Table S1. Rotational constants and vibrational frequencies of Reactants, Complexes, Transition States and Products Computed at the MP2/6-311G(d,p) level.

Species	I_a, I_b, I_c (GHZ)	Frequencies (cm^{-1})
Acetone	10.1, 8.5, 4.9	**79.1**, **138.9**, 376.7, 481.3, 534.4, 803.4, 889.0, 906.0, 1091.3, 1121.2, 1253.8, 1395.4, 1405.8, 1482.3, 1486.2, 1491.5, 1506.8, 1787.6, 3075.2, 3080.0, 3158.2, 3163.1, 3204.2, 3205.3
OH	0.0, 570.9, 570.9	3857.1
RC1	9.2, 2.3, 1.9	35.5, 47.5, 104.1, 162.4, 166.9, 386.5, 481.2, 487.3, 543.0, 550.1, 807.1, 896.3, 937.1, 1093.7, 1118.2, 1266.3, 1400.8, 1410.5, 1482.0, 1485.9, 1495.7, 1511.1, 1776.7, 3078.0, 3084.1, 3160.8, 3171.4, 3202.9, 3209.1, 3731.8
TS1a	9.4, 2.8, 2.3	2122.1***i***, 47.5, **143.6**, 170.6, 278.1, 338.6, 439.8, 486.9, 532.7, 737.4, 815.9, 885.5, 935.8, 979.4, 1108.2, 1129.2, 1233.2, 1275.8, 1401.4, 1451.8, 1483.1, 1495.6, 1558.6, 1789.3, 3078.6, 3124.3, 3163.1, 3206.5, 3208.8, 3779.6
TS2a	7.0, 2.8, 2.3	1745.0***i***, 53.4, 90.5, **131.8**, 139.4, 354.9, 372.6, 513.7, 523.3, 748.1, 823.1, 859.4, 895.9, 989.5, 1099.8, 1145.8, 1249.1, 1305.3, 1399.3, 1442.9, 1461.4, 1492.0, 1499.2, 2124.0, 3081.3, 3131.2, 3170.3, 3213.4, 3230.2, 3840.8
TS3a	5.2, 4.9, 4.3	853.7***i***, **170.4**, **234.9**, 250.4, 268.1, 317.4, 402.0, 503.0, 530.2, 814.6, 892.4, 908.7, 964.9, 1056.2, 1096.9, 1275.6, 1406.1, 1414.7, 1481.7, 1487.3, 1488.6, 1507.5, 1620.8, 3086.5, 3092.1, 3180.0, 3186.5, 3214.4, 3223.6, 3799.9
TS4a	5.3, 4.9, 4.5	816.8***i***, 168.6, 252.0, 282.7, 290.4, 421.2, 471.5, 542.0, 588.8, 760.6, 801.8, 840.4, 992.0, 1007.6, 1166.9, 1181.6, 1341.0, 1408.2, 1452.1, 1469.1, 1498.1, 1500.2, 1603.2, 3100.0, 3131.5, 3196.1, 3223.1, 3298.4, 3310.0, 3842.8
TS5a	9.2, 2.3, 1.9	1551.2***i***, 100.8, 143.7, 161.3, 178.1, 254.3, 302.0, 402.6, 507.9, 553.7, 911.5, 972.0, 996.2, 1074.9, 1176.7, 1234.0, 1240.0, 1381.1, 1382.4, 1399.1, 1481.5, 1488.6, 1970.6, 3080.9, 3087.2, 3186.4, 3207.2, 3267.7, 3305.8, 3855.0
IM1	5.4, 5.1, 4.8	192.2, 242.5, 261.0, 314.3, 337.6, 444.1, 458.2, 545.3, 796.6, 923.1, 952.5, 965.8, 996.3, 1119.8, 1201.6, 1260.9, 1377.3, 1396.1, 1420.8, 1494.2, 1498.2, 1513.0, 1523.7, 3086.9,

		3097.0, 3182.9, 3197.1, 3203.4, 3208.5, 3878.9
PC1a	10.2, 2.3, 1.9	56.2, 96.9, 129.5, 165.4, 186.0, 316.5, 351.8, 399.4, 539.8, 552.1, 677.7, 701.4, 835.8, 923.6, 1045.8, 1094.5, 1292.0, 1404.1, 1478.5, 1489.7, 1495.4, 1708.3, 2060.0, 3084.3, 3169.6, 3198.1, 3220.8, 3336.6, 3771.6, 3964.2
EMK	9.5, 3.6, 2.8	68.5, 108.7, **221.1**, 252.3, 400.7, 469.5, 595.5, 762.7, 782.0, 955.8, 965.8, 1019.1, 1124.8, 1139.0, 1205.2, 1296.6, 1381.5, 1406.8, 1432.7, 1471.8, 1487.8, 1499.1, 1516.3, 1520.6, 1781.4, 3066.8, 3077.9, 3090.3, 3112.4, 3161.5, 3179.2, 3187.3, 3202.2
EMK-RC1	6.3, 1.6, 1.3	28.5, 49.6, 85.3, 123.8, 146.0, 224.7, 270.5, 411.8, 473.3, 501.5, 549.1, 597.5, 762.7, 788.1, 962.7, 995.9, 1021.1, 1123.8, 1137.5, 1208.8, 1297.8, 1390.3, 1409.9, 1434.5, 1466.5, 1491.9, 1510.4, 1516.2, 1520.9, 1768.9, 3066.5, 3084.0, 3092.3, 3110.0, 3172.3, 3182.9, 3187.4, 3198.2, 3727.2
EMK-RC2	4.1, 1.9, 1.4	41.0, 74.3, 93.2, 129.1, 153.7, 232.0, 268.8, 402.6, 455.1, 475.1, 564.1, 606.1, 761.2, 789.3, 961.6, 975.6, 1025.6, 1127.7, 1140.0, 1212.9, 1297.8, 1386.6, 1413.1, 1439.7, 1470.4, 1485.1, 1499.1, 1521.4, 1532.7, 1778.0, 3066.0, 3079.2, 3092.5, 3115.9, 3163.3, 3176.1, 3204.0, 3205.9, 3752.0
TS1b	7.8, 1.7, 1.4	2101.1***i***, 38.7, 89.3, 147.8, **223.6**, 254.7, 294.6, 368.7, 436.3, 477.8, 593.9, 727.7, 762.5, 821.6, 930.5, 973.3, 1018.7, 1030.3, 1129.0, 1132.4, 1229.0, 1240.7, 1298.8, 1391.8, 1433.3, 1456.1, 1467.8, 1516.1, 1520.5, 1561.5, 1783.6, 3068.5, 3092.2, 3113.0, 3125.6, 3182.8, 3188.7, 3211.1, 3781.3
TS2b	4.4, 2.0, 1.6	1726.4***i***, 50.7, 67.8, 92.0, 136.2, **218.1**, 247.9, 357.3, 394.8, 498.5, 586.7, 749.1, 777.0, 824.0, 878.9, 952.9, 1021.4, 1023.4, 1128.1, 1151.8, 1210.5, 1290.0, 1301.6, 1393.5, 1433.0, 1450.6, 1465.6, 1479.2, 1516.2, 1520.3, 2067.8, 3070.6, 3091.4, 3127.0, 3131.9, 3181.8, 3187.7, 3229.2, 3840.2
TS3b	3.3, 2.7, 1.9	1446.4***i***, 43.2, 87.7, **136.7**, 147.0, **190.5**, 219.5, 253.3, 400.8, 466.8, 597.0, 691.1, 782.3, 852.1, 921.0, 972.5, 1005.0, 1059.1, 1131.1, 1156.5, 1213.9, 1261.0, 1385.4, 1410.3,

		1431.6, 1473.2, 1488.9, 1500.3, 1510.5, 1515.2, 1895.3, 3079.5, 3084.3, 3132.2, 3167.7, 3169.1, 3192.6, 3206.2, 3828.8
TS4b	7.7, 1.4, 1.2	1645.9***i***, 48.1, 62.4, 83.2, **113.0**, 116.8, 218.2, 357.8, 409.2, 468.9, 593.2, 740.4, 770.3, 841.6, 895.5, 961.6, 984.4, 1074.6, 1134.6, 1143.2, 1199.9, 1292.4, 1322.3, 1376.6, 1404.4, 1470.6, 1471.6, 1486.6, 1493.8, 1498.4, 1780.1, 3075.3, 3080.3, 3125.8, 3135.6, 3162.8, 3203.1, 3214.9, 3847.4
TS5b	5.2, 2.1, 1.7	1901.9***i***, 53.6, 112.2, **138.7**, 157.9, 243.6, 364.6, 402.4, 460.3, 473.6, 597.1, 704.6, 766.2, 851.7, 957.2, 971.6, 1004.4, 1038.8, 1120.0, 1148.2, 1209.2, 1264.6, 1323.4, 1388.0, 1414.5, 1456.5, 1479.6, 1484.9, 1498.9, 1510.9, 1779.4, 3064.9, 3078.9, 3111.4, 3131.3, 3162.7, 3205.8, 3214.9, 3799.6
PC1b	6.8, 1.5, 1.3	49.4, 64.6, 114.8, 149.3, 183.9, 218.0, 279.0, 315.9, 351.1, 421.9, 513.5, 608.6, 676.2, 682.0, 797.1, 824.5, 980.8, 1029.9, 1095.4, 1128.7, 1231.0, 1292.6, 1402.2, 1434.5, 1466.0, 1483.6, 1514.6, 1520.2, 1707.9, 2051.6, 3071.6, 3094.3, 3117.8, 3185.2, 3192.5, 3196.9, 3335.2, 3772.8, 3964.0
PC2b	4.2, 1.9, 1.3	24.5, 61.5, 104.6, 119.5, 142.4, 156.6, 236.2, 264.6, 293.0, 420.7, 527.6, 606.6, 619.8, 644.7, 795.8, 967.5, 986.0, 1050.4, 1058.2, 1162.0, 1230.1, 1391.0, 1418.2, 1454.1, 1483.4, 1494.7, 1514.1, 1522.9, 1709.8, 2035.5, 3056.2, 3082.7, 3125.9, 3167.8, 3207.5, 3217.9, 3228.0, 3814.0, 3963.4
PC3b	4.4, 1.8, 1.3	34.3, 70.6, 107.0, 129.5, 139.4, 155.8, 255.2, 275.2, 287.2, 408.3, 440.4, 484.6, 557.7, 605.8, 774.6, 809.0, 971.4, 1031.8, 1036.3, 1139.2, 1199.7, 1208.7, 1385.6, 1412.9, 1449.2, 1485.0, 1495.8, 1499.4, 1700.0, 1790.8, 3005.7, 3076.2, 3079.8, 3163.9, 3206.0, 3221.8, 3347.4, 3856.5, 3971.4
P1b	10.0, 3.8, 2.9	67.9, 212.4, 252.5, 261.3, 405.3, 497.6, 599.2, 623.4, 783.5, 824.6, 956.6, 1026.5, 1095.6, 1124.9, 1206.2, 1292.4, 1394.5, 1433.4, 1467.8, 1475.4, 1514.3, 1519.9, 2121.6, 3071.0, 3093.4, 3117.7, 3184.0, 3191.9, 3202.8, 3336.5

P2b	10.1, 3.6, 2.8	64.6, 77.4, 129.9, 257.1, 413.6, 513.6, 606.9, 614.2, 782.5, 959.2, 981.3, 1048.7, 1052.1, 1158.1, 1218.3, 1385.8, 1405.4, 1444.8, 1484.2, 1495.5, 1501.9, 1505.9, 2090.5, 3059.0, 3081.9, 3124.0, 3167.7, 3194.0, 3215.9, 3229.1
P3b	9.6, 3.8, 2.8	76.9, 124.0, 171.9, 269.3, 373.1, 409.1, 462.6, 594.4, 766.7, 810.8, 963.5, 1024.9, 1035.3, 1137.1, 1196.2, 1203.4, 1380.3, 1407.7, 1451.2, 1474.6, 1486.9, 1499.3, 1802.6, 3011.1, 3076.7, 3079.5, 3161.8, 3203.4, 3219.8, 3343.3
iPMKgt	4.7, 3.1, 2.1	61.3, **140.8**, **215.5**, **235.4**, 263.1, 315.8, 353.1, 434.6, 559.3, 621.5, 737.2, 920.6, 938.5, 976.3, 982.1, 1005.6, 1130.3, 1161.8, 1184.3, 1234.0, 1330.8, 1376.2, 1401.7, 1418.3, 1435.3, 1487.8, 1497.4, 1506.2, 1509.5, 1525.3, 1529.4, 1770.5, 3059.6, 3069.8, 3079.1, 3080.3, 3157.0, 3164.4, 3169.0, 3169.8, 3179.6, 3198.6
RC1c	4.2, 1.3, 1.1	29.4, 46.4, 69.2, 140.6, 146.4, 214.5, 240.7, 257.7, 314.3, 349.3, 442.4, 510.8, 556.0, 581.6, 627.3, 747.0, 920.2, 940.7, 982.5, 997.8, 1016.8, 1131.0, 1156.6, 1183.8, 1236.2, 1327.9, 1387.6, 1406.4, 1420.1, 1436.1, 1493.2, 1503.3, 1506.7, 1510.4, 1525.0, 1529.5, 1759.3, 3069.6, 3072.9, 3081.5, 3085.7, 3162.4, 3169.2, 3173.1, 3173.5, 3178.3, 3198.6, 3723.0
RC2c	2.8, 1.6, 1.2	26.5, 61.9, 91.9, 113.0, 152.1, 219.5, 243.4, 273.7, 307.7, 348.8, 436.6, 458.1, 556.7, 573.9, 629.5, 745.1, 921.7, 939.6, 979.8, 991.8, 1011.5, 1133.3, 1160.1, 1183.7, 1236.3, 1328.9, 1385.0, 1405.6, 1420.5, 1439.5, 1487.7, 1497.2, 1508.2, 1515.9, 1527.3, 1532.6, 1766.5, 3068.2, 3072.4, 3082.1, 3083.7, 3161.9, 3167.8, 3170.2, 3171.3, 3189.1, 3201.8, 3753.1
TS1c	4.5, 1.4, 1.2	2074.4***i***, 40.7, 68.7, 147.7, **212.1**, **226.7**, 248.5, 300.2, 328.4, 340.1, 418.3, 440.5, 570.0, 620.3, 723.9, 799.8, 916.0, 934.5, 948.4, 984.5, 992.3, 1045.4, 1128.9, 1165.4, 1198.9, 1240.7, 1246.5, 1327.4, 1385.0, 1418.3, 1436.0, 1458.4, 1503.6, 1508.8, 1524.1, 1528.0, 1561.4, 1782.0, 3065.5, 3071.2, 3081.9, 3126.8, 3160.6, 3168.2, 3173.2, 3180.2, 3213.1, 3781.1
TS2c	2.8, 1.8, 1.4	1764.3***i***, 39.8, 58.0, 101.4, 125.1, **213.4**, **231.5**, 269.2, 316.6, 341.0, 363.3, 443.4, 544.2, 617.9, 724.0, 800.1, 909.9, 925.6,

		940.2, 955.0, 984.9, 1015.2, 1133.2, 1168.6, 1185.9, 1234.0, 1301.5, 1335.1, 1382.6, 1416.5, 1429.2, 1435.4, 1455.9, 1504.4, 1510.3, 1524.9, 1531.0, 1923.1, 3069.6, 3080.0, 3083.4, 3126.7, 3157.3, 3168.6, 3174.5, 3181.2, 3218.3, 3834.7
TS3c	2.3, 2.0, 1.8	1006.1***i***, 38.6, 82.0, 96.8, **164.3**, 181.3**, 203.6**, **222.4**, 273.7, 318.2, 355.5, 426.9, 549.7, 591.8, 684.5, 722.9, 900.4, 945.7, 968.3, 981.70, 1019.5, 1043.0, 1152.9, 1178.8, 1210.3, 1251.2, 1344.7, 1399.1, 1415.5, 1423.1, 1437.4, 1488.1, 1497.1, 1503.3, 1506.0, 1520.1, 1529.2, 1875.4, 3066.0, 3076.5, 3081.7, 3153.3, 3162.2, 3171.0, 3179.9, 3185.1, 3203.6, 3830.5
TS4c	3.0, 1.9, 1.3	1845.9***i***, 54.5, 75.6, 151.8, **157.2**, **225.6**, 256.7, 308.0, 320.0, 385.8, 425.1, 438.5, 554.8, 622.6, 728.1, 796.0, 915.3, 945.1, 972.7, 986.0, 995.6, 1023.2, 1136.6, 1161.7, 1171.9, 1231.1, 1299.6, 1322.7, 1384.6, 1408.3, 1422.2, 1474.9, 1485.3, 1498.5, 1504.5, 1520.3, 1525.1, 1768.7, 3069.4, 3073.7, 3080.9, 3120.7, 3162.5, 3166.6, 3172.9, 3202.2, 3206.1, 3816.1
TS5c	4.3, 1.3, 1.1	1575.4***i***, 58.8, 61.3, 93.8, 117.9, **145.9**, 220.9, **245.5**, 304.8, 335.1, 402.4, 434.1, 555.5, 611.4, 734.5, 817.3, 898.4, 940.0, 957.8, 984.9, 989.8, 1045.2, 1139.4, 1165.9, 1184.3, 1236.3, 1321.5, 1332.1, 1377.1, 1401.3, 1423.9, 1467.2, 1481.7, 1487.5, 1498.5, 1521.9, 1532.1, 1768.4, 3061.4, 3074.2, 3079.9, 3126.6, 3163.3, 3166.3, 3182.8, 3199.5, 3206.7, 3842.8
TS6c	3.2, 1.8, 1.5	1925.9***i***, 49.6, 122.1, **152.3**, 165.1, 223.9, **241.6**, 276.9, 320.7, 395.9, 440.1, 518.4, 601.1, 609.6, 715.7, 798.8, 912.7, 947.4, 978.4, 986.0, 1019.0, 1031.1, 1139.9, 1162.1, 1177.4, 1217.7, 1304.4, 1333.8, 1384.4, 1410.9, 1421.9, 1474.1, 1481.8, 1497.2, 1499.2, 1515.9, 1529.4, 1772.9, 3064.7, 3075.6, 3077.3, 3118.1, 3160.3, 3164.6, 3185.2, 3202.2, 3204.7, 3769.4
TS7c	3.1, 1.8, 1.2	1614.3***i***, 38.9, 80.3, 130.4, **179.2**, 192.5, **234.2**, 243.7, 294.0, 331.6, 379.1, 438.0, 555.4, 620.6, 698.4, 768.8, 901.5, 944.4, 964.7, 979.5, 998.1, 1021.7, 1125.8, 1156.7, 1182.6, 1223.0, 1316.6, 1339.2, 1368.3, 1406.0, 1425.2, 1440.8, 1487.8,

		1494.5, 1504.4, 1512.0, 1514.4, 1771.1, 3066.2, 3080.0, 3082.0, 3106.8, 3169.7, 3172.8, 3183.5, 3186.9, 3212.9, 3842.7
PC1c	4.4, 1.2, 1.1	40.5, 49.2, 113.6, 147.8, 183.7, 208.1, 234.0, 255.7, 313.3, 322.4, 341.2, 361.1, 451.7, 609.6, 640.8, 681.6, 754.9, 799.5, 927.6, 944.5, 984.2, 1002.9, 1116.9, 1155.5, 1198.4, 1243.8, 1333.3, 1398.7, 1421.5, 1434.6, 1481.8, 1504.1, 1507.6, 1522.2, 1529.6, 1708.8, 2041.0, 3071.3, 3082.2, 3084.5, 3164.1, 3168.5, 3172.3, 3186.6, 3196.3, 3334.3, 3767.5, 3963.6
PC2c	3.2, 1.5, 1.0	18.3, 66.6, 82.1, 101.0, 143.4, 157.6, 182.5, 228.7, 281.5, 293.1, 301.3, 370.6, 451.3, 554.1, 579.1, 643.6, 701.3, 945.0, 963.1, 988.4, 1002.4, 1013.8, 1065.7, 1172.5, 1311.7, 1369.6, 1411.1, 1420.3, 1428.0, 1481.5, 1490.6, 1500.3, 1508.8, 1518.8, 1523.5, 1711.5, 1980.9, 3045.0, 3050.0, 3083.4, 3116.8, 3125.9, 3168.5, 3186.5, 3215.7, 3218.5, 3811.3, 3962.7
PC3c	2.9, 1.5, 1.1	27.2, 56.7, 103.6, 112.3, 140.2, 176.6, 228.5, 264.3, 270.1, 272.4, 315.1, 355.8, 443.4, 539.6, 565.3, 580.1, 632.4, 739.4, 925.0, 966.2, 989.5, 1008.9, 1072.5, 1124.9, 1165.7, 1211.3, 1301.0, 1387.7, 1407.4, 1415.1, 1488.5, 1494.9, 1498.5, 1517.8, 1519.8, 1702.5, 1777.5, 3059.7, 3074.0, 3082.7, 3167.2, 3170.9, 3174.6, 3201.1, 3209.4, 3336.3, 3851.6, 3969.7
PC4c	2.8, 1.7, 1.4	52.2, 84.2, 113.1, 144.3, 153.1, 181.5, 208.0, 234.5, 273.4, 281.4, 323.7, 336.0, 440.5, 538.3, 571.7, 599.0, 617.6, 763.7, 934.8, 945.7, 978.6, 1033.4, 1075.3, 1147.5, 1187.3, 1222.4, 1322.1, 1371.2, 1399.9, 1422.2, 1481.4, 1484.1, 1497.4, 1516.5, 1529.5, 1693.0, 1792.6, 3076.0, 3084.7, 3095.5, 3161.1, 3171.5, 3196.2, 3204.4, 3210.2, 3324.3, 3818.9, 3969.9
P1c	4.9, 3.0, 2.3	51.3, 203.9, 222.1, 243.2, 277.4, 302.1, 340.1, 437.6, 576.5, 603.4, 738.9, 786.4, 925.5, 942.9, 964.7, 995.6, 1115.1, 1154.3, 1186.4, 1231.8, 1332.5, 1394.0, 1419.0, 1434.1, 1473.3, 1503.8, 1507.4, 1522.3, 1528.9, 2105.2, 3070.6, 3078.8, 3082.2, 3162.7, 3166.8, 3171.3, 3185.3, 3202.1, 3335.1

P2c	4.7, 3.2, 2.0	61.5, 80.0, 94.5, 182.1, 273.9, 282.3, 359.2, 444.6, 556.2, 580.5, 692.7, 943.1, 953.3, 985.4, 992.5, 1013.5, 1066.5, 1170.4, 1312.9, 1356.2, 1403.2, 1409.4, 1425.5, 1481.3, 1486.9, 1498.7, 1503.5, 1512.6, 1515.6, 2036.8, 3040.5, 3050.0, 3082.6, 3112.3, 3123.2, 3168.2, 3181.8, 3202.3, 3214.2
P3c	4.8, 3.2, 2.1	45.3, 149.2, 151.1, 230.1, 276.8, 303.1, 343.3, 404.5, 457.5, 553.8, 627.1, 732.6, 921.6, 971.2, 974.2, 995.6, 1081.1, 1121.7, 1169.8, 1197.5, 1300.6, 1368.9, 1402.7, 1417.0, 1470.0, 1487.7, 1498.5, 1518.6, 1523.5, 1789.4, 3013.9, 3074.6, 3080.2, 3165.8, 3168.3, 3171.0, 3200.0, 3213.4, 3340.4
P4c	4.8, 3.1, 2.2	56.1, 104.3, 180.5, 235.2, 239.4, 294.4, 350.7, 421.8, 485.1, 560.6, 624.0, 745.1, 914.5, 946.5, 976.5, 1004.5, 1076.8, 1156.8, 1185.0, 1218.7, 1285.6, 1365.5, 1397.5, 1426.5, 1484.2, 1489.7, 1498.1, 1513.3, 1514.9, 1776.2, 3062.8, 3080.7, 3085.4, 3167.2, 3179.3, 3181.7, 3195.3, 3199.7, 3314.2
iPMK-g	4.5, 2.7, 2.4	57.4, 154.3, 211.8, 241.9, 277.2, 279.7, 334.1, 494.4, 530.1, 599.1, 739.2, 923.1, 944.5, 959.4, 982.9, 1028.4, 1104.6, 1153.3, 1205.3, 1278.4, 1347.5, 1362.9, 1398.8, 1412.0, 1433.7, 1482.9, 1496.9, 1507.1, 1514.5, 1526.9, 1529.8, 1769.0, 3067.7, 3068.8, 3080.5, 3104.9, 3155.5, 3158.3, 3161.4, 3164.4, 3166.3, 3201.6
iPMK-g-RC1	4.5, 1.1, 1.1	29.4, 40.2, 66.6, 136.1, 155.6, 201.9, 250.5, 258.8, 280.6, 338.4, 494.9, 512.9, 540.8, 555.7, 611.5, 743.0, 926.8, 946.7, 975.2, 984.5, 1027.9, 1103.4, 1150.2, 1205.7, 1290.7, 1353.7, 1362.6, 1404.4, 1413.9, 1435.4, 1484.4, 1505.3, 1506.2, 1514.5, 1526.5, 1530.6, 1758.3, 3070.8, 3071.6, 3085.9, 3109.7, 3160.8, 3162.4, 3164.4, 3166.2, 3173.8, 3204.5, 3724.1
iPMK-g-RC2	2.8, 1.7, 1.3	55.7, 67.7, 73.4, 161.8, 175.6, 229.5, 234.4, 281.4, 290.5, 340.3, 495.2, 502.0, 540.0, 570.6, 605.5, 745.2, 925.6, 948.5, 968.0, 986.7, 1031.2, 1110.1, 1157.7, 1207.7, 1287.7, 1344.0, 1383.6, 1403.0, 1416.4, 1439.9, 1480.9, 1496.4, 1509.8, 1515.6, 1527.8, 1533.7, 1758.2, 3070.3, 3071.5, 3082.7, 3105.8, 3158.5, 3161.4, 3164.5, 3166.9, 3176.0, 3205.7,

		3713.1
TS1d	4.2, 1.3, 1.3	2096.7***i***, 37.9, 61.5, 161.3, 203.5, 234.8, 246.5, 261.9, 290.9, 335.4, 449.7, 480.7, 534.7, 606.9, 712.9, 794.1, 922.0, 936.6, 947.1, 983.1, 996.2, 1026.2, 1143.9, 1148.3, 1206.6, 1233.6, 1294.1, 1348.3, 1361.9, 1413.6, 1435.0, 1449.9, 1504.4, 1513.0, 1525.1, 1528.1, 1554.0, 1771.0, 3069.7, 3071.4, 3108.5, 3126.8, 3159.6, 3161.8, 3163.9, 3167.4, 3211.8, 3775.5
TS2d	3.3, 1.7, 1.4	1807.8***i***, 39.2, 57.5, 116.2, 191.4, 234.1, 249.4, 272.9, 305.2, 333.8, 379.1, 488.0, 532.6, 584.2, 737.4, 816.8, 925.9, 947.2, 954.5, 969.0, 992.4, 1066.4, 1115.5, 1146.7, 1205.6, 1261.4, 1300.3, 1351.7, 1360.4, 1415.2, 1437.0, 1474.7, 1503.0, 1511.3, 1525.3, 1527.0, 1534.7, 1894.5, 3069.6, 3073.7, 3108.9, 3144.7, 3158.8, 3162.8, 3164.0, 3173.7, 3240.0, 3818.9
TS3d	2.6, 2.1, 1.6	1610.3***i***, 54.0, 88.9, 158.6, 163.0, 209.3, 228.0, 261.5, 277.9, 327.1, 436.3, 453.3, 527.5, 602.2, 636.5, 747.3, 931.4, 954.4, 968.3, 976.8, 993.1, 1043.0, 1127.8, 1153.1, 1214.9, 1255.5, 1310.6, 1398.9, 1409.3, 1429.7, 1480.4, 1493.9, 1499.3, 1500.3, 1507.1, 1520.2, 1533.6, 1766.3, 3063.0, 3064.4, 3080.8, 3150.3, 3151.8, 3165.3, 3168.3, 3175.0, 3203.9, 3779.2
TS4d	2.67, 1.8, 1.4	1605.9***i***, 47.9, 89.0, 110.9, 156.9, 214.8, 230.6, 243.7, 280.8, 315.3, 396.5, 490.6, 528.3, 597.1, 688.0, 750.9, 907.0, 939.9, 965.4, 984.8, 1017.5, 1053.2, 1113.5, 1162.9, 1216.2, 1269.5, 1322.8, 1342.2, 1370.4, 1396.3, 1414.1, 1459.3, 1482.5, 1498.1, 1506.1, 1516.2, 1518.5, 1774.9, 3068.1, 3080.4, 3109.6, 3114.5, 3158.5, 3169.8, 3170.8, 3190.9, 3203.7, 3838.4
PC1d	4.7, 1.1, 1.1	35.2, 53.6, 114.1, 156.5, 182.0, 199.9, 249.3, 256.1, 288.7, 326.5, 338.3, 364.3, 509.9, 542.9, 647.0, 685.5, 762.4, 809.0, 934.0, 948.9, 971.6, 992.6, 1108.3, 1140.5, 1207.6, 1315.7, 1352.5, 1366.1, 1415.3, 1437.4, 1485.2, 1502.5, 1513.0, 1526.2, 1528.2, 1709.4, 2033.4, 3071.3, 3072.2, 3121.2, 3161.1, 3164.7, 3165.7, 3167.6, 3201.8, 3338.3, 3764.0, 3963.4
PC2d	3.2, 1.5, 1.0	18.3, 66.6, 82.1, 101.0, 143.4, 157.6, 182.5, 228.7, 281.5,

		293.1, 301.3, 370.6, 451.3, 554.1, 579.1, 643.6, 701.3, 945.0, 963.1, 988.4, 1002.4, 1013.8, 1065.7, 1172.5, 1311.7, 1369.6, 1411.1, 1420.3, 1428.0, 1481.5, 1490.6, 1500.3, 1508.8, 1518.8, 1523.5, 1711.5, 1980.9, 3045.0, 3050.0, 3083.4, 3116.8, 3125.9, 3168.5, 3186.5, 3215.7, 3218.5, 3811.3, 3962.7
PC3d	2.8, 1.7, 1.3	43.8, 82.2, 91.6, 136.0, 157.5, 172.2, 225.8, 227.6, 273.2, 286.0, 327.6, 343.8, 462.3, 512.3, 533.9, 587.2, 609.0, 755.8, 922.1, 948.0, 967.1, 1035.0, 1070.2, 1156.4, 1195.6, 1253.4, 1307.3, 1367.9, 1399.6, 1425.6, 1470.1, 1481.7, 1496.8, 1519.8, 1525.0, 1701.1, 1774.8, 3073.8, 3082.7, 3117.3, 3163.9, 3168.2, 3170.7, 3199.3, 3204.2, 3331.9, 3805.6, 3970.0

Table S2. Predicted Morse parameters for the processes we investigated.

Complex	Scan range (Å)	De (kcal•mol^{-1})	B (Å^{-1})
RC1a	1.908•••7.908	7.60	1.04
RC1b	1.951•••7.201	8.00	1.18
RC2b	1.960•••7.960	7.48	1.21
RC1c	1.946•••7.946	7.57	1.12
RC2c	1.961•••7.961	7.44	1.21

Coordinates of the species obtained at MP2/6-311G(d,p) level:

RC1a

6	0.661482000	-0.094142000	-0.048385000
8	-0.101064000	-1.044327000	-0.136672000
6	0.158462000	1.335539000	-0.064173000
1	0.920533000	2.028840000	-0.425899000
1	-0.742489000	1.412373000	-0.674685000
1	-0.101917000	1.616704000	0.962172000
6	2.150796000	-0.290079000	0.112645000
1	2.662485000	0.084548000	-0.780168000
1	2.514863000	0.293210000	0.964139000
1	2.376186000	-1.347174000	0.251964000
8	-2.831043000	-0.106106000	0.101896000
1	-1.997235000	-0.592945000	-0.019835000

TS1a

6	0.608718000	-0.129756000	0.058282000
8	0.173633000	-1.263959000	0.160426000
6	-0.292075000	1.077900000	0.178478000
1	-0.028528000	1.895481000	-0.494758000
1	-1.421206000	0.718634000	-0.103153000
1	-0.347909000	1.422798000	1.213640000
6	2.077642000	0.148619000	-0.172844000
1	2.207321000	0.581348000	-1.170438000
1	2.443344000	0.882495000	0.551453000
1	2.646968000	-0.777906000	-0.096363000
8	-2.416767000	-0.042094000	-0.195079000
1	-1.920630000	-0.854999000	-0.006644000

TS2a

6	0.823517000	-0.136603000	0.029343000
8	1.706744000	-0.734183000	-0.538354000
6	-0.365658000	-0.864008000	0.627219000
1	-0.567370000	-0.565451000	1.657918000
1	-1.299640000	-0.493925000	-0.025855000
1	-0.295115000	-1.944077000	0.502856000
6	0.806754000	1.369740000	0.186171000
1	-0.157084000	1.759394000	-0.151133000
1	0.919578000	1.624762000	1.245378000
1	1.624623000	1.807094000	-0.385869000
8	-2.327737000	0.161477000	-0.490027000
1	-2.844729000	0.179074000	0.327363000

TS3a

6	0.170142000	0.037602000	0.231732000
8	-0.545761000	-0.082213000	1.242553000
6	0.570187000	1.415689000	-0.251866000
1	0.792538000	1.416784000	-1.319718000
1	-0.226257000	2.124461000	-0.025215000
1	1.470188000	1.709336000	0.299112000
6	1.061772000	-1.106264000	-0.203922000
1	1.253251000	-1.076863000	-1.277503000
1	2.012672000	-0.998888000	0.328272000
1	0.593895000	-2.048392000	0.077805000
8	-1.290647000	-0.329862000	-0.796360000
1	-2.017618000	0.087998000	-0.307962000

TS4a

6	0.176741000	-0.156622000	0.163313000
8	-0.192877000	-0.481568000	1.297663000

6	1.157434000	0.988308000	-0.073639000
1	0.879699000	1.845879000	0.537879000
1	2.137427000	0.623387000	0.244545000
1	1.208798000	1.260537000	-1.127834000
6	-1.443895000	0.642079000	-0.380089000
1	-1.604851000	1.466218000	0.305157000
1	-1.182673000	0.910174000	-1.399361000
1	-2.157865000	-0.168198000	-0.287277000
8	0.364287000	-1.125050000	-0.812322000
1	0.006501000	-1.927647000	-0.413347000

TS5a

6	0.925976000	-0.221806000	-0.021071000
8	1.411136000	-1.303385000	0.012644000
6	-0.879540000	-0.020054000	-0.085090000
1	-0.839378000	0.882027000	-0.682270000
1	-0.979676000	-0.984838000	-0.565074000
1	-0.836602000	0.059403000	0.999067000
6	1.637030000	1.112716000	0.036073000
1	1.521561000	1.606002000	-0.932906000
1	1.164385000	1.742682000	0.792757000
1	2.694332000	0.959933000	0.258276000
8	-2.649775000	0.191861000	-0.003744000
1	-2.916309000	-0.598149000	0.479486000

RC1b

6	-0.160019000	0.267742000	-0.066866000
8	0.303953000	-0.859372000	-0.159613000
6	0.737745000	1.488295000	-0.008461000
1	1.178964000	1.541179000	0.992416000
1	1.555548000	1.379691000	-0.724071000
1	0.190159000	2.412677000	-0.200948000
6	-1.652936000	0.504156000	0.021410000
1	-1.831887000	1.137285000	0.900659000
1	-1.930840000	1.120949000	-0.844015000
6	-2.470221000	-0.779640000	0.076119000
1	-3.538086000	-0.554033000	0.128817000
1	-2.283114000	-1.390374000	-0.809318000
1	-2.194386000	-1.373670000	0.950111000
8	3.180648000	-0.669635000	0.096969000
1	2.249409000	-0.924964000	-0.025715000

RC2b

6	-0.858410000	-0.310055000	-0.022936000
8	0.089330000	-1.028341000	-0.300522000

6	-2.263383000	-0.865580000	0.063437000
1	-2.819094000	-0.555115000	-0.828186000
1	-2.231750000	-1.954471000	0.106650000
1	-2.787186000	-0.460981000	0.934041000
6	-0.704275000	1.174834000	0.249426000
1	-1.548385000	1.695848000	-0.218392000
1	-0.840000000	1.304357000	1.332421000
6	0.632884000	1.749731000	-0.203968000
1	0.691309000	2.814428000	0.034141000
1	1.464276000	1.237252000	0.280135000
1	0.752832000	1.631567000	-1.284210000
8	2.965942000	-0.877308000	0.200075000
1	2.034926000	-0.961272000	-0.068776000

TS1b

6	0.091652000	0.097398000	0.103934000
8	-0.111817000	-1.095364000	0.258999000
6	-1.030213000	1.104966000	0.195040000
1	-0.902788000	1.977390000	-0.447955000
1	-2.048034000	0.535968000	-0.151641000
1	-1.207757000	1.398118000	1.232241000
6	1.478531000	0.649219000	-0.164014000
1	1.447041000	1.119094000	-1.156344000
1	1.654761000	1.468806000	0.544484000
6	2.572539000	-0.408292000	-0.085530000
1	3.549489000	0.032778000	-0.297851000
1	2.600382000	-0.858601000	0.909141000
1	2.382953000	-1.208020000	-0.804001000
8	-2.875689000	-0.407443000	-0.273182000
1	-2.251052000	-1.102828000	-0.011185000

TS2b

6	-0.214046000	0.653554000	0.089343000
8	-0.792363000	1.484335000	-0.573359000
6	1.214664000	0.862113000	0.548998000
1	1.846010000	0.079373000	-0.101278000
1	1.591522000	1.853648000	0.299341000
1	1.367954000	0.597108000	1.596854000
6	-0.845030000	-0.666787000	0.495701000
1	-0.131568000	-1.457552000	0.236994000
1	-0.917406000	-0.666805000	1.591939000
6	-2.207149000	-0.895007000	-0.146626000
1	-2.632993000	-1.847292000	0.179276000
1	-2.895715000	-0.090470000	0.118957000
1	-2.118116000	-0.905957000	-1.235107000

8	2.450766000	-0.994306000	-0.537390000
1	2.932451000	-1.205525000	0.274525000

TS3b

6	-0.752819000	-0.363113000	0.063734000
8	-0.836579000	-1.017088000	1.085540000
6	-1.928069000	0.375695000	-0.538034000
1	-2.166241000	-0.046632000	-1.519668000
1	-2.793487000	0.293337000	0.119904000
1	-1.654905000	1.425215000	-0.680833000
6	0.571957000	-0.195257000	-0.652895000
1	0.439016000	-0.102097000	-1.735362000
1	0.893480000	0.902355000	-0.343183000
6	1.653031000	-1.172685000	-0.240558000
1	2.609543000	-0.914007000	-0.700149000
1	1.764921000	-1.179214000	0.845069000
1	1.380627000	-2.187584000	-0.546866000
8	0.999608000	2.053881000	0.356207000
1	0.958202000	1.646440000	1.233637000

TS4b

6	1.306622000	0.103490000	-0.041533000
8	1.542668000	1.293524000	-0.140428000
6	2.406748000	-0.939154000	-0.002950000
1	2.161564000	-1.787794000	-0.647936000
1	3.352068000	-0.489084000	-0.307734000
1	2.500695000	-1.319187000	1.020120000
6	-0.118048000	-0.427200000	0.058538000
1	-0.323661000	-0.997157000	-0.856635000
1	-0.164899000	-1.153848000	0.878299000
6	-1.143229000	0.672068000	0.239456000
1	-2.208226000	0.145491000	0.253147000
1	-1.060415000	1.189623000	1.196693000
1	-1.132541000	1.392048000	-0.579001000
8	-3.323870000	-0.488459000	-0.072764000
1	-3.587527000	0.124161000	-0.772484000

TS5b

6	0.905945000	-0.165067000	0.075179000
8	0.396735000	-1.155299000	0.573125000
6	2.383109000	-0.109871000	-0.249344000
1	2.885062000	0.521020000	0.492351000
1	2.808613000	-1.113059000	-0.216344000
1	2.546048000	0.344075000	-1.231022000
6	0.105209000	1.086137000	-0.249253000

1	0.715460000	1.959503000	0.016793000
1	-0.005012000	1.115226000	-1.341550000
6	-1.252546000	1.137814000	0.419614000
1	-1.811671000	2.043248000	0.177643000
1	-1.924951000	0.247527000	-0.022717000
1	-1.208149000	0.973614000	1.496905000
8	-2.304443000	-0.895229000	-0.486765000
1	-1.594035000	-1.381011000	-0.040109000

RC1c

6	0.126699000	0.037188000	-0.256417000
8	0.721977000	-0.973363000	0.091727000
6	0.883888000	1.309322000	-0.592523000
1	1.285614000	1.735207000	0.332237000
1	1.733040000	1.059769000	-1.233143000
1	0.254449000	2.052684000	-1.084017000
6	-1.389147000	0.080313000	-0.322443000
1	-1.652394000	0.512236000	-1.298129000
6	-2.001548000	-1.308589000	-0.184969000
1	-1.742272000	-1.741946000	0.784442000
1	-3.091051000	-1.249886000	-0.263680000
1	-1.629041000	-1.982621000	-0.960330000
6	-1.899223000	1.035056000	0.771338000
1	-1.493495000	2.044730000	0.661471000
1	-2.989950000	1.100964000	0.727469000
1	-1.620185000	0.655298000	1.759759000
8	3.525977000	-0.325075000	0.379052000
1	2.637648000	-0.718668000	0.317770000

RC2c

6	0.555897000	-0.712649000	-0.215886000
8	-0.544838000	-1.243678000	-0.207484000
6	1.806703000	-1.544883000	-0.007354000
1	2.013780000	-1.600583000	1.066788000
1	1.628620000	-2.557447000	-0.372442000
1	2.677786000	-1.106387000	-0.499364000
6	0.738715000	0.787552000	-0.380758000
1	1.493829000	0.925621000	-1.167262000
6	-0.557188000	1.482633000	-0.783054000
1	-1.318350000	1.363365000	-0.009614000
1	-0.377340000	2.550804000	-0.934657000
1	-0.955920000	1.062728000	-1.710515000
6	1.309437000	1.366195000	0.925925000
1	2.275817000	0.925577000	1.186278000
1	1.446066000	2.446350000	0.823566000

1	0.611809000	1.189451000	1.751368000
8	-3.233923000	-0.353874000	0.514612000
1	-2.387384000	-0.692147000	0.175590000

TS1c

6	0.189724000	-0.087203000	0.046714000
8	0.573124000	-1.109459000	0.592801000
6	1.129726000	1.078834000	-0.161461000
1	1.228359000	1.677021000	0.746787000
1	2.233709000	0.602004000	-0.338286000
1	0.897781000	1.700946000	-1.027349000
6	-1.247570000	0.091191000	-0.415289000
1	-1.198495000	0.382789000	-1.474293000
6	-2.045911000	-1.199416000	-0.270108000
1	-2.098529000	-1.494907000	0.781027000
1	-3.063143000	-1.057680000	-0.646704000
1	-1.576076000	-2.017137000	-0.821422000
6	-1.890605000	1.250182000	0.364203000
1	-1.355314000	2.192568000	0.217623000
1	-2.923797000	1.392239000	0.035028000
1	-1.903470000	1.022189000	1.435327000
8	3.208349000	-0.184720000	-0.169241000
1	2.695005000	-0.848132000	0.319423000

TS2c

6	0.096366000	0.843728000	0.117346000
8	0.689731000	1.894353000	-0.028765000
6	-1.318526000	0.837451000	0.664504000
1	-1.358732000	0.511082000	1.706957000
1	-1.796796000	1.808058000	0.534223000
1	-1.959580000	0.003128000	0.095488000
6	0.711280000	-0.505025000	-0.227255000
1	0.091247000	-0.912583000	-1.037055000
6	2.152032000	-0.346210000	-0.699713000
1	2.775246000	0.049263000	0.107609000
1	2.555473000	-1.314395000	-1.010430000
1	2.216960000	0.350548000	-1.538042000
6	0.596819000	-1.470231000	0.962136000
1	-0.444911000	-1.687422000	1.210816000
1	1.085629000	-2.417161000	0.716295000
1	1.092800000	-1.054070000	1.846205000
8	-2.565230000	-0.809409000	-0.731464000
1	-2.681164000	-0.174282000	-1.452344000

TS3c

6	0.919931000	-0.310198000	-0.168986000
8	1.322527000	-1.075116000	-1.025808000
6	1.853646000	0.623677000	0.575622000
1	1.997236000	0.264811000	1.599852000
1	2.817624000	0.641408000	0.065813000
1	1.423351000	1.627344000	0.622459000
6	-0.559758000	-0.226988000	0.180115000
1	-0.854364000	0.847784000	-0.177301000
6	-1.400620000	-1.230889000	-0.587462000
1	-1.160630000	-2.247219000	-0.257160000
1	-2.464412000	-1.047534000	-0.413079000
1	-1.196397000	-1.179933000	-1.658722000
6	-0.832126000	-0.224978000	1.682200000
1	-0.331367000	0.602469000	2.189869000
1	-1.906171000	-0.136719000	1.866987000
1	-0.486940000	-1.165840000	2.128099000
8	-0.949526000	2.101319000	-0.773485000
1	-0.708374000	1.800064000	-1.661403000

TS4c

6	0.539358000	-0.705754000	0.105421000
8	-0.216932000	-1.340367000	0.822745000
6	1.835960000	-1.316409000	-0.390113000
1	2.653943000	-1.005588000	0.268367000
1	1.754194000	-2.403403000	-0.354851000
1	2.075256000	-0.982690000	-1.403219000
6	0.248488000	0.731405000	-0.312859000
1	0.175469000	0.721123000	-1.409724000
6	-1.056865000	1.235686000	0.268189000
1	-1.094574000	1.159599000	1.356318000
1	-1.303606000	2.245090000	-0.069076000
1	-1.952118000	0.554645000	-0.143033000
6	1.423826000	1.645563000	0.080104000
1	2.355146000	1.348765000	-0.409234000
1	1.204539000	2.677041000	-0.208931000
1	1.578322000	1.622303000	1.164009000
8	-2.677912000	-0.460605000	-0.498027000
1	-2.232415000	-1.072056000	0.107185000

TS5c

6	1.345783000	-0.306331000	-0.092474000
8	1.638474000	-1.419629000	0.306614000
6	2.412394000	0.693532000	-0.503423000
1	2.624659000	1.356785000	0.341688000
1	3.325542000	0.155062000	-0.760863000

1	2.083392000	1.313538000	-1.341668000
6	-0.105132000	0.161494000	-0.177403000
1	-0.287403000	0.429952000	-1.228260000
6	-1.054827000	-0.948243000	0.230598000
1	-0.970367000	-1.207598000	1.288363000
1	-2.160341000	-0.534406000	0.111152000
1	-0.968387000	-1.845305000	-0.384207000
6	-0.318850000	1.423011000	0.673103000
1	0.294692000	2.258512000	0.326157000
1	-1.369094000	1.718404000	0.620136000
1	-0.067496000	1.219686000	1.719778000
8	-3.263829000	0.073098000	-0.334924000
1	-3.178553000	-0.233153000	-1.248203000

TS6c

6	0.951891000	-0.415717000	0.062227000
8	0.427915000	-1.489842000	-0.189402000
6	2.454991000	-0.247492000	0.043421000
1	2.923525000	-1.113236000	-0.425444000
1	2.735213000	0.671419000	-0.479476000
1	2.808903000	-0.155824000	1.076461000
6	0.136049000	0.828590000	0.389993000
1	0.766047000	1.484846000	1.006852000
6	-0.181518000	1.558906000	-0.927657000
1	-0.838954000	0.932874000	-1.535144000
1	-0.698036000	2.499801000	-0.716387000
1	0.726777000	1.787018000	-1.493613000
6	-1.134515000	0.499230000	1.154386000
1	-0.971923000	-0.136667000	2.026780000
1	-1.704061000	1.393760000	1.417831000
1	-1.878586000	-0.116293000	0.435857000
8	-2.384512000	-0.903585000	-0.453206000
1	-1.577526000	-1.441383000	-0.507072000

TS7c

6	0.739418000	0.819230000	-0.037173000
8	1.859738000	1.180765000	0.276120000
6	-0.412284000	1.805839000	-0.110820000
1	-0.932873000	1.802683000	0.853719000
1	-0.008231000	2.805713000	-0.275807000
1	-1.136907000	1.537739000	-0.880539000
6	0.433317000	-0.645113000	-0.346357000
1	0.077574000	-0.680712000	-1.386235000
6	1.687164000	-1.508605000	-0.208096000
1	2.037197000	-1.506971000	0.827691000

```
1       1.472392000     -2.538559000     -0.507013000
1       2.494955000     -1.117625000     -0.830191000
6      -0.691670000     -1.168348000      0.545274000
1      -1.733219000     -0.734885000      0.181101000
1      -0.823958000     -2.247979000      0.440983000
1      -0.565491000     -0.905987000      1.599927000
8      -2.905461000     -0.248211000     -0.229690000
1      -3.051331000      0.308124000      0.547954000
```

Variflex input for channel 1b in EMK + OH with USTTSP:

```
!  Multiwell Test Calculation and Sample Input

*Title

& EMK + OH_TS1 (G3_MP2) E/J Resolved Test Case

*CalculationType

 AssociationP
 NeutralP
 EJResP
 HighPresP
 ChannelsD
    1

*CalculationRanges

   ! Range of temperatures

  TRangeP  ListDQ
     11
     ValuesL
500
600
700
800
900
1000
1200
1400
1600
1800
2000
```

```
 DZeroRangeP StepDQ
   10982.15, 100.0, 1

*ConvolutionRanges

 ERangeP StepDQ
  -10982.15, 150., 800

 JRangeP StepDQ
   1, 10, 25

*Complex    !PC1

!***************** Structure Input ****************

! The following lines are typical input for the molecular structure
!   input module, in this case giving input for the complex.

 NearProlateP     !Molecule type

 NElecStatesD     !Number of states
   1
  ElecStatesL     !List of electronic state degeneracies and energies
   2, 0.0

 NModesD      !Number of modes, correction factor
   39, 0.9496
  ModesL      !List of mode frequencies
49.4, 64.6, 114.8, 149.3, 183.9, 218.0, 279.0, 315.9, 351.1, 421.9,
513.5, 608.6,
676.2, 682.0, 797.1, 824.5, 980.8, 1029.9, 1095.4, 1128.7, 1231.0,
1292.6, 1402.2,
1434.5, 1466.0, 1483.6, 1514.6, 1520.2, 1707.9, 2051.6, 3071.6, 3094.3,
3117.8,
3185.2, 3192.5, 3196.9, 3335.2, 3772.8, 3964.0

SigRotD      !Rotational symmetry number for molecule
   1.0

 RotConstP
 MassD
 89.0

 RotConstD !Rotational constants (cm-1)
   0.2267, 0.0500, 0.0433
```

```
!*********************


 EVCStepD      ! step size for complex density of states
   1.0

!End of complex input
*Channel1

*Fragments

!************************************************
! Structure data for OH fragment
!************************************************

LinearP
NElecStatesD
    2
  ElecStatesL
     2, 0.0
     2, 137.
NModesD
  1, 0.9496
    ModesL
      3857.1
SigRotD
   1.0
CartesianP
NAtomsD
   2
PositionL
    1.00000      .000000      .000000      .917779
    15.9949      .000000      .000000     -.573795E-01

!************************************************
! Structure data for EMK fragment
!************************************************

NearprolateP
NElecStatesD
    1
   ElecStatesL
     1, 0.0
NModesD
```

```
  32, 0.9496
   ModesL
68.58, 108.71, 252.3, 400.7, 469.5, 595.5, 762.7, 782.0, 955.8, 965.8,
1019.1, 1124.8, 1139.0, 1205.2, 1296.6, 1381.5, 1406.8, 1432.7, 1471.8,
1487.8, 1499.1, 1516.3, 1520.6, 1781.4, 3066.8, 3077.9, 3090.3, 3112.4,
3161.5, 3179.2, 3187.3, 3202.2

HindRotorD
1

!HindTypeD !Methyl 108.71
!1
!HindParL
!5.6 153.89 3

HindTypeD ! Methyl 221.20
1
HindParL
5.6 860.38 3

SigRotD
   1.00
CartesianP
NAtomsD
    13
   PositionL
    16.0000      .214588E-01   1.30830      .422583
    12.0000      .206906E-01   .937513E-01   .505941
    12.0000     -.456053E-01  -.619781      1.84341
    1.00000      .668532     -1.44746      1.88033
    1.00000      .150492      .881401E-01   2.64933
    1.00000     -1.04777     -1.04324      1.97170
    12.0000      .740843E-01  -.797903     -.725669
    1.00000      1.02695     -1.34301     -.687838
    1.00000     -.707645     -1.56179     -.626983
    12.0000     -.612228E-01  -.227709E-01  -2.03039
    1.00000      .143733E-02  -.695476     -2.88957
    1.00000     -1.01819      .502880     -2.06673
    1.00000      .727492      .727620     -2.11105

*TransState
USTTSP
VibAdiabaticP
 StepscaleD
1.0  40  80
```

```
!StepSizeD
!2.0   10.0

 ElecAdiabaticP
  NElecStatesD
   1
   ElecStatesL
    2   0

  VRCP

  Bondrefp
  RRangeP  TotalPPSetsPQ  StepDQ
   2.3   0.2   30
NPPSetsd
1
 PPSetsL
 0 0 0 0 0 0
 MinEPathD
  -100, 2000, 2

  IntegrationParP
   MonteCarloEJD
   -5000,  5000,  2

SigRotD
   1.0
*Potential
TerminalAtom1p
CentralAtom2p
 VStretchP

!De=8.03   kcal/mol(without ZPE )

MorseD
2808.4925
1.18
1.951

! De, Beta, Re

AnisotropicP
 PowerD
  2
 onesided1P
```

```
 onesided2P
 Theta1D
  162.51
 Theta2D
  113.84

*SecondTS            !ts1_G3
  NElecStatesD
     1
    ElecStatesL
       2, 0.0

 RRHOP

 NearProlateP

 NModesD
 37, 0.9496
 ModesL
38.7, 89.33, 147.8, 254.7, 294.6, 368.7, 436.3, 477.8, 593.9,
727.7, 762.5, 821.6, 930.5, 973.3, 1018.7, 1030.3, 1129.0, 1132.4,
1229.0,
 1240.7, 1298.8, 1391.8, 1433.3, 1456.1, 1467.8, 1516.1, 1520.5, 1561.5,
1783.6,
3068.5, 3092.2, 3113.0, 3125.6, 3182.8, 3188.7, 3211.1, 3781.3

HindRotorD
1

HindTypeD ! Methyl 223.70, 2.5 kal/mol
1
HindParL
5.49 874.38 3

!HindTypeD ! Ethyl 89.33
!4
!HindParL
!0.97, 3.07, -1953.64, 1924.98

 SigRotD
 1.0

 RotConstP
 MassD
 89.0
```

```
 RotConstD
 0.2600, 0.0567, 0.0467
 EckTunD
2101.1,  2588.15, 10142.75 !G3

 TSEnergyD
734.475   !2.1*349.64

*ThirdTS    !RC1
  NElecStatesD
     1
    ElecStatesL
       2, 0.0

 RRHOP

 NearProlateP     !Molecule type

 NModesD      !Number of modes, correction factor
   39, 0.9496
  ModesL      !List of mode frequencies
28.5, 49.6, 85.3, 123.8, 146.0, 224.7, 270.5, 411.8, 473.3, 501.5,
549.1,
597.5, 762.7, 788.1, 962.7, 995.9, 1021.1, 1123.8, 1137.5, 1208.8,
1297.8,
1390.3, 1409.9, 1434.5, 1466.5, 1491.9, 1510.4, 1516.2, 1520.9, 1768.9,
3066.5, 3084.0, 3092.3, 3110.0, 3172.3, 3182.9, 3187.4, 3198.2, 3727.2

 SigRotD
    1.0

 RotConstP
 MassD
 89.0

 RotConstD !Rotational constants (cm-1)
   0.2100, 0.0533, 0.0433

 TSEnergyD
 -1853.675   !-5.3*349.64

!End of channel 1 input

*End
```

Variflex output for channel 1b in EMK + OH with USTTSP:

```
 ******************************************************
 *                                                    *
 *  VARIFLEX: VERSION 1.00; (July 16, 1999)           *
 *  S. J. Klippenstein, A. F. Wagner, R. C. Dunbar,   *
 *  D. M. Wardlaw, and S. H. Robertson                *
 *                                                    *
 ******************************************************


 EMK + OH_TS1 (G3_MP2) E/J Resolved Test Case

 ****** Calculation Type ******

 Thermal assocation rate constants will be evaluated
 for  1 channels in a radical-radical reaction
 The component rates will be evaluated at the E/J resolved level
 for the high stabilization efficiency (high P) limit

 ****** Calculation Ranges ******

 Temperatures (K)
    500.00   600.00   700.00   800.00   900.00  1000.00
   1200.00  1400.00  1600.00  1800.00  2000.00

 D0 values (cm-1)
 ranging from  10982.15 to  10982.15 in steps of    100.00

 ****** Convolution Ranges ******

 Energy values relative to separated fragments (cm-1)
 ranging from -10982.15 to 108867.85 in steps of    150.00

 The total angular momentum J will
  cover the range from    1 to   241 in steps of    10

 ****** Complex Data ******

 Electronic state degeneracies and energies (cm-1)
     2  .00000

 Corrected Vibrational frequencies (cm-1)
    46.9   61.3  109.0  141.8  174.6  207.0  264.9  300.0  333.4
400.6
```

```
   487.6  577.9  642.1  647.6  756.9  782.9  931.4  978.0 1040.2
1071.8
  1169.0 1227.5 1331.5 1362.2 1392.1 1408.8 1438.3 1443.6 1621.8 1948.2
  2916.8 2938.3 2960.7 3024.7 3031.6 3035.8 3167.1 3582.7 3764.2

 Zero point energy =   26360.    cm-1

 Rotational symmetry number is   1.00

 The complex is a near prolate top with
 rotational constants of   .2267      .5000E-01  .4330E-01 (cm-1)
 and symmetrized rotational constants of   .2267      .4665E-01 (cm-1)

 vib. step size for complex density  of states =    1.00 cm-1
 Warning in complex: The complex data is irrelevant since
 a high pressure association is being considered

 ****** Data for fragment 1 of channel   1 ******

 Electronic state degeneracies and energies (cm-1)
    2  .00000
    2  137.00

 Corrected Vibrational frequencies (cm-1)
  3662.7

 Zero point energy =   1831.4    cm-1

 Rotational symmetry number is   1.00

 Fragment1 is linear with
 a rotational constant of   18.84     (cm-1)

 ****** Data for fragment 2 of channel   1 ******

 Electronic state degeneracies and energies (cm-1)
    1  .00000

 Corrected Vibrational frequencies (cm-1)
   65.1  103.2  239.6  380.5  445.8  565.5  724.3  742.6  907.6
917.1
  967.7 1068.1 1081.6 1144.5 1231.3 1311.9 1335.9 1360.5 1397.6 1412.8
 1423.5 1439.9 1444.0 1691.6 2912.2 2922.8 2934.5 2955.5 3002.2 3019.0
 3026.7 3040.8
```

```
 Zero point energy =   23608.    cm-1

    1mode(s) will be treated as 1-dhindered rotors
For mode   1 A type   1 treatment with data =    5.600      860.4
3.000

 Rotational symmetry number is   1.00

 Fragment2 is a near prolate top with
 rotational constants of   .3164     .1207     .9195E-01 (cm-1)

 ****** Orientation tests for each fragment ******

 Fragment1 is a Linear top
 Mass(g/mol)     Ref.x(Ang)    Ref.y(Ang)     Ref.z(Ang) for fragment
1
   1.00000      .000000      .000000      .917779
   15.9949      .000000      .000000     -.573795E-01
 Moments(amu*A**2):   .894980      .894980      .000000

 Fragment2 is a prolate Asymmetric top
 Mass(g/mol)     Ref.x(Ang)    Ref.y(Ang)     Ref.z(Ang) for fragment
2
   16.0000      .214588E-01   1.30830      .422583
   12.0000      .206906E-01   .937510E-01   .505941
   12.0000     -.456053E-01  -.619781      1.84341
   1.00000      .668532     -1.44746      1.88033
   1.00000      .150492      .881398E-01   2.64933
   1.00000     -1.04777     -1.04324      1.97170
   12.0000      .740843E-01  -.797903     -.725669
   1.00000      1.02695     -1.34301     -.687838
   1.00000     -.707645     -1.56179     -.626983
   12.0000     -.612228E-01  -.227712E-01  -2.03039
   1.00000      .143732E-02  -.695476     -2.88957
   1.00000     -1.01819      .502880     -2.06673
   1.00000      .727492      .727620     -2.11105
 Moments(amu*A**2):   183.329      139.719      53.2846

 ****** Transition State Treatment Data ******

 An effective number of states calculation using
 the inverse of 1/N_inner + 1/N_outer - 1/N_max will be performed

 An adiabatic treatment of the conserved mode vibrational
 contribution to the transition state partition functions will
```

```
 be performed

 The vibrational step size for the evaluation of the
 number of states =    1.00 cm-1
 The transitional mode number of states will be evaluated
 on a grid of   80 points starting at   40.000     cm-1
and with the step size increasing with energy
 Interpolation of these values will provide the
 transitional mode numbers for the vibrational grid

 An adiabatic treatment of the electronic state contributions
 will be performed
 for all   1 electronic states in the transition state region

 For effective TS location   1
  of electronic state   1 in channel   1
 the number of states will be evaluated according to
 Variable Reaction Coordinate Flexible Transition State Theory

 ****** VRC data ******

 The pivot points are defined relative to the bonding atoms

 A direct product of the following pivot  point separations (A)

 ranging from     2.30 to     8.10 in steps of      .20
 with the following vectors of pivot point definitions

   d_1    alpha_1   beta_1    d_2    alpha_2    beta_2
      .000     .000     .000     .000     .000     .000
 will be sampled over

    2000 configurations will be sampled in the determination of each
 point along the minimum energy path.  The initial seed for the random
 number generator used in these determinations is   -100

 The phase space integrals will be  evaulated via Monte Carlo
integration with
 Monte Carlo seed = -5000 # M.C. PTS. =    5000 # per Config. =   2

 Rotational symmetry number =   1.0000

***** Potential Parameters for Effective TS Location  1
     of Electronic State  1 in Channel  1 *****
```

```
 A Morse potential is used with parameters
   De =   2808.49  Beta =    1.1800  Re =   1.95

 Using an anisotropic bonding potential

Angular exponent is  2
 Fragment 1 has a one-sided bond
 Fragment 2 has a one-sided bond
Fragment 1 bond angle is  162.510 deg
Fragment 2 bond angle is  113.840 deg

 A statistical treatment of the conserved  mode vibrational
 contribution to the transition state partition functions
 will be performed

 The default step size of   1.00 cm-1 will be used for the
 convolution of the conserved mode vibrations
 and the default step size of   50.00 cm-1 will
 be used for the generation of the transitional mode number of states

 A statistical treatment of the electronic state contributions
 will be performed
 for all   1 electronic states in the transition state region

 For effective TS location   2
  of electronic state   1 in channel   1
 the number of states will be evaluated according to
 Rigid Rotor Harmonic Oscillator assumptions for the energetics

 ****** RRHO data ******


 Corrected Vibrational frequencies (cm-1)
    36.7   84.8  140.4  241.9  279.8  350.1  414.3  453.7  564.0
691.0
   724.1  780.2  883.6  924.2  967.4  978.4 1072.1 1075.3 1167.1 1178.2
  1233.3 1321.7 1361.1 1382.7 1393.8 1439.7 1443.9 1482.8 1693.7 2913.8
  2936.4 2956.1 2968.1 3022.4 3028.0 3049.3 3590.7

 Zero point energy =   25112.    cm-1

    1mode(s) will be treated as 1-dhindered rotors
For mode   1 A type   1 treatment with data =    5.490      874.4
3.000
```

```
 Rotational symmetry number is   1.00
 The TS is a near prolate top
 rot. constants   .26000      .56700E-01  .46700E-01(cm-1)
 symm. rot. constants   .26000      .51700E-01(cm-1)
 With an Eckart tunneling correction
 for an imaginary barrier frequency of    2101.     cm-1
 and with the reactants and products located    2588.
and    .1014E+05
 cm-1 below the barrier

 Delta H_0 for channel     1 TS relative to channel 1 is   734.48     cm-1

 A statistical treatment of the conserved  mode vibrational
 contribution to the transition state partition functions
 will be performed

 The default step size of    1.00 cm-1 will be used for the
 convolution of the conserved mode vibrations
 and the default step size of   50.00 cm-1 will
 be used for the generation of the transitional mode number of states

 A statistical treatment of the electronic state contributions
 will be performed
 for all   1 electronic states in the transition state region

 For effective TS location   3
  of electronic state   1 in channel   1
 the number of states will be evaluated according to
 Rigid Rotor Harmonic Oscillator assumptions for the energetics

 ****** RRHO data ******


 Corrected Vibrational frequencies (cm-1)
    27.1   47.1   81.0  117.6  138.6  213.4  256.9  391.0  449.4
476.2
   521.4  567.4  724.3  748.4  914.2  945.7  969.6 1067.2 1080.2 1147.9
  1232.4 1320.2 1338.8 1362.2 1392.6 1416.7 1434.3 1439.8 1444.2 1679.7
  2911.9 2928.6 2936.4 2953.3 3012.4 3022.5 3026.8 3037.0 3539.3

 Zero point energy =   26157.    cm-1

 Rotational symmetry number is   1.00
 The TS is a near prolate top
 rot. constants   .21000      .53300E-01  .43300E-01(cm-1)
```

```
 symm. rot. constants   .21000      .48300E-01(cm-1)

 Delta H_0 for channel     1 TS relative to channel 1 is  -1853.7     cm-1

 ****** End of all input ******

 ***** Minimum Energy Path results for:
 effective TS location   1 of electronic state   1 in channel   1 *****
```

rmep(A)	Vmep(cm-1)	R(A)	d1(A)	Theta1	Phi1	d2(A)	Theta2	Phi2
2.300	-2471.	2.300	.000	.00	.00	.000	.00	.00
2.500	-2167.	2.500	.000	.00	.00	.000	.00	.00
2.700	-1827.	2.700	.000	.00	.00	.000	.00	.00
2.900	-1526.	2.900	.000	.00	.00	.000	.00	.00
3.100	-1249.	3.100	.000	.00	.00	.000	.00	.00
3.300	-1020.	3.300	.000	.00	.00	.000	.00	.00
3.500	-829.1	3.500	.000	.00	.00	.000	.00	.00
3.700	-661.8	3.700	.000	.00	.00	.000	.00	.00
3.900	-534.1	3.900	.000	.00	.00	.000	.00	.00
4.100	-423.8	4.100	.000	.00	.00	.000	.00	.00
4.300	-339.0	4.300	.000	.00	.00	.000	.00	.00
4.500	-268.9	4.500	.000	.00	.00	.000	.00	.00
4.700	-214.8	4.700	.000	.00	.00	.000	.00	.00
4.900	-170.3	4.900	.000	.00	.00	.000	.00	.00
5.100	-134.2	5.100	.000	.00	.00	.000	.00	.00
5.300	-106.7	5.300	.000	.00	.00	.000	.00	.00
5.500	-84.38	5.500	.000	.00	.00	.000	.00	.00
5.700	-66.18	5.700	.000	.00	.00	.000	.00	.00
5.900	-52.89	5.900	.000	.00	.00	.000	.00	.00
6.100	-41.71	6.100	.000	.00	.00	.000	.00	.00
6.300	-33.02	6.300	.000	.00	.00	.000	.00	.00
6.500	-26.04	6.500	.000	.00	.00	.000	.00	.00
6.700	-20.61	6.700	.000	.00	.00	.000	.00	.00
6.900	-16.31	6.900	.000	.00	.00	.000	.00	.00
7.100	-12.85	7.100	.000	.00	.00	.000	.00	.00
7.300	-10.11	7.300	.000	.00	.00	.000	.00	.00
7.500	-7.988	7.500	.000	.00	.00	.000	.00	.00
7.700	-6.349	7.700	.000	.00	.00	.000	.00	.00
7.900	-4.976	7.900	.000	.00	.00	.000	.00	.00
8.100	-3.962	8.100	.000	.00	.00	.000	.00	.00

```
 Note: d1, theta1, and phi1 are the spherical polar coordinates defining
 the vector from the reference point (either the center-of-mass or
 the bonding atom) to the pivot point in fragment 1.
 Similar definitions hold for fragment 2.
```

Vmep and rmep are the minimum potential and corresponding coordinate for the TS dividing surface defined by R and these pivot point vectors

rmep(A)	Vmep(cm-1)	R(A)	x1(A)	y1(A)	z1(A)	x2(A)	y2(A)	z2(A)
2.300	-2471.	2.300	.000	.000	.918	.021	1.308	.423
2.500	-2167.	2.500	.000	.000	.918	.021	1.308	.423
2.700	-1827.	2.700	.000	.000	.918	.021	1.308	.423
2.900	-1526.	2.900	.000	.000	.918	.021	1.308	.423
3.100	-1249.	3.100	.000	.000	.918	.021	1.308	.423
3.300	-1020.	3.300	.000	.000	.918	.021	1.308	.423
3.500	-829.1	3.500	.000	.000	.918	.021	1.308	.423
3.700	-661.8	3.700	.000	.000	.918	.021	1.308	.423
3.900	-534.1	3.900	.000	.000	.918	.021	1.308	.423
4.100	-423.8	4.100	.000	.000	.918	.021	1.308	.423
4.300	-339.0	4.300	.000	.000	.918	.021	1.308	.423
4.500	-268.9	4.500	.000	.000	.918	.021	1.308	.423
4.700	-214.8	4.700	.000	.000	.918	.021	1.308	.423
4.900	-170.3	4.900	.000	.000	.918	.021	1.308	.423
5.100	-134.2	5.100	.000	.000	.918	.021	1.308	.423
5.300	-106.7	5.300	.000	.000	.918	.021	1.308	.423
5.500	-84.38	5.500	.000	.000	.918	.021	1.308	.423
5.700	-66.18	5.700	.000	.000	.918	.021	1.308	.423
5.900	-52.89	5.900	.000	.000	.918	.021	1.308	.423
6.100	-41.71	6.100	.000	.000	.918	.021	1.308	.423
6.300	-33.02	6.300	.000	.000	.918	.021	1.308	.423
6.500	-26.04	6.500	.000	.000	.918	.021	1.308	.423
6.700	-20.61	6.700	.000	.000	.918	.021	1.308	.423
6.900	-16.31	6.900	.000	.000	.918	.021	1.308	.423
7.100	-12.85	7.100	.000	.000	.918	.021	1.308	.423
7.300	-10.11	7.300	.000	.000	.918	.021	1.308	.423
7.500	-7.988	7.500	.000	.000	.918	.021	1.308	.423
7.700	-6.349	7.700	.000	.000	.918	.021	1.308	.423
7.900	-4.976	7.900	.000	.000	.918	.021	1.308	.423
8.100	-3.962	8.100	.000	.000	.918	.021	1.308	.423

Note: x1, y1, and z1 are the Cartesian coordinates for the pivot point in fragment 1 in the reference Cartesian coordinate system.
Similar definitions hold for fragment 2.
Vmep and rmep are the minimum potential and corresponding coordinate for the TS dividing surface defined by R and these pivot point vectors

***** Partition function results *****

The partition functions for the complex and the fragments are evaluated relative to their respective zero-point levels. That for

```
 the TS is instead evaluated relative to the zero-point level of
 the fragments. The partition function for the fragments includes the
 contribution from relative translational motions.  Those for the
 complex and the TS do not contain any translational contributions

 Temp Q_Fragments  Q_TS   (Monte Carlo err)
  (K)    (cm-3)          (%; 0==>quadrature)
 500.  .193E+37  .147E+11   4.4
 600.  .176E+38  .123E+12   4.6
 700.  .139E+39  .100E+13   4.8
 800.  .980E+39  .767E+13   4.9
 900.  .624E+40  .544E+14   5.0
1000.  .364E+41  .358E+15   5.0
1200.  .994E+42  .123E+17   5.1
1400.  .210E+44  .325E+18   5.0
1600.  .358E+45  .672E+19   4.9
1800.  .505E+46  .113E+21   4.9
2000.  .605E+47  .157E+22   4.8

****** High pressure limit rate constants ******

 For D0 =   10982.    cm-1

 Temp  k_bi-TST  MonteCarlo error
  (K)   (cm3/s)    rel(%) [0 error==>quadrature]
 500.  .7937E-13  4.37
 600.  .8700E-13  4.59
 700.  .1047E-12  4.77
 800.  .1304E-12  4.90
 900.  .1637E-12  4.98
1000.  .2046E-12  5.03
1200.  .3107E-12  5.05
1400.  .4506E-12  5.02
1600.  .6258E-12  4.95
1800.  .8366E-12  4.87
2000.  .1083E-11  4.79
```

Variflex input for channel 1b in EMK + OH without USTTSP:

```
!  Multiwell Test Calculation and Sample Input

*Title

& EMK + OH_TS1 (G3_MP2) E/J Resolved Test Case

*CalculationType
```

```
 AssociationP
 NeutralP
 EJResP
 HighPresP
 ChannelsD
    1

*CalculationRanges

   ! Range of temperatures

  TRangeP  ListDQ
     11
     ValuesL
500
600
700
800
900
1000
1200
1400
1600
1800
2000

 DZeroRangeP StepDQ
   10982.15, 100.0, 1

*ConvolutionRanges

 ERangeP StepDQ
  -10982.15, 150., 800

 JRangeP StepDQ
   1, 10, 25

*Complex    !PC1

!***************** Structure Input ***************

! The following lines are typical input for the molecular structure
!   input module, in this case giving input for the complex.
```

```
 NearProlateP      !Molecule type

 NElecStatesD      !Number of states
   1
  ElecStatesL      !List of electronic state degeneracies and energies
   2, 0.0

 NModesD       !Number of modes, correction factor
   39, 0.9496
  ModesL       !List of mode frequencies
49.4, 64.6, 114.8, 149.3, 183.9, 218.0, 279.0, 315.9, 351.1, 421.9,
513.5, 608.6,
676.2, 682.0, 797.1, 824.5, 980.8, 1029.9, 1095.4, 1128.7, 1231.0,
1292.6, 1402.2,
1434.5, 1466.0, 1483.6, 1514.6, 1520.2, 1707.9, 2051.6, 3071.6, 3094.3,
3117.8,
3185.2, 3192.5, 3196.9, 3335.2, 3772.8, 3964.0

SigRotD       !Rotational symmetry number for molecule
   1.0

 RotConstP
 MassD
 89.0

 RotConstD !Rotational constants (cm-1)
   0.2267, 0.0500, 0.0433

!*********************


 EVCStepD       ! step size for complex density of states
   1.0

!End of complex input
*Channel1

*Fragments

!************************************************
! Structure data for OH fragment
!************************************************

LinearP
NElecStatesD
```

```
    2
  ElecStatesL
    2, 0.0
    2, 137.
NModesD
  1, 0.9496
   ModesL
     3857.1
SigRotD
   1.0
CartesianP
NAtomsD
   2
PositionL
    1.00000      .000000      .000000      .917779
    15.9949      .000000      .000000     -.573795E-01

!************************************************
! Structure data for EMK fragment
!************************************************

NearprolateP
NElecStatesD
    1
   ElecStatesL
    1, 0.0
NModesD
  32, 0.9496
   ModesL
68.58, 108.71, 252.3, 400.7, 469.5, 595.5, 762.7, 782.0, 955.8, 965.8,
1019.1, 1124.8, 1139.0, 1205.2, 1296.6, 1381.5, 1406.8, 1432.7, 1471.8,
1487.8, 1499.1, 1516.3, 1520.6, 1781.4, 3066.8, 3077.9, 3090.3, 3112.4,
3161.5, 3179.2, 3187.3, 3202.2

!FreeRotorD
!1
!FreeRotorL
!5.56

HindRotorD
1

!HindTypeD !Methyl 108.71
!1
!HindParL
```

```
!5.6 153.89 3

HindTypeD ! Methyl 221.20
1
HindParL
5.6 860.38 3

!HindTypeD ! Ethyl 68.58
!4
!HindParL
!1.183 905.63, 1664.8, -1563.27

SigRotD
   1.00
CartesianP
NAtomsD
    13
   PositionL
    16.0000      .214588E-01   1.30830      .422583
    12.0000      .206906E-01   .937513E-01   .505941
    12.0000     -.456053E-01  -.619781      1.84341
    1.00000      .668532     -1.44746      1.88033
    1.00000      .150492      .881401E-01   2.64933
    1.00000     -1.04777     -1.04324      1.97170
    12.0000      .740843E-01  -.797903     -.725669
    1.00000      1.02695     -1.34301     -.687838
    1.00000     -.707645     -1.56179     -.626983
    12.0000     -.612228E-01  -.227709E-01  -2.03039
    1.00000      .143733E-02  -.695476     -2.88957
    1.00000     -1.01819      .502880     -2.06673
    1.00000      .727492      .727620     -2.11105

*TransState           !ts1_G3
  NElecStatesD
     1
    ElecStatesL
       2, 0.0

 RRHOP

 NearProlateP

 NModesD
 37, 0.9496
 ModesL
```

```
38.7, 89.33, 147.8, 254.7, 294.6, 368.7, 436.3, 477.8, 593.9,
727.7, 762.5, 821.6, 930.5, 973.3, 1018.7, 1030.3, 1129.0, 1132.4,
1229.0,
 1240.7, 1298.8, 1391.8, 1433.3, 1456.1, 1467.8, 1516.1, 1520.5, 1561.5,
1783.6,
3068.5, 3092.2, 3113.0, 3125.6, 3182.8, 3188.7, 3211.1, 3781.3

HindRotorD
1

HindTypeD ! Methyl 223.70, 2.5 kal/mol
1
HindParL
5.49 874.38 3

!HindTypeD ! Ethyl 89.33
!4
!HindParL
!0.97, 3.07, -1953.64, 1924.98

 SigRotD
 1.0

 RotConstP
 MassD
 89.0
 RotConstD
 0.2600, 0.0567, 0.0467
 EckTunD
2101.1,  2588.15, 10142.75 !G3

 TSEnergyD
734.475   !2.1*349.64

!End of channel 1 input

*End
```

Variflex output for channel 1b in EMK + OH without USTTSP:

```
 ***************************************************
 *                                                 *
 *  VARIFLEX: VERSION 1.00; (July 16, 1999)        *
 *  S. J. Klippenstein, A. F. Wagner, R. C. Dunbar,  *
```

```
 *  D. M. Wardlaw, and S. H. Robertson              *
 *                                                  *
 ****************************************************


 EMK + OH_TS1 (G3_MP2) E/J Resolved Test Case

 ****** Calculation Type ******

 Thermal assocation rate constants will be evaluated
 for  1 channels in a radical-radical reaction
 The component rates will be evaluated at the E/J resolved level
 for the high stabilization efficiency (high P) limit

 ****** Calculation Ranges ******

 Temperatures (K)
    500.00   600.00   700.00   800.00   900.00  1000.00
   1200.00  1400.00  1600.00  1800.00  2000.00

 D0 values (cm-1)
 ranging from  10982.15 to  10982.15 in steps of    100.00

 ****** Convolution Ranges ******

 Energy values relative to separated fragments (cm-1)
 ranging from -10982.15 to 108867.85 in steps of    150.00

 The total angular momentum J will
  cover the range from    1 to   241 in steps of    10

 ****** Complex Data ******

 Electronic state degeneracies and energies (cm-1)
     2  .00000

 Corrected Vibrational frequencies (cm-1)
    46.9   61.3  109.0  141.8  174.6  207.0  264.9  300.0  333.4
400.6
   487.6  577.9  642.1  647.6  756.9  782.9  931.4  978.0 1040.2
1071.8
  1169.0 1227.5 1331.5 1362.2 1392.1 1408.8 1438.3 1443.6 1621.8 1948.2
  2916.8 2938.3 2960.7 3024.7 3031.6 3035.8 3167.1 3582.7 3764.2

 Zero point energy =   26360.    cm-1
```

```
 Rotational symmetry number is   1.00

 The complex is a near prolate top with
 rotational constants of   .2267     .5000E-01  .4330E-01 (cm-1)
 and symmetrized rotational constants of   .2267     .4665E-01 (cm-1)

 vib. step size for complex density  of states =    1.00 cm-1
 Warning in complex: The complex data is irrelevant since
 a high pressure association is being considered

 ****** Data for fragment 1 of channel   1 ******

 Electronic state degeneracies and energies (cm-1)
    2  .00000
    2  137.00

 Corrected Vibrational frequencies (cm-1)
  3662.7

 Zero point energy =   1831.4    cm-1

 Rotational symmetry number is   1.00

 Fragment1 is linear with
 a rotational constant of   18.84     (cm-1)

 ****** Data for fragment 2 of channel   1 ******

 Electronic state degeneracies and energies (cm-1)
    1  .00000

 Corrected Vibrational frequencies (cm-1)
   65.1  103.2  239.6  380.5  445.8  565.5  724.3  742.6  907.6
917.1
  967.7 1068.1 1081.6 1144.5 1231.3 1311.9 1335.9 1360.5 1397.6 1412.8
 1423.5 1439.9 1444.0 1691.6 2912.2 2922.8 2934.5 2955.5 3002.2 3019.0
 3026.7 3040.8

 Zero point energy =   23608.    cm-1

    1mode(s) will be treated as 1-dhindered rotors
For mode   1 A type   1 treatment with data =    5.600      860.4
3.000
```

```
 Rotational symmetry number is   1.00

 Fragment2 is a near prolate top with
 rotational constants of   .3164      .1207      .9195E-01 (cm-1)

 ****** Orientation tests for each fragment ******

 Fragment1 is a Linear top
 Mass(g/mol)     Ref.x(Ang)    Ref.y(Ang)     Ref.z(Ang) for fragment
1
    1.00000       .000000       .000000       .917779
    15.9949       .000000       .000000     -.573795E-01
 Moments(amu*A**2):   .894980       .894980       .000000

 Fragment2 is a prolate Asymmetric top
 Mass(g/mol)     Ref.x(Ang)    Ref.y(Ang)     Ref.z(Ang) for fragment
2
    16.0000       .214588E-01   1.30830       .422583
    12.0000       .206906E-01   .937510E-01   .505941
    12.0000      -.456053E-01  -.619781       1.84341
    1.00000       .668532      -1.44746       1.88033
    1.00000       .150492       .881398E-01   2.64933
    1.00000      -1.04777      -1.04324       1.97170
    12.0000       .740843E-01  -.797903      -.725669
    1.00000       1.02695      -1.34301      -.687838
    1.00000      -.707645      -1.56179      -.626983
    12.0000      -.612228E-01  -.227712E-01  -2.03039
    1.00000       .143732E-02  -.695476      -2.88957
    1.00000      -1.01819       .502880      -2.06673
    1.00000       .727492       .727620      -2.11105
 Moments(amu*A**2):   183.329      139.719      53.2846

 ****** Transition State Treatment Data ******

 A statistical treatment of the conserved  mode vibrational
 contribution to the transition state partition functions
 will be performed

 The default step size of    1.00 cm-1 will be used for the
 convolution of the conserved mode vibrations
 and the default step size of   50.00 cm-1 will
 be used for the generation of the transitional mode number of states

 A statistical treatment of the electronic state contributions
 will be performed
```

```
 for all   1 electronic states in the transition state region

 For effective TS location   1
  of electronic state   1 in channel   1
 the number of states will be evaluated according to
 Rigid Rotor Harmonic Oscillator assumptions for the energetics

 ****** RRHO data ******


 Corrected Vibrational frequencies (cm-1)
    36.7   84.8  140.4  241.9  279.8  350.1  414.3  453.7  564.0
691.0
   724.1  780.2  883.6  924.2  967.4  978.4 1072.1 1075.3 1167.1 1178.2
  1233.3 1321.7 1361.1 1382.7 1393.8 1439.7 1443.9 1482.8 1693.7 2913.8
  2936.4 2956.1 2968.1 3022.4 3028.0 3049.3 3590.7

 Zero point energy =   25112.    cm-1

    1mode(s) will be treated as 1-dhindered rotors
For mode   1 A type   1 treatment with data =    5.490      874.4
3.000

 Rotational symmetry number is   1.00
 The TS is a near prolate top
 rot. constants   .26000     .56700E-01  .46700E-01(cm-1)
 symm. rot. constants   .26000     .51700E-01(cm-1)
 With an Eckart tunneling correction
 for an imaginary barrier frequency of    2101.     cm-1
 and with the reactants and products located    2588.
and    .1014E+05
 cm-1 below the barrier

 Delta H_0 for channel     1 TS relative to channel 1 is   734.48     cm-1

 ****** End of all input ******

 ***** Partition function results *****

 The partition functions for the complex and the fragments are
 evaluated relative to their respective zero-point levels.  That for
 the TS is instead evaluated relative to the zero-point level of
 the fragments. The partition function for the fragments includes the
 contribution from relative translational motions.  Those for the
 complex and the TS do not contain any translational contributions
```

```
Temp Q_Fragments  Q_TS   (Monte Carlo err)
 (K)    (cm-3)           (%; 0==>quadrature)
 500.  .193E+37  .147E+11    .0
 600.  .176E+38  .123E+12    .0
 700.  .139E+39  .100E+13    .0
 800.  .980E+39  .765E+13    .0
 900.  .624E+40  .543E+14    .0
1000.  .364E+41  .356E+15    .0
1200.  .994E+42  .123E+17    .0
1400.  .210E+44  .323E+18    .0
1600.  .358E+45  .668E+19    .0
1800.  .505E+46  .112E+21    .0
2000.  .605E+47  .156E+22    .0

****** High pressure limit rate constants ******

For D0 =   10982.     cm-1

Temp  k_bi-TST  MonteCarlo error
 (K)   (cm3/s)    rel(%) [0 error==>quadrature]
 500.  .7953E-13  .000
 600.  .8694E-13  .000
 700.  .1046E-12  .000
 800.  .1302E-12  .000
 900.  .1632E-12  .000
1000.  .2039E-12  .000
1200.  .3092E-12  .000
1400.  .4480E-12  .000
1600.  .6217E-12  .000
1800.  .8305E-12  .000
2000.  .1075E-11  .000
```