Electronic Supplementary Information:

Effects of Ambient Gas on Cold Atmospheric Plasma Discharge in the Decomposition of Trifluoromethane

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S1. Record and measure of electrical power by an oscilloscope (Tektronix TDS2012B, 2 channels)

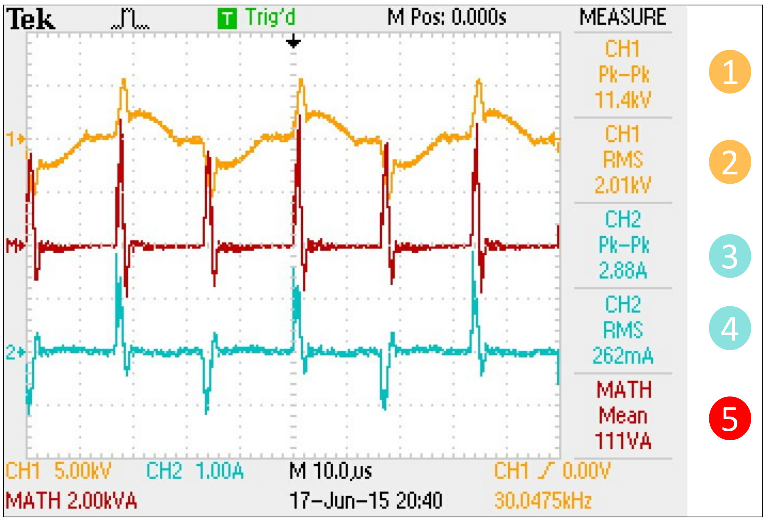

Fig. S1. Electrical waveforms of AC pulse power supplied and five parameter measurements: 1= applied voltage waveform, 2= total current waveform, M= active power, M1= peak to peak of voltage, M2= root mean square of applied voltage, M3= peak to peak of current, M4= root mean square of total current, M5= mean of active power (applied voltage = 6.0 kVp; frequency = 30 kHz total; flow rate = 1000 ml/min; $CHF_3/O_2/N_2$= 2/10/988 ml/min).

S2. Comparison of the phase angle between voltage and current for Ar and He as dilution gases

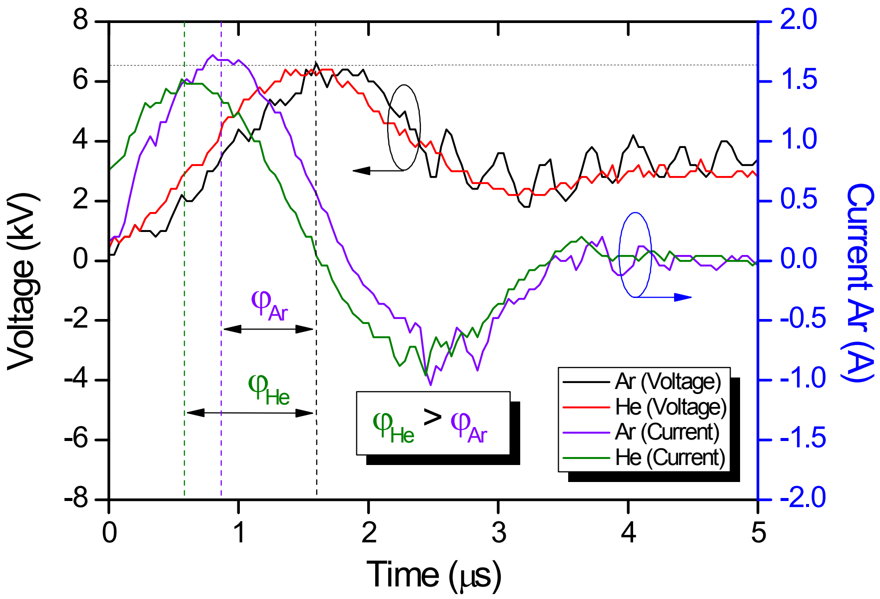

Fig. S2. Diagram of the phase angles between voltage and current for Ar and He as dilution gases (flow rate of CHF_3, O_2 and total flow rate 2, 10 and 1000 ml/min, respectively; frequency= 30 kHz; applied voltage= 6.5 kVp).

S3. Identification of spectra of plasma discharges with the changing composition of the feed gas

Although there was an absence of N_2 in the feed gases with Ar or He dilution, these spectra present N_2 lines in the second positive system ($C^3\Pi_u \rightarrow B^3\Pi_g$). A possible explanation for this might be that there was an N_2 contaminant in our plasma system under these conditions. This phenomenon also presented in the previous reports.[1, 2]

All spectra have a high intensity of the emission line of gas dilution:

Ar dilution gas: from 680 to 1000 nm (Ar I)

He dilution gas: from 380 to 850 nm (He I)

N_2 dilution gas: from 300 to 500 nm (second positive system, $C^3\Pi_u \rightarrow B^3\Pi_g$)

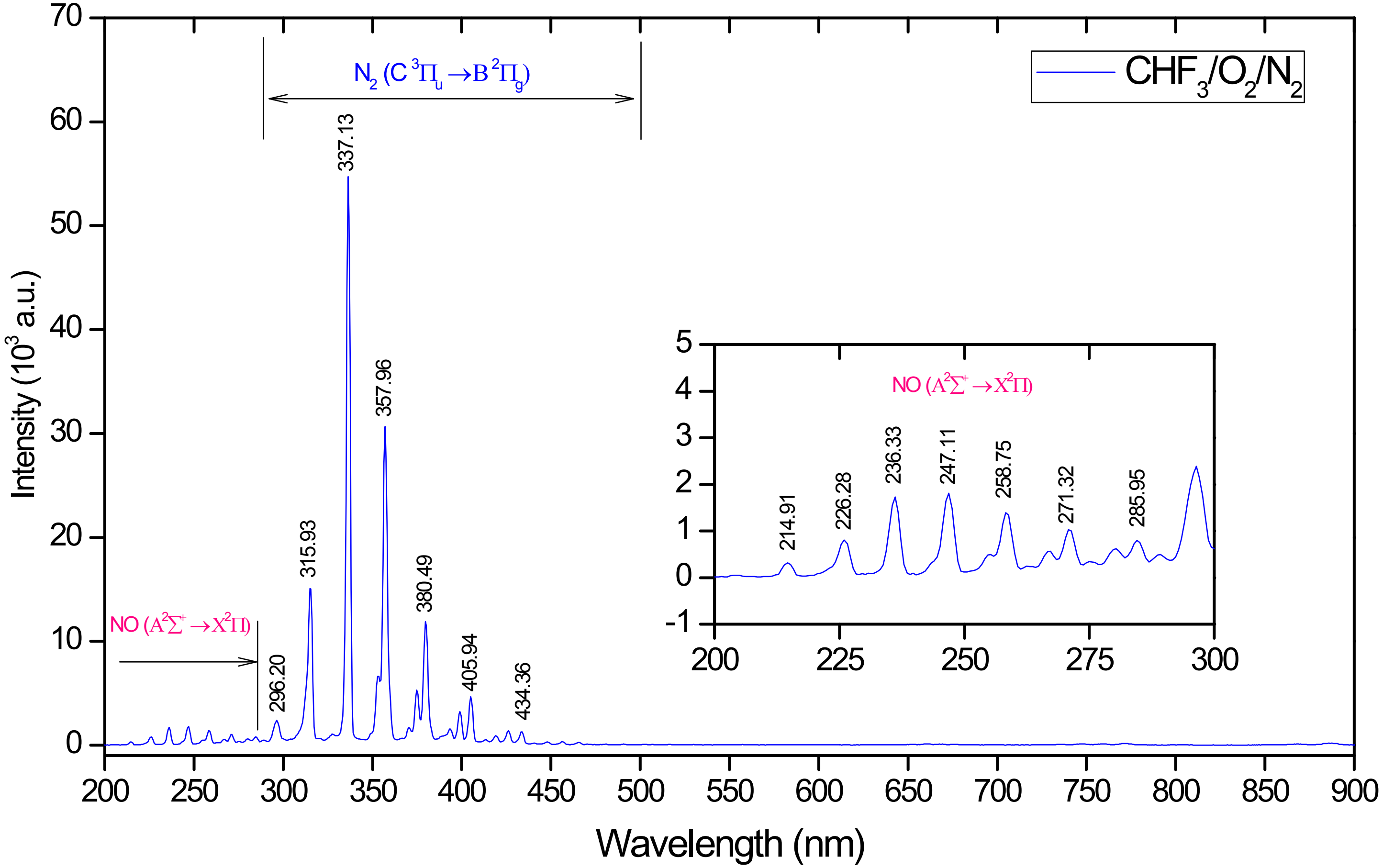

Fig. S3. Emission spectrum of $CHF_3/O_2/N_2$ plasma in a dielectric barrier discharge at atmospheric pressure (flow rate of $CHF_3/O_2/N_2$ = 2/10/988 ml/min; frequency= 30 kHz; active power= 60 W).

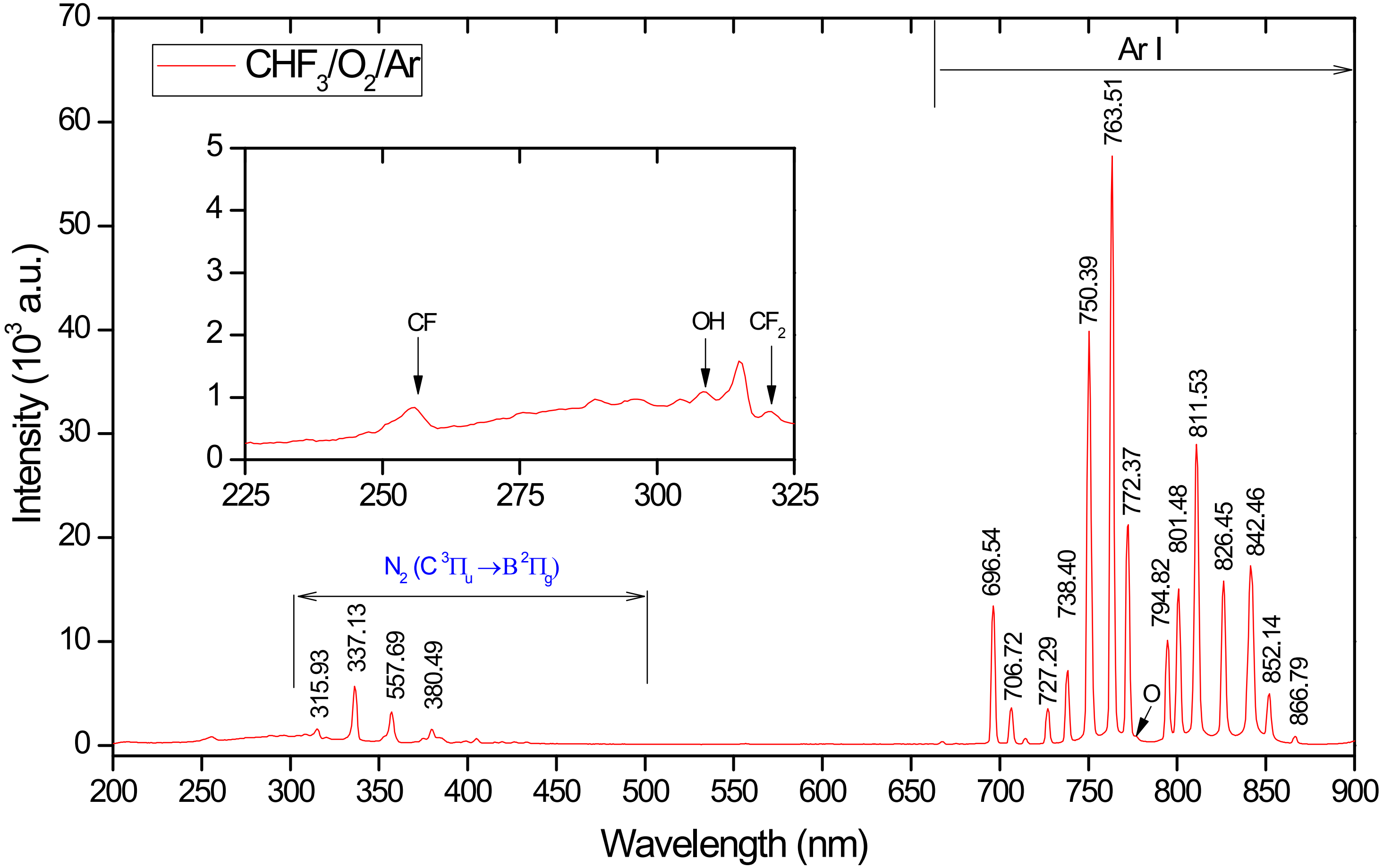

Fig. S4. Emission spectrum of $CHF_3/O_2/Ar$ plasma in a dielectric barrier discharge at atmospheric pressure (flow rate of $CHF_3/O_2/Ar$ = 2/10/988 ml/min; frequency= 30 kHz; active power= 60 W).

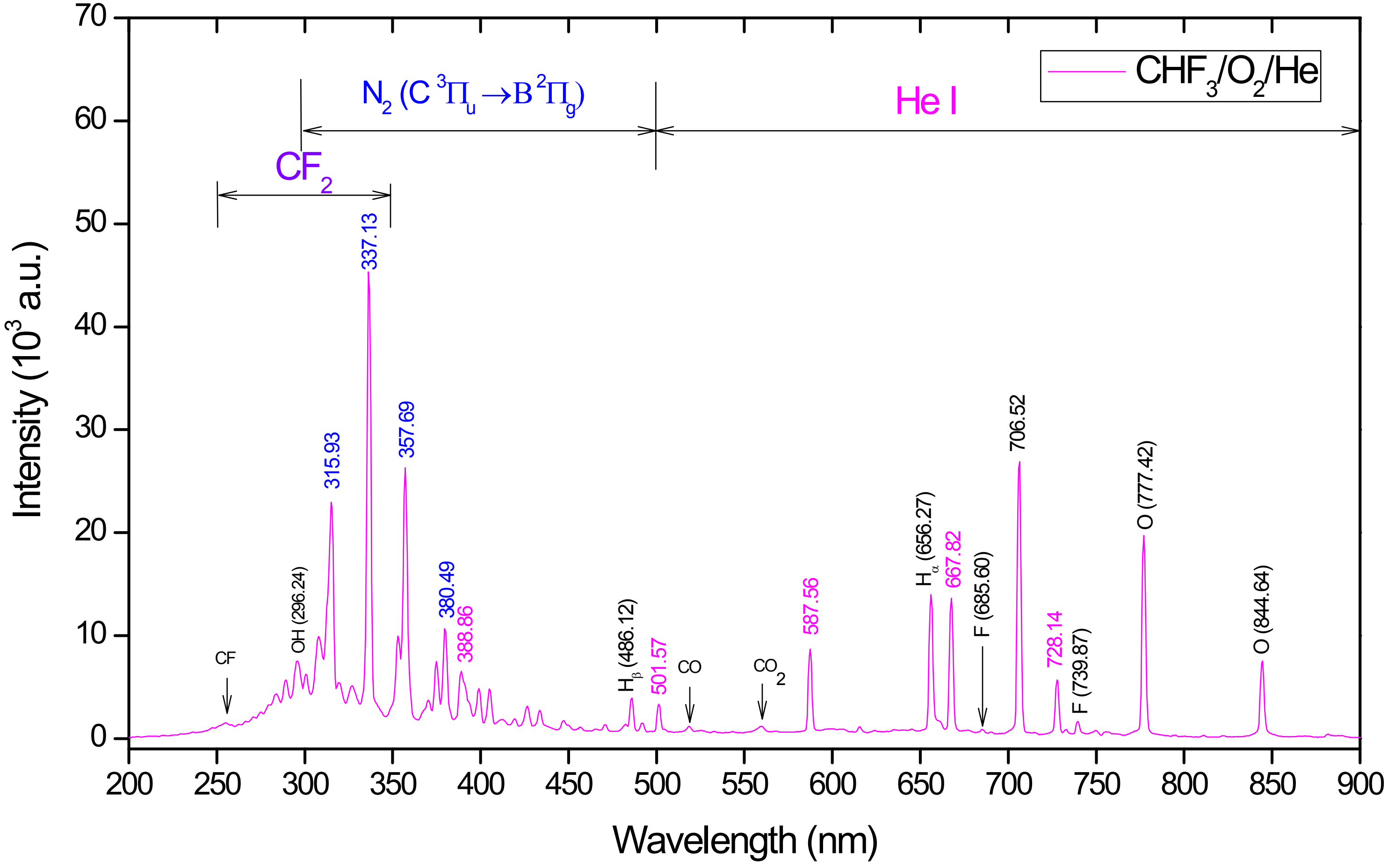

Fig. S5. Emission spectrum of $CHF_3/O_2/He$ plasma in a dielectric barrier discharge at atmospheric pressure (flow rate of $CHF_3/O_2/He$ = 2/10/988 ml/min; frequency= 30 kHz; active power= 60 W).

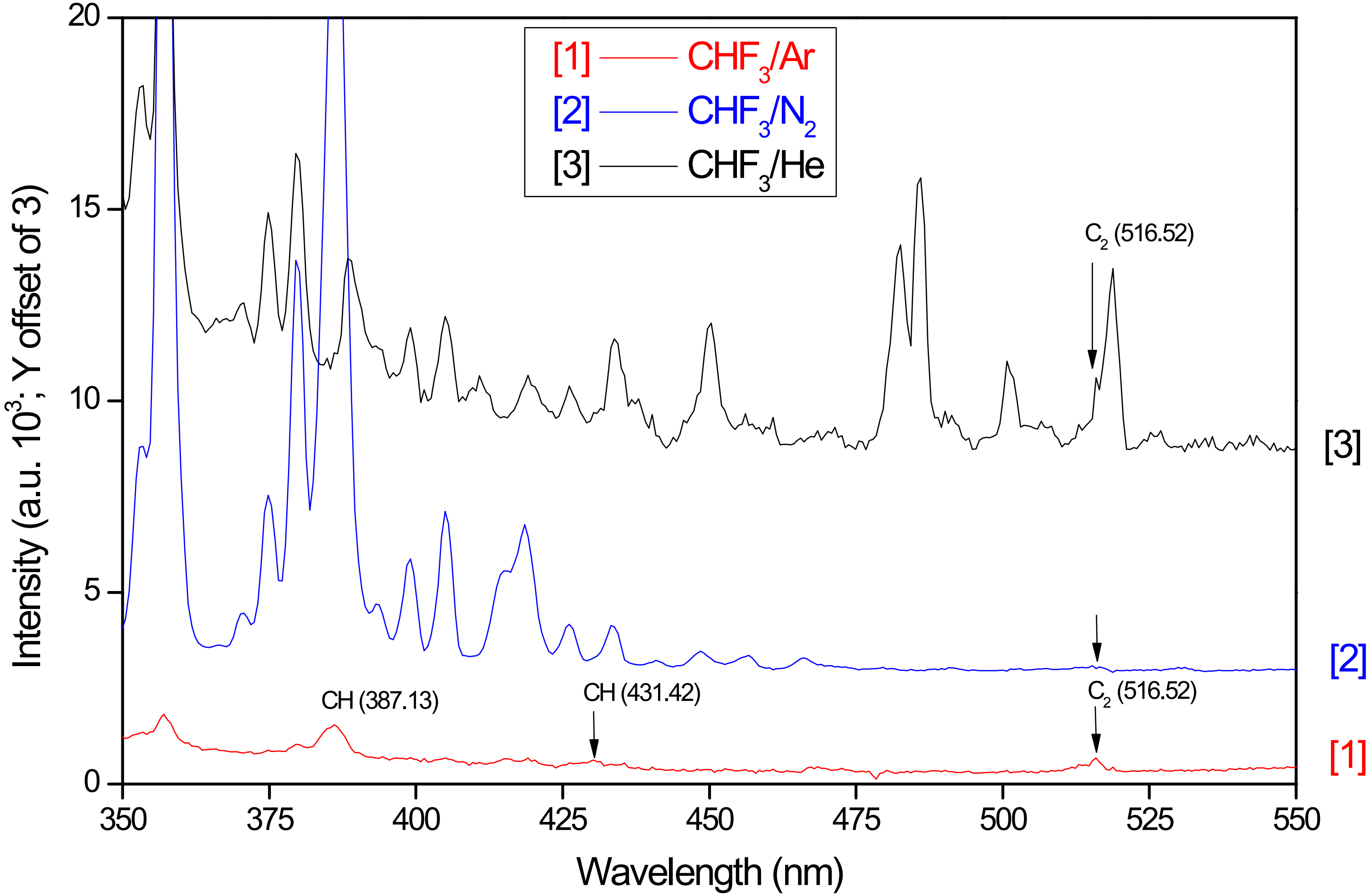

Fig. S6. Emission spectrum of CHF_3/X plasma in a dielectric barrier discharge at atmospheric pressure (flow rate of CHF_3/X = 8/988 ml/min, X stands for Ar, He or N_2; frequency= 30 kHz; active power= 60 W).

S4. Possible chemical reactions for the CHF_3 decompositions in the atmospheric plasma

Possible chemical reactions in plasma discharge were categorized into several groups by the reactants, as shown below. In each group of reactants, the kinetics of the chemical reactions are flowing largest to smallest at a temperature around 300 K. However, several rate constants of chemical reaction were recorded at high temperature because we did not find the rate constant of chemical reaction at the low temperature in the chemical kinetics database.[3]

The electron-impact reaction dissociated radicals or gas molecules. The kinetics of these reactions depended on electron energy. This can be described by an electron-impact cross section (σ).[4, 5] The kinetics of the reaction between excited species (M) with radicals and gases molecules also depend on the energy of the excited species.

Chemical Reaction	Rate Constant		Ref.
	k (cm^3/molecule s)	T (K)	
CHF_3 Reactant			
CHF_3 + e/M → Products	*σ (*)*		5
CHF_3 + ·F → ·CF_3 + HF	1.56E-13	300	6
CHF_3 + CF_3O → CF_3OH + ·CF_3	5.99E-16	296	7
CHF_3 + ·OH → ·CF_3 + H_2O	3.06E-16	300	8
CHF_3 + H· → H_2 + ·CF_3	7.36E-19	300	9
CHF_3 → ·CF_2 + HF	1.70E-19	1150	10
CHF_3 + O· → ·CF_3 + ·OH	9.89E-20	298	11
CHF_3 + ·CF_2 → ·CF_3 + ·CHF_2	4.62E-21	973	12
CHF_3 + H· → ·CHF_2 + HF	4.26E-40	300	13
CHF_3 + H· → CH_2F_2 + ·F	8.49E-58	300	13
·CF_3 Reactant			
·CF_3 + e/M → Products	*σ*		5
·CF_3 + ·CHF_2 → CHF_3 + ·CF_2	8.79E-02	300	14
·CF_3 + O· → COF_2 + ·F	3.32E-11	298	15
·CF_3 + NO → CF_3NO	2.01E-11	253-373	16
·CF_3 + H· → ·CF_2 + HF	9.10E-11	298	17
·CF_3 + ·OH → COF_2 + HF	2.61E-11	300	8
·CF_3 + NO_2 → NO + CF_3O	2.51E-11	300	18
·CF_3 + N → Other Products + ·F	1.79E-11	293	19
·CF_3 + NO_2 → COF_2 + FNO	1.53E-11	298	20
·CF_3 + ·CF_3 → C_2F_6	1.30E-11	300	21
·CF_3 + FCO → CF_3COF	6.91E-12	298	22
·CF_3 + ·CF_2 → C_2F_5	6.42E-12	940	23
·CF_3 + ·CF_3 → Products	1.80E-12	290	24
·CF_3 + O_3 → O_2 + CF_3O	9.30E-13	298	25
·CF_3 + F_2 → CF_4 + ·F	6.60E-14	300	26
·CF_3 + O_2 → O· + CF_3O	2.93E-17	700	27
·CF_3 → ·CF_2 + ·F	1.91E-17	1600	28
·CF_3 + H_2 → CHF_3 + H·	1.73E-18	350	29
·CF_3 + N_2O → N_2 + CF_3O	2.78E-20	589	30
·CF_3 + ·F → CF_4	1.47E-28	290	24

Chemical Reaction	Rate Constant		Ref.
	k (cm^3/molecule s)	T (K)	
$\cdot CF_3 + O_2 \rightarrow CF_3O_2$ (n=3)	2.93E-29	300	31
$\cdot CF_3 + O_2 + M \rightarrow M + CF_3O_2$	1.90E-29	300	32
$\cdot CF_3 + O\cdot \rightarrow CF_3O$			33
$\cdot CF_3 + H_2O \rightarrow CHF_3 + \cdot OH$			34
$\cdot CHF_2$ Reactant			
$\cdot CHF_2$ + e/M → Products	σ		5
$\cdot CHF_2 + H\cdot \rightarrow HF + \cdot CHF$	1.25E+00	298	35
$\cdot CHF_2 + \cdot CHF_2 \rightarrow CH_2F_2 + \cdot CF_2$	1.30E-01	300-400	36
$\cdot CHF_2 + H\cdot \rightarrow H_2 + \cdot CF_2$	3.32E-11	600-1400	37
$\cdot CHF_2 + O\cdot \rightarrow COF_2 + H\cdot$	1.66E-11	600-700	37
$\cdot CHF_2 + H_2 \rightarrow CH_2F_2 + H\cdot$	6.93E-20	300	9
$CO + \cdot CHF_2 \rightarrow FC{\equiv}CF + \cdot OH$			38
$CO + \cdot CHF_2$ → Products			38
$CO + \cdot CHF_2 \rightarrow CHF_2CO$			38
$CO + \cdot CHF_2 \rightarrow CFCFOH$			38
$CO + \cdot CHF_2 \rightarrow CF_2CHO$			38
$CO + \cdot CHF_2 \rightarrow CF_2COH$			38
$\cdot CF_2$ Reactant			
$\cdot CF_2$ + e/M → Products	σ		5
$\cdot CF_2 + \cdot OH$ → Products	4.98E-11	1800	39
$\cdot CF_2 + \cdot F \rightarrow \cdot CF_3$	4.15E-11	298	40
$\cdot CF_2 + O\cdot \rightarrow FCO + \cdot F$	4.07E-11	2000-2430	41
$\cdot CF_2 + H\cdot \rightarrow CF + HF$	3.90E-11	298	17
$\cdot CF_2 + H\cdot$ → Products	3.32E-11	1800	39
$\cdot CF_2 + \cdot OH \rightarrow COF_2 + H\cdot$	2.06E-11	300	42
$\cdot CF_2 + O\cdot$ → Products	1.66E-11	298	15
$\cdot CF_2$ + N → Products	7.21E-12	293	43
$\cdot CF_2 + \cdot CF_2 \rightarrow C_2F_4$	3.70E-14	300	44
$\cdot CF_2 + NO \rightarrow CF_2NO$	1.52E-14	1600	45
$\cdot CF_2 + NO_2 \rightarrow COF_2 + NO$	7.52E-15	298	46
$\cdot CF_2 + O_2$ → Other Products + CO	6.42E-15	1200	47
$\cdot CF_2 + F_2 \rightarrow \cdot CF_3 + \cdot F$	2.01E-15	295	48

Chemical Reaction	Rate Constant		Ref.
	k (cm^3/molecule s)	T (K)	
$\cdot CF_2 + N_2O \rightarrow$ Products	8.30E-16	298	46
$\cdot CF_2 + O_2 \rightarrow COF_2 + O\cdot$	4.72E-16	1200	49
$\cdot CF_2 + O_2 \rightarrow$ Products	8.30E-18	803	50
$H_2 + \cdot CF_2 \rightarrow$ Products	5.00E-19	873	51
$\cdot CF_2 + O_3 \rightarrow$ Products	1.39E-19	300	50
$\cdot CF_2 + H\cdot \rightarrow \cdot CHF_2$	1.80E-21	673	52
$H_2 + \cdot CF_2 \rightarrow CH_2F_2$	4.43E-23	673	52
COF_2 Reactant			
$COF_2 + H\cdot \rightarrow CHF_2O(\cdot)$	1.96E+00	600	53
O(1D) + $COF_2 \rightarrow$ Products	7.41E-11	298	54
O(1D) + $COF_2 \rightarrow CO_2 + F_2$	2.09E-11	298	54
COF_2 + CO $\rightarrow$ FCO + FCO	3.83E-14	2200	55
$COF_2 + \cdot F \rightarrow CF_3O$	9.10E-16	484	56
$COF_2 + \cdot F \rightarrow FCO + F_2$	2.66E-16	2200	55
$COF_2 \rightarrow FCO + \cdot F$	9.76E-17	2600	57
$COF_2 + H_2 \rightarrow$ Products	1.31E-17	1900	57
$COF_2 + \cdot OH \rightarrow HF + FC(O)O\cdot$	8.98E-22	600	53
$COF_2 + H\cdot \rightarrow FCO + HF$	5.29E-25	600	53
$COF_2 + H_2O \rightarrow HF + FC(O)OH$	4.33E-25	600	53
$COF_2 + H_2O \rightarrow CF_2(OH)2$	1.20E-25	600	53
·COF Reactant			
·COF + e/M $\rightarrow$ Products	σ		5
FCO + O· $\rightarrow$ Products	9.96E-11	300-2000	15
FCO + H· $\rightarrow$ CO + HF	4.15E-11	600-1400	37
FCO + FCO $\rightarrow COF_2$ + CO	1.80E-11	295	58
FCO + ·F $\rightarrow COF_2$	5.00E-12	298	59
FCO + ·F $\rightarrow CO + F_2$	4.52E-13	2200	55
FCO + $F_2 \rightarrow COF_2 + \cdot F$	4.00E-14	298	59
FCO $\rightarrow$ CO + ·F	5.98E-16	951	60
FCO + $O_2 \rightarrow$ Products	4.00E-16	800	60

Chemical Reaction	**Rate Constant**		**Ref.**
	k (cm³/molecule s)	**T (K)**	
·CHF Reactant			
·CHF + e/M → Products	σ		[5]
·CHF + O· → CO + HF	1.20E+00	298	[61]
H· + ·CHF → Products	4.90E-10	293	[62]
·CHF + O· → Products	1.50E-10	295	[63]
·CHF + N → Products	2.51E-11	295	[63]
NO + ·CHF → Products	7.04E-12	293	[64]
O_2 + ·CHF → Products	5.00E-16	295	[63]
CF Reactant			
CF + e/M → Products	σ		[5]
CF + NO_2 → Products	4.00E-11	294	[65]
CF + N → CN + ·F	3.90E-11	294	[65]
CF + O· → CO + ·F	3.90E-11	294	[65]
CF + NO → Products	2.09E-11	294	[66]
CF + H· → C + HF	1.91E-11	298	[17]
CF + O· → Products	1.20E-11	293	[43]
CF + F_2 → Products	4.37E-12	300	[67]
CF + N → Products	3.40E-12	293	[43]
CF + O_2 → Products	1.60E-12	294	[66]
CF + ·F → ·CF_2	1.00E-13	294	[65]
H_2 + CF → Products	1.00E-14	284	[66]
CO_2 + CF → Products	1.00E-14	284	[66]
CF_4 + CF → Products	1.00E-14	284	[66]
CF + N_2O → Products	1.00E-14	294	[65]
CF + N_2 → Products	1.00E-14	294	[65]
CF + H· → ·CH + ·F	1.11E-24	300	[68]
CF + ·F → C + F_2	8.12E-63	300	[68]

Chemical Reaction	Rate Constant		Ref.
	k (cm³/molecule s)	T (K)	
CO_2 Reactant			
CO_2 + e/M → Products	σ		5
N(^{2}D) + CO_2 → CO + NO	3.60E-13		69
N(^{2}P) + CO_2 → Products	3.60E-13		69
CO_2 + NO → CO + NO_2	5.00E-15	3000	70
CO_2 + N → CO + NO	1.07E-15	300	71
CO_2 → CO + O·	1.42E-18	2620	72
CO_2 + H· → CO + ·OH	1.40E-29	300	73
CO_2 + O· → CO_3	1.22E-49	300	73
CO_2 + H_2 → CO + H_2O			74
CO Reactant			
CO + e/M → Products	σ		5
O(1D) + CO → CO_2	8.00E-11	100-2100	75
CO + ·F → FCO	5.50E-13	295	76
CO + ·OH → Products	2.41E-13	200-300	31
CO + ·OH → CO_2 + H·	1.49E-13	298	77
CO + CF_3O → Products	6.84E-14	300	78
CO + CF_3O → COF_2 + FCO	2.01E-15	298	78
CO + O· → CO_2	4.98E-16	300	79
CO + CF_3O → CO_2 + ·CF_3	4.00E-16	298	78
CO + OF → CO_2 + ·F	3.65E-17	550	80
CO + O_3 → Products	1.00E-21	298	81
CO + F_2 → FCO + ·F	3.11E-22	273-315	82
CO + O_3 → CO_2 + O_2	4.00E-25	296	83
CO + H· → HCO (**)	1.54E-34	300	84
CO + NO_2 → CO_2 + NO	3.63E-35	300	85

(*): the rate constant depends on the electron energy, and has been described by an electron-impact cross section (σ).

(**): The reaction order: 3; the unit of k(T) is cm^6/molecule^2 s.

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