

**Atmospheric Oxidation of 2-fluoropropene (CH₃CF=CH₂) with Cl Atom and Aerial
Degradation of its Product Radicals from Computational Study**

Nand Krishor Gour, Ramesh Chandra Deka and Subrata Paul*

Department of Chemical Sciences, Tezpur University, Tezpur, Assam -784028, India

*Corresponding Authors: spdsk@tezu.ernet.in

Telephone: +91-7002093921, FAX: +91-3712-267005

Table S1: The Zero-point corrected Total energy (E₀), Enthalpy (H) and Gibbs free energy (G) of all species at MP2/6-31+G(d,p) level of theory. All values are in Hartree.

species	E ₀	H	G
CH ₃ CF=CH ₂	-216.4680828	-216.458211	-216.490484
Cl	-459.5540907	-459.55173	-459.569768
IM_add	-676.0294841	-676.017862	-676.055914
TS1	-676.0067416	-675.995797	-676.034258
TS2a	-675.9854581	-675.974123	-676.013453
TS2b	-675.9861608	-675.974856	-676.013896
TS3	-676.023646	-676.012668	-676.049196
TS4	-676.0263633	-676.015118	-676.052811
P1	-215.8253588	-215.816661	-215.848709
P2	-215.8773544	-215.868363	-215.900969
P3	-676.0481208	-676.036805	-676.073641
P4	-676.0454971	-676.034061	-676.071845
HCl	-460.2009457	-460.197223	-460.218391

Table S2: Cartesian coordinates (in Å) of all species at MP2/6-31+G(d,p) level of theory.

Species	Cartesian Coordinate			
	At. No.	X	Y	Z
CH ₃ CF=CH ₂	6	1.345916000	-0.428778000	-0.000017000
	6	-0.093973000	-0.055816000	-0.000002000
	1	1.838787000	-0.020342000	-0.881980000
	1	1.838791000	-0.020394000	0.881968000
	1	1.454137000	-1.510964000	-0.000050000
	6	-1.175377000	-0.835902000	-0.000042000
	1	-2.166326000	-0.409836000	-0.000026000
	1	-1.058941000	-1.907743000	-0.000092000
	9	-0.262872000	1.310250000	0.000061000
TS1	6	-0.213253000	-0.255112000	1.070279000
	6	-1.272473000	-0.044456000	0.103228000
	1	0.893733000	-0.119267000	0.428296000
	1	-0.113337000	0.523771000	1.819478000
	1	-0.146733000	-1.267251000	1.452798000
	6	-1.981388000	-0.968081000	-0.518212000
	1	-2.746844000	-0.698394000	-1.228481000
	1	-1.797802000	-2.009882000	-0.311923000
	9	-1.492034000	1.273113000	-0.171513000
	17	2.243646000	-0.016535000	-0.267549000
TS2a	6	-2.685633000	-0.303385000	0.000340000
	6	-1.212345000	-0.068465000	0.000171000
	1	-3.120032000	0.159888000	0.885115000
	1	-3.120254000	0.160018000	-0.884259000
	1	-2.907092000	-1.367043000	0.000289000
	6	-0.273855000	-0.957872000	-0.000016000
	1	1.142055000	-0.422090000	-0.000164000
	1	-0.248565000	-2.032467000	-0.000097000

	9	-0.911822000	1.258721000	0.000232000
	17	2.440664000	0.008914000	-0.000349000
TS2	6	1.098745000	1.376199000	0.000038000
	6	1.218793000	-0.104976000	0.000017000
	1	1.595789000	1.774062000	0.883538000
	1	1.595800000	1.774089000	-0.883444000
	1	0.055604000	1.676828000	0.000036000
	6	0.295824000	-1.010478000	0.000005000
	1	0.240780000	-2.085007000	0.000004000
	1	-1.126133000	-0.474498000	-0.000038000
	9	2.532887000	-0.505680000	0.000014000
	17	-2.402235000	0.018893000	-0.000034000
IM _{add}	6	-1.354613000	1.243076000	0.159430000
	6	-0.853413000	-0.153089000	0.152022000
	1	-1.015980000	1.758661000	-0.736992000
	1	-2.445125000	1.233181000	0.164090000
	1	-0.990475000	1.769009000	1.037718000
	6	-0.226428000	-0.836944000	1.141372000
	1	0.012029000	-1.881561000	1.018400000
	1	0.005224000	-0.337115000	2.067490000
	9	-1.187475000	-0.827281000	-0.973852000
	17	1.748725000	0.199123000	-0.206057000
TS3	6	1.179448000	1.236254000	-0.350915000
	6	0.699977000	-0.145058000	-0.078636000
	1	0.855244000	1.902041000	0.443195000
	1	2.269886000	1.215927000	-0.379257000
	1	0.793165000	1.588273000	-1.302675000
	6	0.393119000	-1.104944000	-0.999058000
	1	0.233353000	-2.123661000	-0.686553000
	1	0.219713000	-0.821916000	-2.023102000
	9	1.001315000	-0.564882000	1.166089000

	17	-1.589321000	0.200338000	0.119132000
TS4	6	-1.507036000	1.199465000	-0.063529000
	6	-0.909492000	-0.124008000	0.215296000
	1	-2.592956000	1.128773000	-0.002657000
	1	-1.141448000	1.937626000	0.643546000
	1	-1.238172000	1.502253000	-1.075289000
	6	0.015127000	-0.451139000	1.138181000
	1	0.301761000	-1.482148000	1.269023000
	1	0.266569000	0.266604000	1.900528000
	9	-1.327208000	-1.077957000	-0.636086000
	17	1.809266000	0.153094000	-0.279415000
P1	6	1.233302000	0.658691000	-0.000024000
	6	0.000000000	0.057266000	-0.000002000
	1	2.134482000	0.069047000	-0.000022000
	1	1.300868000	1.733860000	-0.000057000
	6	-1.233305000	0.658685000	0.000018000
	1	-2.134483000	0.069039000	0.000002000
	1	-1.300878000	1.733855000	0.000025000
	9	0.000003000	-1.317072000	0.000012000
P2	6	-1.358253000	-0.281051000	-0.000023000
	6	0.124716000	-0.122565000	-0.000017000
	1	-1.777144000	0.203311000	0.885956000
	1	-1.777161000	0.203543000	-0.885868000
	1	-1.627387000	-1.337081000	-0.000158000
	6	1.024418000	-1.044139000	-0.000146000
	1	2.093123000	-1.164049000	-0.000172000
	9	0.482588000	1.197867000	0.000152000
	P3	6	0.985996000	1.262807000
6		0.375585000	-0.055559000	-0.005183000
1		0.615310000	2.055465000	0.228043000
1		2.068057000	1.188541000	-0.319351000

	1	0.730453000	1.489144000	-1.450249000
	6	0.796465000	-1.224926000	-0.799284000
	1	0.745683000	-2.202152000	-0.347431000
	1	0.884577000	-1.129066000	-1.869420000
	9	0.703756000	-0.287097000	1.335447000
	17	-1.430950000	0.075765000	-0.054778000
P4	6	-1.576740000	1.140835000	-0.133592000
	6	-0.957748000	-0.118060000	0.345898000
	1	-1.172414000	1.422831000	-1.110632000
	1	-2.653667000	1.016333000	-0.232438000
	1	-1.372962000	1.947278000	0.568484000
	6	0.394110000	-0.211291000	0.918315000
	1	0.585353000	-1.213114000	1.291613000
	1	0.519254000	0.520129000	1.711911000
	9	-1.298744000	-1.211118000	-0.407733000
	17	1.683847000	0.137512000	-0.314298000
HCl	17	0.000000000	0.000000000	0.070556000
	1	0.000000000	0.000000000	-1.199459000
CH ₃ CFCICH ₂ (OO [•])	6	-0.527004000	1.455567000	-0.852917000
	6	-0.486108000	0.256634000	0.060791000
	1	-1.431167000	2.025751000	-0.653915000
	1	0.345195000	2.077105000	-0.659915000
	1	-0.524064000	1.137342000	-1.893689000
	6	0.719366000	-0.646574000	-0.103766000
	1	0.734457000	-1.411156000	0.669524000
	1	0.749169000	-1.090404000	-1.096449000
	9	-0.491247000	0.709445000	1.379944000
	17	-1.929897000	-0.765533000	-0.159400000
	8	1.898848000	0.196692000	0.054689000
	8	2.990947000	-0.509610000	-0.142176000
	6	0.192302000	1.466718000	-0.708625000

CH ₃ CFCICH ₂ (O [•])	6	-0.013574000	0.192514000	0.071482000
	1	-0.553227000	2.197777000	-0.405175000
	1	1.188402000	1.851776000	-0.498587000
	1	0.097510000	1.274516000	-1.775428000
	6	0.957455000	-0.944024000	-0.277614000
	1	0.775928000	-1.761527000	0.423215000
	1	0.759321000	-1.256042000	-1.305972000
	9	0.137190000	0.476412000	1.426193000
	17	-1.666606000	-0.433563000	-0.155907000
	8	2.251569000	-0.439362000	-0.141853000
TS5	6	0.111153000	1.461945000	-0.806581000
	6	-0.170281000	0.310651000	0.097423000
	1	-0.653659000	2.225523000	-0.656303000
	1	1.092537000	1.856953000	-0.560076000
	1	0.097221000	1.136918000	-1.843716000
	6	1.292324000	-1.021376000	-0.187560000
	1	0.923799000	-1.635788000	0.648748000
	1	0.905917000	-1.318287000	-1.176662000
	9	-0.043130000	0.623568000	1.407479000
	17	-1.639200000	-0.568052000	-0.178925000
8	2.311197000	-0.340983000	-0.082158000	
CH ₃ C [•] FCI	6	-1.339692000	-0.988853000	0.051220000
	6	-0.372333000	0.083408000	-0.303339000
	1	-1.415858000	-1.096289000	1.136720000
	1	-2.318611000	-0.727078000	-0.344974000
	1	-1.018008000	-1.935413000	-0.374898000
	9	-0.782872000	1.329585000	0.067311000
	17	1.298263000	-0.163224000	0.028828000
HCHO	6	0.539880000	0.000000000	-0.000015000
	1	1.117703000	-0.934258000	0.000030000
	1	1.117702000	0.934258000	0.000030000

	8	-0.684335000	0.000000000	0.000004000
CH ₃ CFCI(OO•)	6	0.916143000	-1.501600000	-0.553466000
	6	0.136413000	-0.371694000	0.056203000
	1	1.874809000	-1.579483000	-0.047883000
	1	0.351788000	-2.421874000	-0.417929000
	1	1.074004000	-1.313936000	-1.612143000
	9	-0.112348000	-0.611530000	1.381898000
	17	0.941245000	1.188356000	-0.079930000
	8	-1.134125000	-0.347610000	-0.625611000
	8	-1.941622000	0.579708000	-0.126483000
CH ₃ CFCI(O•)	6	-1.155265000	1.160211000	-0.231399000
	6	-0.349297000	-0.086216000	0.070526000
	1	-0.959070000	1.449257000	-1.260595000
	1	-2.211449000	0.925701000	-0.114726000
	1	-0.870228000	1.959197000	0.445998000
	9	-0.676454000	-1.066934000	-0.860908000
	17	1.409699000	0.169707000	-0.057804000
	8	-0.601083000	-0.507593000	1.328175000
TS6	6	-1.203602000	1.308421000	-0.224805000
	6	-0.269923000	-0.323446000	0.178288000
	1	-0.777016000	1.513425000	-1.196534000
	1	-2.222932000	0.953791000	-0.207316000
	1	-0.908421000	1.956984000	0.585828000
	9	-0.592541000	-1.001998000	-0.983608000
	17	1.425116000	0.205037000	0.005457000
	8	-0.768073000	-0.600212000	1.232105000
CFCIO	6	0.000000000	-0.496037000	0.000000000
	9	-1.337281000	-0.689390000	0.000000000
	17	0.334230000	1.191539000	0.000000000
	8	0.794203000	-1.384429000	0.000000000
	6	0.000000000	0.000000000	0.000000000

•CH ₃	1	0.000000000	1.075251000	0.000000000
	1	0.931195000	-0.537626000	0.000000000
	1	-0.931195000	-0.537626000	0.000000000
CH ₃ CF(OO•)CH ₂ Cl	6	0.259617000	1.759764000	-0.457509000
	6	0.461275000	0.350428000	0.024059000
	1	-0.691827000	2.132800000	-0.089133000
	1	1.067011000	2.379905000	-0.074392000
	1	0.263062000	1.786350000	-1.545634000
	6	-0.513393000	-0.700926000	-0.470541000
	1	-0.244497000	-1.659279000	-0.037680000
	1	-0.462385000	-0.750360000	-1.555740000
	9	0.488065000	0.325943000	1.406472000
	17	-2.180011000	-0.314048000	0.001005000
	8	1.797755000	-0.011208000	-0.438817000
	8	2.138652000	-1.231254000	-0.054785000
CH ₃ CF(O•)CH ₂ Cl	6	1.044003000	1.382809000	-0.350936000
	6	0.821027000	-0.085812000	-0.015213000
	1	0.257135000	1.963709000	0.122383000
	1	2.009112000	1.691858000	0.043477000
	1	1.020444000	1.526907000	-1.428314000
	6	-0.462514000	-0.708293000	-0.574134000
	1	-0.504932000	-1.750564000	-0.267742000
	1	-0.443621000	-0.636662000	-1.657933000
	9	0.771334000	-0.201820000	1.388886000
	17	-1.915265000	0.109914000	0.026104000
	8	1.858033000	-0.797453000	-0.514238000
	TS7	6	1.012636000	1.600991000
6		0.863844000	-0.343788000	-0.036557000
1		0.110231000	1.884752000	0.322204000
1		1.946728000	1.750386000	0.319064000
1		1.035263000	1.747235000	-1.269701000

	6	-0.482697000	-0.647278000	-0.691553000
	1	-0.592304000	-1.727935000	-0.612283000
	1	-0.422375000	-0.364929000	-1.737664000
	9	0.736097000	-0.377135000	1.354384000
	17	-1.899051000	0.110808000	0.047663000
	8	1.902345000	-0.679821000	-0.556634000
CF(O)CH ₂ Cl	6	1.007363000	-0.106176000	0.039473000
	6	-0.283441000	-0.627422000	0.611230000
	1	-0.342948000	-0.349880000	1.661641000
	1	-0.294915000	-1.706472000	0.500275000
	9	1.068537000	1.257206000	0.135206000
	17	-1.685366000	0.062599000	-0.231490000
	8	1.916091000	-0.740137000	-0.418458000
O ₂	8	0.000000000	0.000000000	0.623220000
	8	0.000000000	0.000000000	-0.623220000
NO	7	0.000000000	0.000000000	-0.609613000
	8	0.000000000	0.000000000	0.533411000
NO ₂	7	0.000000000	0.000000000	0.333077000
	8	0.000000000	1.118348000	-0.145721000
	8	0.000000000	-1.118348000	-0.145721000

Table S3: Vibrational frequencies (in cm⁻¹) of all species at MP2/6-31+G (d,p) level of theory.

CH ₃ CF=CH ₂	196	390	460	466	749	821	860	965	1046	1087
	1297	1438	1473	1513	1536	1764	3128	3216	3243	3268
	3378									
TS1	1656i	68	92	385	428	467	495	558	782	899
	965	980	989	1049	1181	1250	1354	1450	1507	1726
	3204	3279	3312	3392						
TS2a	593i	69	71	215	367	431	489	577	671	766
	888	931	1059	1084	1211	1288	1451	1512	1525	2033

	3135	3232	3257	3390						
TS2b	520i	81	96	199	408	411	449	535	736	785
	869	911	1056	1110	1194	1322	1463	1518	1526	2049
	3140	3232	3268	3381						
IM _{add}	109	175	189	275	392	472	682	760	866	975
	1031	1052	1263	1377	1433	1496	1510	1547	1691	3133
	3227									
TS3	457i	190	242	286	349	397	481	660	855	890
	993	1043	1077	1341	1424	1479	1509	1524	1606	3137
	3240	3275	3286	3414						
TS4	298i	107	143	177	400	482	493	860	890	979
	998	1051	1080	1349	1437	1473	1504	1522	1724	3133
	3223	3267	3284	3401						
P1	413	480	510	575	646	740	747	913	971	1060
	1241	1389	1509	1570	3278	3285	3401	3403		
P2	215	392	442	532	786	804	905	1049	1094	1196
	1428	1492	1502	1976	3091	3175	3209	3373		
P3	217	276	289	320	391	414	471	594	669	866
	963	1005	1125	1250	1314	1456	1502	1529	1530	
P4	94	156	193	359	423	533	688	810	928	1013
	1065	1173	1314	1346	1374	1461	1506	1515	1531	3100
	3184									
HCl	3112									
CH ₃ CFCICH ₂ (OO [•])	21	123	164	267	306	318	373	419	426	525
	753	886	964	1008	1015	1154	1182	1248	1279	1315
	1418	1459	1518	1529						
CH ₃ CFCICH ₂ (O [•])	136	225	273	314	341	393	430	484	716	875
	980	1020	1088	1151	1244	1296	1353	1460	1498	1526
	1533	1562	3112	3140						

TS5	739i	116	182	226	258	306	355	414	428	659
	726	969	1023	1175	1221	1250	1282	1447	1510	1514
	1535	1667	2994	3085						
CH ₃ CFCI	213	330	403	437	698	967	1087	1188	1246	1456
	1516	1522	3109	3212	3255					
HCHO	1211	1282	1570	1760	3040	3123				
CH ₃ CFCI(OO•)	130	244	258	313	379	420	444	628	691	874
	955	1129	1181	1205	1263	1462	1523	1525	3149	3258
	3267									
CH ₃ CFCI(O)	228	256	298	413	432	523	685	896	960	1113
	1170	1244	1444	1522	1527	3148	3256	3275		
TS6	692i	206	241	277	406	461	560	687	762	783
	980	1174	1475	1490	1740	3190	3375	3387		
CFCIO	417	508	663	765	1087	1885				
•CH ₃	471	1479	1479	3230	3428	3428				
CH ₃ CF(OO•)CH ₂ Cl	94	130	189	225	269	338	385	415	509	634
	775	855	892	942	1003	1140	1169	1219	1292	1356
	1384	1465	1511	1530						
CH ₃ CF(O•)CH ₂ Cl	106	202	235	307	330	434	479	567	761	844
	911	967	980	1119	1200	1231	1295	1377	1436	1508
	1528	1534	3147	3180						
TS7	683i	104	184	203	270	277	425	507	589	695
	742	770	851	940	1107	1159	1241	1350	1474	1485
	1500	1772	3175	3190						
CF(O)CH ₂ Cl	58	205	406	557	669	823	860	980	1170	1278
	1366	1509	1880	3180	3269					
O ₂	1410									
NO	3854									
NO ₂	752	1370	2307							

Table S4: The Zero-point corrected Total energy (E_0), Enthalpy (H) and Gibbs free energy (G) of all species at MP2/6-31+G(d,p) level of theory. All values are in Hartree.

Species	E_0	H	G
CH ₃ CF(Cl)CH ₂ (OO [•])	-826.0355788	-826.021829	-826.065055
CH ₃ CF(Cl)CH ₂ O [•]	-751.0597881	-751.047596	-751.086113
TS5	-751.0314715	-751.019099	-751.058683
CH ₃ C [•] FCI	-636.8878474	-636.879563	-636.913443
HCHO	-114.1669317	-114.161511	-114.186998
CH ₃ CFCl(OO [•])	-786.8818208	-786.871387	-786.909523
CH ₃ CFCl(O [•])	-711.9170101	-711.907733	-711.943498
TS6	-711.8915039	-711.882275	-711.918335
CFCl(O)	-672.2567218	-672.251472	-672.282894
NO	-129.5586345	-129.554812	-129.578096
NO ₂	-204.5650909	-204.560617	-204.587915
O ₂	-149.9544284	-149.950927	-149.974267
CH ₃ CF(OO [•])CH ₂ Cl	-826.0415878	-826.028058	-826.06966
CH ₃ CF(O [•])CH ₂ Cl	-751.0762481	-751.06404	-751.102893
TS7	-751.0508943	-751.038598	-751.078079
CF(O)CH ₂ Cl	-711.412285	-711.403856	-711.439472
[•] CH ₃	-39.6673649	-39.661515	-39.683653