New Journal of Chemistry

Supporting Information

$CHF_2CF_2OCHF_2$: Conformational Analysis, Direct Dynamics Study of its Reaction with Cl Atoms and Atmospheric Fate

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Table S1. Structural parameters of the conformers generated at the M06-2X/6-311++G(d,p) level. Bond lengths and angles are given in Å and degrees respectively.

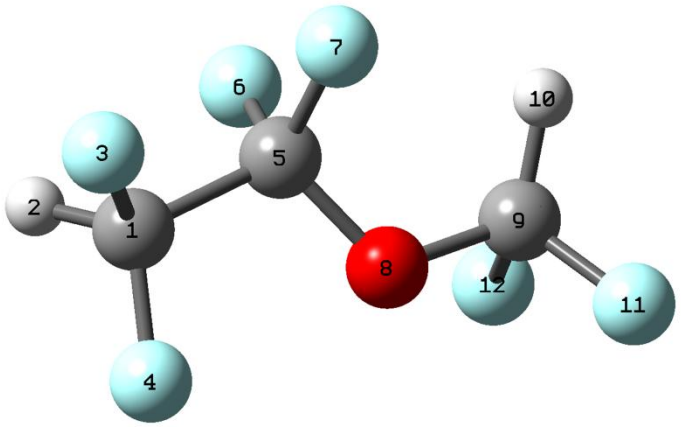
	CF1	CF2	CF3	CF4	CF5	CF6	CF7	CF8	CF9	CF10
C1-H2	1.0910	1.0920	1.0919	1.0911	1.0912	1.0912	1.0897	1.0909	1.0918	1.0915
C1-F3	1.3430	1.3425	1.3443	1.3518	1.3441	1.3400	1.3459	1.3436	1.3437	1.3526
C1-F4	1.3446	1.3432	1.3437	1.3417	1.3445	1.3523	1.3457	1.3454	1.3440	1.3396
C1-C5	1.5304	1.5300	1.5313	1.5349	1.5320	1.5351	1.5375	1.5422	1.5376	1.5402
C5-F6	1.3453	1.3528	1.3446	1.3456	1.3438	1.3526	1.3291	1.3354	1.3432	1.3306
C5-F7	1.3477	1.3486	1.3426	1.3306	1.3356	1.3317	1.3414	1.3368	1.3386	1.3445
C5-O8	1.3618	1.3550	1.3675	1.3720	1.3744	1.3645	1.3849	1.3834	1.3744	1.3731
O8-C9	1.3893	1.3897	1.3825	1.3861	1.3834	1.3877	1.3724	1.3742	1.3796	1.3821
C9-H10	1.0899	1.0902	1.0868	1.0890	1.0870	1.0892	1.0866	1.0867	1.0868	1.0909
C9-F11	1.3404	1.3392	1.3417	1.3332	1.3411	1.3342	1.3391	1.3379	1.3421	1.3268
C9-F12	1.3322	1.3321	1.3407	1.3442	1.3400	1.3401	1.3540	1.3515	1.3407	1.3515
C1-C5-O8	108.2	110.2	109.1	113.4	107.2	115.4	112.7	115.8	117.8	115.3
C5-O8-C9	116.5	116.4	119.7	118.7	119.6	118.7	120.3	121.9	122.4	119.5
H2-C1-C5-O8	58.2	-179.6	-178.6	53.6	-56.7	175.0	67.8	-46.6	169.7	70.8
C9-O8-C5-C1	-177.0	-176.4	-160.2	68.6	-160.2	66.2	-84.6	-49.5	53.2	-35.8
H10-C9-O8-C5	-25.3	-25.9	-163.2	22.0	-163.6	22.9	166.6	-169.3	166.2	71.7

Table S2. Relative energies (in kJ mol^{-1}) for all the conformers and transition states involved calculated at the M06-2X/6-311++G(d,p) level.

System	ΔE_{rel}
CF1	0
CF2	1.55
CF3	4.60
CF4	5.06
CF5	5.19
CF6	5.98
CF7	8.28
CF8	12.60
CF9	12.60
CF10	16.65
TS12c	16.23
TS23a	12.17
TS34c	20.12
TS39b	27.86
TS47b	10.63
TS48b	18.90
TS96a	23.70
TS85a	23.70
TS10-7a	18.62
TS56c	22.97

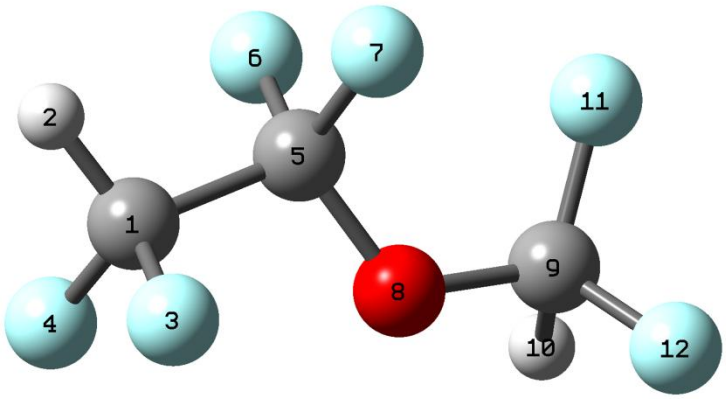
Structures, Imaginary frequency and Cartesian Coordinates of Transition states

TS12c



Imaginary frequency	**69.67*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	1.80937500	0.21042600	-0.40361200
2	H	2.21175900	-0.28483400	-1.28852000
3	F	2.67786700	0.08583300	0.61333000
4	F	1.63686700	1.51445900	-0.65793100
5	C	0.45506400	-0.44679800	-0.00442200
6	F	0.19589600	-1.44908900	-0.87862300
7	F	0.54706800	-1.03271800	1.20364800
8	O	-0.54017200	0.47440300	-0.02026900
9	C	-1.82296500	-0.00660400	0.21694000
10	H	-1.82860500	-0.93497200	0.78795300
11	F	-2.47251600	0.95103800	0.87714300
12	F	-2.44191800	-0.19369700	-0.95653600

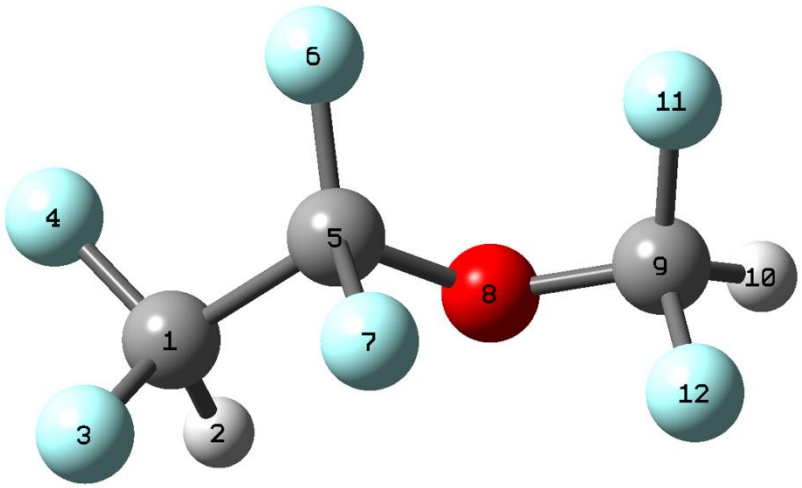
TS 23a



Imaginary frequency	**76.42*i***

Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-1.85183600	-0.03473400	0.09151800
2	H	-2.51229900	0.71141900	0.53784200
3	F	-1.97169200	-1.20093300	0.74667000
4	F	-2.18479300	-0.22494900	-1.19738300
5	C	-0.39687100	0.43869100	0.16674000
6	F	-0.30365000	1.61826200	-0.48116600
7	F	-0.09160500	0.66911100	1.45535500
8	O	0.40254400	-0.50646800	-0.39190000
9	C	1.77416000	-0.30499500	-0.53396500
10	H	2.03580900	-0.26146800	-1.58938700
11	F	2.17449200	0.81340000	0.08363600
12	F	2.38873900	-1.34066800	0.04188800

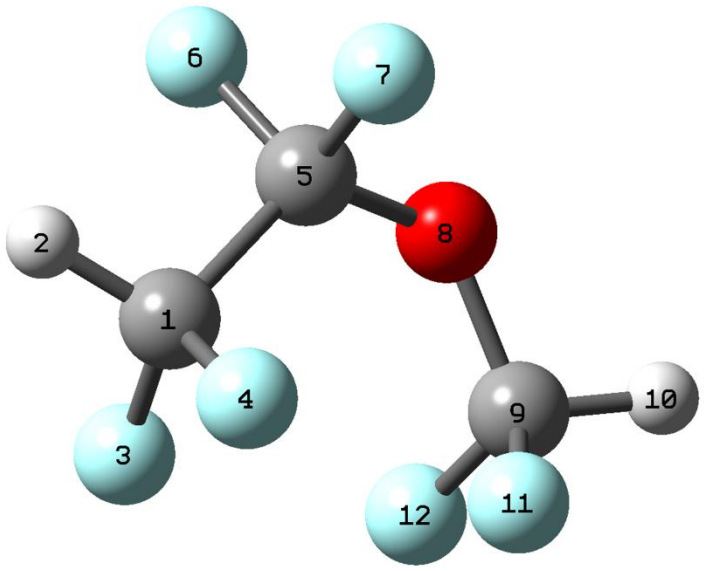
TS 34c



Imaginary frequency	**66.82*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-1.69734300	-0.26969500	-0.47765500
2	H	-1.57515700	-0.61455400	-1.50427500
3	F	-2.20396200	-1.26145400	0.27305300
4	F	-2.55463200	0.76353300	-0.44936300
5	C	-0.32517700	0.17498600	0.11587100
6	F	-0.38125600	1.44818100	0.52091100
7	F	-0.00128600	-0.56763600	1.17865900
8	O	0.60280700	0.03144300	-0.89593000

9	C	1.95204700	0.00163400	-0.58723300
10	H	2.49918000	0.20866400	-1.50357700
11	F	2.25598000	0.90343300	0.35554300
12	F	2.29364100	-1.20685800	-0.11553700

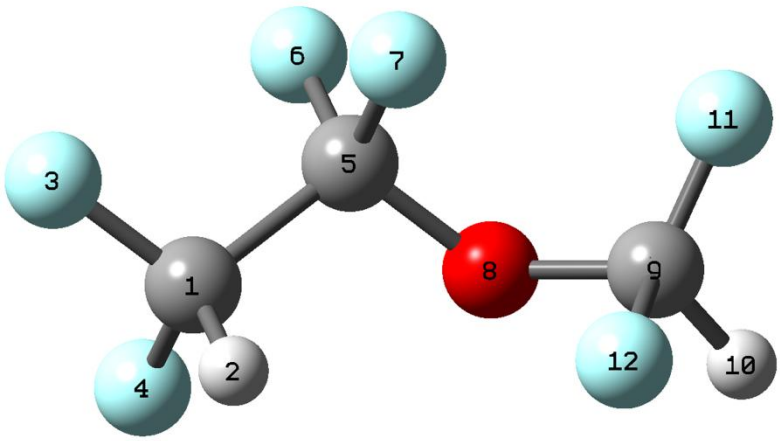
TS 39b



Imaginary frequency	**67.45*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-0.93434800	0.92794300	0.38576000
2	H	-1.91741200	1.09508500	0.83011500
3	F	0.02148600	1.21560700	1.28570200
4	F	-0.79213600	1.72765300	-0.68053400

5	C	-0.84959300	-0.56531800	-0.01031200
6	F	-1.48468100	-1.24478600	0.96189600
7	F	-1.56949300	-0.71917400	-1.13371400
8	O	0.35802900	-1.19599800	-0.17605900
9	C	1.58034100	-0.59087700	-0.37072600
10	H	2.20615400	-1.30158700	-0.90461400
11	F	1.45728000	0.54414600	-1.07338400
12	F	2.15294800	-0.28522500	0.80166100

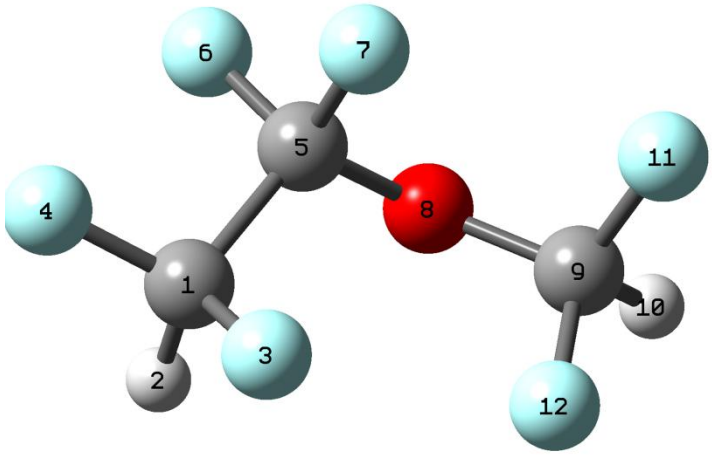
TS 47b



Imaginary frequency	**49.95*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-1.49325300	-0.55648300	0.24972500
2	H	-1.13922100	-1.38158400	0.87152400
3	F	-2.44430500	0.13396400	0.90321400
4	F	-2.01726500	-1.03324300	-0.89298200
5	C	-0.34066400	0.39398800	-0.08991900
6	F	-0.78360300	1.41964600	-0.81605900
7	F	0.16219900	0.87595200	1.05420200

8	O	0.60552300	-0.28884000	-0.83544700
9	C	1.88445500	-0.46945000	-0.36566400
10	H	2.42426600	-1.03700900	-1.11906000
11	F	2.49786000	0.70043400	-0.13974800
12	F	1.87039800	-1.14997700	0.79873500

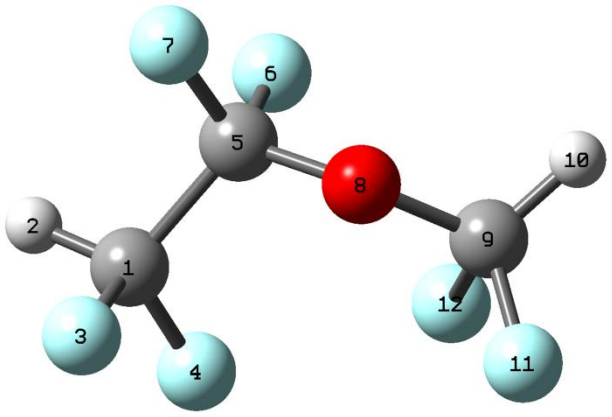
TS 48b



Imaginary frequency	**51.24*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	1.31066300	0.63883300	-0.33972500
2	H	1.32866700	0.88210100	-1.40360900
3	F	0.81605600	1.67041100	0.36235500
4	F	2.56278700	0.40128900	0.09447000
5	C	0.46656900	-0.62447800	-0.07772900
6	F	1.17071100	-1.67697000	-0.50265500
7	F	0.24892700	-0.75896200	1.23163600

8	O	-0.70972700	-0.67151100	-0.80895400
9	C	-1.86593000	-0.02285800	-0.43441500
10	H	-2.61380300	-0.26699000	-1.18474400
11	F	-2.28460500	-0.40957800	0.77702500
12	F	-1.68108200	1.30803200	-0.38825400

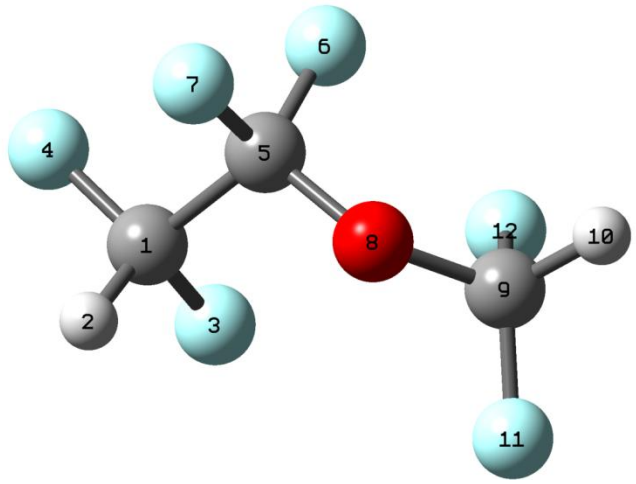
TS 96a



Imaginary frequency	**84.10*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-1.35869400	0.67731500	0.32486500
2	H	-2.26317100	0.50109600	0.91019800
3	F	-1.66962000	1.31616800	-0.81627000
4	F	-0.50489400	1.44443000	1.02370300
5	C	-0.67965700	-0.65248200	-0.03599900
6	F	-0.46312600	-1.35255600	1.09126800
7	F	-1.54290000	-1.34951100	-0.78438100
8	O	0.45675100	-0.52367500	-0.78793700

9	C	1.73139200	-0.32516600	-0.26555000
10	H	2.34126000	-1.21152100	-0.43054200
11	F	2.26032600	0.71220100	-0.91985500
12	F	1.71017600	-0.02608500	1.03708400

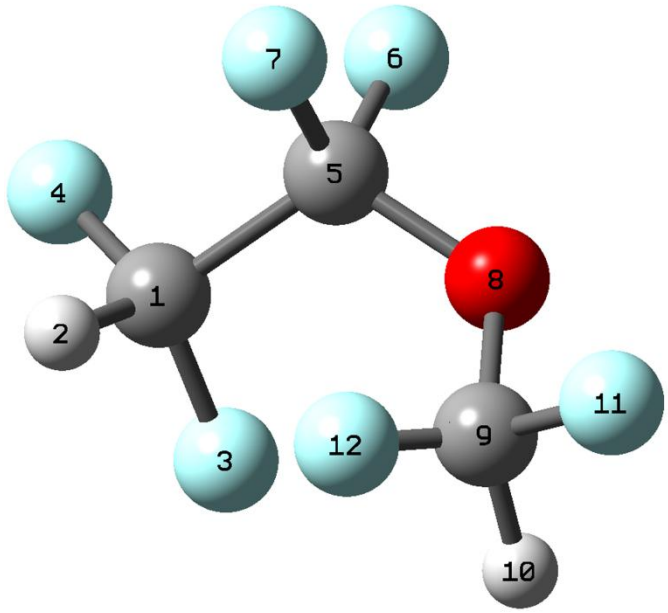
TS 85a



Imaginary frequency	**83.08*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-1.22902400	0.66378300	-0.51690900
2	H	-1.30632900	0.66236400	-1.60566000
3	F	-0.49209900	1.71383100	-0.11471200
4	F	-2.45400300	0.76405900	0.02897500
5	C	-0.58011000	-0.64054200	-0.03272900
6	F	-0.62264500	-0.73183000	1.30009200

7	F	-1.30044600	-1.65091700	-0.53756900
8	O	0.69309700	-0.80871900	-0.52422600
9	C	1.84560200	-0.31994600	0.08443500
10	H	2.45088200	-1.14720600	0.45021000
11	F	2.52269600	0.34986900	-0.85532600
12	F	1.57892600	0.52552400	1.08303700

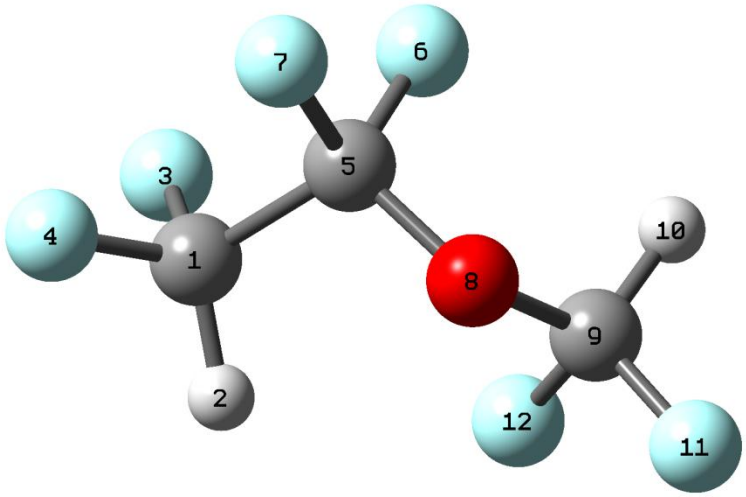
TS 10-7a



Imaginary frequency	**63.52*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	-1.21692900	-0.66474300	0.28746600

2	H	-0.91995000	-1.07559400	1.25006100
3	F	-0.95413300	-1.56109500	-0.69039800
4	F	-2.53402100	-0.41151800	0.29257100
5	C	-0.46169900	0.65104100	-0.03395700
6	F	-1.21415100	1.42173000	-0.81398800
7	F	-0.26692300	1.30319200	1.12799700
8	O	0.72085900	0.49449400	-0.71309200
9	C	1.69038600	-0.40183900	-0.30399000
10	H	1.80583500	-1.20396100	-1.03024600
11	F	2.83685700	0.26657300	-0.17555400
12	F	1.38533700	-0.92812100	0.90246200

TS 56c



Imaginary frequency	**63.16*i***			
Cartesian Coordinates				
Serial No.	**Atoms**	**X**	**Y**	**Z**
1	C	1.24360300	-0.60043100	-0.42075700
2	H	0.62049000	-1.18188300	-1.09872200
3	F	1.68644500	-1.39021300	0.57182600
4	F	2.30615300	-0.12238400	-1.08909700
5	C	0.44144300	0.60025300	0.18695700

6	F	0.33761200	0.45581700	1.52050000
7	F	1.06804500	1.74350800	-0.05589800
8	O	-0.81595300	0.72102100	-0.37470000
9	C	-1.82296800	-0.06248800	0.15453200
10	H	-1.99808900	0.11886500	1.21315800
11	F	-2.91151900	0.20361200	-0.55762500
12	F	-1.51642900	-1.37135800	-0.01650900

Table S3. M06-2X/6-311++G(d,p) optimized parameters of $CHF_2CF_2OCHF_2$(CF1) , transition states (TS A_1 and TS B_1) for hydrogen abstraction by Cl atom and $CHF_2CF_2OC•F_2$ (Rad A_1), and $C•F_2CF_2OCHF_2$ (Rad B_1) radicals. Bond lengths and angles are given in Å and degrees respectively.

Bond lengths (r)	$CHF_2CF_2OCHF_2$ (CF1)	TS A_1	TS B_1	$CHF_2CF_2OC•F_2$ (Rad A_1)	$•CF_2CF_2OCHF_2$ (Rad B_1)
C_1–C_5/C_1-C_4	1.5304	1.5321	1.5296	1.5321	1.5296
C_5–O_8/C_4-O_7	1.3618	1.3847	1.3530	1.3847	1.3530
O_8-C_9/O_7-C_8	1.3893	1.3580	1.3959	1.3580	1.3959
C_1–H_2	1.0910	1.0914	1.4285	1.0914	-
C_1–F_3/ C_1–F_2	1.3430	1.3428	1.3119	1.3428	1.3119
C_1–F_4/ C_1–F_3	1.3446	1.3424	1.3141	1.3424	1.3141
C_5–F_6/ C_4–F_5	1.3453	1.3326	1.3473	1.3326	1.3473
C_5–F_7/ C_4–F_6	1.3476	1.3369	1.3439	1.3369	1.3439
C_9–H_{10}/ C_8–H_9	1.0899	1.4501	1.0903	-	1.0903
C_9–F_{11}/ C_9–F_{10}/ C_8–F_{10}	1.3404	1.3106	1.3286	1.3106	1.3286
C_9–F_{12}/C_9–F_{11}/ C_8–F_{11}	1.3322	1.3176	1.3373	1.3176	1.3373
H.....Cl	-	1.4272	1.4346	-	-
Bond Angle (°)					
$C_1C_5O_8$/ $C_1C_4O_7$	108.2	107.1	108.0	107.1	108.0
$C_5O_8C_9$/ $C_4O_7C_8$	116.5	118.8	116.4	118.8	116.4
Dihedral Angle (°)					
$C_1C_5O_8C_9$/ $C_1C_4O_7C_8$	177.0	-163.4	-176.4	-163.4	-176.4

Table S4. M06-2X/6-311++G(d,p) optimized parameters of $CHF_2CF_2OCHF_2$(CF2) , transition states (TS A_2 and TS B_2) for hydrogen abstraction by Cl atom and $CHF_2CF_2OC•F_2$ (Rad A_2), and

C•$F_2CF_2OCHF_2$ (Rad B_2) radicals. Bond lengths and angles are given in Á and degrees respectively.

Bond lengths (r)	$CHF_2CF_2OCHF_2$ (CF2)	TS A_2	TS B_2	$CHF_2CF_2OC•F_2$ (Rad A_2)	$•CF_2CF_2OCHF_2$ (Rad B_2)
C_1–C_5/C_1-C_4	1.5230	1.5311	1.5303	1.5304	1.5133
C_5–O_8/C_4-O_7	1.3550	1.3783	1.3580	1.3676	1.3644
O_8-C_9/O_7-C_8	1.3897	1.3574	1.3965	1.3629	1.3914
C_1–H_2	1.0920	1.0919	1.4318	1.0919	-
C_1–F_3/ C_1–F_2	1.3432	1.3420	1.3121	1.3430	1.3127
C_1–F_4/ C_1–F_3	1.3425	1.3426	1.3125	1.3430	1.3132
C_5–F_6/ C_4–F_5	1.3486	1.3388	1.3440	1.3431	1.3479
C_5–F_7/ C_4–F_6	1.3528	1.3374	1.3404	1.3432	1.3442
C_9–H_{10}/ C_8–H_9	1.0902	1.4471	1.0903	-	1.0902
C_9–F_{11}/ C_9–F_{10}/ C_8–F_{10}	1.3321	1.3096	1.3365	1.3110	1.3388
C_9–F_{12}/C_9–F_{11}/ C_8–F_{11}	1.3392	1.3186	1.3299	1.3183	1.3322
H.....Cl		1.4296	1.4338		
Bond Angle (°)					
$C_1C_5O_8$/ $C_1C_4O_7$	110.2	108.9	108.6	109.4	109.7
$C_5O_8C_9$/ $C_4O_7C_8$	116.4	118.8	116.4	116.0	116.5
Dihedral Angle (°)					
$C_1C_5O_8C_9$/ $C_1C_4O_7C_8$	176.4	163.3	-175.6	176.5	-175.7

Table S5 Harmonic vibrational frequencies (cm^{-1}) and rotational constants (GHz, within brackets) calculated at M06-2X/6-311++G(d,p) level for $CHF_2CF_2OCHF_2$ (CF1) + Cl system

System	Frequencies (cm^{-1})
$CHF_2CF_2OCHF_2$ (CF1)	37,57,79,132,232,261,318,376,446,488,586,587,597,682,810,904,1096,1162,1180,1187,1197,1223,1268,1333,1390,1402,1447,1479,3150,3167 [2.49156, 0.81885, 0.72938]
TS A_1	727*i*,27,54,66,85,115,139,224,261,330,334,376,450, 505, 570, 592, 640, 748, 826, 900, 905, 939,1131, 1184,1190,1208,1232,1266,1320,1361, 1391,1470, 3147 [1.38325, 0.58272, 0.48083]
TS B_1	809*i*, 24, 34, 60, 70, 95, 130, 227, 246, 322, 335, 382, 437, 493, 578, 608,642, 682, 855, 870, 889, 993,1087, 1165,1196, 1212, 1241,1287,1332,1404,1415, 1449, 3164 [1.12895, 0.62174, 0.49291]

CR A_1	25, 35, 50,58,75, 86,129, 239, 263, 325, 373, 435, 485, 566, 590, 633, 667, 809, 900, 1088, 1162, 1175, 1192, 1203, 1210, 1269, 1331, 1390, 1407, 1447, 1477, 3148, 3165 [0.96105,0.68085,0.48052]
CR B_1	16, 41, 59, 63,76, 89, 132, 234, 262, 325, 372, 443, 482, 568, 591,634, 664, 810, 906, 1086, 1169, 1176, 1193,1201, 1207, 1254, 1339, 1391, 1402, 1445, 1476, 3154, 3169 [0.98921, 0.72286,0.52164]
CP A_1	20, 37, 46, 57, 76, 79, 127, 231, 243, 257, 326, 350, 374, 447,488, 567, 597, 627, 657, 810, 904, 1055, 1181, 1184, 1200, 1226, 1288, 1318, 1351, 1391, 1473, 2980, 3147 [1.15873, 0.58117, 0.45532]

Table S6 Harmonic vibrational frequencies (cm^{-1}) and rotational constants (GHz, within brackets) calculated at M06-2X/6-311++G(d,p) level for $CHF_2CF_2OCHF_2$ (CF2) + Cl system

System	Frequencies (cm^{-1})
$CHF_2CF_2OCHF_2$ (CF2)	32, 59, 78, 129, 218, 245, 362, 370, 455, 507, 552, 589, 629, 667, 748, 935, 1117, 1161, 1176, 1183, 1207, 1212, 1239, 1356, 1390, 1401, 1452, 1478, 3138, 3164 [2.04169, 0.86673, 0.83844]
TS A_2	746*i*, 15, 58, 64, 79, 97, 136, 218, 234, 330, 363, 374, 477, 517, 558, 595, 637, 713, 777, 853, 918, 955, 1138, 1177, 1197, 1205, 1236, 1282,1313, 1340, 1391, 1478, 3142, [1.35712, 0.57971, 0.51311]
TS B_2	791*i*, 27, 39, 51, 69, 95, 134, 214, 241, 309, 363, 371, 457, 510, 570, 608, 639, 676, 815, 873, 898, 989, 1106, 1171, 1197, 1217, 1239, 1268, 1334, 1404, 1414, 1451, 3167,[1.70418, 0.47090, 0.45174]
CR A_2	29, 32, 47, 61, 74, 87, 130, 220, 244, 359, 369, 447, 506, 545, 587, 628, 666, 744, 932, 1107, 1130, 1169, 1179, 1205, 1211, 1224, 1359, 1392, 1405, 1457, 1478, 3140, 3166, [0.94895, 0.64760, 0.48133]
CR B_2	18, 34, 42, 63, 66, 90, 133, 218, 246, 361, 371, 456,506, 551, 589, 629, 667, 747, 932, 1114, 1156, 1175, 1180, 1205, 1210, 1241, 1358, 1395, 1403, 1453, 1479, 3140, 3165 [1.16489, 0.53278, 0.45176]
CP A_2	19, 38, 44, 59, 70, 80, 127, 189, 222, 234, 344, 365,371, 465, 511, 550, 586, 627, 670, 745, 922, 1084, 1176, 1182, 1206, 1216, 1275, 1321, 1361, 1393, 1478, 2981,3143 [1.57941, 0.42234, 0.40152]

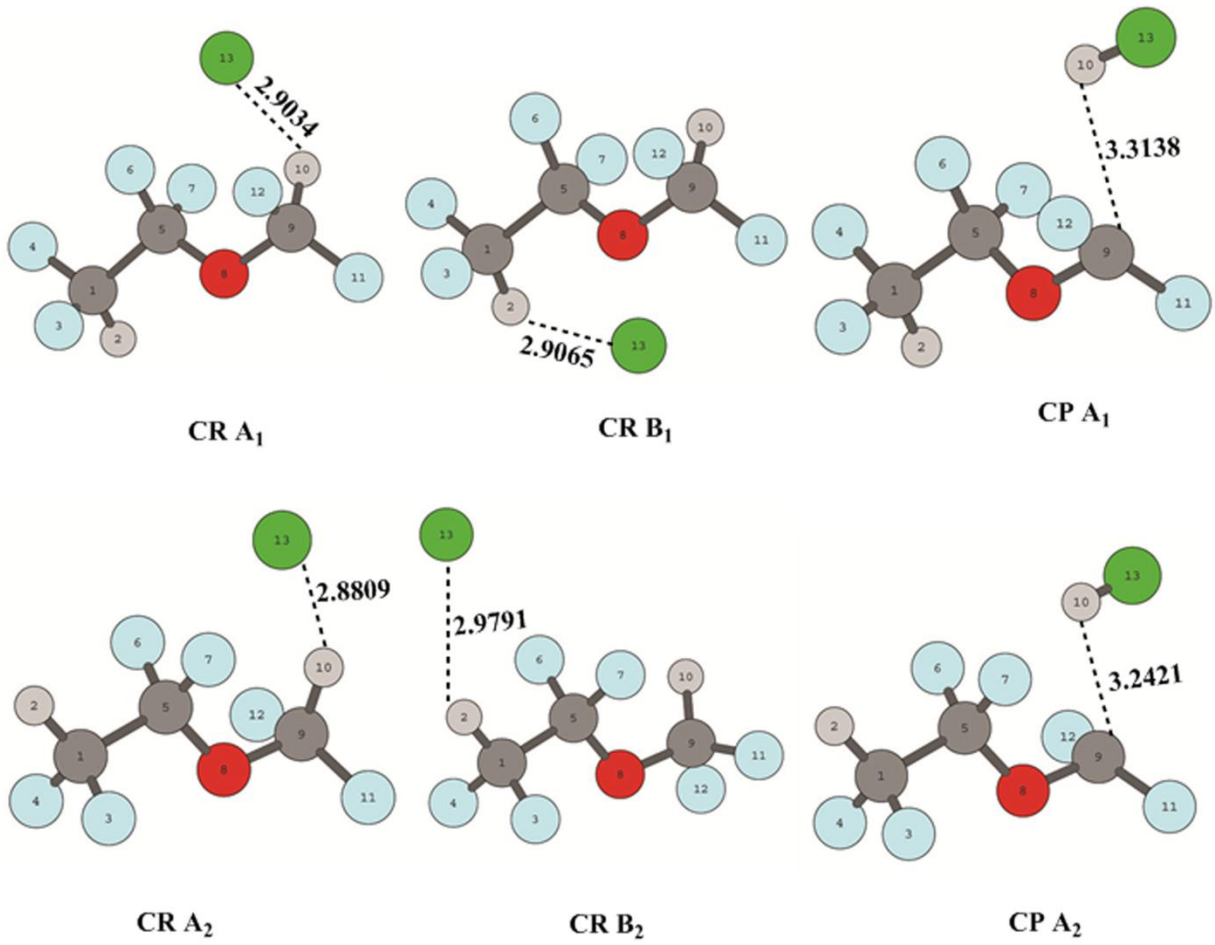


Fig. S1 Optimized structures of the pre- and post-reaction complexes at the M06-2X/6-311++G(d,p) level. Bond lengths are given in Å

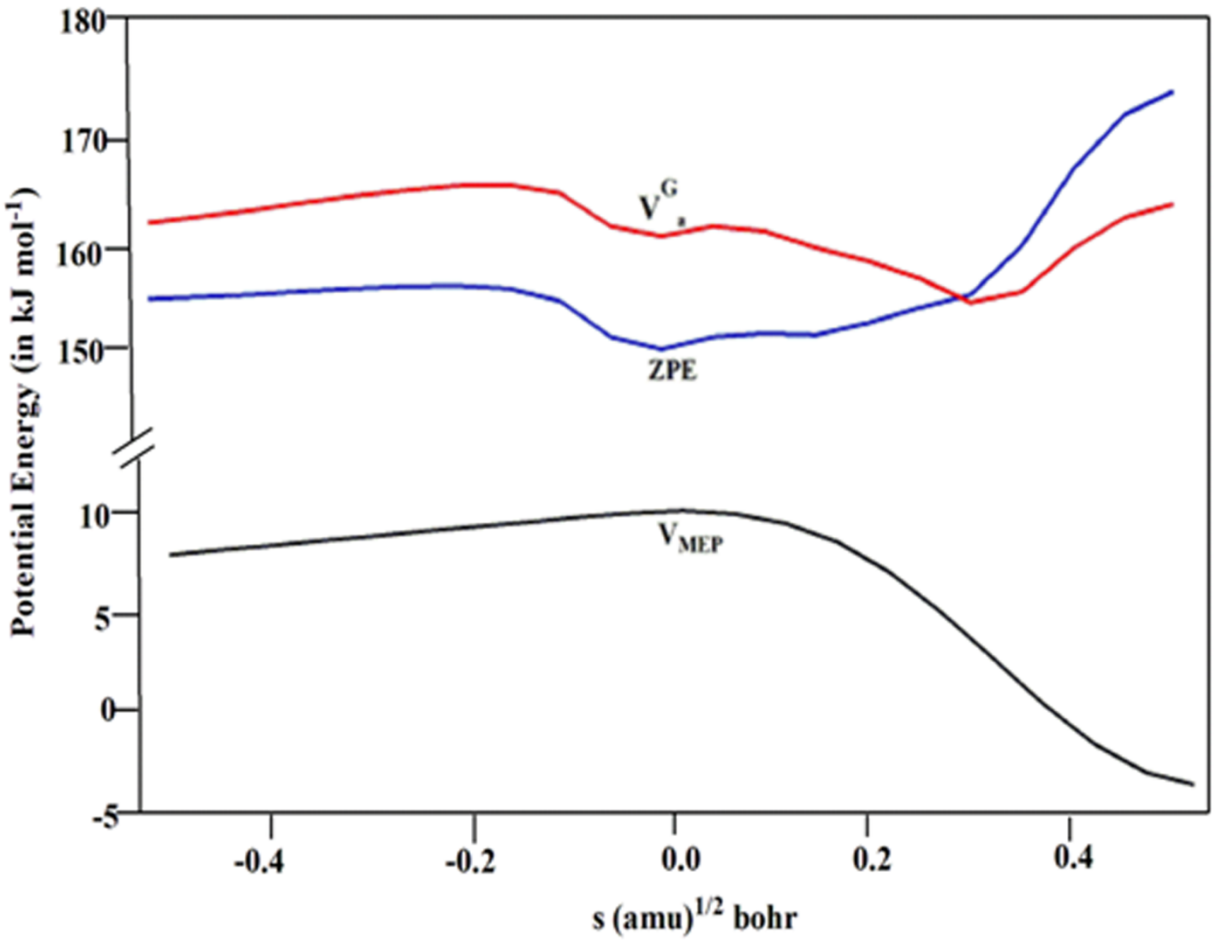


Fig. S2 Classical potential energy curve (V_{MEP}), ground-state vibrationally adiabatic energy curve (V_a^G), and zero-point energy curve (ZPE) as function of s $(amu)^{1/2}$ bohr at the M06-2X/6-311++G(d,p) level for reaction channel R2 via TS B_1 for $CHF_2CF_2OCHF_2$ (CF1) + Cl.

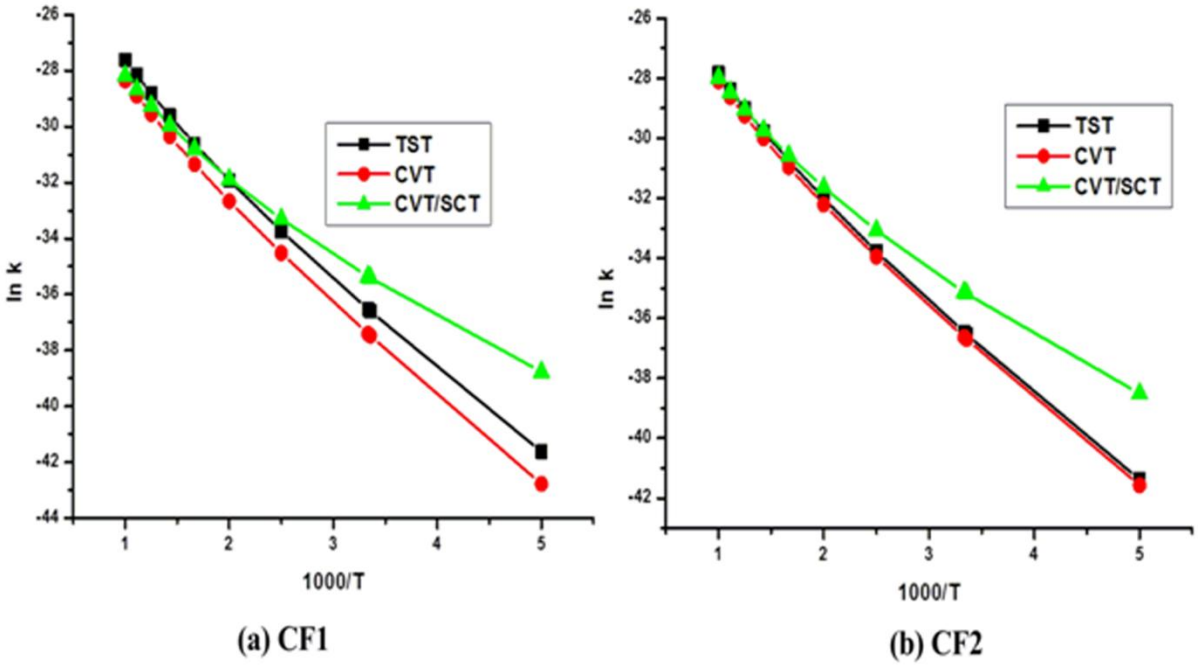


Fig. S3 (a) TST, CVT, and CVT/SCT rate coefficients of $CHF_2CF_2OCHF_2$ (CF1)+ Cl (b) TST, CVT, and CVT/SCT rate coefficients of $CHF_2CF_2OCHF_2$ (CF1)+ Cl.

Table S7 TST/SCT, CVT and CVT/SCT rate coefficient values (in cm^3 $molecule^{-1}$ s^{-1}) for hydrogen abstraction reactions of $CHF_2CF_2OCHF_2$ with Cl atom as calculated using M06-2X/6-311++G(d,p) level and the available estimated results at 298 K.

T	TST(CF1)	CVT(CF1)	CVT/SCT (CF1)	TST(CF2)	CVT(CF2)	CVT/SCT (CF2)
200	8.42×10^{-19}	2.65×10^{-19}	1.46×10^{-17}	1.07×10^{-18}	8.89×10^{-19}	1.89×10^{-17}
298	1.27×10^{-16}	5.28×10^{-17}	4.19×10^{-16}	1.36×10^{-16}	1.16×10^{-16}	5.26×10^{-16}
300	1.37×10^{-16}	5.69×10^{-17}	4.41×10^{-16}	1.46×10^{-16}	1.24×10^{-16}	5.53×10^{-16}
400	2.23×10^{-15}	1.02×10^{-15}	3.44×10^{-15}	2.16×10^{-15}	1.81×10^{-15}	4.32×10^{-15}
500	1.37×10^{-14}	6.51×10^{-15}	1.43×10^{-14}	1.26×10^{-14}	1.03×10^{-14}	1.81×10^{-14}
600	5.06×10^{-14}	2.43×10^{-14}	4.22×10^{-14}	4.45×10^{-14}	3.59×10^{-14}	5.27×10^{-14}
700	1.38×10^{-13}	6.63×10^{-14}	9.88×10^{-14}	1.17×10^{-13}	9.32×10^{-14}	1.23×10^{-13}
800	3.05×10^{-13}	1.46×10^{-13}	1.98×10^{-13}	2.54×10^{-13}	1.99×10^{-13}	2.44×10^{-13}
900	5.88×10^{-13}	2.81×10^{-13}	3.53×10^{-13}	4.80×10^{-13}	3.71×10^{-13}	4.35×10^{-13}
1000	1.02×10^{-13}	4.85×10^{-13}	5.81×10^{-13}	8.20×10^{-13}	6.27×10^{-13}	7.10×10^{-13}

Table S8 Cartesian coordinates (in Å) of different important species in the degradation path of $CHF_2CF_2OCHF_2$. Optimization was done at the M06-2X/6-311++G(d,p) level.

•$OOCF_2CF_2OCHF_2$

Atoms	X	Y	Z
C	2.16183500	0.15288700	0.11623300
O	0.84209900	0.28519000	-0.31718700
C	-0.09824600	-0.34995000	0.42328100
C	-1.45668500	-0.23300200	-0.31318800
H	2.23312200	-0.05212800	1.18486100
F	2.74655000	-0.82989800	-0.57636300
F	2.77258200	1.29581600	-0.18333400
F	-0.18275400	0.16037100	1.66021400
F	0.17986900	-1.65770900	0.56939200
F	-1.45258300	-1.01627900	-1.37690500
F	-2.43013600	-0.59214100	0.51159300
O	-1.70928200	1.06217300	-0.81851000
O	-1.70485500	1.95152100	0.13767400

•$OCF_2CF_2OCHF_2$

Atoms	X	Y	Z
C	2.03521600	0.03699000	0.13763700
O	0.74832200	0.42606800	-0.23812200
C	0.27486300	-0.21577500	0.37405000
C	-1.61868900	0.25684200	-0.26895400
H	2.07760100	-0.33425600	1.16215100
F	2.46987400	-0.90540300	-0.70509300
F	2.80440700	1.11212900	-0.00418000
F	-0.30154400	0.03933400	1.69277300
F	-0.19092100	-1.54436900	0.23737700
F	-1.65799500	-0.15881600	-1.54252000
F	-2.62677200	-0.34821800	0.37895200
O	-1.67345000	1.58818200	-0.15366900

•CF_2OCHF_2

Atoms	X	Y	Z
C	-1.27257300	-0.08679500	-0.38747000
O	0.03881700	-0.20611800	-0.79220900
C	0.97475800	-0.03954400	0.17758400
H	-1.90346400	-0.19355600	-1.26547900
F	-1.56805100	-1.02956500	0.52190600
F	-1.47934100	1.10287200	0.20034500
F	1.50702600	1.16855800	0.17741900
F	1.91590200	-0.95291800	0.08504800

•$OOCF_2OCHF_2$

Atoms	X	Y	Z
C	1.40021200	0.20830000	0.19811500
O	0.32061800	0.03336000	-0.66610400
C	-0.83399100	-0.40312700	-0.11670100
H	1.09256500	0.51011900	1.20055900
F	2.09844800	-0.93110900	0.26466200
F	2.16921800	1.13878400	-0.35723900
F	-0.68060000	-1.51246500	0.59636900
F	-1.69754100	-0.60056600	-1.08573000
O	-1.62507000	1.67380000	0.27696300
O	-1.38250200	0.51872100	0.83269000

•OCF_2OCHF_2

Atoms	X	Y	Z
C	-1.25451800	-0.02129000	0.20495500
O	-0.13502800	-0.22952200	-0.60259500
C	1.08332200	-0.06355700	-0.00398100
H	-1.01366600	-0.04084300	1.26744400
F	-1.79257700	1.15736500	-0.12177300
F	-2.13233600	-0.97592400	-0.09654400
F	1.15440100	1.07956600	0.69950200
F	1.99796500	-0.00347700	-0.96040200
O	1.25925000	-1.11645800	0.83255300

•OCF_2OCF_2

Atoms	X	Y	Z
C	-0.95301700	-0.00000100	-0.00006800
O	0.00002300	-0.00035800	-1.01512000
C	0.95297800	-0.00000500	0.00012200
F	-1.72310600	1.06740000	0.00002900
F	-1.72361800	-1.06703600	-0.00004900
F	1.72310200	1.06753600	-0.00005800
F	1.72358400	-1.06718800	-0.00004600
O	0.00004900	-0.00043700	1.01521800

COF_2

Atoms	X	Y	Z
C	-0.14316500	0.00000400	0.00034700
F	0.62961300	1.05806900	-0.00007000
F	0.62955200	-1.05810400	-0.00007000
O	-1.30918700	0.00003600	-0.00010400