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Trifluoroacetic Acid Formation from HFC-134a under Atmospheric Conditions

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Supplementary Information

Table T1. RMSD of each candidate method with respect to benchmark CCSD(T)-F12/cc-pVTZ-F12//M06-2X-D3/cc-pVTZ level of theory.

Method	RMSD (kcal/mol)
M06-2X-D3/cc-pVTZ	1.3
M06-2X-D3/aug-cc-pVTZ	1.1
M06-2X-D3/def2-TZVP	1.2

Cartesian coordinates of the optimized geometries at M06-2X-D3/cc-pVTZ level of theory

1. OH radical initiated oxidation of HFC-134a (Figure 1)

CF_3CH_2F

C	-0.35536930	-0.09585730	0.17222935
C	1.15588527	-0.11377169	0.20445999
F	-0.83260635	-0.73345862	-0.89500633
F	-0.83266779	1.14716721	0.15248045
F	-0.82635005	-0.70494639	1.26578588
F	1.63028514	0.50845487	-0.91380044
H	1.49261615	-1.14992117	0.22289639
H	1.49257418	0.41688396	1.09462433

OH

O	-0.10488356	0.00000000	0.00000000
H	0.86658441	0.00000000	0.00000000

CF_3CHF

C	0.01982531	-0.29856452	-0.24804042
C	-0.37770475	0.22226406	1.08671351
F	1.34691999	-0.25810357	-0.43958120
F	-0.53665674	0.40505769	-1.23292786
F	-0.36506286	-1.57069443	-0.35840248
F	-0.16874767	1.51518936	1.26044583
H	-0.32930760	-0.39896538	1.96789279

H_2O

H	0.70122546	0.36625080	-0.42154886
H	-0.52380007	-0.53017972	-0.49810161
O	-0.02040093	0.01885708	0.10576970

CF_3CHFOH

C	-0.05440573	0.14632489	-0.59333421
C	-0.41483959	-0.20451334	0.85043000

F 1.26570826 0.02933473 -0.77842373
F -0.41171730 1.38752135 -0.89651500
F -0.66328505 -0.68506555 -1.43491325
F 0.12582185 0.78023046 1.63090594
H -1.49718534 -0.20096170 0.97194489
O 0.05891579 -1.43354878 1.20001935
H 1.00565269 -1.47567205 1.01727039

CFH_2
C -0.18799630 0.35897955 0.51627587
F 0.20500857 -0.41070576 -0.49961918
H -1.25708284 0.47341833 0.60692246
H 0.51970026 1.12115778 0.80353614

CF_3OH
C -0.00767936 0.01691895 0.01039406
F -0.39432142 1.22362870 -0.35589526
F -0.76534021 -0.88337267 -0.62445354
F 1.24659700 -0.17481166 -0.41132949
O -0.11364632 -0.08178521 1.34499572
H 0.17919679 -0.95685797 1.62300979

CF_3
C 0.03190182 0.08974947 0.31174287
F -0.35542300 1.14318929 -0.36830674
F -0.86756261 -0.86446527 0.26247357
F 1.20177275 -0.33828484 -0.10116402

CFH_2OH
C -0.02374807 -0.17345597 0.48249471
F 1.08871908 -0.28994843 -0.32249291
H -0.33931855 -1.19114552 0.72458896
H 0.26515664 0.37639887 1.37566219
O -1.00594159 0.55177356 -0.14724191
H -1.35970535 0.03957112 -0.87952354

i1
C -0.20957074 0.17146712 -0.45984653
C -0.55431171 0.51604967 0.96993442
F 1.11027131 0.10105816 -0.65169599
F -0.69565392 1.06217059 -1.31961515
F -0.72785973 -1.02658629 -0.77031223
F -0.04675627 1.75221944 1.25393307
H -0.10943781 -0.23355508 1.62131920
H -1.63892438 0.53117175 1.06954366
O 1.40976672 -2.09196068 1.03102999
H 1.22531770 -2.41342158 0.13184541

i2
C -0.08654271 0.36008840 -0.47539222
C -0.52006943 0.44881866 0.94339359
F 1.20768064 0.00093748 -0.60554762
F -0.22314689 1.52461551 -1.10432282
F -0.81192851 -0.55874602 -1.12027623
F -0.05384037 1.50775825 1.58579253
H 1.20443282 -2.26024938 0.47969302
H -0.69144036 -0.44467729 1.52276609
O 0.33194629 -2.52726297 0.78004147

H -0.12998449 -2.78797984 -0.02039051

i3
C -0.06782489 0.48710536 -1.06232742
C -0.03385412 -0.80537397 3.19041484
F -0.45216548 1.69295456 -1.44295472
F -0.83268727 -0.41500812 -1.68754702
F 1.18335803 0.28891815 -1.49247487
F 0.35710940 -1.56092398 2.14564067
H -1.10314479 -0.71093936 3.28792095
H 0.67051363 -0.03686003 3.46445679
O -0.16697727 0.40205731 0.26943787
H 0.11350510 -0.47391994 0.57132331

i4
C 0.22787410 0.44457890 -1.09818564
C -0.24745690 -0.60462108 2.24350890
F -0.15814300 1.49638123 -1.78314451
F -0.66543341 -0.52487937 -1.19753162
F 1.40701073 0.03115809 -1.48768213
F 0.83813673 -0.76370076 1.40165075
H -0.57757877 -1.60926409 2.51142445
H 0.08877035 -0.04755463 3.11419225
O -1.23021342 0.13231545 1.63098549
H -1.64567247 -0.39840353 0.94470867

ts-1-2
C -0.27796012 0.15166825 -0.62073585
C -0.37979160 0.26736272 0.88095679
F 0.98777082 -0.05370849 -0.99872990
F -0.70718680 1.25536621 -1.22978411
F -1.01198284 -0.87460966 -1.04335163
F 0.34246203 1.31955322 1.31547240
H 0.09106179 -0.74689263 1.32554020
H -1.41448302 0.32113722 1.21704347
O 0.83446561 -1.80698936 1.53560344
H 1.57292061 -1.60350021 0.93797816

ts-1-3
C 0.01481389 -0.02020693 -0.51729814
C -0.08996527 -0.15716570 1.46588646
F 1.30064014 0.39408708 -0.34775670
F -0.74522311 1.04270382 -0.68413514
F 0.13190875 -0.65449744 -1.70269505
F 0.63357146 0.86178283 1.90776259
H 0.35065258 -1.11364505 1.70369496
H -1.14618799 0.00171197 1.61215941
O -1.24839509 -1.30697565 -0.05290794
H -0.94010761 -2.01887852 -0.62973992

ts-1-p2
C -0.14775407 -0.21849517 -0.62017144
C -0.03830639 -0.25122672 0.90130718
F 0.59126518 0.73747118 -1.15694387
F -1.41535995 -0.01469364 -0.97620882
F 0.23128662 -1.39098443 -1.13800645
F -0.73043653 0.86575101 1.38592656
H 0.97978655 -1.12016075 1.03387635

H -0.67694100 -1.06488039 1.28860000
O 1.45944258 0.36386068 1.30490073
H 1.43838693 0.34796874 2.27405118

ts-2-p2
C -0.09325947 0.15580196 -0.56688769
C -0.35719160 -0.45898712 0.80940806
F 1.18494619 0.05041993 -0.91789621
F -0.46119275 1.42701844 -0.61972444
F -0.81323405 -0.51992684 -1.46989301
F 0.74434629 0.55896039 1.56261163
H -0.68393427 0.18582661 2.15328933
H -1.44957869 -0.54294795 0.88881729
O 0.18127100 -1.67405949 0.99222293
H 1.13656056 -1.61048622 0.85911601

ts-3-4
C -0.00365024 0.44124839 -1.09198720
C -0.14350848 -0.41423204 2.33130016
F -0.02620079 1.74349898 -0.92871302
F -1.03684490 0.06201015 -1.82632784
F 1.11837273 0.08083045 -1.69087256
F 0.87704101 -1.23076809 2.64457036
H -1.10287387 -0.86671665 2.55227876
H 0.02188899 0.59891709 2.66892079
O -0.10369304 -0.18736633 0.55782890
H -0.06190078 -1.12749207 0.33241328

ts-4-p2
C 0.40624005 0.09725496 -0.51430543
C -0.28280142 -0.47399168 1.02900773
F 1.49958179 0.80150585 -0.29324397
F -0.47275734 0.84352648 -1.18550277
F 0.71388759 -0.95726765 -1.26320133
F -0.36523588 0.81554795 1.55228943
H 0.67382086 -1.05011690 1.11067491
H -0.44739036 -0.99476333 2.19858936
O -1.45505412 -1.04517825 0.56654487
H -1.72148653 -0.64034391 -0.26827584

2. O_2 addition to CF_3CHF radical (Figure 4)

O_2
O -0.59492910 -0.00000000 -0.00000000
O 0.59492910 0.00000000 0.00000000

CF_3COOH (TFA)
C -0.07597853 0.26310716 -0.53272566
C 0.01911774 -0.37967366 0.86694592
F 1.06529859 0.19741319 -1.20255243
F -0.42168611 1.53865307 -0.40769373
F -1.01595896 -0.36100964 -1.23506528
H 1.19334656 -1.32221929 1.96865305
O 1.20586977 -0.93513145 1.08118673
O -0.89847036 -0.35651063 1.62386742

CF_3CFO (TFAF)
C -0.22383118 -0.00310054 -0.54399275
C 0.46986896 -0.13306878 0.82249789

F	-0.03288360	1.21790703	-1.03068107
F	-1.52924560	-0.20540406	-0.40633671
F	0.26617903	-0.88790305	-1.38863576
F	-0.03666872	0.76022697	1.65945353
O	1.31493869	-0.89342771	1.10279720

i5

C	-0.26343107	0.26683155	-0.83855095
C	-0.25023066	-0.08464260	0.64750466
F	0.85401894	0.87898647	-1.19982758
F	-1.29193577	1.06980355	-1.08978813
F	-0.40265634	-0.84021335	-1.56058284
F	-0.12633724	1.04713976	1.36226504
H	-1.15189975	-0.62091195	0.93933496
O	0.73673930	-1.59068404	1.96543687
O	0.87888352	-0.90103764	0.86440760

i6

C	-0.09341379	0.30577616	-0.81058251
C	0.61902556	0.17279280	0.54663175
F	0.39307450	1.38404953	-1.42848526
F	-1.39845511	0.45883610	-0.67140733
F	0.15083836	-0.75634210	-1.55465170
F	0.02724989	0.93222109	1.45481803
H	-0.52081538	-2.30178129	1.70636219
O	-0.95211130	-1.91762199	0.92304586
O	1.59242526	-0.44947470	0.74892698

i7

C	-0.37875848	0.08441250	-0.71043169
C	-0.28745074	-0.57130830	0.68398399
F	0.74979284	-0.01866077	-1.39536396
F	-0.67863490	1.36943455	-0.57026195
F	-1.34963362	-0.50210582	-1.40189064
F	1.88671709	1.10260666	1.11200063
H	0.92291953	-1.43393456	1.82383947
O	0.92838660	-1.06389438	0.92816054
O	-1.21891703	-0.61028648	1.42022926

i8

C	-0.23326303	0.01088239	-0.72221336
C	0.18906575	-0.00708333	0.76673689
O	1.54803486	0.08571124	0.92759896
F	-1.55203796	0.08748120	-0.83529014
F	0.19398838	-1.07682234	-1.33906114
F	0.30969410	1.07616322	-1.31464589
F	-0.19215804	-1.18962230	1.27724247
H	1.85248154	0.93099980	0.57483632
O	-0.39295412	1.04414845	1.39858337

ts-5-6

C	-0.22351179	0.23969683	-0.79476951
C	0.03074575	0.04097771	0.69652544
F	0.75550633	0.95937780	-1.33410131
F	-1.36999038	0.88029425	-0.98089639
F	-0.27727889	-0.93394473	-1.40319245
F	-0.05902877	1.18378065	1.36394932
H	-0.71856338	-0.93565614	1.18835400

O 0.20813523 -1.73049621 1.57033694
O 1.10061343 -0.71835117 1.00057351

ts-6-7
C -0.31361697 0.19365652 -0.70820905
C -0.08330214 -0.18551081 0.76379317
F 0.79382700 0.16581538 -1.43079496
F -0.83362275 1.40928415 -0.75982508
F -1.17967315 -0.66972302 -1.22994113
F 1.26840716 0.61083461 1.11669061
H 1.11013194 -1.52561627 1.68784492
O 1.04021852 -1.28057308 0.74270559
O -0.91182678 -0.23102530 1.59933329

ts-6-8
C -0.29036414 0.01471983 -0.72624429
C -0.08355387 0.02691640 0.79885972
O 1.75207016 0.07546324 0.86243253
F -1.59609983 0.00155121 -0.97659046
F 0.26046536 -1.04526257 -1.29053662
F 0.23293790 1.11166219 -1.26027588
F -0.29656869 -1.18178137 1.29285660
H 1.98782466 0.97657163 0.57765075
O -0.18438065 1.02562936 1.47192505

ts-8-7
C -0.04857198 -0.01773445 -0.78158880
C 0.18603374 0.31606541 0.70327071
O 1.43623961 0.11854560 1.04492281
F -1.33478854 -0.01020830 -1.06259144
F 0.46898715 -1.19255030 -1.09964312
F 0.55539657 0.92220985 -1.51190563
F -0.80387351 -1.13370467 1.40822592
H 1.55579101 0.40096717 1.96413835
O -0.63147773 0.94941573 1.37315902

3. Hydrolysis of CF_3CFO (Figure 6)

HF
F -0.08101537 0.00114694 0.03980559
H 0.74327428 -0.01052254 -0.36519577

CF_3H
C -0.06303550 0.23463053 0.23875733
F -0.64726201 0.56797512 -0.90940839
F -0.52858129 -0.95329634 0.61683649
F 1.24603591 0.12426639 0.02710357
H -0.26485272 0.98409503 1.00150036

FCOOH
C -0.08621024 0.14229055 -0.01475972
O 1.19942768 0.16064075 -0.32566639
F -0.44853728 -1.08910207 0.37676270
H 1.58559491 -0.71394114 -0.20060574
O -0.83588587 1.04343599 -0.05948395

i9
C -0.16652089 0.03776011 -0.78519177
C -0.65377373 -0.04576781 0.67049848

O	1.79649991	0.42193893	1.24601595
F	-1.19128754	-0.30482840	-1.57345689
F	0.83241171	-0.79513621	-1.03217268
F	0.19746736	1.26878896	-1.08185061
F	-0.54006407	-1.28797700	1.12283222
H	1.77783726	0.96075684	2.04050306
O	-1.16109786	0.82320929	1.27119576
H	2.37093167	-0.32128949	1.44292149

i10

C	-0.03184047	0.21736765	-0.74399541
C	-0.05538262	0.62142686	0.74290046
O	1.17344334	0.59538898	1.25066764
F	-1.20674850	-0.24287400	-1.12244879
F	0.89312923	-0.71768835	-0.99802903
F	0.26931821	1.28688412	-1.47841338
F	-0.11135267	-2.04652538	1.13573971
H	1.11740938	0.87776286	2.17455826
O	-1.04800003	0.96673926	1.29552466
H	0.56738365	-2.25469022	0.54746805

i11

C	0.10677547	0.54303307	-1.38810111
C	-0.26176861	-0.18524087	1.71536634
O	1.03371532	-0.13963371	1.45592052
F	-0.46472826	0.88516314	-2.53768323
F	-0.38443643	-0.64891533	-1.02114855
F	1.41393188	0.39669908	-1.59611358
F	-0.62773382	-1.41328642	2.08426568
H	1.42510735	-1.01977947	1.51315254
O	-1.01392637	0.71626241	1.64100009
H	-0.08675902	1.28305312	-0.61599725

ts-9-10

C	-0.07753808	0.10376777	-0.80826114
C	-0.21860847	0.24772216	0.71311606
O	1.27614629	0.17019077	1.29454637
F	-1.21758502	-0.33527697	-1.30895573
F	0.90100972	-0.71203506	-1.16130711
F	0.17946892	1.30955489	-1.30968312
F	-0.16225490	-1.43869650	1.13007800
H	1.25082707	0.68068649	2.11759800
O	-0.99838513	0.89452736	1.29909069
H	0.94697267	-0.86454072	1.45939816

ts-9-11

C	0.15717637	0.11308052	-0.90268520
C	-0.36125578	-0.09747407	1.13418496
O	1.01525335	0.52618501	1.50123153
F	-0.44537374	1.23260166	-1.31253699
F	-0.58079157	-0.91897814	-1.32636785
F	1.33608672	0.03236994	-1.58428385
F	-0.16055452	-1.40169848	1.25461477
H	1.59141083	-0.14454678	1.90416578
O	-1.34277400	0.49799642	1.33718435
H	0.98742242	0.42670280	0.38554351

4. NO radical addition to CF_3CHFO_2 (Figure 7)

NO

O	-0.53062987	-0.00000000	0.00000000
N	0.60683418	0.00000000	-0.00000000

HONO

H	-1.03243785	1.27709875	-0.62613359
O	0.63866159	-0.79349911	0.44123787
O	-0.41721133	0.55157424	-0.78855085
N	-0.10708201	0.09566994	0.48862925

HNO_2

H	1.13664693	-0.42951280	-0.58276815
O	-0.24816346	-0.85878498	0.64878741
N	0.25928949	-0.09785566	-0.13300776
O	-0.11665173	0.99656682	-0.46171548

CF_3CHFO

C	-0.17534804	-0.17243542	-0.53764669
C	0.04485403	0.60159635	0.78286842
F	0.49171122	0.41507427	-1.52224376
F	-1.46653417	-0.17629604	-0.84172626
F	0.24556318	-1.42383964	-0.42497085
F	1.38994918	0.70621119	0.97320638
H	-0.37910820	1.61164353	0.64754418
O	-0.60181058	0.01938171	1.77694972

NO_2

O	-0.78914308	0.29164330	0.70728678
N	0.06189662	0.28830631	-0.11120587
O	0.73505600	-0.54358279	-0.61011022

CF_3CHO

C	0.15568700	-0.21248044	-0.24476404
C	0.03812982	0.81191424	0.89263728
F	0.79577474	-1.29607056	0.20238031
F	0.88227227	0.31059947	-1.23585204
F	-1.02025333	-0.57368365	-0.71896472
H	1.01109177	1.12960638	1.30220412
O	-1.01253288	1.21100789	1.27946118

NO_2F

F	1.02031417	-0.70084574	-0.08904353
N	-0.14318698	0.09848482	0.01240665
O	-0.26007930	0.58832493	1.07000662
O	-0.76385289	0.11535975	-0.98087599

i12

C	-0.22419441	0.22827162	-1.52127342
C	-0.25109223	0.56475177	-0.02966210
F	0.67938115	-0.70111813	-1.79394463
F	0.07331491	1.32617072	-2.21008220
F	-1.41861456	-0.20346867	-1.91265485
F	0.95936915	1.06923217	0.31852038
H	-1.01641869	1.31242008	0.17871532
O	-0.50359454	-0.62021527	0.63174377
O	1.22203950	-0.99811205	2.34668211
O	-0.82346417	-0.29933970	1.96122766

N 0.28517236 -0.59152425 2.86184977

i13
C -0.14102813 0.04503385 -1.26337359
C 0.96910427 0.43314323 -0.27031730
F 0.36337497 0.12933285 -2.49631157
F -1.18211038 0.85945753 -1.18649312
F -0.53428682 -1.19407243 -1.04875013
F 0.99046165 1.74894790 -0.09560999
H -1.15457914 1.09688901 2.15324820
O 1.74181365 -0.30202485 0.21265068
O -0.33897898 -1.66369330 2.09231809
O -0.91157233 0.31928150 1.63445095
N -0.65397495 -0.67553585 2.60203269

i14
C -0.03487580 0.32886173 -1.28529586
C 0.97224084 0.56239526 -0.14509289
F 0.56315718 0.64640998 -2.43298677
F -1.11501521 1.07176754 -1.15203472
F -0.37351609 -0.94970509 -1.32324311
F 1.02325512 1.83415448 0.18058737
H 0.36041327 -1.49824210 1.47674826
O -1.07267379 -1.93769152 2.66595287
O 1.66933573 -0.26369454 0.32314782
N -0.56419987 -1.20867310 1.86214877
O -0.99745345 -0.15909132 1.43875705

i15
C 0.23786290 0.15546621 -1.23288829
C 0.45567050 0.93566161 0.09301445
F 0.51319736 0.99067578 -2.24037596
F -1.03049756 -0.22236464 -1.35509793
F 1.02522102 -0.89373303 -1.35758096
F 1.66727025 0.63315852 0.59539436
H 0.41262371 1.99823989 -0.14105398
O -1.61032765 -0.55369331 2.36450653
O -0.54870674 0.79234298 1.04971530
N -0.78449240 -0.53048843 1.52157179
O -0.13925633 -1.39690308 1.02525435

i16
C 1.26135853 0.11784705 -1.02051416
C 1.14498079 1.14648347 0.11397586
F 1.86938754 -0.97819804 -0.56685898
F 2.01830419 0.63407127 -1.99305167
F 0.08731481 -0.21087003 -1.52107149
F -0.63257598 -1.20903952 1.07766573
H 2.11580559 1.52134334 0.47553662
O 0.09413728 1.50038285 0.54647193
N -1.80701537 -0.39844769 1.17761821
O -1.91886953 0.08339997 2.23670631
O -2.42359959 -0.38903435 0.18561459

ts-12-13
C -0.26635430 0.26645377 -1.58672199
C 0.55046564 0.41239828 -0.27096750
F 0.54258070 0.29428542 -2.63487928

F -1.14352237 1.25477729 -1.70224104
F -0.91762434 -0.88626596 -1.57074424
F 1.06292764 1.67405262 -0.22124077
H -0.32934768 0.37014661 0.58220748
O 1.27218307 -0.54211311 0.07944309
O -0.38486145 -1.41040893 3.79868522
O -0.02315258 -0.57050264 1.83338594
N -0.62487571 -0.72300755 2.87375047

ts-12-14
C 0.08648166 0.39457422 -1.44298549
C 0.32509856 0.38789767 0.07902214
F 1.22673499 0.50908522 -2.10655441
F -0.69715135 1.41330153 -1.77247146
F -0.51015995 -0.73614307 -1.79637407
F 0.81188112 1.60122402 0.46304068
H -0.71161890 0.25754519 0.55567603
O 0.26462580 -1.29527349 1.92133493
O 1.02815609 -0.62874096 0.46160227
N -0.86056300 -0.83938606 1.93370051
O -1.69794450 -1.08854873 2.74417818

ts-12-15
C 0.30010720 0.51673068 -1.67278766
C 0.37516546 0.68530942 -0.13833630
F 0.79847951 1.58828255 -2.28679261
F -0.97080925 0.38106269 -2.04699924
F 0.97710611 -0.54932262 -2.07824610
F 1.70043142 0.94788384 0.15186872
H -0.19242833 1.60362096 0.10338253
O -0.93420101 -0.15914707 2.27556809
O -0.10106616 -0.36930539 0.47606762
N -1.00409324 -1.27581442 2.53873504
O -1.36273893 -2.02017199 3.37109183

ts-15-16
C 1.09622028 -0.05767085 -0.91482578
C 0.72241013 0.52532298 0.45359347
F 1.87671369 -1.13018660 -0.81261593
F 1.77125555 0.86957337 -1.60216250
F 0.01770307 -0.38668039 -1.62602201
F -0.02000202 -0.90271221 1.05480797
H 1.57749583 0.51975002 1.14185753
O -0.15643979 1.40082000 0.50398040
N -1.78414020 -0.02830160 1.04864145
O -1.86016279 0.29070009 2.12313968
O -2.18346875 -0.32373583 0.04120042

5. HO_2 radical addition to CF_3CHFO_2 (Figure 8)

HO_2
H -1.18042809 0.35156175 -0.00531493
O -0.31127642 0.27480415 -0.43353215
O 0.46105744 -0.32140472 0.43893356

O_3
O 0.86093659 -0.25277124 -0.59768340
O -0.03971743 -0.34608278 0.23817468

O -0.82121916 0.59885402 0.35950872

$CF_3CHFOOH$
C -0.34978994 0.56584146 -0.70656737
C -0.17766546 -0.21966122 0.59310700
F 0.81163666 1.01504617 -1.16248782
F -1.14945338 1.60673082 -0.48929773
F -0.90657810 -0.20381092 -1.63609201
F 0.32057915 0.62866084 1.53723209
H -1.13804541 -0.60144892 0.94111371
O 0.70977994 -1.23061020 0.33125782
O 0.64306428 -2.13627488 1.42016097
H 1.39299651 -1.84938225 1.95871305

CF_3CFO_2
C -0.23102027 -0.19386281 -0.91099868
C 0.04174413 0.21323389 0.52635430
F 0.00336014 0.83805840 -1.71130734
F -1.50615470 -0.53855286 -1.03460812
F 0.53611263 -1.20530830 -1.25788231
F -0.65791195 1.18930173 0.98236507
O 0.88752565 -0.36773393 1.19949238
O 1.09008435 0.04071513 2.48293969

H_2O_2
H -1.24341349 0.34773516 -0.02631330
O -0.40804934 0.30190637 -0.50419391
O 0.42422669 -0.34705397 0.45136395
H 1.04203947 0.35823578 0.67289881

i17
C 0.05342362 0.13048867 -1.67867358
C -0.60619818 0.14124919 -0.29874119
F 1.27323185 0.65076956 -1.63418862
F -0.68161380 0.84476628 -2.52481852
F 0.13404957 -1.11417835 -2.13601398
F -0.74369363 1.43315255 0.09068009
H -1.58923922 -0.32794079 -0.34187123
O 0.24185709 -0.54822309 0.54541728
O -0.50335535 -1.00766434 1.65864790
O -0.45270508 -0.01914670 2.61982315
O 0.77346993 -0.13549790 3.27599193
H 1.34971164 0.42230878 2.73335838

i18
C 0.05754942 0.05938068 -1.62833667
C -1.15796003 -0.22078164 -0.73108597
F 1.20092608 -0.12905725 -0.99428312
F 0.01668232 1.29529727 -2.11140974
F 0.00574313 -0.78626641 -2.66710768
F -0.31042093 1.81638144 0.63385522
H -2.07847225 0.29324926 -1.04598104
O -1.09564221 -0.97674008 0.18813226
O 1.24610277 -0.78269692 1.85108204
O 0.35671926 -0.88218543 2.68079643
O -0.43155290 0.07064965 2.80334838
H -0.23714312 1.28843151 1.39704796

i19

C	-0.48545046	0.70489597	-1.47725955
C	-0.28311012	-0.08153540	-0.18298372
F	0.66367705	1.16675898	-1.95207189
F	-1.29297130	1.73763877	-1.24677340
F	-1.04979973	-0.07042709	-2.39778237
F	0.22030327	0.77807279	0.75589496
H	-1.23194540	-0.47411688	0.18389238
O	0.61293369	-1.07837701	-0.45278876
O	0.52332920	-2.02846008	0.59496144
O	-0.03729579	-0.48806695	3.26994620
O	1.13133107	-0.66420641	3.15709086
H	1.15763925	-1.67928896	1.23977835

i20

C	-0.03917298	0.18903405	-1.37457010
C	0.22806802	0.57945613	0.07368025
F	0.31636090	1.20175211	-2.16428994
F	-1.33378077	-0.03544949	-1.53281197
F	0.65499688	-0.88214077	-1.69534458
F	-0.56970378	1.44601267	0.57981873
H	-1.94313316	-1.01904106	1.62109273
O	1.20839404	0.13867747	0.66426390
O	1.29023728	0.46642710	2.02929600
O	-1.11630057	-1.11777378	1.12355559
O	-0.26368349	-1.76461949	2.06344705
H	0.32503810	-1.01371701	2.32932369

ts-17-18

C	-0.02215268	0.14594873	-1.63328548
C	-0.15150075	-0.30025411	-0.16734983
F	1.21944371	0.45870085	-1.93818358
F	-0.81823407	1.17158589	-1.88773466
F	-0.40972822	-0.88010934	-2.39229140
F	0.31461318	1.33978260	0.52838642
H	-1.16190740	-0.18396175	0.25480172
O	0.63258284	-1.12797671	0.26429922
O	0.13609355	-1.38372844	2.11905238
O	-0.69648043	-0.53126944	2.40419068
O	-0.15536465	0.67866615	2.71899258
H	0.14326185	1.11816914	1.61791224

ts-17-19

C	-0.53318319	0.66104047	-1.60497061
C	-0.25188647	0.32876776	-0.14152445
F	0.58884387	0.78233184	-2.29861463
F	-1.20057377	1.80998684	-1.67229616
F	-1.27870083	-0.29221034	-2.15339091
F	0.48414973	1.33645378	0.39482285
H	-1.18164810	0.23177182	0.42168019
O	0.46811980	-0.85428432	-0.12019079
O	0.63887674	-1.23061405	1.16748215
O	-0.04115307	-1.60800164	3.10166939
O	1.11813471	-1.14190520	3.21717443
H	1.16245572	-0.50282808	2.38709864

ts-17-20

C	-0.22641115	0.24667190	-1.49418349

C -0.05221525 0.10654018 0.01420893
F -0.69476580 1.44605349 -1.81503341
F -1.08645940 -0.67060181 -1.91957498
F 0.93666223 0.06351423 -2.10418124
F -1.21714485 0.33591220 0.63444523
H 0.29342573 -0.95252429 0.40397286
O 0.96378877 0.88808943 0.44962100
O 1.09563111 0.75003656 1.73969705
O 0.67684820 -1.60998088 1.70144015
O -0.27010889 -1.38780748 2.59466770
H 0.09578164 -0.68964896 3.16633605

6. NO_2 radical addition to CF_3CHFO_2 (Figure 9)

NO2
N -0.00736102 0.17614629 -0.27035576
O -0.53929456 -0.86861702 -0.41058673
O 0.54020558 0.71922116 0.62373118

HO-NO2
H -0.91396751 -0.74918223 -1.25717018
O 0.20538931 -1.11093750 0.51732088
N 0.08488608 0.01376524 0.11426384
O 0.50620428 1.03027664 0.55532964
O -0.65596747 0.15945973 -1.03934417

CF3COOOH
C 0.03593981 0.25300569 -0.71926274
C -0.74759555 -0.02554596 0.59050649
F 1.05185590 1.08901081 -0.49315247
F -0.78293786 0.82858782 -1.58037279
F 0.50251429 -0.86090218 -1.26551210
H 1.77557564 -0.20990065 1.77861924
O -0.05865772 -0.52805501 1.63996468
O 1.26970492 -0.87985234 1.29843789
O -1.90164332 0.20924730 0.69762727

NOF
F 0.88104126 0.08983153 -0.64439186
N -0.39121806 0.38761402 0.00703682
O -0.65969319 -0.43975556 0.72568379

CF3COO-ONO
C 0.21308719 -0.60817289 -1.52951665
C -0.16449854 0.27139573 -0.31667793
F 1.40395823 -0.24963957 -1.99746550
F -0.68643083 -0.45770096 -2.48128983
F 0.26452681 -1.88881030 -1.17960597
O 0.72645386 0.01711096 0.66982081
O 0.53085931 0.87059275 1.75456983
O -1.07380537 1.02386691 -0.28305308
N -0.60967050 0.31438319 2.51011964
O -0.79591041 0.97677264 3.42137586

HO-ONO
H 1.24236323 0.24467647 0.26413681
O 1.21252405 -0.40101497 -0.46897368
O -0.16642633 -0.59247690 -0.64763793

N	-0.94818608	0.12481922	0.19412893
O	-0.36065549	0.80512805	0.95225337

i21

C	-0.58934139	0.75675872	-1.63663592
C	-0.43522440	0.59738082	-0.12601067
F	0.41273094	0.18226552	-2.28989453
F	-0.60863000	2.05415204	-1.93683295
F	-1.73615822	0.21002180	-2.03515549
F	0.69075058	1.23462555	0.27363027
H	-1.30030580	1.02659975	0.39895280
O	-0.34069486	-0.77097040	0.10213376
O	-0.50378062	-0.97738664	1.46727208
O	1.76180520	-1.12251777	1.37128979
N	0.82714319	-1.17935551	2.08598287
O	0.68652813	-1.38242211	3.24298317

i22

C	-0.62242854	0.65892547	-1.68026455
C	-0.25077928	0.82221898	-0.20480738
F	0.21578012	-0.15678352	-2.30391695
F	-0.58279200	1.84608099	-2.27681814
F	-1.85488464	0.17401586	-1.78842556
F	0.97332095	1.39714767	-0.13793534
H	-0.97645280	1.45980520	0.30116780
O	-0.23997214	-0.44984716	0.33498677
O	-0.39633270	-0.33592325	1.73606577
O	0.86351056	-0.27029232	2.28893299
N	1.40251442	-1.63482734	2.51584103
O	0.71546392	-2.46240452	2.13441336

i23

C	-0.05991082	0.12016854	-1.60676108
C	0.02756188	0.78280086	-0.23106640
F	-0.48700496	1.02222823	-2.48005579
F	-0.92681548	-0.87144204	-1.55195766
F	1.12044502	-0.32709175	-1.97126439
F	-1.07453090	1.19118639	0.26198174
H	0.63408386	0.07919595	2.41533457
O	1.11080325	0.95376636	0.31278048
O	1.07664985	1.50196906	1.59977440
N	-0.28600623	-1.25916313	1.51072593
O	-0.75154642	-2.32999355	1.60980983
O	0.29048874	-0.82601974	2.64862941

i24

C	-0.07900205	0.24231023	-1.56918453
C	0.93765296	0.48551656	-0.44324994
F	0.48678470	0.54166225	-2.73793807
F	-1.16145238	0.99225057	-1.41876351
F	-0.43493202	-1.03954940	-1.58695444
F	1.04591672	1.78157141	-0.20264999
H	-1.43099511	-1.44114411	0.73807473
O	1.56749648	-0.34730159	0.10195852
O	-0.33348906	-1.80145992	2.55266034
N	-0.45072577	-0.67940439	2.14983040
O	-0.01462013	0.34466796	2.56779697
O	-1.21867287	-0.52581047	1.00274219

i25

C	0.21154865	0.10521724	-1.09564053
C	0.18079093	-0.26688238	0.41589243
F	1.43957394	0.30416692	-1.54580881
F	-0.47182317	1.23915344	-1.27256292
F	-0.36910672	-0.84662068	-1.80793030
F	1.11550802	0.50665504	1.02593903
H	2.29712165	-1.78517544	0.65727003
O	0.43265700	-1.59889638	0.65646657
O	1.62612353	-1.95045498	-0.01952151
O	-1.06130260	-0.07463812	0.95518977
N	-1.31326245	1.36606305	1.30867268
O	-2.36927537	1.45739013	1.71607313

i26

C	0.08960224	-0.17655510	-1.53441815
C	-0.67004378	-0.46126643	-0.21089091
F	1.10815161	0.65648186	-1.34962742
F	-0.75448178	0.38864951	-2.38192448
F	0.53712436	-1.30191488	-2.07619995
F	0.82062105	1.23198631	1.50104577
H	1.64345683	-0.48203037	0.96197847
O	-0.04647848	-1.20347941	0.72279894
O	1.34754709	-1.28605086	0.49941644
O	-1.77881334	-0.08081876	-0.02361577
N	-0.53833767	1.53351408	2.20767550
O	-0.77973347	0.70829542	2.90690835

i27

C	0.06014496	-0.89945723	-1.51200544
C	-0.33687705	-0.06366169	-0.27607904
F	1.25254178	-0.52935155	-1.95398769
F	-0.83233942	-0.72378996	-2.46651195
F	0.10593318	-2.19130913	-1.19544202
F	1.28237642	2.21441896	-0.33826629
H	0.98495000	2.28613933	0.53240650
O	0.55588502	-0.33059529	0.71238079
O	0.38464035	0.55208545	1.77555359
O	-1.26541742	0.66200066	-0.21014120
N	-0.77430281	0.03892040	2.56970861
O	-0.95397245	0.74867060	3.44107141

i28

C	0.79944460	0.04716469	-1.43670330
C	0.15686200	0.97926811	-0.39380233
F	1.92222533	-0.49103197	-0.99166539
F	1.07978555	0.76889056	-2.52224408
F	-0.04780801	-0.90829147	-1.76608714
F	1.08675865	1.55065184	0.36032131
H	0.20149647	-0.57114136	2.07669732
O	-0.98808136	1.21325210	-0.30306356
O	0.15508118	-1.10554428	1.25768001
O	-1.21886482	-1.37781651	1.13762948
N	-2.00860462	-0.63980403	1.97526375
O	-1.42141345	0.07115840	2.69720391

ts-21-22

C -0.62657524 0.78457957 -1.72872261
C -0.45052718 0.68434014 -0.21599587
F 0.32721295 0.12667093 -2.37639527
F -0.58142089 2.06269460 -2.09980864
F -1.80654989 0.28747433 -2.08767826
F 0.73819542 1.26878428 0.10119964
H -1.25266097 1.20441456 0.30714473
O -0.44032922 -0.65478723 0.10982570
O -0.68504037 -0.79773550 1.43821488
O 1.72346252 -0.75078524 1.74918919
N 1.34635363 -1.62077413 2.39658481
O 0.70619826 -1.86406021 3.32463610

ts-21-23
C 0.13974240 0.14244091 -1.74599892
C 0.02288484 0.28992819 -0.22942027
F -0.31919519 1.21974900 -2.36714276
F -0.57141890 -0.90708304 -2.13036115
F 1.40884155 -0.04224931 -2.07983046
F -1.22208884 0.57160761 0.13479033
H 0.34064966 -0.64743173 0.38629836
O 0.92573341 1.24821265 0.19289242
O 0.66353206 1.71947520 1.34077600
N -0.65071369 -1.27102307 2.31151096
O -0.87013348 -1.78225631 3.36020663
O 0.46340741 -1.30457303 1.75916062

ts-21-24
C -0.10602800 0.18844346 -1.74637644
C 0.32687709 0.32559568 -0.26979008
F 0.94003689 0.29123793 -2.55288427
F -0.96628613 1.14843174 -2.04896447
F -0.68103851 -0.98802320 -1.92635643
F 0.80536317 1.57133402 -0.02681304
H -0.70535223 0.19822487 0.36517613
O 1.04873499 -0.64163161 0.14825259
O 0.51968169 -1.28833163 1.70406291
N -0.33206261 -0.50318165 2.29012998
O -0.15054639 -0.13546982 3.40248423
O -1.31580557 -0.17181617 1.57862752

ts-22-25
C 0.00109783 0.16518450 -1.48861462
C -0.06692579 0.44680860 0.01077248
F -0.41736912 1.21828497 -2.17993260
F -0.77090189 -0.86756358 -1.77611782
F 1.25088289 -0.10780162 -1.83451064
F -1.29956918 0.71082010 0.41548007
H 0.32913138 -0.44433986 0.73469318
O 0.85197179 1.36310859 0.37538818
O 0.71413452 1.73640398 1.59305146
O -0.62790662 -2.16885677 1.08111413
N -0.08307747 -1.86076417 2.08903469
O 0.53622320 -0.78906518 2.18312410

ts-23-24
C 0.60377731 0.34637840 -2.34049427
C 0.18094747 0.19532607 -0.87161849

F 1.74824646 -0.26471769 -2.55577308
F 0.72780708 1.63535172 -2.62768413
F -0.33255558 -0.17693935 -3.12044420
F -0.94721852 0.77890773 -0.62865987
H -2.21876206 -0.87883740 4.19673026
O 0.83180049 -0.39367145 -0.06427779
O 0.16321320 -0.41712831 1.44974131
N -0.63006784 -0.50388449 3.27368024
O -0.16269830 -0.40799584 4.34116098
O -1.95081703 -0.80584865 3.26127717

ts-25-26
C 0.19177110 0.01527947 -1.20991854
C -0.27792033 -0.53299899 0.16584248
F 1.46193100 0.36140500 -1.32163910
F -0.54284176 1.09131151 -1.49166194
F -0.07070870 -0.91946599 -2.12330385
F 0.64674832 0.71793458 1.11115593
H 2.00101261 -0.88369499 0.83422654
O 0.31019607 -1.63852688 0.64704503
O 1.68860653 -1.65782969 0.33396149
O -1.45447136 -0.35498824 0.48953778
N -1.16415016 1.54203307 1.30132508
O -1.43103998 1.44498623 2.33977654

ts-26-27
C 0.02552107 -1.08180226 -1.52786547
C 0.12067385 -0.44359490 -0.12716520
F 1.21224190 -1.31537142 -2.05767757
F -0.64945268 -0.26489805 -2.32979784
F -0.63860712 -2.22850067 -1.44101279
F 0.56369103 2.53780313 1.33244331
H 1.07623562 1.64936913 1.37097456
O 1.32215182 -0.18843306 0.22460210
O 1.42361733 0.35182948 1.52459635
O -0.92028524 -0.24174888 0.48423898
N -0.97538219 0.93535505 2.18571647
O -1.77173824 1.61356080 1.96178469

ts-27-28
C 0.84365851 -0.03443570 -1.44379089
C -0.20954952 0.38322375 -0.40931663
F 1.91235794 -0.57460753 -0.89322323
F 1.19755490 1.03370543 -2.13660773
F 0.28272812 -0.91760066 -2.25714883
F 0.80347290 1.16395206 0.74020921
H 0.42963845 0.14063712 1.27091889
O -1.26544459 0.83874200 -0.54205031
O -0.05605589 -0.82776519 0.82126079
O -1.32962266 -1.16457204 1.27011310
N -1.77942009 -0.38158339 2.36464451
O -1.02743728 0.41557906 2.72581639