

This is supplementary information for the paper titled “A Systematic Study of Rate Constants of the Important Reactions for Ether Oxidation.”

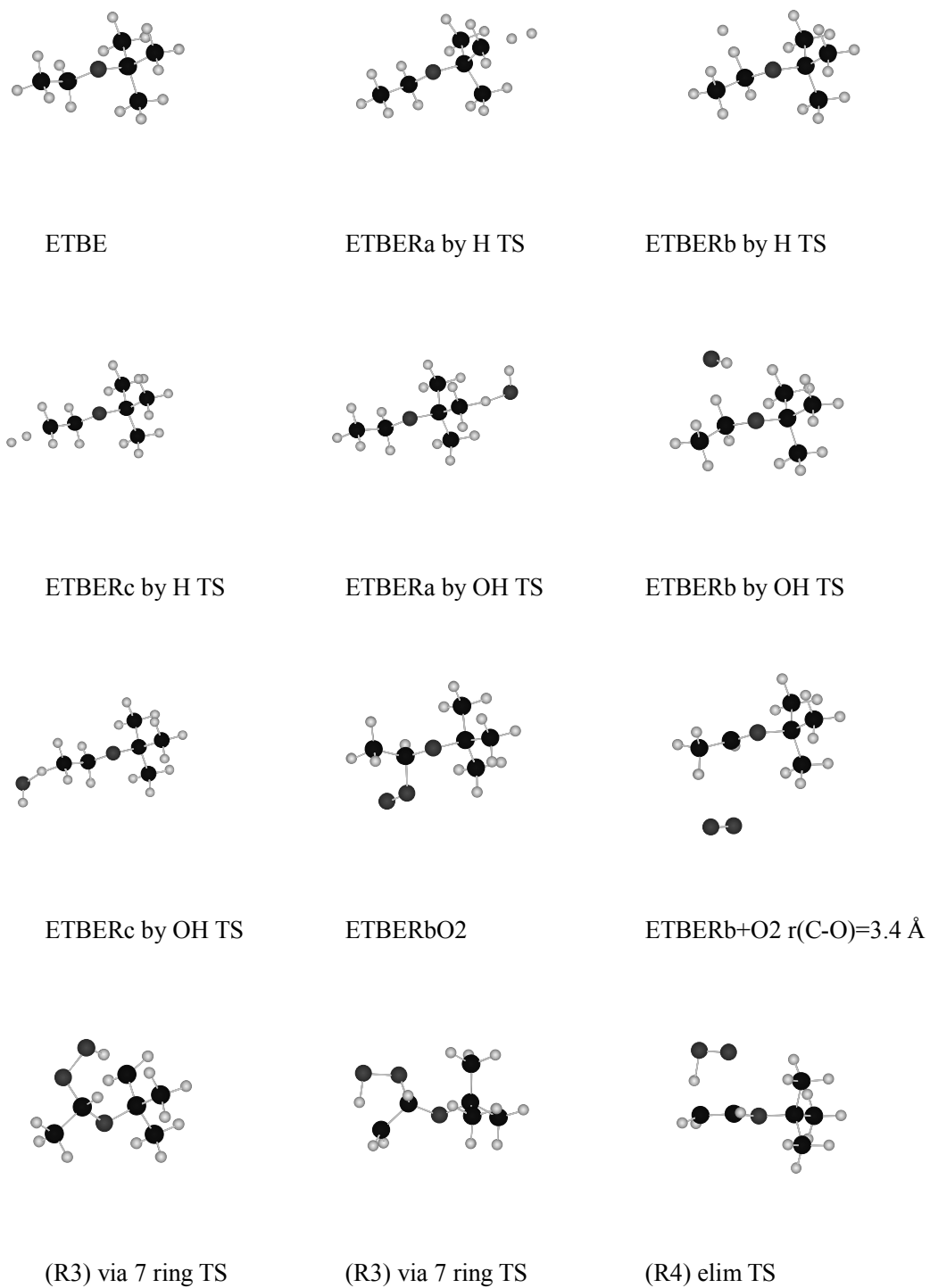


Fig. A The B3LYP/6-31G(d) optimized geometries for species related (R1-4) for ETBE.

Table A. The B3LYP/6-31G(d) unscaled harmonic vibrational frequencies, the rotational constants, and the G3MP2B3 energies at 0 K for species related (R1-4) for ETBE.

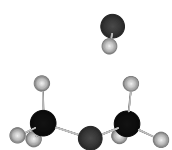
Species	Energies (hatee)	Rotational Constants (GHz)	Frequencies (cm ⁻¹)					
ETBE	-311.743576	4.05705	40.2761,	104.6543,	195.7651,	213.2811,	256.7075,	265.3654,
		1.54910	276.7453,	329.0799,	343.0597,	356.0810,	447.6345,	458.4671,
		1.52354	514.9152,	746.1530,	835.9531,	859.1761,	917.7222,	929.0219,
			971.8189,	977.3312,	1052.5800,	1058.2118,	1106.5741,	1158.1388,
			1198.0656,	1242.8764,	1266.9397,	1289.9366,	1317.8712,	1418.4005,
			1424.5142,	1427.9729,	1449.0682,	1453.5892,	1504.9477,	1513.8465,
			1515.6689,	1517.8403,	1529.3622,	1532.1441,	1534.6190,	1547.9425,
			1563.7454,	3000.0185,	3027.8449,	3051.2287,	3052.8521,	3057.2172,
			3060.8056,	3116.6565,	3121.1270,	3124.2251,	3125.6592,	3127.6726,
			3132.6178,	3133.0295,	3134.3562			
ETBERa by H TS	-312.227118	4.05147	-1193.9664,	-3.3400,	58.7620,	136.5363,	181.3259,	240.8258,
		1.47103	263.8531,	271.0339,	288.4766,	330.5494,	335.4546,	373.5464,
		1.44870	447.8519,	456.6517,	531.0108,	600.9830,	749.2966,	835.3994,
			852.9108,	918.8991,	943.0344,	969.2848,	976.1907,	1026.1371,
			1049.9872,	1091.2504,	1150.4660,	1191.3128,	1198.8042,	1228.6717,
			1240.3856,	1274.0398,	1296.9324,	1313.5302,	1417.8321,	1425.5594,
			1437.1139,	1449.9842,	1482.9817,	1513.3929,	1513.9606,	1522.6348,
			1530.0730,	1534.6681,	1541.0261,	1561.2297,	1804.2083,	3002.9697,
			3032.5316,	3054.8156,	3057.5976,	3059.6640,	3114.6737,	3123.0825,
			3127.2511,	3127.7363,	3129.3203,	3131.2491,	3135.7155,	3198.3222,
ETBERb by H TS	-312.237176	3.83773	-1029.4885,	49.1921,	109.6928,	196.4068,	203.1378,	226.0420,
		1.53291	254.9431,	269.8127,	319.5872,	332.8309,	339.1149,	370.6450,
		1.48832	385.0967,	449.5366,	463.8577,	518.3915,	746.5563,	858.2266,
			889.8509,	922.2449,	932.6750,	972.5432,	990.6501,	1055.2937,
			1060.3089,	1105.7867,	1169.8777,	1191.0332,	1235.4479,	1272.8227,
			1291.9152,	1296.8700,	1347.2635,	1411.0673,	1425.1227,	1427.6113,
			1434.4381,	1452.3289,	1458.2720,	1503.6055,	1510.0957,	1513.0623,
			1516.4530,	1526.2839,	1529.3533,	1531.2459,	1547.7671,	3040.4937,
			3051.6041,	3054.9300,	3056.5651,	3063.7606,	3118.5044,	3120.1859,
			3125.9518,	3128.3331,	3133.7179,	3134.9867,	3136.4326,	3138.3014

ETBERc	-312.226824	4.00467	-1204.3880,	33.3689,	81.6430,	134.5086,	170.3632,	212.9021,
by H TS		1.44932	255.6327,	271.4229,	286.7334,	342.0113,	344.4929,	360.0075,
		1.42137	454.4277,	465.1758,	513.8719,	591.7841,	752.0191,	838.4695,
			874.6255,	918.0805,	930.3571,	972.0834,	989.7373,	1052.0906,
			1053.0543,	1084.7169,	1100.3731,	1193.4693,	1237.3267,	1237.5429,
			1240.8785,	1267.1801,	1288.5708,	1315.7702,	1412.0617,	1425.8615,
			1431.4807,	1452.7357,	1497.9729,	1504.5421,	1514.0713,	1517.4874,
			1532.0862,	1532.5450,	1546.3696,	1556.7464,	1761.5689,	3009.6994,
			3040.5851,	3052.4890,	3053.3124,	3061.3079,	3116.2269,	3119.3653,
			3121.0880,	3124.7246,	3126.0776,	3133.3965,	3134.4909,	3202.7013
ETBERa	-387.397325	3.95485	-1170.2837,	41.5334,	95.0872,	136.5363,	181.3259,	240.8258,
by OH		0.88041	263.8531,	271.0339,	288.4766,	330.5494,	335.4546,	373.5464,
TS		0.86925	447.8519,	456.6517,	531.0108,	600.9830,	749.2966,	835.3994,
			852.9108,	918.8991,	943.0344,	969.2848,	976.1907,	1026.1371,
			1049.9872,	1091.2504,	1150.4660,	1191.3128,	1198.8042,	1228.6717,
			1240.3856,	1274.0398,	1296.9324,	1313.5302,	1417.8321,	1425.5594,
			1437.1139,	1449.9842,	1482.9817,	1513.3929,	1513.9606,	1522.6348,
			1530.0730,	1534.6681,	1541.0261,	1561.2297,	1804.2083,	3002.9697,
			3032.5316,	3054.8156,	3057.5976,	3059.6640,	3114.6737,	3123.0825,
			3127.2511,	3127.7363,	3129.3203,	3131.2491,	3135.7155,	3198.3222
ETBERb	-387.400922	2.26389	-158.2527,	61.5925,	89.5197,	96.6129,	143.1015,	194.5047,
by OH		1.29938	207.9510,	242.1737,	255.9714,	264.1427,	311.6528,	335.5402,
TS		1.04452	347.2676,	354.2351,	441.1794,	463.8590,	511.3456,	642.6192,
			744.7525,	818.7139,	855.5175,	924.9845,	931.1124,	972.7125,
			976.7306,	1054.1197,	1061.1702,	1105.3215,	1144.6959,	1180.0758,
			1233.8233,	1270.2696,	1292.7221,	1296.1990,	1399.1568,	1426.6031,
			1431.4937,	1440.6235,	1456.4633,	1495.5922,	1505.2121,	1511.8928,
			1514.2445,	1516.1992,	1527.4287,	1530.5127,	1532.9869,	1547.0380,
			2490.8206,	3033.1842,	3052.8446,	3055.5680,	3059.1036,	3063.0751,
			3117.7269,	3123.0596,	3128.0864,	3128.6808,	3130.4319,	3135.2628,
			3137.2190,	3145.0874,	3661.8053			
ETBERc	-387.396095	3.64211	-1259.4768,	22.4198,	43.2212,	58.2846,	108.5530,	120.8348,
by OH		0.77709	191.8189,	210.3741,	258.0327,	272.3794,	306.6763,	338.0052,
TS		0.75637	350.6275,	394.4851,	444.7182,	452.8226,	505.8881,	669.9822,
			747.9614,	819.1798,	848.1122,	907.9599,	917.5007,	929.7065,
			970.0673,	988.9045,	1050.3564,	1055.5940,	1086.0558,	1124.8180,

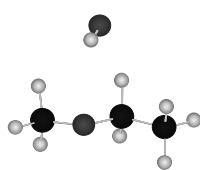
			1197.3679, 1236.4231, 1249.8351, 1268.2904, 1290.5182, 1311.5971, 1415.0468, 1422.8975, 1431.5887, 1448.8955, 1451.0252, 1498.9854, 1502.7777, 1515.0254, 1517.9646, 1530.3250, 1531.5213, 1547.1453, 1557.2158, 3018.9498, 3047.7821, 3053.2390, 3056.7904, 3061.2395, 3100.8796, 3117.1197, 3121.8238, 3124.5341, 3127.2885, 3133.1049, 3133.8544, 3176.0608, 3687.2006
ETBERb	-461.323073	2.5133436	43.6674, 62.4007, 116.1011, 195.4875, 213.5449, 247.2532,
O2		1.0539884	263.0098, 283.5659, 286.1068, 312.4978, 331.9974, 368.4906,
		0.9180796	399.1014, 446.7447, 473.1844, 516.8258, 572.3425, 745.8508,
			811.9332, 862.3206, 924.1778, 935.9391, 975.9937, 982.5220,
			1057.9311, 1063.0114, 1085.2583, 1157.0626, 1201.6160, 1213.4071,
			1237.2752, 1277.1646, 1299.5665, 1351.7513, 1403.6651, 1427.0520,
			1430.6191, 1438.6711, 1455.9066, 1504.2483, 1512.1170, 1516.0663,
			1516.5461, 1517.8152, 1530.4421, 1532.5993, 1547.3722, 3052.9232,
			3058.5107, 3065.0863, 3072.5244, 3090.3307, 3118.9268, 3127.3319,
			3129.4935, 3136.5367, 3136.8867, 3147.0751, 3148.5787, 3161.2578
ETBERb	-461.961718	2.1921046	-86.6146, 29.5815, 49.3606, 69.3826, 117.3455, 143.6009,
+O2	(B3LYP	0.7794439	188.0203, 190.7641, 218.9365, 234.4242, 258.0559, 269.0751,
r(C-O)=	Energy)*	0.6784351	325.1849, 338.7542, 359.4959, 372.2150, 456.5732, 459.5120,
3.4 Å			521.8090, 748.4338, 857.6981, 926.6546, 936.8304, 976.8937,
			978.1704, 1025.7846, 1058.9864, 1063.3098, 1158.5403, 1211.2036,
			1258.0697, 1276.2454, 1298.4674, 1423.5456, 1428.6856, 1431.8345,
			1455.4456, 1459.4364, 1491.8616, 1494.9561, 1503.5816, 1512.0202,
			1515.0524, 1525.3112, 1528.6321, 1535.4400, 1545.1517, 2863.8654,
			3057.8746, 3060.5133, 3067.3524, 3070.3748, 3124.9594, 3127.2403,
			3131.2261, 3133.7513, 3137.8541, 3138.5631, 3142.9017, 3213.3191
(R3) via	-461.286112	2.23368	-1515.3695, 98.9427, 144.9837, 201.5339, 210.7699, 227.7565,
7 ring TS		1.30497	275.9843, 287.1751, 297.8995, 312.7542, 362.7623, 417.5634,
		1.03807	439.8745, 467.2742, 524.3416, 551.5622, 621.6843, 654.5668,
			759.0027, 851.0001, 867.2490, 908.7414, 919.7059, 951.2724,
			972.8041, 988.2274, 1019.8226, 1054.5897, 1110.3149, 1139.3403,
			1174.5606, 1209.1080, 1235.6799, 1269.9522, 1281.7253, 1373.6141,
			1406.7130, 1421.7790, 1434.8697, 1439.5410, 1464.6073, 1503.9460,
			1507.2857, 1513.1132, 1516.4424, 1519.6893, 1526.2934, 1545.3682,
			3054.8758, 3061.9892, 3076.4407, 3077.5155, 3114.0473, 3124.7089,
			3130.7478, 3140.8462, 3148.2396, 3155.4873, 3158.5360, 3207.5873

(R3) via	-461.265152	2.91292	-2012.4700,	47.9470,	89.1560,	130.2852,	199.5118,	218.1208,
5 ring TS		0.9669	257.2017,	265.7531,	298.2075,	323.8206,	346.4538,	392.7432,
		0.88424	404.0190,	464.3867,	496.5945,	531.1705,	584.5722,	672.6971,
			758.4408,	874.0999,	877.6044,	925.4665,	936.5312,	956.2972,
			976.7358,	983.1219,	1022.1545,	1059.6747,	1062.7542,	1089.5653,
			1130.0644,	1186.5311,	1230.6600,	1275.9592,	1297.4979,	1341.0025,
			1409.9643,	1430.9881,	1432.7668,	1457.3663,	1478.5688,	1503.5167,
			1510.7326,	1516.0017,	1528.9458,	1532.1729,	1545.8377,	1734.7021,
			3044.3325,	3056.1406,	3058.4548,	3065.5966,	3121.0375,	3127.7733,
			3129.6641,	3135.1619,	3136.2527,	3138.1845,	3145.1625,	3230.4551
(R4)	-461.277106	2.51922	-1072.7784,	41.5195,	94.2556,	127.0954,	134.5690,	196.8480,
elim TS		0.92802	207.2587,	257.6517,	267.3532,	329.3860,	340.6159,	344.6520,
		0.82085	356.0999,	447.3493,	463.6307,	476.0098,	536.6834,	591.9307,
			646.7190,	751.9511,	852.7958,	915.4278,	928.7612,	936.0337,
			978.6794,	1004.6410,	1059.9902,	1062.7732,	1065.8070,	1208.4625,
			1254.8964,	1280.0592,	1296.5259,	1301.4975,	1326.9565,	1338.6983,
			1430.1553,	1433.7365,	1458.5650,	1464.3977,	1502.1919,	1508.5351,
			1514.1841,	1528.1131,	1530.8403,	1543.9857,	1610.4688,	1639.6454,
			3057.5460,	3062.5676,	3070.1256,	3125.2907,	3132.3460,	3133.6956,
			3136.6786,	3139.7582,	3141.1677,	3157.6091,	3207.0481,	3224.5487

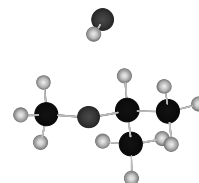
* Energy of effective TS of ETBERb+O2 was calculated by only B3LYP/6-31G(d) method. Activation energy was calculated as the difference of the sum of SPE and ZPE by B3LYP/6-31G(d) method between effective TS and ETBERbO2.



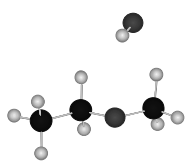
DME(p)



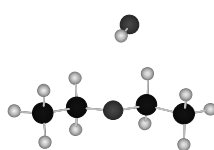
EME(s)



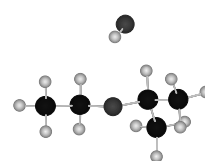
IPME(t)



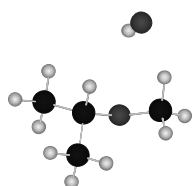
EME(p)



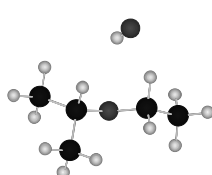
DEE(s)



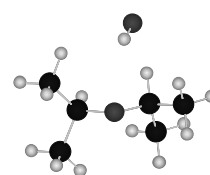
IPEE(t)



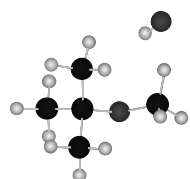
IPME(p)



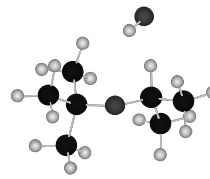
IPEE(s)



DIPE(t)



MTBE(p)



IPTBE(t)

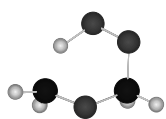
Fig. B The B3LYP/6-31G(d) optimized geometries for TS of (R1) by OH radical for ethers except for ETBE.

Table B. The B3LYP/6-31G(d) unscaled harmonic vibrational frequencies, the rotational constants, and the energies at 0 K by each calculation methods for TS of (R1) by OH radical for ethers except for ETBE.

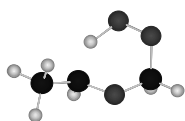
Species	Energies (hatee)	Rotational Constants (GHz)	Frequencies (cm ⁻¹)					
DME(p)	-230.436290	9.30460	-133.0808,	104.8811,	139.8082,	240.8709,	278.9559,	304.9217,
	(G3MP2B3)	4.16162	423.3807,	517.6553,	952.3093,	1119.3937,	1171.9944,	1197.5728,
	-230.40252	3.23164	1211.6640,	1276.0249,	1477.0133,	1486.3442,	1507.7669,	1517.7512,
	(CBS-QB3)		1520.5387,	1542.6966,	2769.6902,	3002.2850,	3018.7558,	3055.5639,
	-230.425821		3137.3776,	3143.2518,	3652.6739			
	(G3MP2)							
EME(s)	-269.678114	4.19139	-150.1805,	74.7710,	138.4028,	148.3401,	223.6611,	252.6703,
	-269.63433	3.68274	297.1638,	322.5548,	472.5933,	575.0359,	826.5312,	876.4242,
	-269.667672	2.17117	1037.5444,	1125.4483,	1149.3221,	1173.9343,	1198.6831,	1248.1789,
			1297.3293,	1408.7457,	1444.7440,	1495.9165,	1512.5529,	1513.3261,
		1516.5065,	1535.7888,	1545.0630,	2677.0035,	2994.5733,	3008.5997,	
		3060.5717,	3062.6047,	3132.5345,	3136.0876,	3142.8615,	3653.1816	
IPME(t)	-308.919989	3.09470	-108.4915,	77.4149,	111.4047,	145.9504,	195.2463,	211.5685,
	-308.86557	2.56677	255.5919,	291.5219,	349.0167,	370.1182,	461.0125,	489.2374,
	-308.908592	1.90816	559.7980,	805.7497,	924.1130,	938.0798,	959.5159,	1104.7883,
			1148.3750,	1167.1997,	1189.4027,	1209.6784,	1238.7858,	1353.2420,
		1384.6690,	1423.0615,	1441.8918,	1493.8024,	1508.1849,	1510.4072,	
		1521.1155,	1526.1510,	1538.3363,	1542.1828,	2686.7756,	3015.5542,	
		3051.9751,	3059.7595,	3075.3700,	3122.5490,	3130.0934,	3132.2808,	
		3136.3049,	3139.6572,	3651.5797				
EME(p)	-269.677567	5.83555	-127.9092,	78.8948,	110.4954,	141.6203,	236.0601,	265.1420,
	-269.63327	2.61968	288.9805,	312.3447,	463.4013,	532.7148,	836.2631,	869.5978,
	-269.665316	1.99344	1038.6182,	1119.8850,	1148.1796,	1178.8793,	1205.2749,	1242.7055,
			1315.5678,	1421.1155,	1451.9081,	1476.7331,	1501.2081,	1514.3396,
		1518.3419,	1531.3140,	1557.6826,	2752.1581,	2990.4354,	3018.5944,	
		3025.0500,	3059.8403,	3130.4859,	3134.8352,	3136.0209,	3654.3840	
DEE(s)	-308.919502	3.60380	-147.6197,	66.7043,	88.4393,	123.0689,	152.2162,	193.7323,
	-308.86533	2.01974	237.0398,	256.7504,	326.0418,	432.2343,	443.1839,	584.2401,
	-308.907121	1.43708	821.5289,	837.7530,	863.8782,	954.2553,	1062.5677,	1106.1557,

			1146.7791,	1170.4598,	1192.3112,	1207.0079,	1295.0857,	1314.6572,
			1392.2308,	1424.8517,	1439.0093,	1462.8138,	1511.8431,	1513.1411,
			1515.1151,	1531.0089,	1535.7063,	1558.0279,	2661.8844,	2992.1666,
			2999.9162,	3033.2626,	3059.4925,	3060.2372,	3130.1831,	3131.7015,
			3134.6723,	3135.6910,	3654.7226			
IPEE(t)	-348.161339	2.54536	-105.4577,	60.6374,	92.4243,	113.1942,	149.5748,	189.2167,
	-348.09674	1.65000	214.5935,	247.5287,	263.6782,	340.0081,	344.8491,	397.7804,
	-348.148129	1.29433	472.8194,	497.2927,	568.3568,	817.5557,	838.6623,	898.6827,
			940.4976,	959.9096,	988.1584,	1096.8528,	1130.4847,	1161.6848,
			1186.2378,	1203.0103,	1209.8926,	1319.6278,	1347.9016,	1382.5702,
			1420.1726,	1427.0066,	1442.7823,	1453.8686,	1509.5132,	1512.2735,
			1514.8572,	1524.6685,	1530.3124,	1537.1195,	1555.2188,	2670.6137,
			3009.8726,	3045.8560,	3053.4114,	3057.7672,	3059.5346,	3122.2040,
			3128.1161,	3129.6351,	3133.3640,	3136.0345,	3139.2631,	3653.1470
IPME	-308.918926	3.91985	-134.0497,	50.6874,	79.6417,	140.9242,	207.5608,	235.4567,
(p)	-308.86426	2.03939	245.0799,	268.2814,	320.6214,	362.8784,	448.8700,	493.0547,
	-308.904929	1.65860	561.5047,	806.6179,	920.4082,	941.4571,	957.2555,	1117.9406,
			1143.7079,	1161.1143,	1176.5483,	1209.2624,	1241.7431,	1389.0161,
			1401.2383,	1431.5510,	1445.7100,	1467.7932,	1500.8361,	1512.5555,
			1514.4013,	1523.1157,	1528.8728,	1538.7088,	2732.8457,	3016.5821,
			3038.2812,	3053.0825,	3057.8766,	3121.9047,	3124.4215,	3128.3590,
			3132.3037,	3134.8589,	3656.0154			
IPEE(s)	-348.161041	2.67439	-156.7611,	44.8671,	69.8315,	90.6577,	149.3033,	199.1737,
	-348.09636	1.60611	222.6578,	246.7023,	265.5652,	309.0565,	343.0722,	414.8360,
	-348.146856	1.21315	467.5501,	478.5392,	606.9437,	818.4202,	822.7900,	896.9864,
			939.4589,	954.6506,	988.8366,	1103.4504,	1132.9591,	1157.6237,
			1176.4450,	1192.4497,	1218.5987,	1291.9500,	1377.0688,	1390.4990,
			1415.8356,	1429.8850,	1441.8667,	1448.2063,	1511.2952,	1512.2716,
			1514.2844,	1515.9384,	1526.6714,	1535.7956,	1541.2837,	2642.2709,
			3018.4618,	3026.1837,	3052.1876,	3057.1335,	3059.2766,	3121.3432,
			3125.1242,	3127.9371,	3130.9280,	3131.8473,	3135.2860,	3655.3915
DIPE(t)	-387.401898	2.01267	-109.9339,	41.2049,	95.7909,	102.3036,	128.1685,	192.8843,
	-387.32652	1.43447	211.9957,	224.6477,	269.8095,	275.7024,	309.3276,	346.8019,
	-387.387399	1.00547	366.3104,	405.2087,	448.1706,	482.9269,	511.5560,	546.3475,
			799.0025,	859.4713,	922.7533,	937.5351,	940.5680,	953.6839,
			958.9316,	1039.3911,	1134.3725,	1158.9603,	1165.8596,	1183.9159,

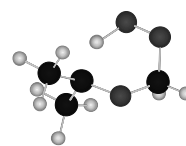
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MTBE	-348.158125	3.35210	-118.3931, 74.4581, 99.8525, 132.3548, 214.1351, 251.0360,
(p)	-348.09380	1.50324	252.4873, 264.7405, 266.5690, 286.2211, 340.6412, 368.0363,
	-348.144256	1.36909	411.5229, 457.2396, 511.6927, 622.2561, 726.5884, 858.2795, 924.6939, 933.0466, 974.0134, 1054.5976, 1058.8167, 1131.5616, 1167.9228, 1214.1863, 1234.4430, 1271.1775, 1299.7743, 1425.8022, 1430.1417, 1451.8997, 1454.8351, 1494.5266, 1503.3563, 1509.7166, 1513.2636, 1516.2753, 1532.2505, 1533.5025, 1546.3669, 2557.1000, 3044.3742, 3054.0148, 3056.7906, 3063.9330, 3118.0220, 3123.6486, 3128.3745, 3130.0343, 3131.3036, 3135.7759, 3146.1337, 3663.8734
IPTBE(t)	-426.639938	1.72510	-98.9462, 75.4042, 105.2105, 114.3415, 135.9114, 191.5233,
	Not found	1.14069	202.6482, 212.3214, 254.1444, 263.8337, 274.9849, 302.3877,
	-426.624648	0.92812	320.6758, 328.0529, 347.6472, 379.2234, 424.0196, 449.6496, 492.5566, 542.0036, 558.3073, 730.8987, 816.9625, 890.2060, 921.6728, 925.9693, 935.5427, 953.9534, 972.0332, 1024.8197, 1055.7984, 1065.6044, 1153.4909, 1168.7130, 1201.3138, 1233.5073, 1268.6299, 1284.5899, 1336.7379, 1383.7105, 1417.6587, 1425.3301, 1431.5533, 1439.5418, 1455.7074, 1502.0043, 1506.8844, 1510.9688, 1514.0908, 1518.9993, 1522.6383, 1527.8707, 1534.5655, 1540.0762, 1548.5361, 2675.9600, 3052.5361, 3054.1768, 3057.5182, 3060.9777, 3066.1385, 3119.5446, 3120.8613, 3122.6878, 3127.4211, 3131.5606, 3134.3607, 3141.9763, 3143.5260, 3145.8170, 3152.3939, 3656.8535



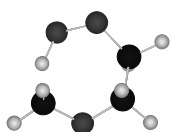
6 ring TS(p)



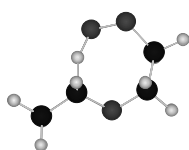
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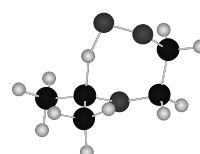
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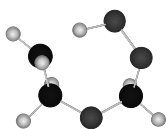
7 ring TS (p adjacent O)



7 ring TS (s ad. O)



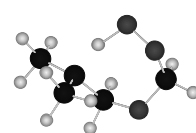
7 ring TS (t ad. O)



7 ring TS(p)



7 ring TS (s)



7 ring TS (t)

Fig. C The B3LYP/6-31G(d) optimized geometries for TS of (R3) for ethers.

Table C. The B3LYP/6-31G(d) unscaled harmonic vibrational frequencies, the rotational constants, and the G3MP2B3 energies at 0 K for TS of (R3) for ethers.

Species	Energies (hatee)	Rotational Constants (GHz)	Frequencies (cm ⁻¹)					
6ringTS (p)	-304.316429	8.51750 5.18355 3.56895	-1672.4016,	252.0411,	402.7260,	470.0935,	476.8851,	590.3327,
			689.1756,	914.0893,	944.6468,	1027.3947,	1121.7986,	1152.6967,
			1191.2151,	1204.2060,	1255.4606,	1315.4217,	1413.8869,	1492.1997,
			1513.1537,	1650.2288,	3047.5093,	3054.0563,	3175.1248,	3204.1187
6ringTS (s)	-343.561495	6.52074 2.60045 2.06880	-1682.6626,	138.5878,	188.6605,	228.9582,	395.2514,	416.4710,
			459.7653,	513.6610,	656.3397,	876.8292,	896.6969,	929.4632,
			989.8373,	1061.1133,	1129.4157,	1152.4328,	1174.0214,	1206.0469,
			1265.9971,	1309.6185,	1376.5500,	1421.8396,	1440.5326,	1503.5745,
			1506.3661,	1517.7162,	1651.8530,	3031.3056,	3035.3146,	3044.6464,
			3107.1558,	3143.1895,	3169.3828			
6ringTS (t)	-382.805835	3.93123 1.90967 1.86759	-1644.9433,	113.9110,	174.0669,	182.5303,	201.7350,	257.8160,
			357.1849,	396.2724,	465.3023,	485.5367,	545.3024,	675.2253,
			814.1023,	924.7024,	947.0141,	952.5139,	985.8046,	998.1509,
			1081.2032,	1148.4105,	1163.0603,	1212.7059,	1245.6840,	1272.5664,
			1309.1318,	1420.2355,	1423.4342,	1437.7556,	1498.6898,	1504.4899,
			1511.7826,	1519.7107,	1525.4922,	1648.6492,	3025.6280,	3034.8350,
			3057.9389,	3106.2002,	3111.0685,	3138.7630,	3145.8017,	3162.9248
7ringTS (p ad. O)	-343.546283	5.09364 3.45524 2.30800	-1786.5145,	169.2307,	212.5476,	343.7003,	378.2386,	448.0274,
			517.2360,	600.1551,	622.2094,	824.2615,	894.0017,	950.2924,
			1022.4283,	1053.5376,	1097.5194,	1127.0994,	1196.8029,	1233.1832,
			1270.5228,	1301.5131,	1334.0511,	1404.2030,	1424.3233,	1478.7154,
			1483.6814,	1513.0827,	1555.6580,	3026.7855,	3039.1213,	3057.5750,
			3113.5034,	3119.4196,	3189.3355			
7ringTS (s ad. O)	-382.791393	4.05765 2.01904 1.46658	-1757.8900,	109.2210,	174.9505,	210.4859,	238.8508,	292.5006,
			348.4909,	398.4092,	479.2130,	550.1426,	597.5373,	825.6750,
			876.5472,	898.6933,	949.1845,	953.5567,	1049.4160,	1082.9122,
			1117.5341,	1130.1764,	1165.5069,	1198.7828,	1283.9334,	1296.5823,
			1327.0344,	1380.7823,	1406.9831,	1430.1935,	1440.2944,	1479.0590,
			1504.2861,	1508.3323,	1519.0285,	1563.5463,	3018.1192,	3024.9925,
			3037.7100,	3055.9190,	3109.0178,	3109.4424,	3115.9598,	3142.4595

7ringTS (t ad. O)	-422.035067	2.85228 1.56940 1.36720	-1711.3793, 291.8896, 556.6738, 956.2292, 1168.3576, 1405.7443, 1507.5001, 3034.1176, 3118.2628,	93.3982, 337.2017, 592.8151, 977.1139, 1197.0484, 1419.8028, 1511.8574, 3049.9425, 3143.3493,	143.7371, 363.4879, 794.0920, 986.5496, 1257.0995, 1428.4926, 1517.9032, 3056.5850,	194.3446, 370.5647, 854.1380, 1047.9693, 1262.0551, 1435.4470, 1535.6787, 3105.5852,	203.7131, 430.1826, 908.8887, 1115.5030, 1296.2583, 1479.1120, 1550.3364, 3109.8395,	215.7472, 490.1410, 953.1252, 1134.1071, 1326.6207, 1497.6173, 3029.5171, 3115.6869, 3146.8033
7ringTS (p)	-343.553885	4.99911 3.56121 2.33879	-1637.8644, 539.3752, 998.7976, 1251.0108, 1491.9560, 3119.9040,	165.0918, 581.1000, 1001.8968, 1310.3638, 1497.0570, 3145.5362,	197.4360, 660.2165, 1044.9339, 1346.8047, 1511.0198,	361.5640, 826.6081, 1119.8944, 1401.7668, 3009.2210,	401.7664, 855.0597, 1140.4649, 1434.3304, 3035.5439,	452.6008, 914.1184, 1187.0968, 1459.8338, 3057.5702, 3213.8130
7ringTS (s)	-382.795115	4.06106 2.00017 1.45914	-1708.5793, 358.8627, 898.0582, 1110.9586, 1338.1965, 1505.2311, 3034.2860,	106.2017, 442.9225, 913.0568, 1119.5997, 1348.6469, 1509.3240, 3052.8292,	159.5503, 472.3452, 929.3208, 1157.8205, 1413.4349, 1515.8368, 3083.3580,	193.9228, 567.3064, 958.8713, 1188.9626, 1433.0626, 1517.9189, 3116.7284,	215.7304, 634.0149, 1005.9258, 1251.9375, 1438.6168, 2999.0294, 3131.4657,	293.4808, 795.3673, 1076.1718, 1298.6820, 1492.5491, 3008.7420, 3143.8660
7ringTS (t)	-422.039489	2.87795 1.54386 1.35462	-1721.0762, 205.1159, 487.6415, 951.1196, 1126.1343, 1348.0043, 1498.3344, 3003.3002, 3098.3027,	100.0718, 265.4990, 559.0843, 966.4895, 1178.0786, 1402.3223, 1503.6295, 3004.2877, 3123.7817,	138.0412, 332.6090, 634.4988, 985.7773, 1213.5403, 1421.6246, 1509.0076, 3010.8903, 3143.5941,	184.2049, 339.1458, 821.8176, 1005.5820, 1231.8817, 1430.2094, 1513.8061, 3035.9784, 3148.1825,	189.2120, 391.3784, 913.1387, 1015.3752, 1281.6233, 1443.6957, 1520.3438, 3054.2884, 3085.5503,	