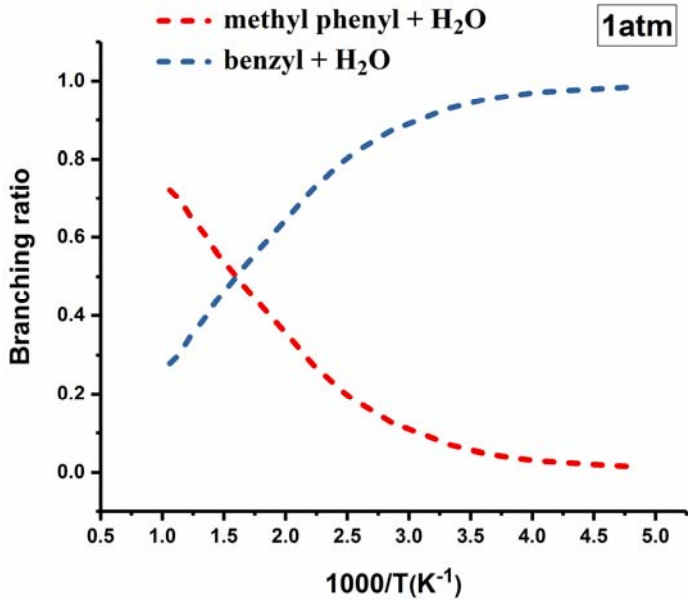
904
905 **13). Figure S3.** The detailed branching ratios for H-abstracton reaction
906



907
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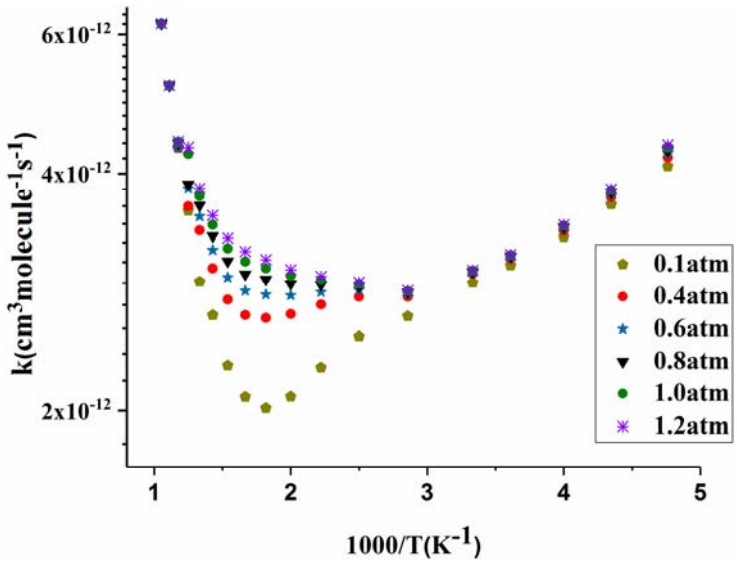
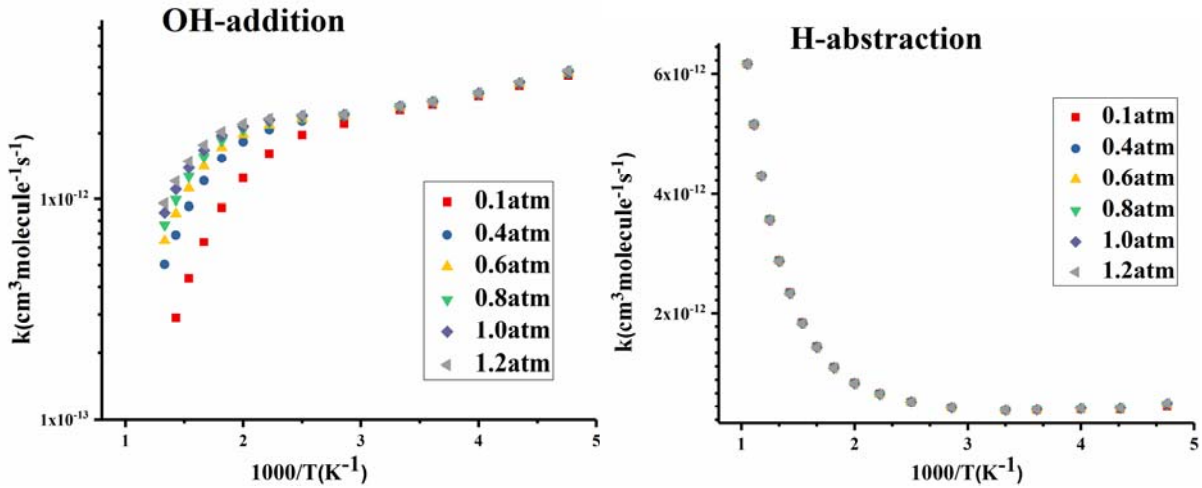
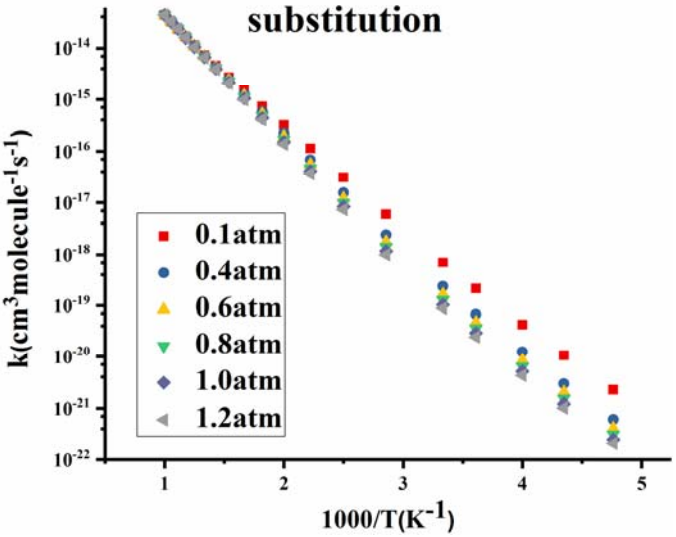
910 **14). Figure S4.** The total rate coefficients at 0.1, 0.4, 0.6, 0.8, 1.0, 1.2 atm

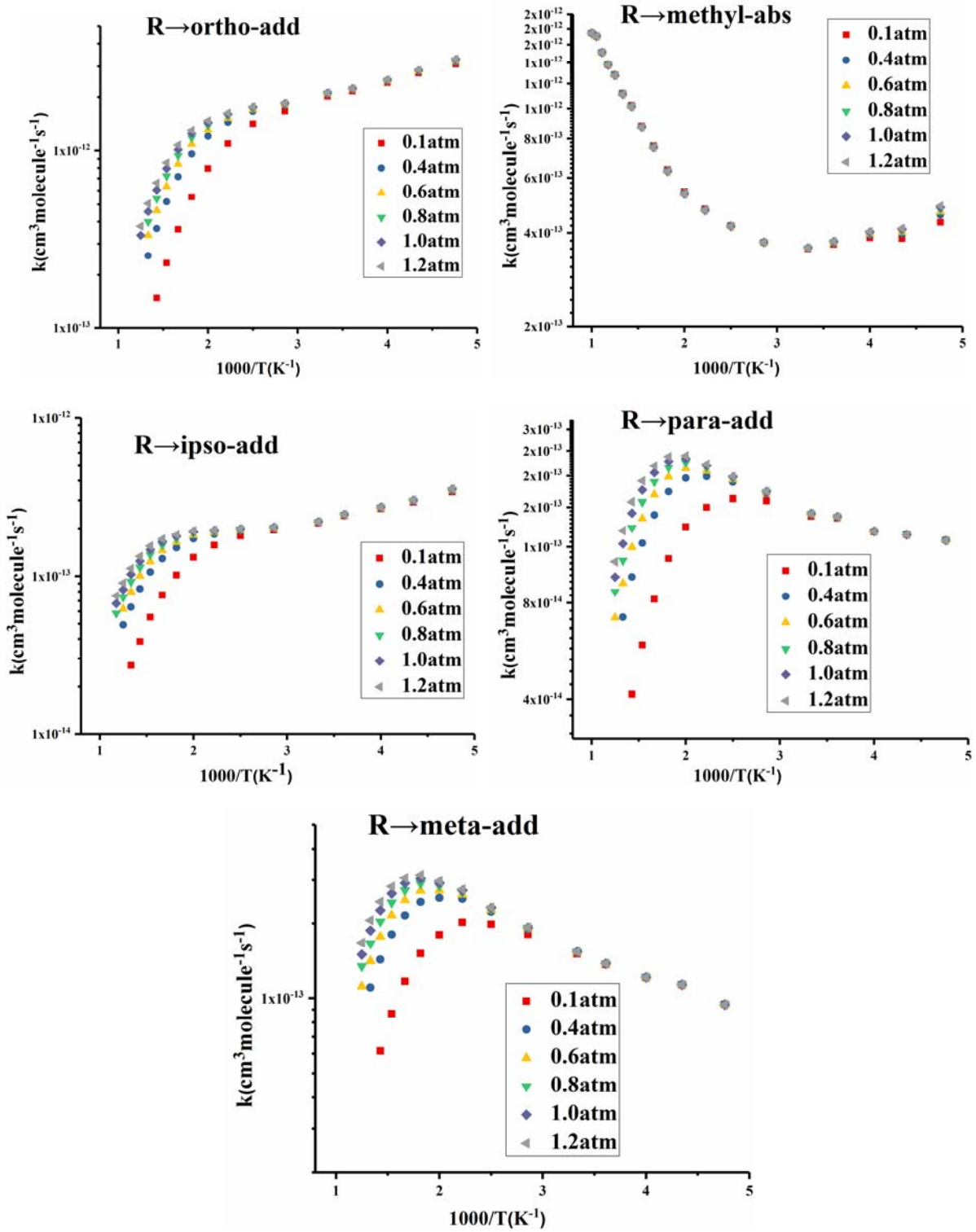


15). Figure S5. The rate coefficients for OH addition, H abstraction and substitution reaction at 0.1, 0.4, 0.6, 0.8, 1.0, 1.2atm

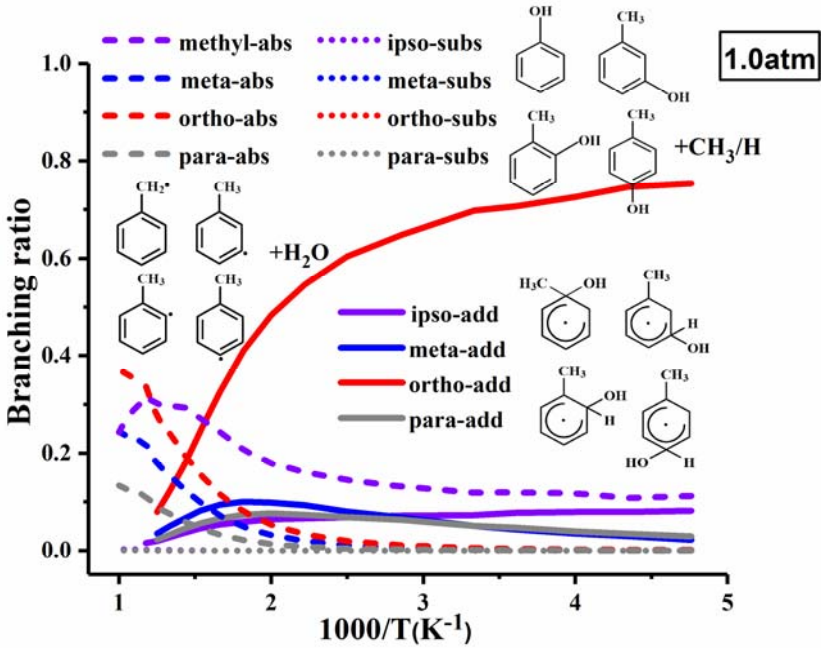




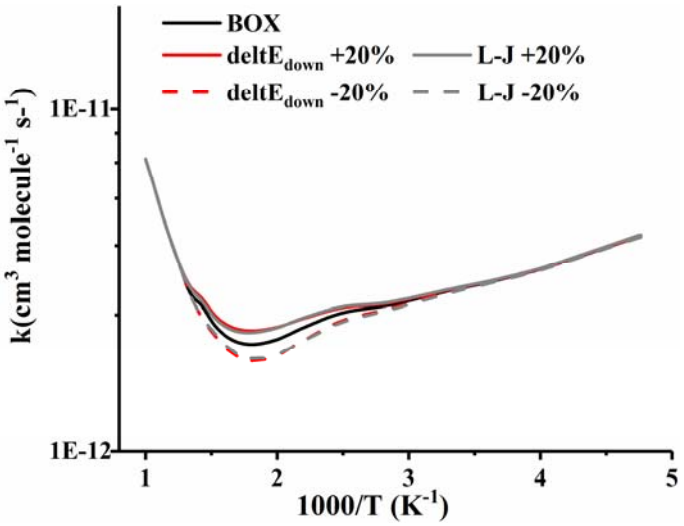
16). Figure S6. The rate coefficients for R-> ortho-add, R-> methyl-abs, R-> ipso-add, R-> para-add and R-> meta-add reactions at 0.1, 0.4, 0.6, 0.8, 1.0, 1.2atm



17). Figure S7. The branching ratio of various channels for OH + toluene.

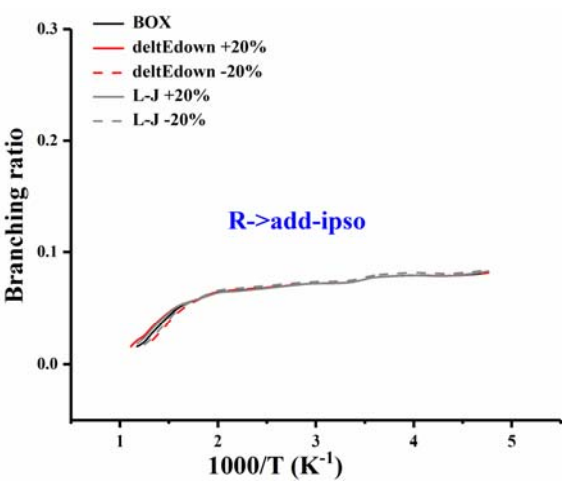


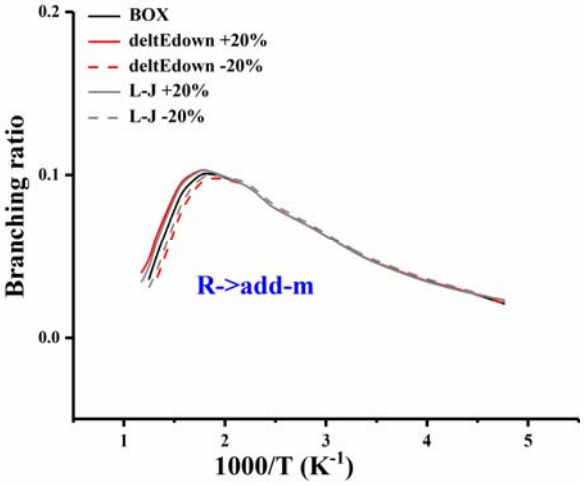
18). Figure S8. The uncertainty evaluation of the total rate coefficients at 0.1atm for collisional parameters



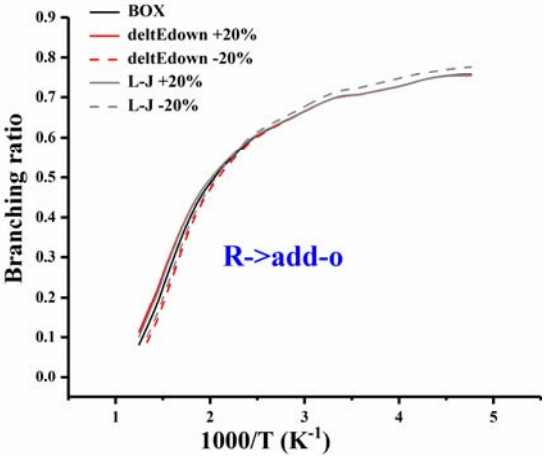
19). Figure S9. The uncertainty evaluation of the branching ratios at 1atm for collisional parameters

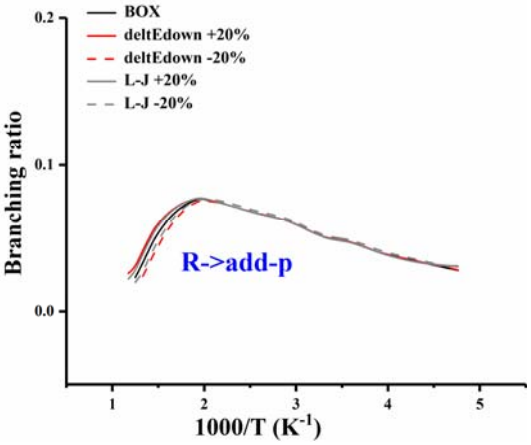
944


BOX
deltEdown +20%
deltEdown -20%
L-J +20%
L-J -20%
R->add-ipso
Branching ratio
1000/T (K-1)

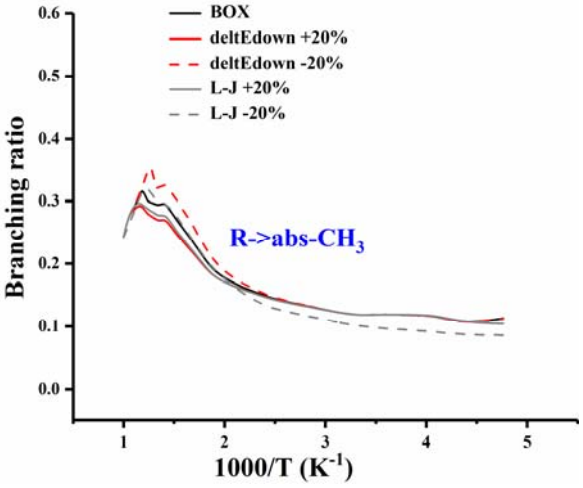

BOX
deltEdown +20%
deltEdown -20%
L-J +20%
L-J -20%
R->add-m
Branching ratio
1000/T (K-1)

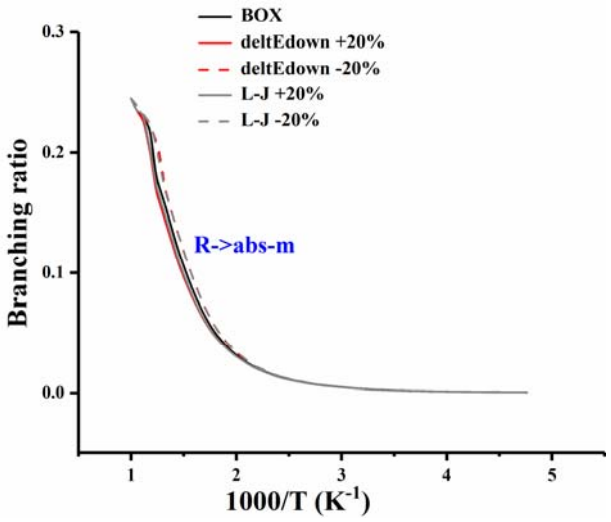
945

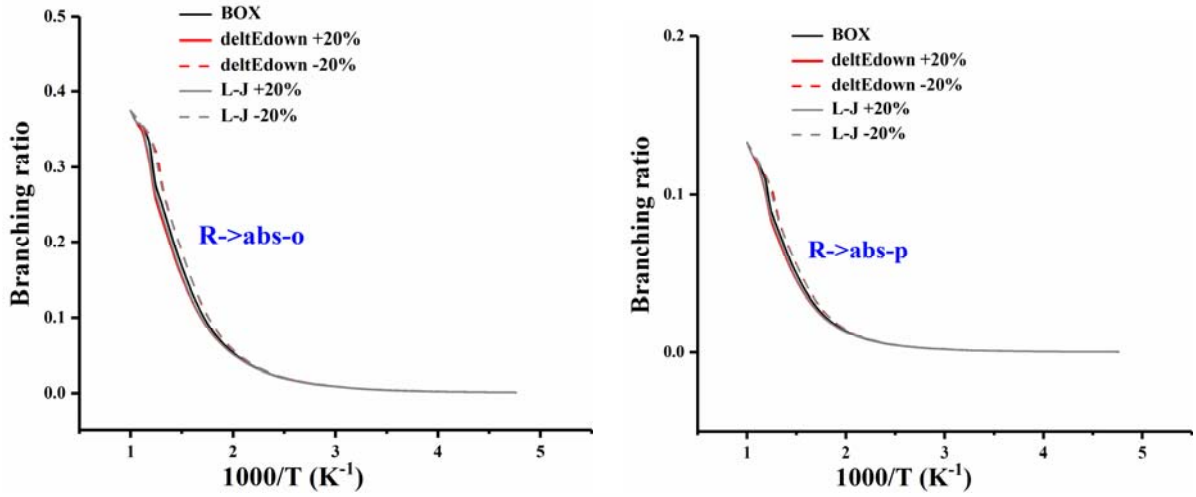

BOX
deltEdown +20%
deltEdown -20%
L-J +20%
L-J -20%
R->add-o
Branching ratio
1000/T (K-1)


BOX
deltEdown +20%
deltEdown -20%
L-J +20%
L-J -20%
R->add-p
Branching ratio
1000/T (K-1)

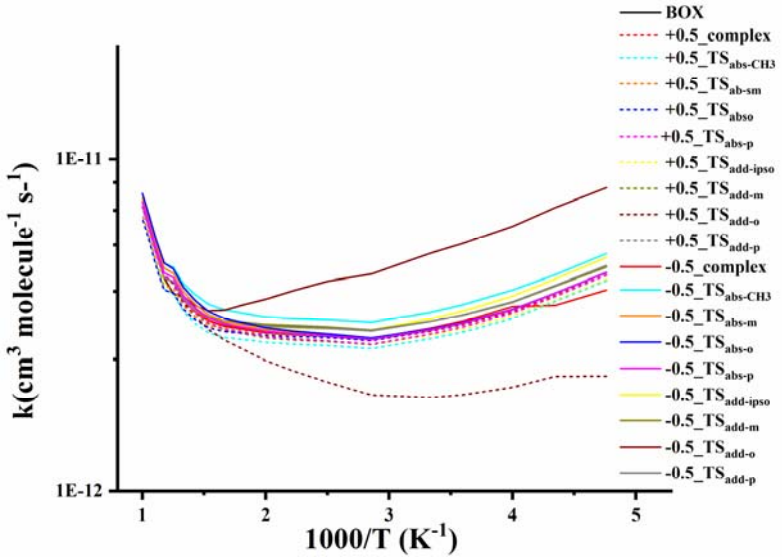
946


BOX
deltEdown +20%
deltEdown -20%
L-J +20%
L-J -20%
R->abs-CH3
Branching ratio
1000/T (K-1)

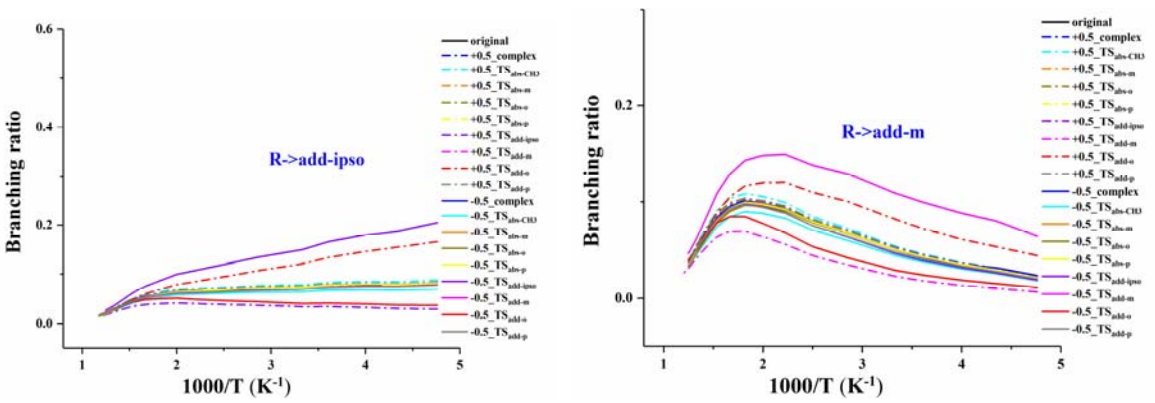

BOX
deltEdown +20%
deltEdown -20%
L-J +20%
L-J -20%
R->abs-m
Branching ratio
1000/T (K-1)

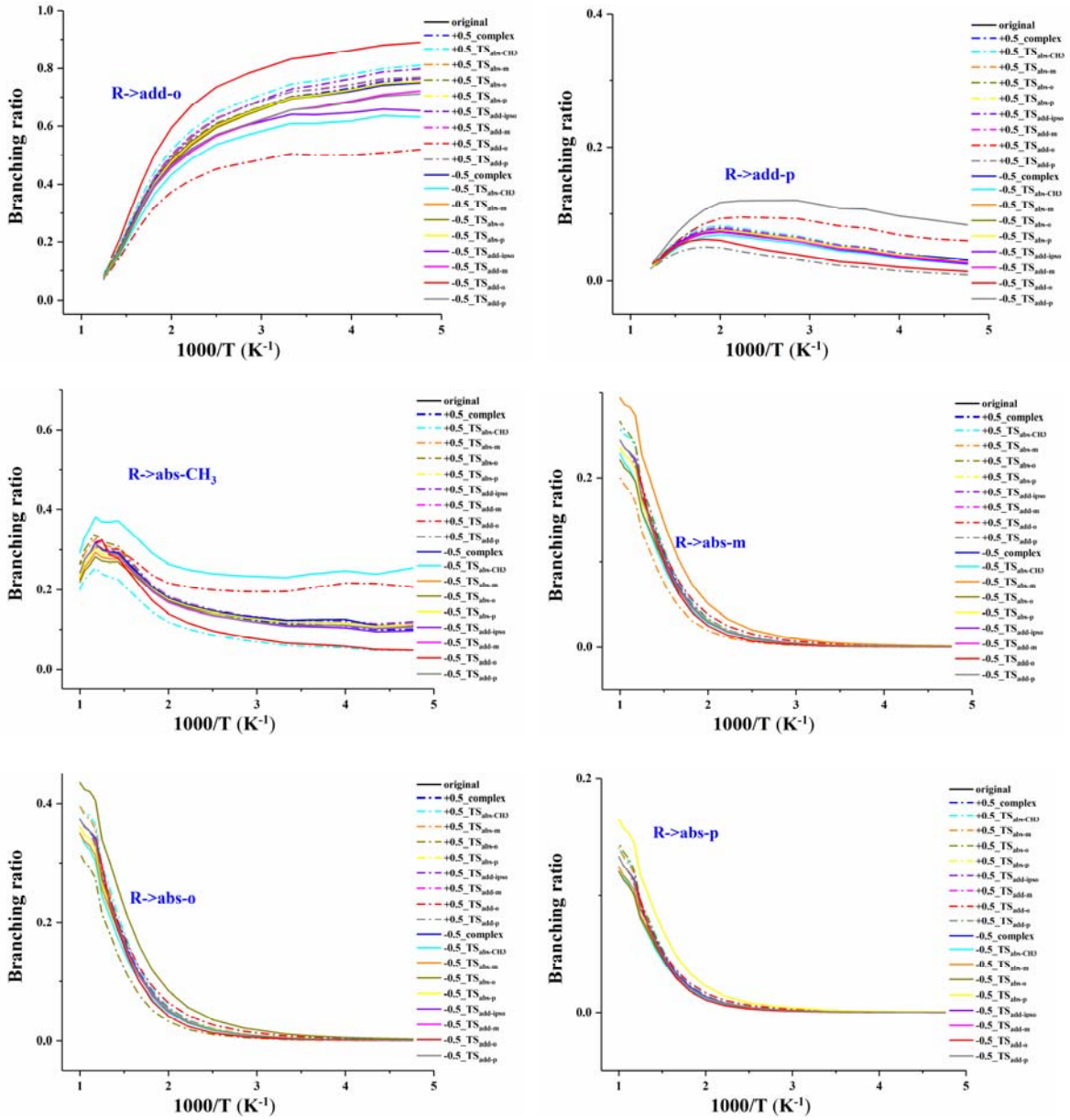


20). Figure S10. The uncertainty evaluation of the rate coefficients at 1atm for energy

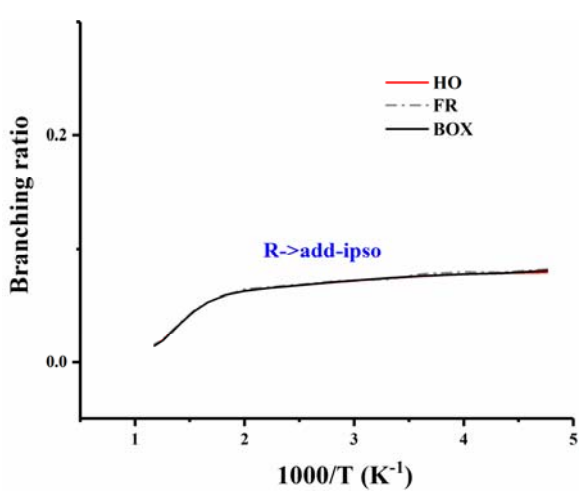


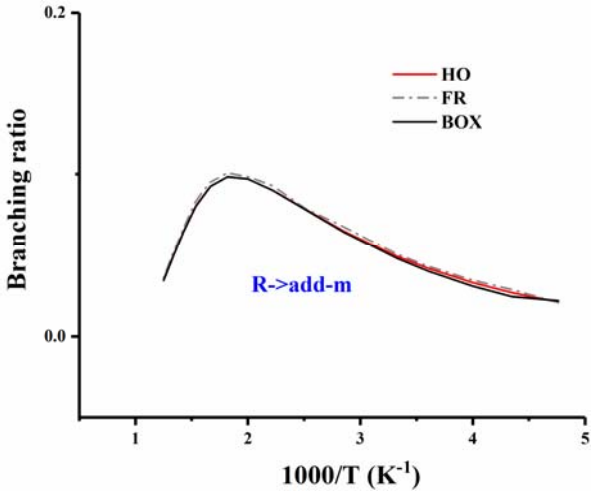
21). Figure S11. The uncertainty evaluation of the branching ratios at 1atm for energy



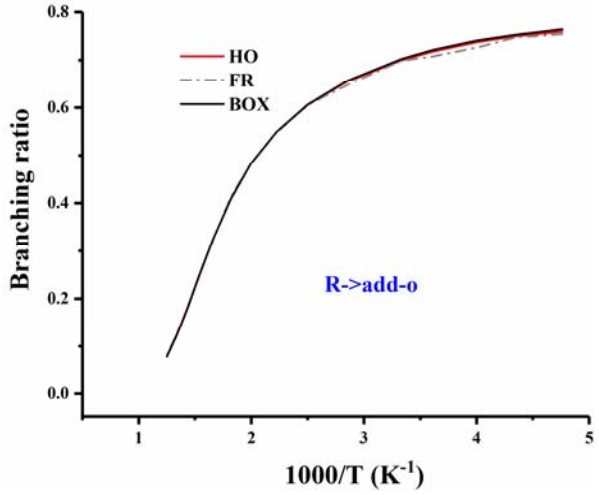


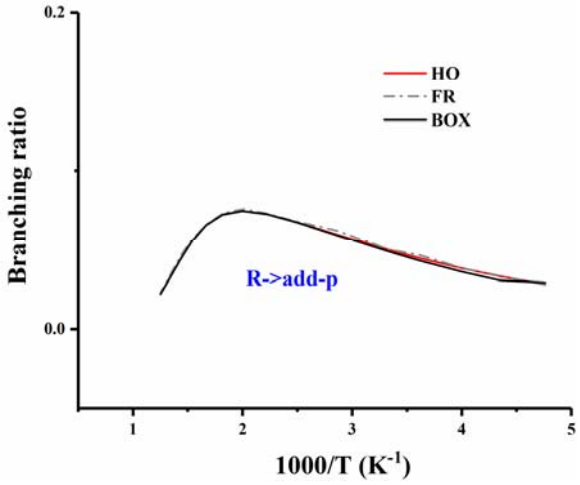
22). Figure S12. The uncertainty evaluation of the branching ratios at 1atm for anharmonic treatment



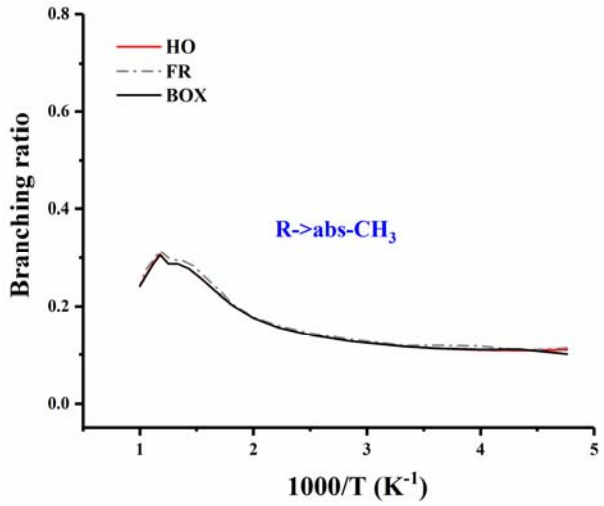


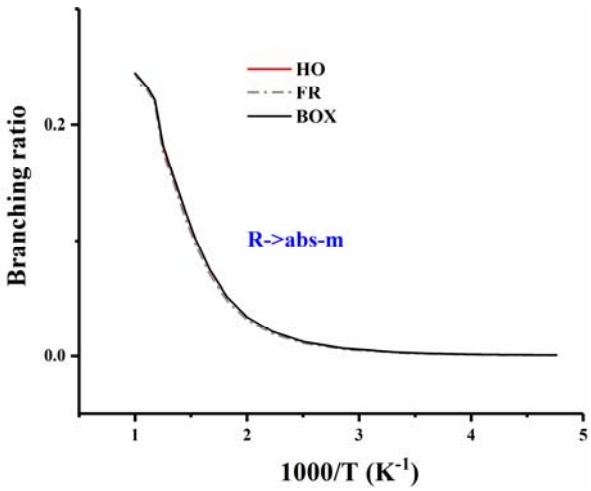
968





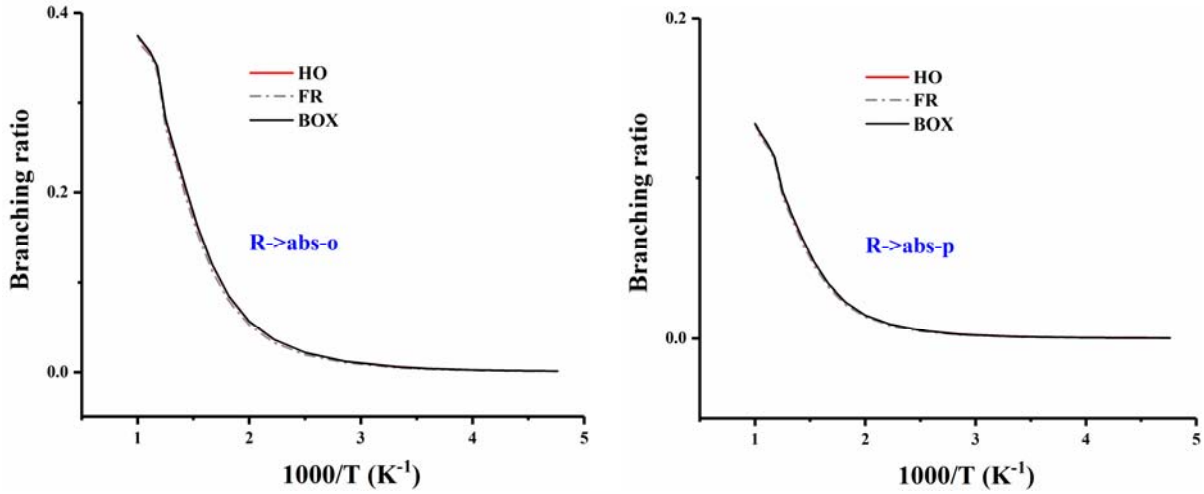
969





970

971



23). Table S11. The input for final rate coefficients for each channels at 300K.

```
!*************************************************
!                    GLOBAL SECTION
!*************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]                    300
PressureList[atm]                     0.1 0.4 0.6 0.8 1.0 1.2
!
!
EnergyStepOverTemperature             .2          ! [Discretization energy step
(global relax matrix)] / T
ExcessEnergyOverTemperature           50          ! [Highest barrier in the model
(global relax matrix)] / T
ModelEnergyLimit[kcal/mol]            400         ! Highest reference energy used
in the calculation ( or ReferenceEnergy[kcal/mol])
!
CalculationMethod                     direct      ! direct or low-eigenvalue
!
WellCutoff                            20          ! well truncation parameter :
Max { dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax                 0.2         ! Max chemical eigenvalue /
Lowest Collision relaxation eigenvalue
!
ReductionMethod                       diagonalization ! [low eigenvalue method
only] diagonalization or projection (default)
!
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!
```

```
!EnergyStepOverTemperature          0.3          #Ratio of discretization energy
step to T
!ExcessEnergyOverTemperature        40
!WellCutoff                         10
!ChemicalEigenvalueMin              1.e-6        #only for direct
diagonalization method
!!!!!!!!test!!!!!!!!!!!!!!!!!!!!!!!!!
RateOutput
rate_toluene+OH.out                        ! -0.5kcal/mol output file name for rate
coefficients
!LogOutput
thf_pyro.log                               ! log file name
!EigenvalueOutput
thf_pyro_eigval.out                        ! eigenvalue output file name
!EigenvectorOutput
thf_pyro_eigvect.out                       ! eigenvector output file name
!PEDOutput
thf_pyro_ped.out                           ! Product energy distributions file name
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!**************************************************
!                 MODEL SECTION
!**************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation                                                  !
Default collisional energy relaxation kernel
     Exponential                                                    !
Currently the only possible energy relaxation model
        Factor[1/cm]                260                             !
(Delta_E_down)^(0) @ standard T (300 K)
        Power                          0.875                        !
Power n in the expression (Delta_E_down) = (Delta_E_down)^(0) (T/T0)^(n)
        ExponentCutoff              10                              ! if
(Delta_E) / (Delta_E_down) > value    transition probability is zero
     End
!
  CollisionFrequency                                                !
Collision frequency model
     LennardJones                                                   !
Currently the only possible collisional frequency model    based on LJ potential
```

```
          Epsilons[K]                          48        561.62                          !
Epsilon_1 and Epsilon_2 N2 and 2-methylphenol
          Sigmas[angstrom]                     3.9       6.36                            !
Sigma_1 and Sigma_2
          Masses[amu]                          28.01     109.15                          !
Masses of the buffer gas molecule and of the complex (check order)
      End
!
!***********************************************
!
!*************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*************************************************
!   REACTANTS
!*************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*************************************************


   Bimolecular        R        # C6H5CH3 + OH
  Fragment REACT1
  RRHO
  Geometry[angstrom]                 15
     C                      -0.00763900   -1.19953600    1.20517200
    C                       -0.00763900    0.19581200    1.20217500
    C                       -0.00388100    0.91356100    0.00000000
    C                       -0.00763900    0.19581200   -1.20217500
    C                       -0.00763900   -1.19953600   -1.20517200
    C                       -0.00648200   -1.90320000    0.00000000
    H                       -0.01220200   -1.73580100    2.14733200
    H                       -0.01234000    0.73486900    2.14413000
    H                       -0.01234000    0.73486900   -2.14413000
    H                       -0.01220200   -1.73580100   -2.14733200
    H                       -0.00930500   -2.98687900    0.00000000
    C                        0.02927600    2.42117200    0.00000000
    H                        1.05986700    2.78965500    0.00000000
    H                       -0.46581000    2.82728400   -0.88435100
    H                       -0.46581000    2.82728400    0.88435100
     Core     RigidRotor
          SymmetryFactor      1.00000000000000
     End
  Rotor                                  Hindered
  Group    13   14   15
  Axis               12              1
  Symmetry             6
```

```
  Potential[kcal/mol]                   6
0.0000
-0.0070
0.0023
0.0044
0.0007
-0.0072
  End
        Frequencies[1/cm]                  38
   202.96       341.60       398.43       447.41       526.70       537.82       634.09
722.96
      800.02       840.70       882.53       915.15       936.50       967.28       977.87
1010.97
      1019.50      1070.19      1137.99      1159.51      1191.28      1296.73      1310.74
1369.93
      1417.20      1442.75      1454.09      1472.11      1565.98      1586.86      2927.97
2986.81
      3009.30      3052.75      3054.42      3067.12      3075.29      3087.53
   ZeroEnergy[kcal/mol]                  0.
   ElectronicLevels[1/cm]                          1
   0.000000000000000E+000     1.00000000000000
  End
  !***********************************
  Fragment REACT2
  RRHO
  Geometry[angstrom]                    2
  O                        0.00000000     0.00000000     0.10800700
  H                        0.00000000     0.00000000    -0.86405300
     Core     RigidRotor
          SymmetryFactor       1.00000000000000
     End
       Frequencies[1/cm]                  1
     3614.32
   ZeroEnergy[kcal/mol]                   0.
   ElectronicLevels[1/cm]                          1
   0.000000000000000E+000     2.00000000000000
  End
  GroundEnergy[kcal/mol] 0.0
  End
  !***********************************
      Well       W              # OHC6H5CH3
      Species
        RRHO
  Geometry[angstrom]                   17
  C                        0.98053000    -0.41677600     0.00000300
```

```
C                  0.26374200    -0.47554900     1.20263700
C                 -1.12900000    -0.58244200     1.20565300
C                 -1.83124600    -0.63613400     0.00000700
C                 -1.12900000    -0.58246600    -1.20564000
C                  0.26374300    -0.47557500    -1.20262800
H                  0.80056000    -0.43321500     2.14440900
H                 -1.66337000    -0.62475800     2.14756700
H                 -2.91142300    -0.71752500     0.00000700
H                 -1.66337100    -0.62480100    -2.14755300
H                  0.80056000    -0.43326100    -2.14440200
C                  2.47848900    -0.24830700     0.00000100
H                  2.92678100    -0.70407000     0.88472600
H                  2.92677900    -0.70407500    -0.88472200
H                  2.74571400     0.81268200    -0.00000200
O                 -0.36116300     2.76685000    -0.00002400
H                 -0.45646600     1.79772300    -0.00003400
   Core      RigidRotor
      SymmetryFactor       0.5                  ! chiral (similarly as below)
   End
       Rotor    Hindered                    !freq=60.98
          Group                                13 14 15
          Axis                                 12 1
          Symmetry                              3
   Potential[kcal/mol]          12
      -0.060 0.732 1.627 2.378 2.749 2.609 2.005 1.135 0.261 -0.389 -0.667 -0.525
      End
              Rotor    Hindered                    !freq=35.62
          Group                                17
          Axis                                 16 1
          Symmetry                              1
   Potential[kcal/mol]          36
        0.000 0.134 0.512 1.079 1.747 2.403 2.958 3.341 3.521 3.520 3.404 3.256
      3.151 3.143 3.254 3.465 3.712 3.914 3.997 3.937 3.752 3.508 3.286 3.155
      3.141 3.230 3.374 3.505 3.533 3.382 3.015 2.459 1.788 1.101 0.520 0.135
      End
     Frequencies[1/cm]                 43
  20.81 102.21 114.15 175.36 219.13 342.17 399.15
  460.29 527.08 631.74 646.79 735.07 800.12 853.75 897.15
  955.48 962.99 969.50 978.45 1010.64 1024.39 1070.20 1138.41
  1160.14 1192.36 1295.95 1308.98 1370.17 1414.50 1443.95 1453.14
  1471.03 1559.81 1582.95 2930.84 2991.98 3013.05 3058.03 3059.31
  3072.02 3079.39 3091.32 3594.43
  ZeroEnergy[kcal/mol]                -3.45
  ElectronicLevels[1/cm]                    1
  0.000000000000000E+000      2.00000000000000
```

```
End
End
!**********************************
  Barrier        B       R        W            # WR-TS
 Variational
   RRHO                                        1
     Geometry[angstrom]                       17
C                    0.00000000     0.00000000     0.00000000
C                    0.00000000     0.00000000     1.40127400
C                    1.19728500     0.00000000     2.12076900
C                    2.42052300     0.00356300     1.44750100
C                    2.43484200     0.00754900     0.05129400
C                    1.23446300     0.00753300    -0.66302900
H                   -0.94549900    -0.00407300     1.93317100
H                    1.17391800    -0.00163700     3.20428000
H                    3.35021200     0.00206200     2.00345300
H                    3.37832000     0.01181100    -0.48197700
H                    1.25566400     0.00935800    -1.74767100
C                   -1.29282800    -0.05335400    -0.77331300
H                   -2.10136800     0.43261200    -0.22420000
H                   -1.19322600     0.43813900    -1.74281700
H                   -1.58951400    -1.09077900    -0.95450900
O                    0.94431800    -3.27694000     0.55275800
H                    1.08798500    -2.31795200     0.64214700
     Core       RigidRotor
       SymmetryFactor                 0.5
     End
          Rotor    Hindered
       Group                                  13 14 15
       Axis                                   12 1
       Symmetry                               3
   Potential[kcal/mol]          12
        -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
     End
                          Rotor    Hindered
       Group                                  17
       Axis                                   16 1
       Symmetry                               1
   Potential[kcal/mol]          36
      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
      End
     Frequencies[1/cm]                        42
   30.74 156.68 157.92 208.66 342.34 400.75 460.03 527.11 635.03
```

```
646.75 735.09 800.37 852.23 898.21 954.38 964.33 969.35 978.58 1011.23
1025.49 1070.28 1140.10 1160.63 1192.79 1296.37 1310.10 1371.27 1416.65 1444.66
1453.53 1471.14 1565.20 1582.71 2930.50 2991.63 3013.39 3058.18 3059.94 3072.00
3079.45 3091.28 3594.39
    ZeroEnergy[kcal/mol]                -3.44
    ElectronicLevels[1/cm]          1
            0          2
End
!**********************************
   RRHO                                        5
    Geometry[angstrom]                  17
C                   0.00000000     0.00000000     0.00000000
C                   0.00000000     0.00000000     1.40127400
C                   1.19728500     0.00000000     2.12076900
C                   2.42052300     0.00356300     1.44750100
C                   2.43484200     0.00754900     0.05129400
C                   1.23446300     0.00753300    -0.66302900
H                  -0.94549900    -0.00407300     1.93317100
H                   1.17391800    -0.00163700     3.20428000
H                   3.35021200     0.00206200     2.00345300
H                   3.37832000     0.01181100    -0.48197700
H                   1.25566400     0.00935800    -1.74767100
C                  -1.29282800    -0.05335400    -0.77331300
H                  -2.10136800     0.43261200    -0.22420100
H                  -1.19322600     0.43813900    -1.74281700
H                  -1.58951400    -1.09077900    -0.95450900
O                   0.92255800    -3.67608700     0.53828700
H                   1.06622500    -2.71709900     0.62767600
    Core      RigidRotor
      SymmetryFactor            0.5
    End
         Rotor   Hindered
        Group                         13 14 15
        Axis                          12 1
        Symmetry                      3
  Potential[kcal/mol]        12
   -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
     End
                           Rotor   Hindered
        Group                         17
        Axis                          16 1
        Symmetry                      1
  Potential[kcal/mol]        36
     0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
     2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
```

```
0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
End
Frequencies[1/cm]	42
16.98 37.93 182.89 206.63 341.89 398.36 456.69 527.02 617.96
634.11 730.87 800.27 848.70 892.70 946.92 949.68 968.57 977.85 1010.57
1023.82 1069.76 1138.86 1159.98 1192.58 1295.80 1309.37 1371.02 1416.01 1444.36
1453.29 1471.00 1563.51 1583.28 2929.98 2990.99 3013.18 3057.39 3059.14 3071.37
3078.92 3090.89 3589.75
ZeroEnergy[kcal/mol]	-3.08
ElectronicLevels[1/cm]	1
0	2
End
!***********************************
RRHO	7
Geometry[angstrom]	17
C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40127400
C	1.19728500	0.00000000	2.12076900
C	2.42052300	0.00356300	1.44750100
C	2.43484200	0.00754900	0.05129400
C	1.23446300	0.00753300	-0.66302900
H	-0.94549900	-0.00407300	1.93317100
H	1.17391800	-0.00163700	3.20428000
H	3.35021200	0.00206200	2.00345300
H	3.37832000	0.01181100	-0.48197700
H	1.25566400	0.00935800	-1.74767100
C	-1.29282800	-0.05335400	-0.77331300
H	-2.10136800	0.43261200	-0.22420100
H	-1.19322600	0.43813900	-1.74281700
H	-1.58951400	-1.09077900	-0.95450900
O	0.91167800	-3.87566000	0.53105100
H	1.05534500	-2.91667100	0.62044000
Core	RigidRotor
SymmetryFactor	0.5
End
Rotor	Hindered
Group	13 14 15
Axis	12 1
Symmetry	3
Potential[kcal/mol]	12
-0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
End
Rotor	Hindered
Group	17
Axis	16 1
```

```
        Symmetry                    1
   Potential[kcal/mol]       36
      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
      End
     Frequencies[1/cm]                 42
 14.96 23.77    193.03 206.46 341.70 398.06 454.57 526.97 598.76
 633.99 728.89 800.22 847.13 890.10 941.38 944.25 968.25 977.62 1010.34 1022.90
 1069.54 1138.48 1159.70 1192.50 1295.51 1309.06 1370.86 1415.84 1444.17 1453.24
 1470.92 1563.24 1583.32 2929.79 2990.74 3013.09 3057.07 3058.81 3071.10
 3078.68 3090.72 3589.23
     ZeroEnergy[kcal/mol]              -2.67
     ElectronicLevels[1/cm]         1
             0        2
End
!**********************************
      RRHO                               8
     Geometry[angstrom]                17
C              0.00000000     0.00000000     0.00000000
C              0.00000000     0.00000000     1.40127400
C              1.19728500     0.00000000     2.12076900
C              2.42052300     0.00356300     1.44750100
C              2.43484200     0.00754900     0.05129400
C              1.23446300     0.00753300    -0.66302900
H             -0.94549900    -0.00407300     1.93317100
H              1.17391800    -0.00163700     3.20428000
H              3.35021200     0.00206200     2.00345300
H              3.37832000     0.01181100    -0.48197700
H              1.25566400     0.00935800    -1.74767100
C             -1.29282800    -0.05335400    -0.77331300
H             -2.10136800     0.43261200    -0.22420100
H             -1.19322600     0.43813900    -1.74281700
H             -1.58951400    -1.09077900    -0.95450900
O              0.90623800    -3.97544600     0.52743300
H              1.04990500    -3.01645800     0.61682200
     Core     RigidRotor
       SymmetryFactor          0.5
     End
        Rotor   Hindered
        Group                       13 14 15
        Axis                        12 1
        Symmetry                    3
   Potential[kcal/mol]       12
     -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
```

```
End
Rotor Hindered
Group 17
Axis 16 1
Symmetry 1
Potential[kcal/mol] 36
0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
End
Frequencies[1/cm] 42
15.09 24.11 197.19 206.26 341.62 397.98 453.48 526.94 588.73
633.94 727.99 800.18 846.42 888.91 937.43 943.10 968.09 977.52 1010.24
1022.45 1069.44 1138.31 1159.56 1192.46 1295.37 1308.93 1370.77 1415.77 1444.07
1453.22 1470.87 1563.15 1583.32 2929.70 2990.63 3013.05 3056.91 3058.66 3070.97
3078.57 3090.64 3589.21
ZeroEnergy[kcal/mol] -2.44
ElectronicLevels[1/cm] 1
0 2
End
!**********************************
RRHO 10
Geometry[angstrom] 17
C 0.00000000 0.00000000 0.00000000
C 0.00000000 0.00000000 1.40127400
C 1.19728500 0.00000000 2.12076900
C 2.42052300 0.00356300 1.44750100
C 2.43484200 0.00754900 0.05129400
C 1.23446300 0.00753300 -0.66302900
H -0.94549900 -0.00407300 1.93317100
H 1.17391800 -0.00163700 3.20428000
H 3.35021200 0.00206200 2.00345300
H 3.37832000 0.01181100 -0.48197700
H 1.25566400 0.00935800 -1.74767100
C -1.29282800 -0.05335400 -0.77331300
H -2.10136800 0.43261200 -0.22420100
H -1.19322600 0.43813900 -1.74281700
H -1.58951400 -1.09077900 -0.95450900
O 0.89535800 -4.17501900 0.52019700
H 1.03902500 -3.21603100 0.60958600
Core RigidRotor
SymmetryFactor 0.5
End
Rotor Hindered
Group 13 14 15
```

```
            Axis                                12 1
            Symmetry                            3
      Potential[kcal/mol]          12
          -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
          End
                                 Rotor    Hindered
            Group                               17
            Axis                                16 1
            Symmetry                            1
      Potential[kcal/mol]          36
          0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
          2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
          0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
          End
        Frequencies[1/cm]                       42
15.51 24.32    204.84 205.50 341.48 397.99 451.46 526.83 569.93
 633.89 726.43 800.13 845.20 886.86 930.51 941.19 967.83 977.35 1010.09
 1021.62 1069.28 1138.05 1159.32 1192.38 1295.12 1308.67 1370.56 1415.69 1443.86
 1453.24 1470.79 1563.03 1583.30 2929.56 2990.43 3012.98 3056.64 3058.38 3070.76
 3078.38 3090.51 3589.69
        ZeroEnergy[kcal/mol]                    -2.02
        ElectronicLevels[1/cm]              1
                0            2
End
!**********************************
       RRHO                                     12
        Geometry[angstrom]                      17
C                  0.00000000       0.00000000       0.00000000
C                  0.00000000       0.00000000       1.40127400
C                  1.19728500       0.00000000       2.12076900
C                  2.42052300       0.00356300       1.44750100
C                  2.43484200       0.00754900       0.05129400
C                  1.23446300       0.00753300      -0.66302900
H                 -0.94549900      -0.00407300       1.93317100
H                  1.17391800      -0.00163700       3.20428000
H                  3.35021200       0.00206200       2.00345300
H                  3.37832000       0.01181100      -0.48197700
H                  1.25566400       0.00935800      -1.74767100
C                 -1.29282800      -0.05335400      -0.77331300
H                 -2.10136800       0.43261200      -0.22420100
H                 -1.19322600       0.43813900      -1.74281700
H                 -1.58951400      -1.09077900      -0.95450900
O                  0.88447900      -4.37459200       0.51296100
H                  1.02814600      -3.41560300       0.60235000
        Core       RigidRotor
```

```
      SymmetryFactor          0.5
    End
        Rotor   Hindered
       Group                    13 14 15
       Axis                     12 1
       Symmetry                 3
  Potential[kcal/mol]     12
      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
     End
                        Rotor   Hindered
       Group                    17
       Axis                     16 1
       Symmetry                 1
  Potential[kcal/mol]     36
     0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
     2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
     0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
     End
    Frequencies[1/cm]               42
  15.78 24 197.35 217.04 341.49 399.57 448.98 526.58 553.99
  633.67 725.34 800.01 844.86 885.80 923.90 942.75 967.78 977.19 1009.90
  1020.84 1069.13 1137.73 1158.97 1192.22 1294.78 1308.40 1370.31 1415.26 1443.52
  1452.92 1470.67 1562.95 1583.22 2929.66 2990.49 3012.76 3056.33 3057.86 3070.58
  3078.15 3090.40 3590.32
    ZeroEnergy[kcal/mol]            -1.71
    ElectronicLevels[1/cm]        1
            0       2
End
!************************************
   RRHO                          14
    Geometry[angstrom]              17
C                0.00000000    0.00000000    0.00000000
C                0.00000000    0.00000000    1.40127400
C                1.19728500    0.00000000    2.12076900
C                2.42052300    0.00356300    1.44750100
C                2.43484200    0.00754900    0.05129400
C                1.23446300    0.00753300   -0.66302900
H               -0.94549900   -0.00407300    1.93317100
H                1.17391800   -0.00163700    3.20428000
H                3.35021200    0.00206200    2.00345300
H                3.37832000    0.01181100   -0.48197700
H                1.25566400    0.00935800   -1.74767100
C               -1.29282800   -0.05335400   -0.77331300
H               -2.10136800    0.43261200   -0.22420100
H               -1.19322600    0.43813900   -1.74281700
```

```
H                    -1.58951400     -1.09077900     -0.95450900
O                     0.87359900     -4.57416500      0.50572500
H                     1.01726600     -3.61517600      0.59511400
      Core      RigidRotor
        SymmetryFactor              0.5
      End
            Rotor   Hindered
          Group                              13 14 15
          Axis                               12 1
          Symmetry                           3
    Potential[kcal/mol]         12
      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
        End
                                     Rotor   Hindered
          Group                              17
          Axis                               16 1
          Symmetry                           1
    Potential[kcal/mol]         36
        0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
        2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
        0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
        End
      Frequencies[1/cm]                 42
  15.87 24.02   198.72 215.03 341.38 399.62 447.98 526.36 544.29
   633.71 724.51 799.98 844.03 884.74 920.69 941.27 967.59 977.08 1009.82
   1020.51 1069.02 1137.55 1158.81 1192.17 1294.61 1308.23 1370.19 1415.22 1443.43
   1452.86 1470.62 1562.89 1583.17 2929.53 2990.31 3012.72 3056.15 3057.69 3070.42
   3078.02 3090.31 3590.81
      ZeroEnergy[kcal/mol]              -1.37
      ElectronicLevels[1/cm]          1
                  0       2
End
!***********************************
      RRHO                                  16
      Geometry[angstrom]                17
C                     0.00000000      0.00000000      0.00000000
C                     0.00000000      0.00000000      1.40127400
C                     1.19728500      0.00000000      2.12076900
C                     2.42052300      0.00356300      1.44750100
C                     2.43484200      0.00754900      0.05129400
C                     1.23446300      0.00753300     -0.66302900
H                    -0.94549900     -0.00407300      1.93317100
H                     1.17391800     -0.00163700      3.20428000
H                     3.35021200      0.00206200      2.00345300
H                     3.37832000      0.01181100     -0.48197700
```

```
H          1.25566400    0.00935800    -1.74767100
C         -1.29282800   -0.05335400    -0.77331300
H         -2.10136800    0.43261200    -0.22420100
H         -1.19322600    0.43813900    -1.74281700
H         -1.58951400   -1.09077900    -0.95450900
O          0.86271900   -4.77373700     0.49848900
H          1.00638600   -3.81474900     0.58787800
     Core      RigidRotor
       SymmetryFactor          0.5
     End
         Rotor   Hindered
         Group                      13 14 15
         Axis                       12 1
         Symmetry                   3
   Potential[kcal/mol]      12
    -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
      End
                          Rotor   Hindered
         Group                      17
         Axis                       16 1
         Symmetry                   1
   Potential[kcal/mol]      36
      0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
      2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
      0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
      End
     Frequencies[1/cm]                42
16.00 24.33   199.41 211.94 341.29 399.79 447.60 526.16 539.30
 633.73 723.98 799.96 843.44 884.05 918.88 940.34 967.46 976.98 1009.76
 1020.32 1068.93 1137.40 1158.69 1192.13 1294.47 1308.07 1370.04 1415.19
 1443.36 1452.83 1470.58 1562.85 1583.12 2929.44 2990.18 3012.67 3056.00 3057.55
 3070.29 3077.91 3090.22 3591.51
     ZeroEnergy[kcal/mol]             -1.09
     ElectronicLevels[1/cm]        1
              0         2
End
!************************************
      RRHO                                19
     Geometry[angstrom]               17
C          0.00000000    0.00000000     0.00000000
C          0.00000000    0.00000000     1.40127400
C          1.19728500    0.00000000     2.12076900
C          2.42052300    0.00356300     1.44750100
C          2.43484200    0.00754900     0.05129400
C          1.23446300    0.00753300    -0.66302900
```

```
H     -0.94549900   -0.00407300    1.93317100
H      1.17391800   -0.00163700    3.20428000
H      3.35021200    0.00206200    2.00345300
H      3.37832000    0.01181100   -0.48197700
H      1.25566400    0.00935800   -1.74767100
C     -1.29282800   -0.05335400   -0.77331300
H     -2.10136800    0.43261200   -0.22420100
H     -1.19322600    0.43813900   -1.74281700
H     -1.58951400   -1.09077900   -0.95450900
O      0.84639900   -5.07309600    0.48763600
H      0.99006600   -4.11410800    0.57702500
      Core     RigidRotor
        SymmetryFactor          0.5
      End
          Rotor   Hindered
        Group                  13 14 15
        Axis                   12 1
        Symmetry               3
    Potential[kcal/mol]      12
      -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
       End
                           Rotor   Hindered
        Group                  17
        Axis                   16 1
        Symmetry               1
    Potential[kcal/mol]      36
       0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
       2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
       0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
       End
      Frequencies[1/cm]                 42
  4.16 6.31 200.10 207.33 341.20 400.12 447.77 526.07 536.79
  633.76 723.46 799.93 842.82 883.43 917.63 939.51 967.31 976.85 1009.68
  1020.25 1068.83 1137.22 1158.52 1192.07 1294.28 1307.88 1369.83 1415.14 1443.30
  1452.79 1470.53 1562.78 1583.06 2929.32 2990.01 3012.60 3055.80 3057.36 3070.13
  3077.78 3090.11 3592.05
      ZeroEnergy[kcal/mol]              -0.73
      ElectronicLevels[1/cm]         1
                 0        2
End
!************************************
       RRHO                                 23
      Geometry[angstrom]                17
C      0.00000000    0.00000000    0.00000000
C      0.00000000    0.00000000    1.40127400
```

```
C                          1.19728500      0.00000000      2.12076900
C                          2.42052300      0.00356300      1.44750100
C                          2.43484200      0.00754900      0.05129400
C                          1.23446300      0.00753300     -0.66302900
H                         -0.94549900     -0.00407300      1.93317100
H                          1.17391800     -0.00163700      3.20428000
H                          3.35021200      0.00206200      2.00345300
H                          3.37832000      0.01181100     -0.48197700
H                          1.25566400      0.00935800     -1.74767100
C                         -1.29282800     -0.05335400     -0.77331300
H                         -2.10136800      0.43261200     -0.22420100
H                         -1.19322600      0.43813900     -1.74281700
H                         -1.58951400     -1.09077900     -0.95450900
O                          0.82463900     -5.47224200      0.47316400
H                          0.96830600     -4.51325300      0.56255300
      Core       RigidRotor
        SymmetryFactor              0.5
      End
          Rotor    Hindered
         Group                               13 14 15
         Axis                                12 1
         Symmetry                            3
    Potential[kcal/mol]          12
       -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
       End
                         Rotor    Hindered
         Group                               17
         Axis                                16 1
         Symmetry                            1
    Potential[kcal/mol]          36
       0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
       2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
       0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
       End
      Frequencies[1/cm]                     42
  9.81 12.62 197.39 202.91 341.11 400.47 448.14 526.18 536.11
  633.78 722.95 799.90 842.17 882.82 916.77 938.70 967.18 976.70 1009.62
  1020.23 1068.72 1137.03 1158.35 1192.01 1294.10 1307.68 1369.55 1415.09 1443.22
  1452.76 1470.46 1562.70 1582.99 2929.22 2989.83 3012.51 3055.59 3057.17 3069.94
  3077.63 3090.01 3592.43
      ZeroEnergy[kcal/mol]                  -0.38
      ElectronicLevels[1/cm]            1
                0          2
End
!**********************************
```

```
      RRHO                              28
    Geometry[angstrom]                  17
C                  0.00000000    0.00000000    0.00000000
C                  0.00000000    0.00000000    1.40127400
C                  1.19728500    0.00000000    2.12076900
C                  2.42052300    0.00356300    1.44750100
C                  2.43484200    0.00754900    0.05129400
C                  1.23446300    0.00753300   -0.66302900
H                 -0.94549900   -0.00407300    1.93317100
H                  1.17391800   -0.00163700    3.20428000
H                  3.35021200    0.00206200    2.00345300
H                  3.37832000    0.01181100   -0.48197700
H                  1.25566400    0.00935800   -1.74767100
C                 -1.29282800   -0.05335400   -0.77331300
H                 -2.10136800    0.43261200   -0.22420100
H                 -1.19322600    0.43813900   -1.74281700
H                 -1.58951400   -1.09077900   -0.95450900
O                  0.79744000   -5.97117400    0.45507400
H                  0.94110700   -5.01218500    0.54446300
    Core     RigidRotor
      SymmetryFactor          0.5
    End
        Rotor   Hindered
        Group                        13 14 15
        Axis                         12 1
        Symmetry                     3
  Potential[kcal/mol]        12
     -0.045 0.736 1.620 2.369 2.747 2.618 2.033 1.186 0.322 -0.342 -0.658 -0.558
     End
                         Rotor   Hindered
        Group                        17
        Axis                         16 1
        Symmetry                     1
  Potential[kcal/mol]        36
     0.000 0.034 0.131 0.281 0.471 0.688 0.919 1.161 1.396 1.609 1.806 1.984
     2.148 2.298 2.438 2.568 2.687 2.799 2.908 3.014 3.111 3.194 3.245 3.230
     0.936 0.930 0.955 1.003 1.068 1.156 1.251 1.027 0.629 0.349 0.151 0.036
     End
    Frequencies[1/cm]                   42
 11.74 15.17 188.86 202.62 341.04 400.63 448.25 526.28 535.56
 633.78 722.42 799.86 841.51 882.17 915.82 937.80 967.05 976.59 1009.54
 1020.23 1068.62 1136.86 1158.21 1191.93 1293.95 1307.50 1369.27 1415.05 1443.14
 1452.75 1470.40 1562.62 1582.91 2929.14 2989.68 3012.42 3055.37 3056.99 3069.77
 3077.50 3089.90 3592.48
    ZeroEnergy[kcal/mol]                -0.11
```

```
        ElectronicLevels[1/cm]              1
                        0          2
End
End
!***********************************
  Bimolecular        P1m          # mCH3Phenyl   +   H2O
Fragment PROD1
RRHO
Geometry[angstrom]                    14
C                       -0.25343300    -1.24974700    -0.00962600
C                        1.12063000    -1.27682000     0.00330000
C                        1.95220100    -0.18048800     0.00814000
C                        1.31803200     1.07076900     0.00208400
C                       -0.07510300     1.15684400    -0.00917700
C                       -0.88065700     0.01164900    -0.01092400
H                        3.03200900    -0.26461200     0.01382700
H                        1.91641500     1.97551800     0.00091800
H                       -0.54683600     2.13347500    -0.01759400
C                       -2.38573500     0.11566100     0.00983300
H                       -2.71946100     1.06725300    -0.40772900
H                       -2.84460900    -0.69006400    -0.56654700
H                       -2.76623800     0.04899600     1.03346600
H                       -0.84688900    -2.15777400    -0.01812600
   Core     RigidRotor
       SymmetryFactor       1
   End
       Rotor                                    Hindered
Group     11 12 13
Axis                  10                 6
Symmetry                      3
Potential[kcal/mol]                    12
       0.000 0.009 0.021 0.032 0.033 0.023 0.011 0.001 -0.004 -0.007 -0.008 -0.004
End
     Frequencies[1/cm]                35
  200.87   344.21   407.23   463.45   517.58   576.53   626.64   738.76
  793.19   836.05   873.07   923.76   996.81   970.24   1017.51 1022.06
  1060.18 1137.13 1173.96 1253.92 1276.21 1367.83 1384.65 1434.92
  1441.41 1445.14 1513.69 1583.68 2929.90 2989.98 3012.02 3054.79
  3060.06 3070.22 3083.44
  ZeroEnergy[kcal/mol]                  0.
  ElectronicLevels[1/cm]                            1
  0.00000000000000E+000     1.00000000000000
End
!***********************************
Fragment PROD2
```

```
RRHO
        Geometry[angstrom]                 3
O                          0.00000000      0.00000000      0.11747400
H                          0.00000000      0.75947900     -0.46989500
H                          0.00000000     -0.75947900     -0.46989500
   Core     RigidRotor
        SymmetryFactor       2.00000000000000
   End
     Frequencies[1/cm]                  3
   1553.79 3699.35 3805.91
  ZeroEnergy[kcal/mol]                  0.
  ElectronicLevels[1/cm]                              1
  0.000000000000000E+000     1.00000000000000
End
GroundEnergy[kcal/mol]     -6.07
End
!***********************************
   Bimolecular        P1o       # oCH3Phenyl   +   H2O
Fragment PROD1
RRHO
Geometry[angstrom]                    14
C                          0.14867000     -1.19274800     -0.00000100
C                         -1.22413800     -1.23410100     -0.00000100
C                         -1.89314700      0.00117300      0.00000300
C                         -1.15453200      1.18376100      0.00000400
C                          0.24221200      1.15341600     -0.00000100
C                          0.94544000     -0.06409400     -0.00000200
H                         -1.77397100     -2.16810700      0.00000000
H                         -2.97702200      0.02887400      0.00000400
H                         -1.66697400      2.13864500      0.00000600
H                          0.80285000      2.08338700      0.00000200
C                          2.45142200     -0.12345000     -0.00000200
H                          2.87884500      0.88047600     -0.00004600
H                          2.82035800     -0.65347300      0.88114100
H                          2.82035100     -0.65354600     -0.88110400
   Core     RigidRotor
        SymmetryFactor       1
   End
        Rotor                                   Hindered
Group     12 13 14
Axis                  11                6
Symmetry                    3
Potential[kcal/mol]                   12
        0.000 0.007 0.031 0.068 0.104 0.131 0.138 0.130 0.102 0.067 0.031 0.008
End
```

```
        Frequencies[1/cm]                    35
      198.31    329.38    402.68    456.67    517.13    530.63    631.41
      731.66 798.40    827.87    898.19    909.03    986.62    968.42    1008.80
      1017.12    1093.50 1132.82 1184.06 1233.02 1288.52 1368.39 1391.00
      1423.69    1436.09 1453.82 1524.91 1583.80 2936.16 2997.04 3014.24
      3048.22    3061.97 3074.98 3085.53
    ZeroEnergy[kcal/mol]                    0.
    ElectronicLevels[1/cm]                              1
    0.000000000000000E+000      1.00000000000000
  End
  !************************************
  Fragment PROD2
  RRHO
        Geometry[angstrom]                  3
  O                        0.00000000      0.00000000      0.11747400
  H                        0.00000000      0.75947900     -0.46989500
  H                        0.00000000     -0.75947900     -0.46989500
    Core      RigidRotor
        SymmetryFactor       2.00000000000000
    End
      Frequencies[1/cm]                   3
  1553.79 3699.35 3805.91
    ZeroEnergy[kcal/mol]                    0.
    ElectronicLevels[1/cm]                              1
    0.000000000000000E+000      1.00000000000000
  End
  GroundEnergy[kcal/mol]     -6.28
  End
  !************************************
    Bimolecular        P1p       # pCH3Phenyl    +    H2O
  Fragment PROD1
  RRHO
  Geometry[angstrom]                    14
  C                       -0.13092100      1.20604100     -0.00869100
  C                        1.27190700      1.22137000      0.00276700
  C                        1.90400500     -0.00017400      0.00939800
  C                        1.27149500     -1.22163000      0.00271600
  C                       -0.13121100     -1.20591500     -0.00879500
  C                       -0.84250300      0.00021200     -0.01101100
  H                        1.81628900     -2.15837200      0.00207300
  H                       -0.67249200     -2.14708300     -0.01797400
  C                       -2.35158600      0.00011300      0.00950600
  H                       -2.75315000     -0.87818200     -0.49955400
  H                       -2.72979200     -0.01103200      1.03624300
  H                       -2.75296000      0.88921700     -0.48047800
```

```
H                          -0.67190900       2.14735800      -0.01781800
H                           1.81690500       2.15799300       0.00217000
    Core      RigidRotor
          SymmetryFactor       1
    End
          Rotor                                        Hindered
Group     10 11 12
Axis                  9                     5
Symmetry                     3
Potential[kcal/mol]                    12
          0.000 0.002 0.010 0.013 0.010 0.002 0.000 0.002 0.011 0.013 0.010 0.002
End
      Frequencies[1/cm]                   35
     216.70    343.63    395.03    444.07    530.64    582.26    615.27
     767.29     786.35    804.70    888.82    932.70    961.92    973.11    1016.78
     1021.61    1072.79 1140.64 1185.65 1259.22 1285.76 1346.06 1371.89
     1429.29    1443.45 1449.61 1546.28 1569.65 2929.45 2988.59 3010.86
     3050.68    3050.92 3076.31 3078.08
  ZeroEnergy[kcal/mol]                    0.
  ElectronicLevels[1/cm]                                  1
  0.000000000000000E+000      1.00000000000000
End
!************************************
Fragment PROD2
RRHO
          Geometry[angstrom]                  3
H                           0.00000000       0.76170000      -0.47894200
O                           0.00000000       0.00000000       0.11973600
H                           0.00000000      -0.76170000      -0.47894200
    Core      RigidRotor
          SymmetryFactor       2.00000000000000
    End
      Frequencies[1/cm]                    3
1553.79 3699.35 3805.91
  ZeroEnergy[kcal/mol]                    0.
  ElectronicLevels[1/cm]                                  1
  0.000000000000000E+000      1.00000000000000
End
GroundEnergy[kcal/mol]      -5.56
End
!************************************
  Barrier          B1m    W      P1m              # TS1m
     RRHO
        Geometry[angstrom]                            17
C                          -1.31246000      -0.41849100       0.01082200
```

```
C                    -1.50905200     0.96848800     0.05567700
C                    -0.43405900     1.85843300     0.02272800
C                     0.87852100     1.37826800    -6.67E-021400
C                     1.05248400     0.00411000    -0.09929300
C                     0.00588600    -0.90158100    -0.06066200
H                    -2.52260600     1.35769800     0.12012900
H                    -0.61567500     2.92977900     0.06015900
H                     1.72584700     2.05701400    -0.07575800
H                     2.24578000    -0.46049100    -0.21722000
H                     0.19667500    -1.97153300    -0.08975100
C                    -2.48278000    -1.37496700     0.01371700
H                    -3.35545700    -0.93687500     0.50923000
H                    -2.78401000    -1.63537000    -1.00962900
H                    -2.23537800    -2.31055900     0.52650800
O                     3.34835000    -0.90256800    -0.01580800
H                     3.36677500    -0.89466900     0.96054400
        Core        RigidRotor
          SymmetryFactor                0.5
        End
        Rotor                                   Hindered
Group     13 14 15
Axis                12                1
Symmetry                3
Potential[kcal/mol]                12
          0.000 -0.100 -0.175 -0.212 -0.205 -0.146 -0.056 0.040 0.110 0.149 0.141 0.082
End
      Rotor                                     Hindered
Group     17
Axis                16                2
Symmetry                1
Potential[kcal/mol]                36
          0.000 -0.060 -0.099 -0.111 -0.092 -0.038 0.063 0.217 0.430 0.701 0.998 1.306
          1.601 1.858 2.072 2.242 2.373 2.473 2.548 2.604 2.643 2.666 2.673 2.648
          0.621 0.657 0.734 0.841 0.972 0.966 0.972 1.005 0.435 0.293 0.176 0.079
End
        Tunneling          Eckart
          ImaginaryFrequency[1/cm]         1264
          WellDepth[kcal/mol]              7.62
          WellDepth[kcal/mol]              10.23
        End
        Frequencies[1/cm]                       42
    99.58     108.27    203.32    338.00    357.71    422.35    466.97    524.13
    557.71    644.34    741.77    770.72    855.45    860.48    887.81    931.90
    1004.59 1010.42 1055.49 1058.85 1099.01 1125.31 1188.74 1218.87
    1270.90 1318.77 1345.62 1423.09 1450.60 1498.37 1501.90 1509.93
```

```
    1600.91 1637.56 3045.41 3108.02 3130.74 3177.03 3189.49 3193.89
    3211.51 3783.29
        ZeroEnergy[kcal/mol]                 4.17
        ElectronicLevels[1/cm]            1
                  0         2
End
!***********************************
    Barrier      B1o   W    P1o          # TS1o
      RRHO
        Geometry[angstrom]                 17
C                    -1.31174500    -0.41955200     0.01115400
C                    -1.50972600     0.96596000     0.06143600
C                    -0.43532800     1.85575500     0.02418400
C                     0.87573700     1.37555800    -0.05560000
C                     1.05353000     0.00136800    -0.11185400
C                     0.00384400    -0.90271700    -0.06541600
H                    -2.52069400     1.35351600     0.13003400
H                    -0.61578500     2.92400600     0.06578700
H                     1.72072800     2.05212900    -0.08316800
H                     2.18564500    -0.43628900    -0.22681400
H                     0.19384500    -1.96974700    -0.10026500
C                    -2.48037900    -1.37337400     0.01489300
H                    -3.33475500    -0.94653200     0.54344200
H                    -2.80044900    -1.59955200    -1.00658700
H                    -2.21770900    -2.31753100     0.49565300
O                     3.35745800    -0.89830100    -0.00666300
H                     3.35391400    -0.89158700     0.96243200
        Core     RigidRotor
          SymmetryFactor             0.5
        End
              Rotor                                    Hindered
Group    13 14 15
Axis              12             1
Symmetry                3
Potential[kcal/mol]              12
        0.000 0.018 0.028 0.023 0.009 -0.015 -0.079 -0.098 -0.088 -0.050 -0.072 -0.044
End
     Rotor                                   Hindered
Group    17
Axis              16             6
Symmetry                1
Potential[kcal/mol]              36
         0.000 0.089 0.205 0.352 0.532 0.746 0.996 1.274 1.558 0.765 0.646 0.658
         0.691 0.737 0.795 0.863 0.921 0.979 0.984 0.987 0.997 1.002 1.031 0.471
         0.324 0.185 0.062 -0.034 -0.083 -0.058 0.060 0.270 0.539 0.812 1.036 1.227
```

```
End
      Tunneling      Eckart
        ImaginaryFrequency[1/cm]      1209
        WellDepth[kcal/mol]           7.30
        WellDepth[kcal/mol]           10.12
      End
      Frequencies[1/cm]                    42
    97.86 127.03 199.18 327.13 372.60 431.70 483.99 532.09 581.53 646.78
   740.84 774.59 829.68 846.16 921.85 935.38 970.04 986.81 1005.74 1020.96
   1049.26 1114.64 1138.48 1178.42 1211.77 1255.92 1295.87 1371.38 1409.63 1439.97
   1444.60 1457.77 1543.34 1573.66 2932.36 2993.19 3026.92 3053.22 3067.96 3079.73
   3089.68 3639.32
      ZeroEnergy[kcal/mol]                 3.85
      ElectronicLevels[1/cm]          1
                  0         2
End
!***********************************
   Barrier      B1p   W    P1p        # TS1p
    RRHO
      Geometry[angstrom]                   17
C                    -1.31174500   -0.41955200    0.01115400
C                    -1.50972600    0.96596000    0.06143600
C                    -0.43532800    1.85575500    0.02418400
C                     0.87573700    1.37555800   -0.05560000
C                     1.05353000    0.00136800   -0.11185400
C                     0.00384400   -0.90271700   -0.06541600
H                    -2.52069400    1.35351600    0.13003400
H                    -0.61578500    2.92400600    0.06578700
H                     1.72072800    2.05212900   -0.08316800
H                     2.18564500   -0.43628900   -0.22681400
H                     0.19384500   -1.96974700   -0.10026500
C                    -2.48037900   -1.37337400    0.01489300
H                    -3.33475500   -0.94653200    0.54344200
H                    -2.80044900   -1.59955200   -1.00658700
H                    -2.21770900   -2.31753100    0.49565300
O                     3.35745800   -0.89830100   -0.00666300
H                     3.35391400   -0.89158700    0.96243200
      Core      RigidRotor
        SymmetryFactor            1
      End
            Rotor                                Hindered
Group    13 14 15
Axis              12              1
Symmetry                3
Potential[kcal/mol]               12
```

```
            0.000 -0.002 0.000 0.002 0.004 0.003 -0.001 0.002 0.004 0.002 0.000 -0.002
End
    Rotor                                       Hindered
Group     17
Axis                  16                4
Symmetry                   1
Potential[kcal/mol]                36
             0.000 0.011 0.039 0.088 0.159 0.241 0.387 0.339 0.390 -0.535 -0.647 -0.711
             -0.733 -0.721 -0.682 -0.617 -0.530 -0.420 -0.286 -0.128 0.061 0.269 0.504 0.773
             1.076 1.390 1.674 1.872 1.981 2.030 2.049 2.050 2.037 2.014 1.976 1.921
End
      Tunneling          Eckart
         ImaginaryFrequency[1/cm]        1298
         WellDepth[kcal/mol]             7.88
         WellDepth[kcal/mol]             9.99
      End
     Frequencies[1/cm]                 42
   86.76 118.23 218.15 344.20 374.22 398.27 443.13 567.43 591.73 627.13
  754.08 791.85 821.76 822.87 908.30 945.54 967.52 982.11 1020.75 1032.33
  1032.39 1091.07 1149.62 1187.01 1219.70 1278.39 1295.49 1365.88 1370.45 1443.19
  1447.81 1462.49 1556.50 1563.74 2930.76 2990.73 3012.90 3056.85 3057.02 3084.51
  3085.59 3641.84
      ZeroEnergy[kcal/mol]                    4.43
      ElectronicLevels[1/cm]               1
                    0           2
End
!***********************************
   Bimolecular       P2        # C6H5CH2    +    H2O
Fragment PROD1
RRHO
Geometry[angstrom]                    14
C                       0.25231700      1.21362000      0.00000600
C                      -1.13207900      1.20859100      0.00001700
C                      -1.83606400      0.00000200     -0.00002900
C                      -1.13208300     -1.20859000     -0.00002600
C                       0.25231300     -1.21362000     -0.00003600
C                       0.98817300     -0.00000100      0.00001100
H                       0.79309900      2.15371800      0.00003900
H                      -1.67301500      2.14795900      0.00001200
H                      -2.91922800      0.00000200     -0.00001700
H                      -1.67302000     -2.14795700     -0.00006000
H                       0.79309500     -2.15371900     -0.00003600
C                       2.40133200     -0.00000200      0.00004900
H                       2.95780500     -0.92793000      0.00002300
H                       2.95780600      0.92792800      0.00008600
```

```
    Core      RigidRotor
         SymmetryFactor       1
    End
          Rotor  Hindered                    ! freq=375
            Group                                13 14
            Axis                                1 12
            Symmetry                             2
    Potential[kcal/mol]          18
          0.000 0.295 1.165 2.555 4.373 6.493 8.752 10.949 12.838 14.049 12.809 10.859
          8.594 6.299 4.190 2.421 1.094 0.276
         End
      Frequencies[1/cm]                35
     192.09 355.22 431.25 456.03 472.36 533.82 623.48 630.07 719.79 829.95
    838.15 876.01 914.62 940.52 976.50 963.58 1009.32 1080.72 1133.11 1141.75
    1232.11 1280.82 1305.32 1429.06 1440.71 1448.76 1546.36 1558.84 3047.04 3059.70
    3062.05 3074.18 3079.56 3092.51 3146.51
    ZeroEnergy[kcal/mol]                  0.
    ElectronicLevels[1/cm]                          1
    0.000000000000000E+000      2.00000000000000
  End
  !***********************************
  Fragment PROD2
  RRHO
         Geometry[angstrom]              3
  O                      0.00000000      0.00000000      0.11747400
  H                      0.00000000      0.75947900     -0.46989500
  H                      0.00000000     -0.75947900     -0.46989500
    Core      RigidRotor
         SymmetryFactor       2.00000000000000
    End
      Frequencies[1/cm]                3
    1553.79 3699.35 3805.91
    ZeroEnergy[kcal/mol]                  0.
    ElectronicLevels[1/cm]                          1
    0.000000000000000E+000      1.00000000000000
  End
  GroundEnergy[kcal/mol]     -28.76
  End
  !***********************************
   Barrier         B2    W      P2            # TS2
  Variational
  RRHO                    !                   1
  Geometry[angstrom]                17
  C                       0.31169200      0.00053800      0.60447400
  C                      -0.35961900      1.21539200      0.31234400
```

```
C        -1.64554000    1.20955000   -0.20059300
C        -2.30030700   -0.00051400   -0.45234400
C        -1.64505900   -1.21007300   -0.19937600
C        -0.35913700   -1.21486200    0.31358800
H         0.14191200    2.15460000    0.51794200
H        -2.14870400    2.14787500   -0.40260200
H        -3.31003500   -0.00091200   -0.84448900
H        -2.14783900   -2.14880400   -0.40044300
H         0.14277200   -2.15365900    0.52013900
C         1.58440400    0.00117000    1.22399800
H         2.05887900    0.93007400    1.51371900
H         2.05965800   -0.92768700    1.51419600
H         2.73551600    0.00014800   -0.36123600
O         3.18568600   -0.00093200   -1.21533300
H         2.46025300   -0.00113400   -1.84483800
   Core     RigidRotor
            SymmetryFactor      0.831548565
End
  Rotor                          Hindered
  Group    13    14     15    16   17
  Axis              12           1
  Symmetry             2
  Potential[kcal/mol]             18
0.000 0.302 1.140 2.508 4.336 6.509 8.874 11.201 13.222 14.572 13.350 11.324
9.051 6.688 4.548 2.744 1.404 0.611
  End
      Rotor                          Hindered
  Group    17
  Axis              16           15
  Symmetry             1
  Potential[kcal/mol]             36
      0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.012 0.022 0.025 0.028 0.032
      0.035 0.035 0.030 0.026 0.024 0.025 0.041 0.025 0.024 0.026 0.031 0.036
      0.035 0.032 0.028 0.025 0.022 0.012 0.000 -0.009 -0.014 -0.015 -0.011 -0.014
  End
     Frequencies[1/cm]            42
    141.24   191.60   213.51   301.96   350.73   384.72   412.49   441.87
    523.56   535.39   630.24   659.89   722.83   835.40   838.16   889.04
    926.71   949.71   980.20   967.38   1010.95 1081.94 1135.80 1144.49
    1228.28 1284.63 1307.39 1430.29 1440.77 1451.49 1550.42 1558.48
    1566.23 3037.39 3062.17 3064.85 3075.81 3082.15 3093.43 3138.95
    3568.48 3751.44
 ZeroEnergy[kcal/mol]    -28.62
  ElectronicLevels[1/cm]                1
    0.0000000000000000          2.0000000000000000
```

```
End
!*******************************************
RRHO                    !                    2
Geometry[angstrom]                  17
C                          0.32029000       0.00054100       0.58667700
C                         -0.35655100       1.21434400       0.30768800
C                         -1.64649500       1.20886300      -0.19630600
C                         -2.30165100      -0.00052600      -0.44876700
C                         -1.64599100      -1.20937200      -0.19511000
C                         -0.35604800      -1.21384400       0.30891900
H                          0.14554500       2.15389900       0.51039000
H                         -2.15115800       2.14765300      -0.39229700
H                         -3.31248900      -0.00092400      -0.83805500
H                         -2.15026600      -2.14856500      -0.39018200
H                          0.14642600      -2.15299300       0.51255200
C                          1.60878200       0.00111900       1.17531600
H                          2.08420800       0.93086700       1.46553600
H                          2.08450600      -0.92812600       1.46673300
H                          2.73019700      -0.00010600      -0.30501500
O                          3.15884900      -0.00088500      -1.17020300
H                          2.41386900      -0.00104100      -1.77535200
    Core     RigidRotor
               SymmetryFactor     0.831548565
End
 Rotor                                        Hindered
 Group     13     14        15     16    17
 Axis                   12                 1
 Symmetry                   2
 Potential[kcal/mol]                  18
0.000 0.373 1.265 2.682 4.551 6.751 9.123 11.433 13.404 14.658 13.177 11.113
8.790 6.473 4.360 2.597 1.310 0.574
 End
          Rotor                                        Hindered
 Group     17
 Axis                   16                 15
 Symmetry                   1
 Potential[kcal/mol]                  36
        0.000 -0.014 -0.012 -0.016 -0.014 -0.009 0.000 0.011 0.021 0.025 0.028 0.032
        0.037 0.037 0.032 0.027 0.024 0.025 0.015 0.026 0.024 0.027 0.032 0.037
        0.036 0.032 0.028 0.025 0.021 0.011 0.000 -0.009 -0.014 -0.016 -0.012 -0.014
 End
     Frequencies[1/cm]                  42
   131.41    194.57    199.39    317.79    350.06    386.39    418.85    442.98
   531.83    535.05    630.38    683.17    723.83    835.92    837.58    890.02
   926.92    950.06    980.66    968.17    1011.54 1081.64 1135.86 1145.02
```

```
      1226.30 1284.56 1307.44 1429.85 1440.20 1452.07 1551.07 1557.07
      1564.38 3035.56 3062.03 3064.67 3075.66 3082.08 3093.39 3136.97
      3554.05 3750.72
  ZeroEnergy[kcal/mol]      -27.44
    ElectronicLevels[1/cm]                              1
      0.0000000000000000             2.0000000000000000
  End
  !*******************************************
  RRHO                    !                       3
  Geometry[angstrom]                  17
  C                          0.32963200       0.00052700       0.57357900
  C                         -0.35562800       1.21119100       0.30716800
  C                         -1.64865400       1.20718100      -0.19387300
  C                         -2.30435900      -0.00052200      -0.44940700
  C                         -1.64815400      -1.20770100      -0.19269100
  C                         -0.35513700      -1.21068900       0.30838100
  H                          0.14588300       2.15222200       0.50488000
  H                         -2.15282600       2.14716300      -0.38536200
  H                         -3.31418900      -0.00092000      -0.84145600
  H                         -2.15193600      -2.14807800      -0.38326700
  H                          0.14676200      -2.15131900       0.50701200
  C                          1.64442000       0.00108300       1.12127400
  H                          2.08856900       0.92910100       1.46413200
  H                          2.08875600      -0.92631400       1.46558500
  H                          2.71573900      -0.00012600      -0.25678200
  O                          3.13187800      -0.00085000      -1.12830000
  H                          2.37845000      -0.00098600      -1.72361400
       Core      RigidRotor
                 SymmetryFactor       0.831548565
  End
    Rotor                                          Hindered
    Group      13      14          15       16    17
    Axis                    12                  1
    Symmetry                      2
    Potential[kcal/mol]                   18
0.000 0.544 1.614 3.189 5.180 7.458 9.836 12.071 13.870 128.213 13.631 22.593
8.744 5.696 3.683 2.063 0.949 0.404
    End
               Rotor                                             Hindered
    Group      17
    Axis                    16                  15
    Symmetry                      1
    Potential[kcal/mol]                   36
          0.000 -0.014 -0.012 -0.016 -0.015 -0.009 -0.001 0.011 0.020 0.025 0.028 0.033
          0.037 0.038 0.033 0.028 0.024 0.026 0.044 0.024 0.025 0.030 0.034 0.037
```

```
        0.037 0.032 0.028 0.025 0.020 0.010 0.000 -0.009 -0.015 -0.016 -0.012 -0.014
  End
       Frequencies[1/cm]              42
     134.58 189.30 211.30 349.31 350.26 393.19 444.43 456.82 533.97 552.31
     630.75 722.71 766.78 834.07 837.83 893.89 927.86 951.69 983.19 971.00
     1013.08 1080.54 1136.27 1145.79 1215.79 1283.70 1307.33 1428.38 1437.07 1453.07
     1550.32 1553.32 1562.26 3026.04 3061.50 3064.02 3075.06 3081.78 3093.09 3125.73
     3485.41 3746.84
ZeroEnergy[kcal/mol]     -24.71
  ElectronicLevels[1/cm]                          1
    0.0000000000000000            2.0000000000000000
End
!*******************************************
RRHO                    !                  4
Geometry[angstrom]                17
C                          0.33049100      0.00052000      0.57033800
C                         -0.35601300      1.20935000      0.30793900
C                         -1.65064800      1.20689900     -0.19387500
C                         -2.30545500     -0.00052000     -0.45009200
C                         -1.65015100     -1.20742200     -0.19269500
C                         -0.35552700     -1.20884400      0.30914200
H                          0.14670100      2.15039600      0.50302000
H                         -2.15440700      2.14706700     -0.38548700
H                         -3.31490200     -0.00092100     -0.84334300
H                         -2.15351800     -2.14798600     -0.38339200
H                          0.14758200     -2.14949000      0.50514100
C                          1.66847700      0.00106200      1.09419200
H                          2.07338200      0.92611000      1.49486100
H                          2.07352900     -0.92325100      1.49641900
H                          2.70434200     -0.00012600     -0.24085400
O                          3.12090600     -0.00083600     -1.11170500
H                          2.36977300     -0.00097100     -1.70758200
     Core     RigidRotor
                SymmetryFactor      0.831548565
End
  Rotor                                         Hindered
  Group     13     14        15     16    17
  Axis                  12                1
  Symmetry                    2
  Potential[kcal/mol]               18
0.000 0.928 2.377 4.270 6.486 8.862 11.160 13.097 14.288 12.649 10.562 8.230
5.921 3.827 2.090 0.835 0.136 0.039
  End
                  Rotor                                         Hindered
  Group     17
```

```
  Axis                16              15
  Symmetry                 1
  Potential[kcal/mol]             36
        0.000 -0.014 -0.012 -0.016 -0.014 -0.009 0.000 0.011 0.021 0.025 0.028 0.032
        0.037 0.038 0.032 0.027 0.024 0.025 0.102 0.027 0.025 0.028 0.032 0.038
        0.037 0.032 0.028 0.025 0.021 0.011 0.000 -0.009 -0.015 -0.016 -0.012 -0.014
  End
      Frequencies[1/cm]             42
   149.28 202.18 228.00 349.10 364.94 397.03 450.20 476.22 533.14 559.54
   631.08 724.78 802.71 831.96 839.39 896.80 928.85 952.39 985.63 973.46
   1013.90 1079.68 1136.80 1145.59 1205.55 1284.04 1307.19 1427.91 1433.20 1453.66
   1546.82 1555.85 1562.53 3017.64 3061.26 3063.77 3074.66 3081.72 3092.83 3115.11
   3419.17 3742.86
ZeroEnergy[kcal/mol]     -22.73
  ElectronicLevels[1/cm]                        1
   0.0000000000000000            2.0000000000000000
End
!*********************************************
RRHO                 !                 5
Geometry[angstrom]             17
C                     0.32635200      0.00052000      0.56881600
C                    -0.35595200      1.20807900      0.30857100
C                    -1.65208800      1.20696600     -0.19435400
C                    -2.30594400     -0.00052000     -0.45045500
C                    -1.65159100     -1.20749000     -0.19317500
C                    -0.35546500     -1.20757300      0.30976700
H                     0.14894600      2.14813400      0.50259300
H                    -2.15567600      2.14713400     -0.38647200
H                    -3.31556400     -0.00091800     -0.84357500
H                    -2.15479000     -2.14805300     -0.38437600
H                     0.14982400     -2.14722800      0.50470600
C                     1.69351900      0.00104100      1.07100500
H                     2.04504000      0.91825800      1.53823900
H                     2.04516200     -0.91530900      1.53985500
H                     2.68173000     -0.00012500     -0.24003000
O                     3.11363500     -0.00082600     -1.09949800
H                     2.35296100     -0.00095400     -1.69088400
    Core     RigidRotor
               SymmetryFactor     0.831548565
End
  Rotor                                    Hindered
  Group    13    14      15    16   17
  Axis               12             1
  Symmetry                 2
  Potential[kcal/mol]             18
```

```
0.000 1.252 2.984 5.091 7.431 9.786 11.906 13.453 12.842 10.914 8.672 6.304
4.107 2.215 0.761 -0.162 -0.498 -0.220
  End
    Rotor                                   Hindered
  Group     17
  Axis                16              15
  Symmetry                1
  Potential[kcal/mol]                36
        0.000 -0.014 -0.011 -0.016 -0.014 -0.009 0.000 0.012 0.022 0.025 0.028 0.032
        0.036 0.036 0.031 0.026 0.024 0.025 0.045 0.016 0.024 0.026 0.031 0.036
        0.036 0.032 0.028 0.025 0.022 0.012 0.000 -0.008 -0.014 -0.016 -0.011 -0.015
  End
      Frequencies[1/cm]                42
 60.94   217.64   247.73   349.43   381.58   398.4    455.17   495.19   531.1    550.45
631.8    727.51   817.1    841.63   872.65   902.42   931.04   952.42   991.65   977.8
1014.84 1078.07 1137.7   1143.22 1187.19 1287.89 1306.79 1426.71 1428.13 1455.09
1546.77 1561.97 1564.39 2996.16 3061.34 3063.99 3074.34 3081.81 3087.27 3092.47
3484.28 3716.41
 ZeroEnergy[kcal/mol]     -19.81
  ElectronicLevels[1/cm]                          1
   0.0000000000000000          2.0000000000000000
 End
 !*****************************************
 RRHO                !                6
 Geometry[angstrom]              17
 C                    0.32302500      0.00051900      0.56859800
 C                   -0.35573500      1.20754800      0.30893200
 C                   -1.65265700      1.20697900     -0.19462300
 C                   -2.30616700     -0.00052000     -0.45058300
 C                   -1.65216000     -1.20750400     -0.19344400
 C                   -0.35525000     -1.20704100      0.31012600
 H                    0.14932500      2.14750200      0.50290300
 H                   -2.15605300      2.14720900     -0.38678800
 H                   -3.31591200     -0.00091800     -0.84353000
 H                   -2.15516700     -2.14812900     -0.38469100
 H                    0.15020300     -2.14659500      0.50501300
 C                    1.70387100      0.00103300      1.06248300
 H                    2.03183400      0.91298700      1.55521400
 H                    2.03194600     -0.91000100      1.55684000
 H                    2.64347000     -0.00009100     -0.20459300
 O                    3.11388100     -0.00082600     -1.09824800
 H                    2.34149500     -0.00094000     -1.67673000
    Core     RigidRotor
              SymmetryFactor       0.831548565
 End
```

```
Rotor                                          Hindered
  Group     13     14        15     16    17
  Axis                    12                 1
  Symmetry                   2
  Potential[kcal/mol]                  18
0     1.376     3.21       5.387     7.754     10.078     12.091   13.427    13.146    10.159    7.821
     5.494
3.359     1.561     0.229     -0.555    -0.743    -0.318
  End
          Rotor                                          Hindered
  Group     17
  Axis                    16                  15
  Symmetry                   1
  Potential[kcal/mol]                  36
            0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.013 0.023 0.026 0.028 0.031
            0.034 0.034 0.030 0.025 0.024 0.025 0.052 0.026 0.023 0.025 0.029 0.033
            0.034 0.031 0.028 0.026 0.023 0.013 0.000 -0.009 -0.014 -0.015 -0.011 -0.015
  End
      Frequencies[1/cm]                  42
  155.16     248.58   283.22   347.65   382.38   401.45   455.56   496.33   531.45   564.85
631.86   727.66   816.37   841.84   873.22   902.82   931.31   952.48   989.68   978.13
1014.9   1077.77 1137.81 1143.39 1186.34 1288.29 1306.79 1424.62 1428.17 1455.41
1556.46 1562.42 1565.38 3004.19 3061.41 3064.09 3074.36 3081.89 3092.47 3095.29
3312.26 3716.93
 ZeroEnergy[kcal/mol]     -17.14
  ElectronicLevels[1/cm]                                 1
    0.0000000000000000              2.0000000000000000
 End
 !*********************************************
 RRHO                    !                    7
 Geometry[angstrom]                 17
 C                          0.32128400       0.00051900       0.56850600
 C                         -0.35556400       1.20726800       0.30912600
 C                         -1.65293600       1.20697800      -0.19477400
 C                         -2.30628400      -0.00052000      -0.45065300
 C                         -1.65244000      -1.20750200      -0.19359600
 C                         -0.35507900      -1.20676100       0.31031800
 H                          0.14938500       2.14729800       0.50314700
 H                         -2.15621500       2.14724800      -0.38691900
 H                         -3.31610700      -0.00091800      -0.84349400
 H                         -2.15532800      -2.14816800      -0.38482200
 H                          0.15026200      -2.14639100       0.50525700
 C                          1.70869000       0.00103000       1.05872700
 H                          2.02532000       0.91074600       1.56399800
 H                          2.02542800      -0.90774200       1.56562900
```

H 2.60183400 -0.00003800 -0.14310800
O 3.11565100 -0.00082800 -1.10070200
H 2.33578700 -0.00093500 -1.67143900
Core RigidRotor
SymmetryFactor 0.831548565
End
Rotor Hindered
Group 13 14 15 16 17
Axis 12 1
Symmetry 2
Potential[kcal/mol] 18
0 1.432 3.313 5.521 7.895 10.199 12.154 13.378 11.821 9.746 7.537
5.105
3.001 1.251 -0.021 -0.739 -0.857 -0.363
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 36
0.000 -0.015 -0.008 -0.014 -0.013 -0.009 0.000 0.013 0.024 0.025 0.025 0.026
0.027 0.026 0.025 0.023 0.023 0.030 0.036 0.034 0.023 0.025 0.025 0.026
0.027 0.027 0.025 0.025 0.024 0.014 0.000 -0.009 -0.013 -0.014 -0.007 -0.015
End
Frequencies[1/cm] 42
197.48 292.79 342.7 397.06 456.08 497.02 526.02 533.24 632.44 665.92
732.09 802.84 842.5 867.96 903.43 932.47 951.35 957.57 975.84 980.89
1015.27 1077.2 1138.93 1145.79 1177.15 1293.04 1306.86 1416.26 1428.43 1429.03
1463.79 1566.62 1567.34 1762.09 2995.95 3061.81 3064.51 3074.34 3081.35 3082.72
3092.47 3668.97
ZeroEnergy[kcal/mol] -13.05
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**
RRHO ! 8
Geometry[angstrom] 17
C 0.31994800 0.00051800 0.56845200
C -0.35541900 1.20705300 0.30927100
C -1.65315600 1.20697700 -0.19490600
C -2.30640600 -0.00052000 -0.45071800
C -1.65266000 -1.20750200 -0.19372700
C -0.35493400 -1.20654600 0.31046300
H 0.14938400 2.14717800 0.50341300
H -2.15635100 2.14728500 -0.38701600

```
H          -3.31628700    -0.00091800    -0.84343900
H          -2.15546500    -2.14820600    -0.38491800
H           0.15026200    -2.14626900     0.50552200
C           1.71224100     0.00102800     1.05616700
H           2.02010500     0.90900800     1.57106800
H           2.02020900    -0.90598900     1.57270400
H           2.56170100     0.00001600    -0.07847300
O           3.11766500    -0.00083100    -1.10391000
H           2.33172300    -0.00093100    -1.66812200
  Core   RigidRotor
      SymmetryFactor    0.831548565
End
 Rotor                         Hindered
 Group   13   14    15   16  17
 Axis          12        1
 Symmetry          2
 Potential[kcal/mol]        18
 0.000 1.474 3.388 5.618 7.995 10.282 12.191 13.325 13.035 9.451 7.113 4.811
 2.732 1.018 -0.208 -0.877 -0.942 -0.397
 End
    Rotor                         Hindered
 Group   17
 Axis          16        15
 Symmetry          1
 Potential[kcal/mol]        36
    0.000 -0.015 -0.009 -0.012 -0.013 -0.009 -0.003 0.007 0.019 0.021 0.021 0.022
    0.022 0.023 0.024 0.026 0.030 0.023 0.027 0.023 0.030 0.025 0.024 0.023
    0.023 0.022 0.021 0.021 0.020 0.007 -0.003 -0.010 -0.013 -0.012 -0.008 -0.015
 End
   Frequencies[1/cm]          42
 167.35   223.1   342.06  398.21  444.75  485.22  528.56  558.15  561.74  632.76
717.27  743.85  822.47  842.93  900.73  931.76  951.23  988.26  980.65  1014.62
1048.79 1053.1  1081.44 1139.52 1155.76 1189.42 1295.3  1307.29 1419.93 1428.4
1462.3  1541.29 1566.75 1574.32 2990.87 3061.69 3064.22 3074.14 3074.47 3082.43
3092.43 3653.4
ZeroEnergy[kcal/mol]   -8.49
 ElectronicLevels[1/cm]                 1
  0.0000000000000000        2.0000000000000000
End
!*******************************************
RRHO           !          9
Geometry[angstrom]         17
C           0.31578600     0.00051800     0.56835900
C          -0.35515500     1.20625100     0.30949000
C          -1.65391400     1.20688600    -0.19555000
```

```
C        -2.30706000   -0.00052100   -0.45097500
C        -1.65341400   -1.20741300   -0.19437000
C        -0.35466700   -1.20574100    0.31067700
H         0.14887400    2.14671000    0.50532200
H        -2.15707900    2.14738200   -0.38739000
H        -3.31728200   -0.00092100   -0.84281000
H        -2.15619000   -2.14830300   -0.38529000
H         0.14975600   -2.14579900    0.50742600
C         1.71917800    0.00102800    1.05732300
H         1.99481200    0.90248700    1.60506100
H         1.99488800   -0.89938600    1.60674900
H         2.46649700    0.00014700    0.11132600
O         3.12707100   -0.00084500   -1.12104500
H         2.31814500   -0.00092200   -1.65715100
   Core     RigidRotor
        SymmetryFactor     0.831548565
End
  Rotor                       Hindered
  Group   13   14     15   16   17
  Axis             12          1
  Symmetry              2
  Potential[kcal/mol]         18
0.000 -1.744 -3.009 -3.719 -3.828 -3.326 -2.251 -0.664 1.326 3.580 5.937 8.128
9.911 10.433 8.888 6.745 4.405 2.108
  End
     Rotor                       Hindered
  Group   17
  Axis             16          15
  Symmetry              1
  Potential[kcal/mol]         36
     0.000 -0.015 -0.009 -0.012 -0.013 -0.009 -0.003 0.007 0.019 0.021 0.021 0.022
     0.023 0.023 0.023 0.025 0.030 0.024 0.027 0.023 0.030 0.025 0.023 0.023
     0.023 0.022 0.022 0.021 0.020 0.008 -0.003 -0.009 -0.013 -0.012 -0.008 -0.015
  End
    Frequencies[1/cm]          42
  158.56   223.21   341.92   398.17   438.86   481.95   530.31   540.68   566.18   632.82
722.91   755.69   825.35   842.79   900.11   931.36   950.12   993.22   980.84   1014.12
1047.2   1071.05 1106     1139.82 1158.01 1191.66 1297.16 1307.71 1419.5   1428.32
1463.28 1487.04 1566.19 1575.34 2987.53 3061.36 3063.62 3069.57 3073.85 3082.16
3092.26 3645.28
 ZeroEnergy[kcal/mol]    0.75
  ElectronicLevels[1/cm]                    1
   0.0000000000000000          2.0000000000000000
 End
 !********************************************
```

RRHO ! 10
Geometry[angstrom] 17
C 0.31345584 0.00052263 0.56897532
C -0.35569416 1.20558463 0.30952832
C -1.65460616 1.20666663 -0.19662668
C -2.30794316 -0.00052037 -0.45161068
C -1.65410116 -1.20719137 -0.19544368
C -0.35519716 -1.20507937 0.31071232
H 0.14740384 2.14610463 0.50798632
H -2.15779816 2.14731963 -0.38806668
H -3.31850716 -0.00092237 -0.84259568
H -2.15690516 -2.14823837 -0.38596468
H 0.14829684 -2.14519537 0.51007832
C 1.71693584 0.00103863 1.07511732
H 1.96572684 0.89800263 1.64334432
H 1.96574884 -0.89478337 1.64514132
H 2.45931984 0.00012463 0.19259932
O 3.13805784 -0.00086037 -1.14354268
H 2.30888884 -0.00091937 -1.64913268
Core RigidRotor
SymmetryFactor 0.831548565
End
Rotor Hindered
Group 13 14 15 16 17
Axis 12 1
Symmetry 2
Potential[kcal/mol] 18
0.000 1.552 3.526 5.794 8.172 10.421 12.233 13.177 11.036 8.882 6.528 4.251
2.222 0.580 -0.560 -1.134 -1.099 -0.459
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 36
0.000 -0.015 -0.008 -0.012 -0.013 -0.009 -0.002 0.010 0.021 0.022 0.022 0.023
0.023 0.024 0.024 0.024 0.028 0.027 0.028 0.027 0.028 0.025 0.024 0.024
0.023 0.023 0.022 0.022 0.021 0.010 -0.002 -0.009 -0.013 -0.013 -0.004 -0.015
End
Frequencies[1/cm] 42
133.64 217.76 339.5 396.69 440.35 490.51 514.99 528.22 596.03 632.47
726.29 770.88 833.92 841.53 896.25 928.39 945.9 997.75 979.96 1012.4
1071.22 1072.8 1140.01 1160.47 1187.03 1200.93 1301.59 1309.49 1381.04 1423.02
1428 1468.18 1563.32 1580.02 2979.51 3056.35 3059.99 3062.63 3072.71 3081.15
3091.56 3633.74

```
ZeroEnergy[kcal/mol]        1.16
  ElectronicLevels[1/cm]                          1
    0.0000000000000000              2.0000000000000000
End
!*******************************************
RRHO                    !                    11
Geometry[angstrom]                    17
C                          0.31159000       0.00051100       0.57079800
C                         -0.35645300       1.20474800       0.30947700
C                         -1.65515700       1.20627100      -0.19878900
C                         -2.30912100      -0.00051100      -0.45300100
C                         -1.65467300      -1.20679000      -0.19761500
C                         -0.35598300      -1.20424600       0.31066500
H                          0.14474600       2.14552500       0.51198000
H                         -2.15823100       2.14719800      -0.38959700
H                         -3.32008800      -0.00090300      -0.84297000
H                         -2.15736900      -2.14810500      -0.38750400
H                          0.14559500      -2.14462300       0.51409100
C                          1.70989700       0.00105900       1.10880100
H                          1.92449000       0.89348600       1.69889000
H                          1.92452000      -0.89020400       1.70064200
H                          2.46649200       0.00023500       0.28381400
O                          3.15353300      -0.00088700      -1.17931400
H                          2.29821900      -0.00093500      -1.64170200
     Core      RigidRotor
                SymmetryFactor       0.831548565
End
  Rotor                                          Hindered
  Group     13      14         15      16    17
  Axis                    12                 1
  Symmetry                       2
  Potential[kcal/mol]                  18
0.000 1.500 3.432 5.674 8.053 10.328 12.208 13.286 11.395 9.274 6.930 4.635
2.572 0.880 -0.319 -0.958 -0.991 -0.416
  End
  Rotor                                          Hindered
  Group     17
  Axis                    16                 15
  Symmetry                       1
  Potential[kcal/mol]                  36
          0.000 -0.015 -0.008 -0.012 -0.013 -0.009 -0.002 0.010 0.021 0.022 0.022 0.023
          0.023 0.024 0.024 0.024 0.028 0.028 0.027 0.028 0.028 0.025 0.024 0.024
          0.024 0.023 0.022 0.022 0.021 0.009 -0.002 -0.009 -0.013 -0.013 -0.004 -0.015
  End
        Frequencies[1/cm]                  42
```

```
 133.63 217.76 339.50 396.69 440.36 490.51 514.98 528.22 596.03 632.47
 726.29 770.88 833.92 841.53 896.25 928.39 945.90 997.75 979.96 1012.40
 1071.22 1072.80 1140.01 1160.47 1187.03 1200.93 1301.59 1309.49 1381.04 1423.02
 1428.00 1468.18 1563.32 1580.02 2979.51 3056.35 3059.99 3062.62 3072.71 3081.15
 3091.56 3633.74
ZeroEnergy[kcal/mol]       0.91
 ElectronicLevels[1/cm]                                1
   0.0000000000000000             2.0000000000000000
End
!*******************************************
RRHO                    !                   12
Geometry[angstrom]                 17
C                          0.31116200      0.00051900      0.57216000
C                         -0.35663700      1.20449800      0.30959000
C                         -1.65507800      1.20612200     -0.19974600
C                         -2.30927600     -0.00051400     -0.45375700
C                         -1.65459200     -1.20664100     -0.19857000
C                         -0.35616100     -1.20399300      0.31077900
H                          0.14381100      2.14540800      0.51344100
H                         -2.15799600      2.14715200     -0.39053800
H                         -3.32030200     -0.00090400     -0.84358400
H                         -2.15713400     -2.14805900     -0.38844300
H                          0.14466400     -2.14450200      0.51555600
C                          1.70677900      0.00106400      1.12127800
H                          1.91173000      0.89246300      1.71649200
H                          1.91175100     -0.88918000      1.71821800
H                          2.47009700      0.00026300      0.30912000
O                          3.15810900     -0.00089800     -1.19175000
H                          2.29561500     -0.00095000     -1.64095500
     Core      RigidRotor
                SymmetryFactor       0.831548565
End
 Rotor                                        Hindered
 Group     13     14        15      16    17
 Axis                   12                 1
 Symmetry                     2
 Potential[kcal/mol]                   18
 0.000 1.444 3.333 5.547 7.922 10.222 12.165 13.366 11.752 9.669 7.338 5.027
 2.930 1.189 -0.071 -0.776 -0.880 -0.372
 End
    Rotor                                        Hindered
 Group     17
 Axis                   16                 15
 Symmetry                     1
 Potential[kcal/mol]                   36
```

```
        0.000 -0.015 -0.009 -0.012 -0.013 -0.010 -0.003 0.006 0.018 0.021 0.021 0.021
        0.022 0.023 0.024 0.026 0.028 0.021 0.008 0.022 0.029 0.025 0.024 0.023
        0.022 0.021 0.021 0.021 0.018 0.005 -0.003 -0.009 -0.013 -0.012 -0.008 -0.015
  End
      Frequencies[1/cm]          42
          59.49 184.96 195.45 343.13 398.94 435.38 509.81 526.71 587.21 633.61
          726.76 805.71 842.92 888.61 922.58 942.28 997.78 975.79 988.66 1010.59
          1070.14 1139.15 1159.64 1193.34 1291.56 1311.59 1361.94 1371.59 1425.92
1430.52
          1470.77 1563.46 1584.46 2470.37 2964.87 3022.83 3055.58 3057.47 3069.20
3077.47
          3088.87 3606.84
 ZeroEnergy[kcal/mol]     0.57
  ElectronicLevels[1/cm]               1
   0.0000000000000000        2.0000000000000000
 End
 !*********************************************
 RRHO          !          13
 Geometry[angstrom]          17
 C                   0.31022100     0.00052600     0.57606700
 C                  -0.35687800     1.20405600     0.31024200
 C                  -1.65446600     1.20584800    -0.20197500
 C                  -2.30902000    -0.00052100    -0.45588300
 C                  -1.65396800    -1.20636600    -0.20079000
 C                  -0.35638300    -1.20354800     0.31143500
 H                   0.14201600     2.14523600     0.51682500
 H                  -2.15690100     2.14707500    -0.39320300
 H                  -3.31994200    -0.00091900    -0.84599400
 H                  -2.15602100    -2.14798400    -0.39109500
 H                   0.14289000    -2.14432200     0.51894700
 C                   1.69990700     0.00108300     1.14682200
 H                   1.88753400     0.89078600     1.75039700
 H                   1.88754500    -0.88746900     1.75209400
 H                   2.47611100     0.00031300     0.35646200
 O                   3.16623500    -0.00091800    -1.21707600
 H                   2.29081800    -0.00098400    -1.64114000
    Core    RigidRotor
           SymmetryFactor     0.831548565
 End
  Rotor                          Hindered
  Group    13    14     15    16   17
  Axis          12          1
  Symmetry          2
  Potential[kcal/mol]          18
0.000 -2.252 -4.619 -6.808 -8.688 -10.125 -11.029 -11.345 -11.047 -10.160 -8.737 -6.868
```

-4.687 -2.344 -0.067 1.889 3.275 2.013
End
Rotor Hindered
Group 17
Axis 16 15
Symmetry 1
Potential[kcal/mol] 36
0.000 -0.015 -0.009 -0.012 -0.013 -0.010 -0.003 0.007 0.018 0.021 0.021 0.022
0.022 0.023 0.024 0.026 0.029 0.022 0.021 0.021 0.029 0.026 0.023 0.023
0.022 0.022 0.021 0.021 0.018 0.006 -0.003 -0.009 -0.013 -0.012 -0.007 -0.015
End
Frequencies[1/cm] 42
197.48 292.79 342.70 397.06 456.08 497.02 526.02 533.24 632.44 665.92
732.09 802.84 842.50 867.96 903.43 932.47 951.35 957.57 975.84 980.89
1015.27 1077.20 1138.93 1145.79 1177.15 1293.04 1306.86 1416.26 1428.43 1429.03
1463.79 1566.62 1567.34 1762.09 2995.95 3061.81 3064.51 3074.34 3081.35 3082.72
3092.47 3668.97
ZeroEnergy[kcal/mol] -0.10
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 14
Geometry[angstrom] 17
C 0.30900400 0.00052700 0.58154200
C -0.35704800 1.20377000 0.31199700
C -1.65302200 1.20556200 -0.20487000
C -2.30790500 -0.00052000 -0.45890700
C -1.65252700 -1.20608400 -0.20368400
C -0.35656000 -1.20325900 0.31319000
H 0.14057500 2.14518300 0.52079500
H -2.15484800 2.14694100 -0.39689100
H -3.31815500 -0.00091900 -0.85080300
H -2.15397100 -2.14785600 -0.39477800
H 0.14144500 -2.14426400 0.52292000
C 1.69234800 0.00110100 1.17259200
H 1.86511400 0.88951900 1.78256100
H 1.86512500 -0.88615700 1.78425000
H 2.47995500 0.00035400 0.39976200
O 3.17277900 -0.00093600 -1.24293200
H 2.28594100 -0.00102000 -1.64306400
Core RigidRotor
SymmetryFactor 0.831548565
End
Rotor Hindered

```
  Group      13      14         15      16    17
  Axis                    12                 1
  Symmetry                     2
  Potential[kcal/mol]                    18
0.000 -1.129 -1.680 -1.616 -0.942 0.298    2.030 3.092 5.369 7.747 9.983 11.766
12.147 10.409 8.243 5.885 3.617 1.602
  End
    Rotor                                          Hindered
  Group      17
  Axis                    16                 15
  Symmetry                     1
  Potential[kcal/mol]                    36
        0.000 -0.015 -0.008 -0.012 -0.013 -0.009 -0.002 0.008 0.020 0.022 0.022 0.022
        0.023 0.023 0.023 0.025 0.029 0.025 0.021 0.026 0.030 0.024 0.024 0.023
        0.023 0.022 0.022 0.022 0.020 0.008 -0.003 -0.010 -0.013 -0.012 -0.007 -0.015
  End
      Frequencies[1/cm]                  42
    60.94 217.64 247.73 349.43 381.58 398.40 455.17 495.19 531.10 550.45
    631.80 727.51 817.10 841.63 872.65 902.42 931.04 952.42 991.65 977.80
    1014.84 1078.07 1137.70 1143.22 1187.19 1287.89 1306.79 1426.71 1428.13 1455.09
    1546.77 1561.97 1564.39 2996.16 3061.34 3063.99 3074.34 3081.81 3087.27 3092.47
    3484.28 3716.41
ZeroEnergy[kcal/mol]     -1.10
  ElectronicLevels[1/cm]                          1
    0.0000000000000000            2.0000000000000000
End
!*******************************************
RRHO                  !                  15
Geometry[angstrom]                 17
C                      0.30730700      0.00053300      0.58930100
C                     -0.35711400      1.20347900      0.31461000
C                     -1.65096700      1.20539500     -0.20799100
C                     -2.30540000     -0.00052200     -0.46372800
C                     -1.65047100     -1.20592200     -0.20680300
C                     -0.35662400     -1.20296100      0.31580400
H                      0.13877300      2.14508900      0.52668100
H                     -2.15172000      2.14691800     -0.40225400
H                     -3.31454000     -0.00092400     -0.85846500
H                     -2.15084000     -2.14784000     -0.40013400
H                      0.13964700     -2.14415800      0.52881000
C                      1.68457800      0.00111800      1.19811500
H                      1.84522800      0.88860000      1.81274200
H                      1.84523400     -0.88519900      1.81442600
H                      2.48113200      0.00038500      0.43910100
O                      3.17740400     -0.00095500     -1.26918800
```

```
H                         2.28035000     -0.00105600     -1.64626100
   Core     RigidRotor
             SymmetryFactor      0.831548565
End
 Rotor                                      Hindered
 Group     13     14        15      16    17
 Axis                 12                1
 Symmetry                   2
 Potential[kcal/mol]                 18
0.000 0.928 2.376 4.269 6.484 8.860 11.158 13.097 14.290 12.656 10.570 8.499
5.929 3.834 2.097 0.841 0.140 0.041
 End
   Rotor                                      Hindered
 Group     17
 Axis                 16                 15
 Symmetry                   1
 Potential[kcal/mol]                 36
        0.000 -0.015 -0.008 -0.014 -0.013 -0.008 0.000 0.014 0.024 0.025 0.026 0.027
        0.027 0.027 0.025 0.023 0.024 0.024 0.046 0.033 0.023 0.024 0.025 0.027
        0.027 0.027 0.026 0.025 0.024 0.014 0.000 -0.009 -0.013 -0.014 -0.008 -0.015
 End
     Frequencies[1/cm]                  42
    62.69 84.04 207.77 351.55 365.36 395.88 449.88 475.99 532.91 560.69
    631.10 724.98 807.79 832.26 839.36 896.74 928.66 952.25 988.65 973.50
    1013.96 1079.89 1136.79 1145.39 1204.86 1284.17 1307.18 1427.85 1434.75 1453.59
    1539.50 1556.05 1562.14 3006.84 3061.17 3063.57 3074.59 3081.80 3092.94 3103.92
    3485.11 3776.42
ZeroEnergy[kcal/mol]       -2.66
 ElectronicLevels[1/cm]                            1
    0.0000000000000000              2.0000000000000000
End
!*******************************************
RRHO                  !                  16
Geometry[angstrom]                17
C                         0.30491100      0.00054100      0.59923800
C                        -0.35731500      1.20324900      0.31868900
C                        -1.64822900      1.20524600     -0.21157600
C                        -2.30163000     -0.00052600     -0.47038400
C                        -1.64773000     -1.20577500     -0.21038500
C                        -0.35682200     -1.20272300      0.31988400
H                         0.13685200      2.14500600      0.53426000
H                        -2.14751600      2.14689400     -0.40906300
H                        -3.30876700     -0.00093200     -0.87020100
H                        -2.14662900     -2.14782400     -0.40693900
H                         0.13773200     -2.14406300      0.53639200
```

```
C                        1.67727200     0.00113300     1.22240100
H                        1.82897900     0.88793000     1.83987100
H                        1.82897500    -0.88449000     1.84156200
H                        2.47630800     0.00040300     0.47578900
O                        3.18011800    -0.00097500    -1.29540800
H                        2.27440600    -0.00108700    -1.65094300
   Core     RigidRotor
            SymmetryFactor      0.831548565
End
   Rotor                                  Hindered
  Group    13    14      15    16   17
  Axis               12              1
  Symmetry                2
  Potential[kcal/mol]               18
0.000 -1.882 -4.115 -6.412 -8.551 -10.347 -11.685 -12.539 -12.827 -12.545 -11.741 -10.400
-8.630 -6.520 -4.246 -2.018 -0.114 1.058
  End
    Rotor                                  Hindered
  Group    17
  Axis               16              15
  Symmetry                1
  Potential[kcal/mol]               36
       0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.013 0.023 0.026 0.028 0.032
       0.035 0.035 0.030 0.026 0.023 0.027 0.285 0.027 0.023 0.026 0.030 0.034
       0.035 0.032 0.028 0.025 0.022 0.013 0.000 -0.009 -0.014 -0.015 -0.011 -0.014
  End
      Frequencies[1/cm]                 42
    125.92 187.63 205.52 342.27 384.02 401.93 461.91 526.82 630.36 633.96
    726.67 799.80 845.37 892.07 945.47 950.94 998.43 977.44 999.72 1011.05
    1069.22 1138.84 1159.91 1189.48 1293.92 1311.05 1375.70 1395.03 1435.01 1436.30
    1471.15 1564.03 1585.03 2871.37 2973.31 3018.60 3054.54 3056.19 3068.57 3076.62
    3088.39 3602.43
ZeroEnergy[kcal/mol]    -3.21
  ElectronicLevels[1/cm]                          1
    0.0000000000000000           2.0000000000000000
End
!********************************************
RRHO                   !                 17
Geometry[angstrom]                17
C                        0.30500100     0.00054500     0.60393900
C                       -0.35664300     1.20309600     0.32176500
C                       -1.64534800     1.20518500    -0.21408000
C                       -2.29760900    -0.00052900    -0.47590600
C                       -1.64484500    -1.20571600    -0.21289000
C                       -0.35614800    -1.20256400     0.32296000
```

```
H                        0.13546100     2.14478800     0.54255800
H                       -2.14207000     2.14708800    -0.41655900
H                       -3.30031200    -0.00094100    -0.88648800
H                       -2.14117800    -2.14802500    -0.41443400
H                        0.13634400    -2.14383400     0.54469300
C                        1.67195900     0.00114700     1.24328100
H                        1.80554300     0.88576600     1.86938500
H                        1.80551800    -0.88227300     1.87108300
H                        2.48498500     0.00042400     0.51830700
O                        3.17800800    -0.00098800    -1.31721600
H                        2.25918100    -0.00117300    -1.64415600
   Core    RigidRotor
          SymmetryFactor     0.831548565
End
 Rotor                                  Hindered
 Group    13    14     15    16   17
 Axis              12          1
 Symmetry            2
 Potential[kcal/mol]          18
0.000 0.572 1.670 3.270 5.280 7.569   9.945 12.166 13.929 14.137 12.366 10.185
7.824 5.566 3.570 1.974 0.889 0.376
 End
   Rotor                                  Hindered
 Group    17
 Axis              16          15
 Symmetry            1
 Potential[kcal/mol]          36
     0.000 -0.014 -0.011 -0.015 -0.014 -0.009 0.000 0.012 0.022 0.026 0.028 0.032
     0.035 0.035 0.030 0.026 0.023 0.026 0.072 0.026 0.024 0.026 0.030 0.035
     0.035 0.032 0.028 0.025 0.022 0.012 0.000 -0.009 -0.014 -0.015 -0.011 -0.015
 End
    Frequencies[1/cm]          42
 124.53 209.75 256.92 343.32 395.69 402.36 462.19 526.49 633.57 634.01
 726.90 798.85 845.88 892.81 946.11 951.65 961.11 977.76 1001.71 1011.12
 1068.99 1138.69 1159.99 1188.07 1293.77 1311.07 1375.51 1396.92 1436.17 1439.67
 1471.06 1564.24 1584.97 2918.60 2980.11 3009.60 3054.37 3055.81 3068.82 3076.81
 3088.88 3574.47
ZeroEnergy[kcal/mol]    -3.39
 ElectronicLevels[1/cm]                   1
  0.0000000000000000          2.0000000000000000
End
!*******************************************
RRHO            !          18
Geometry[angstrom]          17
C                        0.30294800     0.00055400     0.61677800
```

```
C                          -0.35588200      1.20306600      0.32681500
C                          -1.64040300      1.20509700     -0.21918200
C                          -2.29118800     -0.00053400     -0.48498000
C                          -1.63989600     -1.20563100     -0.21799200
C                          -0.35538200     -1.20252500      0.32800900
H                           0.13496900      2.14500900      0.54932500
H                          -2.13705900      2.14689100     -0.42252600
H                          -3.29407900     -0.00094700     -0.89530800
H                          -2.13615900     -2.14783400     -0.42040400
H                           0.13586100     -2.14404300      0.55145700
C                           1.66428100      0.00116100      1.26604600
H                           1.79868400      0.88713400      1.89021800
H                           1.79864300     -0.88360000      1.89195000
H                           2.48055400      0.00041500      0.53434700
O                           3.17279600     -0.00100300     -1.33983500
H                           2.24818500     -0.00124800     -1.65029800
    Core     RigidRotor
             SymmetryFactor      0.831548565
End
 Rotor                                     Hindered
 Group    13    14      15    16   17
 Axis                 12            1
 Symmetry                 2
 Potential[kcal/mol]               18
0.000 0.462 1.451 2.953 4.889 7.133   9.511 11.785 13.661 14.731 13.669 10.700
8.355 6.062 4.001 2.312 1.116 0.482
 End
   Rotor                                     Hindered
 Group    17
 Axis                 16            15
 Symmetry                 1
 Potential[kcal/mol]               36
      0.000 -0.015 -0.009 -0.014 -0.013 -0.008 0.000 0.014 0.024 0.025 0.026 0.028
      0.029 0.028 0.026 0.023 0.023 0.028 0.014 0.025 0.023 0.024 0.026 0.028
      0.029 0.028 0.027 0.025 0.025 0.015 0.000 -0.009 -0.013 -0.014 -0.008 -0.015
 End
    Frequencies[1/cm]              42
  108.83 184.72 214.71 298.47 352.85 384.10 406.05 440.58 528.93 535.40
  630.20 659.75 722.22 835.10 838.40 888.32 926.11 949.18 982.32 967.16
  1010.84 1082.16 1135.77 1144.33 1229.14 1284.77 1307.37 1430.37 1442.74 1451.46
  1550.32 1559.04 1568.64 3029.90 3062.14 3064.85 3075.81 3082.11 3093.42 3130.72
  3571.46 3767.05
ZeroEnergy[kcal/mol]    -3.61
 ElectronicLevels[1/cm]                        1
  0.0000000000000000          2.0000000000000000
```

```
End
        Tunneling       Eckart
      ImaginaryFrequency[1/cm]       1192.8499999999999
      WellDepth[kcal/mol]              4.62
      WellDepth[kcal/mol]              29.93
End
End
!***********************************
 Bimolecular        P3        # C6H5OH   +   CH3
Fragment PROD1
RRHO
Geometry[angstrom]                 13
 C                    0.24040500      1.21022500     -0.01434700
C                    -1.15490900      1.20699800      0.00591300
C                    -1.85625000      0.00030700      0.01602100
C                    -1.15540600     -1.20666300      0.00606000
C                     0.23991700     -1.21049000     -0.01396500
C                     0.93254700     -0.00029900     -0.00920900
H                     0.79975300      2.13770300     -0.03780300
H                    -1.69266800      2.14793200      0.00425000
H                    -2.93948400      0.00053700      0.02829300
H                    -1.69355000     -2.14737500      0.00464300
H                     0.79899500     -2.13812800     -0.03685700
O                     2.32049600     -0.00105500     -0.08827700
H                     2.68515900      0.00729800      0.80085400
    Core     RigidRotor
         SymmetryFactor       1.00000000000000
    End
     Rotor            Hindered
          Group                              13
          Axis                               6 12
          Symmetry                           1
    Potential[kcal/mol]          36
          0.000 -0.116 -0.453 -0.953 -1.549 -2.171 -2.740 -3.185 -3.446 -3.512 -3.386 -
3.062
         -2.572 -1.977 -1.356 -0.783 -0.327 -0.053 -0.015 -0.216 -0.607 -1.129 -1.718 -
2.307
         -2.829 -3.225 -3.454 -3.512 -3.401 -3.117 -2.676 -2.127 -1.530 -0.955 -0.467 -
0.129
         End
      Frequencies[1/cm]                32
  223.27   405.88   409.85   453.28   529.68   533.30   628.39   739.04
  823.15   830.30   882.52   913.59   936.76   978.39   1004.00 1051.70
  1133.65 1136.74 1148.69 1225.40 1275.53 1307.53 1425.90 1469.04
  1570.30 1579.22 3063.25 3071.71 3082.77 3088.27 3093.65 3709.39
```

```
  ZeroEnergy[kcal/mol]                0.
  ElectronicLevels[1/cm]                              1
  0.000000000000000E+000      1.00000000000000
End
!***********************************
Fragment PROD2
RRHO
        Geometry[angstrom]                4
C                        0.00000000      0.00000000     -0.00008100
H                        0.00000000      1.07906800      0.00016200
H                       -0.93450000     -0.53953400      0.00016200
H                        0.93450000     -0.53953400      0.00016200
    Core      RigidRotor
        SymmetryFactor       6.00000000000000
    End
      Frequencies[1/cm]                6
   513.14 1369.86 1369.86 3012.76 3190.07 3190.09
  ZeroEnergy[kcal/mol]                0.
  ElectronicLevels[1/cm]                              1
  0.000000000000000E+000      2.00000000000000
End
GroundEnergy[kcal/mol]       -5.56
End
!***********************************
  Well         W32                  # ipsoOHC6H5CH3
    Species
      RRHO
        Geometry[angstrom]                17
C                        0.03666100     -1.24694500      0.01494200
C                        1.39748600     -1.22569600     -0.03284600
C                        2.11019800     -0.00000300     -0.07136700
C                        1.39748600      1.22569300     -0.03284100
C                        0.03666200      1.24695000      0.01495800
C                       -0.80174700      0.00000900      0.02675100
H                       -0.50761800     -2.18452300      0.05611300
H                        1.94977000     -2.15899900     -0.03381000
H                        3.19194200      0.00000100     -0.10777300
H                        1.94977800      2.15899100     -0.03380600
H                       -0.50758400      2.18454700      0.05615000
C                       -1.79326700      0.00000300     -1.14188200
H                       -2.42709900      0.88757200     -1.08419800
H                       -1.26004800      0.00001600     -2.09355000
H                       -2.42708400     -0.88757500     -1.08420000
O                       -1.64992300      0.00000200      1.21042100
H                       -1.06355300     -0.00011200      1.97541100
```

```
    Core         RigidRotor
                  SymmetryFactor                  1
    End
     Rotor    Hindered                    !freq=257
              Group                                13 14 15
              Axis                                 6 12
              Symmetry                             3
    Potential[kcal/mol]          12
        0.000 0.215 0.806 1.639 2.509 3.177 3.427 3.167 2.495 1.622 0.798 0.217
        End
         Rotor    Hindered                  !freq=340
            Group                              17
            Axis                               6 16
            Symmetry                           1
    Potential[kcal/mol]          36
        0.000 0.106 0.413 0.878 1.435 1.994 2.485 2.849 3.053 3.106 3.058 2.977
        2.914 2.907 2.980 3.105 3.255 3.383 3.437 3.401 3.285 3.135 3.002 2.925
        2.907 2.960 3.041 3.102 3.075 2.898 2.549 2.057 1.486 0.911 0.429 0.113
        End
        Frequencies[1/cm]               43
    82.89     228.40    342.33    386.17    393.06    454.57    536.45    582.65
586.16     692.09    733.83    772.25    819.87    898.42    961.48    966.98
970.32     980.93    994.23    1020.80 1056.54 1083.45 1099.19 1158.20
1250.17    1272.03 1278.69 1350.94 1351.56 1401.96 1436.99 1445.50
1497.81    1560.77 2935.53 3012.38 3022.72 3056.44 3057.95 3074.17
3075.36    3096.04 3673.71
             ZeroEnergy[kcal/mol]              -18.38
             ElectronicLevels[1/cm]            1
                0      2
End
End
!***********************************
 Barrier        B33      W32      P3                # TS33
    RRHO
       Geometry[angstrom]                    17
C                        1.39903800      1.21170600     -0.08840500
C                        0.02710300      1.21406900     -0.26806800
C                       -0.71588100     -0.00042000     -0.30898500
C                        0.02735300     -1.21470400     -0.26617000
C                        1.39926500     -1.21181400     -0.08659200
C                        2.09366800      0.00009700      0.00260400
H                        1.93789900      2.15004300     -0.03114500
H                       -0.51321200     -2.15117500     -0.34037500
H                        1.93833000     -2.14995300     -0.02800700
H                        3.16876200      0.00030200      0.13786800
```

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O                -1.34603100    0.00187400    1.59411600
H                -0.50542900    0.00251800    2.07618900
H                -0.51365500    2.15032200   -0.34361900
C                -2.11935100   -0.00111900   -0.85695500
H                -2.65971300    0.88340700   -0.52045800
H                -2.09198900   -0.00296700   -1.95048100
H                -2.65991400   -0.88438600   -0.51748300
      Core     RigidRotor
        SymmetryFactor          1
      End
      Tunneling        Eckart
        ImaginaryFrequency[1/cm]      411.60
        WellDepth[kcal/mol]           24.77
        WellDepth[kcal/mol]           11.94
      End
      Frequencies[1/cm]             44
106.81 146.65 171.39 218.37 265.42 338.04 407.51 408.71 529.67 622.56
646.63 739.16 785.77 805.41 839.48 920.97 973.90 979.14 968.14 971.61
1007.68 1016.53 1080.70 1129.01 1156.24 1192.19 1268.01 1299.69 1367.04 1407.06
1443.02 1447.98 1450.60 1539.91 1567.93 2938.29 3009.51 3036.00 3064.73 3070.54
3079.13 3085.37 3093.07 3634.88
      ZeroEnergy[kcal/mol]                6.38
      ElectronicLevels[1/cm]            1
                  0         2
End
!************************************
Barrier B32   W   W32
Variational
RRHO              !              1
Geometry[angstrom]            17
C                 1.37576800    1.20658100   -0.09419400
C                 0.01683500    1.20342600   -0.40859100
C                -0.68587100   -0.00089600   -0.56928200
C                 0.01719300   -1.20462000   -0.40593600
C                 1.37617400   -1.20672400   -0.09125000
C                 2.06111000    0.00016800    0.06515600
H                 1.89739400    2.14827200    0.03049900
H                -0.51153100   -2.14497600   -0.51738800
H                 1.89803800   -2.14800700    0.03584800
H                 3.11574900    0.00061800    0.31444800
O                -1.38465100    0.00278100    1.96078100
H                -0.44175100   -0.00109100    2.18192000
H                -0.51219300    2.14337400   -0.52230300
C                -2.13975400   -0.00118200   -0.96697100
H                -2.65464900    0.87510200   -0.57123500
```

```
H                        -2.23719900     0.01123200    -2.05655300
H                        -2.64758600    -0.89000400    -0.59167400
   Core     RigidRotor
            SymmetryFactor      0.856940376
End
 Rotor                                   Hindered
 Group     15 16 17
 Axis               14              3
 Symmetry                 3
 Potential[kcal/mol]              12
   0.000 -0.691 -0.632 -0.626 -0.663 -0.728 -0.820 -0.910 -0.975 -0.988 -0.953 -0.879
 End
   Rotor                                   Hindered
 Group     12
 Axis               11              3
 Symmetry                 1
 Potential[kcal/mol]              36
   0.000 0.011 -0.874 -0.961 -0.989 -0.955 -0.864 -0.731 -0.566 -0.377 -0.170 0.049
   0.276 0.079 0.010 -0.090 -0.164 -0.213 -0.243 -0.257 -0.253 -0.232 -0.194 -0.130
   -0.037 0.093 0.980 0.136 -0.746 -0.876 -0.960 -0.990 -0.962 -0.883 -0.760 -0.606
 End
    Frequencies[1/cm]              42
  79.80     101.23   205.52   338.44   341.33   401.59   452.43   526.62
  631.87   638.80   728.25   798.80   844.75   896.86   956.02   959.69
  969.58   978.23   1009.73 1024.03 1070.67 1137.09 1159.01 1190.78
  1295.56 1307.20 1369.72 1413.01 1442.81 1449.80 1467.67 1558.96
  1581.68 2934.74 2999.46 3025.66 3059.12 3062.56 3071.25 3079.73
  3089.22 3657.23
ZeroEnergy[kcal/mol]     -3.56
 ElectronicLevels[1/cm]                          1
  0.0000000000000000           2.0000000000000000
End
!********************************************
RRHO                 !                2
Geometry[angstrom]               17
C                         1.38193000     1.20707600    -0.09955700
C                         0.01903400     1.20442600    -0.39015700
C                        -0.68679000    -0.00071300    -0.54053400
C                         0.01937900    -1.20540200    -0.38822600
C                         1.38226200    -1.20721000    -0.09758800
C                         2.06962500     0.00014900     0.04865300
H                         1.90631000     2.14880800     0.01535600
H                        -0.51185300    -2.14485300    -0.49530300
H                         1.90690400    -2.14861100     0.01884500
H                         3.12859400     0.00048200     0.27922400
```

```
O                    -1.40419800     0.00237000     1.90855800
H                    -0.47859000     0.00197400     2.19152500
H                    -0.51246300     2.14355500    -0.49873000
C                    -2.13804700    -0.00124600    -0.93944400
H                    -2.64918100     0.88180900    -0.55636700
H                    -2.23384100    -0.00085600    -2.02970500
H                    -2.64820500    -0.88513900    -0.55706900
   Core     RigidRotor
            SymmetryFactor     0.856940376
End
 Rotor                                   Hindered
 Group     15 16 17
 Axis                14                3
 Symmetry                  3
 Potential[kcal/mol]                 12
   0.000 -0.690 -0.632 -0.627 -0.665 -0.731 -0.823 -0.913 -0.976 -0.988 -0.952 -0.877
 End
   Rotor                                 Hindered
 Group     12
 Axis                11                3
 Symmetry                  1
 Potential[kcal/mol]                 36
   0.000 -0.741 -0.876 -0.962 -0.989 -0.954 -0.861 -0.727 -0.561 -0.372 -0.165 0.054
   0.281 0.079 0.614 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.193 -0.128
   -0.034 0.097 0.089 0.137 -0.750 -0.879 -0.962 -0.990 -0.961 -0.881 -0.757 -0.602
 End
    Frequencies[1/cm]                 42
  82.84     115.27    208.24    340.34    363.52    401.33    452.19    527.99
  631.41    638.55    729.12    800.04    845.20    898.48    957.37    960.11
  970.30    978.37    1009.23 1024.20 1072.08 1137.15 1159.59 1193.86
  1294.92 1307.12 1370.63 1413.89 1441.61 1450.53 1467.19 1557.24
  1583.54 2934.09 3000.86 3032.19 3058.13 3062.17 3071.10 3078.13
  3087.89 3664.29
ZeroEnergy[kcal/mol]     -3.36
 ElectronicLevels[1/cm]                          1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                  !                  3
Geometry[angstrom]                 17
C                     1.38627900     1.20743200    -0.09997800
C                     0.02045200     1.20526800    -0.37447700
C                    -0.69022400    -0.00067100    -0.51364900
C                     0.02078400    -1.20620300    -0.37259400
C                     1.38659500    -1.20756100    -0.09808000
```

```
C        2.07648500    0.00014000    0.03677300
H        1.91216100    2.14872400    0.01387700
H       -0.51152000   -2.14566400   -0.47498300
H        1.91274400   -2.14852600    0.01728700
H        3.13883500    0.00045400    0.25630900
O       -1.41066300    0.00221400    1.84950500
H       -0.50207700    0.00237400    2.18455500
H       -0.51211900    2.14441400   -0.47835400
C       -2.14271000   -0.00117700   -0.91455400
H       -2.65055600    0.88122600   -0.52338500
H       -2.24910800   -0.00216500   -2.00547100
H       -2.65033100   -0.88297200   -0.52179700
   Core    RigidRotor
           SymmetryFactor    0.856940376
End
 Rotor                       Hindered
 Group    15 16 17
 Axis          14        3
 Symmetry           3
 Potential[kcal/mol]        12
 0.000 -0.696 -0.634 -0.624 -0.659 -0.722 -0.812 -0.903 -0.971 -0.988 -0.956 -0.884
 End
   Rotor                       Hindered
 Group    12
 Axis          11        3
 Symmetry           1
 Potential[kcal/mol]        36
   0.000 0.022 -0.877 -0.962 -0.989 -0.953 -0.861 -0.727 -0.561 -0.371 -0.164 0.055
   0.282 0.592 0.007 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.192 -0.128
   -0.034 0.097 0.089 0.138 -0.750 -0.879 -0.962 -0.990 -0.961 -0.880 -0.756 -0.602
 End
    Frequencies[1/cm]        42
  79.97   146.01   218.51   340.68   402.24   418.35   455.42   528.45
  630.87   639.85   732.36   798.44   845.82   902.72   959.26   963.12
  972.04   978.21   1008.90 1028.25 1072.78 1137.79 1159.67 1191.27
  1291.98 1305.67 1372.57 1413.35 1443.07 1450.86 1465.42 1555.01
  1582.39 2922.82 2993.37 3024.44 3054.83 3061.31 3067.57 3076.70
  3083.86 3657.25
ZeroEnergy[kcal/mol]    -3.17
 ElectronicLevels[1/cm]              1
  0.0000000000000000         2.0000000000000000
End
!*******************************************
RRHO          !          4
Geometry[angstrom]        17
```

```
C        1.38683800    1.20713300   -0.09906300
C        0.01763700    1.20456300   -0.35870100
C       -0.69072900   -0.00065000   -0.50327000
C        0.01795900   -1.20545200   -0.35683900
C        1.38713800   -1.20726300   -0.09719200
C        2.07833500    0.00012800    0.02533800
H        1.91396500    2.14837900    0.00468000
H       -0.51637200   -2.14493100   -0.44582200
H        1.91451400   -2.14820700    0.00800600
H        3.14425500    0.00041300    0.22070300
O       -1.41035100    0.00217200    1.82178400
H       -0.50299000    0.00243400    2.17096300
H       -0.51693800    2.14376200   -0.44912900
C       -2.14111000   -0.00117700   -0.90912300
H       -2.65333700    0.88175100   -0.52653300
H       -2.22775100   -0.00251100   -1.99950900
H       -2.65329700   -0.88320400   -0.52438600
   Core    RigidRotor
           SymmetryFactor    0.856940376
End
 Rotor                    Hindered
 Group     15 16 17
 Axis          14          3
 Symmetry           3
 Potential[kcal/mol]          12
 0.000 -0.693 -0.633 -0.625 -0.661 -0.726 -0.817 -0.908 -0.973 -0.988 -0.955 -0.881
 End
  Rotor                    Hindered
 Group     12
 Axis          11          3
 Symmetry           1
 Potential[kcal/mol]          36
  0.000 0.022 0.034 -0.962 -0.989 -0.953 -0.861 -0.727 -0.560 -0.371 -0.164 0.055
  0.282 0.079 0.006 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.192 -0.128
  -0.034 0.098 0.321 0.615 0.367 -0.879 -0.962 -0.990 -0.961 -0.880 -0.756 -0.601
  End
    Frequencies[1/cm]          42
  83.54   207.76   217.83   339.93   402.60   446.19   504.08   530.51
  630.89   637.58   728.95   799.81   844.21   901.60   958.35   960.46
  970.71   979.41   1010.26 1025.70 1072.10 1136.97 1159.42 1192.18
  1294.13 1305.20 1370.02 1412.56 1442.54 1449.75 1466.48 1558.35
  1582.38 2936.73 3003.21 3030.00 3059.90 3063.88 3072.50 3080.01
  3089.58 3608.29
ZeroEnergy[kcal/mol]    -2.55
 ElectronicLevels[1/cm]                1
```

```
  0.0000000000000000  2.0000000000000000
End
!*****************************************
RRHO  !  5
Geometry[angstrom]  17
C  1.38705400  1.20748900  -0.09864800
C  0.01656800  1.20527900  -0.34752400
C  -0.69408800  -0.00063100  -0.48607000
C  0.01688100  -1.20614500  -0.34565300
C  1.38734500  -1.20761800  -0.09677000
C  2.07961700  0.00012100  0.01865000
H  1.91519600  2.14850100  0.00302600
H  -0.51853800  -2.14519800  -0.43188400
H  1.91573200  -2.14833300  0.00637500
H  3.14721800  0.00039700  0.20602900
O  -1.40651600  0.00212700  1.78911800
H  -0.51089000  0.00242300  2.16427100
H  -0.51909200  2.14405800  -0.43521600
C  -2.14182300  -0.00115800  -0.90122700
H  -2.65538000  0.88172800  -0.52007300
H  -2.22399500  -0.00247600  -1.99259900
H  -2.65533300  -0.88315000  -0.51794900
  Core  RigidRotor
  SymmetryFactor  0.856940376
End
 Rotor  Hindered
 Group  15 16 17
 Axis  14  3
 Symmetry  3
 Potential[kcal/mol]  12
 0.000 -0.697 -0.635 -0.623 -0.658 -0.721 -0.811 -0.902 -0.970 -0.988 -0.957 -0.886
 End
  Rotor  Hindered
 Group  12
 Axis  11  3
 Symmetry  1
 Potential[kcal/mol]  36
  0.000 -0.742 -0.877 -0.962 -0.989 -0.953 -0.861 -0.726 -0.560 -0.371 -0.164 0.056
  0.282 0.079 0.006 -0.093 -0.166 -0.214 -0.243 -0.257 -0.253 -0.231 -0.192 -0.128
  -0.034 0.098 0.089 0.138 -0.750 -0.879 -0.962 -0.990 -0.961 -0.880 -0.756 -0.601
 End
  Frequencies[1/cm]  42
 88.39  176.06  222.57  339.58  402.87  445.66  513.93  533.70
 630.46  637.81  730.28  799.75  844.38  903.91  959.63  961.93
 971.31  979.61  1010.16 1026.72 1072.85 1137.07 1159.59 1192.24
```

```
   1292.45 1304.38 1370.59 1412.64 1442.61 1450.02 1465.63 1557.45
   1582.84 2933.19 3001.07 3029.42 3059.41 3064.21 3072.18 3079.74
   3088.53 3622.43
ZeroEnergy[kcal/mol]     -2.20
 ElectronicLevels[1/cm]                    1
   0.0000000000000000          2.0000000000000000
End
!*******************************************
RRHO              !             6
Geometry[angstrom]              17
C                    1.38689900      1.20769900     -0.09807900
C                    0.01478000      1.20566600     -0.33485600
C                   -0.69712300     -0.00061000     -0.46930500
C                    0.01508500     -1.20650100     -0.33298500
C                    1.38718000     -1.20782700     -0.09620700
C                    2.08027600      0.00011300      0.01097200
H                    1.91624600      2.14847500     -0.00151500
H                   -0.52164400     -2.14519400     -0.41398000
H                    1.91676600     -2.14831800      0.00181700
H                    3.14986100      0.00037500      0.18614100
O                   -1.40206000      0.00208400      1.75758500
H                   -0.51540900      0.00244000      2.15340000
H                   -0.52218100      2.14409600     -0.41730600
C                   -2.14153400     -0.00114800     -0.89511700
H                   -2.65798000      0.88194100     -0.51870300
H                   -2.21213200     -0.00255700     -1.98708100
H                   -2.65798000     -0.88326700     -0.51643000
    Core     RigidRotor
           SymmetryFactor      0.856940376
End
 Rotor                          Hindered
 Group     15 16 17
 Axis            14            3
 Symmetry            3
 Potential[kcal/mol]            12
 0.000 -0.827 -0.919 -0.973 -0.989 -0.952 -0.873 -0.777 -0.691 -0.638 -0.622 -0.660
 End
   Rotor                          Hindered
 Group     12
 Axis            11            3
 Symmetry            1
 Potential[kcal/mol]            36
   0.000 -0.461 -0.877 -0.963 -0.989 -0.953 -0.861 -0.726 -0.560 -0.370 -0.163 0.056
   0.283 0.079 0.006 -0.093 -0.166 -0.214 -0.244 -0.257 -0.253 -0.231 -0.192 -0.128
   -0.033 0.098 0.089 0.138 -0.751 -0.879 -0.962 -0.990 -0.960 -0.880 -0.756 -0.601
```

```
End
    Frequencies[1/cm]                42
  94.77   187.48   226.29   339.06   403.29   443.47   525.97   552.67
  630.12   637.58   730.65   800.15   844.17   905.88   960.65   962.67
  971.31   980.14   1010.60 1026.60 1073.37 1136.93 1159.67 1192.66
  1291.55 1303.64 1370.06 1412.55 1442.47 1449.88 1465.28 1558.02
  1583.31 2934.69 3002.69 3030.82 3060.34 3065.15 3073.13 3080.62
  3089.41 3621.73
ZeroEnergy[kcal/mol]    -1.74
  ElectronicLevels[1/cm]                        1
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO                !                7
Geometry[angstrom]              17
C                    1.38647800     1.20803800    -0.09776700
C                    0.01318300     1.20632600    -0.32296800
C                   -0.70081200    -0.00058900    -0.45065900
C                    0.01348000    -1.20713300    -0.32109400
C                    1.38675000    -1.20816500    -0.09590100
C                    2.08037900     0.00010700     0.00425800
H                    1.91712500     2.14854100    -0.00578100
H                   -0.52441700    -2.14537800    -0.39832200
H                    1.91763100    -2.14839300    -0.00245900
H                    3.15156200     0.00035700     0.16939800
O                   -1.39662700     0.00204200     1.72605100
H                   -0.51952400     0.00245100     2.14174300
H                   -0.52494100     2.14431600    -0.40165200
C                   -2.14116200    -0.00114000    -0.88951800
H                   -2.66059400     0.88211300    -0.51769800
H                   -2.20039000    -0.00261000    -1.98230500
H                   -2.66062700    -0.88337100    -0.51532400
   Core      RigidRotor
             SymmetryFactor       0.856940376
End
  Rotor                                  Hindered
  Group     15 16 17
  Axis                14                3
  Symmetry                3
  Potential[kcal/mol]                12
  0.000 -0.705 -0.639 -0.623 -0.653 -0.713 -0.801 -0.893 -0.965 -0.990 -0.962 -0.895
  End
    Rotor                                  Hindered
  Group     12
  Axis                11                3
```

```
  Symmetry                 1
  Potential[kcal/mol]                 36
    0.000 -0.100 0.064 -0.963 -0.989 -0.953 -0.860 -0.726 -0.559 -0.370 -0.163 0.057
    0.283 0.079 0.006 -0.093 -0.166 -0.215 -0.244 -0.257 -0.253 -0.231 -0.192 -0.128
    -0.033 0.099 0.090 0.138 -0.751 -0.880 -0.962 -0.990 -0.960 -0.880 -0.755 -0.600
  End
     Frequencies[1/cm]                 42
   96.80   188.30   231.15   338.58   403.86   440.52   528.29   580.63
   629.65   638.09   731.82   800.28   844.29   908.58   962.37   964.29
   971.53   980.47   1010.93 1026.80 1074.19 1136.81 1159.77 1193.04
   1289.71 1302.89 1369.89 1412.57 1442.47 1449.88 1464.58 1558.15
   1583.73 2934.00 3002.77 3031.37 3060.78 3065.96 3073.88 3081.10
   3089.67 3625.02
 ZeroEnergy[kcal/mol]    -1.27
  ElectronicLevels[1/cm]                          1
   0.0000000000000000          2.0000000000000000
 End
 !*****************************************
 RRHO                 !                 8
 Geometry[angstrom]                17
 C                      1.38582500     1.20841200    -0.09781600
 C                      0.01159700     1.20705800    -0.31165300
 C                     -0.70498100    -0.00056500    -0.43026000
 C                      0.01188600    -1.20783700    -0.30977700
 C                      1.38608900    -1.20853900    -0.09596100
 C                      2.07988000     0.00010100    -0.00147100
 H                      1.91792200     2.14859600    -0.01183500
 H                     -0.52704500    -2.14564500    -0.38392000
 H                      1.91841500    -2.14846100    -0.00853600
 H                      3.15244800     0.00034000     0.15403700
 O                     -1.39055600     0.00200200     1.69503500
 H                     -0.52214500     0.00246800     2.12799300
 H                     -0.52755500     2.14462100    -0.38724700
 C                     -2.14042100    -0.00113500    -0.88452800
 H                     -2.66357600     0.88235300    -0.51871200
 H                     -2.18503900    -0.00268400    -1.97801800
 H                     -2.66365100    -0.88353800    -0.51620700
    Core      RigidRotor
              SymmetryFactor      0.856940376
 End
  Rotor                                  Hindered
  Group      15 16 17
  Axis                  14                  3
  Symmetry                  3
  Potential[kcal/mol]                 12
```

```
0.000 -0.096 -0.189 -0.249 -0.271 -0.242 -0.167 -0.072 0.017 0.074 0.097 0.067
End
  Rotor                                  Hindered
Group     12
Axis                 11              3
Symmetry                   1
Potential[kcal/mol]              36
  0.000 -0.501 -0.878 -0.963 -0.989 -0.953 -0.860 -0.725 -0.559 -0.369 -0.162 0.058
  0.284 0.079 0.005 -0.094 -0.166 -0.215 -0.244 -0.257 -0.253 -0.231 -0.192 -0.127
  -0.033 0.099 0.090 0.138 -0.752 -0.880 -0.962 -0.990 -0.960 -0.879 -0.755 -0.600
End
   Frequencies[1/cm]             42
 101.69   193.80   236.49   338.08   404.64   436.23   529.50   614.80
 629.10   639.24   733.22   800.18   844.48   911.75   964.52   966.29
 971.58   980.59   1011.36 1026.60 1075.11 1136.53 1159.77 1193.40
 1287.38 1302.23 1369.43 1412.55 1442.51 1449.79 1463.72 1558.32
 1583.71 2934.13 3003.54 3032.29 3061.59 3066.94 3074.83 3081.95
 3090.38 3626.87
ZeroEnergy[kcal/mol]     -0.80
 ElectronicLevels[1/cm]                              1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                  !            9
Geometry[angstrom]             17
C                      1.38494800      1.20878400     -0.09849400
C                      0.01027000      1.20813500     -0.30156400
C                     -0.70995500     -0.00054000     -0.40736200
C                      0.01055400     -1.20888300     -0.29968800
C                      1.38520500     -1.20891500     -0.09665100
C                      2.07901600      0.00009700     -0.00567000
H                      1.91861600      2.14869400     -0.01897200
H                     -0.52918800     -2.14626900     -0.37180800
H                      1.91909900     -2.14857500     -0.01570000
H                      3.15259400      0.00032700      0.14233300
O                     -1.38397200      0.00196400      1.66459600
H                     -0.52381300      0.00248400      2.11303100
H                     -0.52968700      2.14528100     -0.37513100
C                     -2.13947700     -0.00113300     -0.88003600
H                     -2.66680700      0.88255400     -0.52084500
H                     -2.16771500     -0.00276300     -1.97414000
H                     -2.66692600     -0.88367200     -0.51820900
   Core     RigidRotor
               SymmetryFactor      0.856940376
End
```

```
  Rotor                                  Hindered
  Group     15 16 17
  Axis               14              3
  Symmetry                3
  Potential[kcal/mol]            12
  0.000 -0.094 -0.189 -0.253 -0.279 -0.256 -0.184 -0.091 0.001 0.061 0.089 0.065
  End
    Rotor                                  Hindered
  Group     12
  Axis               11              3
  Symmetry                1
  Potential[kcal/mol]            36
    0.000 -0.744 -0.879 -0.963 -0.989 -0.952 -0.859 -0.724 -0.558 -0.368 -0.161 0.059
    0.285 0.079 0.193 -0.078 -0.155 -0.212 -0.244 -0.258 -0.252 -0.228 -0.184 -0.114
    -0.014 0.126 0.090 0.139 -0.752 -0.881 -0.963 -0.990 -0.960 -0.879 -0.754 -0.599
   End
     Frequencies[1/cm]             42
   104.36   199.28   242.65   337.67   405.69   430.93   530.24   628.32
   640.90   653.95   735.32   799.33   844.92   915.41   967.59   969.35
   971.51   980.09   1011.67 1025.93 1076.26 1136.04 1159.65 1193.52
   1284.11 1301.67 1368.99 1412.44 1442.70 1449.68 1462.31 1557.59
   1582.82 2933.87 3004.10 3032.94 3062.02 3067.68 3075.95 3082.37
   3090.69 3629.17
ZeroEnergy[kcal/mol]     -0.67
  ElectronicLevels[1/cm]                       1
   0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO               !              10
Geometry[angstrom]            17
C                   1.38400900     1.20963200    -0.09849600
C                   0.00955400     1.20917900    -0.29365000
C                  -0.71621300    -0.00051600    -0.38163700
C                   0.00982000    -1.20992500    -0.29177500
C                   1.38424500    -1.20974300    -0.09667200
C                   2.07771400     0.00009600    -0.00935000
H                   1.91952400     2.14906900    -0.02790500
H                  -0.53029300    -2.14705400    -0.36379400
H                   1.91998800    -2.14894700    -0.02467800
H                   3.15213100     0.00030500     0.13248000
O                  -1.37703300     0.00193000     1.63509500
H                  -0.52421600     0.00250300     2.09673000
H                  -0.53077400     2.14607000    -0.36709900
C                  -2.13873000    -0.00113100    -0.87591200
H                  -2.67052100     0.88295700    -0.52462700
```

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H                    -2.14810500     -0.00285800     -1.97027500
H                    -2.67068800     -0.88400300     -0.52183500
   Core     RigidRotor
            SymmetryFactor     0.856940376
End
 Rotor                               Hindered
 Group     15 16 17
 Axis                14                  3
 Symmetry                  3
 Potential[kcal/mol]                12
 0.000 -0.090 -0.188 -0.257 -0.288 -0.272 -0.206 -0.114 -0.020 0.044 0.077 0.061
 End
   Rotor                               Hindered
 Group     12
 Axis                11                  3
 Symmetry                  1
 Potential[kcal/mol]                36
   0.000 -0.745 -0.879 -0.964 -0.989 -0.952 -0.859 -0.724 -0.557 -0.367 -0.160 0.060
   0.286 0.079 0.004 -0.095 -0.167 -0.215 -0.244 -0.257 -0.253 -0.230 -0.191 -0.127
   -0.032 0.100 0.090 0.139 -0.753 -0.881 -0.963 -0.990 -0.960 -0.878 -0.753 -0.598
 End
    Frequencies[1/cm]                42
  109.02    206.41    249.32    337.46    407.10    424.63    530.51    627.23
  644.69    698.51    737.69    797.26    844.85    919.68    971.24    973.50
  971.08    978.89    1011.54 1024.08 1077.68 1134.92 1159.12 1193.05
  1279.81 1301.37 1368.27 1411.83 1442.88 1449.48 1459.95 1555.48
  1579.99 2934.52 3005.40 3034.21 3062.94 3068.70 3076.53 3083.47
  3091.44 3630.78
ZeroEnergy[kcal/mol]     -0.55
 ElectronicLevels[1/cm]                                1
  0.0000000000000000             2.0000000000000000
End
!*********************************************
RRHO                   !                   11
Geometry[angstrom]                17
C                      1.38290200      1.21043400     -0.10022500
C                      0.00936400      1.21117600     -0.28688500
C                     -0.72396000     -0.00047100     -0.35320300
C                      0.00962500     -1.21186700     -0.28501100
C                      1.38313600     -1.21057700     -0.09842000
C                      2.07679300      0.00008100     -0.01064500
H                      1.92008000      2.14937500     -0.03661900
H                     -0.53073200     -2.14868100     -0.35806300
H                      1.92052400     -2.14930800     -0.03348200
H                      3.15167400      0.00029000      0.12717300
```

```
O                -1.37022200    0.00190100    1.60705800
H                -0.52394000    0.00253000    2.07980000
H                -0.53119000    2.14777200   -0.36128600
C                -2.13764100   -0.00114100   -0.87288700
H                -2.67379500    0.88320500   -0.52920400
H                -2.12847400   -0.00299700   -1.96699500
H                -2.67399200   -0.88420200   -0.52621500
   Core    RigidRotor
           SymmetryFactor    0.856940376
End
  Rotor                          Hindered
  Group    15 16 17
  Axis            14            3
  Symmetry              3
  Potential[kcal/mol]           12
  0.000 -0.086 -0.185 -0.261 -0.298 -0.292 -0.233 -0.143 -0.048 0.023 0.062 0.055
  End
    Rotor                          Hindered
  Group    12
  Axis            11            3
  Symmetry              1
  Potential[kcal/mol]           36
    0.000 -0.745 -0.879 -0.964 -0.989 -0.952 -0.858 -0.723 -0.556 -0.366 -0.159 0.061
    0.287 0.079 0.004 -0.095 -0.167 -0.215 -0.244 -0.257 -0.252 -0.230 -0.191 -0.126
    -0.031 0.101 0.090 0.139 -0.754 -0.881 -0.963 -0.990 -0.959 -0.878 -0.753 -0.598
  End
     Frequencies[1/cm]           42
   117.67   209.55   256.29   337.14   406.03   415.86   530.42   625.42
   647.98   741.00   749.48   793.31   843.65   923.64   971.66   975.94
   969.99   975.96   1010.42 1021.39 1079.25 1132.72 1158.04 1192.75
   1274.21 1300.72 1367.69 1410.15 1443.15 1448.89 1456.08 1549.61
   1575.23 2936.33 3007.40 3035.32 3063.60 3069.47 3077.55 3084.30
   3092.11 3633.12
ZeroEnergy[kcal/mol]   -0.35
  ElectronicLevels[1/cm]                    1
   0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO              !            12
Geometry[angstrom]            17
C                 1.38170060    1.21168903   -0.10213541
C                 0.00976560    1.21405203   -0.28179841
C                -0.73321840   -0.00043697   -0.32271541
C                 0.01001560   -1.21472097   -0.27990041
C                 1.38192760   -1.21183097   -0.10032241
```

```
C                        2.07633060      0.00008003     -0.01112641
H                        1.92056160      2.15002603     -0.04487541
H                       -0.53054940     -2.15119197     -0.35410541
H                        1.92099260     -2.14996997     -0.04173741
H                        3.15142460      0.00028503      0.12413759
O                       -1.36336840      0.00185703      1.58038559
H                       -0.52276640      0.00250103      2.06245859
H                       -0.53099240      2.15030503     -0.35734941
C                       -2.13668840     -0.00113597     -0.87068541
H                       -2.67705040      0.88339003     -0.53418841
H                       -2.10932640     -0.00298397     -1.96421141
H                       -2.67725140     -0.88440297     -0.53121341
   Core     RigidRotor
              SymmetryFactor       0.856940376
End
 Rotor                                         Hindered
 Group     15 16 17
 Axis                  14                  3
 Symmetry                    3
 Potential[kcal/mol]                  12
 0.000 0.765 1.637 2.397 2.813 2.733 2.182 1.343 0.471 -0.214 -0.557 -0.493
 End
   Rotor                                         Hindered
 Group     12
 Axis                  11                  3
 Symmetry                    1
 Potential[kcal/mol]                  36
   0.000 0.065 0.339 0.789 1.352 1.931 2.447 2.831 3.046 3.101 3.054 2.972
   2.910 2.902 2.975 3.098 3.248 3.377 3.432 3.397 3.282 3.133 2.999 2.921
   2.902 2.955 3.036 3.097 3.072 2.904 2.573 2.105 1.557 0.991 0.498 0.153
 End
    Frequencies[1/cm]                  42
  134.65   217.72   265.14   337.80   407.22   408.56   529.67   622.56
  646.49   738.98   785.81   805.82   839.30   920.82   973.75   978.98
  968.10   971.62   1007.64 1016.53 1080.61 1128.85 1156.12 1192.10
  1267.93 1299.60 1367.02 1406.97 1442.93 1447.91 1450.50 1539.83
  1567.88 2938.20 3009.43 3035.91 3064.67 3070.47 3079.06 3085.30
  3093.01 3634.70
ZeroEnergy[kcal/mol]     -0.66
 ElectronicLevels[1/cm]                          1
  0.0000000000000000            2.0000000000000000
End
!*******************************************
RRHO                  !                  13
Geometry[angstrom]                  17
```

```
C        1.38049900    1.21294400   -0.10404600
C        0.01016700    1.21692800   -0.27671200
C       -0.74247700   -0.00040300   -0.29222800
C        0.01040600   -1.21757500   -0.27479000
C        1.38071900   -1.21308400   -0.10222500
C        2.07586900    0.00007900   -0.01160800
H        1.92104300    2.15067700   -0.05313200
H       -0.53036700   -2.15370200   -0.35014800
H        1.92146200   -2.15063200   -0.04999200
H        3.15117500    0.00028000    0.12110200
O       -1.35651500    0.00181300    1.55371300
H       -0.52159300    0.00247200    2.04511700
H       -0.53079400    2.15283800   -0.35341300
C       -2.13573500   -0.00113100   -0.86848400
H       -2.68030600    0.88357500   -0.53917300
H       -2.09017900   -0.00297100   -1.96142800
H       -2.68051100   -0.88460400   -0.53621200
   Core    RigidRotor
        SymmetryFactor    0.856940376
End
 Rotor                          Hindered
 Group    15 16 17
 Axis          14         3
 Symmetry           3
 Potential[kcal/mol]          12
 0.000 0.721 1.588 2.389 2.887 2.910 2.440 1.637 0.753 0.016 -0.401 -0.418
 End
   Rotor                          Hindered
 Group    12
 Axis          11         3
 Symmetry           1
 Potential[kcal/mol]          36
   0.000 0.065 0.341 0.791 1.354 1.933 2.448 2.832 3.046 3.102 3.054 2.972
   2.910 2.903 2.975 3.099 3.249 3.377 3.432 3.397 3.282 3.133 2.999 2.921
   2.903 2.956 3.037 3.098 3.072 2.903 2.572 2.104 1.555 0.990 0.497 0.153
 End
    Frequencies[1/cm]          42
  169.46   229.70   276.20   339.65   402.26   408.31   528.67   619.08
  639.67   734.95   779.61   831.74   862.73   913.61   973.73   978.98
  965.94   966.96   1004.31 1013.49 1081.43 1123.93 1153.87 1191.21
  1264.64 1297.97 1366.45 1402.36 1441.29 1446.32 1446.70 1530.43
  1559.49 2938.31 3010.30 3035.97 3065.42 3071.13 3080.37 3086.04
  3093.66 3634.53
ZeroEnergy[kcal/mol]    -1.34
 ElectronicLevels[1/cm]                  1
```

```
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO              !              14
Geometry[angstrom]             17
C                   1.37917300    1.21456400   -0.10598100
C                   0.01106800    1.22055900   -0.27297300
C                  -0.75290500   -0.00036700   -0.26042600
C                   0.01128900   -1.22119100   -0.27101800
C                   1.37938400   -1.21469800   -0.10413800
C                   2.07588900    0.00008100   -0.01158400
H                   1.92140200    2.15161300   -0.06096100
H                  -0.52970300   -2.15696600   -0.34721600
H                   1.92180200   -2.15157200   -0.05775600
H                   3.15122300    0.00027800    0.11947300
O                  -1.34977900    0.00176000    1.52838600
H                  -0.51942700    0.00240900    2.02689900
H                  -0.53010600    2.15611200   -0.35057400
C                  -2.13482000   -0.00111800   -0.86701400
H                  -2.68343600    0.88371600   -0.54450000
H                  -2.07163400   -0.00286700   -1.95904000
H                  -2.68362500   -0.88480400   -0.54167900
   Core    RigidRotor
           SymmetryFactor     0.856940376
End
 Rotor                               Hindered
 Group    15 16 17
 Axis              14            3
 Symmetry                3
 Potential[kcal/mol]            12
 0.000 0.666 1.518 2.354 2.933 3.067 2.692 1.941 1.053 0.267 -0.227 -0.332
 End
   Rotor                               Hindered
 Group    12
 Axis              11            3
 Symmetry                1
 Potential[kcal/mol]            36
   0.000 0.066 0.341 0.792 1.355 1.934 2.449 2.833 3.047 3.102 3.054 2.972
   2.910 2.903 2.975 3.099 3.249 3.378 3.432 3.397 3.282 3.132 2.998 2.921
   2.903 2.956 3.037 3.098 3.072 2.903 2.571 2.103 1.554 0.989 0.497 0.152
 End
    Frequencies[1/cm]            42
  188.50   240.14   288.99   342.86   396.66   409.89   527.88   614.55
  630.98   730.48   771.62   820.78   900.52   920.51   972.60   977.78
  961.61   962.76   999.07   1012.91 1081.60 1117.27 1151.48 1191.07
```

```
    1262.02 1295.26 1365.68 1395.44 1435.96 1445.07 1445.09 1519.98
    1551.53 2938.59 3011.23 3035.39 3066.26 3071.67 3081.87 3086.85
    3094.59 3635.25
  ZeroEnergy[kcal/mol]     -2.61
   ElectronicLevels[1/cm]                          1
    0.0000000000000000             2.0000000000000000
  End
  !****************************************
  RRHO                !                 15
  Geometry[angstrom]                17
  C                      1.37757600      1.21625800     -0.10790600
  C                      0.01235000      1.22442100     -0.27006600
  C                     -0.76408900     -0.00033200     -0.22791100
  C                      0.01256200     -1.22503800     -0.26807900
  C                      1.37777800     -1.21638800     -0.10604900
  C                      2.07632600      0.00008000     -0.01124100
  H                      1.92154000      2.15259900     -0.06852400
  H                     -0.52860000     -2.16054000     -0.34515400
  H                      1.92192500     -2.15256500     -0.06530000
  H                      3.15156300      0.00027300      0.11872000
  O                     -1.34318900      0.00171500      1.50380700
  H                     -0.51682000      0.00236600      2.00825000
  H                     -0.52898900      2.15970100     -0.34855100
  C                     -2.13365000     -0.00110900     -0.86585900
  H                     -2.68618400      0.88385600     -0.54992900
  H                     -2.05442200     -0.00281800     -1.95653900
  H                     -2.68636100     -0.88497800     -0.54717500
     Core      RigidRotor
               SymmetryFactor       0.856940376
  End
   Rotor                                    Hindered
   Group     15 16 17
   Axis                14                3
   Symmetry                    3
   Potential[kcal/mol]                 12
   0.000 0.601 1.429 2.289 2.944 3.188 2.919 2.233 1.352 0.526 -0.044 -0.239
   End
     Rotor                                    Hindered
   Group     12
   Axis                11                3
   Symmetry                    1
   Potential[kcal/mol]                 36
     0.000 0.066 0.341 0.791 1.355 1.934 2.449 2.833 3.047 3.102 3.054 2.972
     2.910 2.903 2.975 3.099 3.249 3.378 3.432 3.397 3.282 3.132 2.998 2.921
     2.903 2.956 3.037 3.098 3.072 2.903 2.571 2.103 1.554 0.989 0.497 0.152
```

```
End
   Frequencies[1/cm]          42
 202.06  248.93  302.52  347.47  391.46  412.26  528.04  609.42
 622.02  726.55  763.93  808.08  886.38  970.03  971.36  976.55
 994.01  996.17  1031.43 1015.35 1080.72 1110.37 1150.24 1193.00
 1260.90 1291.51 1364.84 1386.83 1429.65 1443.50 1445.22 1510.88
 1547.57 2939.88 3012.67 3033.96 3066.58 3071.39 3083.01 3087.03
 3095.47 3637.14
ZeroEnergy[kcal/mol]   -4.66
 ElectronicLevels[1/cm]                    1
 0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO            !          16
Geometry[angstrom]           17
C                  1.37598600    1.21792700   -0.10983600
C                  0.01336100    1.22806000   -0.26726900
C                 -0.77516200   -0.00029700   -0.19530900
C                  0.01356500   -1.22866200   -0.26525500
C                  1.37618900   -1.21805600   -0.10796700
C                  2.07689400    0.00008000   -0.01070200
H                  1.92170200    2.15359500   -0.07642100
H                 -0.52729800   -2.16422900   -0.34386300
H                  1.92207900   -2.15357300   -0.07318600
H                  3.15202200    0.00027100    0.11830900
O                 -1.33652500    0.00167200    1.47924900
H                 -0.51404200    0.00232900    1.98949300
H                 -0.52767600    2.16340400   -0.34728900
C                 -2.13232400   -0.00110300   -0.86457200
H                 -2.68925200    0.88396500   -0.55577800
H                 -2.03706700   -0.00278400   -1.95368800
H                 -2.68942500   -0.88511300   -0.55306800
   Core   RigidRotor
          SymmetryFactor    0.856940376
End
 Rotor                     Hindered
 Group   15 16 17
 Axis        14          3
 Symmetry          3
 Potential[kcal/mol]           12
 0.000 0.533 1.329 2.199 2.918 3.263 3.101 2.488 1.626 0.770 0.133 -0.147
 End
   Rotor                     Hindered
 Group   12
 Axis        11          3
```

```
  Symmetry                 1
  Potential[kcal/mol]                 36
    0.000 0.066 0.342 0.792 1.356 1.935 2.450 2.833 3.047 3.102 3.053 2.972
    2.910 2.903 2.975 3.099 3.249 3.378 3.432 3.397 3.282 3.132 2.998 2.921
    2.903 2.956 3.037 3.098 3.072 2.902 2.570 2.102 1.553 0.988 0.496 0.152
  End
     Frequencies[1/cm]                 42
   212.26   250.41   303.64   339.72   373.26   400.53   509.61   581.87
   591.33   696.03   730.24   766.21   839.19   933.83   938.97   950.28
   954.04   973.13   987.45  1021.37 1077.91 1105.17 1150.54 1196.77
  1260.18 1286.75 1364.07 1377.80 1423.69 1442.36 1445.83 1504.29
  1547.95 2940.38 3013.47 3031.19 3066.04 3070.15 3083.26 3086.29
  3096.04 3638.82
ZeroEnergy[kcal/mol]    -7.19
  ElectronicLevels[1/cm]                          1
    0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO                !                17
Geometry[angstrom]                17
C                      1.37456300      1.21947800     -0.11181900
C                      0.01373300      1.23121500     -0.26406500
C                     -0.78573800     -0.00025800     -0.16306800
C                      0.01392800     -1.23180200     -0.26202500
C                      1.37476200     -1.21960500     -0.10993800
C                      2.07737100      0.00008000     -0.01005500
H                      1.92195100      2.15456400     -0.08533100
H                     -0.52599300     -2.16789800     -0.34304200
H                      1.92232000     -2.15455300     -0.08208600
H                      3.15247100      0.00027000      0.11788100
O                     -1.32965700      0.00162800      1.45432100
H                     -0.51145500      0.00229700      1.97073600
H                     -0.52635900      2.16708600     -0.34649500
C                     -2.13076400     -0.00109600     -0.86293200
H                     -2.69276100      0.88402800     -0.56236400
H                     -2.01835200     -0.00275400     -1.95011100
H                     -2.69293300     -0.88520200     -0.55969100
   Core      RigidRotor
             SymmetryFactor       0.856940376
End
  Rotor                                  Hindered
  Group      15 16 17
  Axis                  14                  3
  Symmetry                  3
  Potential[kcal/mol]                 12
```

```
  0.000 0.466 1.223 2.095 2.863 3.295 3.235 2.698 1.865 0.990 0.295 -0.062
  End
    Rotor                                   Hindered
  Group     12
  Axis                 11                 3
  Symmetry                   1
  Potential[kcal/mol]                 36
    0.000 0.067 0.343 0.794 1.358 1.937 2.452 2.834 3.047 3.102 3.053 2.972
    2.910 2.903 2.976 3.100 3.250 3.378 3.432 3.397 3.281 3.132 2.998 2.921
    2.903 2.956 3.038 3.098 3.072 2.902 2.569 2.100 1.552 0.986 0.495 0.151
   End
     Frequencies[1/cm]                 42
   234.06   274.03   327.50   358.56   386.31   421.82   532.38   600.62
   608.71   719.80   756.47   786.56   860.21   969.61   975.22   983.31
   986.29   977.31   1005.43 1030.72 1073.64 1102.14 1151.91 1203.37
   1258.87 1281.34 1363.38 1369.45 1418.14 1441.73 1446.57 1499.68
   1549.88 2940.34 3014.11 3027.60 3064.64 3068.08 3082.26 3084.53
   3096.17 3641.49
 ZeroEnergy[kcal/mol]     -9.97
  ElectronicLevels[1/cm]                              1
   0.0000000000000000              2.0000000000000000
 End
 !********************************************
 RRHO                    !                 18
 Geometry[angstrom]                 17
 C                          1.37326800       1.22084700     -0.11392200
 C                          0.01341600       1.23385500     -0.26012400
 C                         -0.79576900     -0.00022100     -0.13154300
 C                          0.01360300     -1.23442400     -0.25805600
 C                          1.37346400     -1.22097300     -0.11202900
 C                          2.07759700       0.00007900     -0.00938900
 H                          1.92224900       2.15538900     -0.09557700
 H                         -0.52499400     -2.17128400     -0.34231700
 H                          1.92260800     -2.15539200     -0.09232100
 H                          3.15277800       0.00026700      0.11716600
 O                         -1.32245100       0.00158300      1.42886000
 H                         -0.50998300       0.00226700      1.95336800
 H                         -0.52534500       2.17049000     -0.34580100
 C                         -2.12883000     -0.00108900     -0.86091200
 H                         -2.69637500       0.88407200     -0.56975800
 H                         -1.99760000     -0.00272300     -1.94567600
 H                         -2.69654700     -0.88527200     -0.56712100
     Core     RigidRotor
               SymmetryFactor      0.856940376
 End
```

```
Rotor                                   Hindered
Group    15 16 17
Axis              14              3
Symmetry                 3
Potential[kcal/mol]               12
0.000 0.401 1.118 1.984 2.789 3.294 3.326 2.864 2.065 1.180 0.439 0.015
End
  Rotor                                   Hindered
Group    12
Axis              11              3
Symmetry                 1
Potential[kcal/mol]               36
  0.000 0.068 0.346 0.797 1.361 1.940 2.455 2.836 3.049 3.102 3.053 2.972
  2.910 2.903 2.977 3.101 3.251 3.379 3.433 3.397 3.281 3.131 2.998 2.921
  2.904 2.957 3.038 3.099 3.071 2.901 2.567 2.098 1.549 0.984 0.493 0.150
End
    Frequencies[1/cm]              42
 289.78   293.77   344.29   363.54   386.16   428.85   536.76   597.19
 604.52   716.36   755.67   778.96   851.19   968.88   974.80   979.16
 981.08   972.19   1020.11 1044.48 1069.14 1100.25 1153.60 1215.03
 1256.51 1275.86 1362.25 1362.76 1413.17 1441.46 1447.29 1496.28
 1550.92 2939.96 3014.94 3024.01 3062.75 3065.63 3080.46 3082.26
 3095.98 3645.30
ZeroEnergy[kcal/mol]     -12.39
 ElectronicLevels[1/cm]                        1
 0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                 !              19
Geometry[angstrom]              17
C                      1.37192500      1.22203800     -0.11623400
C                      0.01254800      1.23612500     -0.25525300
C                     -0.80528300     -0.00018400     -0.10092600
C                      0.01272600     -1.23667400     -0.25315600
C                      1.37211400     -1.22216300     -0.11432900
C                      2.07748200      0.00007900     -0.00881300
H                      1.92248900      2.15598300     -0.10721700
H                     -0.52454300     -2.17425700     -0.34124000
H                      1.92283400     -2.15600300     -0.10394800
H                      3.15284300      0.00026400      0.11588700
O                     -1.31492600      0.00153400      1.40293500
H                     -0.51013500      0.00224100      1.93802100
H                     -0.52487600      2.17348300     -0.34475900
C                     -2.12628900     -0.00108100     -0.85860100
H                     -2.69959500      0.88415400     -0.57793600
```

```
H                          -1.97465100     -0.00268900     -1.94040300
H                          -2.69976600     -0.88538100     -0.57533900
   Core     RigidRotor
               SymmetryFactor        0.856940376
End
 Rotor                                      Hindered
 Group     15 16 17
 Axis                14                 3
 Symmetry                  3
 Potential[kcal/mol]                12
 0.000 0.342 1.018 1.874 2.704 3.269 3.383 2.990 2.229 1.340 0.563 0.082
 End
    Rotor                                      Hindered
 Group     12
 Axis                11                 3
 Symmetry                    1
 Potential[kcal/mol]                36
    0.000 0.069 0.348 0.801 1.365 1.944 2.458 2.838 3.050 3.102 3.053 2.971
    2.910 2.904 2.978 3.102 3.252 3.380 3.433 3.397 3.280 3.131 2.997 2.921
    2.904 2.958 3.039 3.099 3.071 2.899 2.565 2.095 1.545 0.980 0.490 0.149
 End
     Frequencies[1/cm]                  42
  304.87    340.49    367.44    386.30    436.74    473.15    547.67    594.02
  603.23    713.69    756.87    772.95    844.61    968.07    974.01    975.46
  975.80    967.57    1028.89 1055.76 1065.06 1098.87 1154.97 1232.49
  1252.72 1271.03 1356.18 1362.19 1408.86 1441.41 1447.97 1493.62
  1551.23 2939.30 3015.92 3020.69 3060.63 3063.06 3078.38 3079.88
  3095.61 3650.55
ZeroEnergy[kcal/mol]     -14.72
 ElectronicLevels[1/cm]                               1
  0.0000000000000000            2.0000000000000000
End
!********************************************
RRHO                    !                    20
Geometry[angstrom]                17
C                           1.37033200       1.22312800     -0.11900500
C                           0.01106700       1.23824400     -0.24889000
C                          -0.81396100     -0.00014600     -0.07162400
C                           0.01123500     -1.23876500     -0.24676000
C                           1.37051300     -1.22325300     -0.11708500
C                           2.07685000       0.00007900     -0.00854600
H                           1.92260600       2.15634400     -0.12104400
H                          -0.52489200     -2.17693600     -0.33903800
H                           1.92293300     -2.15638500     -0.11775500
H                           3.15252800       0.00025900       0.11336800
```

```
O                    -1.30734000     0.00147900     1.37676800
H                    -0.51183500     0.00221500     1.92416600
H                    -0.52520400     2.17618800    -0.34260400
C                    -2.12255300    -0.00107100    -0.85609300
H                    -2.70197700     0.88435900    -0.58751600
H                    -1.94802200    -0.00264500    -1.93429200
H                    -2.70214600    -0.88561900    -0.58496800
   Core      RigidRotor
             SymmetryFactor       0.856940376
End
 Rotor                                  Hindered
 Group     15 16 17
 Axis                14                  3
 Symmetry              3
 Potential[kcal/mol]                   12
 0.000 0.290 0.930 1.773 2.621 3.233 3.413 3.081 2.356 1.469 0.665 0.138
 End
      Rotor                                  Hindered
 Group     12
 Axis                11                  3
 Symmetry               1
 Potential[kcal/mol]                   36
   0.000 0.069 0.348 0.801 1.365 1.944 2.458 2.838 3.050 3.102 3.053 2.971
   2.910 2.904 2.978 3.102 3.252 3.380 3.433 3.397 3.280 3.131 2.997 2.921
   2.904 2.958 3.039 3.099 3.071 2.899 2.565 2.095 1.545 0.980 0.490 0.149
 End
      Frequencies[1/cm]                   42
  318.01   347.40   369.88   387.17   444.88   532.41   589.47   590.86
  647.98   714.38   766.58   768.56   840.78   967.05   970.92   971.03
  974.48   963.56  1038.47 1061.56 1062.30 1097.88 1155.69 1247.27
 1253.61 1267.70 1351.33 1362.03 1405.28 1441.58 1448.62 1491.59
 1551.32 2937.75 3015.92 3017.22 3058.16 3060.23 3076.06 3077.29
 3095.03 3657.48
ZeroEnergy[kcal/mol]     -16.55
 ElectronicLevels[1/cm]                        1
  0.0000000000000000            2.0000000000000000
End
!*****************************************
RRHO                 !                  21
Geometry[angstrom]                  17
C                     1.36801300     1.22437600    -0.12319300
C                     0.00837200     1.24071100    -0.23866800
C                    -0.82022000    -0.00010700    -0.04552700
C                     0.00852300    -1.24119300    -0.23648600
C                     1.36817800    -1.22449700    -0.12124100
```

```
C 2.07488800 0.00007700 -0.00991800
H 1.92260100 2.15651600 -0.14103800
H -0.52736800 -2.17950600 -0.33217500
H 1.92289300 -2.15658600 -0.13769800
H 3.15129800 0.00024700 0.10589000
O -1.30102100 0.00140600 1.35222000
H -0.51547000 0.00218200 1.91193000
H -0.52764300 2.17880200 -0.33583300
C -2.11505900 -0.00105500 -0.85447000
H -2.70170300 0.88496600 -0.60203800
H -1.91060400 -0.00256600 -1.92796000
H -2.70185800 -0.88627700 -0.59958000
   Core RigidRotor
      SymmetryFactor 0.856940376
End
  Rotor Hindered
  Group 15 16 17
  Axis 14 3
  Symmetry 3
  Potential[kcal/mol] 12
  0.000 0.259 0.875 1.710 2.565 3.204 3.423 3.129 2.427 1.543 0.725 0.172
  End
    Rotor Hindered
  Group 12
  Axis 11 3
  Symmetry 1
  Potential[kcal/mol] 36
    0.000 0.075 0.358 0.815 1.381 1.959 2.470 2.847 3.054 3.103 3.052 2.970
    2.910 2.916 2.981 3.107 3.257 3.383 3.434 3.396 3.278 3.128 2.996 2.921
    2.905 2.961 3.042 3.101 3.070 2.894 2.556 2.083 1.532 0.968 0.481 0.143
  End
     Frequencies[1/cm] 42
   325.35 351.03 371.20 387.95 452.49 539.20 587.84 592.08
   698.85 731.42 766.43 816.26 851.10 965.35 968.88 969.23
   974.73 997.62 1052.03 1059.10 1069.60 1097.57 1155.89 1242.41
   1266.58 1274.13 1348.44 1363.51 1402.87 1442.26 1449.39 1490.67
   1551.93 2933.18 3011.10 3012.81 3054.64 3056.58 3073.30 3073.98
   3093.80 3667.88
ZeroEnergy[kcal/mol] -17.65
  ElectronicLevels[1/cm] 1
   0.0000000000000000 2.0000000000000000
End
!*******************************************
RRHO ! 22
Geometry[angstrom] 17
```

```
C                 1.36554400     1.22581100     -0.12920700
C                 0.00469300     1.24326600     -0.22417900
C                -0.81754000    -0.00007900     -0.03811400
C                 0.00482300    -1.24369100     -0.22191900
C                 1.36568500    -1.22592700     -0.12718300
C                 2.07136400     0.00007100     -0.01926200
H                 1.92323700     2.15659600     -0.17492800
H                -0.53394700    -2.18136400     -0.31087900
H                 1.92346400    -2.15671900     -0.17141600
H                 3.14988900     0.00021600      0.07796700
O                -1.30680500     0.00132500      1.35516300
H                -0.52024700     0.00209100      1.90836700
H                -0.53414800     2.18074600     -0.31476900
C                -2.09927100    -0.00102800     -0.86284200
H                -2.69505800     0.88706200     -0.63624300
H                -1.84505700    -0.00235000     -1.93016300
H                -2.69515000    -0.88853300     -0.63406400
   Core     RigidRotor
            SymmetryFactor      0.856940376
End
 Rotor                                 Hindered
 Group     15 16 17
 Axis                 14                3
 Symmetry                3
 Potential[kcal/mol]            12
 0.000 0.288 0.927 1.770 2.617 3.231 3.413 3.084 2.360 1.473 0.669 0.141
 End
   Rotor                                 Hindered
 Group     12
 Axis                 11                3
 Symmetry                1
 Potential[kcal/mol]             36
   0.000 0.081 0.370 0.830 1.398 1.975 2.483 2.856 3.058 3.104 3.051 2.969
   2.910 2.918 2.985 3.112 3.262 3.387 3.435 3.394 3.274 3.125 2.993 2.921
   2.907 2.964 3.045 3.102 3.068 2.887 2.545 2.069 1.517 0.954 0.470 0.138
 End
    Frequencies[1/cm]              42
  294.53   349.31   374.97   388.78   454.94   538.63   587.67   592.75
  702.83   734.13   769.74   819.82   856.20   969.38   969.48   973.02
  978.27   996.45   1056.23 1060.24 1072.69 1099.67 1156.23 1247.97
  1268.82 1273.72 1351.20 1368.66 1403.94 1444.70 1450.64 1492.44
  1553.90 2911.13 2985.71 3005.44 3046.49 3048.78 3069.01 3069.67
  3090.12 3704.82
ZeroEnergy[kcal/mol]     -17.36
 ElectronicLevels[1/cm]                        1
```

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    0.0000000000000000           2.0000000000000000
End
 !***********************************
        Tunneling     Eckart
       ImaginaryFrequency[1/cm]        411.6
       WellDepth[kcal/mol]             3.18
       WellDepth[kcal/mol]             18.11
End
End
!***********************************
 Bimolecular        P4m          # mOHC6H4CH3 + H
Fragment PROD1
RRHO
Geometry[angstrom]                   16
C                      0.03828900    -0.98332300    -0.01103200
C                     -1.21419400    -0.36747800     0.00155700
C                     -1.31683100     1.02422600     0.00783400
C                     -0.15108900     1.79118800     0.00251200
C                      1.10089000     1.18051600    -0.00905900
C                      1.20539600    -0.21732100    -0.01208300
H                     -2.29153300     1.50193700     0.01367200
H                     -0.22618900     2.87251300     0.00277400
H                      1.99944500     1.78707000    -0.01692600
O                     -2.31206400    -1.18783600     0.00152300
H                     -3.10835700    -0.64861900     0.00128900
H                      0.08363700    -2.06635100    -0.01979200
C                      2.55658700    -0.88788300     0.01051600
H                      2.91140200    -1.01152500     1.03818800
H                      2.51470600    -1.87797900    -0.44695700
H                      3.29911700    -0.29390900    -0.52590100
   Core     RigidRotor
       SymmetryFactor      0.5
   End
              Rotor   Hindered                    ! freq=50
          Group                              14 15 16
          Axis                               6 13
          Symmetry                           3
   Potential[kcal/mol]        12
          0.000 0.005 0.012 0.021 0.018 0.008 0.001 0.001 0.008 0.015 0.012 0.004
         End
        Rotor   Hindered                     !freq=244
          Group                              11
          Axis                               2 10
          Symmetry                           1
   Potential[kcal/mol]        36
```

```
          0.000 0.092 0.389 0.864 1.452 2.084 2.683 3.172 3.487 3.568 3.400 3.028
        2.516 1.924 1.325 0.786 0.367 0.116 0.040 0.136 0.405 0.837 1.382 1.980
        2.565 3.067 3.426 3.574 3.472 3.122 2.616 2.009 1.378 0.800 0.343 0.070
          End
        Frequencies[1/cm]                40
      198.61   222.19   295.05   427.33   445.22   521.41   538.70   546.11
      558.40   741.48   743.99   834.52   847.66   912.44   947.09   974.50
      988.51   1018.59 1071.93 1134.08 1143.48 1165.80 1255.31 1287.04
      1319.62 1369.79 1428.64 1443.52 1462.20 1467.25 1572.12 1598.85
      2929.96 2989.47 3012.20 3051.32 3063.99 3075.65 3081.82 3706.83
    ZeroEnergy[kcal/mol]                0.
    ElectronicLevels[1/cm]                          1
    0.000000000000000E+000     1.00000000000000
  End
  !***********************************
  Fragment PROD2
  RRHO
        Geometry[angstrom]                1
H                          0.00000000      0.00000000      0.00000000
    Core     RigidRotor
        SymmetryFactor      1.00000000000000
    End
    ZeroEnergy[kcal/mol]                0.
    ElectronicLevels[1/cm]                          1
    0.000000000000000E+000     2.00000000000000
  End
  GroundEnergy[kcal/mol]     1.02
  End
  !***********************************
    Bimolecular       P4o       # oOHC6H4CH3 + H
  Fragment PROD1
  RRHO
  Geometry[angstrom]                16
  C                        -0.58741200    -0.62124200    -0.00003100
  C                        -0.39709600     0.76973300    -0.00000600
  C                         0.88413500     1.32167300     0.00001700
  C                         1.99797900     0.48646800     0.00001400
  C                         1.83489000    -0.89976800    -0.00004700
  C                         0.54852700    -1.43744100    -0.00007500
  H                         0.98536700     2.40000700     0.00003400
  H                         2.99111300     0.91992900     0.00003400
  H                         2.69768500    -1.55439500    -0.00007200
  H                         0.41480900    -2.51417900    -0.00013200
  O                        -1.44958500     1.64859900     0.00011500
  H                        -2.27720700     1.15968200    -0.00069600
```

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C                    -1.97801700    -1.20387200     0.00007400
H                    -2.54736500    -0.90051000     0.88608300
H                    -2.54800600    -0.89932200    -0.88512400
H                    -1.93774900    -2.29330800    -0.00072200
   Core    RigidRotor
      SymmetryFactor    0.5
   End
    Rotor  Hindered                ! freq=94
         Group                          14 15 16
         Axis                           1 13
         Symmetry                       3
   Potential[kcal/mol]        12
         0.000 0.071 0.296 0.643 1.024 1.322 1.445 1.347 1.064 0.686 0.330 0.089
        End
     Rotor   Hindered               !freq=150
         Group                          12
         Axis                           2 11
         Symmetry                       1
   Potential[kcal/mol]        36
      0.000 0.053 0.246 0.591 1.055 1.583 2.124 2.609 2.963 3.155 3.106 2.798
      2.296 1.666 0.998 0.368 -0.128 -0.445 -0.548 -0.447 -0.133 0.362 0.991 1.659
      2.289 2.794 3.104 3.156 2.966 2.614 2.130 1.589 1.061 0.596 0.249 0.054
       End
    Frequencies[1/cm]              40
    186.29   259.01   301.30   424.19   434.14   512.90   529.95   581.51
    591.00   746.70   758.39   835.09   850.50   903.58   918.78   963.53
    1011.53 1018.60 1082.58 1134.16 1146.18 1191.56 1239.63 1281.99
    1328.43 1368.32 1428.31 1438.52 1462.05 1470.31 1568.76 1599.29
    2908.11 2955.21 3014.00 3057.11 3070.55 3085.32 3093.61 3713.37
  ZeroEnergy[kcal/mol]             0.
  ElectronicLevels[1/cm]                   1
  0.000000000000000E+000    1.00000000000000
 End
 !***********************************
 Fragment PROD2
 RRHO
      Geometry[angstrom]             1
H                    0.00000000     0.00000000     0.00000000
   Core    RigidRotor
      SymmetryFactor    1.00000000000000
   End
  ZeroEnergy[kcal/mol]             0.
  ElectronicLevels[1/cm]                   1
  0.000000000000000E+000    2.00000000000000
 End
```

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GroundEnergy[kcal/mol]     0.71
End
!**********************************
  Bimolecular          P4p        # pOHC6H4CH3 + H
Fragment PROD1
RRHO
Geometry[angstrom]                   16
C                        0.72793300     -1.21888100     -0.00140500
C                        1.43852100     -0.01733900      0.00327400
C                        0.74887800      1.19466900     -0.00111900
C                       -0.64762000      1.19870300     -0.00908100
C                       -1.37951600      0.00884900     -0.00977600
C                       -0.66342400     -1.19615200     -0.00894900
H                        1.29558600      2.13295400     -0.00313800
H                       -1.17062800      2.14924600     -0.01586800
O                        2.80767300     -0.09363200      0.00788400
H                        3.17287700      0.79589800      0.00413700
H                        1.27506500     -2.15356700     -0.00346800
H                       -1.20434700     -2.13691500     -0.01568900
C                       -2.88816700      0.01551700      0.01221100
H                       -3.27078800     -0.15261500      1.02360800
H                       -3.28284400      0.97204200     -0.33574400
H                       -3.29593400     -0.77018500     -0.62783500
    Core     RigidRotor
        SymmetryFactor     1
    End
                    Rotor    Hindered                        ! freq=45
            Group                                  14 15 16
            Axis                                   5 13
            Symmetry                               3
    Potential[kcal/mol]          12
            0.000 0.001 0.032 0.054 0.061 0.051 0.016 -0.002 -0.001 -0.004 -0.005 -0.003
           End
         Rotor    Hindered                        !freq=242.8
            Group                                  10
            Axis                                   2 9
            Symmetry                               1
    Potential[kcal/mol]          36
        0.000 0.079 0.323 0.750 1.287 1.862 2.405 2.853 3.145 3.228 3.086 2.758
        2.297 1.761 1.211 0.709 0.315 0.083 0.000 0.070 0.302 0.674 1.170 1.721
        2.254 2.723 3.064 3.224 3.161 2.884 2.447 1.910 1.335 0.792 0.353 0.078
        End
      Frequencies[1/cm]                 40
      139.99    305.27    317.85    405.67    425.02    465.80    492.40    539.38
      655.70    747.07    781.78    814.56    851.84    874.72    927.98    971.97
```

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        992.28    1019.39 1087.49 1151.12 1152.28 1192.89 1233.22 1291.99
        1322.85 1371.40 1404.16 1441.86 1454.47 1491.65 1576.32 1598.79
        2926.43 2983.71 3006.69 3045.99 3057.34 3065.82 3089.47 3708.61
    ZeroEnergy[kcal/mol]                    0.
    ElectronicLevels[1/cm]                          1
    0.000000000000000E+000      1.00000000000000
  End
  !**********************************
  Fragment PROD2
  RRHO
        Geometry[angstrom]              1
H                       0.00000000      0.00000000      0.00000000
    Core    RigidRotor
        SymmetryFactor      1.00000000000000
    End
    ZeroEnergy[kcal/mol]                    0.
    ElectronicLevels[1/cm]                          1
    0.000000000000000E+000      2.00000000000000
  End
  GroundEnergy[kcal/mol]    1.61
  End
  !**********************************
    Well        W4m2                # mHOC6CH5CH3
     Species
       RRHO
        Geometry[angstrom]              17
  C                       0.14099700    -0.97869900    -0.32239800
  C                       1.21099700    -0.18524500    -0.03819900
  C                       1.01290600     1.21583700     0.15518800
  C                      -0.28100600     1.78068600     0.06851000
  C                      -1.37041600     1.01057500    -0.21359600
  C                      -1.26403800    -0.46815400    -0.42165900
  H                       1.86322500     1.84760900     0.38399600
  H                      -0.40260700     2.84570600     0.23380800
  H                      -2.36371900     1.44077000    -0.26934000
  C                       2.60530400    -0.74771900     0.08222800
  H                       2.61160600    -1.82600200    -0.08195000
  H                       3.27417400    -0.28656500    -0.64966000
  H                       3.01997100    -0.54980900     1.07447700
  O                      -2.13809300    -1.18196200     0.49153600
  H                      -1.81337900    -0.99991100     1.38073800
  H                      -1.68362200    -0.73293100    -1.40072400
  H                       0.27063700    -2.04685600    -0.46407300
            Core        RigidRotor
              SymmetryFactor              0.5
```

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                End
  Rotor Hindered                !freq=122
                Group                           11 12 13
                Axis                            2 10
                Symmetry                        3
    Potential[kcal/mol]         12
        0.000 0.047 0.171 0.353 0.552 0.702 0.756 0.700 0.546 0.356 0.174 0.050
        End
         Rotor   Hindered                !freq=290
            Group                           15
            Axis                            6 14
            Symmetry                        1
    Potential[kcal/mol]         36
      0.000 0.100 0.406 0.870 1.428 1.986 2.449 2.752 2.871 2.841 2.712 2.557
     2.440 2.397 2.430 2.520 2.632 2.724 2.762 2.731 2.647 2.535 2.440 2.397
     2.431 2.536 2.676 2.789 2.812 2.688 2.400 1.968 1.443 0.904 0.434 0.118
        End
            Frequencies[1/cm]           43
     91.89    175.96   330.34   371.13   435.12   466.20   495.93   535.98   619.64
     699.25   762.67   786.67   847.46   897.67   950.54   961.86   986.66
     989.91   1024.75 1040.74 1084.71 1133.73 1161.11 1175.99 1272.16
     1282.10 1324.70 1344.54 1369.46 1389.61 1437.26 1449.26 1515.76
     1577.37 2898.68 2929.59 2986.09 3014.93 3058.36 3060.12 3075.37
     3084.80 3670.76
            ZeroEnergy[kcal/mol]            -16.64
            ElectronicLevels[1/cm]          1
              0     2
End
End
!***********************************
 Barrier        B4m3    W4m2    P4m             # TS4m3
   RRHO
     Geometry[angstrom]             17
C                   -0.05072100    -0.97334300    -0.01973500
C                   -1.22376700    -0.22700800    -0.01481400
C                   -1.13291700     1.17672500    -0.00966100
C                    0.11461100     1.81011600    -0.03017800
C                    1.28954600     1.07397300    -0.02420500
C                    1.22096500    -0.34003500     0.08041800
H                   -2.04231800     1.77201500    -0.01640800
H                    0.16514000     2.89520600    -0.06675600
H                    2.26645400     1.54472200    -0.05273600
C                   -2.57297900    -0.90803600    -0.01993900
H                   -3.04075900    -0.86432200     0.97231300
H                   -3.26148700    -0.42565600    -0.72290500
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H                    -2.49022500    -1.96356100    -0.29816800
O                     2.38642900    -1.02527200    -0.17468600
H                     2.24484800    -1.96376100     0.02515200
H                     1.29299000    -0.40571800     1.82435600
H                    -0.09450600    -2.06110000    -0.03868200
      Core      RigidRotor
        SymmetryFactor              0.5
      End
      Tunneling       Eckart
        ImaginaryFrequency[1/cm]      1207.49
        WellDepth[kcal/mol]           26.61
        WellDepth[kcal/mol]           8.95
      End
      Frequencies[1/cm]                   44
    59.26    202.24   207.01   274.54   296.67   416.91   453.07   504.34
    518.52   525.68   583.48   677.41   693.96   752.96   802.40   858.55
    913.03   950.31   983.14   975.51   990.57   1025.98 1069.44 1130.44
    1144.81 1161.71 1238.16 1287.10 1302.23 1370.47 1405.74 1442.05
    1453.30 1475.50 1567.40 1585.66 2932.14 2992.28 3013.28 3051.30
    3064.63 3080.30 3101.60 3703.68
      ZeroEnergy[kcal/mol]                9.97
      ElectronicLevels[1/cm]              1
                    0          2
End
!***********************************
Barrier B4m2     W     W4m2
    Variational
RRHO                !                 1
Geometry[angstrom]              17
C                    -1.25487500    -0.10749200    -0.08864300
C                    -0.92487200     1.17583000     0.36987000
C                     0.34591800     1.71263800     0.15496300
C                     1.31251200     0.97161300    -0.52571200
C                     0.99973600    -0.31269200    -0.98121800
C                    -0.27669200    -0.84096900    -0.76677600
H                    -1.67018500     1.75915400     0.90335100
H                     0.57987900     2.70693900     0.51952300
H                     2.29977600     1.38247800    -0.69710700
H                     1.73601500    -0.89042500    -1.52628700
H                    -0.51147600    -1.83534300    -1.13050200
C                    -2.62651800    -0.68526300     0.16034300
H                    -3.39771000     0.09829500     0.13342000
H                    -2.87587100    -1.44078800    -0.59097900
H                    -2.67776800    -1.16889800     1.14838200
O                     2.13502100    -1.42370600     1.23441500
```

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H                    1.50457500    -0.80183300     1.61895800
   Core    RigidRotor
           SymmetryFactor     0.412697798
End
 Rotor                               Hindered
 Group    13 14 15
 Axis              12              1
 Symmetry                3
 Potential[kcal/mol]               12
   0.000 0.004 -0.001 -0.002 0.003 0.016 0.041 0.062 0.066 0.061 0.051 0.021
 End
      Rotor                               Hindered
 Group    17
 Axis              16              5
 Symmetry                1
 Potential[kcal/mol]               36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
    Frequencies[1/cm]              42
   55.88    208.60   222.55   240.66   349.70   403.20   460.94   525.79
   632.67   639.46   735.05   799.77   851.50   893.72   951.95   960.42
   977.82   981.40   1009.91 1034.23 1071.31 1139.40 1160.28 1190.52
   1297.17 1309.81 1380.54 1416.87 1447.56 1457.23 1470.35 1562.22
   1582.77 2875.14 2927.28 2977.50 3045.42 3063.48 3068.44 3082.02
   3095.05 3697.13
ZeroEnergy[kcal/mol]    -3.42
 ElectronicLevels[1/cm]                       1
  0.0000000000000000          2.0000000000000000
End
!*******************************************
RRHO               !               2
Geometry[angstrom]              17
C                   -1.25857400    -0.10438000    -0.08687800
C                   -0.93949200     1.18916100     0.35189900
C                    0.33231200     1.72513900     0.14845600
C                    1.31309700     0.97329600    -0.50381500
C                    1.00969900    -0.31811700    -0.94333000
C                   -0.26852600    -0.84624000    -0.74053300
H                   -1.69646400     1.78145400     0.85655100
H                    0.55463400     2.72935200     0.48950700
H                    2.30249400     1.38409000    -0.66479700
H                    1.76501500    -0.90983700    -1.44895000
H                   -0.49108400    -1.84996900    -1.08535100
```

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C                    -2.63164000   -0.67969200    0.15723600
H                    -3.41159400    0.04315200   -0.09140300
H                    -2.79534600   -1.57568500   -0.44229500
H                    -2.76029900   -0.95425300    1.20821600
O                     2.14312700   -1.44553800    1.18255300
H                     1.60951600   -0.79590400    1.66347100
   Core    RigidRotor
          SymmetryFactor     0.412697798
End
 Rotor                              Hindered
 Group    13 14 15
 Axis             12          1
 Symmetry               3
 Potential[kcal/mol]            12
   0.000 -0.005 -0.005 0.000 0.016 0.041 0.061 0.062 0.056 0.032 0.014 -0.005
 End
       Rotor                                  Hindered
 Group    17
 Axis             16          5
 Symmetry               1
 Potential[kcal/mol]            36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
    Frequencies[1/cm]             42
   18.02    86.18    202.73    308.70    340.71    402.56    454.12    525.71
   629.17    632.99    733.97    799.69    850.13    889.21    948.95    954.69
   965.30    979.24    1008.60 1019.13 1069.51 1139.15 1160.51 1191.02
   1294.94 1308.87 1370.26 1416.13 1440.38 1453.96 1469.56 1559.77
   1583.22 2932.71 2990.47 3017.47 3052.49 3061.03 3072.29 3077.97
   3090.65 3657.74
ZeroEnergy[kcal/mol]     -2.98
 ElectronicLevels[1/cm]                     1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO              !              3
Geometry[angstrom]              17
C                    -1.25367800   -0.10846300   -0.07572700
C                    -0.94563900    1.19907100    0.33023000
C                     0.32995800    1.73136300    0.14052200
C                     1.32564200    0.96328400   -0.46417500
C                     1.03507800   -0.34233600   -0.87323800
C                    -0.24848400   -0.86810200   -0.67764700
```

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H                    -1.71520100     1.80565700     0.79814300
H                     0.54534400     2.74275100     0.46589500
H                     2.31842000     1.36910000    -0.61490400
H                     1.78935600    -0.93582200    -1.37084300
H                    -0.46137900    -1.88200200    -0.99845000
C                    -2.63449800    -0.67424600     0.14617500
H                    -3.40270500     0.00144400    -0.23786100
H                    -2.74952500    -1.63747900    -0.35303400
H                    -2.83165000    -0.82376900     1.21170500
O                     2.10728400    -1.41091800     1.07109600
H                     1.53984800    -0.87735200     1.64927100
   Core    RigidRotor
            SymmetryFactor    0.412697798
End
 Rotor                                  Hindered
 Group    13 14 15
 Axis              12              1
 Symmetry            3
 Potential[kcal/mol]              12
 0.000 -0.004 0.000 0.009 0.032 0.056 0.066 0.063 0.054 0.026 0.005 0.005
 End
       Rotor                                  Hindered
 Group    17
 Axis              16              5
 Symmetry            1
 Potential[kcal/mol]              36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
    Frequencies[1/cm]              42
  59.05    147.90   204.78   340.88   401.37   451.17   460.14   524.99
  625.00   633.41   736.43   800.59   852.31   888.86   943.07   954.58
  965.76   981.14   1009.56 1020.08 1068.81 1138.63 1159.51 1191.52
  1294.33 1308.07 1370.50 1414.70 1439.39 1454.14 1469.27 1561.92
  1583.34 2929.97 2987.05 3012.49 3050.02 3065.79 3071.78 3086.95
  3106.97 3636.83
ZeroEnergy[kcal/mol]    -2.55
 ElectronicLevels[1/cm]                        1
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO              !              4
Geometry[angstrom]              17
C                    -1.25094700    -0.11078300    -0.07092500
```

```
C        -0.94581600    1.20039400    0.32422400
C         0.33131400    1.73074300    0.14038100
C         1.33020700    0.95888400   -0.45261600
C         1.03988900   -0.34765400   -0.85932000
C        -0.24256800   -0.87476600   -0.66134500
H        -1.71911900    1.81156200    0.77898400
H         0.54421600    2.74527400    0.45713100
H         2.32554100    1.36113400   -0.59529700
H         1.79562200   -0.94240800   -1.35455300
H        -0.45101500   -1.89332000   -0.96946900
C        -2.63408400   -0.67367400    0.14328600
H        -3.39728600    0.00429900   -0.24650300
H        -2.74848100   -1.63631100   -0.35725200
H        -2.83930900   -0.82269100    1.20722300
O         2.09248200   -1.39680800    1.04235700
H         1.52368500   -0.88147100    1.63872500
    Core    RigidRotor
        SymmetryFactor    0.412697798
End
  Rotor                    Hindered
  Group    13 14 15
  Axis          12          1
  Symmetry          3
  Potential[kcal/mol]          12
  0.000 -0.004 0.000 0.008 0.030 0.054 0.065 0.063 0.054 0.026 0.005 0.005
  End
        Rotor                    Hindered
  Group    17
  Axis          16          5
  Symmetry          1
  Potential[kcal/mol]          36
  0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
  2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
  2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
  End
      Frequencies[1/cm]          42
    163.24   182.49   205.48   340.68   403.67   455.59   513.69   525.04
    624.58   633.55   738.87   801.16   854.59   888.96   945.51   954.64
    965.89   981.84   1010.31 1020.28 1069.05 1139.25 1160.10 1192.08
    1294.53 1307.97 1370.42 1415.09 1439.58 1453.99 1469.85 1562.98
    1584.54 2930.58 2987.96 3012.49 3052.93 3067.33 3073.16 3087.13
    3102.49 3611.30
ZeroEnergy[kcal/mol]    -2.19
  ElectronicLevels[1/cm]                1
    0.0000000000000000          2.0000000000000000
```

```
End
!****************************************
RRHO                    !                   5
Geometry[angstrom]                  17
C                       -1.24833100     -0.11357200     -0.06638500
C                       -0.94560700      1.20152200      0.31770200
C                        0.33399000      1.72902800      0.14318100
C                        1.33376400      0.95562000     -0.44537400
C                        1.04750800     -0.35631600     -0.83950800
C                       -0.23832200     -0.87993600     -0.64949900
H                       -1.72117800      1.81565800      0.76471000
H                        0.54457400      2.74606200      0.45305300
H                        2.33028000      1.35595400     -0.58442200
H                        1.80048800     -0.94838800     -1.34127200
H                       -0.44444500     -1.90086400     -0.95087700
C                       -2.63374900     -0.67346800      0.14096200
H                       -3.39355000      0.00640000     -0.25208400
H                       -2.74772400     -1.63557400     -0.36068000
H                       -2.84446400     -0.82263800      1.20382900
O                        2.07614900     -1.38074800      1.01391200
H                        1.51597300     -0.88410600      1.63293400
   Core      RigidRotor
                SymmetryFactor    0.412697798
End
 Rotor                                      Hindered
 Group     13 14 15
 Axis                  12                  1
 Symmetry                  3
 Potential[kcal/mol]                 12
 0.000 -0.004 -0.001 0.007 0.028 0.053 0.065 0.063 0.055 0.027 0.006 0.006
 End
        Rotor                                       Hindered
 Group     17
 Axis                  16                  5
 Symmetry                  1
 Potential[kcal/mol]                 36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
    Frequencies[1/cm]                 42
  169.06   173.46   205.83   340.55   404.48   457.20   524.68   539.94
  627.10   635.48   742.31   801.58   857.62   890.74   951.53   956.51
  965.89   982.76  1010.50 1020.53 1069.01 1139.09 1160.12 1192.47
 1293.44 1307.41 1370.44 1414.84 1439.65 1453.84 1469.69 1563.32
```

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  1585.14 2930.57 2988.01 3012.61 3052.72 3068.72 3074.07 3088.60
  3105.16 3617.28
ZeroEnergy[kcal/mol]      -1.73
 ElectronicLevels[1/cm]                      1
  0.0000000000000000          2.0000000000000000
End
!******************************************
RRHO                    !                6
Geometry[angstrom]                17
C                     -1.24593900    -0.11597900    -0.06292300
C                     -0.94493300     1.20196900     0.31277300
C                      0.33586100     1.72816300     0.14330800
C                      1.33807300     0.95166100    -0.43524900
C                      1.05426600    -0.36404900    -0.82136800
C                     -0.23370400    -0.88595800    -0.63537400
H                     -1.72316800     1.81952500     0.75035100
H                      0.54444800     2.74728000     0.44765900
H                      2.33543400     1.35039200    -0.57216900
H                      1.80433000    -0.95326100    -1.32987000
H                     -0.43777400    -1.90866900    -0.93178800
C                     -2.63336600    -0.67305100     0.13818700
H                     -3.38985300     0.00869300    -0.25789500
H                     -2.74706600    -1.63462000    -0.36452500
H                     -2.84915600    -0.82246300     1.20000700
O                      2.06009100    -1.36494900     0.98517400
H                      1.50751300    -0.88551200     1.62379200
   Core     RigidRotor
           SymmetryFactor      0.412697798
End
 Rotor                                Hindered
 Group    13 14 15
 Axis                12               1
 Symmetry                 3
 Potential[kcal/mol]               12
 0.000 -0.005 -0.002 0.005 0.026 0.051 0.065 0.063 0.055 0.028 0.007 0.006
 End
       Rotor                                Hindered
 Group    17
 Axis                16               5
 Symmetry                   1
 Potential[kcal/mol]               36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
```

```
   Frequencies[1/cm]                 42
  162.20   176.25   205.85   340.44   403.22   458.44   524.49   565.08
  611.14   634.61   746.63   802.32   861.61   893.31   954.30   960.71
  966.02   983.70   1010.71 1020.81 1068.93 1138.97 1160.13 1192.97
  1292.15 1306.79 1370.46 1414.54 1439.89 1453.72 1469.66 1563.77
  1585.92 2930.67 2988.19 3012.76 3052.81 3069.82 3074.41 3089.77
  3108.30 3619.77
ZeroEnergy[kcal/mol]     -1.27
 ElectronicLevels[1/cm]                          1
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO                !                 7
Geometry[angstrom]                17
C                    -1.24361500     -0.11841400     -0.05975500
C                    -0.94399700      1.20199300      0.30841600
C                     0.33756700      1.72744300      0.14288100
C                     1.34228700      0.94790100     -0.42517000
C                     1.06141800     -0.37216600     -0.80190900
C                    -0.22947500     -0.89163000     -0.62213200
H                    -1.72474900      1.82272200      0.73680100
H                     0.54380200      2.74900900      0.44044000
H                     2.34046100      1.34512700     -0.55987000
H                     1.80789000     -0.95763300     -1.31968000
H                    -0.43161900     -1.91596400     -0.91393000
C                    -2.63297200     -0.67258800      0.13553700
H                    -3.38621400      0.01111800     -0.26322800
H                    -2.74668600     -1.63360200     -0.36821500
H                    -2.85328000     -0.82218200      1.19638100
O                     2.04410000     -1.34923100      0.95650600
H                     1.49937800     -0.88598000      1.61324300
   Core      RigidRotor
             SymmetryFactor       0.412697798
End
 Rotor                                  Hindered
 Group     13 14 15
 Axis                12                1
 Symmetry                3
 Potential[kcal/mol]                12
 0.000 -0.005 -0.002 0.004 0.025 0.050 0.064 0.063 0.055 0.028 0.008 0.006
 End
        Rotor                                   Hindered
 Group     17
 Axis                16                5
 Symmetry                1
```

```
 Potential[kcal/mol]                36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
     Frequencies[1/cm]                42
  164.02 170.33 206.89 340.32 403.01 460.70 524.24 596.97
  625.31 644.24 752.37 803.12 866.17 896.99 961.06 972.91
  966.09 984.44 1010.85 1021.79 1068.86 1138.99 1160.18 1193.36
  1290.38 1306.33 1370.48 1414.30 1440.04 1453.51 1469.70 1563.99
  1586.67 2930.88 2988.55 3012.94 3053.47 3070.89 3075.09 3090.76
  3108.87 3620.72
ZeroEnergy[kcal/mol]      -0.63
 ElectronicLevels[1/cm]                          1
  0.0000000000000000            2.0000000000000000
End
!********************************************
RRHO                    !                 8
Geometry[angstrom]                17
C                        -1.24150900     -0.12073400     -0.05747700
C                        -0.94269900      1.20151300      0.30514700
C                         0.33907300      1.72702900      0.14162500
C                         1.34626400      0.94463300     -0.41549600
C                         1.06954600     -0.38131300     -0.78011200
C                        -0.22597100     -0.89684600     -0.61031100
H                        -1.72555000      1.82476700      0.72584900
H                         0.54272500      2.75121600      0.43182100
H                         2.34484800      1.34093700     -0.54924100
H                         1.81052700     -0.96082700     -1.31194700
H                        -0.42679600     -1.92209000     -0.89951700
C                        -2.63260300     -0.67209100      0.13308200
H                        -3.38322600      0.01327500     -0.26764200
H                        -2.74660900     -1.63279100     -0.37118300
H                        -2.85606000     -0.82157900      1.19327100
O                         2.02822200     -1.33364200      0.92809500
H                         1.49241100     -0.88541700      1.60197500
    Core      RigidRotor
              SymmetryFactor       0.412697798
End
 Rotor                                          Hindered
 Group      13 14 15
 Axis                  12                  1
 Symmetry                    3
 Potential[kcal/mol]                12
 0.000 -0.005 -0.002 0.004 0.024 0.049 0.064 0.063 0.055 0.029 0.009 0.006
```

```
End
    Rotor                                   Hindered
Group   17
Axis            16          5
Symmetry            1
Potential[kcal/mol]          36
0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
End
  Frequencies[1/cm]          42
  126.24   172.22   208.33   340.21   401.73   462.42   523.80   626.15
  629.16   670.66   759.84   804.11   871.70   901.49   967.28   991.34
  966.32   984.75   1010.65 1023.09 1068.70 1138.87 1159.87 1193.47
  1287.64 1305.91 1370.49 1413.76 1440.20 1453.20 1469.43 1563.21
  1586.82 2931.06 2988.90 3013.16 3054.11 3071.96 3075.67 3091.76
  3109.49 3622.01
ZeroEnergy[kcal/mol]   -0.02
 ElectronicLevels[1/cm]                  1
  0.0000000000000000        2.0000000000000000
End
!*******************************************
RRHO            !           9
Geometry[angstrom]          17
C              -1.23974700    -0.12282100    -0.05637800
C              -0.94119100     1.20059800     0.30326800
C               0.34033900     1.72683600     0.13959300
C               1.34983200     0.94211800    -0.40671200
C               1.07905300    -0.39176200    -0.75558300
C              -0.22329200    -0.90132100    -0.60040000
H              -1.72563400     1.82568400     0.71811900
H               0.54125900     2.75381300     0.42140000
H               2.34821700     1.33855600    -0.54108000
H               1.81295800    -0.96322300    -1.30692400
H              -0.42363300    -1.92679000    -0.88894700
C              -2.63233500    -0.67161600     0.13094200
H              -3.38111900     0.01500800    -0.27096600
H              -2.74702000    -1.63233800    -0.37310500
H              -2.85719300    -0.82046400     1.19089900
O               2.01268400    -1.31843400     0.90026800
H               1.48625200    -0.88407800     1.58991100
   Core   RigidRotor
         SymmetryFactor    0.412697798
End
 Rotor                              Hindered
```

```
    Group      13 14 15
    Axis                  12                  1
    Symmetry                  3
    Potential[kcal/mol]                  12
    0.000 0.000 0.000 0.000 0.001 0.002 0.003 0.003 0.002 0.001 0.000    0.000
    End
            Rotor                                        Hindered
    Group      17
    Axis                  16                  5
    Symmetry                  1
    Potential[kcal/mol]                  36
    0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
    2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
    2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
    End
       Frequencies[1/cm]                  42
     102.16   176.13   210.46   340.14   398.85   463.75   523.09   627.72
     649.36   707.78   768.73   805.74   878.52   906.59   974.07   964.78
     975.77   983.66   1011.20 1024.72 1068.62 1138.91 1159.21 1193.04
     1283.97 1305.69 1370.41 1412.86 1440.36 1452.71 1468.76 1560.74
     1585.66 2931.30 2989.33 3013.43 3054.89 3072.46 3076.54 3091.48
     3104.21 3624.13
  ZeroEnergy[kcal/mol]    0.55
   ElectronicLevels[1/cm]                          1
     0.0000000000000000            2.0000000000000000
  End
  !*****************************************
  RRHO                  !                  10
  Geometry[angstrom]                  17
  C                    -1.23848100    -0.12495100    -0.05663400
  C                    -0.94007900     1.19985900     0.30265600
  C                     0.34179800     1.72691900     0.13720200
  C                     1.35272500     0.94164500    -0.39971700
  C                     1.09127900    -0.40477200    -0.72789400
  C                    -0.22258200    -0.90504500    -0.59294500
  H                    -1.72545300     1.82592300     0.71404300
  H                     0.54018300     2.75625900     0.41191900
  H                     2.35044200     1.33885800    -0.53617600
  H                     1.81296900    -0.96272900    -1.30811800
  H                    -0.42309800    -1.93006000    -0.88276200
  C                    -2.63222100    -0.67123900     0.12924400
  H                    -3.38006600     0.01617200    -0.27301400
  H                    -2.74781400    -1.63231800    -0.37386100
  H                    -2.85699300    -0.81898600     1.18937800
  O                     1.99799000    -1.30401800     0.87364800
```

```
H 1.48159600 -0.88221000 1.57767000
  Core RigidRotor
    SymmetryFactor 0.412697798
End
 Rotor Hindered
 Group 13 14 15
 Axis 12 1
 Symmetry 3
 Potential[kcal/mol] 12
 0.000 -0.005 -0.003 0.003 0.023 0.048 0.064 0.063 0.055 0.029 0.009 0.007
 End
   Rotor Hindered
 Group 17
 Axis 16 5
 Symmetry 1
 Potential[kcal/mol] 36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
   Frequencies[1/cm] 42
  125.93 175.13 214.19 340.32 395.86 463.88 521.66 626.01
  658.97 750.90 776.81 810.94 884.53 910.69 980.97 963.82
  977.14 987.01 1014.89 1026.71 1067.69 1138.17 1156.07 1191.52
  1277.87 1304.83 1370.41 1409.72 1440.47 1451.89 1465.61 1554.14
  1581.11 2931.44 2989.56 3013.79 3056.10 3073.42 3077.25 3092.43
  3104.36 3628.74
ZeroEnergy[kcal/mol] 0.81
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
End
!**********************************************
RRHO ! 11
Geometry[angstrom] 17
C -1.23755777 -0.12736542 -0.05754242
C -0.93946377 1.19957058 0.30283958
C 0.34360223 1.72739458 0.13493258
C 1.35528823 0.94297158 -0.39422542
C 1.10556723 -0.41965942 -0.69864742
C -0.22344377 -0.90855742 -0.58737942
H -1.72537477 1.82604058 0.71215558
H 0.53954923 2.75877558 0.40353358
H 2.35231223 1.34098258 -0.53268742
H 1.81085923 -0.95977842 -1.31419342
H -0.42426977 -1.93299342 -0.87868642
```

```
C -2.63230377 -0.67101242 0.12786958
H -3.37949577 0.01704058 -0.27449742
H -2.74890577 -1.63256242 -0.37400542
H -2.85623677 -0.81733742 1.18839058
O 1.98397723 -1.29029842 0.84822658
H 1.47652523 -0.87987042 1.56464358
  Core RigidRotor
    SymmetryFactor 0.412697798
End
  Rotor Hindered
  Group 13 14 15
  Axis 12 1
  Symmetry 3
  Potential[kcal/mol] 12
  0.000 -0.068 -0.034 0.084 0.264 0.454 0.611 0.683 0.659 0.535 0.351 0.154
  End
    Rotor Hindered
  Group 17
  Axis 16 5
  Symmetry 1
  Potential[kcal/mol] 36
  0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
  2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
  2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
  End
    Frequencies[1/cm] 42
   133.14 183.20 219.98 340.72 393.10 462.63 519.32 622.61
   655.11 773.07 786.70 836.66 885.74 911.87 984.66 997.21
   966.56 991.57 1019.32 1028.18 1065.74 1137.02 1150.06 1189.03
   1270.46 1303.25 1370.36 1404.04 1440.45 1450.80 1458.79 1543.18
   1573.43 2931.54 2989.71 3014.26 3057.97 3074.65 3078.03 3093.76
   3105.19 3631.89
ZeroEnergy[kcal/mol] 0.35
  ElectronicLevels[1/cm] 1
   0.0000000000000000 2.0000000000000000
End
!********************************************
RRHO ! 12
Geometry[angstrom] 17
C -1.23663500 -0.12978000 -0.05845000
C -0.93884900 1.19928200 0.30302400
C 0.34540600 1.72787000 0.13266300
C 1.35785200 0.94429800 -0.38873400
C 1.11985600 -0.43454700 -0.66940100
C -0.22430600 -0.91206900 -0.58181400
```

```
H        -1.72529700   1.82615800   0.71026800
H         0.53891500   2.76129200   0.39514800
H         2.35418300   1.34310700  -0.52919800
H         1.80875000  -0.95682800  -1.32026900
H        -0.42544200  -1.93592700  -0.87461100
C        -2.63238700  -0.67078600   0.12649500
H        -3.37892600   0.01790900  -0.27598100
H        -2.74999800  -1.63280700  -0.37415000
H        -2.85548000  -0.81568900   1.18740300
O         1.96996500  -1.27657900   0.82280500
H         1.47145400  -0.87753100   1.55161700
   Core     RigidRotor
       SymmetryFactor     0.412697798
End
  Rotor                 Hindered
   Group     13 14 15
  Axis          12          1
  Symmetry          3
  Potential[kcal/mol]          12
  0.000 -0.068 -0.034 0.084 0.264 0.454 0.611 0.683 0.659 0.536 0.351 0.154
  End
      Rotor                 Hindered
  Group    17
  Axis          16          5
  Symmetry          1
  Potential[kcal/mol]          36
  0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
  2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
  2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
  End
     Frequencies[1/cm]          42
   151.22   207.97   228.36   341.12   391.04   461.57   516.59   617.49
   646.72   769.89   792.41   870.58   888.71   913.56   984.99   990.43
   961.58   998.47   1028.57 1033.24 1065.62 1137.22 1142.88 1186.66
   1266.18 1301.87 1370.18 1398.15 1440.29 1449.56 1450.53 1532.54
   1565.88 2931.59 2989.81 3014.71 3059.49 3073.65 3078.43 3086.56
   3099.89 3630.11
ZeroEnergy[kcal/mol]     -0.54
  ElectronicLevels[1/cm]              1
   0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO          !          13
Geometry[angstrom]          17
C        -1.23590500  -0.13251300  -0.05971000
```

```
C                -0.93873100    1.19944800    0.30376000
C                 0.34756000    1.72859100    0.13053800
C                 1.36016300    0.94707000   -0.38439200
C                 1.13555300   -0.45067500   -0.63941600
C                -0.22641700   -0.91545100   -0.57764000
H                -1.72544300    1.82635200    0.70977500
H                 0.53868300    2.76383500    0.38755300
H                 2.35594900    1.34649600   -0.52620800
H                 1.80477300   -0.95185400   -1.32986200
H                -0.42778400   -1.93884900   -0.87150200
C                -2.63257900   -0.67067200    0.12532300
H                -3.37852500    0.01866000   -0.27721000
H                -2.75127600   -1.63319400   -0.37398100
H                -2.85449400   -0.81391000    1.18673000
O                 1.95661300   -1.26356800    0.79853300
H                 1.46545900   -0.87443300    1.53723300
   Core     RigidRotor
         SymmetryFactor     0.412697798
End
 Rotor                     Hindered
 Group     13 14 15
 Axis          12         1
 Symmetry          3
 Potential[kcal/mol]          12
 0.000 -0.068 -0.034 0.085 0.265 0.455 0.612 0.683 0.659 0.536 0.351 0.154
 End
      Rotor                     Hindered
 Group     17
 Axis          16         5
 Symmetry           1
 Potential[kcal/mol]          36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
    Frequencies[1/cm]          42
  166.56   227.74   243.71   342.15   391.46   461.30   513.36   610.50
  638.08   762.05   792.79   862.43   888.70   934.94   982.28   989.39
  995.58   1003.63 1028.66 1052.37 1080.94 1133.42 1137.93 1183.63
  1263.22 1299.67 1369.73 1390.25 1437.76 1440.12 1449.24 1522.79
  1559.65 2931.50 2989.71 3015.14 3059.62 3061.88 3078.54 3079.68
  3099.22 3630.56
ZeroEnergy[kcal/mol]    -2.20
 ElectronicLevels[1/cm]              1
  0.0000000000000000       2.0000000000000000
```

```
End
!****************************************
RRHO                    !                   14
Geometry[angstrom]                  17
C                       -1.23517100     -0.13545500     -0.06120800
C                       -0.93900500      1.19985300      0.30481100
C                        0.34998700      1.72924300      0.12834700
C                        1.36218200      0.95047600     -0.38055900
C                        1.15190100     -0.46730300     -0.60910300
C                       -0.22912100     -0.91856500     -0.57402000
H                       -1.72581300      1.82659500      0.71001800
H                        0.53853500      2.76638800      0.37986400
H                        2.35754100      1.35055400     -0.52342700
H                        1.79922500     -0.94565300     -1.33807300
H                       -0.43075500     -1.94168000     -0.86862400
C                       -2.63275600     -0.67055900      0.12421400
H                       -3.37827300      0.01935400     -0.27825000
H                       -2.75261300     -1.63365400     -0.37363300
H                       -2.85356200     -0.81194900      1.18617700
O                        1.94370600     -1.25101000      0.77470500
H                        1.45910600     -0.87055400      1.52156100
   Core      RigidRotor
                SymmetryFactor       0.412697798
End
 Rotor                                      Hindered
 Group     13 14 15
 Axis                  12                  1
 Symmetry                  3
 Potential[kcal/mol]                 12
 0.000 -0.068 -0.033 0.086 0.266 0.456 0.613 0.684 0.659 0.535 0.350 0.154
 End
          Rotor                                      Hindered
 Group     17
 Axis                  16                  5
 Symmetry                  1
 Potential[kcal/mol]                 36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
    Frequencies[1/cm]                 42
  173.55   240.90   264.51   344.01   395.85   462.42   510.52   602.90
  631.86   753.90   791.78   848.18   875.26   940.78   979.73   989.97
  967.82   1011.88 1028.50 1052.43 1114.39 1131.65 1143.12 1180.25
  1262.71 1296.73 1368.72 1380.68 1423.92 1439.66 1448.85 1517.30
```

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    1558.82 2931.03 2989.08 3015.25 3043.34 3063.52 3077.86 3079.00
    3098.60 3634.44
ZeroEnergy[kcal/mol]     -4.80
 ElectronicLevels[1/cm]                              1
  0.0000000000000000             2.0000000000000000
End
!****************************************
RRHO                 !                 15
Geometry[angstrom]                 17
C                      -1.23451700     -0.13816200     -0.06261200
C                      -0.93930400      1.20021800      0.30600300
C                       0.35221100      1.73001200      0.12609400
C                       1.36443700      0.95310000     -0.37657000
C                       1.16789000     -0.48349400     -0.57889100
C                      -0.23095300     -0.92185900     -0.57010000
H                      -1.72624700      1.82682800      0.71045500
H                       0.53811800      2.76932700      0.37123000
H                       2.35901300      1.35505600     -0.52095000
H                       1.79361100     -0.93975300     -1.34193400
H                      -0.43398600     -1.94456100     -0.86581700
C                      -2.63301700     -0.67042800      0.12299300
H                      -3.37817400      0.01998800     -0.27941900
H                      -2.75413600     -1.63418900     -0.37326700
H                      -2.85276900     -0.80985600      1.18552900
O                       1.93062800     -1.23835200      0.75042100
H                       1.45249400     -0.86639300      1.50520400
   Core      RigidRotor
             SymmetryFactor      0.412697798
End
 Rotor                                    Hindered
 Group      13 14 15
 Axis                  12                 1
 Symmetry                3
 Potential[kcal/mol]                   12
 0.000 -0.067 -0.032 0.087 0.267 0.457 0.614 0.684 0.659 0.535 0.350 0.154
 End
        Rotor                                    Hindered
 Group      17
 Axis                  16                 5
 Symmetry                1
 Potential[kcal/mol]                   36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
```

```
   Frequencies[1/cm]                 42
  179.20   260.00   283.83   346.89   404.53   465.73   508.89   596.86
  628.75   747.75   790.51   835.08   863.79   934.13   977.65   986.77
  979.09   1027.62 1034.53 1049.97 1109.40 1136.77 1174.88 1187.08
  1262.47 1293.63 1364.50 1373.24 1411.70 1439.32 1448.69 1514.90
  1561.62 2930.37 2988.21 3015.03 3028.54 3064.03 3075.55 3078.36
  3096.46 3636.98
 ZeroEnergy[kcal/mol]     -7.90
  ElectronicLevels[1/cm]                 1
   0.0000000000000000          2.0000000000000000
 End
 !*****************************************
 RRHO                !                16
 Geometry[angstrom]                17
 C                    -1.23388400    -0.14049400    -0.06371200
 C                    -0.93939400     1.20034700     0.30718800
 C                     0.35406100     1.73087800     0.12369300
 C                     1.36713500     0.95443400    -0.37189700
 C                     1.18302000    -0.49872300    -0.54929300
 C                    -0.23137400    -0.92553000    -0.56521800
 H                    -1.72661800     1.82697600     0.71070200
 H                     0.53721900     2.77272800     0.36092600
 H                     2.36052700     1.35936600    -0.51856700
 H                     1.78846300    -0.93451700    -1.34178900
 H                    -0.43673800    -1.94765900    -0.86250700
 C                    -2.63339400    -0.67024100     0.12152000
 H                    -3.37814500     0.02060100    -0.28101300
 H                    -2.75585100    -1.63475100    -0.37302100
 H                    -2.85230400    -0.80764500     1.18457600
 O                     1.91699500    -1.22530100     0.72532500
 H                     1.44649000    -0.86294200     1.48892100
    Core      RigidRotor
              SymmetryFactor       0.412697798
 End
  Rotor                                  Hindered
  Group     13 14 15
  Axis                12                1
  Symmetry                3
  Potential[kcal/mol]                12
  0.000 -0.067 -0.031 0.088 0.268 0.458 0.614 0.685 0.659 0.535 0.349 0.153
  End
         Rotor                                  Hindered
  Group     17
  Axis                16                5
  Symmetry                1
```

```
Potential[kcal/mol]                36
0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
End
   Frequencies[1/cm]                42
 273.13   294.03   304.02   351.30   418.63   473.30   508.32   594.13
 627.57   744.17   788.96   824.35   856.47   924.46   975.92   984.15
 981.27   1027.64 1042.54 1071.41 1104.14 1137.21 1172.87 1233.93
 1261.49 1290.91 1355.52 1371.13 1402.51 1439.06 1448.61 1513.38
 1563.85 2929.73 2987.43 3013.40 3014.69 3063.08 3071.85 3077.59
 3093.22 3640.41
ZeroEnergy[kcal/mol]     -10.72
 ElectronicLevels[1/cm]                        1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                  !                 17
Geometry[angstrom]              17
C                      -1.23306200    -0.14265200    -0.06442000
C                      -0.93916200     1.20016500     0.30824000
C                       0.35565300     1.73173000     0.12096900
C                       1.37026200     0.95472000    -0.36614600
C                       1.19712300    -0.51277300    -0.52082000
C                      -0.23061800    -0.92963600    -0.55887500
H                      -1.72683700     1.82699900     0.71039700
H                       0.53575500     2.77643600     0.34875600
H                       2.36233600     1.36274800    -0.51575200
H                       1.78345700    -0.92944600    -1.33954900
H                      -0.43820800    -1.95122100    -0.85778800
C                      -2.63387200    -0.66995700     0.11968900
H                      -3.37797800     0.02130600    -0.28338400
H                      -2.75762200    -1.63525000    -0.37307100
H                      -2.85246500    -0.80528200     1.18313800
O                       1.90266000    -1.21179200     0.69941100
H                       1.44214800    -0.86142100     1.47389400
    Core     RigidRotor
             SymmetryFactor      0.412697798
End
 Rotor                                   Hindered
 Group     13 14 15
 Axis                 12                 1
 Symmetry                  3
 Potential[kcal/mol]                12
0.000 -0.067 -0.031 0.088 0.269 0.459 0.615 0.685 0.659 0.535 0.349 0.153
```

```
    End
          Rotor                                  Hindered
    Group     17
    Axis                16               5
    Symmetry                  1
    Potential[kcal/mol]               36
    0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
    2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
    2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
    End
       Frequencies[1/cm]              42
    289.64   315.49   356.61   406.74   451.74   508.01   526.07   608.28
    629.55   746.02   786.98   815.77   852.82   914.27   974.34   982.11
    980.26   1027.26 1039.33 1088.52 1117.86 1137.13 1170.66 1258.49
    1278.44 1290.96 1346.70 1370.34 1395.91 1438.87 1448.58 1512.29
    1565.02 2929.21 2986.79 2995.60 3014.28 3061.41 3067.93 3076.67
    3089.96 3644.68
  ZeroEnergy[kcal/mol]     -13.34
    ElectronicLevels[1/cm]                       1
      0.0000000000000000           2.0000000000000000
  End
  !*********************************************
  RRHO                   !                  18
  Geometry[angstrom]               17
  C                    -1.23188000    -0.14505000    -0.06443300
  C                    -0.93845400     1.19956400     0.30896600
  C                     0.35717600     1.73268100     0.11749900
  C                     1.37412700     0.95423800    -0.35837500
  C                     1.20942600    -0.52477600    -0.49445500
  C                    -0.22877500    -0.93469300    -0.54981600
  H                    -1.72689000     1.82694800     0.70874400
  H                     0.53343600     2.78079600     0.33357400
  H                     2.36505200     1.36484600    -0.51109600
  H                     1.77778600    -0.92361900    -1.33619800
  H                    -0.43765000    -1.95620200    -0.84940000
  C                    -2.63447700    -0.66947900     0.11713100
  H                    -3.37715400     0.02239600    -0.28759400
  H                    -2.75945600    -1.63561600    -0.37374800
  H                    -2.85413800    -0.80235000     1.18071800
  O                     1.88774900    -1.19812400     0.67245600
  H                     1.43835500    -0.86170100     1.45837900
     Core     RigidRotor
               SymmetryFactor      0.412697798
  End
    Rotor                                  Hindered
```

```
    Group      13 14 15
    Axis                  12                  1
    Symmetry                  3
    Potential[kcal/mol]                  12
    0.000 -0.067 -0.031 0.088 0.268 0.458 0.614 0.685 0.659 0.535 0.349 0.153
    End
    Rotor                                       Hindered
    Group      17
    Axis                  16                  5
    Symmetry                  1
    Potential[kcal/mol]                  36
    0.000 0.025 0.263 0.684 1.220 1.775 2.261 2.606 2.779 2.788 2.690 2.548
    2.433 2.381 2.408 2.494 2.606 2.699 2.744 2.721 2.640 2.529 2.429 2.381
    2.407 2.510 2.660 2.801 2.859 2.786 2.546 2.142 1.624 1.069 0.567 0.191
    End
       Frequencies[1/cm]                  42
     295.45   324.39   362.86   424.26   462.16   507.64   563.04   624.35
     698.00   781.65   788.53   809.84   856.38   905.60   973.06   980.61
     978.41  1026.80 1036.33 1086.24 1136.79 1145.81 1172.59 1257.55
    1284.03 1322.78 1339.83 1369.78 1391.46 1438.76 1448.62 1511.97
    1566.06 2928.74 2978.51 2986.22 3013.89 3059.04 3064.13 3075.51
    3086.81 3653.26
  ZeroEnergy[kcal/mol]    -15.22
   ElectronicLevels[1/cm]                              1
     0.0000000000000000             2.0000000000000000
  End
  !*******************************************
  RRHO                  !                  19
  Geometry[angstrom]                  17
  C                      -1.23066700     -0.15223200     -0.04775600
  C                      -0.94284200      1.20459600      0.29288000
  C                       0.35326800      1.74283600      0.10588900
  C                       1.38097900      0.95897700     -0.32694200
  C                       1.21188100     -0.52239100     -0.47404900
  C                      -0.22304500     -0.95103300     -0.49800000
  H                      -1.74156100      1.84134600      0.65629200
  H                       0.51884800      2.79156300      0.30917800
  H                       2.37895500      1.35940700     -0.45852200
  H                       1.74686700     -0.88890500     -1.35878400
  H                      -0.41207500     -1.98989900     -0.74670000
  C                      -2.64194700     -0.66293500      0.10140800
  H                      -3.35460800      0.01283700     -0.38291400
  H                      -2.74827600     -1.65227600     -0.34854400
  H                      -2.92450100     -0.73625700      1.15799500
  O                       1.89083600     -1.19871700      0.61687300
```

```
H                          1.44095800     -0.97640000      1.46174600
   Core     RigidRotor
                SymmetryFactor       0.412697798
End
 Rotor                                      Hindered
 Group     13 14 15
 Axis                 12                1
 Symmetry              3
 Potential[kcal/mol]                  12
 0.000 -0.050 0.002 0.134 0.321 0.508 0.652 0.706 0.661 0.524 0.332 0.141
 End
   Rotor                                      Hindered
 Group     17
 Axis                 16                5
 Symmetry              1
 Potential[kcal/mol]                  36
 0.000 0.144 0.489 0.986 1.543 2.070 2.484 2.737 2.815 2.757 2.626 2.492
 2.408 2.401 2.463 2.569 2.675 2.745 2.754 2.696 2.593 2.483 2.408 2.399
 2.470 2.603 2.757 2.860 2.852 2.689 2.355 1.879 1.330 0.794 0.354 0.074
 End
     Frequencies[1/cm]                42
  302.82   350.52   434.28   467.52   501.56   561.06   586.96   625.70
  711.47   784.71   798.81   842.83   897.76   949.09   961.26   984.05
  983.70  1030.92 1037.71 1086.60 1134.25 1161.13 1209.29 1268.11
 1282.40 1340.56 1363.02 1373.07 1387.09 1439.68 1450.73 1516.45
 1575.47 2912.50 2920.49 2967.35 3001.69 3064.21 3069.14 3078.76
 3103.43 3437.38
ZeroEnergy[kcal/mol]    -15.80
 ElectronicLevels[1/cm]                          1
  0.0000000000000000          2.0000000000000000
End
 !***********************************
        Tunneling      Eckart
      ImaginaryFrequency[1/cm]        449.63
      WellDepth[kcal/mol]             4.20
      WellDepth[kcal/mol]             17.38
End
End
!***********************************
    Well       W4o2                  # oHOC6CH5CH3
    Species
      RRHO
        Geometry[angstrom]              17
C                       0.72707500    -0.56931700     0.11837200
C                      -0.23304100    -1.49219200    -0.18886700
```

```
C                          -1.60934300     -1.16231400     -0.22480300
C                          -2.02716900      0.15946600      0.07390800
C                          -1.11888800      1.12448100      0.38666100
C                           0.35577700      0.86978400      0.37224100
H                           0.06630600     -2.51384400     -0.40152900
H                          -2.34081200     -1.91973100     -0.47590700
H                          -3.08484700      0.39817000      0.05694200
H                          -1.43232400      2.13779500      0.61109000
C                           2.18409800     -0.90674900      0.19889500
H                           2.56334100     -0.72514800      1.21144700
H                           2.36617300     -1.95252200     -0.05359700
H                           2.76721900     -0.27131000     -0.47271800
O                           1.00495600      1.74222300     -0.59603100
H                           0.57819900      1.57286500     -1.44396200
H                           0.80604800      1.19698700      1.31803800
          Core        RigidRotor
            SymmetryFactor              0.5
          End
      Rotor  Hindered                 !freq=150
          Group                              12 13 14
          Axis                               1 11
          Symmetry                           3
    Potential[kcal/mol]        12
       0.000 0.065 0.274 0.583 0.931 1.219 1.338 1.237 0.966 0.627 0.312 0.094
       End
        Rotor   Hindered                !freq=323
          Group                              16
          Axis                               6 15
          Symmetry                           1
    Potential[kcal/mol]        36
      0.000 0.089 0.377 0.810 1.301 1.754 2.099 2.306 2.380 2.352 2.283 2.224
     2.208 2.245 2.328 2.431 2.524 2.579 2.589 2.563 2.537 2.547 2.632 2.809
     3.072 3.383 3.670 3.856 3.847 3.596 3.099 2.447 1.735 1.057 0.501 0.137
       End
          Frequencies[1/cm]           43
     77.96    220.62   267.37   377.09   401.02   485.87   507.54   567.10
     632.51   697.17   766.85   795.22   876.05   910.95   962.75   972.28
     997.92   984.75   1010.78 1025.34 1085.97 1138.84 1162.89 1175.05
     1263.16 1294.47 1342.65 1364.06 1374.74 1383.84 1426.23 1444.83
     1504.05 1569.86 2902.16 2914.34 2972.35 3012.16 3051.22 3060.36
     3078.5   3093.82 3667.04
          ZeroEnergy[kcal/mol]               -17.79
          ElectronicLevels[1/cm]          1
            0    2
End
```

```
End
!***********************************
 Barrier        B4o3     W4o2     P4o            # TS4o3
   RRHO
     Geometry[angstrom]                  17
C                      0.57534600    -0.66804400    -0.02000100
C                     -0.57107100    -1.45073500    -0.01224800
C                     -1.84920600    -0.88642800    -0.00578300
C                     -1.99427800     0.50136700    -0.03766100
C                     -0.87381400     1.31428600    -0.05503100
C                      0.41333500     0.74135900     0.08055000
H                     -0.46295400    -2.52986600    -0.03341900
H                     -2.72330900    -1.52576600    -0.00002100
H                     -2.98130500     0.94627900    -0.07947800
H                     -0.97040700     2.39450500    -0.08857200
C                      1.95781800    -1.24791000    -0.02879400
H                      2.53690000    -0.86961700    -0.87442800
H                      2.49775400    -0.96016600     0.87872200
H                      1.91960800    -2.33642500    -0.08480100
O                      1.55225300     1.48958600    -0.13565200
H                      1.36508400     2.41059200     0.06877600
H                      0.45181400     0.73040100     1.77224700
     Core       RigidRotor
       SymmetryFactor              0.5
     End
     Tunneling          Eckart
       ImaginaryFrequency[1/cm]        1156.69
       WellDepth[kcal/mol]             26.36
       WellDepth[kcal/mol]             7.87
     End
     Frequencies[1/cm]                   44
    152.38   163.32
    249.66   274.75   290.19   408.53   445.67   495.21   536.66   565.02
    582.06   673.28   717.45   756.64   806.77   848.00   880.92   950.43
    981.69   973.56   1027.50 1033.31 1079.50 1136.20 1147.73 1194.93
    1215.66 1280.65 1300.48 1368.76 1411.86 1429.87 1454.07 1474.94
    1565.42 1588.92 2928.12 2985.80 3018.19 3057.53 3062.49 3077.57
    3092.48 3706.17
       ZeroEnergy[kcal/mol]            8.58
       ElectronicLevels[1/cm]          1
                    0          2
End
!***********************************
Barrier B4o2     W     W4o2
Variational
```

```
RRHO                    !                   1
Geometry[angstrom]                  17
C                       -0.13262800     -1.44097100      0.35089000
C                        0.75568900     -0.55899100     -0.27630100
C                        0.23879200      0.62098600     -0.83791300
C                       -1.12864200      0.90785600     -0.76922400
C                       -2.00067500      0.02270800     -0.13598000
C                       -1.49692700     -1.15504700      0.42366000
H                        0.24820600     -2.35756100      0.79183600
H                        0.90580600      1.30473200     -1.34676800
H                       -1.50514600      1.82383600     -1.21121500
H                       -3.06018500      0.24325500     -0.08232400
H                       -2.16680400     -1.85107400      0.91789300
C                        2.23419700     -0.84036200     -0.31771400
H                        2.74445900     -0.29063000      0.47627700
H                        2.43995600     -1.90375200     -0.18659900
H                        2.66706300     -0.52319400     -1.26697600
O                        0.98934700      1.96220800      1.18870500
H                        0.24476200      1.51086900      1.64766800
   Core      RigidRotor
             SymmetryFactor       0.423178412
End
 Rotor                                  Hindered
 Group     13 14 15
 Axis                12                  2
 Symmetry                3
 Potential[kcal/mol]                12
   0.000 0.089 0.183 0.251 0.287 0.278 0.217 0.128 0.030 -0.042 -0.076 -0.064
 End
   Rotor                                  Hindered
 Group     17
 Axis                16                  3
 Symmetry                1
 Potential[kcal/mol]                36
 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
 End
    Frequencies[1/cm]                42
   70.51   208.67   341.57   405.43   446.33   460.62   526.88   609.17
   632.18   640.15   733.98   799.87   853.32   890.79   951.97   962.79
   965.93   977.85   1010.07 1018.29 1069.37 1138.55 1159.73 1192.33
   1295.00 1308.61 1365.13 1414.68 1439.37 1453.41 1469.73 1559.12
   1580.88 2942.49 3006.64 3019.43 3047.68 3062.07 3068.37 3083.85
   3092.58 3461.52
```

```
ZeroEnergy[kcal/mol]      -3.74
  ElectronicLevels[1/cm]                                1
    0.0000000000000000              2.0000000000000000
End
!*****************************************
RRHO                    !                   2
Geometry[angstrom]                  17
C                        -0.13466400     -1.45077700      0.33866200
C                         0.75770100     -0.56265800     -0.26693500
C                         0.24687300      0.63237000     -0.80592600
C                        -1.12254700      0.91783400     -0.74674800
C                        -1.99839200      0.02472900     -0.13297200
C                        -1.50015200     -1.16362100      0.40657300
H                         0.24184100     -2.37267600      0.77113000
H                         0.91286000      1.31143800     -1.32032700
H                        -1.49538300      1.83817700     -1.18235500
H                        -3.05896800      0.24253100     -0.08691100
H                        -2.17432100     -1.86735500      0.88331200
C                         2.23521800     -0.84336100     -0.31840800
H                         2.76926200     -0.17939700      0.37102700
H                         2.45151500     -1.88075200     -0.04453700
H                         2.62970400     -0.66494000     -1.32532100
O                         0.98021600      1.95636400      1.16252800
H                         0.21706000      1.64201700      1.65071800
   Core      RigidRotor
                SymmetryFactor       0.423178412
End
  Rotor                                       Hindered
  Group      13 14 15
  Axis                   12                   2
  Symmetry                    3
  Potential[kcal/mol]                   12
     0.000 0.063 0.153 0.246 0.313 0.349 0.340 0.278 0.190 0.091 0.020 -0.014
  End
     Rotor                                       Hindered
  Group      17
  Axis                   16                   3
  Symmetry                    1
  Potential[kcal/mol]                   36
  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
  End
      Frequencies[1/cm]                   42
    73.57     173.29    200.10    248.89    347.55    406.96    459.19    526.45
```

631.98 640.44 734.60 800.58 853.81 890.87 953.53 959.69
972.25 983.00 1011.88 1027.32 1069.92 1138.86 1159.17 1192.53
1296.98 1308.58 1371.05 1415.30 1440.75 1458.34 1470.96 1561.16
1581.34 2906.64 2967.51 2984.26 3050.60 3063.21 3070.43 3084.28
3099.94 3777.83
ZeroEnergy[kcal/mol] -3.64
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 3
Geometry[angstrom] 17
C -0.13630300 -1.45877600 0.32311000
C 0.75965000 -0.56227800 -0.26429200
C 0.25239200 0.64224900 -0.78766600
C -1.11614900 0.93153400 -0.72261300
C -1.99453600 0.03281400 -0.12013100
C -1.50077600 -1.16781700 0.39542900
H 0.23644100 -2.38992800 0.73719600
H 0.92084200 1.32649500 -1.29274500
H -1.48424000 1.86313500 -1.13674100
H -3.05253400 0.25904600 -0.05851300
H -2.17708100 -1.87602900 0.86203800
C 2.23843300 -0.83639500 -0.29996900
H 2.76119900 -0.12017100 0.33945800
H 2.46315900 -1.84456300 0.05201700
H 2.63636600 -0.73024500 -1.31261500
O 0.96529800 1.93355300 1.11855900
H 0.20382600 1.62404800 1.63359000
Core RigidRotor
SymmetryFactor 0.423178412
End
Rotor Hindered
Group 13 14 15
Axis 12 2
Symmetry 3
Potential[kcal/mol] 12
0.000 0.043 0.123 0.218 0.300 0.350 0.365 0.325 0.248 0.148 0.062 0.011
End
Rotor Hindered
Group 17
Axis 16 3
Symmetry 1
Potential[kcal/mol] 36
0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358

```
3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
End
   Frequencies[1/cm]            42
  78.37   140.78   214.33   343.34   406.25   458.74   494.04   526.53
  631.70   643.67   736.02   800.78   856.29   893.79   955.16   960.55
  966.68   981.65   1011.83 1020.72 1069.01 1138.46 1159.08 1192.85
  1295.44 1308.00 1365.43 1414.82 1436.77 1457.07 1470.42 1561.00
  1581.32 2931.09 2992.44 3011.87 3054.18 3065.92 3073.39 3085.23
  3097.56 3635.75
ZeroEnergy[kcal/mol]   -3.32
 ElectronicLevels[1/cm]                 1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO              !            4
Geometry[angstrom]            17
C                  -0.13631900    -1.46183100     0.31706800
C                   0.76374900    -0.55762600    -0.25028500
C                   0.26042900     0.65583000    -0.75908300
C                  -1.10780700     0.94850500    -0.69185400
C                  -1.99062200     0.03996100    -0.11262800
C                  -1.50118800    -1.17112800     0.38140000
H                   0.23196600    -2.40078700     0.71624900
H                   0.92991600     1.33891700    -1.26506400
H                  -1.47015200     1.89050800    -1.08602300
H                  -3.04855800     0.26612700    -0.05343900
H                  -2.18231100    -1.88918300     0.82440200
C                   2.24192700    -0.83136500    -0.28687500
H                   2.76532300    -0.10203000     0.33649000
H                   2.46998900    -1.83263800     0.08171700
H                   2.63435900    -0.74259700    -1.30322600
O                   0.94249600     1.90234500     1.06021700
H                   0.21239800     1.59039300     1.61892400
   Core    RigidRotor
         SymmetryFactor     0.423178412
End
 Rotor                       Hindered
 Group    13 14 15
 Axis           12          2
 Symmetry             3
 Potential[kcal/mol]           12
 0.000 0.031 0.106 0.199 0.287 0.343 0.368 0.341 0.270 0.172 0.080 0.021
 End
   Rotor                       Hindered
```

```
  Group      17
  Axis                  16                  3
  Symmetry                    1
  Potential[kcal/mol]                   36
  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
  End
      Frequencies[1/cm]                   42
    80.87   187.12   218.33   343.00   406.89   461.12   526.12   570.81
    631.28   644.34   738.82   801.38   859.94   900.48   956.92   961.79
    965.72   982.58   1012.88 1020.02 1069.12 1138.18 1159.24 1193.64
    1294.02 1307.50 1364.24 1414.43 1435.84 1456.76 1470.70 1562.15
    1582.37 2932.58 2994.21 3013.99 3057.60 3068.88 3076.77 3086.80
    3095.98 3622.96
ZeroEnergy[kcal/mol]     -2.56
  ElectronicLevels[1/cm]                              1
    0.0000000000000000              2.0000000000000000
End
!*****************************************
RRHO                  !                  5
Geometry[angstrom]                  17
C                      -0.13572400     -1.46177000      0.31656200
C                       0.76598600     -0.55437600     -0.24130800
C                       0.26494500      0.66489700     -0.74026400
C                      -1.10462200      0.95592200     -0.67840200
C                      -1.98902500      0.04246800     -0.11163500
C                      -1.50084700     -1.17185900      0.37531600
H                       0.23025800     -2.40498600      0.70751500
H                       0.93341700      1.34392000     -1.25324700
H                      -1.46436800      1.90212900     -1.06447500
H                      -3.04780200      0.26593400     -0.05894600
H                      -2.18413600     -1.89443200      0.80708000
C                       2.24328200     -0.82973200     -0.28330300
H                       2.77017300     -0.09819400      0.33438800
H                       2.47255300     -1.83004600      0.08706300
H                       2.62983000     -0.74448100     -1.30223400
O                       0.93123300      1.88527900      1.03094800
H                       0.21714800      1.57344300      1.61036700
    Core      RigidRotor
              SymmetryFactor       0.423178412
End
  Rotor                                    Hindered
  Group      13 14 15
  Axis                  12                  2
```

```
    Symmetry                    3
    Potential[kcal/mol]                 12
    0.000 0.027 0.098 0.190 0.280 0.339 0.368 0.346 0.277 0.182 0.088 0.025
    End
      Rotor                                     Hindered
    Group     17
    Axis                16                3
    Symmetry                1
    Potential[kcal/mol]                 36
    0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
    3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
    2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
    End
       Frequencies[1/cm]                42
     82.94   205.13   219.46   342.94   405.77   462.60   525.93   608.30
     631.61   648.91   741.21   801.76   862.61   906.88   959.99   964.49
     965.45   983.28   1013.86 1020.03 1069.26 1138.24 1159.41 1194.10
     1293.10 1307.26 1363.71 1414.10 1435.44 1456.49 1471.27 1563.01
     1583.18 2932.70 2994.37 3014.55 3058.64 3069.78 3077.86 3087.02
     3095.59 3618.88
  ZeroEnergy[kcal/mol]   -1.92
    ElectronicLevels[1/cm]                          1
     0.0000000000000000          2.0000000000000000
  End
  !*****************************************
  RRHO                !                6
  Geometry[angstrom]                17
  C                    -0.13456000    -1.46086000     0.31760800
  C                     0.76823100    -0.55195200    -0.23360600
  C                     0.27046800     0.67704500    -0.71662200
  C                    -1.10269000     0.96158300    -0.66916200
  C                    -1.98751200     0.04528900    -0.11036900
  C                    -1.50032300    -1.17258100     0.36922500
  H                     0.22923600    -2.40798300     0.70101600
  H                     0.93596000     1.34795300    -1.24332800
  H                    -1.46082600     1.90988700    -1.05117300
  H                    -3.04736700     0.26529500    -0.06440900
  H                    -2.18500700    -1.89778400     0.79437000
  C                     2.24443000    -0.82901300    -0.28156600
  H                     2.77393100    -0.09647200     0.33279400
  H                     2.47455700    -1.82930900     0.08816000
  H                     2.62597900    -0.74416000    -1.30255100
  O                     0.92006000     1.86741100     1.00262400
  H                     0.22063300     1.56415400     1.60324900
     Core      RigidRotor
```

```
            SymmetryFactor      0.423178412
End
  Rotor                                 Hindered
  Group    13 14 15
  Axis                12              2
  Symmetry                  3
  Potential[kcal/mol]             12
  0.000 0.023 0.093 0.184 0.276 0.336 0.367 0.349 0.282 0.188 0.093 0.027
  End
    Rotor                                 Hindered
  Group    17
  Axis                16              3
  Symmetry                  1
  Potential[kcal/mol]             36
  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
  End
      Frequencies[1/cm]             42
    86.12   200.20   215.12   343.00   403.92   465.46   525.63   627.21
    641.00   669.05   744.88   801.97   866.33   916.79   965.11   974.03
    965.61   984.08   1014.66 1020.86 1068.90 1138.15 1159.17 1194.02
    1290.80 1306.36 1363.06 1413.10 1435.07 1456.01 1471.55 1562.44
    1582.93 2932.10 2993.47 3015.13 3058.82 3070.24 3078.77 3087.78
    3096.97 3623.14
ZeroEnergy[kcal/mol]     -1.74
  ElectronicLevels[1/cm]                        1
    0.0000000000000000           2.0000000000000000
End
!*******************************************
RRHO                  !               7
Geometry[angstrom]              17
C                      -0.13353100     -1.46059200      0.31703300
C                       0.77043000     -0.54907800     -0.22485500
C                       0.27624100      0.69002300     -0.69205800
C                      -1.10104600      0.96718900     -0.65965300
C                      -1.98624100      0.04685100     -0.11172300
C                      -1.49929200     -1.17204200      0.36622000
H                       0.22830200     -2.41162700      0.69229700
H                       0.93846100      1.35136500     -1.23572400
H                      -1.45847900      1.91603500     -1.04077900
H                      -3.04711100      0.26311100     -0.07360000
H                      -2.18541300     -1.90013100      0.78388600
C                       2.24519100     -0.82863500     -0.28039400
H                       2.77837800     -0.09588300      0.33056000
```

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H                      2.47613100    -1.82929500     0.08766400
H                      2.62061600    -0.74357900    -1.30372800
O                      0.90930800     1.84982000     0.97484100
H                      0.22364400     1.55255200     1.59338000
   Core     RigidRotor
            SymmetryFactor      0.423178412
End
 Rotor                                  Hindered
 Group     13 14 15
 Axis                12                2
 Symmetry                3
 Potential[kcal/mol]                12
0.000 0.019 0.086 0.176 0.269 0.332 0.366 0.352 0.287 0.196 0.099 0.031
 End
   Rotor                                  Hindered
 Group     17
 Axis                16                3
 Symmetry                1
 Potential[kcal/mol]                36
 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
 End
    Frequencies[1/cm]                42
  87.49   196.02   208.13   343.04   400.67   468.80   525.28   628.65
  663.08   709.50   750.59   801.75   871.91   930.26   974.42   990.80
  972.14   985.22   1015.46 1022.97 1068.50 1137.86 1158.88 1193.50
  1288.10 1305.91 1362.34 1411.62 1434.84 1455.40 1471.90 1560.91
  1581.80 2931.67 2992.81 3015.81 3059.55 3070.86 3078.80 3085.99
  3095.23 3626.04
ZeroEnergy[kcal/mol]    -1.29
 ElectronicLevels[1/cm]                          1
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO                !                8
Geometry[angstrom]                17
C                     -0.13220900    -1.46056200     0.31576500
C                      0.77247800    -0.54787500    -0.21748700
C                      0.28358800     0.70603100    -0.66451400
C                     -1.10108500     0.97164100    -0.65249200
C                     -1.98516900     0.04828500    -0.11383400
C                     -1.49841700    -1.17146600     0.36490700
H                      0.22785400    -2.41496200     0.68397500
H                      0.93952500     1.35148200    -1.23393700
```

```
H                    -1.45851500     1.91970800    -1.03533500
H                    -3.04698800     0.26085600    -0.08279100
H                    -2.18550100    -1.90125200     0.77781500
C                     2.24572600    -0.82875400    -0.27978000
H                     2.78147200    -0.09567000     0.32866500
H                     2.47778100    -1.82977700     0.08644100
H                     2.61648500    -0.74266400    -1.30493700
O                     0.89926400     1.83280700     0.94833000
H                     0.22512000     1.54402900     1.58243200
    Core      RigidRotor
                SymmetryFactor       0.423178412
  End
   Rotor                                  Hindered
   Group     13 14 15
   Axis                12                  2
   Symmetry                3
   Potential[kcal/mol]                    12
  -0.011
 0.076
 0.173
 0.246
 0.287
 0.277
 0.214
 0.122
 0.024
-0.045
-0.077
-0.063
   End
     Rotor                                    Hindered
   Group     17
   Axis                16                  3
   Symmetry                1
   Potential[kcal/mol]                    36
   0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
   3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
   2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
   End
      Frequencies[1/cm]                   42
    88.99   194.94   206.11   343.37   398.00   472.89   524.41   627.73
    679.75   746.32   760.67   801.00   875.20   941.24   978.62   992.37
    981.98   988.98   1015.21 1024.60 1066.34 1137.03 1157.08 1191.12
    1283.44 1304.26 1361.75 1408.42 1434.40 1454.35 1471.38 1554.86
    1578.25 2930.70 2991.35 3016.26 3060.35 3071.54 3079.73 3086.45
```

```
   3095.73 3630.62
ZeroEnergy[kcal/mol]    -0.80
 ElectronicLevels[1/cm]                              1
  0.0000000000000000              2.0000000000000000
End
!****************************************
RRHO                 !                  9
Geometry[angstrom]                 17
C                      -0.13058910     -1.46087721      0.31433670
C                       0.77454390     -0.54827021     -0.21138930
C                       0.29227690      0.72434779     -0.63550730
C                      -1.10260910      0.97554079     -0.64719030
C                      -1.98441610      0.04994079     -0.11617230
C                      -1.49792110     -1.17121221      0.36465870
H                       0.22780290     -2.41824421      0.67631570
H                       0.93939990      1.34884479     -1.23688530
H                      -1.46027910      1.92247979     -1.03226830
H                      -3.04711810      0.25889679     -0.09151630
H                      -2.18569810     -1.90191721      0.77440470
C                       2.24635590     -0.82912721     -0.27937330
H                       2.78366690     -0.09547921      0.32719770
H                       2.47991590     -1.83039721      0.08505470
H                       2.61345490     -0.74151321     -1.30600130
O                       0.88971790      1.81639179      0.92295470
H                       0.22603090      1.53522779      1.57058570
   Core      RigidRotor
             SymmetryFactor       0.423178412
End
 Rotor                                    Hindered
 Group     13 14 15
 Axis                12                2
 Symmetry                 3
 Potential[kcal/mol]                 12
 0.000 0.152 0.407 0.727 1.040 1.258 1.292 1.116 0.793 0.441 0.152 -0.012
 End
   Rotor                                    Hindered
 Group     17
 Axis                16                3
 Symmetry                 1
 Potential[kcal/mol]                 36
 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
 End
    Frequencies[1/cm]                 42
```

```
   96.47    198.78    208.09    344.00    395.36    476.42    522.79    625.47
   680.95    753.77    792.97    812.94    875.74    949.38    980.32    991.33
   983.73    998.09    1013.18 1025.21 1062.22 1134.75 1153.82 1186.83
   1277.29 1301.81 1361.13 1403.55 1433.74 1452.83 1469.32 1542.77
   1572.09 2929.28 2989.29 3016.58 3061.32 3072.21 3081.15 3087.34
   3096.51 3633.76
ZeroEnergy[kcal/mol]      -1.45
  ElectronicLevels[1/cm]                          1
   0.0000000000000000              2.0000000000000000
End
!*******************************************
RRHO                    !                    10
Geometry[angstrom]                   17
C                            -0.12896900     -1.46119200       0.31290900
C                             0.77660900     -0.54866600      -0.20529200
C                             0.30096600      0.74266500      -0.60650000
C                            -1.10413300      0.97944000      -0.64188800
C                            -1.98366300      0.05159700      -0.11851100
C                            -1.49742500     -1.17095800       0.36441000
H                             0.22775200     -2.42152600       0.66865600
H                             0.93927500      1.34620700      -1.23983300
H                            -1.46204300      1.92525100      -1.02920100
H                            -3.04724800      0.25693700      -0.10024100
H                            -2.18589500     -1.90258200       0.77099500
C                             2.24698600     -0.82950100      -0.27896600
H                             2.78586100     -0.09528800       0.32573100
H                             2.48205000     -1.83101700       0.08366800
H                             2.61042500     -0.74036300      -1.30706600
O                             0.88017200      1.79997700       0.89758000
H                             0.22694200      1.52642600       1.55873900
     Core      RigidRotor
                    SymmetryFactor       0.423178412
End
  Rotor                                          Hindered
  Group      13 14 15
  Axis                    12                    2
  Symmetry                       3
  Potential[kcal/mol]                    12
  0.000 0.146 0.397 0.715 1.030 1.256 1.301 1.134 0.815 0.463 0.169 -0.003
  End
      Rotor                                          Hindered
  Group      17
  Axis                    16                    3
  Symmetry                       1
  Potential[kcal/mol]                    36
```

```
  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
  End
     Frequencies[1/cm]                42
   112.04   208.01   219.98   344.92   392.68   478.57   520.74   622.18
   674.31   752.55   792.56   858.50   876.08   950.37   986.11   990.25
   985.35   1009.17 1012.42 1031.70 1058.19 1130.67 1151.08 1182.93
   1273.82 1300.37 1360.49 1399.06 1432.78 1451.27 1466.17 1530.16
   1564.76 2927.60 2986.95 3016.80 3061.79 3070.72 3075.27 3084.83
   3095.61 3632.15
 ZeroEnergy[kcal/mol]     -2.24
  ElectronicLevels[1/cm]                          1
   0.0000000000000000          2.0000000000000000
 End
 !*****************************************
 RRHO                !                11
 Geometry[angstrom]                17
 C                    -0.12705800     -1.46172100      0.31148900
 C                     0.77866400     -0.55048100     -0.20024500
 C                     0.31072800      0.76258700     -0.57675700
 C                    -1.10687400      0.98290700     -0.63806500
 C                    -1.98314100      0.05355600     -0.12093100
 C                    -1.49735400     -1.17109700      0.36487500
 H                     0.22805000     -2.42473000      0.66160700
 H                     0.93807900      1.34098100     -1.24677500
 H                    -1.46508100      1.92763900     -1.02736200
 H                    -3.04754800      0.25536400     -0.10859200
 H                    -2.18633000     -1.90310700      0.76929300
 C                     2.24769100     -0.83002200     -0.27865300
 H                     2.78771400     -0.09516800      0.32446400
 H                     2.48460700     -1.83167900      0.08225700
 H                     2.60809100     -0.73914900     -1.30803000
 O                     0.87110400      1.78430000      0.87336800
 H                     0.22717200      1.51665200      1.54555200
    Core      RigidRotor
              SymmetryFactor       0.423178412
 End
  Rotor                                    Hindered
  Group     13 14 15
  Axis                12                2
  Symmetry                  3
  Potential[kcal/mol]                12
  0.000 0.142 0.389 0.705 1.022 1.253 1.307 1.148 0.833 0.480 0.182 0.005
  End
```

```
    Rotor                                   Hindered
  Group     17
  Axis                16              3
  Symmetry                  1
  Potential[kcal/mol]              36
  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
  End
      Frequencies[1/cm]              42
   151.28   216.05   232.76   346.56   391.07   480.59   517.89   617.63
   666.91   747.65   788.66   859.96   904.94   944.08   986.36   997.14
   989.32   1005.89 1016.33 1052.54 1064.44 1123.28 1148.75 1179.24
   1271.20 1298.91 1360.07 1394.25 1431.64 1449.42 1459.77 1516.23
   1557.68 2925.48 2984.06 3016.76 3054.08 3062.29 3073.09 3085.60
   3095.72 3632.45
ZeroEnergy[kcal/mol]     -3.31
  ElectronicLevels[1/cm]                        1
   0.0000000000000000            2.0000000000000000
End
!*******************************************
RRHO                 !                 12
Geometry[angstrom]               17
C                      -0.12483100    -1.46210800     0.30990000
C                       0.78056100    -0.55316700    -0.19574800
C                       0.32119100     0.78327200    -0.54664100
C                      -1.11032100     0.98593100    -0.63492800
C                      -1.98259200     0.05574700    -0.12345700
C                      -1.49765000    -1.17155700     0.36575500
H                       0.22858100    -2.42773300     0.65473800
H                       0.93556600     1.33385800    -1.25374400
H                      -1.46879800     1.92975500    -1.02593600
H                      -3.04786300     0.25391100    -0.11696900
H                      -2.18695800    -1.90361400     0.76867900
C                       2.24830700    -0.83055100    -0.27839800
H                       2.79023800    -0.09553500     0.32307600
H                       2.48719800    -1.83236300     0.08082300
H                       2.60616600    -0.73810400    -1.30895600
O                       0.86235000     1.76914900     0.84977100
H                       0.22656200     1.50706400     1.53119000
    Core     RigidRotor
               SymmetryFactor      0.423178412
End
  Rotor                                   Hindered
    Group     13 14 15
```

```
Axis 12 2
Symmetry 3
Potential[kcal/mol] 12
0.000 0.138 0.382 0.696 1.014 1.250 1.311 1.158 0.847 0.494 0.193 0.011
End
Rotor Hindered
Group 17
Axis 16 3
Symmetry 1
Potential[kcal/mol] 36
0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
End
Frequencies[1/cm] 42
208.86 230.88 242.26 349.05 391.30 483.02 514.66 612.66
661.61 741.38 784.69 847.81 924.38 936.11 983.83 966.42
1000.19 1001.98 1017.93 1046.63 1111.64 1113.71 1149.05 1176.32
1270.07 1297.49 1360.25 1390.01 1430.54 1446.46 1449.67 1505.95
1555.25 2922.84 2980.55 3015.97 3037.20 3062.01 3072.12 3086.92
3095.76 3635.78
ZeroEnergy[kcal/mol] -5.74
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!********************************************
RRHO ! 13
Geometry[angstrom] 17
C -0.12266300 -1.46261500 0.30824800
C 0.78237100 -0.55525800 -0.19120200
C 0.33150700 0.80371700 -0.51660900
C -1.11318300 0.98920300 -0.63160100
C -1.98214500 0.05775300 -0.12598500
C -1.49807500 -1.17203000 0.36681500
H 0.22909300 -2.43110500 0.64722800
H 0.93255700 1.32700300 -1.25702500
H -1.47282300 1.93176100 -1.02480000
H -3.04833000 0.25212000 -0.12608700
H -2.18769200 -1.90411700 0.76839400
C 2.24904700 -0.83116700 -0.27817700
H 2.79359300 -0.09650700 0.32163600
H 2.48998900 -1.83319300 0.07923900
H 2.60434800 -0.73716800 -1.30987400
O 0.85347100 1.75396000 0.82590200
H 0.22567800 1.49714100 1.51621400
```

```
      Core      RigidRotor
                SymmetryFactor       0.423178412
   End
    Rotor                                   Hindered
    Group     13 14 15
    Axis                12                2
    Symmetry                3
    Potential[kcal/mol]                12
    0.000 0.134 0.374 0.688 1.007 1.247 1.315 1.170 0.862 0.508 0.204 0.017
    End
      Rotor                                   Hindered
    Group     17
    Axis                16                3
    Symmetry                1
    Potential[kcal/mol]                36
    0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
    3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
    2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
    End
       Frequencies[1/cm]                42
     215.92   246.33   260.66   352.08   394.65   486.68   511.87   608.45
     659.42   736.54   781.29   834.91   926.68   935.09   981.68   967.59
     996.73   1011.83 1027.67 1046.33 1104.13 1139.45 1169.24 1176.80
     1268.51 1296.43 1360.67 1386.43 1428.82 1433.71 1446.81 1501.32
     1556.88 2920.33 2977.21 3014.73 3022.46 3060.62 3070.26 3087.49
     3095.12 3638.05
   ZeroEnergy[kcal/mol]     -8.69
    ElectronicLevels[1/cm]                          1
     0.0000000000000000             2.0000000000000000
   End
   !*****************************************
   RRHO                !                14
   Geometry[angstrom]                17
   C                      -0.12074500     -1.46330100      0.30654600
   C                       0.78420700     -0.55610200     -0.18613500
   C                       0.34123700      0.82331200     -0.48705000
   C                      -1.11492800      0.99307000     -0.62745000
   C                      -1.98176300      0.05940500     -0.12850200
   C                      -1.49846400     -1.17231100      0.36787400
   H                       0.22944500     -2.43504600      0.63844700
   H                       0.92946700      1.32086400     -1.25682100
   H                      -1.47664300      1.93387000     -1.02362200
   H                      -3.04886600      0.24974200     -0.13654200
   H                      -2.18848500     -1.90460600      0.76790700
   C                       2.25001600     -0.83189600     -0.27796700
```

```
H                2.79809900   -0.09824300    0.32010900
H                2.49288600   -1.83430600    0.07730000
H                2.60228700   -0.73632800   -1.31085700
O                0.84411100    1.73845600    0.80138700
H                0.22555700    1.48723500    1.50148000
   Core    RigidRotor
          SymmetryFactor    0.423178412
End
 Rotor                         Hindered
 Group   13 14 15
 Axis          12          2
 Symmetry           3
 Potential[kcal/mol]        12
 0.000 0.129 0.365 0.677 0.997 1.243 1.320 1.182 0.880 0.526 0.218 0.025
 End
   Rotor                         Hindered
 Group   17
 Axis          16          3
 Symmetry           1
 Potential[kcal/mol]        36
 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
 End
    Frequencies[1/cm]        42
  229.05   257.55   285.69   356.13   402.58   491.49   509.78   605.65
  659.19   734.32   778.21   823.93   921.91   935.71   979.90   965.88
  992.79   1013.39 1028.94 1073.43 1096.41 1141.26 1171.15 1219.53
  1266.10 1295.80 1361.05 1383.06 1417.12 1430.05 1445.63 1499.55
  1559.02 2918.30 2974.40 3006.12 3013.66 3058.57 3067.79 3086.44
  3094.29 3640.81
ZeroEnergy[kcal/mol]    -11.53
 ElectronicLevels[1/cm]                1
  0.0000000000000000        2.0000000000000000
End
!********************************************
RRHO          !          15
Geometry[angstrom]         17
C               -0.11907500   -1.46406500    0.30474200
C                0.78615900   -0.55577400   -0.18016200
C                0.35028600    0.84174500   -0.45836500
C               -1.11567900    0.99758800   -0.62206900
C               -1.98127400    0.06080100   -0.13110500
C               -1.49869200   -1.17231000    0.36877100
H                0.22949300   -2.43947900    0.62821300
```

```
H                  0.92628400     1.31516700    -1.25418100
H                 -1.47957400     1.93640200    -1.02176500
H                 -3.04926200     0.24673100    -0.14846400
H                 -2.18928000    -1.90505400     0.76677500
C                  2.25122200    -0.83270700    -0.27773900
H                  2.80392100    -0.10078900     0.31845300
H                  2.49561900    -1.83579200     0.07482400
H                  2.59966700    -0.73552500    -1.31201600
O                  0.83402700     1.72259900     0.77615200
H                  0.22750600     1.47816300     1.48840000
   Core     RigidRotor
            SymmetryFactor     0.423178412
End
  Rotor                             Hindered
  Group     13 14 15
  Axis              12          2
  Symmetry               3
  Potential[kcal/mol]          12
  0.000 0.123 0.354 0.663 0.985 1.237 1.325 1.197 0.901 0.547 0.235 0.034
  End
    Rotor                             Hindered
  Group     17
  Axis              16          3
  Symmetry               1
  Potential[kcal/mol]          36
  0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
  3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
  2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
  End
     Frequencies[1/cm]          42
   263.12   301.79   356.67   384.93   466.01   497.11   509.90   606.67
   661.95   737.59   775.01   815.59   918.00   932.82   978.28   963.20
   989.13   1013.61 1025.05 1090.52 1110.31 1140.79 1169.39 1259.04
   1270.11 1295.50 1361.29 1380.00 1404.32 1429.61 1444.75 1498.79
   1560.39 2916.59 2971.98 2988.60 3012.25 3056.28 3065.13 3084.26
   3093.67 3644.25
ZeroEnergy[kcal/mol]     -14.16
  ElectronicLevels[1/cm]                 1
   0.0000000000000000        2.0000000000000000
End
!*******************************************
RRHO               !          16
Geometry[angstrom]          17
C                 -0.11749200    -1.46491000     0.30271000
C                  0.78843600    -0.55450300    -0.17255300
```

```
C 0.35834700 0.85840800 -0.43108000
C -1.11569200 1.00307700 -0.61475700
C -1.98055500 0.06216300 -0.13404800
C -1.49867500 -1.17199800 0.36928700
H 0.22908300 -2.44462800 0.61601100
H 0.92265200 1.30901100 -1.25018900
H -1.48124300 1.94007400 -1.01803400
H -3.04941600 0.24301500 -0.16240300
H -2.19010600 -1.90556100 0.76423600
C 2.25276200 -0.83364200 -0.27743100
H 2.81186300 -0.10452800 0.31649500
H 2.49820400 -1.83788600 0.07139100
H 2.59591700 -0.73461800 -1.31353100
O 0.82308800 1.70675500 0.75010800
H 0.23214200 1.46872300 1.47647000
  Core RigidRotor
      SymmetryFactor 0.423178412
End
 Rotor Hindered
 Group 13 14 15
 Axis 12 2
 Symmetry 3
 Potential[kcal/mol] 12
 0.000 0.115 0.340 0.646 0.969 1.229 1.329 1.215 0.927 0.573 0.256 0.046
 End
   Rotor Hindered
 Group 17
 Axis 16 3
 Symmetry 1
 Potential[kcal/mol] 36
 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
 End
    Frequencies[1/cm] 42
  265.57 316.50 363.21 398.26 502.53 504.12 574.30 630.84
  680.94 765.81 771.53 813.05 915.29 928.90 976.82 997.74
  985.54 1013.36 1021.56 1086.23 1139.07 1146.66 1168.05 1258.91
  1295.32 1310.28 1361.43 1377.34 1393.92 1429.42 1444.09 1498.61
  1561.59 2914.92 2969.59 2970.49 3010.80 3053.61 3062.22 3081.66
  3093.06 3650.36
ZeroEnergy[kcal/mol] -16.24
 ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
End
```

```
!******************************************
RRHO                    !                    17
Geometry[angstrom]                  17
C                          -0.11578400     -1.46638400       0.30037400
C                           0.79183700     -0.55221300     -0.16037100
C                           0.36374700       0.86989100     -0.40811000
C                          -1.11496700       1.01128300     -0.60238100
C                          -1.97965400       0.06384200     -0.13795300
C                          -1.49821400     -1.17129600       0.36809800
H                           0.22736400     -2.45238200       0.59905900
H                           0.91738200       1.29909200     -1.24754800
H                          -1.48018500       1.94818500     -1.00684800
H                          -3.04956200       0.23776800     -0.18136800
H                          -2.19139800     -1.90700600       0.75612400
C                           2.25537500     -0.83508800     -0.27677400
H                           2.82607800     -0.11177900       0.31363900
H                           2.50122500     -1.84195500       0.06471800
H                           2.58854300     -0.73304900     -1.31618600
O                           0.81083700       1.69326900       0.72285500
H                           0.24300000       1.45352300       1.46612000
   Core     RigidRotor
           SymmetryFactor       0.423178412
End
 Rotor                                   Hindered
 Group     13 14 15
 Axis                   12                   2
 Symmetry                    3
 Potential[kcal/mol]                  12
 0.000 0.103 0.319 0.619 0.943 1.214 1.333 1.238 0.964 0.611 0.287 0.064
 End
   Rotor                                   Hindered
 Group     17
 Axis                   16                   3
 Symmetry                    1
 Potential[kcal/mol]                  36
 0.000 0.091 0.413 0.936 1.597 2.310 2.980 3.516 3.818 3.872 3.717 3.443
 3.131 2.854 2.658 2.557 2.535 2.556 2.585 2.584 2.537 2.451 2.347 2.258
 2.211 2.217 2.269 2.339 2.380 2.331 2.151 1.831 1.394 0.904 0.452 0.131
 End
    Frequencies[1/cm]                  42
  263.77   327.66   372.56   402.89   501.43   509.55   584.21   646.17
  706.23   767.82   798.21   881.23   915.40   939.34   975.78   994.84
  983.18   1012.84 1019.98 1083.73 1138.32 1164.68 1179.74 1258.57
  1295.87 1344.59 1362.05 1375.71 1387.99 1429.37 1443.82 1499.50
  1563.31 2912.53 2953.14 2966.61 3008.60 3049.09 3058.32 3079.22
```

```
   3091.68 3653.77
ZeroEnergy[kcal/mol]     -17.26
 ElectronicLevels[1/cm]                          1
  0.0000000000000000             2.0000000000000000
End
!****************************************
RRHO                !                 18
Geometry[angstrom]                17
C                      -0.13228000     -1.50496400      0.24654200
C                       0.78404600     -0.55794900     -0.11270800
C                       0.34907300      0.85939100     -0.39359300
C                      -1.13483900      1.03361400     -0.47926400
C                      -1.99969200      0.04645200     -0.11634400
C                      -1.52144800     -1.23217100      0.27097700
H                       0.21094200     -2.50128500      0.50504000
H                       0.83108300      1.21086800     -1.31611200
H                      -1.49370500      2.01362200     -0.77375600
H                      -3.06796500      0.23214400     -0.12778400
H                      -2.21811000     -2.00501700      0.56750200
C                       2.25444500     -0.82884800     -0.19336700
H                       2.80712900     -0.14195300      0.45437300
H                       2.48793000     -1.85497100      0.09499900
H                       2.62057800     -0.66378600     -1.21414100
O                       0.88694200      1.77376300      0.60742100
H                       0.42354600      1.56965000      1.43028800
   Core      RigidRotor
             SymmetryFactor       0.423178412
End
 Rotor                                  Hindered
 Group     13 14 15
 Axis                12                2
 Symmetry                    3
 Potential[kcal/mol]                   12
 0.000 0.093 0.299 0.594 0.919 1.198 1.333 1.257 0.995 0.644 0.315 0.081
 End
 Rotor                                  Hindered
 Group     17
 Axis                16                3
 Symmetry                    1
 Potential[kcal/mol]                   36
 0.000 0.154 0.534 1.101 1.785 2.496 3.139 3.622 3.854 3.846 3.649 3.358
 3.049 2.791 2.620 2.542 2.536 2.563 2.588 2.574 2.516 2.421 2.319 2.238
 2.205 2.225 2.286 2.354 2.376 2.294 2.077 1.722 1.263 0.774 0.348 0.073
 End
    Frequencies[1/cm]                  42
```

```
    264.31 342.22 395.17 402.36 490.31 509.88 571.74 635.54
    698.85 767.50 797.42 880.05 911.25 960.65 970.57 994.64
    984.96 1012.12 1024.20 1085.11 1139.31 1164.15 1183.09 1265.23
    1295.20 1349.02 1363.95 1374.47 1385.32 1427.31 1444.81 1504.57
    1570.70 2896.12 2909.89 2965.91 3010.04 3056.21 3060.58 3078.08
    3098.25 3643.05
  ZeroEnergy[kcal/mol]     -18.29
   ElectronicLevels[1/cm]                          1
    0.0000000000000000            2.0000000000000000
  End
   !***********************************
        Tunneling       Eckart
       ImaginaryFrequency[1/cm]         406
       WellDepth[kcal/mol]              2.68
       WellDepth[kcal/mol]              17.02
  End
  End
  !***********************************
     Well        W4p2                  # pHOC6CH5CH3
     Species
       RRHO
        Geometry[angstrom]               17
  C                     0.70827100     1.24600900    -0.30063200
  C                    -0.63855300     1.21997800    -0.10413700
  C                    -1.36430000     0.00032000    -0.00082100
  C                    -0.63866600    -1.21968600    -0.10425800
  C                     0.70800700    -1.24599300    -0.30064900
  C                     1.53505900    -0.00006800    -0.37954300
  H                    -1.18469100    -2.15502600    -0.02613300
  H                     1.24027100    -2.18763800    -0.37457500
  O                     2.56611500    -0.00021400     0.64458400
  H                     2.10928400    -0.00002200     1.49352900
  H                     2.12595000    -0.00014600    -1.30348800
  H                     1.24070600     2.18755300    -0.37455300
  H                    -1.18433700     2.15543700    -0.02593900
  C                    -2.84079900    -0.00008900     0.26276900
  H                    -3.32083100    -0.88095900    -0.16944000
  H                    -3.05106300    -0.01072200     1.33947900
  H                    -3.31831500     0.89040200    -0.15192000
            Core        RigidRotor
              SymmetryFactor              1
            End
            Rotor    Hindered                !freq=15.76
           Group                             15 16 17
           Axis                               3 14
```

```
                Symmetry                                3
        Potential[kcal/mol]          12
            0.000 -0.001 0.003 -0.001 0.000 -0.001 -0.002 0.000 -0.001 0.000 0.003 -0.001
            End
             Rotor    Hindered                    !freq=268.95
                Group                                10
                Axis                                 6 9
                Symmetry                             1
        Potential[kcal/mol]          36
            0.000 0.106 0.407 0.872 1.424 1.973 2.418 2.711 2.837 2.819 2.704 2.564
            2.461 2.424 2.457 2.537 2.635 2.711 2.734 2.702 2.621 2.524 2.448 2.425
            2.474 2.586 2.726 2.830 2.831 2.689 2.393 1.954 1.420 0.880 0.416 0.107
            End
                Frequencies[1/cm]               43
         72.37     214.82    330.97    361.72    395.45    453.35    492.38    600.78
         626.33    748.09    762.53    766.19    871.29    953.40    960.88    968.20
         986.61    971.90    996.28    1019.91 1127.94 1150.12 1177.04 1205.34
         1223.74 1295.01 1344.94 1365.69 1366.55 1419.02 1434.20 1437.59
         1485.01 1571.82 2905.71 2908.24 2968.89 3005.24 3047.94 3048.96
         3076.11 3078.07 3669.76
                ZeroEnergy[kcal/mol]                -16.88
                ElectronicLevels[1/cm]          1
                  0     2
    End
    End
    !***********************************
     Barrier        B4p3     W4p2     P4p          # TS4p3
       RRHO
          Geometry[angstrom]                 17
    C                      0.69740100    -1.22292600    -0.03502200
    C                     -0.68505400    -1.19954000    -0.03932500
    C                     -1.40195500     0.00567400    -0.02000200
    C                     -0.67362900     1.20190200    -0.04259800
    C                      0.71062700     1.20612300    -0.05191700
    C                      1.41917400    -0.01294000     0.08290300
    H                     -1.20475800     2.14685600    -0.08732100
    H                      1.26080600     2.14042400    -0.08507200
    O                      2.77762500    -0.08966600    -0.14790800
    H                      3.19031600     0.73067600     0.13826000
    H                      1.46461900     0.00862900     1.77073400
    H                      1.25091600    -2.15301500    -0.05705100
    H                     -1.22766500    -2.13812000    -0.08112700
    C                     -2.90808000     0.01209500     0.01956800
    H                     -3.32062200    -0.84569100    -0.51582700
    H                     -3.27440100    -0.03614000     1.04992200
```

```
H                  -3.31110500    0.92138900   -0.43089100
    Core     RigidRotor
      SymmetryFactor          0.5
    End
    Tunneling       Eckart
      ImaginaryFrequency[1/cm]      1196.85
      WellDepth[kcal/mol]           27.20
      WellDepth[kcal/mol]           8.71
    End
  Frequencies[1/cm]                 44
  55.86    131.99
  250.17   303.19   314.70   393.25   427.27   448.62   510.65   531.54
  651.35   656.58   709.66   758.72   823.29   837.48   881.46   965.16
  976.72   972.21   988.36   1024.64 1092.88 1142.86 1153.44 1198.79
  1217.56 1268.16 1310.57 1370.56 1412.85 1441.40 1451.98 1473.50
  1553.42 1597.62 2925.43 2983.17 3008.09 3055.98 3061.47 3072.62
  3096.32 3705.05
    ZeroEnergy[kcal/mol]             10.31
    ElectronicLevels[1/cm]           1
              0        2
End
!************************************
Barrier B4p2    W    W4p2
Variational
RRHO                 !              1
Geometry[angstrom]            17
C                   1.31381800    0.00001300   -0.84727900
C                   0.63772100    1.20709800   -0.63958100
C                  -0.68966700    1.20375100   -0.21237700
C                  -1.37128900   -0.00000900    0.01354300
C                  -0.68967600   -1.20374300   -0.21243800
C                   0.63772600   -1.20707100   -0.63966100
H                   2.33854000    0.00002800   -1.18817700
H                   1.15088900    2.14701800   -0.80592200
H                  -1.20471000    2.14521700   -0.05060200
H                  -1.20471700   -2.14521500   -0.05072000
H                   1.15088400   -2.14698500   -0.80607700
C                  -2.79240300    0.00002500    0.51786100
H                  -2.81515400    0.00151200    1.61213400
H                  -3.33381000    0.88436200    0.17725400
H                  -3.33317100   -0.88568400    0.17967300
O                   2.56838600   -0.00003800    1.45983500
H                   1.65914500   -0.00041300    1.81477500
   Core     RigidRotor
         SymmetryFactor     0.843552272
```

```
End
 Rotor                                   Hindered
 Group    13 14 15
 Axis                 12                4
 Symmetry                3
 Potential[kcal/mol]               12
   0.000 0.005 0.006 0.003 0.001 0.001 0.001 -0.001 0.002 0.003 0.006 0.003
 End
   Rotor                                   Hindered
 Group    17
 Axis                 16                1
 Symmetry                1
 Potential[kcal/mol]                36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]                42
   105.59   208.96   282.85   341.35   401.35   453.14   473.70   526.91
   632.26   641.75   732.23   799.86   845.64   891.40   944.45   954.22
   966.56   976.99   1008.16 1020.08 1068.71 1138.21 1159.98 1191.80
   1293.91 1308.79 1369.45 1416.26 1442.42 1452.52 1467.92 1557.09
   1583.13 2928.88 2988.26 3014.16 3055.44 3055.54 3078.99 3080.57
   3117.01 3563.62
ZeroEnergy[kcal/mol]     -3.44
 ElectronicLevels[1/cm]                              1
  0.0000000000000000             2.0000000000000000
End
!********************************************
RRHO                 !                  2
Geometry[angstrom]                 17
C                          1.31834700     -0.00001200     -0.81844800
C                          0.64270200      1.20712300     -0.61222500
C                         -0.68893700      1.20384700     -0.19927500
C                         -1.37412000      0.00000800      0.01365600
C                         -0.68895400     -1.20384200     -0.19927800
C                          0.64268400     -1.20713700     -0.61222600
H                          2.34510100     -0.00001900     -1.16180900
H                          1.15702600      2.14679700     -0.77509200
H                         -1.20724600      2.14518700     -0.04885500
H                         -1.20727800     -2.14517500     -0.04885900
H                          1.15699400     -2.14681900     -0.77509600
C                         -2.80633500      0.00001300      0.48642300
H                         -2.85260100     -0.00015100      1.58016300
H                         -3.33971200      0.88518000      0.13508200
```

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H                         -3.33980900    -0.88499200     0.13481600
O                          2.56995100     0.00000000     1.40287400
H                          1.68060100    -0.00000900     1.81062400
   Core     RigidRotor
              SymmetryFactor      0.843552272
End
 Rotor                                        Hindered
 Group     13 14 15
 Axis                  12                 4
 Symmetry                    3
 Potential[kcal/mol]                 12
    0.000 0.005 0.006 0.003 0.002 0.001 0.001 -0.001 0.002 0.003 0.006 0.003
 End
    Rotor                                        Hindered
 Group     17
 Axis                  16                 1
 Symmetry                    1
 Potential[kcal/mol]                 36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
     Frequencies[1/cm]                 42
    124.67   215.15   338.84   342.50   401.34   458.24   523.81   534.37
    632.74   641.01   739.81   799.89   844.64   896.58   947.90   953.92
    967.20   977.45   1008.92 1020.49 1069.79 1141.23 1159.91 1191.58
    1294.30 1310.30 1369.49 1417.46 1442.53 1453.12 1467.88 1559.48
    1583.29 2927.52 2987.26 3013.41 3056.91 3057.20 3076.89 3082.49
    3097.22 3534.20
ZeroEnergy[kcal/mol]     -2.76
 ElectronicLevels[1/cm]                              1
   0.0000000000000000              2.0000000000000000
End
!******************************************
RRHO                  !                    3
Geometry[angstrom]                17
C                          1.32397300    -0.00001100    -0.80113400
C                          0.65002100     1.20750200    -0.58920400
C                         -0.68272200     1.20404200    -0.18200900
C                         -1.37065900     0.00000800     0.02031400
C                         -0.68273900    -1.20403800    -0.18200900
C                          0.65000300    -1.20751500    -0.58920200
H                          2.34934400    -0.00001900    -1.14893400
H                          1.16878100     2.14685300    -0.73831600
H                         -1.20066300     2.14521600    -0.03049800
```

```
H                     -1.20069200   -2.14520500   -0.03049700
H                      1.16875100   -2.14687300   -0.73831300
C                     -2.81346100    0.00001300    0.45934400
H                     -2.89159100   -0.00018800    1.55102400
H                     -3.33643500    0.88467500    0.09126200
H                     -3.33653700   -0.88445500    0.09093500
O                      2.54763100   -0.00000200    1.34544900
H                      1.68073000    0.00001300    1.79321700
   Core     RigidRotor
            SymmetryFactor      0.843552272
End
 Rotor                              Hindered
 Group     13 14 15
 Axis              12            4
 Symmetry               3
 Potential[kcal/mol]          12
 0.000 0.004 0.006 0.003 0.002 0.001 0.001 -0.001 0.002 0.003 0.005 0.004
 End
   Rotor                              Hindered
 Group     17
 Axis              16            1
 Symmetry               1
 Potential[kcal/mol]           36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]             42
  138.95   219.93   287.85   341.91   400.54   458.75   523.99   540.20
  632.57   640.42   744.05   800.25   843.69   898.63   949.49   954.22
  967.82   977.97   1008.96 1020.66 1069.99 1141.63 1160.07 1192.27
  1294.02 1310.51 1369.78 1417.67 1442.94 1453.03 1467.48 1559.89
  1584.05 2928.54 2988.38 3012.50 3058.42 3058.73 3077.74 3084.12
  3097.08 3565.66
ZeroEnergy[kcal/mol]    -2.45
 ElectronicLevels[1/cm]                          1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                 !             4
Geometry[angstrom]             17
C                      1.33553800   -0.00001100   -0.77186800
C                      0.65877200    1.20842400   -0.56520200
C                     -0.67609800    1.20463800   -0.16929500
C                     -1.36616400    0.00000800    0.02362500
```

```
C        -0.67611400    -1.20463300    -0.16929500
C         0.65875500    -1.20843700    -0.56520100
H         2.35503000    -0.00001800    -1.13182500
H         1.17975300     2.14699000    -0.71093400
H        -1.19539200     2.14531000    -0.01968600
H        -1.19542000    -2.14529800    -0.01968500
H         1.17972300    -2.14701000    -0.71093100
C        -2.81526100     0.00001200     0.43939700
H        -2.91176400    -0.00019300     1.52953000
H        -3.33194500     0.88468400     0.06268100
H        -3.33204200    -0.88446300     0.06234700
O         2.51235900    -0.00000200     1.28087000
H         1.67758400     0.00001600     1.77860300
   Core     RigidRotor
         SymmetryFactor      0.843552272
End
  Rotor                                   Hindered
  Group     13 14 15
  Axis            12            4
  Symmetry                3
  Potential[kcal/mol]              12
  0.000 0.003 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.004
  End
    Rotor                                   Hindered
  Group     17
  Axis            16            1
  Symmetry                1
  Potential[kcal/mol]              36
  0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
  2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
  2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
  End
     Frequencies[1/cm]              42
   153.71   185.72   226.22   341.99   400.19   458.46   523.86   550.53
   631.83   640.18   749.37   801.06   843.23   900.72   951.12   955.49
   968.04   978.58   1008.26 1020.37 1069.84 1140.44 1160.54 1193.80
   1292.18 1309.62 1369.92 1417.91 1442.86 1452.65 1466.35 1558.58
   1585.45 2929.17 2988.99 3012.99 3059.30 3059.38 3082.22 3085.27
   3107.46 3610.97
ZeroEnergy[kcal/mol]    -1.81
  ElectronicLevels[1/cm]                     1
   0.0000000000000000         2.0000000000000000
End
!*********************************************
RRHO                  !              5
```

```
Geometry[angstrom]        17
C     1.34261400   -0.00001100   -0.75386300
C     0.66311500    1.20907800   -0.55307200
C    -0.67330900    1.20507600   -0.16536100
C    -1.36410700    0.00000900    0.02340100
C    -0.67332400   -1.20506900   -0.16536100
C     0.66309800   -1.20909200   -0.55307100
H     2.35822400   -0.00001700   -1.12234700
H     1.18511800    2.14707600   -0.69811300
H    -1.19365000    2.14542800   -0.01679700
H    -1.19367900   -2.14541300   -0.01679600
H     1.18508900   -2.14709700   -0.69811000
C    -2.81479000    0.00001100    0.43228800
H    -2.91573900   -0.00019300    1.52209700
H    -3.32998900    0.88476400    0.05375500
H    -3.33008400   -0.88454400    0.05341900
O     2.49351200   -0.00000300    1.24831600
H     1.67514700    0.00001700    1.77002400
  Core   RigidRotor
         SymmetryFactor    0.843552272
End
 Rotor                          Hindered
 Group    13 14 15
 Axis           12          4
 Symmetry            3
 Potential[kcal/mol]         12
 0.000 0.003 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.004
 End
   Rotor                          Hindered
 Group    17
 Axis           16          1
 Symmetry            1
 Potential[kcal/mol]         36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]        42
  135.64   158.11   228.28   342.08   400.36   457.73   524.45   567.44
  631.38   640.68   753.93   801.55   843.29   903.54   954.11   956.72
  968.12   978.86   1007.54 1020.30 1069.83 1139.67 1160.88 1194.81
  1290.42 1309.18 1370.01 1418.19 1442.79 1452.47 1465.51 1557.68
  1586.26 2928.91 2988.71 3013.17 3058.94 3058.99 3083.97 3086.28
  3113.33 3626.75
ZeroEnergy[kcal/mol]    -1.54
```

```
 ElectronicLevels[1/cm]                  1
   0.0000000000000000        2.0000000000000000
End
!*******************************************
RRHO              !           6
Geometry[angstrom]            17
C                      1.34974500    -0.00001100    -0.73374600
C                      0.66724300     1.20965300    -0.54103800
C                     -0.67103800     1.20536400    -0.16326300
C                     -1.36211000     0.00000900     0.02168200
C                     -0.67104900    -1.20535500    -0.16326400
C                      0.66722900    -1.20966900    -0.54103600
H                      2.36193700    -0.00001600    -1.11173800
H                      1.19133700     2.14720300    -0.68080600
H                     -1.19326800     2.14550000    -0.02017100
H                     -1.19329500    -2.14548300    -0.02017200
H                      1.19131000    -2.14722700    -0.68080100
C                     -2.81320700     0.00001200     0.42753500
H                     -2.91480700    -0.00019500     1.51725600
H                     -3.32783000     0.88495900     0.04870600
H                     -3.32792500    -0.88473700     0.04836700
O                      2.47487400    -0.00000300     1.21618000
H                      1.66877100     0.00001700     1.75751700
   Core    RigidRotor
           SymmetryFactor     0.843552272
End
 Rotor                             Hindered
 Group    13 14 15
 Axis            12          4
 Symmetry             3
 Potential[kcal/mol]       12
 0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.004
 End
   Rotor                             Hindered
 Group    17
 Axis            16          1
 Symmetry             1
 Potential[kcal/mol]        36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]          42
   156.09   175.26   227.05   342.19   400.81   456.06   525.46   610.09
   631.16   643.69   760.51   802.24   843.57   908.60   958.86   962.02
```

```
  968.45   979.40   1006.96 1020.34 1070.25 1139.77 1161.33 1196.07
  1289.00 1309.38 1369.90 1418.91 1442.67 1452.50 1464.96 1558.11
  1587.17 2929.08 2988.91 3013.42 3059.27 3059.35 3084.74 3087.25
  3112.30 3618.85
ZeroEnergy[kcal/mol]     -0.94
 ElectronicLevels[1/cm]                    1
  0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                 !              7
Geometry[angstrom]             17
C                   1.35933300    -0.00000800    -0.70780600
C                   0.67022800     1.21043700    -0.53256000
C                  -0.66866200     1.20577600    -0.16102400
C                  -1.36074500     0.00000600     0.01872100
C                  -0.66868600    -1.20577900    -0.16102600
C                   0.67020500    -1.21044000    -0.53255100
H                   2.36491200    -0.00002300    -1.10236300
H                   1.19534300     2.14765500    -0.66995900
H                  -1.19334300     2.14558300    -0.02506700
H                  -1.19337700    -2.14558000    -0.02507000
H                   1.19531000    -2.14766400    -0.66994600
C                  -2.81158000     0.00001100     0.42426400
H                  -2.91131200    -0.00019700     1.51420800
H                  -3.32636100     0.88525400     0.04637000
H                  -3.32645500    -0.88503200     0.04602900
O                   2.45645300    -0.00000300     1.18499100
H                   1.66667100     0.00001800     1.74899700
   Core    RigidRotor
           SymmetryFactor     0.843552272
End
 Rotor                              Hindered
 Group    13 14 15
 Axis              12            4
 Symmetry               3
 Potential[kcal/mol]            12
0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005   0.003
 End
   Rotor                              Hindered
 Group    17
 Axis              16            1
 Symmetry               1
 Potential[kcal/mol]             36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
```

```
  2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
  End
     Frequencies[1/cm]                42
   124.75   172.38   221.21   342.29   402.09   453.11   525.65   630.71
   640.01   661.50   768.51   802.87   844.36   916.09   963.53   979.25
   968.58   979.85   1005.23 1020.75 1070.24 1139.24 1161.70 1197.20
   1285.77 1309.32 1369.56 1419.51 1442.57 1452.33 1463.63 1556.89
   1586.91 2928.86 2988.80 3013.75 3059.71 3059.84 3086.07 3088.46
   3113.58 3623.17
 ZeroEnergy[kcal/mol]     -0.39
  ElectronicLevels[1/cm]                          1
   0.0000000000000000          2.0000000000000000
 End
 !*****************************************
 RRHO                !              8
 Geometry[angstrom]              17
 C                    1.36951000    -0.00000900    -0.68115300
 C                    0.67326300     1.21128700    -0.52286500
 C                   -0.66703700     1.20617000    -0.16180400
 C                   -1.35908900     0.00001000     0.01758400
 C                   -0.66706200    -1.20616500    -0.16180300
 C                    0.67323800    -1.21129500    -0.52285800
 H                    2.36761700    -0.00002000    -1.09583300
 H                    1.19831000     2.14836400    -0.66106600
 H                   -1.19403200     2.14570200    -0.03359700
 H                   -1.19406800    -2.14569000    -0.03359800
 H                    1.19827800    -2.14837800    -0.66105500
 C                   -2.80981500     0.00000600     0.42237200
 H                   -2.90822400    -0.00020700     1.51248300
 H                   -3.32462900     0.88554800     0.04526400
 H                   -3.32471400    -0.88534100     0.04491700
 O                    2.43861000    -0.00000300     1.15441600
 H                    1.66317700     0.00001700     1.73732800
    Core      RigidRotor
              SymmetryFactor       0.843552272
 End
  Rotor                                  Hindered
  Group     13 14 15
  Axis                12                4
  Symmetry                    3
  Potential[kcal/mol]              12
  0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.005 0.003
  End
    Rotor                                  Hindered
  Group     17
```

```
 Axis 16 1
 Symmetry 1
 Potential[kcal/mol] 36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
 Frequencies[1/cm] 42
 110.17 167.90 216.06 342.54 401.66 446.98 525.54 630.18
 655.26 706.07 781.49 803.20 846.50 928.83 970.57 968.57
 968.83 986.33 1002.98 1022.18 1070.08 1139.26 1161.90 1198.42
 1281.70 1309.80 1369.14 1420.33 1442.62 1452.22 1461.75 1554.51
 1584.52 2928.66 2988.59 3014.12 3060.46 3060.57 3086.03 3089.32
 3108.13 3625.80
ZeroEnergy[kcal/mol] -0.08
 ElectronicLevels[1/cm] 1
 0.0000000000000000 2.0000000000000000
End
!********************************************
RRHO ! 9
Geometry[angstrom] 17
C 1.38277300 -0.00000400 -0.65103500
C 0.67491900 1.21297000 -0.51525200
C -0.66547600 1.20678200 -0.16341600
C -1.35809900 0.00000500 0.01730300
C -0.66548700 -1.20678000 -0.16341800
C 0.67490600 -1.21297400 -0.51524700
H 2.36761600 -0.00001100 -1.09599000
H 1.19921700 2.14997900 -0.65624000
H -1.19476900 2.14595800 -0.04261800
H -1.19478800 -2.14595300 -0.04262100
H 1.19920000 -2.14998500 -0.65623300
C -2.80847600 0.00000500 0.42132400
H -2.90631800 -0.00020900 1.51163100
H -3.32332500 0.88583900 0.04489500
H -3.32341500 -0.88563100 0.04454600
O 2.42193800 -0.00000400 1.12522500
H 1.66035700 0.00001700 1.72514200
 Core RigidRotor
 SymmetryFactor 0.843552272
End
 Rotor Hindered
 Group 13 14 15
 Axis 12 4
 Symmetry 3
```

```
Potential[kcal/mol]              12
0.000 0.004 0.005 0.003 0.002 -0.001 0.001 -0.001 0.002 0.003 0.006 0.003
End
  Rotor                                   Hindered
Group    17
Axis                16               1
Symmetry                  1
Potential[kcal/mol]              36
0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
End
    Frequencies[1/cm]              42
  121.14    168.61    220.42    342.58    404.05    446.67    525.91    628.61
  678.33    746.47    792.54    802.72    845.74    942.51    977.73    966.01
  968.15    993.88    1007.02 1021.80 1068.52 1137.70 1162.42 1199.51
  1274.53 1310.02 1368.83 1420.94 1442.30 1451.43 1458.03 1545.63
  1582.15 2927.83 2987.80 3014.20 3061.01 3061.21 3086.96 3090.26
  3107.83 3630.52
ZeroEnergy[kcal/mol]     0.38
 ElectronicLevels[1/cm]                        1
  0.0000000000000000           2.0000000000000000
End
!********************************************
RRHO                   !                 10
Geometry[angstrom]              17
C                        1.39846073     -0.00000400     -0.61907474
C                        0.67558273      1.21567800     -0.50938874
C                       -0.66381827      1.20791700     -0.16517974
C                       -1.35773527      0.00000500      0.01751126
C                       -0.66382927     -1.20791500     -0.16518174
C                        0.67556973     -1.21568100     -0.50938274
H                        2.36516573     -0.00001100     -1.10150174
H                        1.19902173      2.15259400     -0.65342174
H                       -1.19542727      2.14660700     -0.05119674
H                       -1.19544527     -2.14660200     -0.05119974
H                        1.19900473     -2.15260000     -0.65341374
C                       -2.80757227      0.00000500      0.42076326
H                       -2.90527027     -0.00020900      1.51130526
H                       -3.32245627      0.88608800      0.04486426
H                       -3.32254627     -0.88588100      0.04451626
O                        2.40602473     -0.00000400      1.09727826
H                        1.65709673      0.00001800      1.71209826
   Core     RigidRotor
            SymmetryFactor      0.843552272
```

```
End
 Rotor                              Hindered
 Group     13 14 15
 Axis                 12                4
 Symmetry                  3
 Potential[kcal/mol]                12
 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
 End
   Rotor                              Hindered
 Group     17
 Axis                 16                1
 Symmetry                  1
 Potential[kcal/mol]                36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]                42
  124.27   178.82   225.52   342.59   406.19   439.05   525.75   625.88
  679.88   778.53   800.70   819.49   840.98   956.17   981.43   994.32
  966.81   991.04   1014.91 1020.64 1064.60 1135.68 1161.96 1200.61
  1264.52 1309.93 1368.41 1421.12 1441.78 1449.50 1452.26 1530.50
  1575.76 2926.42 2986.45 3014.07 3061.45 3061.74 3088.31 3091.39
  3108.36 3633.75
ZeroEnergy[kcal/mol]     -0.06
 ElectronicLevels[1/cm]                          1
  0.0000000000000000             2.0000000000000000
End
!********************************************
RRHO                  !                 11
Geometry[angstrom]                17
C                         1.41414900     -0.00000400     -0.58711400
C                         0.67624700      1.21838600     -0.50352500
C                        -0.66216100      1.20905200     -0.16694300
C                        -1.35737100      0.00000500      0.01772000
C                        -0.66217100     -1.20905000     -0.16694500
C                         0.67623400     -1.21838800     -0.50351900
H                         2.36271600     -0.00001100     -1.10701300
H                         1.19882600      2.15520900     -0.65060300
H                        -1.19608500      2.14725600     -0.05977500
H                        -1.19610300     -2.14725100     -0.05977800
H                         1.19881000     -2.15521500     -0.65059400
C                        -2.80666800      0.00000500      0.42020200
H                        -2.90422200     -0.00020900      1.51097900
H                        -3.32158800      0.88633700      0.04483400
```

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H                    -3.32167700    -0.88613100     0.04448600
O                     2.39011200    -0.00000400     1.06933100
H                     1.65383600     0.00001900     1.69905400
   Core    RigidRotor
            SymmetryFactor      0.843552272
End
 Rotor                                  Hindered
 Group    13 14 15
 Axis               12              4
 Symmetry           3
 Potential[kcal/mol]            12
 0.000 -0.001 0.003 -0.001 0.000 0.000 -0.002 0.000 -0.001 0.000 0.002 -0.001
 End
   Rotor                                  Hindered
 Group    17
 Axis               16              1
 Symmetry           1
 Potential[kcal/mol]            36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]              42
  159.71   206.37   231.78   342.61   408.31   429.10   525.44   622.72
  673.39   784.08   798.47   831.70   866.03   965.77   981.29   993.73
  965.25   989.40   1016.41 1033.76 1059.42 1135.66 1160.83 1201.52
  1256.11 1310.54 1367.77 1421.14 1441.02 1446.79 1446.96 1515.72
  1567.74 2924.72 2984.89 3013.84 3061.41 3061.74 3083.75 3092.18
  3099.05 3631.79
ZeroEnergy[kcal/mol]    -0.74
 ElectronicLevels[1/cm]                 1
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO                !              12
Geometry[angstrom]             17
C                     1.43163600    -0.00000500    -0.55414400
C                     0.67605600     1.22197700    -0.49907800
C                    -0.66035600     1.21063900    -0.16871200
C                    -1.35758900     0.00000600     0.01822900
C                    -0.66036400    -1.21063400    -0.16871400
C                     0.67604600    -1.22198200    -0.49907500
H                     2.35806400    -0.00001000    -1.11673200
H                     1.19786700     2.15869100    -0.64875900
H                    -1.19661400     2.14824800    -0.06788800
```

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H                    -1.19663000    -2.14824000    -0.06789000
H                     1.19785100    -2.15870000    -0.64875100
C                    -2.80609100     0.00000500     0.41996700
H                    -2.90391000    -0.00020700     1.51101800
H                    -3.32107200     0.88653400     0.04498500
H                    -3.32116200    -0.88632800     0.04464000
O                     2.37496300    -0.00000400     1.04267300
H                     1.64955700     0.00001700     1.68447400
   Core      RigidRotor
             SymmetryFactor       0.843552272
End
 Rotor                                   Hindered
  Group      13 14 15
 Axis                12                4
 Symmetry                 3
 Potential[kcal/mol]                12
 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 -0.001 0.000 0.003 -0.001
 End
   Rotor                                   Hindered
 Group      17
 Axis                16                1
 Symmetry                 1
 Potential[kcal/mol]                36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]                42
  195.77   228.31   237.73   342.55   411.55   418.37   525.10   618.49
  666.30   781.60   794.35   817.81   900.18   966.89   979.39   962.85
  964.23   991.76   1012.87 1052.31 1069.57 1135.99 1159.35 1202.84
  1246.62 1311.01 1367.11 1420.65 1439.41 1441.78 1441.81 1499.60
  1560.39 2922.20 2982.67 3013.28 3060.73 3061.11 3065.99 3092.82
  3095.43 3631.94
ZeroEnergy[kcal/mol]     -2.45
 ElectronicLevels[1/cm]                          1
  0.0000000000000000          2.0000000000000000
End
!*****************************************
RRHO                !                13
Geometry[angstrom]                17
C                     1.45007200    -0.00000500    -0.52066600
C                     0.67527500     1.22591800    -0.49535500
C                    -0.65833600     1.21231000    -0.17055600
C                    -1.35828700     0.00000700     0.01890800
```

```
C        -0.65834300    -1.21230500    -0.17055700
C         0.67526600    -1.22592300    -0.49535200
H         2.35122700    -0.00000900    -1.12593200
H         1.19643600     2.16258200    -0.64721500
H        -1.19708500     2.14926500    -0.07607600
H        -1.19710000    -2.14925600    -0.07607900
H         1.19642000    -2.16259200    -0.64720800
C        -2.80564500     0.00000500     0.41992900
H        -2.90461200    -0.00020700     1.51127300
H        -3.32082700     0.88665100     0.57600
H        -3.32091700    -0.88644600     0.04483200
O         2.36045800    -0.00000400     1.01665000
H         1.64456200     0.00001600     1.66833000
   Core    RigidRotor
        SymmetryFactor    0.843552272
End
 Rotor                          Hindered
 Group    13 14 15
 Axis           12          4
 Symmetry            3
 Potential[kcal/mol]          12
 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
 End
   Rotor                          Hindered
 Group    17
 Axis           16          1
 Symmetry            1
 Potential[kcal/mol]          36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]          42
  222.77   241.16   246.77   342.39   409.38   416.33   525.00   613.69
  661.43   778.03   789.52   802.16   912.64   966.78   977.24   997.41
  968.66   1004.94 1011.39 1043.99 1117.54 1135.88 1159.87 1205.11
  1237.64 1310.85 1366.81 1417.61 1434.89 1434.91 1439.98 1487.63
  1558.42 2918.73 2979.59 3012.00 3046.67 3059.85 3060.93 3092.58
  3094.55 3635.66
ZeroEnergy[kcal/mol]    -5.01
 ElectronicLevels[1/cm]              1
  0.0000000000000000         2.0000000000000000
End
!********************************************
RRHO           !          14
```

```
Geometry[angstrom]                 17
C                      1.46813400     -0.00000500     -0.48732300
C                      0.67509500      1.22949500     -0.49140500
C                     -0.65650000      1.21392800     -0.17244200
C                     -1.35895700      0.00000700      0.01964900
C                     -0.65650900     -1.21392400     -0.17244300
C                      0.67508400     -1.22950000     -0.49140100
H                      2.34381400     -0.00001000     -1.13105500
H                      1.19476400      2.16667700     -0.64605100
H                     -1.19785000      2.15029300     -0.08517000
H                     -1.19786600     -2.15028500     -0.08517300
H                      1.19474800     -2.16668600     -0.64604500
C                     -2.80534000      0.00000400      0.42000900
H                     -2.90589700     -0.00020700      1.51158300
H                     -3.32075800      0.88669700      0.04530400
H                     -3.32084700     -0.88649400      0.04496100
O                      2.34588200     -0.00000400      0.99027000
H                      1.63921900      0.00001600      1.65147100
   Core      RigidRotor
             SymmetryFactor       0.843552272
End
 Rotor                                    Hindered
 Group     13 14 15
 Axis                 12                4
 Symmetry                  3
 Potential[kcal/mol]                12
 0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
 End
   Rotor                                    Hindered
 Group     17
 Axis                 16                1
 Symmetry                  1
 Potential[kcal/mol]                36
 0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
 2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
 2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
 End
    Frequencies[1/cm]                42
  240.81   241.86   272.22   342.46   405.42   423.20   525.11   609.51
  659.64   775.24   786.32   788.51   913.21   966.65   975.31   994.21
  968.53   1005.14 1035.68 1037.78 1135.32 1148.39 1179.27 1208.23
  1229.91 1309.61 1366.78 1407.27 1429.99 1431.66 1439.16 1482.03
  1560.59 2915.28 2976.52 3010.40 3031.53 3057.62 3058.65 3090.66
  3092.50 3637.82
ZeroEnergy[kcal/mol]    -8.08
```

```
  ElectronicLevels[1/cm]                    1
    0.0000000000000000          2.0000000000000000
End
!********************************************
RRHO                 !                   15
Geometry[angstrom]                 17
C                          1.48513800     -0.00000500     -0.45466000
C                          0.67596900      1.23243300     -0.48657400
C                         -0.65496800      1.21536700     -0.17440900
C                         -1.35930800      0.00000700      0.02037800
C                         -0.65497700     -1.21536200     -0.17441000
C                          0.67595900     -1.23243900     -0.48657000
H                          2.33655400     -0.00001000     -1.13210500
H                          1.19332000      2.17061000     -0.64496100
H                         -1.19899300      2.15120500     -0.09580600
H                         -1.19901000     -2.15119600     -0.09580900
H                          1.19330300     -2.17062000     -0.64495500
C                         -2.80513600      0.00000500      0.42016000
H                         -2.90747900     -0.00020700      1.51183700
H                         -3.32073500      0.88668800      0.04531700
H                         -3.32082400     -0.88648500      0.04497500
O                          2.33079800     -0.00000400      0.96311900
H                          1.63454600      0.00001500      1.63464800
    Core     RigidRotor
              SymmetryFactor      0.843552272
End
  Rotor                                        Hindered
  Group     13 14 15
  Axis                  12                  4
  Symmetry                    3
  Potential[kcal/mol]                 12
  0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
  End
     Rotor                                        Hindered
  Group     17
  Axis                  16                  1
  Symmetry                    1
  Potential[kcal/mol]                   36
  0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
  2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
  2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
  End
      Frequencies[1/cm]                  42
    254.29    256.52    296.85    343.09    409.31    431.84    525.40    606.12
    660.35    772.36    777.89    786.30    907.32    966.25    973.47    991.29
```

966.97 1003.03 1028.05 1074.89 1134.55 1151.30 1203.98 1223.60
1230.96 1307.55 1366.84 1394.01 1425.39 1431.35 1438.52 1479.80
1562.44 2912.61 2974.05 3008.87 3016.51 3054.96 3055.99 3087.37
3089.19 3640.99
ZeroEnergy[kcal/mol] -10.94
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!***
RRHO ! 16
Geometry[angstrom] 17
C 1.50088600 -0.00000500 -0.42315400
C 0.67773300 1.23484800 -0.48047500
C -0.65355500 1.21658200 -0.17654800
C -1.35926000 0.00000700 0.02102300
C -0.65356300 -1.21657700 -0.17654900
C 0.67772300 -1.23485400 -0.48047100
H 2.32929500 -0.00001000 -1.13078200
H 1.19267100 2.17397700 -0.64330300
H -1.20039500 2.15182800 -0.10805000
H -1.20041200 -2.15181800 -0.10805200
H 1.19265400 -2.17398600 -0.64329700
C -2.80494500 0.00000400 0.42030800
H -2.90900800 -0.00020700 1.51199500
H -3.32063400 0.88666000 0.04521400
H -3.32072200 -0.88645700 0.04487200
O 2.31499100 -0.00000500 0.93515000
H 1.63210800 0.00001400 1.61954100
Core RigidRotor
SymmetryFactor 0.843552272
End
Rotor Hindered
Group 13 14 15
Axis 12 4
Symmetry 3
Potential[kcal/mol] 12
0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
End
Rotor Hindered
Group 17
Axis 16 1
Symmetry 1
Potential[kcal/mol] 36
0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421

```
  2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
  End
     Frequencies[1/cm]                42
   260.81   314.54   340.87   380.46   435.91   479.11   523.81   595.57
   659.32   759.53   759.88   781.63   887.15   953.48   959.27   976.22
   964.82  1001.34 1021.20 1113.37 1133.65 1151.24 1205.85 1218.71
  1276.06 1305.11 1366.82 1382.14 1421.42 1431.61 1437.99 1478.78
  1563.16 2910.73 2972.16 2999.08 3007.56 3052.25 3053.29 3083.79
  3085.64 3644.71
 ZeroEnergy[kcal/mol]     -13.64
  ElectronicLevels[1/cm]                          1
   0.0000000000000000          2.0000000000000000
 End
 !*****************************************
 RRHO                !                17
 Geometry[angstrom]                17
 C                     1.51465000     -0.00000500     -0.39353600
 C                     0.68031800      1.23709300     -0.47227700
 C                    -0.65206800      1.21769700     -0.17908500
 C                    -1.35875100      0.00000700      0.02144200
 C                    -0.65207500     -1.21769200     -0.17908700
 C                     0.68030800     -1.23709800     -0.47227300
 H                     2.32117800     -0.00001000     -1.12805000
 H                     1.19332200      2.17685600     -0.63976100
 H                    -1.20209300      2.15216300     -0.12256000
 H                    -1.20210900     -2.15215300     -0.12256300
 H                     1.19330500     -2.17686600     -0.63975500
 C                    -2.80459000      0.00000400      0.42034500
 H                    -2.91027500     -0.00020600      1.51200100
 H                    -3.32032900      0.88663500      0.04497300
 H                    -3.32041700     -0.88643300      0.04463200
 O                     2.29863500     -0.00000500      0.90627300
 H                     1.63138100      0.00001200      1.60465000
    Core      RigidRotor
              SymmetryFactor       0.843552272
 End
  Rotor                                  Hindered
  Group     13 14 15
  Axis                12                4
  Symmetry                    3
  Potential[kcal/mol]                12
  0.000 -0.002 0.002 0.000 -0.001 0.000 -0.002 0.000 -0.001 -0.001 0.002 -0.001
  End
    Rotor                                    Hindered
  Group     17
```

```
  Axis                    16                  3
  Symmetry                 1
  Potential[kcal/mol]                 36
  0.000 0.091 0.413 0.936 1.597 2.310 2.980 3.516 3.818 3.872 3.717 3.443
  3.131 2.854 2.658 2.557 2.535 2.556 2.585 2.584 2.537 2.451 2.347 2.258
  2.211 2.217 2.269 2.339 2.380 2.331 2.151 1.831 1.394 0.904 0.452 0.131
  End
     Frequencies[1/cm]                 42
   267.76   329.58   350.49   394.80   451.23   518.12   600.34   613.96
   711.80   763.46   766.66   817.52   890.33   965.20   969.58   986.37
   962.33  1000.01 1015.09 1132.50 1146.11 1154.04 1205.81 1215.41
  1302.40 1317.94 1366.76 1372.61 1418.24 1432.11 1437.52 1478.58
  1563.69 2909.31 2970.57 2981.77 3006.34 3049.25 3050.30 3080.20
  3082.08 3652.88
ZeroEnergy[kcal/mol]    -15.68
  ElectronicLevels[1/cm]                          1
   0.0000000000000000          2.0000000000000000
End
!*******************************************
RRHO                  !                 18
Geometry[angstrom]                17
C                      1.52228100    -0.00000500    -0.37025000
C                      0.68431000     1.24013700    -0.45793400
C                     -0.65060200     1.21924600    -0.18261200
C                     -1.35731300     0.00000800     0.02028500
C                     -0.65061000    -1.21924000    -0.18261300
C                      0.68430100    -1.24014200    -0.45792900
H                      2.30828300    -0.00001000    -1.12915700
H                      1.19779200     2.17954000    -0.62754600
H                     -1.20508800     2.15237600    -0.14197300
H                     -1.20510400    -2.15236500    -0.14197600
H                      1.19777600    -2.17955000    -0.62753900
C                     -2.80333700     0.00000400     0.41956600
H                     -2.91004700    -0.00020500     1.51121300
H                     -3.31935400     0.88662700     0.04425700
H                     -3.31944100    -0.88642700     0.04391800
O                      2.28311100    -0.00000500     0.87613200
H                      1.63264900     0.00000900     1.58892000
   Core      RigidRotor
             SymmetryFactor       0.843552272
End
  Rotor                                  Hindered
  Group     13 14 15
  Axis                12                  4
  Symmetry                 3
```

```
    Potential[kcal/mol]                 12
    0.000 -0.001 0.003 0.000 0.000 0.000 -0.002 0.000 0.000 0.000 0.003 -0.001
    End
    Rotor                                       Hindered
    Group     17
    Axis                16              1
    Symmetry                1
    Potential[kcal/mol]                 36
    0.000 0.079 0.358 0.806 1.353 1.907 2.369 2.682 2.828 2.825 2.718 2.578
    2.468 2.422 2.448 2.523 2.621 2.701 2.731 2.707 2.630 2.533 2.452 2.421
    2.462 2.567 2.707 2.819 2.835 2.711 2.435 2.012 1.484 0.940 0.463 0.132
    End
       Frequencies[1/cm]                42
     266.74   333.14   358.49   397.52   459.99   515.24   597.96   636.48
     753.53   760.40   769.25   870.61   936.84   965.37   967.88   985.25
     961.14   998.93   1012.17 1131.46 1148.72 1181.49 1205.08 1215.14
     1301.06 1351.11 1366.77 1368.14 1416.68 1433.04 1437.07 1479.84
     1565.07 2908.21 2961.04 2969.09 3005.10 3045.13 3046.24 3077.59
     3079.46 3660.77
  ZeroEnergy[kcal/mol]    -16.56
   ElectronicLevels[1/cm]                          1
    0.0000000000000000          2.0000000000000000
  End
   !**********************************
          Tunneling      Eckart
        ImaginaryFrequency[1/cm]        427.07
        WellDepth[kcal/mol]             3.80
        WellDepth[kcal/mol]             17.23
  End
  End
End
```