DFT-B3LYP//6-311G** optimized geometries and frequencies
of low-temperature species involved in low-temperature
combustion of dimethyl ether for the following articles:

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).

Species involved in chain propagation

CH3OCH2

angstroms

atom	x	y	z
O	-0.4665751434	0.1346058325	0.2216339500
C	0.5947417668	0.9713260374	-0.2195043858
C	-0.2643114621	-1.1938754361	0.0390163366
H	0.2756476278	2.0001546495	-0.0585898778
H	1.5081829191	0.7762177609	0.3528897907
H	0.7967260721	0.8154514643	-1.2864817408
H	-1.1060427041	-1.8019197379	0.3396765442
H	0.4019695664	-1.5097787809	-0.7596834124

harmonic vibrational frequencies(cm^-1):

184.71 325.11 431.25 612.44 960.93 1137.72 1168.87
1250.68 1286.16 1457.74 1486.63 1496.34 1502.71 2996.43
3053.66 3094.96 3130.83 3247.89

O2

angstroms

atom	x	y	z
O	0.0000000000	0.0000000000	0.6028505537
O	0.0000000000	0.0000000000	-0.6028505537

harmonic vibrational frequencies (cm^-1):

1642.22

CH3OCH2OO (helix)

angstroms

atom	x	y	z
O	-0.0004333524	0.0042663523	0.0005842595
O	0.0001774689	-0.0004029801	1.3223977136
C	1.3702658392	-0.0015199912	1.8518494632
O	1.9630582605	1.2322567520	1.7763091947
C	1.4124518695	2.2125960768	2.6582893527
H	1.4462946166	1.8643959813	3.6982377961
H	2.0313443258	3.1018179117	2.5541787690
H	0.3807428944	2.4525296121	2.3881746341
H	1.9477914215	-0.6954609590	1.2444916910
H	1.2246000825	-0.3515057110	2.8815609098

harmonic vibrational frequencies(cm^-1):

86.46 138.94 195.26 330.21 467.45 602.52 833.41
945.62 1100.96 1155.21 1173.49 1194.47 1237.73 1322.47
1406.96 1469.16 1487.35 1493.06 1508.40 3002.82 3018.69
3077.97 3140.98 3146.21

CH3OCH2OO (chair)

angstroms

atom	x	y	z
O	-0.0170445193	0.0082425880	0.0067975215
O	0.0020665553	-0.0021467549	1.3289063231
C	1.3777472253	-0.0020795829	1.8461231616
O	1.8532725159	-1.2747844384	2.0303150084
C	2.2223126644	-1.9669150722	0.8339246866
H	2.9369396058	-1.3770351076	0.2482926930
H	2.6891895517	-2.8968883436	1.1541533547
H	1.3484996013	-2.1873411178	0.2156256707
H	1.9633039938	0.5883812246	1.1327847842
H	1.2914498582	0.4684704811	2.8242833272

harmonic vibrational frequencies(cm^-1):

110.42 135.87 188.13 383.76 445.29 575.37 829.87
943.90 1116.84 1131.22 1174.34 1211.11 1239.53 1325.62
1405.58 1469.22 1485.83 1494.89 1505.56 3011.81 3030.16
3083.03 3138.05 3143.55

p-TS1

angstroms

atom	x	y	z
O	-0.0011368371	-0.0020139337	0.0022973560
O	-0.0020859608	0.0064394816	1.4234612531
C	2.3724278218	0.0017158850	0.4997553789
O	2.0796626935	1.0910464941	1.2882236090
C	0.7490832382	1.1069487262	1.8358256864
H	1.1994461603	-0.1558652983	-0.1508196305
H	2.4101501887	-0.9630983405	1.0168781627
H	3.2121411572	0.2259042803	-0.1518857325
H	0.3028932999	2.0476995274	1.5028749189

H	0.7921212058	1.0335876421	2.9254366307

harmonic vibrational frequencies(cm^-1):

-1718.22 168.53 328.22 444.50 562.57 598.94 709.80
899.95 910.73 1025.02 1098.57 1117.94 1162.30 1201.82
1255.71 1269.55 1410.85 1473.34 1489.44 1669.97 3023.54
3042.75 3105.42 3174.13

CH2OCH2OOH (helix)

angstroms

atom	x	y	z
O	-0.0011731590	0.0025118537	0.0004646966
O	-0.0005269804	-0.0000350668	1.4600196736
C	1.3349532539	0.0000810117	1.8769841699
O	2.0016566758	1.2235315085	1.6961469882
C	1.5519388981	2.2684971339	2.4484862889
H	-0.6501001051	-0.6974811526	-0.1519059577
H	2.1684667636	3.1511057720	2.3818507668
H	0.8970652502	2.0660590730	3.2873029509
H	1.2582219091	-0.2476797185	2.9438401942
H	1.9127539789	-0.7403631285	1.3235771872

harmonic vibrational frequencies(cm^-1):

86.75 144.79 168.98 246.61 327.21 422.94 477.84
612.01 867.56 966.37 1028.25 1109.59 1211.35 1244.27
1331.19 1389.96 1420.21 1456.41 1486.19 3012.59 3117.00
3130.70 3284.54 3784.34

CH2OCH2OOH (syn-chair)

angstroms

atom	x	y	z
H	-0.0206612738	-0.0998437554	0.0274659637
O	-0.0014995373	-0.0170329835	0.9939952995
O	1.4266194390	-0.0083564215	1.2478065961
C	1.8687663107	1.3190850124	1.2246997059
O	2.0531734736	1.8202806981	-0.0849662687
C	0.9337223481	2.2487686376	-0.7355692680
H	1.1449496608	2.6552719698	-1.7148513978
H	0.1092281515	2.6213958885	-0.1345972765
H	2.8583678726	1.2823632268	1.6800077058
H	1.1778880513	1.9578568146	1.7860455819

frequencies(cm^-1) harmonic vibrational:

138.46 164.35 270.00 375.31 389.20 449.43 607.89
687.85 874.40 950.94 1023.71 1121.76 1221.64 1233.35
1331.50 1395.47 1414.94 1457.78 1486.83 3029.78 3102.80
3134.22 3252.75 3720.87

CH2OCH2OOH (anti-chair)

angstroms

atom	x	y	z
H	-0.0070834741	0.0606705133	0.0005364439
O	-0.0127206815	-0.0377277379	0.9622342795
O	1.4267849600	0.0040793949	1.2111142815
C	1.7473731730	-1.0661506115	2.0558026965
O	1.5132404018	-0.8238902369	3.4200367773
C	0.2347407448	-0.9889066751	3.8698906175
H	0.1416181602	-0.9344397726	4.9435110959
H	-0.4856294827	-1.4815850162	3.2302448111
H	2.8286652929	-1.1649058421	1.9501615537
H	1.2176535067	-1.9679422501	1.7270360009

frequencies(cm^-1) harmonic vibrational:

115.17 141.24 148.47 249.12 386.36 412.22 443.54
583.65 861.03 963.51 1020.34 1113.13 1215.29 1240.00
1342.84 1379.31 1419.44 1451.61 1484.25 3018.05 3120.01
3138.91 3288.78 3781.30

p-TS2

angstroms

atom	x	y	z
O	0.0104060420	-0.0183066139	-0.0057323495
O	0.0096763497	0.0002014508	1.4636165306
C	1.2885402168	0.0087752026	1.8678938896
O	2.0311130544	1.7687839804	1.4943455643
C	1.2119255459	2.7074968278	1.3151688097
H	-0.8546985235	-0.4286246817	-0.1463996772
H	0.6684850925	2.8145213550	0.3680863652
H	0.9647534239	3.4058202225	2.1273760946
H	1.3337393436	0.0425203128	2.9480667131
H	1.9928789707	-0.5859545583	1.2999536181

harmonic vibrational frequencies(cm^-1):

-470.48 89.90 97.47 149.56 187.98 222.95 388.57
495.60 623.50 806.58 897.93 934.79 1145.04 1190.88
1217.46 1347.84 1409.48 1455.61 1555.43 2965.04 3049.95
3131.25 3269.22 3781.19

p-TS2'

angstroms

atom	x	y	z
O	0.0138610060	0.0221755058	-0.0152916730
O	0.0020498726	-0.0053031584	1.4371560665
C	1.2709577422	-0.0169538388	1.8819849193
O	1.8778373090	-1.9076141661	1.8038613495
C	0.9897478977	-2.7717802717	1.6064862663
H	-0.2900084898	-0.8785564297	-0.2023286855
H	0.4021852492	-3.1977686016	2.4314419734

H	0.7392383923	-3.1100020088	0.5877497355
H	1.2967437907	0.1400174135	2.9528017476
H	2.0289023047	0.4008928568	1.2346145838

harmonic vibrational frequencies(cm^-1):

-409.43 65.30 97.85 181.20 205.11 247.91 394.79
503.56 621.49 869.37 888.07 920.91 1153.23 1203.75
1214.93 1366.04 1382.76 1449.53 1563.12 2938.98 3020.52
3140.26 3279.41 3754.62

p-TS2"

angstroms

atom	x	y	z
O	-0.0129006504	0.0153311079	0.0076360970
O	-0.0034891798	0.0112400829	1.7553139226
C	2.6475610889	-0.0147459444	1.7503219724
O	2.0781280482	1.1469511073	1.9357502182
C	0.5955214736	1.1486867476	2.0716684212
H	-0.8009658906	-0.5431686343	-0.0448434359
H	2.0431781193	-0.8820600871	1.5290730784
H	3.7280969960	-0.0036662427	1.7593569789
H	0.3002141458	2.0113117351	1.4696377030
H	0.4434331086	1.3307480720	3.1427133705

harmonic vibrational frequencies(cm^-1):

-782.31 97.64 171.55 184.37 333.52 363.06 420.11
608.54 643.18 751.49 997.31 1041.72 1097.86 1206.52
1237.78 1268.46 1400.81 1431.77 1503.36 3023.05 3090.10
3152.08 3299.80 3796.92

H2C=O (singlet)

angstroms

atom	x	y	z
C	0.0000000000	0.0000000000	0.5997605406
O	0.0000000000	0.0000000000	-0.6001999456
H	0.0000000000	0.9385984800	1.1921813425
H	0.0000000000	-0.9385984800	1.1921813425

harmonic vibrational frequencies(cm^-1):

1202.24 1270.31 1539.49 1827.02 2869.42 2918.82

OH

angstroms

atom	x	y	z
O	0.0000000000	0.0000000000	-0.0577973418
H	0.0000000000	0.0000000000	0.9172857576

harmonic vibrational frequencies(cm^-1):

3705.51

p-TS3

angstroms

atom	x	y	z
O	0.0045699190	0.0005660698	0.0076552873
C	-0.0009925315	-0.0007479623	1.9441687245
C	1.0892519545	0.0000617228	-0.6211006486
H	-1.0535516233	0.1959345742	2.0921986964
H	0.3399535608	-1.0054494635	2.1574418737
H	0.6799958806	0.8090391310	2.1739667546
H	1.5895113059	-0.9398536770	-0.8953023465
H	1.6126434375	0.9382183623	-0.8556562817

harmonic vibrational frequencies(cm^-1):

-535.47 82.90 169.35 299.99 655.40 694.27 935.43
996.58 1217.67 1355.36 1425.83 1431.60 1559.17 2954.78
3032.70 3095.30 3254.42 3266.80

CH3

angstroms

atom	x	y	z
C	0.0000000000	0.0000000000	0.0000000000
H	1.0804984808	0.0000000000	0.0000000000
H	-0.5402492404	0.9357391331	0.0000000000
H	-0.5402492404	-0.9357391331	0.0000000000

harmonic vibrational frequencies(cm^-1):

543.16 1403.59 1403.62 3103.97 3283.04 3283.20

p-TS4

angstroms

atom	x	y	z
C	2.7896590000	-1.3957540000	-4.5267740000
C	3.6387000000	-1.4699980000	-2.5743210000
O	3.7141120000	-2.7485540000	-2.7858390000
O	2.6698350000	-0.9929980000	-3.2969510000
O	4.2293910000	-3.2883040000	-1.8499830000
H	2.0321750000	-1.3891110000	-5.0989620000
H	3.6264880000	-1.7195860000	-4.8357860000
H	3.7272590000	-3.2052300000	-1.1682990000
H	4.4647240000	-1.0586260000	-2.8017290000
H	3.4417320000	-1.3066680000	-1.6594990000

harmonic vibrational frequencies(cm^-1):

-704.96 127.62 180.75 220.28 259.02 353.78 523.53
679.38 892.65 987.02 1003.23 1097.24 1124.60 1157.71

1168.24 1208.52 1378.98 1506.92 1541.26 2994.13 3087.93
3110.26 3222.32 3800.34

1,3-dioxetane

angstroms

atom	x	y	z
O	1.0366404970	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	-0.9832144912
O	-1.0366404970	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	0.9832144912
H	0.0000000000	0.9038034940	1.6062647055
H	0.0000000000	-0.9038034940	1.6062647055
H	0.0000000000	0.9038034940	-1.6062647055
H	0.0000000000	-0.9038034940	-1.6062647055

harmonic vibrational frequencies(cm^-1):

170.21 892.15 943.05 995.28 1058.46 1074.54 1111.66
1116.89 1122.38 1171.32 1339.17 1439.26 1544.79 1581.08
2977.24 2994.78 3026.12 3029.32

p-TS5

angstroms

atom	x	y	z
C	2.7896590000	-1.3957540000	-4.5267740000
C	3.6387000000	-1.4699980000	-2.5743210000
O	3.7141120000	-2.7485540000	-2.7858390000
O	2.6698350000	-0.9929980000	-3.2969510000
O	4.2293910000	-3.2883040000	-1.8499830000
H	2.0321750000	-1.3891110000	-5.0989620000
H	3.6264880000	-1.7195860000	-4.8357860000
H	3.7272590000	-3.2052300000	-1.1682990000
H	4.4647240000	-1.0586260000	-2.8017290000
H	3.4417320000	-1.3066680000	-1.6594990000

harmonic vibrational frequencies(cm^-1):

-1001.29 81.01 166.00 264.55 319.02 387.50 488.64
575.38 702.57 907.35 969.81 1013.35 1156.39 1204.68
1227.75 1330.47 1337.54 1459.14 1502.24 3006.28 3013.34
3094.75 3129.76 3770.76

ethylene oxide

angstroms

atom	x	y	z
O	0.0000000000	0.0000000000	0.8013197857
C	0.0000000000	-0.7336818737	-0.4253149423
C	0.0000000000	0.7336818737	-0.4253149423
H	0.9195555813	1.2701370988	-0.6473055486
H	-0.9195555813	1.2701370988	-0.6473055486
H	-0.9195555813	-1.2701370988	-0.6473055486

H 0.9195555813 -1.2701370988 -0.6473055486

harmonic vibrational frequencies(cm^-1):

819.18 844.51 890.93 1040.31 1140.63 1143.45 1168.71
1173.01 1301.61 1505.61 1541.20 3075.36 3082.91 3155.81
3171.47

HOO

angstroms

atom	x	y	z
H	0.6158019581	1.1195311814	0.0000000000
O	0.6515857355	0.1485623674	0.0000000000
O	-0.6903868571	-0.2191030096	0.0000000000

harmonic vibrational frequencies(cm^-1):

990.58 1203.02 3718.70

Species involved in chain branching

OOCH2OCH2OOH ("W")

angstroms

atom	x	y	z
C	2.7586631005	3.7845751983	1.8592812671
C	1.7854533950	2.3808485339	0.2277016270
O	2.0008515072	3.6741858791	0.7107942937
O	4.1764450506	3.8990755641	1.4862569095
O	4.9030461578	4.0798779148	2.5682359927
O	3.0061759245	1.9325886997	-0.3517971610
O	2.7566202282	0.5452297781	-0.7058273561
H	2.9646486599	0.5751341235	-1.6495051137
H	1.4949627132	1.6896974867	1.0297586734
H	1.0002838020	2.4531606660	-0.5282041125
H	2.6741738119	2.9166446865	2.5200127757
H	2.4940921541	4.7122467482	2.3640829018

harmonic vibrational frequencies(cm^-1):

50.87 66.36 94.42 119.01 191.13 282.08 354.90
402.72 488.47 559.86 923.72 943.40 1010.90 1054.67
1085.89 1167.77 1186.92 1208.79 1265.18 1301.63 1376.80
1408.19 1439.67 1496.62 1530.62 3001.48 3044.54 3087.49
3140.37 3781.08

OOCH2OCH2OOH ("helix")

angstroms

atom	x	y	z

C	2.8673450420	0.8573154218	0.6317080504
C	0.6270122120	0.1627407753	0.9210241408
O	3.0151101537	3.0059842932	1.4402683887
O	2.6435942974	2.2827222977	0.3966597143
O	1.9146427394	0.3220948167	1.4824991407
O	0.5890673581	-0.7268511300	-0.1584301187
O	0.7887226234	-2.0712111595	0.3748785420
H	0.0471568673	-2.5184836002	-0.0561079328
H	-0.0046157742	-0.1820940188	1.7388201987
H	0.2610471813	1.0996173316	0.4879337561
H	3.8373377951	0.7494970161	1.1103982605
H	2.8313928813	0.4265049207	-0.3709263428

harmonic vibrational frequencies(cm^-1):

54.29 65.08 104.37 193.45 206.58 251.11 418.71
463.98 605.39 623.51 847.05 867.60 952.25 1026.55
1077.76 1142.53 1162.55 1206.52 1303.16 1332.92 1389.53
1403.13 1429.83 1475.06 1489.86 3046.46 3076.52 3131.09
3166.54 3775.84`

OOCH2OCH2OOH ("ring")

angstroms

atom	x	y	z
C	-0.0009760889	-0.0001793469	0.0008999964
C	0.0008896230	0.0027636445	2.3536734084
O	0.7500290611	-0.0001982580	1.1719982797
O	-0.5513440364	-1.3105975230	2.4855405369
O	-1.6427788485	-1.1991475490	3.4333862107
O	0.3349150024	2.1488228446	-0.7308467688
O	-0.5758074104	1.3111907139	-0.2619656074
H	0.6705143260	-0.2397281778	-0.8194226335
H	-0.8684460665	-0.6590519259	0.0575761826
H	-0.8163858170	0.7290169015	2.3375206868
H	0.7021061322	0.2169017489	3.1632219392
H	-1.2903487937	-1.7193933427	4.1689055015

harmonic vibrational frequencies(cm^-1):

-30.64 72.44 106.65 168.85 244.10 260.81 362.13
449.92 538.28 602.80 864.47 943.49 980.06 1020.87
1400.60 1433.70 1487.96 1534.51 3040.82 3085.45 3101.79
1099.09 1147.08 1174.96 1205.30 1270.77 1322.33 1377.19
3172.88 3767.77

b-TS1

angstroms

atom	x	y	z
C	0.0050339813	0.0071963334	-0.0034853525
C	0.0024010413	-0.0243777101	2.3557837282
O	0.7649020530	-0.0277411122	1.2162466285
O	0.6241247354	0.8256647941	3.2579758196

O	0.1126363693	0.4886418009	4.5680924004
O	-1.9065019634	0.6891574416	0.9707052370
O	-0.9030753556	1.0596564611	0.0299494451
H	0.7200276123	0.2206312181	-0.7956235353
H	-0.5157783015	-0.9451434039	-0.1466470457
H	-0.2139941881	-1.0058021279	2.7967123149
H	-1.1765149935	0.4449537950	1.9173585724
H	-0.2153895237	1.3556401721	4.8460769987

harmonic vibrational frequencies(cm^-1):

-1556.68 38.48 90.12 180.89 212.01 340.27 409.86
445.65 514.47 550.81 663.08 910.31 925.43 973.77
1022.46 1105.25 1131.01 1153.04 1184.98 1248.53 1299.37
1336.79 1402.98 1421.96 1488.10 1661.56 3016.83 3036.83
3152.81 3773.13

HOOCH2OCH(=O)H---OH [ap,ap]

angstroms

atom	x	y	z
C	0.0665777673	0.0199696262	-0.0411638788
C	0.0411391580	-0.1355209578	2.3249491750
O	0.7698249589	-0.0052814889	1.1998436569
O	0.5417871173	-0.0679025609	3.4130200092
O	-1.8620470976	-0.8683664671	4.7095749346
O	-1.1015701165	1.9495336776	0.2923131726
O	-0.0808637139	1.3119585385	-0.5276892328
H	0.6972010577	-0.4795080242	-0.7753427217
H	-0.9048223168	-0.4737151835	0.0637704050
H	-1.0297617201	-0.3254639421	2.1561884570
H	-0.6110478466	2.7259684901	0.5983365495
H	-0.9333864232	-0.5687156292	4.5915534646

harmonic vibrational frequencies(cm^-1):

37.63 63.61 88.77 148.84 176.47 204.18 253.87
346.64 424.81 505.24 538.34 608.69 697.77 878.15
1021.82 1050.13 1058.23 1114.04 1199.50 1322.12 1393.78
1407.53 1434.91 1482.91 1817.42 3017.67 3043.72 3145.62
3569.76 3771.46

HOOCH2OC(=O)H---OH [sp,ap]

angstroms

atom	x	y	z
C	2.4438728312	-1.2968373603	0.0589354963
C	3.5018189783	0.7799336497	0.4991627383
O	2.4208146975	0.0245678176	0.6730440962
O	4.4836506494	0.4535866919	-0.1256404181
O	5.7751212335	2.9209356930	0.4587145219
O	0.1765474162	-1.5815271773	0.0932842989
O	1.4422670710	-2.0510456396	0.6273394447
H	2.3121347916	-1.1783005754	-1.0172852960

H	3.3798672578	-1.7993490787	0.3042821237
H	3.3862286079	1.7457897531	1.0048780683
H	-0.1155016763	-0.9989816034	0.8099622087
H	5.6333557079	2.0210582870	0.0902181126

harmonic vibrational frequencies(cm^-1):

20.66 51.93 65.16 135.15 148.04 256.15 269.63
326.88 419.94 500.65 550.22 610.98 782.70 879.65
921.04 1061.77 1104.66 1139.29 1236.75 1290.42 1389.06
1394.87 1416.00 1477.67 1767.36 3073.84 3074.86 3146.40
3573.65 3755.25

HOOCH2OC(=O)H [ap,ap]

angstroms

atom	x	y	z
C	0.0314310000	0.0930210000	-0.0224240000
C	0.0759960000	-0.0955960000	2.3456710000
O	0.7581290000	0.1572910000	1.1285310000
O	-0.3082130000	1.0792870000	2.9898330000
O	-1.4243050000	1.6244510000	2.2315060000
H	-0.9931870000	-0.2820600000	0.1397700000
O	0.4864460000	0.4017850000	-1.0780110000
H	-1.0521330000	2.4790920000	1.9699070000
H	-0.7907920000	-0.7428640000	2.1747490000
H	0.7899460000	-0.5546360000	3.0285330000

harmonic vibrational frequencies(cm^-1):

85.05 133.24 189.97 269.94 340.28 423.19 536.13
695.27 877.28 1023.00 1029.71 1044.94 1091.48 1181.90
1318.59 1388.73 1409.49 1431.74 1482.65 1860.98 2981.54
3036.35 3139.98 3767.09

HOOCH2OC(=O)H [sp,ap]

angstroms

atom	x	y	z
C	-0.0034487853	-0.0187032113	-0.0011357373
C	-0.0055498881	0.0018361192	2.3663084077
O	0.7358391962	-0.0342171335	1.2470382559
O	-1.2027112958	0.0636195292	2.4057220871
O	1.5346801353	-1.2612976802	-1.1513583988
O	0.9076476192	0.0425302941	-1.0361015832
H	-0.6298347934	-0.9102099578	-0.0537130938
H	-0.5945694164	0.8958418604	-0.0713724662
H	0.6604221062	-0.0298882190	3.2403132300
H	2.3278080068	-1.1275117709	-0.6120627345

harmonic vibrational frequencies(cm^-1):

28.20 134.53 223.83 263.05 324.53 409.29 548.99

783.78 880.59 936.03 1038.80 1094.16 1140.78 1196.45
1287.79 1387.36 1398.47 1415.87 1479.99 1807.81 3033.37
3069.33 3137.29 3756.43

HOOCH2OC(=O)H [sp,sp]

angstroms

atom	x	y	z
C	1.4046397726	0.9544900423	-0.5532954107
C	0.4975615198	-0.6832233815	0.9973097955
O	-0.7240729464	1.8590826276	-0.6708812847
O	0.2946314476	1.0908100329	-1.3582496993
O	1.4772862525	-0.3216037672	0.1715911273
O	-0.5445974935	-0.1074913249	1.1937931024
H	1.4675174366	1.7703640041	0.1676452063
H	2.2751663957	0.8991192190	-1.2041601087
H	0.7744373658	-1.6215318669	1.4947277530
H	-1.0169347857	1.2115297651	0.0033759486

harmonic vibrational frequencies(cm^-1):

105.72 206.77 257.21 304.75 438.96 543.68 610.96
786.15 835.96 896.06 1046.18 1079.41 1150.94 1200.73
1311.58 1404.36 1425.64 1468.68 1501.30 1779.45 3056.71
3079.31 3158.37 3552.90

b-TS2

angstroms

atom	x	y	z
C	0.0071176626	-0.0058183177	0.0016969874
C	-0.0020255528	0.0089701100	2.6512679265
O	1.0030368050	0.0055528253	1.9244000425
O	0.4630561248	0.9988726679	-0.6250631829
O	-1.2064933302	0.0123248406	2.2105450518
O	-0.4179340439	2.1992380018	-0.3990447316
H	0.2375149570	2.8897535895	-0.5834196913
H	-0.9758612828	0.0138424518	1.0700551568
H	0.6264273119	-0.8613266744	-0.2861764582
H	0.1076762272	0.0026699059	3.7462624744

harmonic vibrational frequencies(cm^-1):

-987.24 93.85 121.82 164.97 220.60 286.02 417.00
507.81 621.44 652.05 843.09 952.07 1062.63 1241.72
1311.53 1337.80 1371.68 1385.53 1418.84 1703.70 1788.15
3014.22 3090.79 3760.18

HC(=O)OH-trans

angstroms

atom	x	y	z
C	-0.1287169044	-0.4039414370	0.0000000000
O	1.0687178641	-0.4038140100	0.0000000000

O	-0.9041274477	0.6963376168	0.0000000000
H	-0.3120148299	1.4651484235	0.0000000000
H	-0.7675443876	-1.2980488531	0.0000000000

harmonic vibrational frequencies(cm^-1):

632.98 699.29 1058.12 1131.67 1310.21 1411.27 1836.57
3042.15 3738.10

HC(=O)OH-cis

angstroms

atom	x	y	z
C	0.3958670863	0.1099062241	0.0000000000
O	0.3955113434	-1.0808533495	0.0000000000
O	-0.7423903452	0.8403568006	0.0000000000
H	-0.5218651617	1.7797831572	0.0000000000
H	1.3135650669	0.7284370165	0.0000000000

harmonic vibrational frequencies(cm^-1):

647.55 674.90 1132.46 1259.56 1294.48 1462.26 1885.85
3092.11 3822.66

HCO

angstroms

atom	x	y	z
H	0.5367808273	1.4506189657	0.0000000000
C	0.5367613093	0.3231217082	0.0000000000
O	-0.4365210463	-0.3338205129	0.0000000000

harmonic vibrational frequencies(cm^-1):

1116.36 1942.87 2628.61

OCH2OC(=O)H

angstroms

atom	x	y	z
O	0.0018140544	0.0009894132	0.0040883380
O	-0.0021603129	0.0001069169	2.3584307702
C	0.7180710825	-0.0011064850	1.1165613272
O	-1.6070580571	-1.0614697279	3.4983806158
C	-0.9455285068	-0.9661958623	2.5128433629
H	1.3522788333	0.9023551239	1.1642322375
H	1.4179461579	-0.8618921207	1.0894515151
H	-1.0284707454	-1.6328084531	1.6373010395

harmonic vibrational frequencies(cm^-1):

117.06 141.60 273.11 509.05 697.68 774.18 996.81
1035.01 1080.21 1128.04 1196.34 1320.78 1372.38 1432.65
1859.53 2876.75 2940.07 2974.42

b-TS3

angstroms

atom	x	y	z
C	-3.1509700000	-0.4279600000	0.4920570000
C	-3.6267610000	-0.7376790000	2.5609270000
O	-2.4305330000	-1.1539240000	2.8746280000
O	-1.6005420000	-0.6222000000	2.1920790000
O	-3.9227790000	-1.0561070000	1.3301830000
O	-2.6344840000	0.7190830000	0.8185930000
H	-0.8316190000	-0.9201960000	2.3968150000
H	-4.2545200000	-1.1495530000	3.1429650000
H	-3.6748670000	0.2053910000	2.6652140000
H	-2.9477590000	-0.8232450000	-0.3474620000

harmonic vibrational frequencies(cm^-1):

-1436.68 64.60 145.05 244.99 266.24 322.64 483.65
539.99 660.35 776.64 922.47 992.86 1040.06 1121.83
1178.15 1243.54 1283.34 1365.97 1396.71 1794.58 1823.00
3006.35 3047.32 3622.67

b-TS3'

angstroms

atom	x	y	z
C	-3.0491650261	-0.6269448772	0.2626957144
C	-3.3176514729	-0.9569376660	2.6153785155
O	-2.3569186748	-1.7932792935	2.7780056425
O	-1.1510060335	-0.2667553263	2.8616347734
O	-3.8944713099	-0.7829335886	1.3334936188
H	-1.9951972405	-0.5531593179	0.5624105979
H	-0.2105777475	-0.0686643405	3.0505686346
H	-4.1287090508	-0.9764433743	3.3569345787
H	-2.6673403593	0.0382126107	2.9047584375
O	-3.4676468506	-0.5647526980	-0.8499391724

harmonic vibrational frequencies(cm^-1):

-1381.74 97.94 139.28 150.89 297.76 335.96 478.13
533.50 665.89 713.47 974.15 1010.81 1045.26 1074.54
1144.89 1242.43 1261.04 1366.66 1427.71 1849.89 1878.22
3017.01 3046.43 3625.82

HC(=O)OC(=O)H [sp,ap]

angstroms

atom	x	y	z
C	0.4539003157	1.2984917204	0.0000000000
C	-0.3052286393	-0.9611008380	0.0000000000
H	0.7692984288	-1.1704516736	0.0000000000
O	-0.5888559542	0.4039636470	0.0000000000
O	1.6139523834	1.0245057992	0.0000000000

O	-1.1870627137	-1.7534642503	0.0000000000
H	0.0310158621	2.3110996217	0.0000000000

harmonic vibrational frequencies(cm^-1):

99.08 230.72 254.30 539.85 780.73 1006.40 1036.52 1051.02 1109.73 1387.02 1407.99 1826.01 1878.51 3058.45 3087.13

HC(=O)OC(=O)H [sp,sp]

angstroms

atom	x	y	z
C	1.2014397434	0.2086169924	-0.3305962391
C	-1.2014397434	-0.2086169924	-0.3305962391
O	-1.3432842247	-0.4843701017	0.8129350763
O	0.0000000000	0.0000000000	-0.9937177228
O	1.3432842247	0.4843701017	0.8129350763
H	-1.9981838072	-0.1050188640	-1.0800061196
H	1.9981838072	0.1050188640	-1.0800061196

harmonic vibrational frequencies(cm^-1):

72.80 214.23 247.48 551.72 809.36 974.82 1013.13 1044.26 1086.13 1398.67 1414.83 1812.27 1901.66 3038.59 3041.59

HC(=O)OC(=O)H [ap,ap]

angstroms

atom	x	y	z
C	0.0000000000	1.1838348136	0.3585813350
C	0.0000000000	-1.1838348136	0.3585813350
H	0.0000000000	-1.0361348976	1.4508743768
O	0.0000000000	0.0000000000	-0.3474459093
H	0.0000000000	1.0361348976	1.4508743768
O	0.0000000000	-2.2361242065	-0.1867168271
O	0.0000000000	2.2361242065	-0.1867168271

harmonic vibrational frequencies(cm^-1):

130.81 176.48 273.79 531.28 709.46 1027.86 1033.94 1058.84 1130.57 1394.69 1444.24 1840.00 1916.65 2979.09 3002.67

H2O

angstroms

atom	x	y	z
O	0.0000000000	0.0000000000	-0.0663835132
H	0.0000000000	0.7571876779	0.5267772642
H	0.0000000000	-0.7571876779	0.5267772642

harmonic vibrational frequencies(cm^-1):

1638.54 3811.42 3908.45

b-TS5

angstroms

atom	x	y	z
C	-0.5705524858	1.0263211178	-0.7815743617
C	-3.2764839041	1.7069207879	-2.1822277938
O	-1.4285930383	2.0253061169	-1.0021622059
O	-2.6071645295	1.8360401947	-3.2425939392
O	-1.7621921269	2.9973017530	-3.1515527390
O	-0.8833708138	-0.0590822869	-0.3747780779
H	-1.3369268950	2.6352511760	-1.9885705562
H	0.4784199156	1.3087779294	-0.9916026991
H	-3.5105356031	2.5627424213	-1.5643266407
H	-3.7549333296	0.7400346044	-2.0503493367

harmonic vibrational frequencies(cm^-1):

-986.41 22.25 114.42 130.90 259.14 393.46 480.72
619.35 747.54 815.41 849.06 1042.65 1084.46 1190.28
1223.99 1359.21 1393.28 1414.62 1568.32 1755.11 1806.39
2943.86 3129.73 3274.83

b-TS5' (HOOCH2OC(=O)H -> CH2OO...HC(=O)OH complex)

angstroms

atom	x	y	z
C	1.5749849470	1.4855674350	-1.2566543565
C	0.3496959389	-0.9055654240	1.2999128640
O	-0.5937993126	1.7429781297	-0.6532190591
O	0.4126538406	1.8227593336	-1.5825699463
O	1.4561481272	-0.4716038613	1.0566493903
O	-0.7936592828	-0.4661593881	0.8166127606
H	1.7688335515	1.0739561994	-0.2660202823
H	2.3044872303	1.5888542747	-2.0531379360
H	0.1831290961	-1.7556772536	1.9775056924
H	-0.6556414842	0.3442663705	0.2384738882

harmonic vibrational frequencies(cm^-1):

-55.68 62.64 148.41 190.00 217.62 259.84 536.96
686.30 705.42 866.11 993.91 1032.60 1087.16 1249.69
1272.01 1402.99 1433.71 1464.76 1562.27 1767.46 3016.44
3047.18 3082.10 3241.07

CO

angstroms

atom	x	y	z
C	0.0000000000	0.0000000000	0.6438514258
O	0.0000000000	0.0000000000	-0.4830420976

harmonic vibrational frequencies(cm^-1):

2220.3

b-TS4

angstroms

atom	x	y	z
C	-2.4337280000	3.6536930000	1.5580160000
C	-3.6073170000	-0.0068910000	-0.4329830000
O	-2.8383430000	0.0329450000	0.5948980000
O	-4.0719450000	1.1038360000	-0.8941500000
H	-3.8564980000	-0.8377960000	-0.8226600000
H	-2.2639960000	-0.5888850000	0.5550960000
O	-2.3450420000	4.9235400000	1.8234730000

harmonic vibrational frequencies(cm^-1):

-1198.24 182.18 222.21 335.97 474.57 763.75 842.77
1068.21 1247.76 1349.83 1385.86 1659.10 1771.38 2191.22
3003.07

CH2OO

angstroms

atom	x	y	z
C	0.4053654977	1.0854217372	0.0000000000
O	0.4049804349	-0.1746370467	0.0000000000
O	-0.7620240715	-0.8387772171	0.0000000000
H	-0.5434614074	1.6114864781	0.0000000000
H	1.3833854848	1.5482026328	0.0000000000

harmonic vibrational frequencies(cm^-1):

534.55 674.73 909.22 934.60 1241.69 1398.04 1527.83
3121.20 3278.41

CH2OO...HC(=O)OH complex

angstroms

atom	x	y	z
C	0.0071998771	-0.0068721963	-0.8050097704
C	0.0179883331	-0.0443855064	2.9607910617
O	2.0553853506	0.2015528194	0.1574284691
O	1.2229449368	0.2801468686	-0.9225399278
O	-0.8235379226	-0.3410951668	2.1387884258
O	1.2642068986	0.3048458197	2.7184464304
H	-0.4041012473	-0.2927991342	0.1659175016
H	-0.5546584187	0.0862506254	-1.7282463773
H	-0.1866050267	-0.0343138986	4.0412824523
H	1.4638795847	0.2671241194	1.7368339306

harmonic vibrational frequencies(cm^-1):

18.95 102.99 163.13 176.87 209.61 243.74 549.17
703.00 710.69 882.39 960.01 1055.24 1083.03 1250.32
1279.11 1406.35 1438.80 1477.80 1559.91 1769.88 3024.54
3027.83 3118.36 3232.98

b-TS6

angstroms

atom	x	y	z
C	0.0387450000	-0.3992270000	-1.3720790000
C	0.1522010000	-0.5777980000	1.0524940000
O	0.8802970000	-0.7081000000	-0.1285930000
O	-0.1559520000	0.7136410000	1.5895240000
O	-1.2779530000	1.5037820000	1.0106660000
O	0.5780030000	-0.6750020000	-2.4245490000
H	-0.6801190000	-0.5599170000	-0.8022660000
H	-1.4185490000	0.7149040000	0.8157200000
H	-0.9081010000	-0.2814550000	1.0736120000
H	0.3663070000	-1.4755850000	1.9583840000

harmonic vibrational frequencies(cm^-1):

-1261.56 58.43 139.93 208.37 220.09 273.50 397.54
570.00 628.63 666.71 874.09 891.83 1028.37 1080.04
1185.99 1220.35 1318.06 1348.22 1416.98 1473.65 2074.17
2242.23 3068.83 3707.24

H2

angstroms

atom	x	y	z
H	0.0000000000	0.0000000000	0.3720733746
H	0.0000000000	0.0000000000	-0.3720733746

harmonic vibrational frequencies(cm^-1):

4421.82

HC(=O)OOH-cis

angstroms

atom	x	y	z
C	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.2013470568
O	1.1067047299	0.0000000000	-0.7591202220
O	2.3010692909	0.0003494682	0.0476811744
H	1.9155167124	-0.0000303462	0.9501829795
H	-0.8718821162	-0.0001725720	-0.6656884766

harmonic vibrational frequencies(cm^-1):

342.34 347.88 477.42 846.25 888.58 1001.36 1143.55
1360.67 1492.47 1796.48 3072.12 3538.56

HC(=O)OOH-trans

angstroms

atom	x	y	z
C	-1.4003944846	2.2648397247	0.4844326853
O	-1.7879949297	2.8228876872	1.4602135525
O	-0.3434578823	2.7692754079	-0.2253978846
O	-0.1241686420	1.9332566528	-1.3925031398
H	0.8244979357	1.7679761394	-1.2971123322
H	-1.7900162418	1.3423904648	0.0302000115

harmonic vibrational frequencies(cm^-1):

191.70 226.52 383.38 609.94 948.70 1035.90 1101.30
1372.12 1401.39 1860.43 3033.97 3776.64

b-TS7

angstroms

atom	x	y	z
C	-0.0038831305	0.0349777771	0.0043968730
C	-0.0073291415	-0.0041455812	2.3576870774
O	0.7011879505	0.0408237120	1.1703639995
O	-1.1913972221	0.0315660548	2.4524333993
O	0.4301829454	-1.9039078515	-0.8074254215
O	0.6441989299	0.0085968389	-1.1001167664
H	-1.0784638276	-0.1068705596	0.0794391505
H	0.2657198050	1.2194539097	-0.7427231995
H	0.7193262424	-0.0684985698	3.1749189057
H	1.2801658235	-2.2443606617	-0.4910536504

harmonic vibrational frequencies(cm^-1):

-1650.24 62.38 159.01 208.82 254.67 346.07 442.88
488.65 559.50 655.08 779.86 795.71 957.62 1023.87
1041.80 1109.02 1336.11 1396.91 1440.52 1679.02 1843.16
3082.42 3173.45 3765.47

HC(=O)OCH(OH)2

angstroms

atom	x	y	z
C	-0.3070523389	-0.2177052225	0.0492446256
C	-0.5015449338	-0.0582730867	2.4484976466
O	0.2882632247	0.0677536243	1.3590213724
O	-1.6655642772	-0.3375550030	2.4582716612
O	-0.1020894104	-1.5174420623	-0.3089527799
O	0.3452047154	0.6139980144	-0.8473863146
H	-1.3810091355	-0.0530225418	0.1259902320
H	0.3773270566	1.5025011760	-0.4764899629
H	0.1044450084	0.1525361419	3.3421936853
H	0.8309998896	-1.6067548583	-0.5452254657

harmonic vibrational frequencies(cm^-1):

34.37 208.47 241.65 266.48 357.78 476.76 532.22
603.95 757.19 886.32 1041.42 1061.84 1145.50 1165.44
1255.06 1363.09 1404.54 1406.10 1477.78 1817.84 3021.73
3126.40 3784.17 3832.57