

Hydrogen-abstraction reactions of methyl ethers,  $\text{H}_3\text{COCH}_{3-x}(\text{CH}_3)_x$ ,  $x=0-2$ , by  $\cdot\text{OH}$ ; Chong-Wen Zhou  $\text{C}^3$

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 ( $\text{cm}^{-1}$ )
<b>DME</b>	38.4, 10.2, 9.0	204.7, 267.2, 425.0, 980.5, 1146.8, 1182.6, 1220.3, 1232.1, 1288.2, 1485.8, 1500.4, 1510.5, 1514.6, 1525.4, 1548.3, 3016.6, 3025.9, 3079.9, 3085.2, 3182.8, 3183.8
<b>OH</b>	0.0, 570.9, 570.9	3857.1
<b>DME-RC</b>	10.4, 3.5, 2.8	27.2, 66, 176.9, 191.5, 265, 424.6, 484.1, 672.0, 966.8, 1141.2, 1182, 1221.4, 1224.0, 1291, 1486.9, 1502.6, 1511, 1514.6, 1524.7, 1546, 3038.6, 3045.3, 3110, 3116.5, 3193.8, 3201, 3704.1
<b>TS1-1</b>	10.7, 4.2, 3.4	1481.6 <i>i</i> , 110.2, 128.5, 229.4, 242.5, 357.0, 433.8, 781.5, 930.5, 986.5, 1154.3, 1199.1, 1227.1, 1277.8, 1326.7, 1379.3, 1489.3, 1502.9, 1508.1, 1536.5, 1570.2, 3045.9, 3062.5, 3124.6, 3197.1, 3198.9, 3838.1
<b>TS1-2</b>	22.5, 3.1, 2.8	1953.0 <i>i</i> , 52.1, 123.1, 210.3, 218.5, 320.9, 357.1, 748.9, 931.8, 1016.9, 1159.1, 1171.6, 1206.2, 1244.5, 1276.5, 1292.1, 1494.0, 1505.7, 1519.8, 1543.7, 1618.6, 3036.9, 3054.1, 3106.9, 3136.3, 3192.6, 3841.6
<b>PC1</b>	13.2, 3.1, 2.5	56.8, 90.5, 148.4, 186.0, 186.9, 201.7, 343.4, 443.3, 556.7, 723.7, 992.1, 1156.2, 1197.4, 1279.7, 1296.1, 1483.5, 1510.4, 1520.6, 1532.1, 1693.9, 3064.5, 3147.7, 3163.8, 3207.4, 3333.7, 3871.9, 3979.7
<b>P1</b>	46.1, 10.9, 9.4	182.4, 316.2, 442.3, 739.9, 998.7, 1161.5, 1197.0, 1278.3, 1310.0, 1487.1, 1510.7, 1528.7, 1531.2, 3056.1, 3135.3, 3149.4, 3203.2, 3310.6
<b>EME</b>	28.0, 4.2, 3.9	103.9, 214.8, 270.5, 292.9, 473.6, 837.2, 890.1, 1061.6, 1135.0, 1186.6, 1190.2, 1223.0, 1258.9, 1318.6, 1411.1, 1453.6, 1500.7, 1501.1, 1504.9, 1524.2, 1533.1, 1559.3, 3010.4, 3024.6, 3051.4, 3085.8, 3088.8, 3181.8, 3182.0, 3188.5
<b>EME-RC</b>	4.0, 3.5, 2.0	45.8, 74.8, 109.5, 173.3, 222.3, 281.2, 302.2, 472.4, 510.6, 693.3, 841.1, 884.3, 1054.5, 1136.5, 1175.5, 1187.8, 1224.3, 1256.5, 1321.2, 1414.5, 1454.6, 1499.8, 1506.8, 1507.3, 1526.4, 1534.3, 1557.3, 3032.6, 3043.2, 3080.3, 3090.5, 3114.9, 3182.7, 3192.2, 3195.6, 3679.3

<b>Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0–2, by ·OH;</b>		Chong-Wen Zhou C <sup>3</sup>
<b>TS2a</b>	4.4, 3.9, 2.3	1246.3 <i>i</i> , 92.1, 103.5, 134.2, 215.0, 249.9, 252.0, 297.3, 479.1, 731.0, 876.1, 899.7, 1001.4, 1079.4, 1138.0, 1183.8, 1202.1, 1244.5, 1265.0, 1360.9, 1394.9, 1439.4, 1496.8, 1498.0, 1507.0, 1517.7, 1538.4, 1600.0, 3043.9, 3049.3, 3085.8, 3121.8, 3178.9, 3188.4, 3194.0, 3836.4
<b>TS2b-1</b>	7.6, 2.3, 1.9	1376.3 <i>i</i> , 58.7, 96.6, 161.7, 179.7, 262.2, 290.0, 356.5, 476.0, 814.6, 841.6, 889.1, 922.4, 1071.9, 1135.9, 1172.0, 1216.8, 1237.5, 1258.5, 1320.4, 1403.1, 1414.7, 1457.9, 1499.5, 1501.5, 1523.6, 1529.6, 1557.0, 3024.8, 3050.2, 3088.2, 3090.3, 3181.3, 3189.1, 3192.1, 3843.3
<b>TS2b-2</b>	11.6, 1.9, 1.7	1941.2 <i>i</i> , 42.1, 97.5, 103.9, 208.3, 261.0, 266.9, 314.7, 444.0, 735.6, 836.8, 904.8, 948.2, 1074.0, 1158.9, 1161.6, 1194.4, 1211.3, 1278.0, 1278.0, 1318.8, 1411.7, 1451.0, 1501.8, 1521.2, 1524.9, 1556.3, 1616.6, 3029.8, 3055.1, 3075.2, 3088.3, 3138.0, 3182.1, 3188.8, 3841.1
<b>TS2c-1</b>	6.8, 2.9, 2.2	1921.6 <i>i</i> , 81.5, 131.7, 172.5, 231.8, 296.2, 386.8, 453.4, 467.8, 696.8, 871.7, 943.9, 996.7, 1059.9, 1162.3, 1175.4, 1188.6, 1210.0, 1258.6, 1289.7, 1324.7, 1434.6, 1472.7, 1499.9, 1506.4, 1527.8, 1548.2, 1578.6, 3022.7, 3037.2, 3073.4, 3105.4, 3134.1, 3189.9, 3222.8, 3791.7
<b>TS2c-2</b>	14.4, 1.7, 1.6	1692.7 <i>i</i> , 61.9, 83.4, 102.3, 115.0, 233.0, 273.5, 391.6, 460.7, 779.4, 843.3, 900.7, 969.2, 1067.8, 1141.7, 1183.3, 1188.2, 1225.0, 1253.0, 1313.7, 1317.1, 1435.6, 1465.3, 1495.6, 1505.0, 1506.6, 1531.5, 1552.9, 3022.5, 3029.7, 3069.8, 3091.5, 3133.9, 3185.3, 3217.7, 3844.7
<b>PC2a</b>	4.3, 3.1, 1.9	53.6, 92.6, 103.9, 146.5, 179.8, 200.1, 230.9, 285.1, 306.0, 484.1, 614.1, 674.8, 903.8, 1062.7, 1091.3, 1152.8, 1197.6, 1214.9, 1289.1, 1394.9, 1447.7, 1495.1, 1507.3, 1509.7, 1527.1, 1533.8, 1700.1, 3039.5, 3064.3, 3141.6, 3147.6, 3160.0, 3193.0, 3205.3, 3839.0, 3971.4
<b>PC2b</b>	2.9, 2.5, 1.9	39.0, 88.9, 114.0, 149.0, 207.2, 264.6, 273.6, 309.2, 317.3, 485.1, 602.1, 728.3, 843.5, 880.4, 1067.4, 1138.1, 1204.8, 1246.0, 1276.8, 1325.2, 1415.0, 1454.7, 1505.1, 1508.4, 1534.7, 1549.9, 1698.0, 3064.7, 3090.5, 3122.8, 3161.4, 3181.6, 3202.7, 3318.8, 3838.8, 3970.8
<b>PC2c</b>	3.9, 2.1, 1.4	54.5, 96.1, 113.2, 156.8, 195.4, 226.0, 265.5, 292.5, 316.2, 477.9, 533.1, 670.5, 855.2, 982.7, 1081.3, 1148.6, 1184.6,

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		1200.3, 1249.7, 1273.2, 1424.4, 1488.8, 1499.6, 1506.1, 1521.9, 1544.6, 1706.2, 2971.5, 3038.7, 3043.8, 3109.4, 3191.6, 3214.2, 3340.8, 3812.7, 3965.2	
<b>P2a</b>	33.8, 4.2, 3.9	109.2, 173.8, 212.5, 293.5, 482.3, 679.5, 906.9, 1056.7, 1096.7, 1147.7, 1196.7, 1217.9, 1300.1, 1396.8, 1448.2, 1489.3, 1503.8, 1509.3, 1522.8, 1533.5, 3042.5, 3052.9, 3131.1, 3133.0, 3143.9, 3181.8, 3199.3	
<b>P2b</b>	30.6, 4.4, 4.1	90.6, 250.4, 302.2, 309.3, 483.9, 735.5, 834.7, 886.9, 1075.3, 1133.7, 1203.7, 1245.6, 1295.3, 1321.2, 1412.9, 1453.7, 1502.5, 1509.9, 1524.9, 1549.2, 3050.5, 3088.6, 3105.0, 3149.8, 3181.9, 3189.1, 3309.3	
<b>P2c</b>	30.7, 4.4, 4.1	102.8, 177.0, 231.5, 297.7, 425.2, 491.7, 854.4, 985.3, 1082.9, 1135.3, 1193.9, 1199.9, 1250.6, 1268.7, 1425.1, 1480.9, 1498.9, 1504.8, 1522.3, 1546.1, 2951.0, 3013.2, 3024.1, 3086.1, 3184.8, 3214.4, 3337.7	
<b>IPME</b>	7.6, 3.8, 2.8	42.7, 195.8, 217.4, 265.5, 306.7, 366.2, 454.3, 507.2, 827.4, 938.5, 946.4, 961.2, 1134.8, 1162.7, 1182.5, 1199.4, 1224.4, 1256.6, 1379.4, 1400.5, 1420.5, 1431.2, 1494.1, 1497.7, 1504.0, 1508.8, 1519.5, 1532.9, 1539.3, 3012.9, 3030.3, 3074.9, 3079.6, 3100.5, 3165.8, 3172.4, 3174.3, 3178.5, 3181.4	
<b>IPME-RC</b>	3.9, 2.1, 1.4	29.4, 69.6, 102.8, 167.3, 196.6, 227.3, 281.3, 305.2, 377.2, 473.9, 497.0, 515.9, 712.9, 823.7, 944.0, 950.3, 963.2, 1121.9, 1161.2, 1185.2, 1201.3, 1221.9, 1257.4, 1384.2, 1401.1, 1424.1, 1436.8, 1495.1, 1501.7, 1504.9, 1514.6, 1520.0, 1536.5, 1539.6, 3028.9, 3047.2, 3077.6, 3083.1, 3130.4, 3169.4, 3175.2, 3176.7, 3186.4, 3190.9, 3667.5	
<b>TS3a</b>	2.8, 2.8, 2.1	836.7 <i>i</i> , 73.9, 94.6, 134.9, 195.0, 220.2, 234.1, 275.4, 308.1, 370.2, 441.2, 493.7, 698.2, 829.5, 938.3, 948.5, 975.9, 1079.5, 1130.8, 1181.5, 1193.6, 1205.0, 1230.7, 1310.4, 1335.1, 1411.7, 1427.6, 1491.0, 1493.2, 1498.8, 1509.1, 1516.6, 1523.8, 1539.9, 1574.0, 3053.6, 3073.0, 3078.4, 3131.7, 3166.1, 3171.0, 3182.8, 3186.1, 3187.6, 3836.7	
<b>TS3b-1</b>	5.3, 1.8, 1.5	1338.2 <i>i</i> , 28.5, 120.3, 168.9, 186.0, 225.2, 270.4, 323.6, 333.6, 362.2, 451.4, 516.2, 746.1, 830.2, 878.5, 944.2, 950.7, 967.3, 1150.5, 1170.0, 1187.8, 1218.4, 1245.1, 1255.0, 1378.7, 1406.8, 1422.8, 1434.1, 1444.4, 1496.8, 1500.3, 1509.5, 1518.9, 1535.5, 1565.0, 3026.1, 3053.6, 3078.1, 3081.0, 3166.3, 3175.6, 3180.6,	

<b>Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;</b>		Chong-Wen Zhou C <sup>3</sup>
		3190.4, 3197.6, 3841.1
<b>TS3b-2</b>	6.0, 1.6, 1.4	1873.8 <i>i</i> , 37.9, 85.9, 131.8, 213.8, 237.1, 254.0, 273.5, 332.3, 363.0, 451.9, 497.7, 728.2, 857.2, 942.0, 942.4, 958.6, 972.4, 1143.9, 1157.8, 1188.4, 1206.9, 1225.0, 1287.0, 1304.7, 1381.3, 1401.1, 1423.3, 1432.5, 1499.5, 1504.3, 1513.5, 1521.0, 1530.9, 1621.7, 3028.3, 3063.2, 3074.9, 3081.4, 3150.9, 3168.7, 3170.6, 3177.3, 3182.5, 3839.8
<b>TS3c-1</b>	3.9, 2.5, 1.7	1904.5 <i>i</i> , 53.5, 87.4, 147.6, 199.2, 254.5, 297.1, 324.6, 381.0, 459.8, 473.2, 505.2, 739.1, 823.1, 935.0, 961.7, 999.8, 1033.2, 1131.3, 1165.7, 1188.5, 1199.9, 1211.2, 1256.6, 1300.3, 1379.2, 1408.4, 1419.2, 1470.3, 1494.9, 1503.8, 1509.7, 1527.1, 1538.6, 1579.1, 3037.5, 3042.5, 3078.0, 3120.1, 3124.1, 3171.5, 3175.9, 3185.0, 3213.6, 3786.7
<b>TS3c-2</b>	6.9, 1.5, 1.4	1634.6 <i>i</i> , 26.8, 56.5, 109.1, 162.2, 204.4, 260.8, 298.1, 340.0, 382.1, 444.6, 507.4, 787.8, 856.9, 902.4, 941.5, 959.2, 995.3, 1129.0, 1160.5, 1182.0, 1197.1, 1222.7, 1253.0, 1303.2, 1392.1, 1401.9, 1422.2, 1460.5, 1483.0, 1495.6, 1506.2, 1518.2, 1527.2, 1538.2, 3030.7, 3035.5, 3079.0, 3105.1, 3123.5, 3172.0, 3182.3, 3185.9, 3208.3, 3842.4
<b>TS3d-1</b>	5.7, 1.7, 1.4	1639.7 <i>i</i> , 42.3, 70.0, 110.3, 164.6, 202.7, 246.1, 295.8, 356.2, 368.0, 447.3, 510.2, 779.2, 868.1, 909.9, 940.3, 949.0, 990.6, 1130.6, 1159.8, 1181.0, 1197.5, 1222.7, 1254.5, 1304.0, 1387.9, 1399.1, 1427.8, 1460.4, 1480.0, 1497.3, 1510.5, 1514.2, 1522.8, 1537.3, 3032.6, 3038.1, 3082.1, 3101.5, 3120.3, 3175.2, 3182.4, 3194.2, 3203.0, 3842.5
<b>TS3d-2</b>	3.9, 2.1, 1.7	1659.9 <i>i</i> , 29.7, 84.8, 114.2, 128.9, 222.0, 247.7, 303.3, 363.3, 385.4, 467.3, 523.2, 797.0, 828.9, 911.7, 926.2, 956.8, 978.8, 1137.4, 1162.5, 1167.9, 1199.9, 1222.9, 1259.2, 1318.1, 1369.2, 1394.6, 1427.2, 1474.1, 1484.3, 1495.2, 1507.8, 1518.7, 1527.7, 1536.8, 2988.6, 3031.0, 3082.4, 3102.4, 3125.5, 3177.2, 3182.6, 3192.1, 3202.3, 3844.4
<b>TS3d-3</b>	3.9, 2.5, 1.7	1903.2 <i>i</i> , 53.4, 87.3, 147.6, 199.2, 254.5, 297.1, 324.7, 381.0, 459.7, 473.2, 505.1, 739.2, 823.1, 935.0, 961.7, 999.8, 1033.1, 1131.2, 1165.7, 1188.6, 1199.9, 1211.2, 1256.6, 1300.5, 1379.2, 1408.4, 1419.2, 1470.3, 1494.9, 1503.8, 1509.7, 1527.1, 1538.6, 1579.3, 3037.5, 3042.5, 3078.0, 3120.2, 3124.1, 3171.5, 3176.0, 3185.0, 3213.6, 3786.7,

<b>Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0–2, by ·OH;</b>		Chong-Wen Zhou C <sup>3</sup>
<b>PC3a</b>	3.7, 2.2, 1.5	29.6, 62.3, 125.6, 174.3, 180.7, 187.1, 230.0, 247.1, 308.3, 317.6, 377.4, 403.0, 501.6, 615.3, 794.5, 959.2, 969.1, 984.9, 1112.0, 1135.4, 1196.1, 1218.3, 1308.4, 1321.4, 1422.5, 1430.6, 1490.5, 1497.5, 1503.7, 1506.7, 1516.6, 1525.5, 1536.3, 1708.2, 3021.9, 3033.2, 3066.9, 3133.6, 3138.9, 3152.4, 3180.7, 3190.1, 3200.9, 3836.0, 3966.9
<b>PC3b</b>	4.3, 3.2, 2.0	68.0, 94.7, 118.6, 153.6, 194.0, 248.5, 277.2, 279.4, 312.7, 333.4, 358.4, 470.0, 521.7, 598.1, 750.7, 822.8, 950.1, 952.7, 966.5, 1148.6, 1181.5, 1218.2, 1253.0, 1272.1, 1380.8, 1397.5, 1424.1, 1440.0, 1500.5, 1502.1, 1515.3, 1518.8, 1538.1, 1696.2, 3061.5, 3081.4, 3084.7, 3153.5, 3174.7, 3180.4, 3186.3, 3189.9, 3310.3, 3828.9, 3969.9
<b>PC3c</b>	4.5, 3.2, 1.9	34.1, 53.3, 93.7, 153.1, 184.2, 207.0, 241.5, 271.2, 296.0, 317.7, 385.3, 448.5, 481.7, 573.2, 691.9, 838.2, 929.9, 970.6, 1070.9, 1127.9, 1172.6, 1189.7, 1199.9, 1244.6, 1361.2, 1388.2, 1415.7, 1481.3, 1495.6, 1505.8, 1511.3, 1525.5, 1538.7, 1706.4, 2964.5, 3046.1, 3081.9, 3124.3, 3174.5, 3182.8, 3187.6, 3209.7, 3337.2, 3796.5, 3963.9
<b>P3a</b>	7.9, 4.0, 2.8	123.3, 167.5, 183.5, 243.9, 310.1, 365.6, 394.8, 500.0, 796.5, 955.2, 968.4, 983.2, 1110.8, 1140.1, 1194.5, 1216.6, 1313.4, 1327.7, 1419.9, 1427.2, 1487.3, 1497.1, 1499.4, 1504.3, 1513.6, 1525.9, 1536.1, 3014.2, 3026.4, 3056.9, 3129.8, 3132.0, 3135.3, 3177.2, 3183.2, 3192.9
<b>P3b</b>	7.8, 4.0, 3.0	113.9, 213.4, 258.5, 279.0, 322.0, 357.3, 467.5, 519.0, 740.2, 829.4, 944.4, 953.4, 967.0, 1150.4, 1177.7, 1212.5, 1249.8, 1285.4, 1381.7, 1399.7, 1422.3, 1435.0, 1498.9, 1503.5, 1506.0, 1513.2, 1529.9, 3045.6, 3076.5, 3081.9, 3142.9, 3169.2, 3177.4, 3179.4, 3182.6, 3306.0
<b>P3c</b>	8.1, 3.9, 2.9	109.8, 203.0, 210.0, 244.6, 289.8, 334.4, 469.3, 475.8, 570.4, 840.5, 931.0, 959.1, 1081.4, 1150.3, 1170.9, 1177.2, 1201.6, 1254.8, 1351.2, 1395.2, 1411.0, 1473.8, 1497.2, 1501.7, 1505.5, 1519.2, 1537.9, 3006.4, 3031.5, 3080.5, 3101.4, 3179.9, 3182.1, 3182.2, 3193.9, 3315.5
<b>H<sub>2</sub>O</b>	784.9, 449.6, 285.8	1667.1, 3905.2, 4013.1

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**Hydrogen-abstraction reactions of methyl ethers,  $\text{H}_3\text{COCH}_{3-x}(\text{CH}_3)_x$ ,  $x=0-2$ , by  $\cdot\text{OH}$ ;** Chong-Wen Zhou  $\text{C}^3$

Table S2. Enthalpies of reaction IR1 and IR2 (in  $\text{kJ mol}^{-1}$ ) at different level at 298 K.

Reactions	CBS-QB3	CBS-APNO	G3	G4	W1BD	average
IR1	-3.38	-0.93	-0.49	-1.51	1.64	$-0.93 \pm 1.82$
IR2	-0.59	-0.47	-0.40	0.96	-0.41	$-0.18 \pm 0.64$

<sup>a</sup> Formation enthalpy  $\Delta H_f(298.15\text{K})$  in  $\text{kJ mol}^{-1}$ :

$\text{CH}_3\text{C}(\text{O})\text{CH}_3 = -217.30 \pm 0.70^1$ ;  $\text{CH}_3\text{OCH}_3 = -183.94 \pm 0.46^2$ ;  $\text{CH}_3\text{C}(\text{O})\dot{\text{C}}\text{H}_2 = -34.9 \pm 1.90^3$ ;  $\text{CH}_3\text{OH} = -201.17 \pm 0.18^2$ ;  $\dot{\text{C}}\text{H}_2\text{OH} = -17.18 \pm 0.37^2$

Combining with the heat formation of the species in the isodesmic reactions shown in Table S2 which are obtained from literatures, we get the final average heat formation of  $\text{CH}_3\text{O}\dot{\text{C}}\text{H}_2$  as  $0.16 \pm 0.85 \text{ kJ mol}^{-1}$ .

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

**EME**

8	0.000000000	-0.602998000	-0.000013000
6	-1.156957000	0.199801000	0.000033000
1	-2.017381000	-0.470123000	0.000040000
1	-1.201580000	0.841637000	0.892127000
1	-1.201625000	0.841674000	-0.892032000
6	1.156957000	0.199801000	-0.000025000
1	1.201625000	0.841637000	0.892067000
1	2.017381000	-0.470123000	-0.000060000
1	1.201580000	0.841674000	-0.892092000

**EME-RC**

8	-0.338825000	-0.086811000	-0.335643000
6	-0.539299000	1.255973000	0.069530000
1	0.329593000	1.821858000	-0.264626000
1	-1.447919000	1.669464000	-0.385514000
1	-0.619337000	1.329997000	1.162043000
6	-1.392160000	-0.920270000	0.108173000
1	-2.350975000	-0.595068000	-0.315442000
1	-1.171076000	-1.930657000	-0.235612000
1	-1.467675000	-0.915767000	1.203676000
8	2.442052000	-0.288749000	0.070839000
1	1.490327000	-0.389567000	-0.112309000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

Chong-Wen Zhou C<sup>3</sup>

**TS1-1**

8	-0.897003000	0.352825000	-0.513431000
6	0.047319000	1.060289000	0.220116000
1	1.057623000	0.454671000	0.288936000
1	0.266302000	1.994462000	-0.296590000
1	-0.254554000	1.232308000	1.262317000
6	-1.308213000	-0.813969000	0.180233000
1	-1.809819000	-0.554526000	1.122049000
1	-2.008205000	-1.339601000	-0.468687000
1	-0.447423000	-1.455711000	0.398965000
8	2.024331000	-0.501168000	0.035106000
1	1.742815000	-0.622782000	-0.882482000

**TS1-2**

8	0.532369000	-0.407283000	-0.000173000
6	-0.150197000	0.810177000	-0.000005000
1	-1.313205000	0.516650000	-0.000230000
1	0.018733000	1.398724000	0.910329000
1	0.018973000	1.399108000	-0.910050000
6	1.934405000	-0.208912000	0.000079000
1	2.256591000	0.342162000	0.893543000
1	2.395766000	-1.196366000	-0.000049000
1	2.256862000	0.342519000	-0.893067000
8	-2.346648000	-0.259730000	0.000036000
1	-1.824734000	-1.074280000	0.000176000

**PC1**

8	-0.445129000	-0.118423000	0.057853000
6	-0.430101000	1.238047000	-0.081278000
1	-1.288656000	1.784668000	0.299057000
1	0.569024000	1.644991000	-0.028922000
6	-1.748533000	-0.681903000	-0.015693000
1	-2.194903000	-0.495208000	-0.996848000
1	-1.638014000	-1.753773000	0.141971000
1	-2.391557000	-0.261018000	0.765602000
8	2.444034000	-0.305236000	-0.087599000
1	1.524467000	-0.548796000	-0.229887000
1	2.500203000	-0.318455000	0.868821000

**EME**

8	0.501016000	-0.512963000	-0.000007000
6	1.797871000	0.039142000	0.000004000
1	2.503402000	-0.792501000	0.000014000
1	1.971704000	0.657793000	-0.892311000
1	1.971687000	0.657800000	0.892318000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

6	-0.482241000	0.502040000	-0.000003000
1	-0.363584000	1.142721000	-0.888471000
1	-0.363576000	1.142719000	0.888466000
6	-1.845328000	-0.161075000	0.000004000
1	-2.637414000	0.592570000	-0.000233000
1	-1.955981000	-0.789201000	-0.886398000
1	-1.956175000	-0.788843000	0.886636000

**EME-RC**

8	-0.495684000	-0.275627000	-0.354982000
6	-1.591507000	-1.099994000	0.001898000
1	-1.476444000	-2.038944000	-0.539947000
1	-1.602605000	-1.301679000	1.081146000
1	-2.540930000	-0.629724000	-0.282975000
6	-0.539322000	0.974449000	0.324690000
1	-0.496105000	0.805043000	1.410830000
1	-1.490813000	1.475967000	0.097526000
6	0.638445000	1.808704000	-0.139004000
1	0.634599000	2.777963000	0.366709000
1	1.574906000	1.295783000	0.087017000
1	0.578665000	1.974141000	-1.217076000
8	2.069040000	-1.399046000	0.105673000
1	1.186185000	-1.060119000	-0.134261000

**TS2a**

8	0.650747000	-0.703699000	-0.434692000
6	1.897263000	-0.263379000	0.079905000
1	2.654307000	-0.518172000	-0.661663000
1	1.887661000	0.820324000	0.244272000
1	2.132511000	-0.766864000	1.026911000
6	-0.400517000	-0.369802000	0.422668000
1	-0.518047000	0.796166000	0.448531000
1	-0.180916000	-0.652477000	1.463784000
6	-1.687714000	-0.970064000	-0.090148000
1	-2.524308000	-0.668871000	0.544876000
1	-1.879303000	-0.628076000	-1.109580000
1	-1.617869000	-2.061222000	-0.096079000
8	-0.472270000	2.132070000	0.004823000
1	-0.236048000	1.871688000	-0.896651000

**TS2b-1**

8	0.346044000	0.835310000	-0.312903000
6	-0.948955000	1.104167000	0.106227000
1	-1.330739000	1.959051000	-0.452487000
1	-1.661536000	0.204509000	-0.153591000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

Chong-Wen Zhou C<sup>3</sup>

1	-1.023099000	1.270226000	1.190578000
6	0.905213000	-0.262243000	0.394509000
1	0.257971000	-1.139975000	0.267826000
1	0.954779000	-0.022530000	1.468495000
6	2.289768000	-0.523978000	-0.161331000
1	2.755688000	-1.362988000	0.362744000
1	2.226231000	-0.764355000	-1.224621000
1	2.918691000	0.360691000	-0.039392000
8	-2.373581000	-0.991414000	-0.211567000
1	-2.353834000	-1.163469000	0.739786000

**TS2b-2**

8	-0.052357000	-0.065139000	-0.000127000
6	0.923271000	0.934205000	-0.000053000
1	1.968987000	0.347980000	-0.000073000
1	0.913434000	1.546253000	-0.910312000
1	0.913411000	1.546132000	0.910287000
6	-1.365561000	0.479989000	0.000117000
1	-1.504870000	1.112194000	-0.889215000
1	-1.504689000	1.111833000	0.889732000
6	-2.349203000	-0.672860000	-0.000020000
1	-3.375447000	-0.295559000	0.000167000
1	-2.201677000	-1.291823000	-0.887659000
1	-2.201489000	-1.292193000	0.887330000
8	2.764271000	-0.673736000	0.000065000
1	2.045991000	-1.321820000	-0.000026000

**TS2c-1**

8	-0.283704000	0.733173000	-0.451439000
6	-1.169054000	1.709935000	0.067359000
1	-0.945453000	2.642691000	-0.451714000
1	-2.218827000	1.451639000	-0.111060000
1	-1.012901000	1.849574000	1.145819000
6	-0.310343000	-0.493879000	0.279918000
1	-0.188797000	-0.264719000	1.350342000
6	0.889273000	-1.285410000	-0.189279000
1	1.048072000	-2.198711000	0.387332000
1	0.863849000	-1.478192000	-1.263571000
1	1.860508000	-0.602006000	0.009367000
6	-1.615054000	-1.255408000	0.060518000
1	-2.475303000	-0.711319000	0.458330000
1	-1.766045000	-1.416999000	-1.010742000
1	-1.571231000	-2.226293000	0.562473000
8	2.513902000	0.499319000	0.176005000
1	1.795610000	1.042973000	-0.184196000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

Chong-Wen Zhou C<sup>3</sup>

**TS2c-2**

8	1.418100000	0.477654000	-0.076962000
6	2.478460000	-0.452075000	-0.012747000
1	3.404952000	0.106688000	-0.148119000
1	2.504401000	-0.964006000	0.959533000
1	2.395192000	-1.209743000	-0.804920000
6	0.171499000	-0.169739000	0.082822000
1	0.133075000	-0.700761000	1.045743000
1	0.020533000	-0.914734000	-0.713344000
6	-0.912003000	0.880153000	0.025144000
1	-1.946236000	0.304791000	0.174433000
1	-0.861207000	1.591918000	0.850285000
1	-0.948379000	1.393478000	-0.936512000
8	-2.931566000	-0.560374000	0.064191000
1	-3.022336000	-0.495905000	-0.896254000

**PC2a**

8	0.566438000	-0.326348000	0.223687000
6	1.704333000	-1.146882000	-0.017119000
1	1.472771000	-2.130770000	0.388977000
1	1.905405000	-1.225843000	-1.089648000
1	2.584185000	-0.738147000	0.492400000
6	0.712299000	0.958379000	-0.238321000
1	1.727922000	1.351722000	-0.186287000
6	-0.459469000	1.831766000	0.051874000
1	-0.362589000	2.781114000	-0.479130000
1	-1.379343000	1.336513000	-0.266013000
1	-0.544816000	2.048087000	1.126739000
8	-2.233039000	-1.101276000	-0.151820000
1	-1.281619000	-0.969384000	-0.074736000
1	-2.532091000	-0.891878000	0.734168000

**PC2b**

8	-0.562559000	-0.464323000	-0.273361000
6	-1.484542000	-1.424510000	0.018594000
1	-1.282324000	-2.366018000	-0.473231000
1	-2.506737000	-1.093945000	0.181376000
6	-0.841260000	0.806153000	0.331329000
1	-0.779255000	0.703035000	1.420355000
1	-1.863097000	1.103772000	0.064212000
6	0.175355000	1.803173000	-0.185301000
1	-0.004845000	2.784070000	0.262183000
1	1.181902000	1.472993000	0.073738000
1	0.095804000	1.892896000	-1.271409000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

8	2.318011000	-0.801222000	0.197563000
1	1.367964000	-0.855127000	0.045790000
1	2.649650000	-0.626208000	-0.684367000

**PC2c**

8	-0.472822000	-0.372939000	-0.231586000
6	-1.526413000	-1.282739000	0.021985000
1	-1.173435000	-2.271333000	-0.272028000
1	-1.795047000	-1.294271000	1.086635000
1	-2.416340000	-1.025746000	-0.567220000
6	-0.837456000	0.953727000	0.128664000
1	-1.162072000	0.964141000	1.186036000
1	-1.698446000	1.281155000	-0.474603000
6	0.329169000	1.853280000	-0.074572000
1	1.321147000	1.465092000	0.111568000
1	0.173746000	2.921405000	-0.146935000
8	2.346071000	-0.836171000	0.144113000
1	1.382755000	-0.805345000	0.093713000
1	2.589898000	-0.707835000	-0.773847000

**IPME**

8	0.690722000	-0.592481000	-0.362610000
6	1.939539000	-0.115588000	0.090547000
1	2.703350000	-0.728717000	-0.389843000
1	2.113171000	0.933965000	-0.178233000
1	2.032058000	-0.218988000	1.181541000
6	-0.412889000	-0.007039000	0.317926000
1	-0.219412000	-0.043822000	1.403465000
6	-1.615218000	-0.877719000	-0.007182000
1	-2.508013000	-0.510333000	0.506902000
1	-1.797121000	-0.862346000	-1.085762000
1	-1.425885000	-1.909335000	0.298129000
6	-0.634163000	1.443947000	-0.101710000
1	0.213925000	2.079873000	0.164028000
1	-0.777039000	1.488701000	-1.185646000
1	-1.524430000	1.849245000	0.388816000

**IPME-RC**

8	0.249113000	0.500534000	-0.299302000
6	0.197640000	1.867263000	0.081101000
1	1.129584000	2.320872000	-0.258792000
1	-0.643771000	2.388583000	-0.386601000
1	0.124186000	1.968126000	1.172123000
6	-0.745914000	-0.312234000	0.334600000
1	-0.666919000	-0.163687000	1.423707000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;** Chong-Wen Zhou C<sup>3</sup>

6	-0.396427000	-1.750417000	-0.009511000
1	-1.084857000	-2.436556000	0.491090000
1	-0.475395000	-1.898996000	-1.090514000
1	0.624384000	-1.981645000	0.300655000
6	-2.149188000	0.061699000	-0.127784000
1	-2.429725000	1.071817000	0.180225000
1	-2.200508000	-0.000199000	-1.219059000
1	-2.878135000	-0.633424000	0.298819000
8	2.886606000	-0.461268000	-0.001633000
1	1.978740000	-0.146876000	-0.174610000

**Ts3a**

8	-0.587932000	-0.589256000	-0.819910000
6	-1.858334000	-0.615600000	-0.186102000
1	-2.595121000	-0.734757000	-0.981300000
1	-1.953587000	-1.455023000	0.511666000
1	-2.043234000	0.323461000	0.348870000
6	0.456445000	-0.154855000	0.017899000
1	0.210503000	0.925156000	0.375318000
6	1.705599000	-0.077505000	-0.835520000
1	2.525712000	0.372142000	-0.270441000
1	1.998653000	-1.083582000	-1.152720000
1	1.514245000	0.524636000	-1.726607000
6	0.636557000	-0.995523000	1.273967000
1	-0.225594000	-0.928680000	1.940607000
1	0.782214000	-2.043496000	0.988415000
1	1.516730000	-0.653011000	1.824210000
8	-0.269354000	2.280173000	0.446225000
1	-0.513837000	2.286722000	-0.490007000

**Ts3b-1**

8	-0.254799000	-0.917862000	-0.452240000
6	1.002159000	-1.241634000	0.040536000
1	1.394108000	-2.077888000	-0.539331000
1	1.787770000	-0.381991000	-0.109975000
1	0.990042000	-1.476299000	1.114226000
6	-0.923407000	0.105527000	0.291195000
1	-0.644275000	0.002177000	1.352312000
6	-2.411987000	-0.153399000	0.134570000
1	-2.991096000	0.606994000	0.666355000
1	-2.676150000	-0.119210000	-0.926219000
1	-2.672228000	-1.139617000	0.525969000
6	-0.516880000	1.485676000	-0.213315000
1	0.564560000	1.619212000	-0.161160000
1	-0.826855000	1.594023000	-1.256667000
1	-1.001043000	2.267324000	0.380799000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

8	2.821613000	0.562831000	0.013995000
1	2.641339000	0.768512000	0.941741000
<b>TS3b-2</b>			
8	-0.260072000	0.140208000	-0.213567000
6	-1.093964000	-0.905491000	0.195554000
1	-2.203614000	-0.472619000	0.115779000
1	-1.065432000	-1.777962000	-0.465700000
1	-0.948512000	-1.177184000	1.247912000
6	1.059906000	0.074909000	0.334329000
1	0.976164000	-0.032625000	1.427878000
6	1.717387000	1.402661000	0.003416000
1	2.726425000	1.443084000	0.422909000
1	1.781229000	1.521602000	-1.081893000
1	1.129794000	2.227971000	0.412070000
6	1.832551000	-1.110299000	-0.231882000
1	1.360369000	-2.060589000	0.031788000
1	1.872335000	-1.031365000	-1.322482000
1	2.854089000	-1.119762000	0.159751000
8	-3.127038000	0.434368000	-0.089319000
1	-2.481250000	1.112156000	-0.333419000
<b>TS3c-1</b>			
8	-0.283704000	0.733173000	-0.451439000
6	-1.169054000	1.709935000	0.067359000
1	-0.945453000	2.642691000	-0.451714000
1	-2.218827000	1.451639000	-0.111060000
1	-1.012901000	1.849574000	1.145819000
6	-0.310343000	-0.493879000	0.279918000
1	-0.188797000	-0.264719000	1.350342000
6	0.889273000	-1.285410000	-0.189279000
1	1.048072000	-2.198711000	0.387332000
1	0.863849000	-1.478192000	-1.263571000
1	1.860508000	-0.602006000	0.009367000
6	-1.615054000	-1.255408000	0.060518000
1	-2.475303000	-0.711319000	0.458330000
1	-1.766045000	-1.416999000	-1.010742000
1	-1.571231000	-2.226293000	0.562473000
8	2.513902000	0.499319000	0.176005000
1	1.795610000	1.042973000	-0.184196000
<b>TS3c-2</b>			
8	-1.434300000	-0.537793000	0.341996000
6	-2.562727000	-0.044591000	-0.352151000
1	-3.433268000	-0.553261000	0.063785000
1	-2.692794000	1.037208000	-0.224290000
1	-2.495924000	-0.267239000	-1.426526000
6	-0.206328000	-0.027419000	-0.167329000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

1	-0.232952000	-0.057894000	-1.268422000
6	0.864166000	-0.979920000	0.324180000
1	1.902363000	-0.613245000	-0.128058000
1	0.949351000	-0.968237000	1.413236000
1	0.730079000	-1.997212000	-0.047072000
6	0.053619000	1.402997000	0.293757000
1	-0.705962000	2.092939000	-0.081332000
1	0.042937000	1.435872000	1.387858000
1	1.029495000	1.734483000	-0.068511000
8	3.029780000	0.011114000	-0.428281000
1	3.250451000	0.263612000	0.478872000

**TS3d-1**

8	1.560750000	0.310007000	0.290342000
6	2.387539000	-0.697912000	-0.255165000
1	3.385472000	-0.541883000	0.156328000
1	2.051153000	-1.707445000	0.013484000
1	2.434964000	-0.622833000	-1.350645000
6	0.229038000	0.266375000	-0.212445000
1	0.256860000	0.053509000	-1.292730000
6	-0.369615000	1.643221000	0.016538000
1	-1.400876000	1.666340000	-0.341973000
1	-0.352332000	1.873370000	1.086404000
1	0.215866000	2.400426000	-0.509246000
6	-0.573812000	-0.819765000	0.487035000
1	-0.216508000	-1.834909000	0.303649000
1	-0.659760000	-0.625106000	1.558708000
1	-1.669003000	-0.806252000	0.022455000
8	-2.921805000	-0.563385000	-0.336585000
1	-3.196290000	-0.179712000	0.507722000

**TS3d-2**

8	-1.117849000	0.017412000	-0.627628000
6	-2.112054000	-0.864124000	-0.149203000
1	-2.733625000	-1.128298000	-1.005474000
1	-1.691081000	-1.784899000	0.273188000
1	-2.738616000	-0.378753000	0.613262000
6	-0.352028000	0.615449000	0.404381000
1	-1.037282000	1.018276000	1.172781000
6	0.415538000	1.757620000	-0.241383000
1	1.008045000	2.292904000	0.506924000
1	1.082667000	1.349652000	-1.004057000
1	-0.278822000	2.456074000	-0.712907000
6	0.583767000	-0.377317000	1.074668000
1	0.092489000	-1.263057000	1.480995000
1	1.308964000	-0.793522000	0.226268000
1	1.203431000	0.093060000	1.841856000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;**

8	2.319661000	-1.041555000	-0.592782000
1	2.957995000	-0.458065000	-0.160338000

**TS3d-3**

8	0.627120000	0.978323000	-0.449839000
6	-0.310165000	1.889566000	0.116358000
1	-0.340052000	2.749761000	-0.553694000
1	-1.308327000	1.451827000	0.200344000
1	0.019087000	2.221914000	1.109932000
6	0.757592000	-0.228256000	0.295790000
1	0.620768000	-0.018149000	1.367536000
6	2.174539000	-0.726610000	0.056229000
1	2.361744000	-1.659199000	0.595133000
1	2.325963000	-0.898506000	-1.012318000
1	2.890574000	0.027585000	0.389325000
6	-0.256188000	-1.259360000	-0.155236000
1	-1.378752000	-0.879607000	0.101513000
1	-0.215498000	-1.409046000	-1.235855000
1	-0.180281000	-2.209992000	0.377120000
8	-2.649056000	-0.591718000	0.149244000
1	-2.814414000	-0.521465000	-0.813126000

**PC3a**

8	0.096882000	0.542177000	-0.516783000
6	-0.086376000	1.892900000	-0.102457000
1	0.697526000	2.467158000	-0.595368000
1	-1.062852000	2.277146000	-0.410935000
1	0.020933000	1.985665000	0.983539000
6	-0.664338000	-0.403535000	0.148631000
6	-0.293997000	-1.780463000	-0.302843000
1	-0.739631000	-2.529686000	0.355879000
1	-0.653935000	-1.968369000	-1.325960000
1	0.791124000	-1.900953000	-0.299683000
6	-2.105848000	-0.081363000	0.407010000
1	-2.239377000	0.812459000	1.021615000
1	-2.646991000	0.077429000	-0.539600000
1	-2.576258000	-0.919021000	0.926243000
8	2.766345000	-0.254750000	0.267366000
1	1.967319000	0.051551000	-0.176136000
1	2.439677000	-0.418034000	1.153694000

**PC3b**

8	0.313711000	0.749318000	-0.514384000
6	1.004533000	1.848467000	-0.101893000
1	0.623373000	2.767299000	-0.527333000
1	2.071219000	1.723168000	0.067495000
6	0.850780000	-0.508543000	-0.051602000

**Hydrogen-abstraction reactions of methyl ethers, H<sub>3</sub>COCH<sub>3-x</sub>(CH<sub>3</sub>)<sub>x</sub>, x=0-2, by ·OH;** Chong-Wen Zhou C<sup>3</sup>

1	1.939055000	-0.472990000	-0.201077000
6	0.238886000	-1.582044000	-0.933247000
1	0.634294000	-2.562365000	-0.653254000
1	-0.846449000	-1.588516000	-0.805717000
1	0.474152000	-1.392646000	-1.983186000
6	0.528321000	-0.702554000	1.423204000
1	0.967541000	0.095058000	2.027614000
1	-0.556537000	-0.691916000	1.550203000
1	0.918305000	-1.663081000	1.772258000
8	-2.518179000	0.264469000	0.031953000
1	-1.654715000	0.589476000	-0.248060000
1	-2.669610000	0.754266000	0.841735000
<b>PC3c</b>			
8	0.121336000	0.575151000	-0.170495000
6	-0.188877000	1.911024000	0.188603000
1	0.659611000	2.522012000	-0.121526000
1	-1.090283000	2.272669000	-0.318126000
1	-0.324086000	2.005052000	1.274271000
6	-0.813347000	-0.381609000	0.341942000
1	-1.011116000	-0.125315000	1.400506000
6	-0.158802000	-1.718866000	0.266197000
1	-0.763172000	-2.613144000	0.348317000
1	0.916863000	-1.784492000	0.357943000
6	-2.134139000	-0.341137000	-0.426751000
1	-2.633666000	0.624706000	-0.320856000
1	-1.940293000	-0.527392000	-1.486111000
1	-2.809042000	-1.114343000	-0.048433000
8	2.863276000	-0.269347000	-0.106051000
1	1.970881000	0.100042000	-0.098357000
1	2.918399000	-0.622698000	-0.995203000

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