

## **Theoretical study of hydroxyl radical (OH·) induced decomposition of *tert*-butyl methyl ether (MTBE)**

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Supporting Information  
(2 Tables, 10 pages)

**Table 1.** Total Energies of Fig. 1 to 3. of the Main Manuscript.

1	-272.560125
2	-347.065142
3	-346.556829
4	-423.406179
5	-345.907158
6	-271.902858
7	-271.912860
8	-422.163366
9	-347.723420
10	-347.078251
TS:1->6	-348.232661
TS:4->9	-423.394292
TS:9->2	-422.718346
TS:9->3	-347.048892
TS:10->3 + H	-347.040432
TS:10->3 + H <sub>2</sub> O	-422.842392
TS:10->C <sub>4</sub> H <sub>9</sub> + HCOOH	-347.063704
TS:5->8	-345.890764
TS:3->5	-422.234089

**Table 2.** GAUSSIAN Archive entries

1

```
1\1\MF(BIN)-SILICIUM\SP\RHF\GFHFB4\C5H12O1\THEIS\28-Jun-2019\0\#\#N Geo
m=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\Ether\0,1\C,0
,-5.2614994882,1.0747142135,-0.0447357322\C,0,-4.0688962578,0.11326790
43,-0.0096298804\O,0,-2.9340968707,0.9933887133,0.0221879129\C,0,-1.65
07802434,0.4148357038,0.0595797527\C,0,-4.1299185507,-0.7579658831,1.2
554635696\C,0,-4.0572288214,-0.7601757126,-1.2746233794\H,0,-6.2067738
038,0.5246808693,-0.0713792587\H,0,-5.2041415591,1.7151525799,-0.92932
96068\H,0,-5.2549471924,1.7167367363,0.8405432369\H,0,-0.9393131471,1.
2450186259,0.0793016377\H,0,-1.4838237094,-0.1993072141,0.9560684121\H
,0,-1.4326468122,-0.2008694513,-0.8247651287\H,0,-3.3151316904,-1.4869
688915,1.291466682\H,0,-5.0701612912,-1.3170264341,1.2861053941\H,0,-4
.0731112297,-0.1316048261,2.1508278744\H,0,-4.9942477809,-1.3192243427
,-1.3583080233\H,0,-3.9489311561,-0.1353668484,-2.1663168183\H,0,-3.24
18333956,-1.4892857424,-1.2624566447\Version=EM64L-G09RevD.01\State=1
-A\HF=-271.292898\RMSD=8.030e-09\Dipole=0.0103494,-0.5424148,0.000789\
Quadrupole=1.7007349,-1.5220703,-0.1786645,-0.3711077,0.0543971,-0.009
4992\PG=C01 [X(C5H12O1)]\@\
```

2

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H11O2(2)\THEIS\03-Aug-2019\0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\ende\0,2\C,0,2.0395739032,-0.7658812038,-0.3112672418\C,0,0.7733524242,0.0269958672,0.0254421858\O,0,-0.2902828356,-0.7663475663,-0.563859254\C,0,-1.5989419598,-0.6288703436,-0.1041047609\C,0,0.6124607105,0.1550158563,1.5462465617\C,0,0.8104078718,1.4084113706,-0.644742728\O,0,-2.1449388902,0.5827946893,0.0041410877\H,0,2.9316722626,-0.2313602964,0.0283893342\H,0,2.1144928149,-0.9141989307,-1.3920140515\H,0,2.017664842,-1.7491677489,0.1673112372\H,0,-1.7219173941,-1.08882738,0.9100920032\H,0,-2.2116836707,-1.2698596285,-0.7706212637\H,0,-0.263751111,0.7499220495,1.8170913527\H,0,1.4918565706,0.653179773,1.9644314404\H,0,0.5294936948,-0.8307624174,2.0160389596\H,0,1.6745841746,1.9814908956,-0.2920646498\H,0,0.8939214435,1.2942875808,-1.729482452\H,0,-0.0985208512,1.9706884331,-0.4265217605\Version=EM64L-G09RevD.01\State=2-A\HF=-345.5666855\S2=0.761719\S2-1=0.\S2A=0.750106\RMSD=2.479e-09\Dipole=0.2665844,-0.1819714,0.3747346\Quadrupole=0.0996311,-0.5453962,0.4457651,2.7649617,0.36713,-0.6604702\PG=C01 [X(C5H11O2)]\@

3

N-N= 3.297496712521D+02 E-N=-1.468618271845D+03 KE= 3.445870724892D+02  
1\1\MF(BIN)-SILICIUM\SP\RHF\GFHFB4\C5H10O2\THEIS\25-Sep-2019\0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\ester\0,1\C,0,-5.4725831359,-0.2354263359,0.3826916028\C,0,-4.0464311829,-0.2929303242,-0.1729232375\O,0,-3.6110371621,1.0583797081,-0.5744160985\C,0,-3.5135015871,2.0497525011,0.3127372652\C,0,-3.0548722178,-0.8795538427,0.8363336383\C,0,-4.004468371,-1.0646160307,-1.4923390473\O,0,-3.74401062,2.015964631,1.4927373629\H,0,-5.8334456412,-1.2530562625,0.5618762856\H,0,-6.1438374987,0.2403066179,-0.3387106871\H,0,-5.5088636138,0.3200444726,1.3197516989\H,0,-3.1726113051,2.9519233625,-0.2229910901\H,0,-2.0386598108,-0.8539090524,0.4313886528\H,0,-3.3145961335,-1.9240521039,1.034990765\H,0,-3.0755623566,-0.3278194965,1.7760742217\H,0,-4.310985899,-2.1019355471,-1.3305591887\H,0,-4.6793369025,-0.6133311941,-2.2249354191\H,0,-2.993320562,-1.0622151034,-1.9087197248\Version=EM64L-G09RevD.01\State=1-A\HF=-345.0496387\RMSD=7.845e-09\Dipole=-0.0187497,-0.5633984,-0.6998235\Quadrupole=1.3373117,1.8231306,-3.1604424,0.7632247,-0.0158327,-3.0836011\PG=C01 [X(C5H10O2)]\@

4

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C5H13O3(2)\THEIS\07-Sep-2019\0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\ende\0,2\C,0,-2.1224210133,1.5620183889,0.1955955026\C,0,-1.1456389123,0.4613591323,-0.2268995485\O,0,0.1335885583,1.1365242402,-0.2407921774\C,0,1.2948167411,0.389865858,-0.4318379656\C,0,-1.1707825987,-0.6902397236,0.7903106876\C,0,-1.4900499587,-0.0437480986,-1.6364177399\O,0,1.92710262

7,0.0238828619,0.785272308\H,0,-3.1470447142,1.1799112898,0.22491346\H,0,-2.0806968529,2.3962390066,-0.5100038565\H,0,-1.8607766116,1.9412682126,1.1871762009\H,0,2.0113364691,1.0454676383,-0.9342625767\H,0,1.1187389575,-0.5022082621,-1.043811024\H,0,-0.4920183124,-1.5023246125,0.5098200678\H,0,-2.1762410609,-1.1184066012,0.8493914487\H,0,-0.9004597302,-0.326424626,1.786487719\H,0,-2.5039349357,-0.4554956822,-1.656445279\H,0,-1.4367890808,0.7789188285,-2.3550539033\H,0,-0.8099436526,-0.8349321452,-1.9657193159\O,0,2.137774536,-2.3549489538,0.6561558834\H,0,1.4070139252,-0.6708213921,1.2138653158\H,0,3.0749356202,-2.1411983599,0.802641793\\Version=EM64L-G09RevD.01\State=2-A\HF=-421.6137136\S2=0.758259\S2-1=0.\S2A=0.75005\RMSD=5.010e-09\Dipole=-0.140444,-0.6842536,-0.2137775\Quadrupole=3.7699864,-3.079143,-0.6908434,-3.1788644,-0.4876651,-1.5109561\PG=C01 [X(C5H13O3)]\\@

5

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H9O2(2)\THEIS\04-Oct-2019\0\#N Geometry=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\Rad\\0,2\C,0,-1.7422621498,0.8820905072,-0.3412400429\C,0,-0.8282353277,-0.1532952211,0.3043488872\O,0,0.5163388426,0.5369526172,0.270386688\C,0,1.5854597569,-0.0442323118,0.7448107899\C,0,-1.2061198429,-0.4170089123,1.7596180117\C,0,-0.7432415253,-1.4322649683,-0.5244882783\O,0,1.7734346515,-1.1071022078,1.2547040251\H,0,-2.7669939678,0.5004369442,-0.3796930851\H,0,-1.416456314,1.1038273262,-1.3608012131\H,0,-1.7400942411,1.812141136,0.2330447789\H,0,-0.5177994524,-1.1230163721,2.2268745151\H,0,-2.2151061164,-0.8399752184,1.8015521548\H,0,-1.2029330505,0.5141653716,2.333051246\H,0,-1.733323861,-1.8967081207,-0.576990967\H,0,-0.4170237525,-1.2094120888,-1.54421903\H,0,-0.0507036495,-2.1485704811,-0.0797104802\\Version=EM64L-G09RevD.01\State=2-A\HF=-344.4180361\S2=0.763002\S2-1=0.\S2A=0.750118\RMSD=7.404e-09\Dipole=-1.2652246,0.2019262,-0.3459859\Quadrupole=-1.3491845,-0.0827257,1.4319102,1.6494975,-1.4839397,1.419605\PG=C01 [X(C5H9O2)]\\@

6

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H11O1(2)\THEIS\25-Sep-2019\0\#N Geometry=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\cdot\\0,2\C,0,-5.5945353167,-0.9072470237,0.0020107175\C,0,-4.1958121566,-0.2609942637,0.0492221199\O,0,-4.4818185732,1.146971761,-0.0134197819\C,0,-3.3705191595,2.0160829236,0.0071972608\C,0,-3.4920276425,-0.6334763539,1.3662031683\C,0,-3.3897379754,-0.69033129,-1.1397398413\H,0,-5.5210416874,-1.9973276129,0.0405871909\H,0,-6.1081379919,-0.6207658741,-0.9190961937\H,0,-6.1907698068,-0.5600941341,0.8520110151\H,0,-3.7539154283,3.0181499156,-0.2031919726\H,0,-2.8687023853,2.03747086,0.9853830912\H,0,-2.6245151148,1.7561066903,-0.7572155688\H,0,-2.4808189974,-0.2209415226,1.4184956355\H,0,-3.4103498041,-1.7210219727,1.4562501708\H,0,-4.0662341356,-0.2585268207,2.2183765678\H,0,-3.6382415912,-0.2948597804,-

2.1185867085\H,0,-2.6724452334,-1.5002095017,-1.0751498709\\Version=EM64L-G09RevD.01\State=2-A\HF=-270.6605599\S2=0.763174\S2-1=0.\S2A=0.750109\RMSD=3.274e-09\Dipole=0.4597893,-0.2562187,0.0488861\Quadrupole=-0.7657497,0.6506161,0.1151336,1.1006165,-0.0575047,-0.110109\PG=C01 [X(C5H11O1)]\@

7

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C5H11O1(2)\THEIS\25-Sep-2019\0\#N  
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\CO dot\0,2  
\C,0,-5.6791741646,-0.7559359745,-0.0103102251\C,0,-4.222943608,-0.285  
911454,0.0031394267\O,0,-4.3305234508,1.1534606311,0.1296300774\C,0,-3  
.1985538072,1.8879592498,0.2478165912\C,0,-3.475207313,-0.8647313583,1  
.211056573\C,0,-3.5300523876,-0.6532603682,-1.3163748786\H,0,-5.731622  
62,-1.8453541486,-0.0922722803\H,0,-6.2140248312,-0.3167244842,-0.8570  
597237\H,0,-6.1847749107,-0.449998073,0.9095256775\H,0,-3.3936448521,2  
.9532488047,0.2840870135\H,0,-2.2775497519,1.525109917,-0.1993925646\H  
,0,-2.4444812598,-0.5031038707,1.2508251252\H,0,-3.4531362939,-1.95736  
64592,1.1546043089\H,0,-3.9733860051,-0.5757958103,2.1408304372\H,0,-3  
.5605349218,-1.7369015864,-1.4645100454\H,0,-4.0387331638,-0.175166046  
5,-2.158344697\H,0,-2.4802236584,-0.3485089689,-1.3285628161\\Version=  
EM64L-G09RevD.01\State=2-A\HF=-270.6677393\S2=0.761598\S2-1=0.\S2A=0.7  
50092\RMSD=9.136e-09\Dipole=0.2727272,-0.4812143,-0.1772782\Quadrupole  
=0.2004547,0.3167597,-0.5172145,0.970445,-0.4082148,-0.3775809\PG=C01  
[X(C5H11O1)]\@

8

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C5H11O3(2)\THEIS\05-Nov-2019\0\#N  
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\perox\0,2\  
C,0,-5.2619416283,1.0567963506,-0.1187340689\C,0,-4.0494789713,0.12537  
30173,-0.0887990782\O,0,-2.9421530542,1.0182525786,-0.4225142623\C,0,-  
1.665350186,0.5564750685,-0.3383712505\C,0,-3.8722814096,-0.4894252978  
,1.3038924029\C,0,-4.1712129072,-0.9562999762,-1.1691230132\O,0,-1.161  
3791511,0.7709270298,1.0419239976\O,0,0.004773102,0.1886084154,1.18951  
45453\H,0,-6.1793546367,0.498101622,0.086359538\H,0,-5.3542293986,1.53  
05085816,-1.0998464352\H,0,-5.1559828965,1.842958226,0.6334293276\H,0,  
-1.5273607896,-0.5108564156,-0.538080469\H,0,-1.0244365242,1.160217498  
9,-0.9865699554\H,0,-3.013602168,-1.1646143511,1.3474523492\H,0,-4.763  
7292463,-1.0680834056,1.5648320072\H,0,-3.7308191151,0.2909214734,2.05  
52287511\H,0,-5.0575504913,-1.5712256313,-0.9867893454\H,0,-4.26515966  
4,-0.4995256312,-2.158287456\H,0,-3.3069998641,-1.6274141534,-1.176771  
5848\\Version=EM64L-G09RevD.01\State=2-A\HF=-420.3818085\S2=0.764525\S  
2-1=0.\S2A=0.75015\RMSD=2.307e-09\Dipole=-0.7790639,-0.584084,-0.61431  
72\Quadrupole=-0.5915749,0.5406355,0.0509395,0.4370929,-3.3722323,-0.1  
348971\PG=C01 [X(C5H11O3)]\@

9

N-N= 3.479799411346D+02 E-N=-1.507908970687D+03 KE= 3.457443122395D+02  
1\1\MF(BIN)-SILICIUM\SP\RHF\GFHFB4\C5H12O2\THEIS\08-Jul-2019\0\#\#N Geo  
m=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\OH add\0,1\C,  
0,-5.2410571292,1.0452976004,-0.0961579028\C,0,-4.0374054518,0.1115638  
944,0.077900094\O,0,-2.925162475,1.0159270712,0.2458136402\C,0,-1.6235  
52682,0.6041070372,-0.0515034217\C,0,-4.2091914464,-0.731832043,1.3519  
904947\C,0,-3.8898910198,-0.7841784103,-1.1603454081\O,0,-1.0785561347  
, -0.3508039102,0.8331749137\H,0,-6.1732439057,0.475505933,-0.156449731  
6\H,0,-5.1351168979,1.6423555398,-1.0063159182\H,0,-5.305916868,1.7299  
282693,0.7537955627\H,0,-1.0183944868,1.5075545743,0.0631040671\H,0,-1  
.5446071896,0.2472681094,-1.0888868254\H,0,-3.3552862289,-1.3924710302  
,1.5143687182\H,0,-5.1158597623,-1.3432973854,1.2923771784\H,0,-4.2893  
549419,-0.0752650019,2.2223660147\H,0,-4.8118331779,-1.3532910346,-1.3  
104464093\H,0,-3.7102017973,-0.1891848285,-2.0610394473\H,0,-3.0774979  
06,-1.5120484847,-1.0602055861\H,0,-1.2745484988,-1.2305039003,0.49817  
69666\Version=EM64L-G09RevD.01\State=1-A\HF=-346.1896177\RMSD=4.730e-  
09\Dipole=-0.4057842,-0.643132,-0.7302569\Quadrupole=-0.7529382,1.2153  
657,-0.4624275,-0.1978834,-2.6566826,0.0885791\PG=C01 [X(C5H12O2)]\#@

10

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H11O2(2)\THEIS\27-Sep-2019\0\#\#N Ge  
om=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\h abs\0,2\C,  
0,-5.1998421542,1.121272368,-0.0240479481\C,0,-4.1099747114,0.05178381  
3,-0.0666303432\O,0,-2.8665388997,0.8371865893,-0.0850621976\C,0,-1.67  
17403652,0.2329495121,-0.0355839782\C,0,-4.1514687893,-0.8304120308,1.  
1836497565\C,0,-4.2114692891,-0.7809787136,-1.3482894972\O,0,-1.178087  
0654,0.1159955585,1.2463526477\H,0,-6.1921036937,0.6604601206,-0.01597  
92042\H,0,-5.1256133065,1.7745735645,-0.8977715226\H,0,-5.0924756373,1  
.7364987249,0.8732228109\H,0,-1.482092368,-0.6148349311,-0.7029456314\  
H,0,-3.3523329269,-1.5763609454,1.1718749469\H,0,-5.1084770856,-1.3595  
313257,1.2395566519\H,0,-4.033717395,-0.222990354,2.0844501915\H,0,-5.  
1740287414,-1.3006613462,-1.3860503612\H,0,-4.1311758767,-0.1383579886  
, -2.2297128598\H,0,-3.4259064058,-1.5407956565,-1.3992295291\H,0,-0.29  
12388022,-0.2567195335,1.1908089999\Version=EM64L-G09RevD.01\State=2-  
A\HF=-345.5659557\S2=0.759804\S2-1=0.\S2A=0.750073\RMSD=9.036e-09\Dipo  
le=-0.0211507,-0.8859129,-0.3054515\Quadrupole=4.3541774,-2.1797546,-2  
.1744229,-2.8543571,-0.1090016,0.0097746\PG=C01 [X(C5H11O2)]\#@

TS:1->6

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C5H13O2(2)\THEIS\06-Jul-2019\0\#\#N  
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\TS\0,2\C,0  
, -5.3724790445,0.9956242947,0.1404553003\C,0,-4.1426652079,0.081880561  
1,0.1314228125\O,0,-3.0372070801,0.9968212595,0.285528189\C,0,-1.73082  
28811,0.4535044509,0.3277901971\C,0,-4.20061162,-0.8968287405,1.301894

0378\C,0,-4.0494919191,-0.67688141,-1.2048075923\O,0,-3.7947704261,0.7  
609238735,3.1238910523\H,0,-6.2841628055,0.4170493331,-0.0338857208\H,  
0,-5.2818768007,1.752508954,-0.6429851663\H,0,-5.4576512262,1.49629885  
99,1.1077677372\H,0,-1.0488043682,1.3052967277,0.3914573744\H,0,-1.570  
1436791,-0.1830192194,1.2078768274\H,0,-1.4830836373,-0.1176717774,-0.  
5757419032\H,0,-3.3827525925,-1.6194599292,1.3383022385\H,0,-5.1664609  
638,-1.3969258694,1.4005914833\H,0,-4.0797451807,-0.224767446,2.326423  
3776\H,0,-4.9554440381,-1.2687133867,-1.3638649933\H,0,-3.9520351925,0  
.0337045136,-2.0314284573\H,0,-3.199908955,-1.3642756692,-1.233327876\  
H,0,-3.4052443819,1.3316936196,2.4374700819\\Version=EM64L-G09RevD.01\  
State=2-A\HF=-346.6796573\S2=0.787122\S2-1=0.\S2A=0.750511\RMSD=5.877e  
-09\Dipole=0.2321999,-0.4070711,-0.7968096\Quadrupole=3.256032,1.24943  
21,-4.5054641,0.5321325,0.7664203,0.4903697\PG=C01 [X(C5H13O2)]\@

#### TS:4->9

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C5H13O3(2)\THEIS\07-Sep-2019\0\#N  
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\H abs\\0,2\  
C,0,-5.1869590009,1.1316634558,0.025007745\C,0,-4.0870019591,0.0643583  
312,0.0049300541\O,0,-2.8779223026,0.8361265301,0.2334456944\C,0,-1.63  
06382113,0.3877834767,-0.1780313955\C,0,-4.2897102831,-0.9234306952,1.  
1646982942\C,0,-4.0734331424,-0.6639450694,-1.344016622\O,0,-0.9941469  
267,-0.5019325785,0.7034214631\H,0,-6.1744631071,0.6731745241,-0.08127  
93017\H,0,-5.0422846076,1.8451190401,-0.7911836899\H,0,-5.1589921089,1  
.6832695806,0.9687711715\H,0,-0.9902663392,1.2786385951,-0.1909704841\  
H,0,-1.6481107809,-0.0475120494,-1.1857244797\H,0,-3.568250481,-1.7428  
326017,1.1342115254\H,0,-5.2916332565,-1.3630226184,1.1174107211\H,0,-  
4.1869022255,-0.4015915946,2.1199183666\H,0,-5.0552322043,-1.115275109  
3,-1.5158797713\H,0,-3.8769130214,0.0321000754,-2.1660517474\H,0,-3.33  
36939904,-1.468475232,-1.3701698533\O,0,-1.4669426567,-2.624271833,0.0  
006917055\H,0,-1.4142610655,-1.4595277097,0.6770125026\H,0,-0.53416032  
87,-2.8769555179,-0.0863628985\\Version=EM64L-G09RevD.01\State=2-A\HF=  
-421.5843105\S2=0.76584\S2-1=0.\S2A=0.750165\RMSD=0.000e+00\Dipole=0.0  
517534,-1.0946516,-0.6952018\Quadrupole=1.3280476,1.4579148,-2.7859624  
, -4.7503625,-2.6224593,-0.6668866\PG=C01 [X(C5H13O3)]\@

#### TS:9->2

N-N= 4.318855465417D+02 E-N=-1.852814219895D+03 KE= 4.202174600354D+02  
1\1\MF(BIN)-CARBON\SP\RHF\GFHFB4\C5H12O3\THEIS\07-Sep-2019\0\#N  
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\TS\\0,1\C,0,1.82  
83564206,-0.954820903,0.0916576614\C,0,0.621595087,-0.0337576372,0.254  
2007513\O,0,-0.5212007784,-0.877715917,-0.0852060272\C,0,-1.87991017,-  
0.3571057445,-0.0291183515\C,0,0.5251835962,0.5104701029,1.6829945939\  
C,0,0.6399998463,1.1027528933,-0.7900788077\O,0,-2.1650230051,0.784845  
4264,0.4154389411\H,0,2.7521646566,-0.3932696623,0.2567351616\H,0,1.85  
75971715,-1.3877559436,-0.9117887481\H,0,1.7819985727,-1.7674802565,0.

8212558018\H,0,-2.1710150892,-0.561652903,-1.0990385652\H,0,-0.3104530  
173,1.2003873759,1.7935823678\H,0,1.4586997411,1.0291200364,1.92330418  
32\H,0,0.3769565184,-0.3250705213,2.3695243117\H,0,1.5123070934,1.7337  
831847,-0.5958209641\H,0,0.7226106296,0.6966097308,-1.8017226726\H,0,-  
0.2583603162,1.7155434678,-0.712175022\H,0,-2.3483469976,-1.2500474183  
,0.5090194117\O,0,-0.88853311,-2.1777327457,1.4773549285\H,0,-0.329429  
8498,-2.9399305655,1.7104040444\\Version=EM64L-G09RevD.01\State=1-A\HF  
=-420.7599204\RMSD=9.227e-09\Dipole=1.6447211,-0.9571109,-0.4034717\Qu  
adрупole=-2.6150239,1.2608283,1.3541956,3.7449342,2.3169067,-1.7235785  
\PG=C01 [X(C5H12O3)]\@

### TS:9->3

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H11O2(2)\THEIS\07-Sep-2019\0\#N Ge  
om=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\TS\0,2\C,0,1  
.9791052118,-0.7469359772,-0.3188705461\C,0,0.7165856887,0.0441989575,  
0.0273708564\O,0,-0.3562849858,-0.8081070808,-0.5043555355\C,0,-1.6547  
950749,-0.4937366961,-0.3227158748\C,0,0.5720151414,0.1993432785,1.544  
8781476\C,0,0.7059921685,1.3964763067,-0.6935960037\O,0,-2.1072331293,  
0.5547411727,0.116473028\H,0,2.8670525196,-0.2042581747,0.0176724773\H  
,0,2.0539576706,-0.8989304944,-1.3990991056\H,0,1.9658763467,-1.726639  
1424,0.1665798065\H,0,-2.0276633941,-1.4722227347,0.9729759202\H,0,-2.  
257587873,-1.2094054401,-0.9114431654\H,0,-0.3231260794,0.7652257735,1  
.8032519785\H,0,1.4456665129,0.7274189599,1.9391163565\H,0,0.523517403  
6,-0.7819705061,2.0268579498\H,0,1.5775208053,1.9824835496,-0.38497439  
47\H,0,0.7615446267,1.2500849395,-1.7764942893\H,0,-0.1969545595,1.960  
7123086,-0.460065606\\Version=EM64L-G09RevD.01\State=2-A\HF=-345.52234  
4\S2=0.837315\S2-1=0.\S2A=0.75063\RMSD=3.989e-09\Dipole=0.6674054,-0.3  
087439,-0.0715999\Quadrupole=-0.8182085,-0.0411748,0.8593833,3.3736347  
,1.5851264,-0.2353167\PG=C01 [X(C5H11O2)]\@

### TS:10->3 + H

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H11O2(2)\THEIS\29-Sep-2019\0\#N Ge  
om=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\ts\0,2\C,0,-  
5.0415491265,1.1646934843,0.012724003\C,0,-4.100958448,-0.0403291617,0  
.0525355653\O,0,-2.8080306014,0.559104897,0.3857513706\C,0,-1.72254154  
11,-0.210587573,0.5224705257\C,0,-4.5232496631,-1.0200665954,1.1535532  
917\C,0,-4.0271475345,-0.7139182897,-1.3228741445\O,0,-0.6205564255,0.  
2951985857,0.7422348362\H,0,-6.0588814482,0.8453084119,-0.2303549267\H  
,0,-4.710444005,1.8823340352,-0.742376842\H,0,-5.0558291558,1.66955162  
24,0.9821016668\H,0,-1.8544442315,-1.2814159724,0.3264208116\H,0,-3.87  
51855914,-1.899965227,1.1931393205\H,0,-5.5436961414,-1.3687299333,0.9  
688826374\H,0,-4.4987903413,-0.5284210717,2.1299371795\H,0,-5.02351983  
07,-1.0484568162,-1.6267411159\H,0,-3.6577118949,-0.0083895802,-2.0721  
826773\H,0,-3.3715208886,-1.5889659574,-1.3190223506\H,0,0.0514488687,  
0.9853551418,-0.3403901511\\Version=EM64L-G09RevD.01\State=2-A\HF=-345



.5089756\S2=0.849052\S2-1=0.\S2A=0.750732\RMSD=4.107e-09\Dipole=-1.779  
3184,-1.0214446,-0.2420836\Quadrupole=-5.2224605,2.5364,2.6860606,-3.4  
222478,-0.3879651,-0.0754762\PG=C01 [X(C5H11O2)]\@\

### TS:10->3 + H<sub>2</sub>O

N-N= 4.290900131548D+02 E-N=-1.847554052137D+03 KE= 4.204782829408D+02  
1\1\MF(BIN)-SILICIUM\SP\RHF\GFHFB4\C5H12O3\THEIS\02-Oct-2019\0\#\#N Geo  
m=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\0,1\C,0,-5  
.1225179903,1.1571455813,0.1630984568\C,0,-4.058928225,0.0697868434,0.  
0093591625\O,0,-2.8272649279,0.7585805767,0.4202503438\C,0,-1.64990636  
31,0.1791005301,0.2738802049\C,0,-4.3287105331,-1.0953559717,0.9668366  
494\C,0,-3.9566674987,-0.3879801261,-1.4484323058\O,0,-0.6259885325,0.  
7829349697,0.7915071501\H,0,-6.1106906991,0.7575596908,-0.0816375566\H  
,0,-4.9090005475,1.9962497598,-0.5039288161\H,0,-5.1407177595,1.530721  
7838,1.1902429736\H,0,-1.6696645313,-0.9138377977,0.1706708327\H,0,-3.  
5706464082,-1.8795192178,0.8829286655\H,0,-5.2975141284,-1.5483750346,  
0.7356357856\H,0,-4.3504802283,-0.7434506328,2.0018136096\H,0,-4.94226  
1865,-0.7116623455,-1.7958508904\H,0,-3.6037221923,0.4285294741,-2.081  
2998643\H,0,-3.2691887363,-1.2296782624,-1.5670252031\H,0,-0.313919080  
1,0.9223413623,-0.3417452332\O,0,-0.9662534485,0.5912801246,-1.3935974  
242\H,0,-0.5708863052,-0.1922763084,-1.7979565407\Version=EM64L-G09Re  
vD.01\State=1-A\HF=-421.0180212\RMSD=6.194e-09\Dipole=-1.1723372,-1.39  
57481,-0.3624502\Quadrupole=0.5222213,0.8953249,-1.4175462,-3.8409943,  
-2.7820789,0.4077557\PG=C01 [X(C5H12O3)]\@\

### TS:10->C<sub>4</sub>H<sub>9</sub> + HCOOH

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C5H11O2(2)\THEIS\29-Sep-2019\0\#\#N  
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\ts\0,2\C,0  
, -5.171481319,1.1433462043,-0.094110839\C,0,-4.1704048574,0.0237131297  
, -0.0356411922\O,0,-2.6420428413,1.028660388,0.0019894643\C,0,-1.51464  
96382,0.493234661,-0.1784503437\C,0,-4.1272683654,-0.7386782057,1.2625  
653669\C,0,-4.0267857476,-0.8051955689,-1.2799996208\O,0,-0.9238189561  
, -0.1728167315,0.8694806112\H,0,-6.1983458979,0.7525324555,-0.06375941  
69\H,0,-5.0583516686,1.7257599749,-1.0125612853\H,0,-5.0444204421,1.81  
73680473,0.7580227831\H,0,-1.0913752642,0.2924201654,-1.1686032649\H,0  
, -3.2803432819,-1.4285171939,1.2932485242\H,0,-5.0475198831,-1.3281151  
04,1.3937111087\H,0,-4.0419062697,-0.0560361728,2.1121883821\H,0,-4.83  
48068928,-1.5458619386,-1.3543918721\H,0,-4.0536259641,-0.1854946447,-  
2.1811309146\H,0,-3.0820393908,-1.3635025053,-1.2727729173\H,0,-0.0896  
813199,-0.5465659607,0.5647294264\Version=EM64L-G09RevD.01\State=2-A\  
HF=-345.5340683\S2=0.884111\S2-1=0.\S2A=0.753616\RMSD=3.181e-09\Dipole  
=0.019227,-0.7414616,-0.5879882\Quadrupole=4.5817588,-2.6564356,-1.925  
3233,-2.3159773,-2.1870552,0.1399407\PG=C01 [X(C5H11O2)]\@\

**TS:5->8**

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H9O2(2)\THEIS\04-Oct-2019\0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\CO2 Tab\0,2\C,0,-1.7547496574,0.9027138198,-0.3518061751\C,0,-0.9516262427,-0.1870498414,0.2974491594\O,0,0.7382385281,0.6675962749,0.2680287463\C,0,1.7361554291,0.1060095713,0.7233302766\C,0,-1.196295903,-0.4046205625,1.7654014628\C,0,-0.7217724622,-1.4221538213,-0.5294543051\O,0,2.1598597163,-0.875465097,1.2460375302\H,0,-2.8072570339,0.5929823522,-0.4323066372\H,0,-1.3933956578,1.1177141181,-1.3607757569\H,0,-1.7234625355,1.8247956968,0.2343639988\H,0,-0.4616713365,-1.08603169,2.2003333781\H,0,-2.1920360044,-0.8510919362,1.9113223176\H,0,-1.176353424,0.5386121054,2.3177084154\H,0,-1.6661583298,-1.9787517877,-0.6317102758\H,0,-0.3794664985,-1.1704320039,-1.5367233568\H,0,0.0065404122,-2.0898611985,-0.637397783\Version=EM64L-G09RevD.01\State=2-A\HF=-344.3866827\S2=0.824575\S2-1=0.\S2A=0.751415\RMSD=6.886e-09\Dipole=-2.0183525,0.0098893,-0.4217611\Quadrupole=-2.9863931,0.703703,2.2826901,1.264202,-1.8584586,1.4086324\PG=C01 [X(C5H9O2)]\@\

**TS:3->5**

1\1\MF(BIN)-CARBON\SP\UHF\GFHFB4\C5H11O3(2)\THEIS\06-Oct-2019\0\#\#N Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\ts\0,2\C,0,-1.8619308007,0.8338268569,-0.2980736181\C,0,-0.7936025692,-0.0799861744,0.3017107358\O,0,0.4173830212,0.7726101533,0.2612544212\C,0,1.5875152449,0.3325276756,0.7022751843\C,0,-1.1242837913,-0.4355721207,1.7529257427\C,0,-0.5766521067,-1.3198714826,-0.5685251254\O,0,1.8616445341,-0.7394789252,1.176669001\H,0,-2.8246556415,0.3155902709,-0.3235297755\H,0,-1.595152514,1.1221628293,-1.3183054801\H,0,-1.9726647267,1.7426287312,0.2995004151\H,0,2.3458053838,1.1429266295,0.5597000446\H,0,-0.3591746642,-1.0788481972,2.1879573031\H,0,-2.0839787856,-0.9605257248,1.7870517101\H,0,-1.2126264261,0.4714837712,2.3582190306\H,0,-1.5118720275,-1.884616,-0.6330597098\H,0,-0.2851244605,-1.0286811351,-1.5819363615\H,0,0.1938073773,-1.9676988769,-0.1499530182\O,0,4.0266299055,1.3443988592,-0.0817420176\H,0,4.2732580471,0.4777878595,0.2923645177\Version=EM64L-G09RevD.01\State=2-A\HF=-420.4691527\S2=0.758518\S2-1=0.\S2A=0.750054\RMSD=2.096e-09\Dipole=-0.5852637,-0.1417734,-0.1017667\Quadrupole=4.1770549,-3.06898,-1.1080749,-0.5771918,0.209041,2.1125995\PG=C01 [X(C5H11O3)]\@\