Tab. A1: Rotational constants B_i and harmonic vibrational wavenumbers ω_i (scaled by 0.961) of stable species and transition states in the chemically activated decomposition of c-$C_6H_{11}O$ calculated with the G3MP2B3 method.

species	B_i / cm^{-1}	ω_i / cm^{-1}
cyclohexoxy chair equatorial	0.142, 0.077, 0.055	148.7, 217.4, 296.5, 317.4, 385.8, 404.7, 438.4, 531.4, 750.3, 760.1, 816.0, 816.9, 845.6, 870.5, 948.9, 955.6, 994.1, 1021.5, 1025.7, 1055.9, 1108.9, 1127.9, 1169.7, 1182.5, 1240.0, 1251.8, 1254.4, 1296.8, 1327.9, 1331.0, 1343.0, 1345.9, 1450.2, 1454.8, 1455.7, 1462.0, 1476.1, 2730.2, 2901.8, 2902.9, 2910.8, 2918.7, 2923.5, 2954.9, 2955.5, 2959.5, 2974.3, 2976.7
hexanal-6-yl	0.333, 0.030, 0.028	51.0, 93.2, 106.7, 112.3, 137.9, 174.7, 217.9, 346.8, 394.3, 451.2, 651.9, 677.2, 708.8, 782.4, 852.5, 875.1, 928.6, 1000.5, 1021.0, 1048.1, 1050.2, 1110.1, 1140.1, 1218.1, 1232.7, 1278.2, 1290.7, 1295.8, 1349.3, 1369.8, 1380.9, 1423.0, 1429.7, 1440.9, 1456.6, 1473.8, 1761.8, 2779.2, 2817.8, 2892.6, 2902.4, 2914.2, 2914.9, 2933.2, 2937.7, 2972.0, 3038.2, 3132.4
hexanal-3-yl	0.314, 0.029, 0.027	25.9, 43.9, 98.2, 128.1, 154.6, 221.0, 234.5, 308.5, 353.5, 399.2, 665.9, 679.7, 715.7, 832.2, 854.6, 881.8, 972.5, 1000.5, 1032.1, 1056.3, 1098.1, 1107.4, 1163.0, 1206.3, 1215.5, 1282.0, 1293.1, 1352.0, 1375.5, 1383.8, 1387.8, 1405.9, 1441.8, 1462.9, 1469.9, 1478.7, 1763.5, 2787.1, 2813.3, 2817.1, 2843.8, 2866.2, 2917.8, 2923.0, 2948.7, 2984.9, 2992.4, 3085.2
hexanal-2-yl	0.260, 0.031, 0.030	33.3, 82.5, 117.5, 142.3, 234.2, 255.8, 271.9, 376.3, 408.5, 643.6, 668.8, 720.0, 783.9, 867.2, 881.2, 935.2, 947.0, 969.1, 1020.6, 1063.3, 1075.1, 1148.7, 1204.6, 1230.7, 1271.7, 1294.9, 1306.7, 1357.0, 1362.7, 1385.6, 1408.5, 1442.7, 1458.1, 1467.8, 1470.4, 1480.8, 1531.9, 2844.0, 2887.0, 2908.3, 2914.8, 2925.4, 2935.8, 2956.9, 2987.7, 2991.1, 2993.1, 3047.6
TS c-β-C-C	0.129, 0.074, 0.052	-310.5, 120.0, 188.5, 273.6, 298.8, 326.5, 373.9, 438.1, 516.8, 602.9, 746.8, 775.3, 794.9, 832.9, 859.8, 867.5, 930.0, 968.1, 981.7, 1034.6, 1064.3, 1106.0, 1151.1, 1172.8, 1231.6, 1241.6, 1307.2, 1331.8, 1347.1, 1349.0, 1353.2, 1430.1, 1432.5, 1439.7, 1457.0, 1464.8, 1554.8, 2758.5, 2852.0, 2900.8, 2907.6, 2913.8, 2934.5, 2954.8, 2960.2, 2966.9, 3027.6, 3116.8
TS c-β-C-H	0.139, 0.078, 0.055	-813.7, 136.1, 201.5, 321.3, 384.4, 385.3, 434.3, 459.5, 483.2, 531.1, 587.0, 719.6, 727.7, 813.6, 841.8, 878.1, 885.6, 965.8, 995.7,1042.4, 1047.1, 1094.4, 1100.7, 1195.5, 1215.0, 1239.0, 1248.1, 1299.9, 1313.7, 1331.0, 1343.2, 1344.6, 1428.7, 1435.3, 1457.1, 1460.0, 1472.8, 1602.2, 2893.3, 2898.9, 2905.4, 2914.0, 2918.0, 2958.7, 2959.1, 2963.3, 2992.2, 2993.1
TS l6-1,4-H	0.208, 0.043, 0.038	-1804.9, 48.6, 96.9, 134.1, 186.5, 226.4, 325.0, 442.9, 513.5, 545.1, 667.6, 718.9, 779.2, 836.7, 851.5, 866.5, 888.7, 930.2, 968.9, 984.3, 1022.8, 1092.9, 1114.1, 1177.2, 1181.0, 1222.1, 1263.9, 1289.1, 1300.0, 1343.4, 1372.2, 1383.3, 1416.3, 1423.8, 1457.4, 1470.3, 1576.0, 1759.3, 2770.0, 2888.9, 2914.0, 2916.4, 2928.6, 2962.1, 2975.8, 2985.0, 2989.5, 3065.2
TS l6-1,5-H	0.145, 0.053, 0.046	-1360.9, 71.3, 111.7, 227.4, 235.6, 286.2, 396.5, 447.4, 450.2, 565.4, 671.4, 768.5, 790.5, 823.6, 846.5, 895.4, 924.8, 942.8, 995.5, 1024.5, 1046.0, 1062.8, 1116.8, 1159.6, 1196.7, 1236.3, 1289.8, 1316.5, 1332.8, 1342.3, 1358.6, 1380.1, 1424.2, 1435.8, 1447.6, 1456.9, 1466.4, 1696.3, 2794.6, 2886.2, 2911.4, 2922.3, 2949.2, 2963.4, 2972.3, 2982.9, 2993.7, 3076.7
TS l6-β-C-H	0.168, 0.042, 0.037	-496.2, 56.9, 73.9, 113.4, 140.2, 217.7, 237.5, 317.9, 363.6, 384.5, 421.1, 607.3, 641.0, 686.2, 777.7, 830.3, 886.0, 893.8, 931.9, 943.4, 995.6, 1030.6, 1052.7, 1108.4, 1180.4, 1216.0, 1263.1, 1282.0, 1285.1, 1340.9, 1349.7, 1382.5, 1411.8, 1417.1, 1451.7, 1469.0, 1601.5, 1760.5, 2783.6, 2897.7, 2921.0, 2921.4, 2932.5, 2974.3, 2992.4, 3025.3, 3038.7, 3119.0
TS l6-β-C-C	0.172, 0.032, 0.029	-350.5, 40.0, 57.8, 78.9, 86.4, 165.6, 198.6, 250.7, 333.9, 368.3, 516.6, 649.5, 666.6, 737.3, 763.0, 793.8, 822.4, 856.3, 912.0, 916.9, 981.2, 1010.5, 1045.5, 1115.3, 1200.5, 1213.5, 1245.4, 1268.8, 1278.0, 1335.0, 1377.6, 1418.5, 1430.0, 1439.4, 1454.2, 1547.0, 1760.4, 2774.9, 2900.3, 2923.6, 2934.4, 2973.7, 3007.7, 3032.2, 3041.5, 3093.4, 3102.0, 3126.0
TS l3-β-C-C(1)	0.123, 0.043, 0.035	-365.4, 16.4, 44.8, 85.6, 141.4, 146.3, 171.9, 204.5, 278.7, 384.7, 524.3, 602.2, 670.0, 744.6, 765.0, 795.0, 819.8, 864.1, 910.3, 963.7, 980.6, 994.7, 1033.6, 1115.5, 1177.1, 1205.5, 1254.8, 1281.5, 1375.1, 1376.5, 1392.7, 1423.3, 1440.8, 1455.3, 1459.5, 1549.6, 1760.5, 2772.0, 2867.9, 2879.0, 2917.6, 2939.5, 2977.1, 3030.7, 3031.7, 3050.2, 3113.4, 3120.1
TS l3-β-C-C(2)	0.116, 0.048, 0.037	-362.2, 48.3, 56.8, 99.2, 106.8, 189.4, 233.6, 275.0, 281.5, 394.8, 419.7, 623.7, 685.6, 725.9, 847.1, 856.7, 906.1, 920.7, 965.8, 1002.9, 1015.5, 1074.0, 1125.5, 1161.7, 1230.2, 1255.5, 1263.3, 1292.4, 1344.9, 1383.0, 1409.7, 1444.6, 1462.4, 1469.1, 1477.5, 1554.2, 1775.1, 2669.8, 2881.7, 2915.6, 2924.0, 2946.0, 2962.2, 2989.0, 2993.2, 3021.2, 3037.1, 3115.7
TS l2-β-C-C	0.181, 0.029, 0.027	-152.8, 31.9, 39.4, 60.6, 82.1, 141.8, 243.8, 276.5, 295.3, 363.1, 412.1, 592.7, 669.8, 693.4, 728.7, 870.8, 874.4, 916.0, 923.8, 960.1, 984.3, 992.9, 1039.8, 1068.1, 1170.6, 1255.7, 1275.0, 1293.6, 1372.0, 1381.1, 1395.1, 1439.4, 1456.4, 1466.1, 1476.8, 1543.2, 1702.6, 2805.7, 2911.9, 2927.9, 2947.1, 2993.8, 3002.9, 3034.7, 3053.1, 3063.7, 3127.8, 3147.1

Tab. 2: Rotational constants B_i and harmonic vibrational wavenumbers ω_i (scaled by 0.961) of stable species and transition states in the chemically activated decomposition of c-$C_8H_{15}O$ calculated with the G3MP2B3 method.

species	B_i / cm^{-1}	ω_i / cm^{-1}
cyclooctoxy boat-chair	0.060, 0.057, 0.041	107.6, 148.8, 194.6, 213.5, 237.2, 308.9, 340.7, 351.3, 404.3, 455.7, 496.0, 592.8, 676.5, 729.0, 763.8, 772.5, 831.4, 839.3, 871.5, 911.8, 923.7, 974.4, 989.3, 1010.8, 1024.4, 1051.1, 1065.2, 1090.8, 1116.7, 1134.9, 1163.6, 1170.7, 1220.7, 1246.3, 1250.3, 1267.8, 1285.3, 1324.7, 1337.0, 1344.5, 1348.2, 1356.5, 1362.5, 1370.6, 1443.8, 1447.0, 1454.6, 1456.8, 1459.9, 1471.8, 1475.3, 2728.4, 2901.7, 2905.4, 2908.3, 2913.2, 2917.6, 2921.5, 2928.7, 2932.7, 2940.8, 2949.9, 2951.8, 2954.9, 2965.4, 2970.2
octanal-8-yl	0.254, 0.013, 0.013	34.9, 56.5, 66.7, 89.3, 113.7, 128.2, 150.0, 153.9, 174.6, 240.3, 293.0, 400.8, 435.6, 465.4, 648.9, 677.2, 703.2, 718.9, 777.6, 849.0, 863.0, 892.0, 959.0, 982.7, 999.6, 1024.8, 1030.6, 1048.9, 1060.1, 1115.1, 1129.9, 1199.1, 1208.7, 1245.9, 1257.2, 1276.5, 1291.4, 1292.6, 1306.9, 1345.7, 1364.8, 1370.3, 1379.8, 1421.0, 1428.2, 1438.9, 1453.9, 1455.1, 1466.3, 1479.1, 1759.8, 2775.5, 2811.6, 2888.5, 2892.6, 2896.2, 2903.0, 2911.0, 2911.3, 2913.5, 2928.0, 2930.8, 2949.9, 2969.2, 3034.8, 3128.5
octanal-5-yl	0.225, 0.013, 0.013	26.8, 42.9, 64.3, 79.2, 106.0, 127.6, 160.3, 175.6, 232.1, 242.9, 287.0, 397.4, 408.9, 452.5, 651.4, 676.9, 713.2, 737.9, 834.7, 863.4, 870.1, 887.5, 976.8, 1005.1, 1019.6, 1022.4, 1041.2, 1068.5, 1101.6, 1113.3, 1144.7, 1201.1, 1215.4, 1244.7, 1256.8, 1281.7, 1284.0, 1307.8, 1348.5, 1366.5, 1381.4, 1383.3, 1388.1, 1423.0, 1437.1, 1447.2, 1462.9, 1465.6, 1469.1, 1478.8, 1761.7, 2778.7, 2800.0, 2805.4, 2884.7, 2890.2,

		2892.7, 2914.3, 2915.5, 2922.9, 2939.5, 2947.0, 2977.6, 2984.9, 2991.3, 3030.8
octanal-4-yl	0.255, 0.013, 0.013	24.8, 37.2, 57.4, 90.5, 118.5, 127.3, 152.5, 171.2, 235.4, 239.4, 298.8, 403.4, 415.7, 452.0, 646.0, 676.1, 710.5, 758.6, 820.0, 862.5, 872.1, 897.7, 973.4, 993.0, 1014.2, 1024.3, 1035.4, 1074.9, 1102.4, 1111.7, 1155.1, 1200.2, 1202.3, 1253.6, 1259.5, 1271.3, 1292.0, 1306.8, 1347.6, 1367.1, 1380.2, 1383.6, 1389.2, 1421.7, 1436.9, 1446.4, 1458.2, 1468.2, 1469.5, 1481.3, 1760.8, 2780.1, 2808.5, 2843.1, 2893.7, 2898.3, 2902.1, 2910.8, 2920.8, 2923.1, 2926.9, 2936.0, 2949.7, 2985.1, 2990.0, 3024.6
TS c-β-C-C	0.060, 0.053, 0.037	-384.7, 85.4, 156.1, 193.4, 202.8, 225.3, 257.4, 303.7, 349.7, 372.5, 427.4, 460.9, 611.6, 667.6, 703.0, 740.1, 750.8, 810.6, 822.9, 830.1, 889.6, 926.4, 945.0, 964.2, 996.7, 1021.3, 1046.9, 1056.2, 1088.6, 1101.3, 1152.9, 1174.9, 1203.8, 1242.2, 1247.7, 1279.8, 1322.9, 1328.0, 1332.1, 1349.2, 1354.3, 1363.3, 1371.0, 1423.2, 1435.9, 1447.5, 1452.4, 1460.9, 1469.3, 1475.7, 1503.5, 2784.5, 2847.0, 2890.0, 2902.7, 2907.6, 2921.8, 2926.3, 2928.3, 2943.3, 2948.3, 2951.7, 2971.3, 2993.8, 3008.4, 3098.5
TS c-β-C-H	0.061, 0.055, 0.039	-953.2, 90.0, 141.7, 196.8, 222.1, 240.2, 307.3, 341.7, 368.2, 429.3, 474.4, 488.1, 490.8, 554.6, 631.0, 685.3, 725.7, 772.8, 792.3, 832.7, 845.6, 892.6, 909.7, 943.9, 979.4, 1010.2, 1038.0, 1071.0, 1075.7, 1089.1, 1148.8, 1178.4, 1182.5, 1224.2, 1244.4, 1252.0, 1274.9, 1317.6, 1320.4, 1330.1, 1347.5, 1350.6, 1359.5, 1368.9, 1438.5, 1445.9, 1454.9, 1456.0, 1459.8, 1473.3, 1478.0, 1580.4, 2904.7, 2911.3, 2920.9, 2923.7, 2927.7, 2931.4, 2938.3, 2942.2, 2950.4, 2956.4, 2966.3, 2974.7, 2984.7, 2988.6
TS l8-1,4-H	0.139, 0.017, 0.016	-1789.8, 37.9, 59.5, 81.3, 109.0, 142.9, 174.2, 183.5, 228.9, 302.1, 382.9, 477.8, 522.3, 552.3, 650.2, 678.0, 737.8, 793.0, 833.4, 856.8, 862.7, 869.5, 906.3, 936.8, 976.7, 997.1, 1007.4, 1024.5, 1061.9, 1077.4, 1120.4, 1156.5, 1176.1, 1199.3, 1223.9, 1251.7, 1268.7, 1284.2, 1294.4, 1310.7, 1346.1, 1365.0, 1379.7, 1383.3, 1421.2, 1423.0, 1446.2, 1455.4, 1465.4, 1468.8, 1578.8, 1759.9, 2775.6, 2846.1, 2889.2, 2903.9, 2911.0, 2911.7, 2922.8, 2934.4, 2944.1, 2955.5, 2964.9, 2972.3, 2983.0, 3062.9
TS l8-1,5-H	0.119, 0.020, 0.019	-1638.2, 38.3, 61.8, 86.1, 126.7, 161.2, 171.2, 245.7, 292.2, 347.4, 415.5, 433.3, 472.8, 563.7, 650.1, 677.8, 777.7, 790.5, 821.5, 825.5, 863.6, 869.5, 918.7, 945.8, 976.4, 1015.7, 1032.0, 1036.6, 1061.8, 1071.9, 1120.6, 1154.3, 1181.1, 1197.4, 1238.0, 1243.4, 1271.7, 1297.3, 1318.0, 1330.8, 1341.0, 1360.0, 1379.7, 1395.3, 1420.6, 1422.2, 1446.1, 1450.3, 1455.0, 1464.0, 1472.9, 1759.2, 2776.0, 2883.3, 2886.9, 2888.6, 2894.2, 2904.4, 2917.1, 2920.2, 2933.1, 2937.7, 2950.9, 2957.7, 2971.4, 3045.4
TS l8-β-C-H	0.196, 0.014, 0.013	-502.4, 35.2, 50.0, 67.3, 89.0, 119.2, 135.2, 172.9, 173.9, 230.1, 322.1, 343.6, 381.8, 418.6, 433.0, 626.4, 649.6, 677.9, 712.5, 758.4, 851.8, 864.2, 881.3, 902.1, 941.8, 984.1, 992.9, 1001.2, 1022.6, 1028.5, 1062.7, 1125.9, 1168.3, 1205.3, 1223.4, 1259.9, 1266.6, 1275.3, 1290.5, 1294.3, 1320.6, 1356.1, 1370.2, 1381.1, 1412.9, 1422.7, 1454.8, 1455.7, 1465.6, 1479.7, 1600.9, 1761.7, 2780.0, 2892.2, 2897.2, 2908.9, 2914.7, 2920.3, 2922.5, 2934.8, 2942.2, 2963.6, 2974.0, 3027.7, 3036.5, 3117.1
TS l8-β-C-C	0.137, 0.014, 0.013	-346.7, 30.4, 40.5, 55.2, 66.6, 107.6, 128.9, 133.5, 172.9, 204.5, 244.2, 345.6, 383.9, 396.5, 515.0, 649.4, 677.2, 712.3, 744.3, 766.5, 793.6, 821.2, 861.5, 869.6, 911.2, 965.2, 969.5, 983.5, 1010.6, 1030.9, 1060.1, 1124.4, 1189.9, 1200.9, 1211.2, 1250.8, 1265.9, 1284.5, 1286.9, 1290.6, 1336.1, 1362.8, 1380.8, 1422.3, 1430.2, 1438.3, 1454.0, 1457.8, 1475.4, 1546.7, 1761.7, 2778.3, 2892.6, 2900.8, 2907.7, 2914.6, 2927.1, 2934.1, 2947.2, 2973.4, 3006.8, 3032.1, 3041.4, 3092.1, 3101.6, 3125.6
TS l5-β-C-C (1)	0.084, 0.017, 0.015	-372.4, 23.4, 32.5, 51.7, 91.4, 106.5, 122.9, 149.0, 159.8, 175.1, 234.0, 286.8, 363.2, 417.4, 516.2, 647.4, 652.8, 690.7, 743.4, 749.4, 800.3, 851.6, 866.7, 885.4, 905.5, 954.0, 993.5, 999.8, 1009.6, 1032.9, 1043.9, 1123.7, 1173.8, 1180.9, 1226.1, 1248.0, 1256.9, 1285.1, 1311.8, 1357.7, 1373.7, 1381.1, 1405.1, 1422.4, 1438.5, 1448.1, 1455.0, 1458.6, 1466.7, 1547.0, 1761.8, 2778.6, 2869.4, 2875.7, 2892.4, 2914.2, 2930.0, 2940.9, 2941.3, 2978.0, 2979.8, 3020.5, 3023.4, 3029.3, 3106.2, 3110.7
TS l5-β-C-C (2)	0.088, 0.016, 0.014	-337.6, 26.3, 28.2, 45.3, 76.4, 91.8, 124.1, 150.5, 191.5, 230.7, 236.6, 281.9, 383.9, 415.0, 494.6, 643.8, 664.8, 671.4, 724.8, 766.8, 827.2, 845.7, 852.9, 872.2, 895.6, 915.2, 960.0, 1003.0, 1014.3, 1048.9, 1072.2, 1104.5, 1161.3, 1229.4, 1243.1, 1251.2, 1263.3, 1270.7, 1289.2, 1344.0, 1374.1, 1381.1, 1405.2, 1413.7, 1440.4, 1448.9, 1462.7, 1468.7, 1478.4, 1548.9, 1763.1, 2762.8, 2879.6, 2883.9, 2911.5, 2916.7, 2922.8, 2932.8, 2953.4, 2986.5, 2991.9, 3018.5, 3028.7, 3036.3, 3107.2, 3122.0
TS l4-β-C-C (1)	0.101, 0.015, 0.014	-343.9, 28.4, 42.0, 48.0, 60.8, 105.6, 120.0, 159.1, 165.5, 247.5, 253.2, 331.0, 354.8, 408.3, 513.1, 648.5, 660.7, 668.1, 728.6, 755.1, 830.4, 866.7, 870.3, 883.6, 888.7, 912.6, 961.6, 991.2, 1000.4, 1026.2, 1072.7, 1120.9, 1176.2, 1185.0, 1245.9, 1250.2, 1271.7, 1279.9, 1302.4, 1340.8, 1373.2, 1378.5, 1406.0, 1419.1, 1438.6, 1448.3, 1455.3, 1467.0, 1476.3, 1548.1, 1760.6, 2778.2, 2900.1, 2906.6, 2913.9, 2922.6, 2927.8, 2938.7, 2969.3, 2986.5, 2995.7, 3010.4, 3017.9, 3032.0, 3094.2, 3112.6
TS l4-β-C-C (2)	0.113, 0.016, 0.014	-406.4, 31.3, 33.8, 55.7, 89.0, 103.7, 130.7, 152.6, 220.5, 241.6, 262.9, 339.6, 365.2, 450.1, 485.4, 668.3, 711.6, 731.0, 773.9, 812.7, 871.2, 889.7, 905.1, 914.8, 959.7, 960.7, 976.3, 987.8, 1020.6, 1026.7, 1083.6, 1125.7, 1162.1, 1209.9, 1236.3, 1243.9, 1275.7, 1294.0, 1313.7, 1358.7, 1367.9, 1386.3, 1405.0, 1433.6, 1446.1, 1457.0, 1467.9, 1470.7, 1480.6, 1529.9, 1620.6, 2795.0, 2881.8, 2904.7, 2912.3, 2925.1, 2927.2, 2938.6, 2956.7, 2987.6, 2992.9, 3026.1, 3032.0, 3043.5, 3118.6, 3142.1

Tab. A3: Reduced moments of inertias $I_{red,i}$, Fourier coefficients a_i, $b_{i,k}$, $c_{i,l}$ for the representation of the 1-D hindrance potentials $V_i(\varphi)^a$ and 1-D harmonic wavenumbers ω^*_i for the 1-D HIRs in the ring-opening product and its transition states in the c-$C_6H_{11}O$ decomposition. The internal rotations are labelled successively starting with the C-C bond adjacent to the O atom. The Fourier coefficients are arranged in ascending order of k and l, with $k_{min} = l_{min} = 1$, respectively.

species	C-C bond i	$I_{red,i}$ / 10^{47} kg m^2	Fourier coefficients			ω^*_i / cm^{-1}
			a_i / cm^{-1}	$b_{i,k}$ / cm^{-1}	$c_{i,l}$ / cm^{-1}	
hexanal-6-yl	1	26.4	453.34	-113.20 -104.47 -201.60 -23.60 12.06 3.08 -1.49	-6.45 0.89	79.6
	2	119.0	706.67	-613.79 422.90 -554.81 28.02 14.04 5.75 -8.78	-12.17 10.89 -5.50	39.6
	3	56.6	788.11	-401.76 178.52 -585.30 18.08 -10.09 15.65 -3.21	-6.43 6.11 -4.41 -0.71 1.00 -0.69	66.8
	4	49.5	706.58	-300.82 185.43 -622.28 5.34 21.09 8.02 -3.37	8.93 -24.65 21.79 -28.26 6.44 -1.85	70.8
	5	2.9	28.22	-2.58 -6.11 -0.96 -3.64 -1.36 -14.26 0.70	1.10 10.56 -4.21 -4.75 -0.88 2.57 -0.68	108.3
TS l6-1,4-H	1	26.5	304.2	-66.6 60.2 -236.6 -60.7 -13.0 11.2 1.4	61.1 -22.8 -4.8 -4.3 5.5 0.9 -0.7	76.7
	2	100.2	525.1	-7.1 -159.2 -403.3 49.6 -5.0	-381.4 -169.5 183.3 51.0 -14.6 4.6 -1.2	44.7
TS l6-1,5-H	1	26.5	1422.4	-149.0 -1222.3 -95.8 15.8 26.0 6.2 -3.2	-23.8 254.5 -120.6 -58.8 9.7 8.0 1.9	98.9
TS l6-β-C-C	1	27.1	421.8	-131.5 -63.0 -189.0 -26.3 -14.8 2.8	12.4 -2.9 -0.8 -0.1 0 0 0	75.78

	2	80.5	701.9	-524.7 339.1 -557.8 22.2 28.2 -9.0	38.5 -11.5 -3.3 -4.5 4.3 -2.3 1.4	48.99
	3	87.8	463.6	-293.7 170.9 -339.0 -25.9 9.0 19.3 -4.2	-7.1 67.4 -55.6 -5.5 13.8 3.8 -7.3	38.89
	4	47.0	130.3	-14.9 -4.4 -106.5 -8.0 1.0 1.7 0.9	-23.1 10.1 14.4 -9.3 -2.2 -0.3 0.9	34.37
TS l6-β-C-H	1	27.1	587.8	-191.0 -176.3 -177.6 -38.3 -11.4 6.2 0.6	112.2 -104.9 24.6 -0.6 7.8 0.4 -0.3	80.52
	2	101.1	672.9	-580.6 427.8 -558.4 29.9 14.2 3.6 -9.5	16.0 -49.7 51.5 -6.9 -1.4 -1.2 3.9	43.47
	3	129.4	783.8	-218.5 -56.7 -570.0 56.7 10.1 4.8 -10.1	94.3 76.5 -123.5 -26.5 39.6 10.4 1.3	45.39
	4	37.5	439.2	-112.3 -41.3 -303.5 -14.1 17.6 16.8 -2.4	-150.9 13.2 22.3 12.9 7.8 -3.5 -0.7	58.69

a:
$$V_i(\varphi_i) = a_i + \sum_k b_{i,k}\cos(k\varphi_i) + \sum_l c_{i,l}\sin(l\varphi_i)$$

Tab. A4: Reduced moments of inertias $I_{red,i}$, Fourier coefficients a_i, $b_{i,k}$, $c_{i,l}$ for the representation of the 1-D hindrance potentials $V_i(\varphi)^a$ and 1-D harmonic wavenumbers ω^*_i for the 1-D HIRs in the ring-opening product and its transition states in the c-$C_8H_{15}O$ decomposition. The internal rotations are labelled successively starting with the C-C bond adjacent to the O atom. The Fourier coefficients are arranged in ascending order of k and l, with $k_{min} = l_{min} = 1$, respectively.

species	C-C bond i	$I_{red,i}$ / 10^{47} kg m^2	Fourier coefficients			ω^*_i / cm^{-1}
			a_i / cm^{-1}	$b_{i,k}$ / cm^{-1}	$c_{i,l}$ / cm^{-1}	
octanal-8-yl	1	27.4	441.3	-108.1 -98.9 -201.5 -23.5 -11.9 3.7 -0.9	4.1 -0.1 1.0 0.5 0 0 0.2	77.0
	2	158.1	698.2	-606.7 426.5 -557.6 29.0 14.8 5.4 -9.5	5.7 -3.2 5.7 -2.6 0 0 -0.9	34.5
	3	97.5	787.5	-386.5 168.4 -587.9 17.8 -9.4 15.0 -5.0	1.70 1.1 1.6 0 -0.6 -1.6 -0.9	51.7
	4	160.4	768.9	-391.8 174.8 -578.7 24.7 -15.3 19.7 -2.2	5.0 -2.6 3.5 -1.2	38.7
	5	141.0	775.2	-407.9 180.2 -570.9 24.4 -16.0 19.5 -4.5	2.6 -5.5 -3.0 3.6 -2.7 2.0 0.8	41.6
	6	41.4	694.6	-294.9 198.0 -618.6 0 13.1 6.0 1.9	-2.1 9.0 -41.2 -4.4 17.6 0 5.2	77.4
	7	2.9	27.2	-3.3 -5.0 0 -3.2 -0.9 -14.8 0	1.9 -9.8 4.5 4.1 0 -3.1 0.7	111.0
TS l8-1,4-H	1	27.4	428.3	-97.7 -97.6 -201.5 -23.0 -11.6 4.0 -0.8	8.4 4.9 -4.3 -0.9 -0.4 0 -0.1	76.4
	2	149.9	675.0	-577.3 413.4 -550.4 30.2 12.2 5.5 -8.8	12.3 19.9 -18.8 2.9 1.7 -0.8 -1.2	35.2

	3	98.5	727.2	-323.2 161.3 -584.6 11.9 -4.2 13.8 -2.2	41.3 -18.0 -0.7 9.4 -8.1 3.3 -1.1	50.4
	4	154.3	583.2	-263.5 99.9 -432.2 8.8 -5.9 11.5 -1.6	90.6 -37.5 -20.3 22.1 -19.5 12.7 -1.8	35.3
TS l8-1,5-H	1	27.0	459.7	-114.6 -118.8 -196.3 -21.4 -11.4 3.6 -0.8	-7.5 -4.0 0.8 1.5 1.3	77.5
	2	165.5	643.0	-334.8 185.9 -507.8 9.8 -7.8 8.9 2.8	-54.6 110.0 -37.0 -26.2 5.9 6.5 -2.7	35.6
	3	87.3	664.5	-316.6 113.9 -468.0 -0.7 -2.1 9.9 -0.9	85.2 -18.0 -27.2 21.9 -21.5 10.4 -2.3	49.5
TS l8-β-C-C	1	27.4	436.1	-108.8 -93.3 -201.4 -23.8 -11.9 4.0 -0.8	3.2 0.9 -0.3 0 -0.4 0 -0.1	76.4
	2	147.2	697.4	-608.1 426.8 -554.8 28.5 14.0 5.1 -8.9	6.6 1.2 -3.2 0.8	65.7
	3	103.1	783.1	-397.7 175.9 -583.3 18.7 -11.1 17.1 -2.7	8.0 -1.6 0.3 0.6	49.1
	4	111.0	741.8	-289.3 138.0 -616.0 20.8 -5.7 14.1 -3.8	12.1 -9.1 1.8 2.2 -1.6 0.3 0.4	49.0
	5	217.6	484.1	-310.6 156.4 -317.8 -22.2 0 10.1 0	-50.6 99.0 -89.3 -6.0 16.9 17.9 -6.5	25.6

	6	48.8	131.5	-16.7 -3.4 -104.8 -7.8 0.6 0.7 0	24.7 -7.5 -16.8 8.5 1.8 0 -0.5	34.9
TS l8-β-C-H	1	27.4	451.9	-117.8 -102.3 -200.4 -22.6 -11.6 3.8 -0.9	0 0.4 0.8 0.2 -0.2 0 -0.1	76.8
	2	158.1	683.8	-592.5 426.6 -557.3 29.2 14.4 4.9 -9.1	-1.5 1.4	34.4
	3	97.5	780.8	-384.0 167.6 -587.2 19.7 -10.9 16.4 -2.3	3.8 -2.6 4.2 0.5 0.4 -0.6	50.7
	4	160.4	775.9	-402.5 181.2 -580.3 24.0 -15.1 19.9 -3.0	-7.7 10.8 -2.1 -3.4 3.9 -1.2 -0.6	38.9
	5	141.0	730.3	-304.8 152.5 -595.3 8.215 -2.3 13.6 -2.2	50.9 -38.7 6.9 9.0 -2.2 -3.2	42.8
	6	41.1	429.9	-107.6 -30.1 -315.4 -6.8 16.0 15.3 -1.4	75.3 44.4 -34.3 -15.0 -4.8 3.8	55.7

a:
$$V_i(\varphi_i) = a_i + \sum_k b_{i,k}\cos(k\varphi_i) + \sum_l c_{i,l}\sin(l\varphi_i)$$