This file contains DFT-B3LYP//6-311G** optimized geometries,
total energies, and harmonic vibrational frequencies of
reactant, product, and transition state species calculated for:

A. Andersen and E. A. Carter,
"First-Principles-Derived Kinetics of the Reactions Involved
in Low-Temperature Dimethyl Ether Oxidation",
Molecular Physics, 106, 367-396 (2008).

The optimized geometries and harmonic
vibrational frequencies of reactant, product, and transition
state species not included here are included in the
supplemental information for:

A. Andersen and E. A. Carter,
"A Hybrid Density Functional Theory Study of the Low-
Temperature Dimethyl Ether Combustion Pathways. I:
Chain-Propagation",
Israel J. Chem., 42, 245-260 (2002).

A. Andersen and E. A. Carter,
"Hybrid Density Functional Theory Predictions fo Low-Temperature
Dimethyl Ether Combustion Pathways. II. Chain-Branching
Energetics and Possible Role of the Criegee Intermediate",
J. Phys. Chem. A, 107, 9463-9478 (2003).

The file for the second and third articles above will be included
with this file along with 1, 10, and 40 atm rate constant
expression for reactions discussed in the kinetics (the first
article listed above).
Note that total energies are included in the text of the
second and third articles above.

OCH2OC(=O)H decomposition:

TS: OCH2OC(=O)H -> HCO + HC(=O)OH

	angstroms		
atom	x	y	z
C	-0.7747298917	1.2333672310	0.2556561950
C	1.6565923323	0.6423365005	0.1487172685
O	0.8934710288	1.2521216868	-0.6465654438
O	-1.1892933111	2.3391915145	0.5097382645
O	1.3084113398	0.1720880188	1.2602515878
H	-0.1058381981	0.6566116933	1.0903054718
H	-1.2619843712	0.5382134632	-0.4436226369
H	2.7066379066	0.5095112167	-0.1552683653

total E: -303.68586473330 hartrees

harmonic vibrational frequencies(cm^-1):

-352.47 177.48 296.39 351.12 503.58 800.30 901.45
1001.70 1047.94 1117.69 1324.33 1333.02 1358.95 1551.51
1684.37 1855.46 2985.44 3007.74

TS: OCH2OC(=O)H -> HOCH2OCO

	angstroms		
atom	x	y	z
C	-1.7205168010	0.2982598540	0.0209027040
C	0.3981045780	0.1724672470	-0.0770593730
O	-0.6142840980	0.9810905460	0.0318876730
O	1.6104618310	0.6356124280	-0.0041189870
O	-1.7997232680	-0.3787799780	-1.0858454700
H	0.2493388060	-0.7570894960	-0.2059270740
H	-1.7306261060	-0.3001464310	0.7585808040
H	-2.4598941800	0.8915339110	0.0840578000

total E: -303.67309363458 hartrees

harmonic vibrational frequencies(cm^-1):

-1194.05 187.60 318.14 459.63 569.77 741.02 848.54
1022.71 1061.94 1134.75 1146.23 1212.31 1404.52 1538.06
1875.49 1968.65 3004.88 3057.05

HOCH2OCO

	angstroms		
atom	x	y	z
C	-1.7652190047	0.1976893861	-0.0340927201
C	0.5822218047	0.3302511794	0.1376373876
O	-0.5503718878	1.0074647193	-0.0593846413
O	1.6849684149	0.7529559718	0.1356104016
O	-1.9384813645	-0.5258012388	-1.1951869359
H	-1.3525058650	-1.2910433491	-1.1784531571
H	-1.7268740519	-0.4264532972	0.8631667538
H	-2.5622817812	0.9331444195	0.0264110155

total E: -303.70873295130 hartrees

harmonic vibrational frequencies(cm^-1):

77.94 224.63 286.35 448.66 484.23 665.20 947.18
1026.03 1095.09 1142.29 1294.21 1410.49 1447.70 1516.31
1884.53 3047.59 3166.36 3810.14

HPMF bimolecular decomposition (by HC(=O)OH and H2O):

TS: HPMF + HC(=O)OH -> HC(=O)OC(=O)H + H2O + HC(=O)OH
[Aplincourt & Ruiz-Lopez, JPCA, 104, 380-388 (2000)]

	angstroms		
atom	x	y	z
C	2.1258387506	-0.8151441215	0.4267199021
C	1.6011971267	-1.4766247488	2.6990611432
O	-0.2550728956	0.1695441365	0.4027637126
O	0.9722416399	-1.0875084096	-0.1029993971
O	2.4551648130	-1.4977869178	1.6744218769
O	0.5163300478	-0.9476577284	2.7386253417
H	2.2199299206	0.3647659457	0.6004224207
H	2.9422719750	-1.0476124625	-0.2697769100
H	2.0349451531	-2.0293611574	3.5409552838
H	-0.2803029830	-0.1846876537	1.3245273886
C	1.9900269273	2.8356981693	0.1417588340
H	3.0928453661	2.9201917376	0.1472297464
O	1.2709337445	3.6884292434	-0.3094974433
O	1.5573726068	1.7133434087	0.7068695339
H	0.3883267491	1.0269135123	0.4725664404

total E: -569.29133394704 hartrees

harmonic vibrational frequencies(cm^-1):

-848.46 36.21 87.90 101.69 133.38 160.30 223.34
252.09 310.65 325.55 424.30 528.33 567.83 675.84
765.14 790.57 843.55 908.31 1034.45 1042.22 1049.01
1093.39 1159.21 1189.37 1255.14 1308.03 1370.55 1398.04
1411.18 1439.59 1554.82 1670.70 1755.55 1766.47 2030.20
2944.31 3032.59 3068.66 3425.06

TS: HPMF + HC(=O)OH -> HC(=O)OC(=O)H + H2O + HC(=O)OH
[This work]

	angstroms		
atom	x	y	z
C	2.1517356293	-0.9829985159	0.5454082724
C	1.5711870418	-1.4985812915	2.8258485951
O	-0.2100590601	0.0383340549	0.4159291993
O	1.0145357994	-1.1844570342	-0.0429723967
O	2.3729799984	-1.7236545692	1.7918303903
O	0.6049812213	-0.7697544939	2.8523075912
H	2.4213716200	0.1991247655	0.7453205604
H	2.9805163197	-1.2629551220	-0.1180919251
H	1.9072232060	-2.0829579008	3.6906692717
H	-0.1063148484	-0.1301240743	1.3836204824
C	2.0049700112	2.3914633315	0.3963211796
H	2.3521183957	3.4377830160	0.3842479316
O	2.8129382244	1.5552597831	0.8870097775
O	0.8677086443	2.1664469469	-0.0806300877

H	0.2903955548	1.0053415106	0.1542700647

total E: -569.30694920096 hartrees

harmonic vibrational frequencies(cm^-1):

-1306.55 66.60 67.56 123.30 162.15 230.43 246.37
251.02 329.75 346.52 376.29 540.51 563.69 704.46
756.01 802.12 832.52 868.32 1007.07 1042.57 1068.91
1101.03 1183.08 1250.76 1300.70 1344.26 1376.86 1397.55
1406.69 1414.87 1479.31 1578.21 1606.29 1753.65 1779.78
2993.71 3034.41 3068.85 3389.98

TS: HPMF + H2O -> HC(=O)OC(=O)H + 2H2O

angstroms

atom	x	y	z
C	2.1569360605	-0.9224692057	0.5466088207
C	1.7899825739	-1.6113365195	2.8813626013
O	-0.0752388163	0.7040424227	0.2653482345
O	1.0687745028	-0.9104248036	-0.1032390243
O	2.2302793705	-1.9061141084	1.6648719710
O	1.3720776887	-0.5489635785	3.2801908778
H	2.3046309121	0.2434210560	1.0268813976
H	3.0839427792	-1.0783950983	-0.0240907128
H	1.8630237677	-2.5035832611	3.5186197062
H	-0.6832748022	0.1300419583	0.7532813448
H	1.7755699805	1.1383707611	2.4328896155
O	1.9547746841	1.4793750096	1.5362688965
H	1.0508388784	1.3895666667	1.0752512805

total E: -455.93265284796 hartrees

harmonic vibrational frequencies(cm^-1):

-832.03 33.64 91.85 188.03 199.81 253.27 265.06
388.34 405.52 445.09 551.84 611.13 689.30 702.76
727.07 827.57 840.06 982.54 1047.70 1061.43 1194.91
1300.59 1397.34 1405.63 1421.26 1531.06 1687.65 1768.20
2784.60 2996.51 3039.86 3645.33 3795.66

Criegee Intermediate (CH2OO) decomposition:

TS: CH2OO -> HCO + OH

angstroms

atom	x	y	z
C	-1.2709476791	-0.5699816938	0.1461857722
O	-0.2941101551	0.1742409238	-0.1079312333

O	0.8114902893	-0.7751600389	-0.0188697114
H	-2.2354738824	-0.0404503339	0.1316243147
H	-0.2973005431	-1.5061971387	0.2446923422

total E: -189.57698905757 hartrees

harmonic vibrational frequencies(cm^-1):

-1780.48 673.19 721.00 893.37 1147.72 1274.09 1528.49 2090.25 3021.13

TS: CH2OO -> c-CH2OO (dioxirane)

angstroms

atom	x	y	z
C	-0.1545282886	-0.7132257191	0.0012297738
H	-0.8834615585	-1.3995470091	-0.4376933157
H	0.8463356948	-1.0385482098	0.2634897774
O	-0.5369438841	0.4647296167	0.2837073061
O	0.6889545623	1.0480845520	-0.3027116382

total E: -189.59867418352 hartrees

harmonic vibrational frequencies(cm^-1):

-696.54 741.28 777.10 1014.51 1200.58 1407.58 1556.64 3052.30 3208.96

c-CH2OO (dioxirane)

angstroms

atom	x	y	z
C	0.0000000000	0.0000000000	0.7866456187
H	0.0000000000	0.9272126995	1.3604949219
H	0.0000000000	-0.9272126995	1.3604949219
O	0.7501799435	0.0000000000	-0.3808094444
O	-0.7501799435	0.0000000000	-0.3808094444

total E: -189.66906444228 hartrees

harmonic vibrational frequencies(cm^-1):

807.86 896.06 1024.69 1182.24 1252.44 1313.40 1550.52 3052.89 3146.87

TS: c-CH2OO (dioxirane) -> OCH2O (methylenebis(oxy))

angstroms

atom	x	y	z
H	0.9108877795	0.0207306437	1.2123485603
C	0.0036803772	0.0030306695	0.5886523012

H	-0.9086728529	-0.0354334111	1.2071994882
O	0.0237383194	0.9984762950	-0.3773175251
O	-0.0266390764	-0.9998232958	-0.3676106846

total E: -189.63596268845 hartrees

harmonic vibrational frequencies(cm^-1):

-747.08 761.59 991.33 1057.73 1167.63 1207.73 1514.86
2923.98 2978.12

OCH2O (methylenebis(oxy))

angstroms

atom	x	y	z
O	0.0010676776	1.1735933767	-0.2728116615
C	-0.0002571942	0.0005196722	0.3663087665
O	-0.0008633386	-1.1738475716	-0.2716921617
H	0.8659919269	0.0002340111	1.0788887559
H	-0.8661725686	-0.0023874011	1.0791799719

total E: -189.66253320943 hartrees

harmonic vibrational frequencies(cm^-1):

491.88 587.77 798.26 910.14 1154.68 1160.31 1238.79
2788.29 2800.66

TS: OCH2O (methylenebis(oxy)) -> H2 + CO2

angstroms

atom	x	y	z
H	-0.6671335119	-0.0081359488	1.2104742442
C	0.0027412541	-0.0034911801	0.2462116313
H	0.6694883335	-0.0043029616	1.2122628706
O	0.0001599122	1.1644125707	-0.2537879460
O	0.0017248800	-1.1719609063	-0.2544321056

total E: -189.65776197261 hartrees

harmonic vibrational frequencies(cm^-1):

-1324.30 565.51 627.63 689.72 966.44 1208.96 1517.98
2350.70 2423.69

CO2

angstroms

atom	x	y	z
O	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	1.1603683349

O	0.0000000000	0.0000000000	2.3207366698

total E: -188.64117135771 hartrees

harmonic vibrational frequencies(cm^-1):

666.67 666.67 1374.38 2435.75

TS: OCH2O (methylenebis(oxy)) -> HC(=O)OH

angstroms

atom	x	y	z
O	0.1393903081	1.1496820109	-0.1457285101
C	-0.1711025235	-0.0533493245	0.3304372305
O	0.0170999826	-1.1776500590	-0.2691127564
H	0.8508098673	0.0843637711	0.8987339562
H	-0.9445575210	-0.0571849227	1.1290608619

total E: -189.65703454854 hartrees

harmonic vibrational frequencies(cm^-1):

-1012.02 461.76 647.71 982.80 1098.96 1285.13 1365.38
2453.43 2878.99

TS: HC(=O)OH -> CO + H2O

angstroms

atom	x	y	z
C	-0.2832338440	-1.3617982490	0.5365793341
O	0.7615501847	-1.2774898120	0.0750207065
O	-1.3554435786	-2.8642139640	0.3084756394
H	-1.4093633388	-1.5308365428	0.7362310009
H	-1.4230341326	-3.0956110415	-0.6299125686

total E: -189.70621416044 hartrees

harmonic vibrational frequencies(cm^-1):

-1639.53 319.42 398.35 576.10 785.90 1048.99 1950.35
2596.53 3764.24

TS: HC(=O)OH -> CO2 + H2

angstroms

atom	x	y	z
C	-0.0002707197	-0.0004787541	0.0001502385
H	0.0003883223	0.0000746265	1.4541195615
H	0.9700998414	-0.0000255198	1.0716560350
O	1.2392062071	-0.0004496080	-0.1959082375
O	-1.0675802422	-0.0004203065	-0.4723268624

total E: -189.70372226662 hartrees

harmonic vibrational frequencies(cm^-1):

-2248.70 608.62 732.66 867.07 1075.44 1339.45 1728.23
2029.02 2136.10

CH2OO bimolecular reactions

TS: CH2OO + H2C=O -> SOZ

angstroms

atom	x	y	z
H1	-2.8716881071	-0.1639775734	-0.6322520355
C1	-2.8868214333	-0.9493584091	0.1395462198
H2	-3.7705010826	-0.9653280903	0.8083574625
O1	-1.9922870708	-1.7495127521	0.2645748914
O2	-1.1343303704	1.4491002447	0.1380019313
O3	0.0820233738	1.0724269627	0.6031870056
C2	0.5485407569	-0.0506357087	0.2834484012
H3	1.5239151154	-0.2689681647	0.7007345653
H4	-0.0411482654	-0.7282264879	-0.3253317239

total E: -304.17935994790 hartrees

-131.79 67.22 106.01 133.45 168.21 216.62 534.83
676.54 902.88 953.90 1191.28 1257.85 1274.90 1415.56
1540.20 1544.73 1798.40 2900.42 3008.35 3114.80 3271.89

SOZ (secondary ozonide)

angstroms

atom	x	y	z
H	-3.2412257935	-0.7662905387	-0.6014733830
C	-2.5339744017	-0.5509871021	0.2022278621
H	-3.0248087029	-0.4990331057	1.1809623597
O	-1.4919511643	-1.5145986568	0.2342610603
O	-1.9095480095	0.6748167784	-0.1212679569
O	-0.6929142477	0.5497225126	0.6784956801
C	-0.2950715676	-0.7541984995	0.3054163745
H	0.3569458530	-1.1235683151	1.0997921859
H	0.2041394219	-0.7521638195	-0.6704450638

total E: -304.25222986071 hartrees

harmonic vibrational frequencies(cm^-1):

171.68 378.90 713.38 755.27 851.05 929.19 958.39

1039.87 1090.97 1143.95 1147.45 1220.05 1224.64 1370.31
1423.86 1520.45 1532.23 3013.85 3016.71 3100.67 3101.95

TS: SOZ -> SOZ-diradical

	angstroms		
atom	x	y	z
H	-3.3756821021	-0.9129192929	-0.2575838091
C	-2.5258853869	-0.5583239536	0.3569235171
H	-2.8631673469	-0.5091904408	1.4051535833
O	-1.4872657909	-1.5243497324	0.2344154766
O	-2.1876192490	0.6409789365	-0.1380593947
O	-0.2936775469	0.3624480839	0.8123799749
C	-0.2461721813	-0.8282150072	0.1977830788
H	0.4856103997	-1.4347106314	0.7654989871
H	0.1082536673	-0.7582355379	-0.8436565973

total E: -304.21730659635 hartrees

harmonic vibrational frequencies(cm^-1):

-279.76 190.03 298.29 541.75 736.69 925.13 940.32
952.00 975.29 1078.68 1107.87 1156.69 1165.12 1330.07
1341.09 1398.58 1410.56 2915.92 2926.45 2954.65 2957.84

SOZ-diradical

	angstroms		
atom	x	y	z
H	-3.5068774458	-0.7405973517	-0.3436902659
C	-2.7814322479	-0.8372139158	0.4816337523
H	-3.2543385369	-1.5053933125	1.2371005646
O	-1.6381317511	-1.4568776772	-0.0738519942
O	-2.5903649095	0.3324196086	1.0950949553
O	-1.0299482503	-2.8018452764	1.7418639563
C	-0.6698494152	-1.8496864648	0.8792059638
H	-0.3639114401	-0.9757826120	1.4994035725
H	0.2226889250	-2.1470232733	0.3038422364

total E: -304.22390702872 hartrees

harmonic vibrational frequencies(cm^-1):

102.81 145.74 267.13 577.11 588.10 773.39 839.87
921.19 1046.28 1074.78 1095.15 1160.13 1225.16 1327.61
1333.10 1348.11 1387.96 2827.48 2840.37 2957.88 2961.46

TS: SOZ-diradical -> HOCH2OC(=O)H

	angstroms		
atom	x	y	z

H	-3.2384750072	-1.5131715985	-0.0087522690
C	-2.5686807895	-0.8875446600	0.6197551731
H	-2.5707858769	-1.6112358139	1.5714887285
O	-1.2251995653	-1.0052874000	0.1754825377
O	-2.9966443693	0.2744908125	0.9113282228
O	-1.3847371184	-2.8387563709	1.5576099590
C	-0.5578381136	-1.9777497072	0.9626989313
H	0.0791542775	-1.4227748008	1.6808809489
H	0.1350874599	-2.5561604985	0.3186137143

total E: -304.21297664059 hartrees

harmonic vibrational frequencies(cm^-1):

-1078.45 118.79 298.17 525.80 574.22 673.83 848.39
920.27 929.30 974.89 1091.01 1166.72 1242.47 1258.43
1298.66 1346.46 1386.30 1954.75 2864.02 2873.76 2899.65

HOCH2OC(=O)H (hydroxymethylformate, HMF)

angstroms

atom	x	y	z
H	-3.4873090772	-1.5751856867	-0.6043312059
C	-2.7023063444	-1.2355806424	0.0651844846
H	-3.0692086441	-0.4680978545	0.7534757641
O	-1.7429849448	-0.5790772163	-0.8255187894
O	-2.1710363854	-2.3317041517	0.7106389814
O	-0.4558400638	-0.1084882130	0.9721302097
C	-0.6830089943	-0.0486083025	-0.2104802360
H	-1.5586795073	-1.9947699636	1.3779980506
H	-0.0389913663	0.4539489453	-0.9448033363

total E: -304.37720464249 hartrees

harmonic vibrational frequencies(cm^-1):

152.13 255.89 315.78 508.95 603.73 806.89 862.06
1043.39 1068.97 1124.27 1192.98 1297.53 1395.51 1422.21
1454.66 1515.31 1782.64 3041.69 3044.58 3162.38 3776.66

TS: HOCH2OC(=O)H -> HC(=O)OH + H2C=O

angstroms

atom	x	y	z
H	-3.3501444632	-1.3309959766	-0.6186265122
C	-2.5956984762	-1.2747690198	0.1695583751
H	-2.8245771928	-0.5747807309	0.9816074228
O	-1.4887151112	0.0154434381	-0.6292212023
O	-1.8578067414	-2.2866040351	0.3754908328
O	0.0531197597	-0.9328925359	0.7102620726
C	-0.3269015349	-0.0853391540	-0.1572394463
H	-0.8240727895	-1.7457955862	0.7585267381

H	0.4269975847	0.6252282815	-0.5226317192

total E: -304.34470135044 hartrees

harmonic vibrational frequencies(cm^-1):

-1138.33 199.91 282.70 422.38 519.51 584.51 829.02
925.68 1064.33 1226.35 1271.42 1348.71 1375.03 1384.85
1436.05 1629.61 1677.24 1790.54 3010.95 3038.89 3107.03

TS: HOOCH2OH -> CH2OO + H2O

angstroms

atom	x	y	z
H	-0.7854357062	0.3192244664	0.4787046756
H	-0.1435621753	-1.1549848099	0.3071542169
O	0.0260450819	-0.2338092654	0.0757779633
O	-1.2153458346	1.3545033416	1.4924604904
O	0.1750676281	1.7813487898	1.4387502297
C	0.8796525704	0.7304144941	1.5675774139
H	1.9259309466	0.8305106048	1.2910526333
H	0.5598431029	-0.0335467410	2.2688447145

total E: -266.08667829759 hartrees

harmonic vibrational frequencies(cm^-1):

-442.11 352.55 414.66 529.16 598.21 702.29 801.82
880.92 1119.63 1207.19 1223.65 1386.93 1531.69 1662.99
2214.37 3100.68 3224.06 3824.00

HOOCH2OH (hydroxymethylhydroperoxide, HMHP)

angstroms

atom	x	y	z
H	-0.8537327941	1.3170359213	2.9798143797
H	0.1564771701	-0.7693330279	1.2961965781
O	0.5393449084	-0.1916417661	0.6276666342
O	0.0597152021	1.0368437454	3.1257292718
O	0.7046810185	1.7108262500	2.0009441863
C	1.3857094176	0.6975360394	1.2896170866
H	1.9427062279	1.2562754587	0.5357067093
H	2.0669925143	0.1805118863	1.9765522365

total E: -266.15824364048 hartrees

harmonic vibrational frequencies(cm^-1):

164.38 213.09 373.22 464.05 612.75 865.81 996.19
1059.36 1092.79 1273.76 1379.72 1399.13 1426.92 1490.50
3012.23 3116.11 3785.43 3827.20

TS: HOOCH2OH + H2O -> 2H2O + HC(=O)OH

	angstroms		
atom	x	y	z
H	1.3083124728	0.0777195827	1.9950590892
H	2.0241661439	-1.2322005599	1.3328430395
O	1.4530636771	-0.9687465436	2.0657774113
H	0.8044588200	1.7771790557	0.9993300773
H	-1.0054704549	-0.3075478527	-0.9391946987
O	-0.6623283501	-1.0349004525	-0.4048961844
O	0.6677832349	1.3119861223	1.8339444831
O	-0.9964702630	0.5530361795	1.2522465328
C	-0.8717527146	-0.6892662493	0.9445278932
H	0.1382990946	-1.1063041056	1.5322428802
H	-1.6371989292	-1.3235284751	1.4293157811

total E: -342.56266117894 hartrees

harmonic vibrational frequencies(cm^-1):

-1136.07 97.70 162.69 290.18 400.50 425.82 444.36
485.00 561.78 598.35 669.84 755.07 831.10 1000.24
1053.42 1139.69 1245.63 1271.22 1333.86 1450.50 1548.96
1681.86 2199.37 2936.45 3789.16 3817.52 3824.40