Supplementary Information for Atmospheric Chemistry of *Z*- and *E*-$CF_3CH{=}CHCF_3$

Freja F. Østerstrøm[1,*], Simone Thirstrup Andersen[1], Theis I. Sølling[1], Ole John Nielsen[1] and Mads P. Sulbaek Andersen[1,2,*]

[1] Copenhagen Center for Atmospheric Research, Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark

[2] Department of Chemistry and Biochemistry, California State University Northridge, 18111 Nordhoff St., Northridge, CA 91330-8262, USA

* Corresponding author: freja.oesterstroem@gmail.com, mpsa@csun.edu

Table of Contents

Table S1: Calculated total energies for three oxidants (Cl, OH, and OD), *Z*-$CF_3CH=CHCF_3$ (Z), and *E*-$CF_3CH=CHCF_3$ (E) as well as complexes, transition states (TS), and formed alkyl radicals of the reactions of Z and E with the oxidants using G4MP2, GAUSSIAN 09 Revision A.02. The numbers in parentheses refer to the compound number in Figures 5 and S11.

Compound	Free energy (Hartree)
Cl	-459.719368
OH	-75.684177
OD	-75.687115
E **(1)**	-752.087388
Z **(2)**	-752.079611
Complex: Z-OH **(5)**	-827.762744
Complex: Z-OD	-827.765758
Complex: E-OH **(3)**	-827.769582
Complex: E-OD	-827.772635
Alkyl radical: Z-OH **(6)**	-827.806622
Alkyl radical: Z-OD	-827.810190
Alkyl radical: E-OH **(4)**	-827.808914
Alkyl radical: E-OD	-827.812441
TS: Z-OH **(5→6)**	-827.760934
TS: Z-OD	-827.763957
TS: E-OH **(3→4)**	-827.762962
TS: E-OD	-827.766099
Alkyl radical: Z-Cl **(7)**	-1211.821839
Alkyl radical: E-Cl **(8)**	-1211.828657

Table S2: GAUSSIAN09 revision A.02 archive entries for OH, *Z*- and *E*-$CF_3CH=CHCF_3$ as well as complexes, transition states (TS), and formed alkyl radicals of the reactions of Z and E with OH radicals as wells as the formed alkyl radicals of the reactions with Cl atoms. The numbers in parentheses refer to the compound number in Figures 5 and S11.

OH
1\1\MF(BIN)-SILICIUM\Mixed\G4MP2\G4MP2\H1O1(2)\THEIS\21-Jun-2016\0\\# G4MP2\\IRCf\\0,2\O,0,-1.8296815811,0.0358435068,0.4275747054\H,0,-1.6954006381,0.2717749423,1.3652049908\\Version=EM64L-G09RevD.01\MP2/GTBas1=-75.5210254\CCSD(T)/GTBas1=-75.5370872\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-75.4181316\MP2/GTMP2LargeXP=-75.6176558\HF/GFHFB3=-75.41952\HF/GFHFB4=-75.4259773\G4MP2=-75.6672482\FreqCoord=-3.4575970987,0.0677344115,0.8079990946,-3.2038428915,0.5135802107,2.5798635478\PG=C*V [C*(H1O1)]\NImag=0\\
***Z*-$CF_3CH=CHCF_3$ (2)**
1\1\MF(BIN)-SILICIUM\SP\RHF\GFHFB4\C4H2F6\THEIS\22-Jun-2016\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\hbind\\0,1\C,0,6.7719487289,-10.6406091733,0.1440093092\C,0,6.2027112945,-9.6379217742,0.7998859767\C,0,5.5155147893,-8.4333836138,0.2043343748\F,0,4.237697111,-8.6950962106,-0.1013344963\F,0,6.1181073241,-7.983441465,-0.9006173011\F,0,5.5179791524,-7.4362165894,1.1024372947\C,0,6.8713318493,-10.8094788855,-1.352922274\F,0,7.0839512908,-12.1036834064,-1.6367225033\F,0,7.8948800436,-10.1128118338,-1.863960619\F,0,5.7589386789,-10.4334101866,-1.9921939707\H,0,7.2422311435,-11.4458151065,0.6977535708\H,0,6.1900828603,-9.6442210386,1.8843569606\\Version=EM64L-G09RevD.01\State=1-A\HF=-749.608701\RMSD=4.783e-09\Dipole=0.3145887,-0.5533293,1.1190408\Quadrupole=-1.2141367,-1.3211932,2.5353299,-0.0296233,1.5462472,-2.808832\PG=C01 [X(C4H2F6)]\\@
***E*-$CF_3CH=CHCF_3$ (1)**
1\1\MF(BIN)-SILICIUM\Mixed\G4MP2\G4MP2\C4H2F6\THEIS\21-Jun-2016\0\\# G4MP2\\IRCf\\0,1\C,0,-0.003500802,0.3669007725,-0.5598333933\C,0,0.3790178189,-0.3692120247,0.4711618243\C,0,1.0966812698,0.203191075,1.6576469494\F,0,0.3966959444,-0.0125395868,2.7813732732\F,0,1.2992064403,1.5212145714,1.5472738369\F,0,2.2920437925,-0.3846503991,1.8146427927\C,0,-0.7214176409,-0.2053880646,-1.7461562973\F,0,-0.0220680669,0.0103965919,-2.8701121401\F,0,-1.9169889524,0.3825383201,-1.9023725337\F,0,-0.9239219444,-1.523425936,-1.6357307887\H,0,0.1808931561,1.4338527792,-0.6073898655\H,0,0.1945292037,-1.436147548,0.5187846459\\Version=EM64L-G09RevD.01\State=1-A\MP2/GTBas1=-750.7937144\CCSD(T)/GTBas1=-750.8635767\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-749.5480341\MP2/GTMP2LargeXP=-751.6742786\HF/GFHFB3=-749.5643645\HF/GFHFB4=-749.6196117\G4MP2=-752.0514708\FreqCoord=-0.0066155571,0.6933419781,-1.0579317933,0.7162398772,-0.6977096117,0.8903668122,2.0724272551,0.3839754844,3.1324987594,0.7496466929,-0.0236963849,5.2560337596,2.4551443622,2.8746789293,2.9239238043,4.3313350524,-0.7268839113,3.4291779072,-1.3632817687,-0

.388127193,-3.2997571872,-0.0417026027,0.0196467113,-5.4237259155,-3.6
225841197,0.7228926603,-3.5949630914,-1.7459594432,-2.8788578028,-3.09
10832178,0.3418385243,2.7095890676,-1.1478005017,0.3676069199,-2.71392
55522,0.9803609026\PG=C01 [X(C4H2F6)]\NImag=0\\

Complex: *Z*-$CF_3CH=CHCF_3$-OH (5)

1\1\MF(BIN)-CARBON\Freq\UB3LYP\6-31G(d)\C4H3F6O1(2)\THEIS\24-Jun-2016\
0\\# b3lyp/6-31* opt=(TS,noraman,noeigen,calcall) scf=qc\\nyt ts\\0,2\
C,0.0069373263,0.3875137002,-0.5154756046\C,0.712858407,-0.3093932064,
0.3732204867\C,-0.8873407773,-0.1477292613,-1.6051503055\F,-0.18461654
36,-0.3824002366,-2.732637853\F,-1.8342122195,0.7609315059,-1.89845862
17\F,-1.5079502404,-1.2955346196,-1.2640686832\C,0.7480221361,-1.80682
69097,0.5348894822\O,-2.8506603994,-0.439684075,1.1477585551\F,-0.3591
105724,-2.2663166984,1.1881741098\F,1.8112433045,-2.1570945726,1.28238
62918\F,0.8261946349,-2.4671309329,-0.629889772\H,0.0783007348,1.47094
67212,-0.5156050765\H,1.3219646602,0.2186680483,1.1003803212\H,-2.0587
044512,-1.0202924629,1.1606006696\\Version=EM64L-G09RevD.01\State=2-A\
HF=-828.3832873\S2=0.751954\S2-1=0.\S2A=0.750002\RMSD=0.000e+00\RMSF=4
.208e-04\ZeroPoint=0.0732015\Thermal=0.0852743\Dipole=1.0870292,0.5675
48,0.2778712\DipoleDeriv=-0.1577127,0.008219,0.0052184,0.006457,0.0190
991,-0.0022298,0.0170307,-0.0530957,-0.1166685,-0.1907711,0.0774812,0.
0547907,0.05445,-0.1556625,0.0568104,0.106001,0.0794538,-0.1368529,1.7
292866,-0.1742163,0.0468686,0.0573196,1.4062677,-0.0065747,0.0492843,-
0.1986339,1.7808281,-0.4666271,0.0519005,0.1555602,0.0081026,-0.254381
4,-0.1486594,0.1618123,-0.0216548,-0.8639423,-0.6302632,0.3176816,-0.1
620919,0.2435439,-0.5312959,0.0762195,-0.1873315,0.1457625,-0.4087792,
-0.4933033,-0.2309397,0.0325923,-0.276004,-0.6356018,0.0953827,0.02313
12,0.0943979,-0.4203471,1.7054696,-0.0836407,-0.0294391,-0.2283568,1.6
385101,-0.3049316,-0.0587878,-0.0365708,1.6192512,-0.2635203,-0.105718
1,0.0234171,-0.1464889,-0.2698675,0.0105274,0.0540545,-0.0123483,-0.37
82657,-0.7509626,-0.106747,0.2791187,-0.0893082,-0.5224792,0.2363156,0
.2541849,0.1112729,-0.4455316,-0.68434,0.1415981,-0.2716043,0.2130767,
-0.4281729,0.1808188,-0.2935332,0.1176354,-0.4870307,-0.2733018,0.0306
513,0.0403065,0.0939209,-0.5632286,-0.1966175,0.0637687,-0.2268956,-0.
6500331,0.0962687,0.0007614,-0.051058,-0.0093192,0.0022188,0.0044667,-
0.0481928,0.0141413,0.0804629,0.0898021,-0.0142988,-0.07028,-0.0048635
,0.0333466,-0.0003614,-0.0741886,-0.0128374,0.057072,0.2899751,0.08726
75,-0.0533993,0.0774697,0.2612477,-0.0011666,-0.0672336,-0.0006273,0.3
698369\Polar=46.9503162,-5.8989738,47.8635718,8.486112,-5.9034251,47.6
330877\PG=C01 [X(C4H3F6O1)]\NImag=0\\

Complex: *E*-$CF_3CH=CHCF_3$-OH (3)

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C4H3F6O1(2)\THEIS\21-Jun-2016\0\\#N
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\Ende R\\0,
2\C,0,-0.0103412406,0.3254316991,-0.6049543101\C,0,0.4513781324,-0.420
9091743,0.3913983107\C,0,1.0856947393,0.1712720011,1.6135085485\F,0,0.

278953618,-0.0029555962,2.6874729768\F,0,1.3136216762,1.480929729,1.49
69874423\F,0,2.2443278567,-0.4325531589,1.8964532313\C,0,-0.6531591583
,-0.2650126736,-1.8288451209\F,0,0.1029951938,-0.0021917592,-2.9088853
12\F,0,-1.8569895229,0.2675054064,-2.0426752652\F,0,-0.7900656612,-1.5
923104182,-1.7411149313\H,0,0.0735288975,1.405152759,-0.6061222979\H,0
,0.3667618329,-1.5011076536,0.3910182\O,0,-2.1467827924,0.4679139209,0
.9188961502\H,0,-1.7521375714,0.3438969186,1.8022093778\\Version=EM64L
-G09RevD.01\State=2-A\HF=-825.039336\S2=0.827984\S2-1=0.\S2A=0.751472\
RMSD=3.214e-09\Dipole=0.2507838,-0.0407366,0.4905278\Quadrupole=-2.105
8307,2.7975691,-0.6917384,-0.1583865,-3.37218,-1.3113491\PG=C01 [X(C4H
3F6O1)]\\@

Alkyl radical: *Z*-$CF_3CH=CHCF_3$-OH (6)

1\1\MF(BIN)-CARBON\Freq\UB3LYP\GTBas3\C4H3F6O1(2)\THEIS\01-Jul-2016\0\
\#N Geom=AllCheck Guess=TCheck SCRF=Check B3LYP/GTBas3 Freq\\ende\\0,2
\C,0.7606810708,-0.3452698684,1.0275858663\C,-0.6250477665,0.229224827
1,1.0565737174\C,-1.5179613021,-0.3541049818,-0.0594929047\F,-1.495353
8345,-1.6929074183,-0.036802887\F,-1.0964583007,0.0508022764,-1.267492
5681\F,-2.7815456536,0.0432469746,0.0871803266\C,1.7298711021,-0.08525
30617,-0.0743380376\F,2.9905742123,-0.1198774052,0.3716263489\F,1.5353
965612,1.1239536112,-0.6514021453\F,1.6296591189,-0.9991006666,-1.0559
49831\O,-0.6619754666,1.6384726811,1.0102989961\H,1.0685840823,-1.0824
042826,1.7576690368\H,-1.1023741102,-0.0591705637,1.997534423\H,-0.172
8817132,1.9234388781,0.2293016586\\Version=EM64L-G09RevD.01\State=2-A\
HF=-828.4916972\S2=0.75393\S2-1=0.\S2A=0.75001\RMSD=0.000e+00\RMSF=3.3
44e-06\ZeroPoint=0.0768763\Thermal=0.0875254\Dipole=0.2016076,-0.19417
94,0.5597438\DipoleDeriv=-0.1098833,-0.0530022,0.0302439,-0.166771,-0.
114925,-0.1161589,0.0568942,-0.1158419,-0.1085456,0.3198837,-0.0403456
,-0.0489924,-0.0501713,0.6166836,0.0120145,-0.0355809,-0.0160529,0.151
1008,1.5940256,-0.0197025,-0.0367698,0.0976505,1.3902424,-0.0165385,0.
0211538,-0.0674073,1.3047525,-0.3320459,-0.0741595,-0.0367434,-0.05088
16,-0.8599197,-0.0032028,-0.0584802,-0.0730779,-0.2839394,-0.3793996,-
0.0679001,0.0598989,-0.0896071,-0.3099894,0.091895,0.1032513,0.1395183
,-0.7548648,-0.9430898,0.1559736,0.0351954,0.103274,-0.2948861,-0.0335
067,-0.056277,-0.0191135,-0.2870192,1.6947824,-0.0147679,0.0162164,-0.
0152027,1.4230473,0.1008527,-0.0988932,0.0908846,1.389044,-0.9576494,0
.0364828,-0.1581309,0.0059999,-0.2461554,-0.0022663,-0.0759409,0.00058
79,-0.3332229,-0.3890956,0.0386395,0.0562289,0.1291855,-0.710397,0.169
6169,0.0293603,0.2487779,-0.4022787,-0.3612329,0.0069767,0.0590406,-0.
0068721,-0.4947152,-0.2606326,0.0965378,-0.3153849,-0.6247928,-0.51284
25,0.0143517,-0.067296,0.028112,-0.838164,-0.0120265,-0.0938171,0.0453
983,-0.3118025,0.0174305,0.0453637,0.0201772,0.0514659,0.0776504,0.062
2805,0.0239745,0.054276,0.0690185,0.0019081,-0.0194818,0.0490543,-0.00
85701,0.0236681,0.0163943,0.0475177,0.0451561,-0.0191611,0.3572089,-0.
0084283,0.0218767,-0.0276121,0.3378601,-0.0087215,0.0402998,-0.0177207

,0.211711\Polar=56.2549832,-1.8900313,48.3383035,-1.7385178,-1.3937129
,47.0689036\PG=C01 [X(C4H3F6O1)]\NImag=0\\

Alkyl radical: *E*-$CF_3CH=CHCF_3$-OH (4)

1\1\MF(BIN)-SILICIUM\SP\UHF\GFHFB4\C4H3F6O1(2)\THEIS\21-Jun-2016\0\\#N
Geom=AllCheck Guess=TCheck SCRF=Check HF/GFHFB4 SCF=Tight\\IRCf\\0,2\
C,0,-0.6016764572,0.2861701262,-0.2440263524\C,0,0.5223219259,-0.44642
70975,0.4111924474\C,0,1.2084263349,0.1969249082,1.5599749035\F,0,0.31
24566345,0.4968663647,2.5446070052\F,0,1.7794676049,1.362796922,1.2156
266119\F,0,2.1443875133,-0.5841673864,2.0961120378\C,0,-0.8082185036,-
0.1865338373,-1.6834083928\F,0,0.2857710719,0.0846155025,-2.4093704328
\F,0,-1.8457643798,0.4292888609,-2.2473361788\F,0,-1.0234172001,-1.505
5986269,-1.7389657055\H,0,-0.3826770244,1.3616477119,-0.2937707746\H,0
,0.6600926988,-1.5088528974,0.2586531348\O,0,-1.8288635678,0.037280755
1,0.4332865663\H,0,-1.6962186514,0.270337694,1.3594931299\\Version=EM6
4L-G09RevD.01\State=2-A\HF=-825.0709275\S2=0.763249\S2-1=0.\S2A=0.7501
16\RMSD=9.008e-09\Dipole=0.233042,0.0434997,0.4477519\Quadrupole=-2.12
08895,3.1842019,-1.0633124,-1.844236,-3.4157449,-0.6436132\PG=C01 [X(C
4H3F6O1)]\\@

TS: *Z*-$CF_3CH=CHCF_3$-OH (5→6)

1\1\MF(BIN)-CARBON\Mixed\G4MP2\G4MP2\C4H3F6O1(2)\THEIS\24-Jun-2016\0\\
G4MP2 scf=qc\\hbind\\0,2\C,0,6.6740855821,-10.6447832118,0.212307040
6\C,0,6.1306747497,-9.5806250326,0.7884398528\C,0,5.5467075584,-8.3635
113323,0.115152188\F,0,4.241162167,-8.5398550733,-0.1352727998\F,0,6.1
416580799,-8.0601284082,-1.047741726\F,0,5.6634913716,-7.3046878972,0.
9214657447\C,0,6.8810868027,-10.8728568091,-1.2635553398\F,0,7.1650478
445,-12.1609470614,-1.484759183\F,0,7.927109909,-10.1548585212,-1.7383
61004\F,0,5.81567539,-10.5556436897,-2.0012649924\O,0,8.8264036973,-7.
8944027026,0.0648403261\H,0,7.0497631493,-11.4546053046,0.8275686144\H
,0,6.0466311643,-9.5430796824,1.8691161538\H,0,8.5430185341,-8.3530542
734,-0.7489358753\\Version=EM64L-G09RevD.01\State=2-A\MP2/GTBas1=-826.
3081866\CCSD(T)/GTBas1=-826.3998758\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM
P2LargeXP=-824.9559614\MP2/GTMP2LargeXP=-827.2829702\HF/GFHFB3=-824.97
28468\HF/GFHFB4=-825.0340811\G4MP2=-827.7214181\FreqCoord=12.612193937
6,-20.1157250143,0.4012021628,11.5852962867,-18.1047574935,1.489935394
,10.4817582246,-15.8047459273,0.2176060989,8.0146349808,-16.1379873031
,-0.2556285448,11.6060517729,-15.2314352875,-1.9799449201,10.702447648
2,-13.8038596119,1.7413178983,13.0033695538,-20.5467216514,-2.38777354
6,13.5399781551,-22.9808594625,-2.8057882291,14.9800667533,-19.1899015
233,-3.2850262177,10.9900337649,-19.9472757299,-3.7818427549,16.679485
7262,-14.9182590906,0.1225304587,13.322121654,-21.646066986,1.56387803
74,11.4264769271,-18.0338070641,3.5321176412,16.1439653776,-15.7849849
498,-1.4152836954\PG=C01 [X(C4H3F6O1)]\NImag=1\\

TS: *E*-$CF_3CH=CHCF_3$-OH (3→4)

1\1\MF(BIN)-CARBON\Mixed\G4MP2\G4MP2\C4H3F6O1(2)\THEIS\21-Jun-2016\0\\

g4mp2 opt=(TS,calcall,noraman,noeigen)\\add\\0,2\C,0,-10.8685826894,
8.1481954231,-2.2945260818\C,0,-10.2638272478,7.3879232217,-1.37102446
55\C,0,-9.605784609,7.9775495626,-0.160696986\F,0,-10.3956567806,7.817
1158421,0.925816742\F,0,-9.3728113799,9.2869296314,-0.2891172973\F,0,-
8.4460343532,7.3683927157,0.1025225987\C,0,-11.4462666071,7.5573848196
,-3.5566600207\F,0,-10.5771741546,7.7635640084,-4.5648240222\F,0,-12.5
949044693,8.1325638607,-3.8975387929\F,0,-11.6410669348,6.2398251438,-
3.4536830586\H,0,-10.8078949474,9.2282646634,-2.2797327702\H,0,-10.285
9607743,6.3058828568,-1.4136986384\O,0,-12.7607882141,8.1606606431,-1.
1352384095\H,0,-12.4276378385,8.1458766075,-0.2202697974\\Version=EM64
L-G09RevD.01\State=2-A\MP2/GTBas1=-826.304012\CCSD(T)/GTBas1=-826.4001
447\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-824.9524226\MP2/GTMP2
LargeXP=-827.2813332\HF/GFHFB3=-824.9691248\HF/GFHFB4=-825.0305953\G4M
P2=-827.7235849\FreqCoord=-20.5386447355,15.3978578268,-4.3360258994,-
19.3958225737,13.9611515797,-2.5908607613,-18.1523022025,15.0753838849
,-0.3036732939,-19.6449442869,14.7722080906,1.7495400916,-17.712046603
3,17.5497536187,-0.5463525122,-15.9606918365,13.9242442722,0.193739634
,-21.6303091314,14.2813875899,-6.7211133869,-19.9879624121,14.67100979
1,-8.6262672468,-23.8009201168,15.3683184549,-7.3652809109,-21.9984284
013,11.7915606388,-6.5265151306,-20.4239615235,17.4388928956,-4.308070
5918,-19.437648877,11.9163916254,-2.671503261,-24.1143949645,15.421413
6789,-2.1452896895,-23.4848319935,15.3934759004,-0.4162495925\PG=C01 [
X(C4H3F6O1)]\NImag=1\\

Alkyl radical: *Z*-$CF_3CH=CHCF_3$-Cl (7)

1\1\MF(BIN)-SILICIUM\Mixed\G4MP2\G4MP2\C4H2Cl1F6(2)\THEIS\08-Jul-2016\
0\\# g4mp2\\Cl produkt\\0,2\C,0,-0.4372637796,0.3939887018,-0.28347599
77\C,0,0.6498264932,-0.3419761051,0.3893873822\C,0,-0.9520342664,-0.19
40773733,-1.6066677532\F,0,0.0781462695,-0.3023581172,-2.4570675231\F,
0,-1.8545500103,0.6199006948,-2.1554152587\F,0,-1.5045951269,-1.394863
1008,-1.4599364115\C,0,0.7299589507,-1.8328467859,0.5115937217\Cl,0,-1
.8593963103,0.579462418,0.8682439134\F,0,-0.4061268038,-2.368007045,0.
9792338279\F,0,1.7194576712,-2.1649459264,1.3501226984\F,0,0.987443176
5,-2.4181120471,-0.6704480379\H,0,-0.1230731365,1.4150963914,-0.498356
6215\H,0,1.3616208728,0.2198132949,0.9799530599\\Version=EM64L-G09RevD
.01\State=2-A\MP2/GTBas1=-1210.3634287\CCSD(T)/GTBas1=-1210.4493302\MP
2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1209.030367\MP2/GTMP2LargeX
P=-1211.3393467\HF/GFHFB3=-1209.0526219\HF/GFHFB4=-1209.1109385\G4MP2=
-1211.7833816\FreqCoord=-0.8263087912,0.7445307458,-0.5356920009,1.227
994106,-0.6462411827,0.7358355119,-1.7990840327,-0.3667530842,-3.03616
20402,0.1476750476,-0.5713740356,-4.6431847086,-3.5045916191,1.1714425
428,-4.0731445416,-2.8432727308,-2.6359092533,-2.7588799891,1.37942250
5,-3.4635784689,0.9667720254,-3.5137497989,1.0950252743,1.640743213,-0
.7674684343,-4.4748847958,1.8504837548,3.2493040956,-4.0911548934,2.55
13621458,1.8659971754,-4.5695695276,-1.2669631779,-0.2325745224,2.6741
446314,-0.9417575312,2.5730905464,0.4153869276,1.8518429062\PG=C01 [X(

C4H2Cl1F6)]\NImag=0\\

Alkyl radical: *E*-$CF_3CH=CHCF_3$-Cl (8)

1\1\MF(BIN)-SILICIUM\Mixed\G4MP2\G4MP2\C4H2Cl1F6(2)\THEIS\16-Aug-2016\
0\\# g4mp2\\Cl produkt\\0,2\C,0,-0.5573190327,0.3252389777,-0.30701862
95\C,0,0.419321209,-0.438260388,0.48004327\C,0,1.2087540385,0.19917508
15,1.5736079423\F,0,0.6143343114,0.0517414788,2.7695257896\F,0,1.36621
69901,1.5154830673,1.3650764084\F,0,2.4240495895,-0.3566808036,1.66336
48375\C,0,-0.7295516781,-0.2278987031,-1.7255679258\F,0,0.4360178273,-
0.1066896285,-2.3775710769\F,0,-1.6556119358,0.4426584634,-2.404592553
8\F,0,-1.0628934349,-1.5205549066,-1.7139536114\Cl,0,-2.192044417,0.27
7642071,0.5398730282\H,0,-0.2992238222,1.3807936181,-0.375098892\H,0,0
.4502583548,-1.518636328,0.4148874135\\Version=EM64L-G09RevD.01\State=
2-A\MP2/GTBas1=-1210.3668481\CCSD(T)/GTBas1=-1210.4527375\MP2/GTBas2=0
.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1209.0365622\MP2/GTMP2LargeXP=-1211.3
441491\HF/GFHFB3=-1209.0591477\HF/GFHFB4=-1209.1175852\G4MP2=-1211.788
6101\FreqCoord=-1.0531803404,0.6146125956,-0.5801811274,0.7924022467,-
0.8281921082,0.9071503121,2.2842140947,0.3763863566,2.9736880514,1.160
9236026,0.0977772246,5.2336452603,2.5817759494,2.8638479563,2.57962056
24,4.5807898567,-0.6740290357,3.143304002,-1.3786528714,-0.4306661349,
-3.2608508034,0.8239542827,-0.201614179,-4.4929581969,-3.128653141,0.8
365032662,-4.5440213879,-2.0085775004,-2.8734323435,-3.2389029301,-4.1
423636193,0.5246674772,1.0202121697,-0.5654510764,2.6093217843,-0.7088
341787,0.8508649797,-2.8698067554,0.7840235876\PG=C01 [X(C4H2Cl1F6)]\N
Imag=0\\

Table S3: Coordinates for the optimized structure of *E*-$CF_3CH=CHCF_3$ calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	1.941566	-0.01141	0.000045
C	0.502527	-0.43489	-0.00024
H	0.343299	-1.50831	-0.0006
C	-0.50258	0.434868	0.000181
H	-0.34333	1.508284	0.000841
C	-1.9416	0.011445	-0.00013
F	2.584762	-0.49878	1.089584
F	2.100236	1.330411	0.000346
F	2.585033	-0.49785	-1.08978
F	-2.58458	0.497002	1.090489
F	-2.10024	-1.33043	-0.00164
F	-2.58515	0.499633	-1.08893

Table S4: Coordinates for the optimized structure of $CF_3CHClC(O)CF_3$ (R) conformer 1 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	1.74718	-0.59101	-0.12377
C	0.521737	0.315627	-0.31568
C	-0.66299	-0.10794	0.572137
C	-2.03924	-0.14682	-0.15271
F	-3.03614	-0.39896	0.691387
F	-2.27779	1.028614	-0.77621
F	-2.01053	-1.1158	-1.09943
F	2.69775	-0.28966	-1.03152
F	2.292137	-0.51031	1.094345
F	1.368255	-1.87495	-0.33735
O	-0.57252	-0.39621	1.733862
Cl	0.919147	2.031611	0.044099
H	0.251416	0.262784	-1.37146

Table S5: Coordinates for the optimized structure of $CF_3CHClC(O)CF_3$ (R) conformer 2 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	0.536248	0.259452	-0.35194
C	-0.606	-0.52186	0.311333
C	-2.05692	-0.15469	-0.14299
F	-2.61637	0.707832	0.724241
F	-2.05905	0.416675	-1.36997
F	-2.81234	-1.25846	-0.19496
O	-0.45351	-1.3718	1.146626
Cl	0.516184	1.942763	0.290284
H	0.369064	0.329649	-1.42851
C	1.910547	-0.3933	-0.14752
F	2.293504	-0.44937	1.1333
F	1.874124	-1.65075	-0.64427
F	2.851292	0.287428	-0.83641

Table S6: Coordinates for the optimized structure of $CF_3CHClC(O)CF_3$ (S) conformer 1 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	-1.91044	-0.39348	-0.14755
C	-0.5362	0.259524	-0.35184
H	-0.36883	0.329657	-1.4284
C	0.606076	-0.52161	0.311541
C	2.056967	-0.15467	-0.14303
F	2.812357	-1.25849	-0.19474
F	2.059121	0.416375	-1.37014
F	2.616445	0.708123	0.72396
F	-2.85125	0.286988	-0.8366
F	-1.8738	-1.65096	-0.6442
F	-2.29356	-0.44948	1.133212
O	0.453682	-1.3713	1.147104
Cl	-0.51664	1.942893	0.290198

Table S7: Coordinates for the optimized structure of $CF_3CHClC(O)CF_3$ (S) conformer 2 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	-1.7472	-0.59107	-0.1238
C	-0.52175	0.315618	-0.31568
H	-0.25143	0.262815	-1.37146
C	0.663001	-0.10793	0.572068
C	2.039297	-0.14686	-0.15276
F	3.036159	-0.39877	0.691477
F	2.010917	-1.11576	-1.09947
F	2.277613	1.028758	-0.77615
F	-1.36826	-1.87501	-0.33764
F	-2.29186	-0.51061	1.094461
F	-2.69794	-0.28958	-1.03123
O	0.572619	-0.39618	1.733803
Cl	-0.91937	2.031579	0.044061

Table S8: Coordinates for the optimized structure of $CF_3CHClC(O)CF_3$ (S) conformer 1 calculated at the ωB97XD/cc-pVTZ level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	1.910955	-0.37723	0.14395
C	0.533954	0.253786	0.359877
H	0.374873	0.326707	1.433025
C	-0.59719	-0.5417	-0.28653
C	-2.04673	-0.15319	0.139697
F	-2.80215	-1.23772	0.194109
F	-2.05917	0.43014	1.342862
F	-2.5736	0.690978	-0.74155
F	2.83823	0.323684	0.798563
F	1.903449	-1.61291	0.651197
F	2.263733	-0.44004	-1.12964
O	-0.44026	-1.41178	-1.08169
Cl	0.482756	1.911202	-0.29184

Table S9: Coordinates for the optimized structure of *Z*-$CF_3CH=CHCF_3$ conformer 1 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	1.603627	0.019025	-0.0012
C	0.666448	1.200652	0.001391
H	1.188658	2.15239	0.012696
C	-0.66643	1.200737	-0.00256
H	-1.18845	2.152568	-0.014
C	-1.60369	0.01909	0.001056
F	2.7934	0.396633	-0.53485
F	1.156196	-1.0268	-0.72299
F	1.856457	-0.42217	1.254448
F	-1.15924	-1.02314	0.73003
F	-1.85105	-0.42834	-1.2534
F	-2.79576	0.39914	0.527777

Table S10: Coordinates for the optimized structure of *Z*-$CF_3CH=CHCF_3$ conformer 2 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01 (Ångstrøm).

Atom	X	Y	Z
C	1.610125	-0.02026	-0.00071
C	0.665121	-1.19847	-0.01357
H	1.179849	-2.15409	-0.02389
C	-0.66774	-1.19216	-0.0111
H	-1.19451	-2.14181	-0.00399
C	-1.60722	-0.01593	-0.00251
F	2.862877	-0.46141	0.280399
F	1.296165	0.903822	0.931525
F	1.671107	0.605052	-1.19858
F	-2.67204	-0.28793	-0.79989
F	-1.06272	1.133892	-0.43676
F	-2.09395	0.201769	1.244996

Figure S1: Pseudo first-order rate coefficients of the reaction O_3 + *E*-$CF_3CH=CHCF_3$ versus O_3 concentration. The inset shows the loss of *E*-$CF_3CH=CHCF_3$ versus time at different O_3 concentrations. The symbols indicate different O_3 concentrations: 1.56 Torr (white circles), 2.28 Torr (gray circles), 2.71 Torr (black circles), 3.96 Torr (white triangles), 4.60 Torr (gray triangles), and 6.09 Torr (black triangles). See text for details.

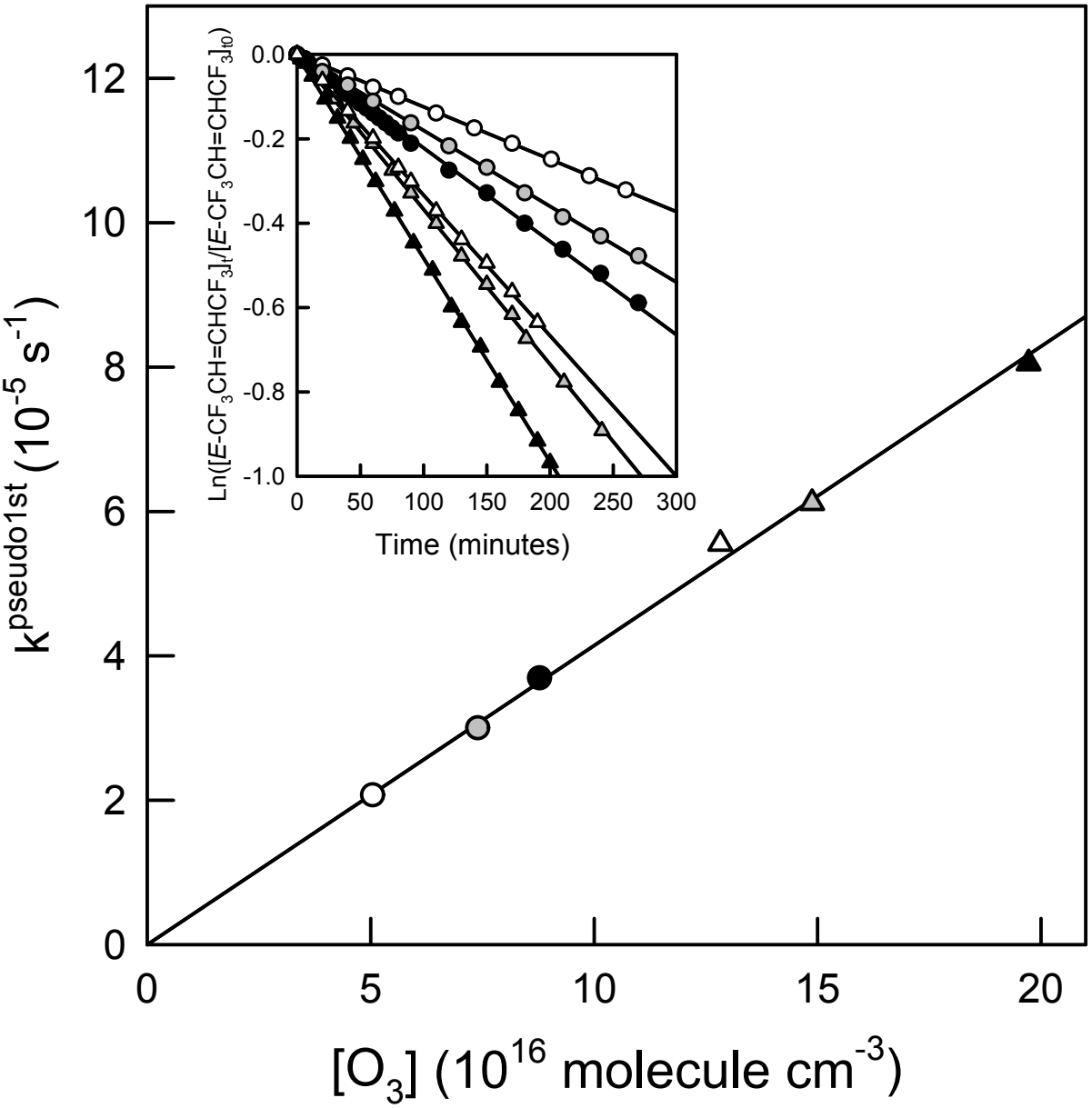


Figure S2: IR spectrum of *E*-$CF_3CH=CHCF_3$ calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

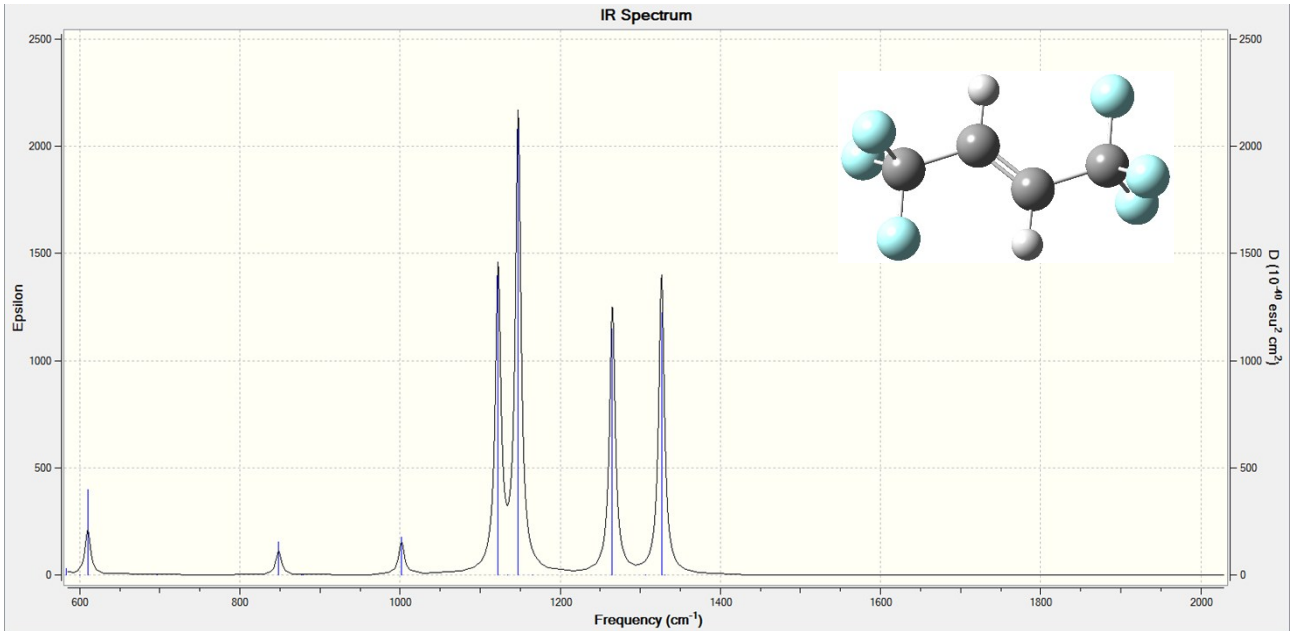


Figure S3: IR spectrum of $CF_3CHClC(O)CF_3$ (R) conformer 1 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

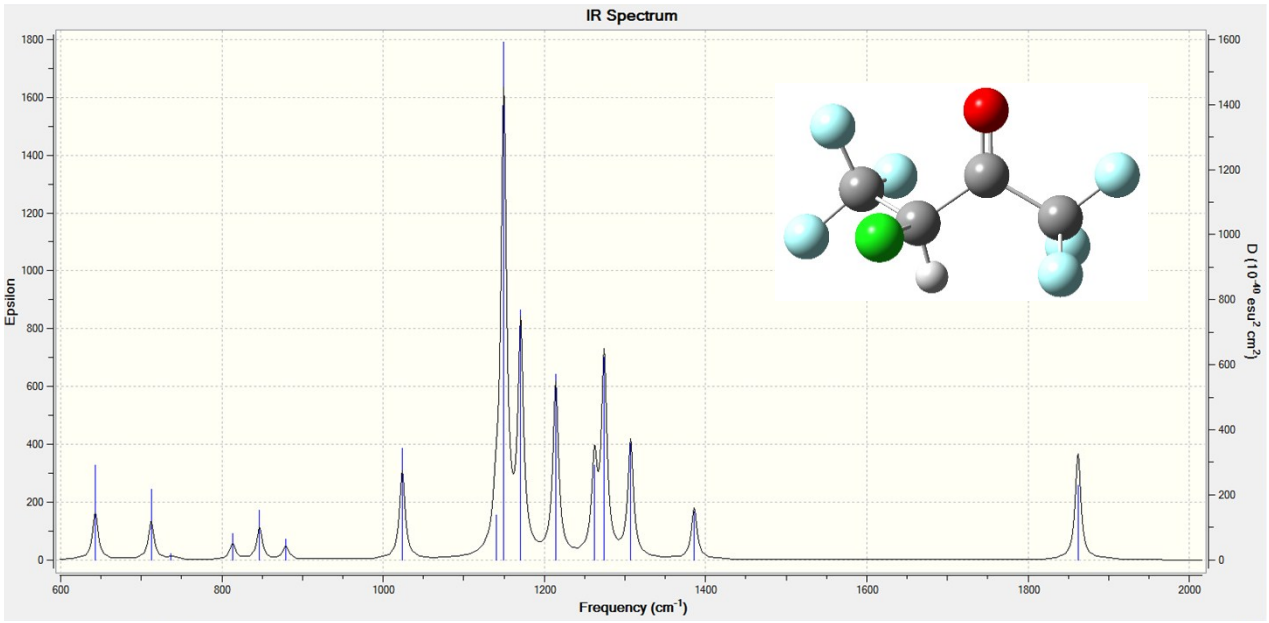


Figure S4: IR spectrum of $CF_3CHClC(O)CF_3$ (R) conformer 2 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

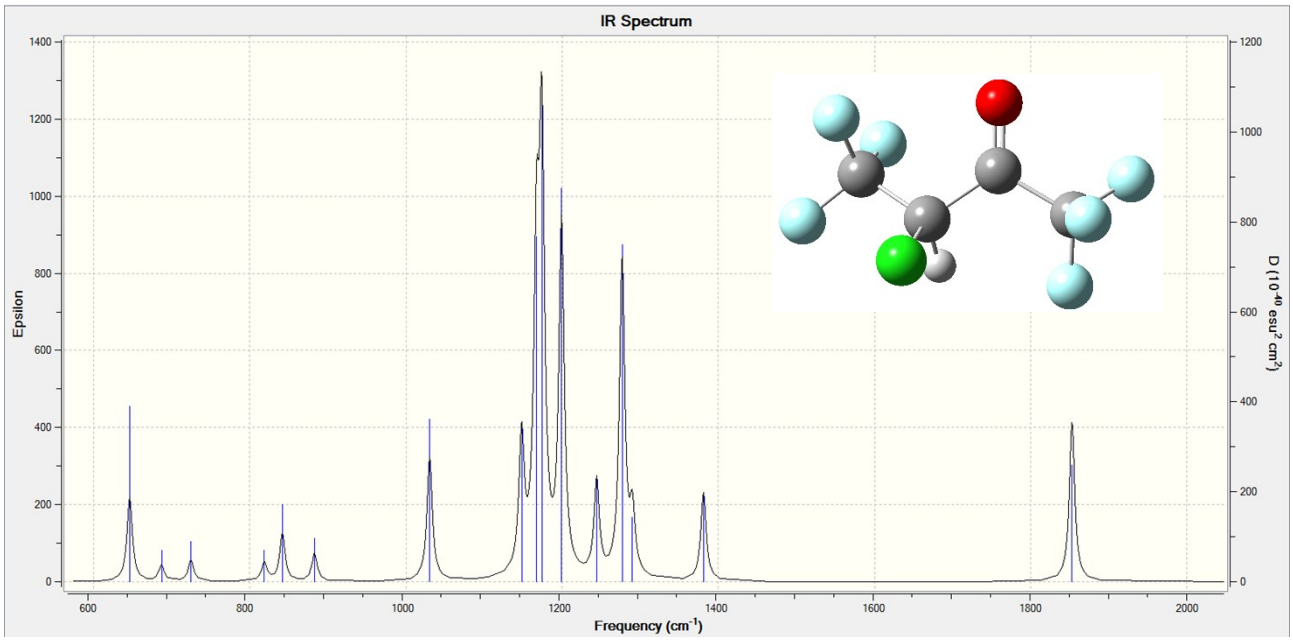


Figure S5: IR spectrum of $CF_3CHClC(O)CF_3$ (S) conformer 1 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

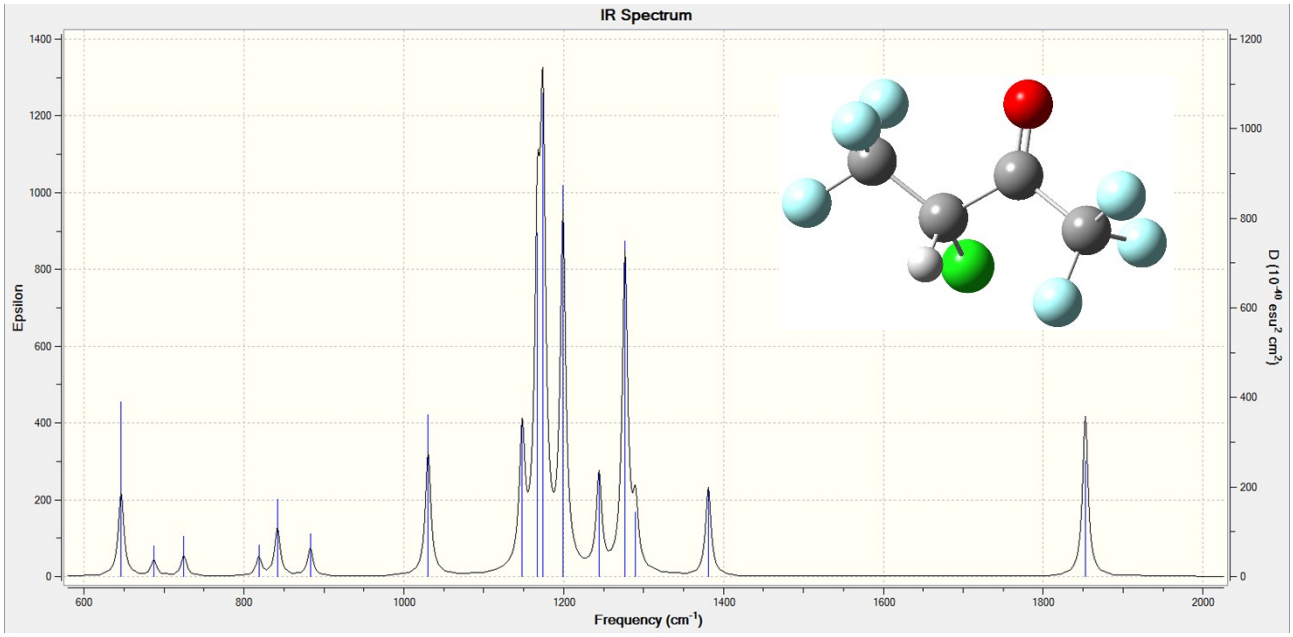


Figure S6: IR spectrum of $CF_3CHClC(O)CF_3$ (S) conformer 2 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

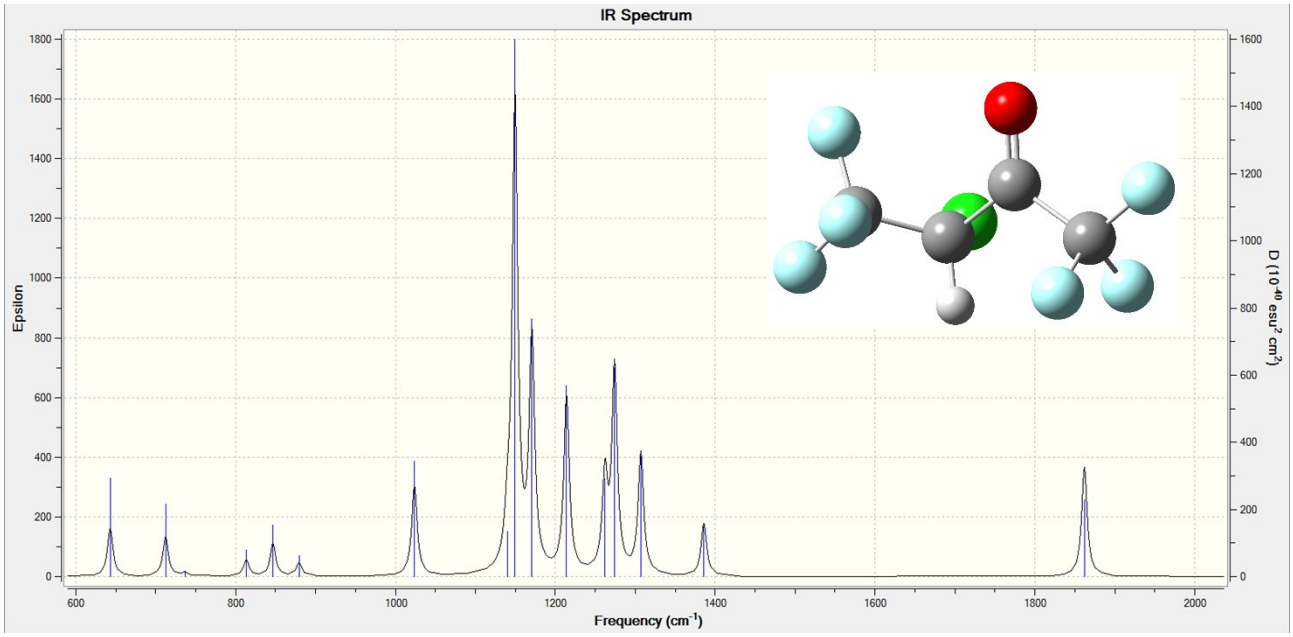


Figure S7: IR spectrum of $CF_3CHClC(O)CF_3$ (S) conformer 1 calculated at the ωB97XD/cc-pVTZ level using GAUSSIAN 09 Revision D.01.

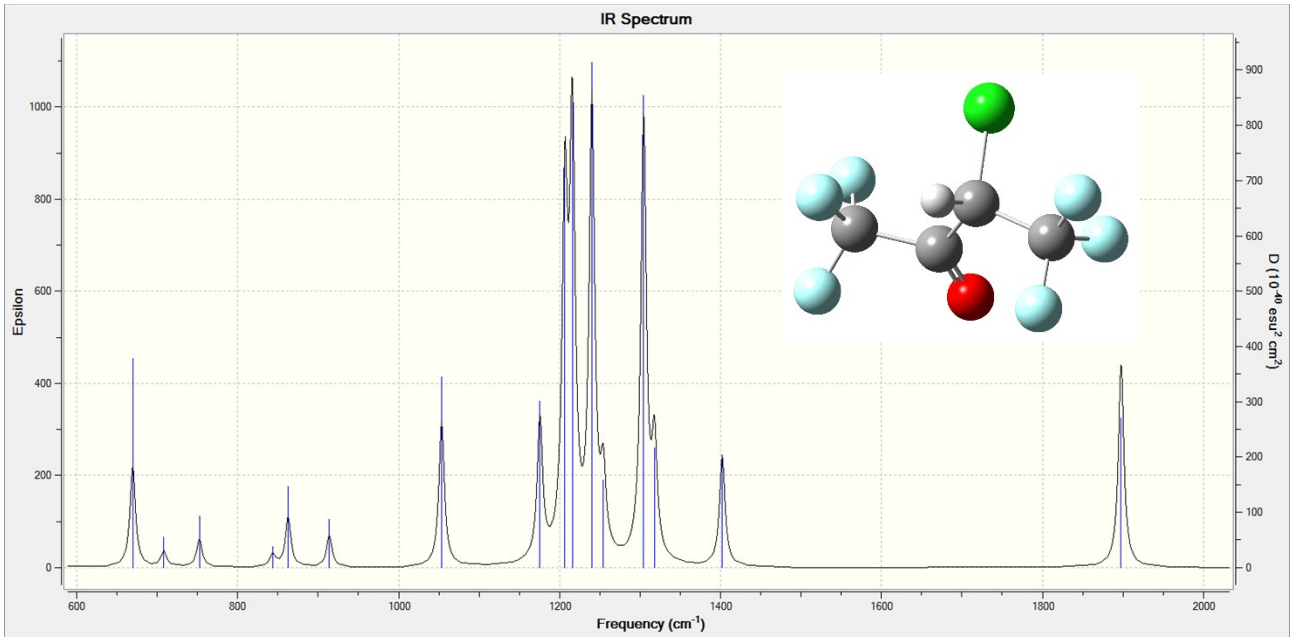


Figure S8: IR spectrum of *Z*-$CF_3CH=CHCF_3$ conformer 1 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

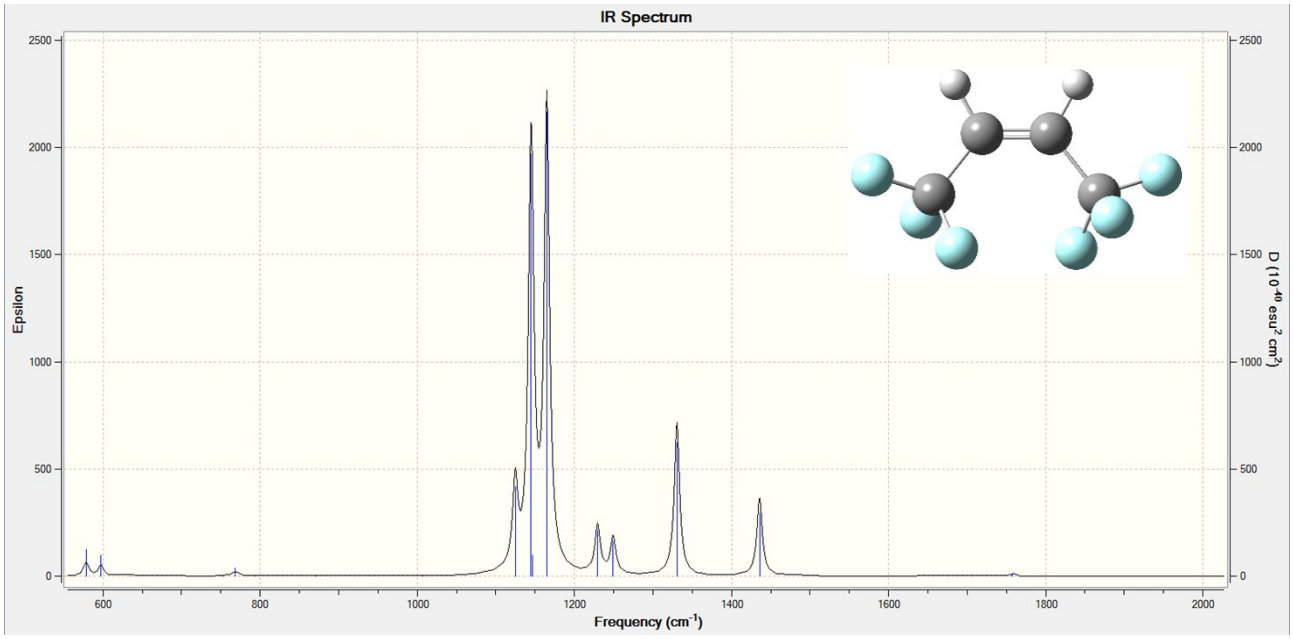


Figure S9: IR spectrum of *Z*-$CF_3CH=CHCF_3$ conformer 2 calculated at the B3LYP/6-31+G(d,p) level using GAUSSIAN 09 Revision D.01.

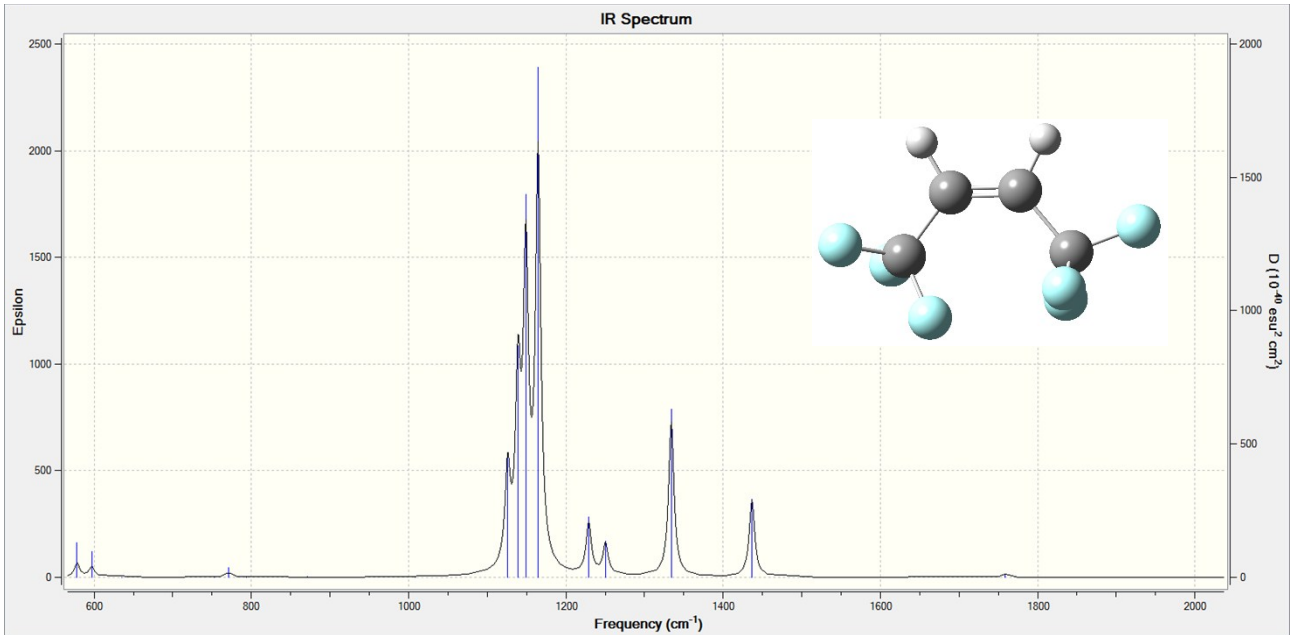
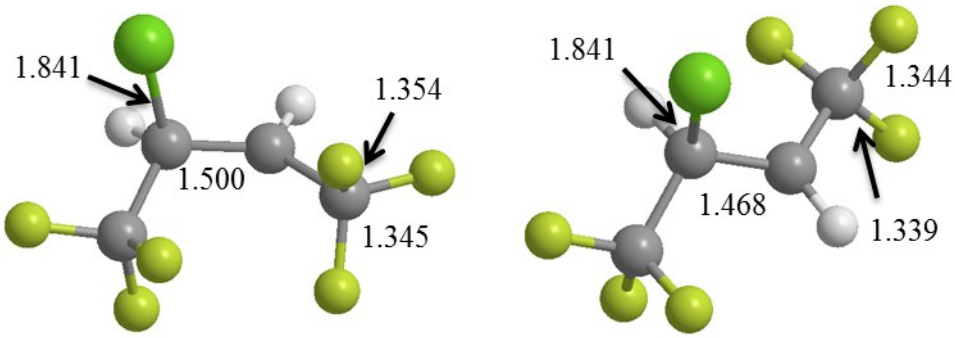


Figure S10: Structures of optimized geometries of alkyl radicals formed in the addition of Cl atoms to *Z*- and *E*-$CF_3CH=CHCF_3$; 7: Alkyl radical formed from Cl + *Z*-$CF_3CH=CHCF_3$ and 8: Alkyl radical formed from Cl + *E*-$CF_3CH=CHCF_3$. Highlighted bond lengths are in units of Ångstrøm.



7 **8**