Supporting Information for

The Mechanism and Kinetic Studies on Oxidation Reaction of Acetofenate Initiated by HOx, NO_3, O_3, and Cl Radical

Lingyan Kang[a], Chenxi Zhang[b], Xiaomin Sun[a*]

[a] Environment Research Institute, Shandong University, Jinan 250100, P. R. China

[b] Department of Resourse and Environment, Binzhou University, Binzhou 256600, PR China

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Table S1C The lifetimes of AF + OH addition reactions according to the rate constants at 200-400K

Table S1C The lifetimes of AF + OH abstraction reactions according to the rate constants at 200-400K

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Table SD The total lifetimes of AF with different oxidants according to the rate constants at 200-400K

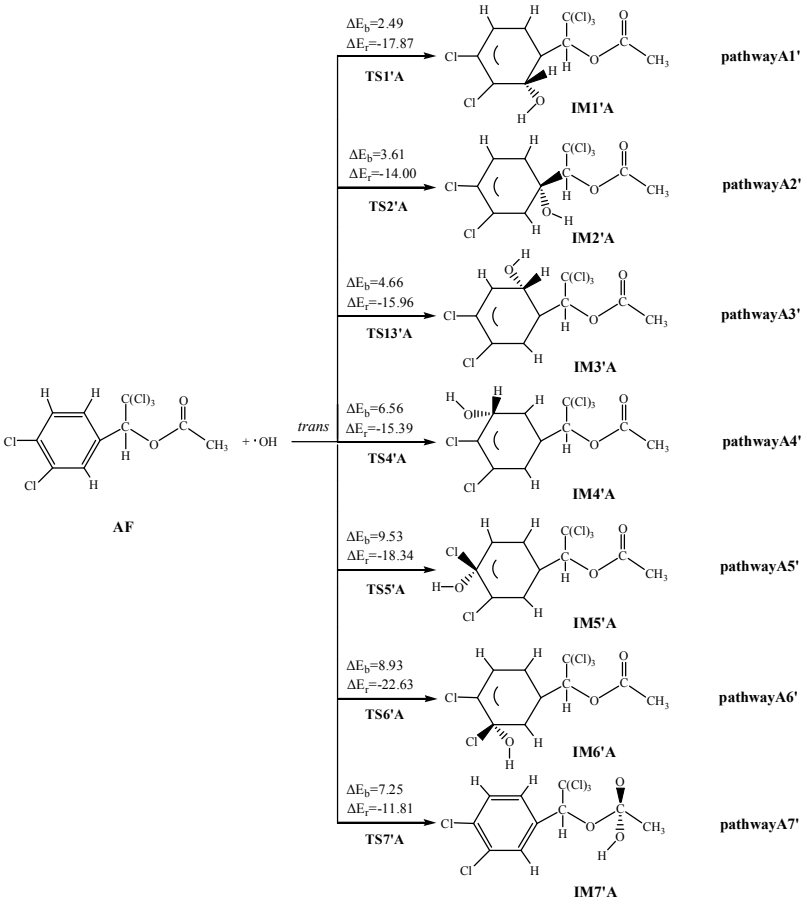

Figure S1 OH radical-initiated *trans*-addition pathways with the potential barriers ΔE_b and reaction heats ΔE_r (kcal/mol)

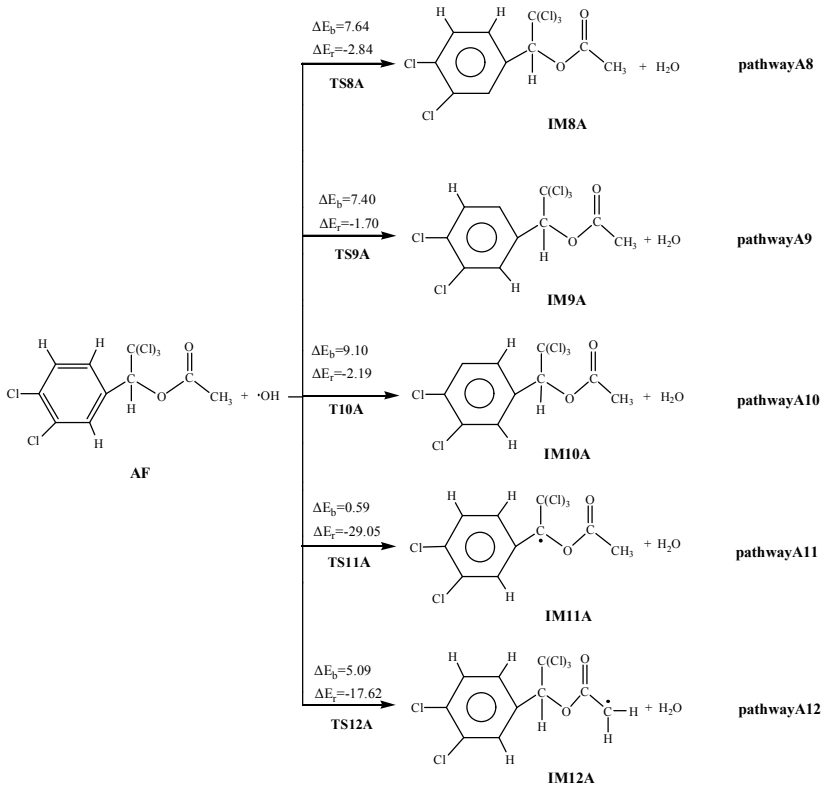

Figure S2 OH initiated H atom abstraction pathways with the potential barriers ΔE_b and reaction heats ΔE_r (kcal/mol)

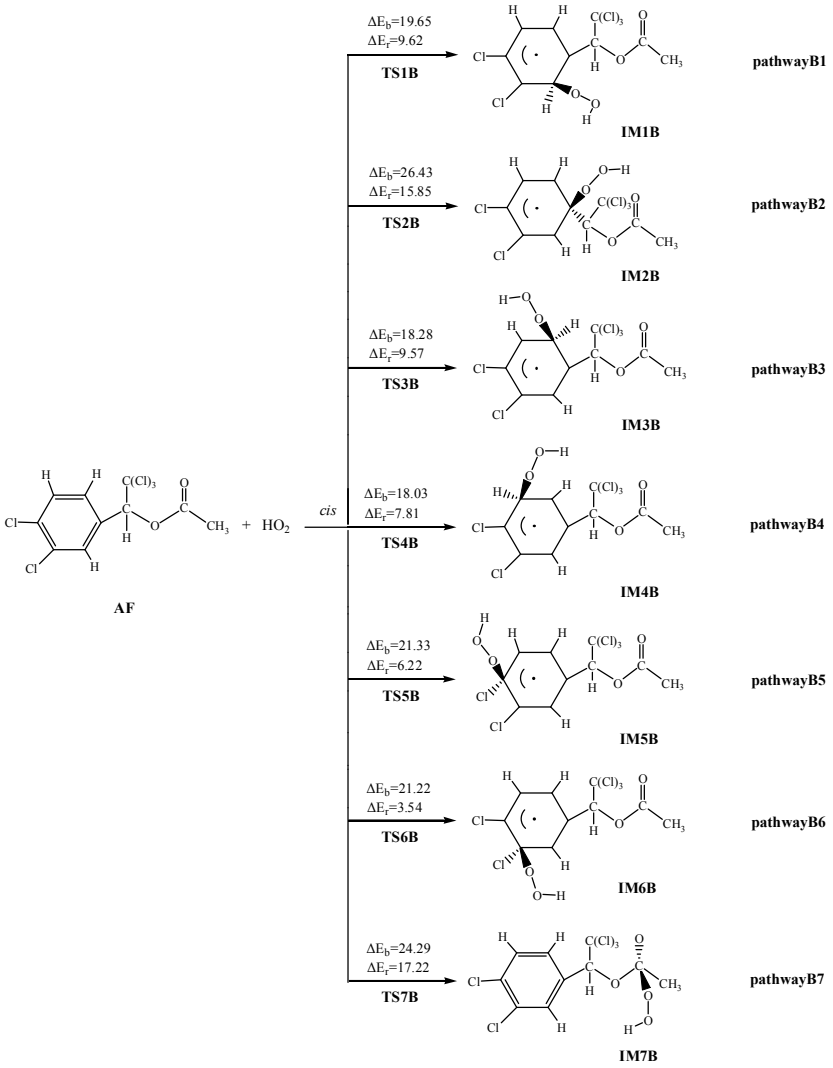

Figure S3 HO_2 radical-initiated *cis*-addition pathways pathways with the potential barriers ΔE_b and reaction heats ΔE_r (kcal/mol)

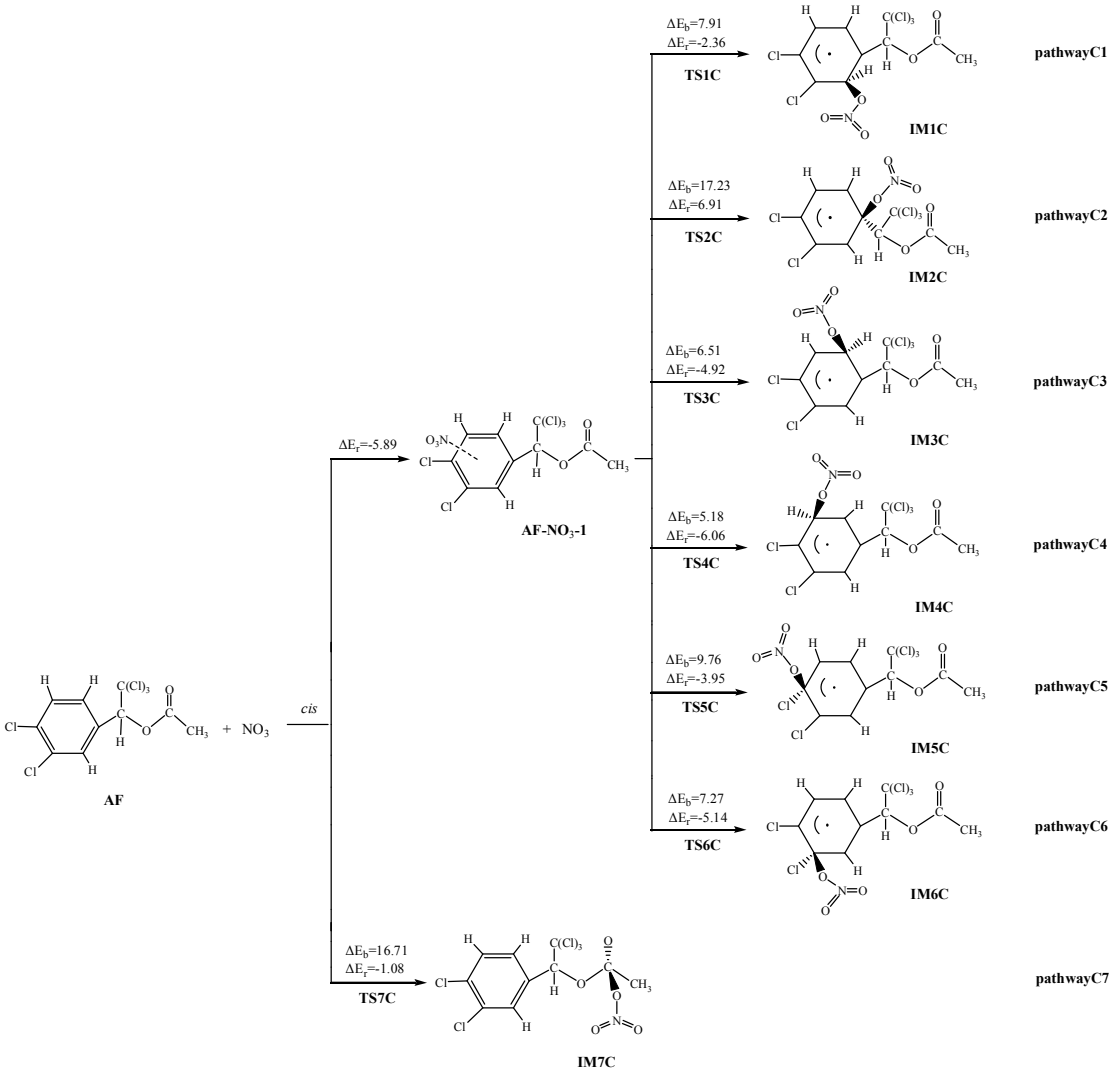

Figure S4 NO_3 radical-initiated *cis*-addition pathways pathways with the potential barriers ΔE_b and reaction heats ΔE_r (kcal/mol)

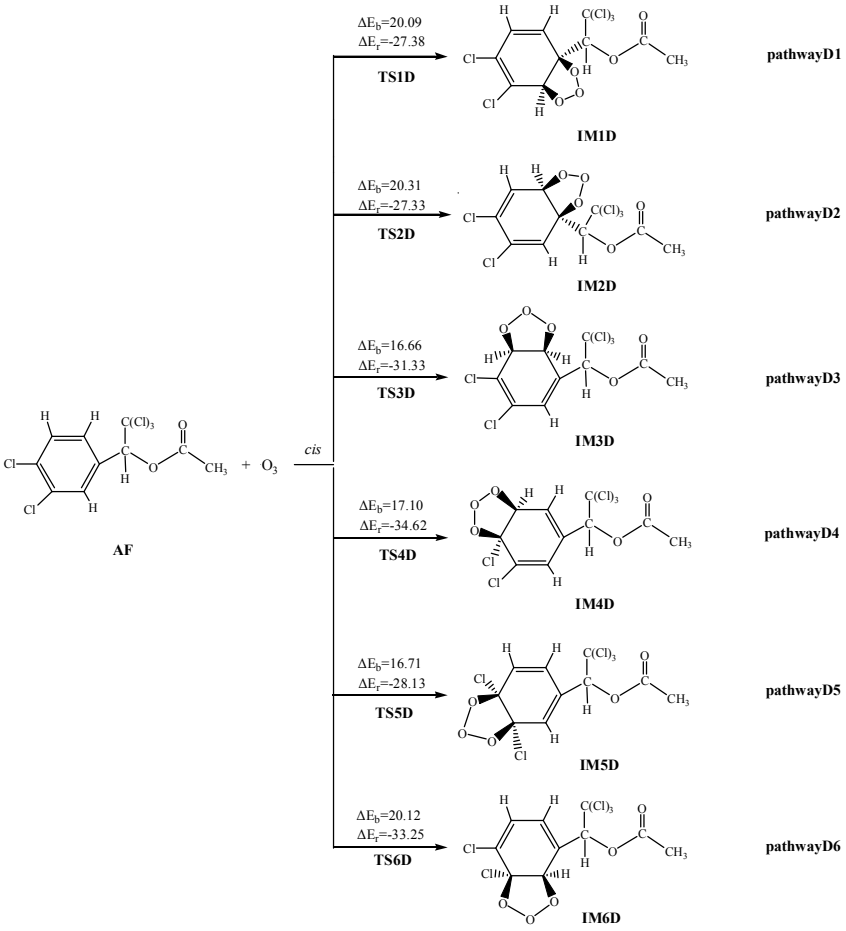

Figure S5 O_3 initiated *cis*-addition pathways pathways with the potential barriers ΔE_b and reaction heats ΔE_r (kcal/mol)

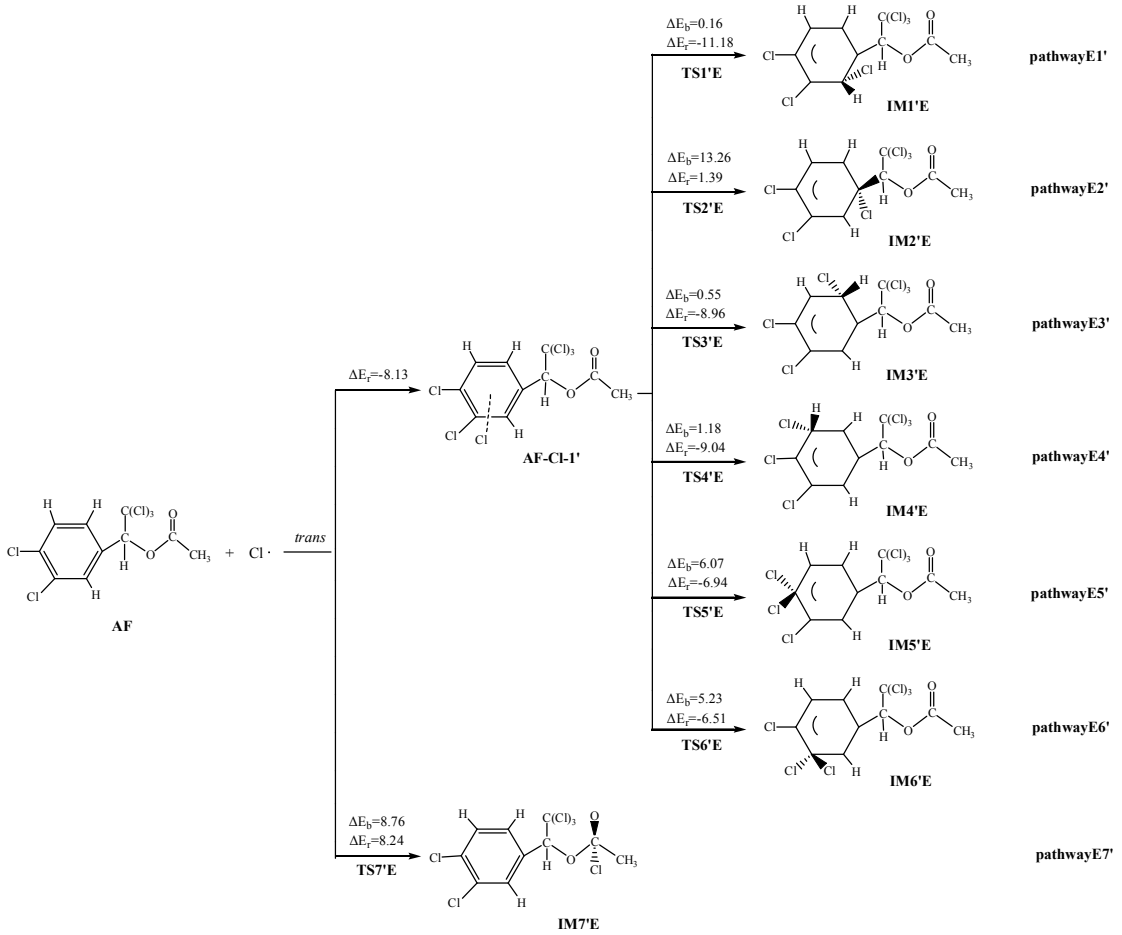

Figure S6 Cl radical-initiated *trans*-addition pathways pathways with the potential barriers ΔE_b and reaction heats ΔE_r (kcal/mol)

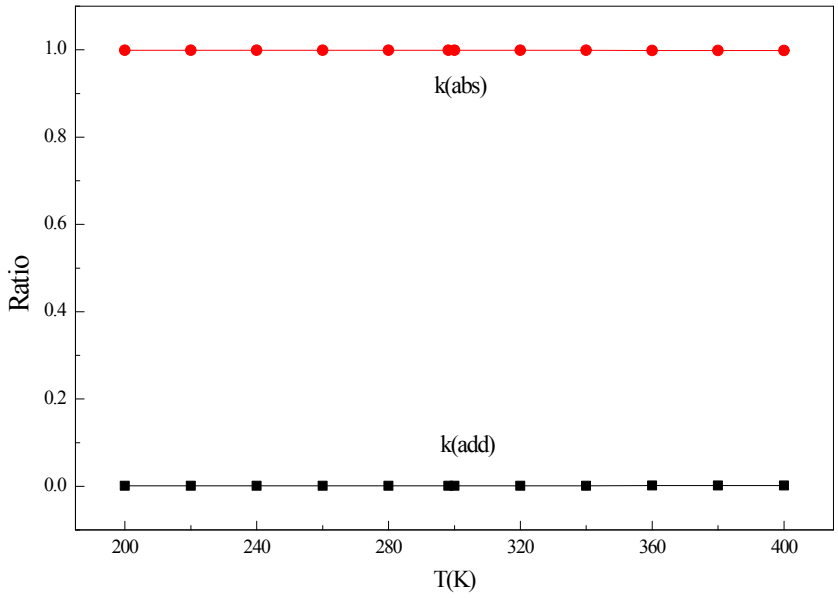

Figure S7 The ratio of the rate constants for addition and abstraction reactions to the total rate constant of AF with OH

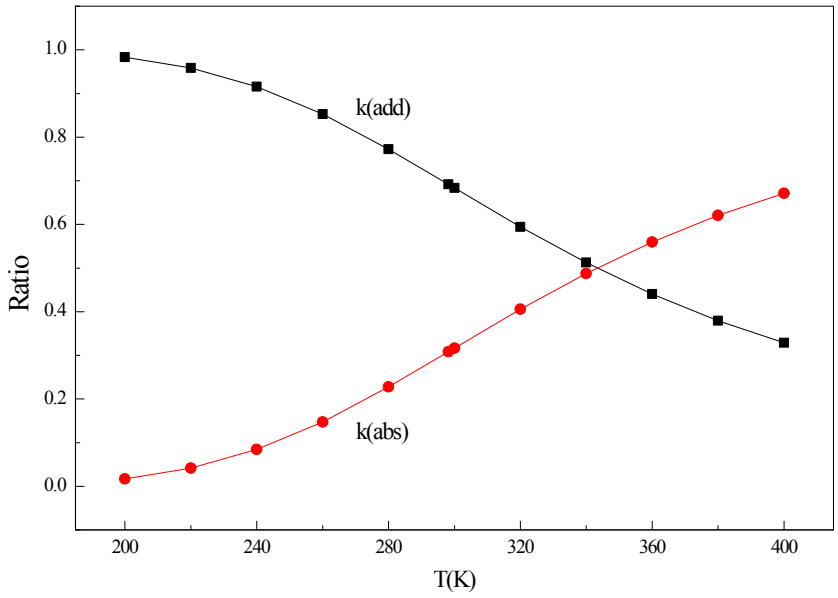

Figure S8 The ratio of the rate constants for addition and abstraction reactions to the total rate constant of AF with NO_3

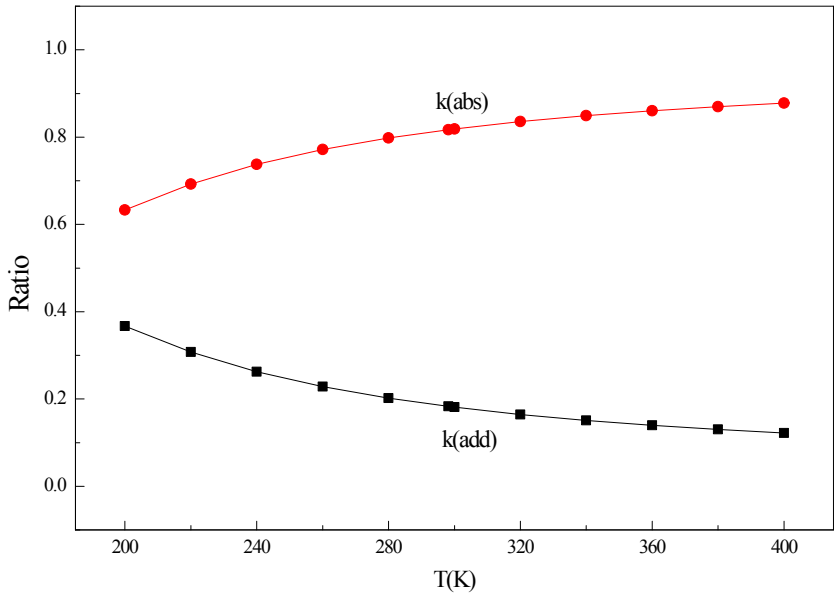

Figure S9 The ratio of the rate constants for addition and abstraction reactions to the total rate constant of AF with Cl

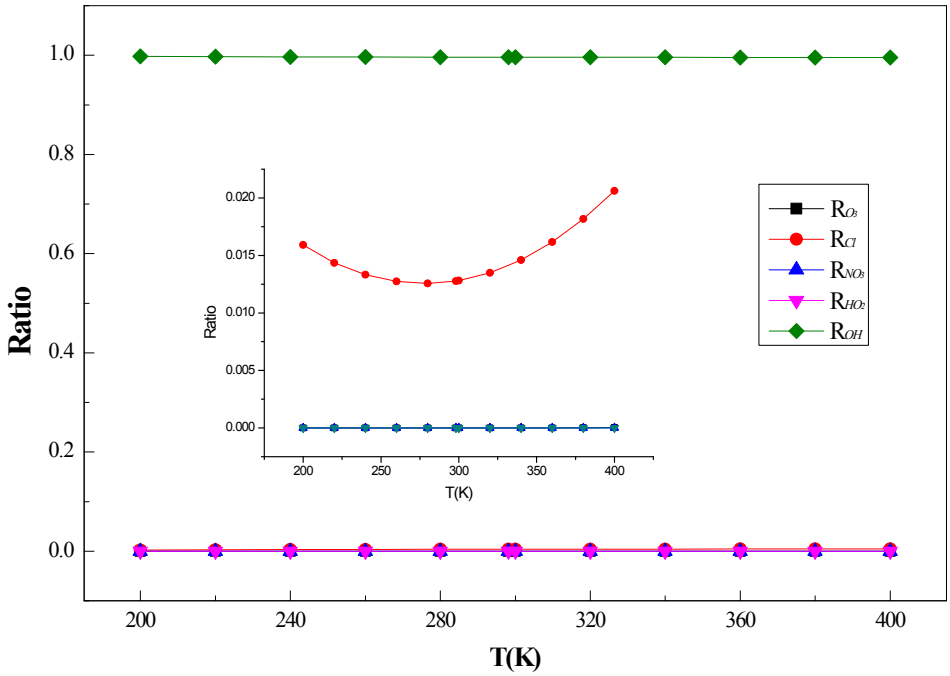

Figure S10 The rate branching ratio of each initiated reactions to the total rate from 200 to 400K

Table S1A The rate constants of addition reactions of AF with OH at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_1	k_2	k_3	k_4	k_5	k_6	k_7	$k_{1'}$	$k_{2'}$	$k_{3'}$	$k_{4'}$	$k_{5'}$	$k_{6'}$	$k_{7'}$
200	3.12E-20	5.71E-26	5.50E-19	8.21E-24	4.74E-19	5.21E-19	1.04E-23	1.91E-18	1.21E-19	3.08E-20	8.88E-22	7.92E-25	1.02E-24	1.04E-23
220	9.58E-20	6.72E-25	1.55E-18	6.75E-23	1.59E-18	1.62E-18	6.62E-23	4.08E-18	3.35E-19	1.08E-19	4.82E-21	8.49E-24	9.49E-24	6.64E-23
240	2.48E-19	5.32E-24	3.74E-18	3.97E-22	4.42E-18	4.23E-18	3.14E-22	7.82E-18	7.94E-19	3.14E-19	2.00E-20	6.22E-23	6.20E-23	3.15E-22
260	5.62E-19	3.11E-23	7.97E-18	1.80E-21	1.06E-17	9.67E-18	1.19E-21	1.37E-17	1.67E-18	7.82E-19	6.77E-20	3.40E-22	3.08E-22	1.19E-21
280	1.14E-18	1.42E-22	1.54E-17	6.64E-21	2.28E-17	1.98E-17	3.76E-21	2.25E-17	3.19E-18	1.73E-18	1.94E-19	1.47E-21	1.23E-21	3.77E-21
298.15	**2.03E-18**	**4.79E-22**	**2.62E-17**	**1.88E-20**	**4.21E-17**	**3.53E-17**	**9.43E-21**	**3.35E-17**	**5.37E-18**	**3.27E-18**	**4.52E-19**	**4.74E-21**	**3.70E-21**	**9.46E-21**
300	2.14E-18	5.38E-22	2.76E-17	2.08E-20	4.47E-17	3.73E-17	1.03E-20	3.48E-17	5.65E-18	3.47E-18	4.90E-19	5.30E-21	4.11E-21	1.03E-20
320	3.73E-18	1.74E-21	4.63E-17	5.70E-20	8.10E-17	6.55E-17	2.51E-20	5.14E-17	9.38E-18	6.44E-18	1.11E-18	1.64E-20	1.19E-20	2.52E-20
340	6.15E-18	4.92E-21	7.36E-17	1.40E-19	1.38E-16	1.08E-16	5.54E-20	7.30E-17	1.48E-17	1.12E-17	2.30E-18	4.47E-20	3.08E-20	5.56E-20
360	9.63E-18	1.25E-20	1.12E-16	3.12E-19	2.23E-16	1.70E-16	1.13E-19	1.01E-16	2.23E-17	1.84E-17	4.42E-18	1.10E-19	7.19E-20	1.13E-19
380	1.45E-17	2.89E-20	1.64E-16	6.43E-19	3.45E-16	2.57E-16	2.14E-19	1.35E-16	3.24E-17	2.90E-17	7.97E-18	2.47E-19	1.55E-19	2.15E-19
400	2.10E-17	6.19E-20	2.32E-16	1.24E-18	5.14E-16	3.75E-16	3.84E-19	1.76E-16	4.57E-17	4.37E-17	1.36E-17	5.14E-19	3.09E-19	3.85E-19

Table S2A The rate constants of abstraction reactions of AF with OH reactions at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_8	k_9	k_{10}	k_{11}	k_{12}
200	6.29E-21	1.66E-20	2.12E-21	1.11E-13	1.52E-17
220	4.38E-20	1.09E-19	2.06E-20	1.54E-13	5.91E-17
240	2.24E-19	5.34E-19	1.39E-19	2.05E-13	1.86E-16
260	9.02E-19	2.07E-18	7.09E-19	2.64E-13	4.96E-16
280	3.01E-18	6.68E-18	2.90E-18	3.32E-13	1.16E-15
298.15	**7.88E-18**	**1.70E-17**	**8.90E-18**	**4.01E-13**	**2.30E-15**
300	8.64E-18	1.86E-17	9.91E-18	4.09E-13	2.46E-15
320	2.19E-17	4.61E-17	2.93E-17	4.94E-13	4.77E-15
340	5.02E-17	1.03E-16	7.68E-17	5.89E-13	8.63E-15
360	1.05E-16	2.13E-16	1.82E-16	6.93E-13	1.47E-14
380	2.06E-16	4.09E-16	3.97E-16	8.06E-13	2.38E-14
400	3.79E-16	7.39E-16	8.03E-16	9.29E-13	3.70E-14

Table S3A The rate constants of AF with HO_2 reactions at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_1	k_2	k_3	k_4	k_5	k_6	k_7	$k_{1'}$	$k_{2'}$	$k_{3'}$	$k_{4'}$	$k_{5'}$	$k_{6'}$	$k_{7'}$
200	5.89E-38	4.12E-46	7.21E-37	1.50E-36	2.67E-39	9.85E-40	4.95E-44	5.55E-33	2.22E-36	1.43E-33	2.58E-35	7.84E-41	1.86E-39	2.91E-44
220	6.40E-36	2.11E-43	5.73E-35	1.12E-34	4.27E-37	1.53E-37	1.56E-41	2.02E-31	1.51E-34	5.81E-32	1.59E-33	1.64E-38	2.46E-37	1.11E-41
240	3.23E-34	3.89E-41	2.23E-33	4.16E-33	2.97E-35	1.04E-35	1.90E-39	4.08E-30	5.19E-33	1.29E-30	4.99E-32	1.42E-36	1.47E-35	1.61E-39
260	9.05E-33	3.26E-39	5.00E-32	8.96E-32	1.09E-33	3.76E-34	1.13E-37	5.27E-29	1.04E-31	1.80E-29	9.35E-31	6.31E-35	4.71E-34	1.10E-37
280	1.59E-31	1.46E-37	7.28E-31	1.26E-30	2.41E-32	8.22E-33	3.76E-36	4.77E-28	1.39E-30	1.75E-28	1.17E-29	1.64E-33	9.33E-33	4.13E-36
298.15	**1.55E-30**	**3.00E-36**	**6.11E-30**	**1.03E-29**	**2.83E-31**	**9.52E-32**	**6.10E-35**	**2.75E-27**	**1.08E-29**	**1.06E-27**	**8.66E-29**	**2.19E-32**	**9.99E-32**	**7.36E-35**
300	1.93E-30	3.99E-36	7.48E-30	1.25E-29	3.57E-31	1.20E-31	7.95E-35	3.25E-27	1.31E-29	1.26E-27	1.05E-28	2.80E-32	1.25E-31	9.68E-35
320	1.72E-29	7.27E-35	5.80E-29	9.46E-29	3.81E-30	1.27E-30	1.16E-33	1.76E-26	9.49E-29	7.19E-27	7.23E-28	3.38E-31	1.23E-30	1.54E-33
340	1.20E-28	9.48E-34	3.55E-28	5.67E-28	3.10E-29	1.02E-29	1.24E-32	7.86E-26	5.47E-28	3.36E-26	4.00E-27	3.06E-30	9.24E-30	1.79E-32
360	6.76E-28	9.36E-33	1.79E-27	2.80E-27	2.01E-28	6.55E-29	1.02E-31	2.99E-25	2.61E-27	1.33E-25	1.84E-26	2.19E-29	5.60E-29	1.59E-31
380	3.20E-27	7.30E-32	7.68E-27	1.18E-26	1.08E-27	3.48E-28	6.82E-31	9.96E-25	1.07E-26	4.60E-25	7.26E-26	1.28E-28	2.82E-28	1.13E-30
400	1.30E-26	4.66E-31	2.86E-26	4.30E-26	4.90E-27	1.57E-27	3.78E-30	2.95E-24	3.79E-26	1.41E-24	2.51E-25	6.28E-28	1.22E-27	6.62E-30

Table S4A The rate constants of addition reactions of AF with NO_3 reactions at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_1	k_2	k_3	k_4	k_5	k_6	k_7	$k_{1'}$	$k_{2'}$	$k_{3'}$	$k_{4'}$	$k_{5'}$	$k_{6'}$	$k_{7'}$
200	4.19E-28	2.84E-37	3.96E-26	3.85E-25	1.27E-28	2.34E-27	1.66E-37	3.45E-21	1.23E-34	5.69E-22	9.86E-23	3.80E-27	4.62E-25	9.35E-36
220	3.09E-27	1.77E-35	2.13E-25	1.53E-24	1.43E-27	1.49E-26	9.21E-36	6.09E-21	4.19E-33	1.16E-21	3.14E-22	3.03E-26	1.98E-24	3.85E-34
240	1.66E-26	5.65E-34	8.77E-25	4.87E-24	1.10E-26	7.11E-26	2.66E-34	9.93E-21	8.08E-32	2.12E-21	8.35E-22	1.74E-25	6.77E-24	8.66E-33
260	7.00E-26	1.07E-32	2.95E-24	1.32E-23	6.22E-26	2.70E-25	4.62E-33	1.52E-20	1.00E-30	3.59E-21	1.94E-21	7.71E-25	1.94E-23	1.22E-31
280	2.42E-25	1.35E-31	8.41E-24	3.13E-23	2.79E-25	8.55E-25	5.41E-32	2.22E-20	8.74E-30	5.69E-21	4.02E-21	2.80E-24	4.84E-23	1.19E-30
298.15	**6.53E-25**	**1.01E-30**	**1.95E-23**	**6.26E-23**	**9.20E-25**	**2.15E-24**	**3.82E-31**	**3.01E-20**	**4.90E-29**	**8.27E-21**	**7.24E-21**	**7.81E-24**	**1.00E-22**	**7.31E-30**
300	7.18E-25	1.22E-30	2.11E-23	6.69E-23	1.03E-24	2.35E-24	4.61E-31	3.10E-20	5.77E-29	8.57E-21	7.66E-21	8.62E-24	1.08E-22	8.69E-30
320	1.87E-24	8.46E-30	4.75E-23	1.31E-22	3.27E-24	5.72E-24	3.03E-30	4.20E-20	3.04E-28	1.24E-20	1.36E-20	2.33E-23	2.19E-22	4.98E-29
340	4.39E-24	4.70E-29	9.80E-23	2.39E-22	9.11E-24	1.27E-23	1.60E-29	5.53E-20	1.32E-27	1.72E-20	2.26E-20	5.63E-23	4.12E-22	2.34E-28
360	9.44E-24	2.18E-28	1.88E-22	4.10E-22	2.28E-23	2.58E-23	7.12E-29	7.10E-20	4.93E-27	2.33E-20	3.59E-20	1.24E-22	7.29E-22	9.32E-28
380	1.88E-23	8.63E-28	3.38E-22	6.69E-22	5.22E-23	4.91E-23	2.71E-28	8.94E-20	1.61E-26	3.06E-20	5.46E-20	2.54E-22	1.22E-21	3.23E-27
400	3.52E-23	2.99E-27	5.77E-22	1.04E-21	1.10E-22	8.81E-23	9.10E-28	1.10E-19	4.69E-26	3.94E-20	8.00E-20	4.86E-22	1.95E-21	9.93E-27

Table S5A The rate constants of abstraction reactions of AF with NO_3 reactions at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_8	k_9	k_{10}	k_{11}	k_{12}
200	2.69E-31	4.04E-31	1.46E-30	9.53E-23	3.72E-28
220	8.51E-30	1.53E-29	5.16E-29	4.23E-22	8.20E-27
240	1.54E-28	3.20E-28	1.02E-27	1.49E-21	1.10E-25
260	1.81E-27	4.26E-27	1.30E-26	4.36E-21	9.96E-25
280	1.51E-26	3.95E-26	1.16E-25	1.11E-20	6.68E-24
298.15	**8.15E-26**	**2.33E-25**	**6.62E-25**	**2.34E-20**	**3.04E-23**
300	9.57E-26	2.76E-25	7.81E-25	2.51E-20	3.51E-23
320	4.86E-25	1.52E-24	4.18E-24	5.19E-20	1.51E-22
340	2.06E-24	6.90E-24	1.85E-23	9.91E-20	5.51E-22
360	7.45E-24	2.67E-23	6.98E-23	1.77E-19	1.75E-21
380	2.37E-23	8.99E-23	2.30E-22	3.00E-19	4.97E-21
400	6.77E-23	2.70E-22	6.78E-22	4.84E-19	1.28E-20

Table S6A The rate constants of AF with O_3 at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_1	k_2	k_3	k_4	k_5	k_6	$k_{1'}$	$k_{2'}$	$k_{3'}$	$k_{4'}$	$k_{5'}$	$k_{6'}$
200	1.54E-39	1.21E-39	3.70E-35	9.40E-36	2.88E-35	3.50E-39	4.00E-33	3.41E-30	2.58E-32	3.77E-35	2.17E-40	6.02E-34
220	1.86E-37	1.53E-37	2.03E-33	5.69E-34	1.60E-33	4.24E-37	1.25E-31	6.21E-29	6.87E-31	2.00E-33	3.60E-38	2.14E-32
240	1.02E-35	8.77E-36	5.80E-32	1.77E-32	4.61E-32	2.34E-35	2.23E-30	7.07E-28	1.07E-29	5.57E-32	2.58E-36	4.27E-31
260	3.07E-34	2.73E-34	1.00E-30	3.28E-31	8.03E-31	7.08E-34	2.60E-29	5.61E-27	1.11E-28	9.41E-31	9.74E-35	5.45E-30
280	5.73E-33	5.25E-33	1.16E-29	4.05E-30	9.40E-30	1.33E-32	2.15E-28	3.35E-26	8.36E-28	1.07E-29	2.21E-33	4.88E-29
298.15	**5.86E-32**	**5.50E-32**	**8.18E-29**	**2.98E-29**	**6.64E-29**	**1.36E-31**	**1.15E-27**	**1.39E-25**	**4.15E-27**	**7.42E-29**	**2.64E-32**	**2.79E-28**
300	7.32E-32	6.88E-32	9.85E-29	3.61E-29	8.00E-29	1.70E-31	1.35E-27	1.59E-25	4.84E-27	8.93E-29	3.34E-32	3.29E-28
320	6.85E-31	6.59E-31	6.44E-28	2.47E-28	5.26E-28	1.60E-30	6.84E-27	6.28E-25	2.27E-26	5.75E-28	3.62E-31	1.76E-27
340	4.97E-30	4.87E-30	3.40E-27	1.36E-27	2.79E-27	1.16E-29	2.88E-26	2.12E-24	8.94E-26	3.00E-27	2.99E-30	7.82E-27
360	2.91E-29	2.90E-29	1.50E-26	6.21E-27	1.24E-26	6.83E-29	1.04E-25	6.30E-24	3.04E-25	1.31E-26	1.97E-29	2.96E-26
380	1.42E-28	1.44E-28	5.70E-26	2.44E-26	4.71E-26	3.35E-28	3.29E-25	1.68E-23	9.16E-25	4.92E-26	1.07E-28	9.78E-26
400	5.97E-28	6.14E-28	1.91E-25	8.38E-26	1.58E-25	1.41E-27	9.34E-25	4.08E-23	2.48E-24	1.63E-25	4.91E-28	2.88E-25

Table S7A The rate constants of addition reactions of AF with Cl at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_1	k_2	k_3	k_4	k_5	k_6	k_7	$k_{1'}$	$k_{2'}$	$k_{3'}$	$k_{4'}$	$k_{5'}$	$k_{6'}$	$k_{7'}$
200	1.07E-13	1.74E-25	2.32E-16	1.23E-12	8.31E-18	1.06E-17	3.17E-22	3.05E-13	1.14E-27	6.88E-14	2.84E-14	9.27E-20	5.06E-19	6.11E-23
220	1.33E-13	2.77E-24	5.46E-16	1.49E-12	2.92E-17	3.41E-17	2.44E-21	3.82E-13	2.86E-26	9.44E-14	4.50E-14	4.50E-19	2.03E-18	5.50E-22
240	1.62E-13	2.83E-23	1.13E-15	1.78E-12	8.45E-17	9.20E-17	1.35E-20	4.69E-13	4.28E-25	1.25E-13	6.71E-14	1.71E-18	6.55E-18	3.48E-21
260	1.94E-13	2.05E-22	2.11E-15	2.09E-12	2.10E-16	2.16E-16	5.86E-20	5.64E-13	4.27E-24	1.60E-13	9.52E-14	5.33E-18	1.79E-17	1.68E-20
280	2.30E-13	1.13E-21	3.66E-15	2.43E-12	4.65E-16	4.52E-16	2.08E-19	6.69E-13	3.10E-23	2.00E-13	1.30E-13	1.43E-17	4.28E-17	6.55E-20
298.15	**2.64E-13**	**4.39E-21**	**5.70E-15**	**2.76E-12**	**8.78E-16**	**8.19E-16**	**5.71E-19**	**7.72E-13**	**1.50E-22**	**2.41E-13**	**1.68E-13**	**3.16E-17**	**8.60E-17**	**1.94E-19**
300	2.68E-13	5.00E-21	5.94E-15	2.79E-12	9.33E-16	8.67E-16	6.29E-19	7.83E-13	1.74E-22	2.45E-13	1.72E-13	3.41E-17	9.19E-17	2.15E-19
320	3.09E-13	1.85E-20	9.17E-15	3.18E-12	1.73E-15	1.55E-15	1.67E-18	9.06E-13	7.97E-22	2.96E-13	2.22E-13	7.33E-17	1.81E-16	6.14E-19
340	3.53E-13	5.94E-20	1.35E-14	3.60E-12	3.01E-15	2.60E-15	3.99E-18	1.04E-12	3.07E-21	3.51E-13	2.79E-13	1.45E-16	3.32E-16	1.56E-18
360	4.00E-13	1.68E-19	1.92E-14	4.04E-12	4.95E-15	4.14E-15	8.69E-18	1.18E-12	1.02E-20	4.12E-13	3.45E-13	2.68E-16	5.72E-16	3.59E-18
380	4.50E-13	4.30E-19	2.65E-14	4.51E-12	7.77E-15	6.32E-15	1.76E-17	1.33E-12	3.03E-20	4.78E-13	4.19E-13	4.67E-16	9.37E-16	7.64E-18
400	5.03E-13	1.00E-18	3.56E-14	5.00E-12	1.17E-14	9.31E-15	3.32E-17	1.49E-12	8.08E-20	5.49E-13	5.02E-13	7.74E-16	1.47E-15	1.51E-17

Table S8A The rate constants of abstraction reactions of AF with Cl at 200-400K (unit: $cm^3molecule^{-1}s^{-1}$)

T(K)	k_8	k_9	k_{10}	k_{11}	k_{12}
200	1.05E-23	2.47E-25	1.14E-24	4.59E-16	7.25E-15
220	2.14E-22	8.31E-24	3.29E-23	1.63E-15	2.58E-14
240	2.67E-21	1.58E-22	5.51E-22	4.75E-15	7.56E-14
260	2.29E-20	1.94E-21	6.07E-21	1.19E-14	1.90E-13
280	1.46E-19	1.68E-20	4.79E-20	2.65E-14	4.23E-13
298.15	**6.37E-19**	**9.32E-20**	**2.48E-19**	**5.02E-14**	**8.04E-13**
300	7.33E-19	1.10E-19	2.90E-19	5.34E-14	8.55E-13
320	3.04E-18	5.74E-19	1.41E-18	9.95E-14	1.59E-12
340	1.07E-17	2.49E-18	5.76E-18	1.73E-13	2.79E-12
360	3.32E-17	9.21E-18	2.02E-17	2.86E-13	4.60E-12
380	9.15E-17	2.99E-17	6.25E-17	4.51E-13	7.26E-12
400	2.29E-16	8.68E-17	1.73E-16	6.82E-13	1.10E-11

Table S1B Arrhenius formulas for elementary reactions of AF with OH over the temperature range of 200-400 K (unit: $cm^3molecule^{-1}s^{-1}$)

	Reactions	$k_{298.15K}$	Arrhenius formulas	R^2
(A1)	AF+OH→TS1A→IM1A	2.03E-18	k=1,32E-14exp(-2606.8/T)	0.9995
(A2)	AF+OH→TS2A→IM2A	4.79E-22	k=6.26E-14exp(-5559.7/T)	0.9999
(A3)	AF+OH→TS3A→IM3A	2.62E-17	k=9.09E-14exp(-2418.2/T)	0.9995
(A4)	AF+OH→TS4A→IM4A	1.88E-20	k=1.75E-13exp(-4771.5/T)	0.9999
(A5)	AF+OH→TS5A→IM5A	4.21E-17	k=5.19E-13exp(-2796.2/T)	0.9996
(A6)	AF+OH→TS6A→IM6A	3.53E-17	k=2.52E-13exp(-2632.7/T)	0.9995
(A7)	AF+OH→TS7A→IM7A	9.43E-21	k=1.32E-14exp(-4207.9/T)	0.9998
(A1')	AF+OH→TS1'A→IM1'A	3.35E-17	k=1.51E-14exp(-1810.8/T)	0.9999
(A2')	AF+OH→TS2'A→IM2'A	5.37E-18	k=1.60E-14exp(-2373.4/T)	0.9994
(A3')	AF+OH→TS3'A→IM3'A	3.27E-18	k=5.78E-14exp(-2904.1/T)	0.9996
(A4')	AF+OH→TS4'A→IM4'A	4.52E-19	k=1.95E-13exp(-3856.9/T)	0.9998
(A5')	AF+OH→TS5'A→IM5'A	4.74E-21	k=3.11E-13exp(-5354.4/T)	0.9999
(A6')	AF+OH→TS6'A→IM6'A	3.70E-21	k=8.78E-14exp(-5051.6/T)	0.9999
(A7')	AF+OH→TS7'A→IM7'A	9.46E-21	k=1.33E-14exp(-4208.2/T)	0.9999
	k_{add}	1.48E-16	k=2.13E-11exp(-4403.8/T)	0.9998
(A8)	AF+OH→TS8A→IM8A+H_2O	7.88E-18	k=3.07E-11exp(-4282.5/T)	0.9998
(A9)	AF+OH→TS9A→IM9A+H_2O	1.70E-17	k=2.84E-10exp(-5139.7/T)	0.9999
(A10)	AF+OH→TS10A→IM10A+H_2O	8.90E-18	k=7.24E-12exp(-850.68/T)	0.9997
(A11)	AF+OH→TS11A→IM11A+H_2O	4.01E-13	k=8.38E-11exp(-3119.5/T)	0.9997
(A12)	AF+OH→TS12A→IM12A+H_2O	2.30E-15	k=4.99E-13exp(-2398.0/T)	0.9978
	k_{abs}	4.03E-13	k=7.69E-12exp(-864.51/T)	0.9942
	k_{total}	4.04E-13	k=7.71E-12exp(-865.03/T)	0.9941

Table S2B Arrhenius formulas for elementary reactions of AF with HO_2 over the temperature range of 200-400 K (unit: $cm^3molecule^{-1}s^{-1}$)

	Reactions	$k_{298.15K}$	Arrhenius formulas	R^2
(B1)	AF+ HO_2→TS1B→IM1B	1.55E-30	k=2.70E-15exp(-10451/T)	1.0000
(B2)	AF+ HO_2→TS2B→IM2B	3.00E-36	k=4.92E-16exp(-13866/T)	1.0000
(B3)	AF+ HO_2→TS3B→IM3B	6.11E-30	k=1.06E-15exp(-9762.7/T)	1.0000
(B4)	AF+ HO_2→TS4B→IM4B	1.03E-29	k=1.51E-15exp(-9633.3/T)	1.0000
(B5)	AF+ HO_2→TS5B→IM5B	2.83E-31	k=8.36E-15exp(-11296/T)	1.0000
(B6)	AF+ HO_2→TS6B→IM6B	9.52E-32	k=2.35E-15exp(-11241/T)	1.0000
(B7)	AF+ HO_2→TS7B→IM7B	6.10E-35	k=2.68E-16exp(-12787/T)	1.0000
(B1')	AF+ HO_2→TS1'B→IM1'B	2.75E-27	k=1.46E-15exp(-8037.9/T)	0.9999
(B2')	AF+ HO_2→TS2'B→IM2'B	1.08E-29	k=6.04E-16exp(-9425.7/T)	1.0000
(B3')	AF+ HO_2→TS3'B→IM3'B	1.06E-27	k=1.29E-15exp(-8284.0/T)	0.9999
(B4')	AF+ HO_2→TS4'B→IM4'B	8.66E-29	k=2.28E-15exp(-9201.1/T)	1.0000
(B5')	AF+ HO_2→TS5'B→IM5'B	2.19E-32	k=4.69E-15exp(-11886/T)	1.0000
(B6')	AF+ HO_2→TS6'B→IM6'B	9.99E-32	k=7.43E-16exp(-10884/T)	1.0000
(B7')	AF+ HO_2→TS7'B→IM7'B	7.36E-35	k=1.41E-15exp(-13225/T)	1.0000
	k_{total}	7.02E-33	k=2.91E-15exp(-8133.1/T)	0.9999

Table S3B Arrhenius formulas for elementary reactions of AF with NO_3 over the temperature range of 200-400 K (unit: $cm^3molecule^{-1}s^{-1}$)

	Reactions	$k_{298.15K}$	Arrhenius formulas	R^2
(C1)	AF+NO_3→AF-NO3-1→TS1C→IM1C	6.53E-25	k=2.76E-18exp(-4537.1/T)	0.9998
(C2)	AF+ NO_3→AF-NO3-1→TS2C→IM2C	1.01E-30	k=2.95E-17exp(-9233.1/T)	1.0000
(C3)	AF+ NO_3→AF-NO3-1→TS3C→IM3C	1.95E-23	k=7.83E-18exp(-3835.6/T)	0.9998
(C4)	AF+ NO_3→AF-NO3-1→TS4C→IM4C	6.26E-23	k=2.64E-18exp(-3163.0/T)	0.9997
(C5)	AF+ NO_3→AF-NO3-1→TS5C→IM5C	9.20E-25	k=8.98E-17exp(-5472.7/T)	0.9999
(C6)	AF+ NO_3→AF-NO3-1→TS6C→IM6C	2.15E-24	k=3.09E-18exp(-4215.6/T)	0.9998
(C7)	AF+ NO_3→TS7C→IM7C	3.82E-31	k=4.65E-18exp(-8970.9/T)	1.0000
(C1')	AF+NO_3→AF-NO3-1'→TS1'C→IM1'C	3.01E-20	k=3.31E-18exp(-1388.4/T)	0.9983
(C2')	AF+NO_3→AF-NO3-1'→TS2'C→IM2'C	4.90E-29	k=1.68E-17exp(-7906.5/T)	0.9999
(C3')	AF+NO_3→AF-NO3-1'→TS3'C→IM3'C	8.27E-21	k=2.55E-18exp(-1696.3/T)	0.9989
(C4')	AF+NO_3→AF-NO3-1'→TS4'C→IM4'C	7.24E-21	k=6.06E-17exp(-2680.8/T)	0.9996
(C5')	AF+NO_3→AF-NO3-1'→TS5'C→IM5'C	7.81E-24	k=5.81E-17exp(-4705.0/T)	0.9999
(C6')	AF+NO_3→AF-NO3-1'→TS6'C→IM6'C	1.00E-22	k=7.67E-18exp(-3340.2/T)	0.9997
(C7')	AF+ NO_3→TS7'C→IM7'C	7.31E-30	k=9.84E-18exp(-8314,6/T)	1.0000
	k_{add}	4.59E-20	k=1.59E-14exp(-7739.4/T)	0.9999
(C8)	AF+ NO_3→TS8C→IM8C+HNO_3	8.15E-26	k=1.68E-13exp(-8128.9/T)	1.0000
(C9)	AF+ NO_3→TS9C→IM9C+HNO_3	2.33E-25	k=2.95E-13exp(-7984.9/T)	0.9999
(C10)	AF+ NO_3→TS10C→IM10C+HNO_3	6.62E-25	k=2.29E-15exp(-3414.1/T)	0.9997
(C11)	AF+ NO_3→TS11C→IM11C+HNO_3	2.34E-20	k=4.09E-13exp(-6941.9/T)	0.9999
(C12)	AF+ NO_3→TS12C→IM12C+HNO_3	3.04E-23	k=1.13E-17exp(-1616.2/T)	0.9942
	k_{abs}	2.34E-20	k=2.37E-15exp(-3422.2/T)	0.9997
	k_{total}	6.93E-20	k=8.85E-17exp(-2067.6/T)	0.9799

Table S4B Arrhenius formulas for elementary reactions of AF with O_3 over the temperature range of 200-400 K (unit: $cm^3molecule^{-1}s^{-1}$)

	Reactions	$k_{298.15K}$	Arrhenius formulas	R^2
(D1)	AF+O_3→TS1D→IM1D	5.86E-32	k=2.15E-16exp(-10673/T)	1.0000
(D2)	AF+ O_3→TS2D→IM2D	5.50E-32	k=2.90E-16exp(-10781/T)	1.0000
(D3)	AF+ O_3→TS3D→IM3D	8.18E-29	k=9.16E-16exp(-8946.6/T)	1.0000
(D4)	AF+ O_3→TS4D→IM4D	2.98E-29	k=6.98E-16exp(-9165.8/T)	1.0000
(D5)	AF+ O_3→TS5D→IM5D	6.64E-29	k=8.07E-16exp(-8970.8/T)	1.0000
(D6)	AF+ O_3→TS6D→IM6D	1.36E-31	k=5.27E-16exp(-10689/T)	1.0000
(D1')	AF+ O_3→TS1'D→IM1'D	1.15E-27	k=2.04E-16exp(-7709.1/T)	0.9999
(D2')	AF+ O_3→TS2'D→IM2'D	1.39E-25	k=4.55E-16exp(-6520.0/T)	0.9999
(D3')	AF+ O_3→TS3'D→IM3'D	4.15E-27	k=2.23E-16exp(-7353.6/T)	0.9999
(D4')	AF+ O_3→TS4'D→IM4'D	7.42E-29	k=6.56E-16exp(-8875.8/T)	1.0000
(D5')	AF+ O_3→TS5'D→IM5'D	2.64E-32	k=1.03E-15exp(-11380/T)	1.0000
(D6')	AF+ O_3→TS6'D→IM6'D	2.79E-28	k=1.29E-16exp(-7996.2/T)	0.9999
	k_{total}	1.45E-25	k=5.38E-16exp(-6555.2/T)	0.9999

Table S5B Arrhenius formulas for elementary reactions of AF with Cl over the temperature range of 200-400 K (unit: $cm^3molecule^{-1}s^{-1}$)

	Reactions	$k_{298.15K}$	Arrhenius formulas	R^2
(E1)	AF+Cl→AF-Cl-1→TS1E→IM1E	2.64E-13	k=2.22E-12exp(-622.06/T)	0.9918
(E2)	AF+Cl→AF-Cl-1→TS2E→IM2E	4.39E-21	k=5.43E-12exp(-6229.8/T)	0.9999
(E3)	AF+Cl→AF-Cl-1→TS3E→IM3E	5.70E-15	k=5.10E-12exp(-2014.4/T)	0.9992
(E4)	AF+Cl→AF-Cl-1→TS4E→IM4E	2.76E-12	k=1.90E-11exp(-563.22/T)	0.9900
(E5)	AF+Cl→AF-Cl-1→TS5E→IM5E	8.78E-16	k=1.54E-11exp(-2901.8/T)	0.9996
(E6)	AF+Cl→AF-Cl-1→TS6E→IM6E	8.19E-16	k=7.63E-12exp(-2712.8/T)	0.9996
(E7)	AF+Cl→TS7E→IM7E	5.71E-19	k=3.25E-12exp(-4625.9/T)	0.9998
(E1')	AF+Cl→AF-Cl-1'→TS1'E→IM1'E	7.72E-13	k=6.77E-12exp(-635.43/T)	0.9921
(E2')	AF+Cl→AF-Cl-1'→TS2'E→IM2'E	1.50E-22	k=5.35E-12exp(-7232.5/T)	0.9999
(E3')	AF+Cl→AF-Cl-1'→TS3'E→IM3'E	2.41E-13	k=4.08E-12exp(-831.94/T)	0.9954
(E4')	AF+Cl→AF-Cl-1'→TS4'E→IM4'E	1.68E-13	k=8.29E-12exp(-1150.8/T)	0.9976
(E5')	AF+Cl→AF-Cl-1'→TS5'E→IM5'E	3.16E-17	k=6.03E-12exp(-3613.5/T)	0.9998
(E6')	AF+Cl→AF-Cl-1'→TS6'E→IM6'E	8.60E-17	k=3.97E-12exp(-3190.5/T)	0.9997
(E7')	AF+Cl→TS7'E→IM7'E	1.94E-19	k=3.49E-12exp(-4968.7/T)	0.9999
	k_{add}	4.21E-12	k=4.66E-09exp(-6759.9/T)	0.9999
(E8)	AF+Cl→AF-Cl-2→TS8E→IM8E+HCl	6.37E-19	k=2.84E-08exp(-7872.0/T)	0.9999
(E9)	AF+Cl→TS9E→IM9E+HCl	9.32E-20	k=2.47E-08exp(-7538.3/T)	0.9999
(E10)	AF+Cl→TS10E→IM10E+HCl	2.48E-19	k=9.45E-10exp(-2922.6/T)	0.9996
(E11)	AF+Cl→AF-Cl-3→TS11E→IM11E+HCl	5.02E-14	k=1.56E-08exp(-2931.0/T)	0.9996
(E12)	AF+Cl→TS11E→IM12E+HCl	8.04E-13	k=3.50E-11exp(-617.51/T)	0.9896
	k_{abs}	8.54E-13	k=9.67E-10exp(-2930.5/T)	0.9896
	k_{total}	5.07E-12	k=7.84E-10exp(-947.77/T)	0.9326

Table S1C The lifetimes of AF+OH addition reactions according to the rate constants at 200-400K

T(K)	τ_1(s)	τ_2(s)	τ_3(s)	τ_4(s)	τ_5(s)	τ_6(s)	τ_7(s)	$\tau_{1'}$(s)	$\tau_{2'}$(s)	$\tau_{3'}$(s)	$\tau_{4'}$(s)	$\tau_{5'}$(s)	$\tau_{6'}$(s)	$\tau_{7'}$(s)
200	9.38E+09	5.76E+21	4.30E+12	8.15E+08	1.20E+14	9.45E+13	3.16E+18	3.28E+09	8.78E+23	1.45E+10	3.53E+10	1.08E+16	1.98E+15	1.64E+19
220	7.52E+09	3.61E+20	1.83E+12	6.72E+08	3.42E+13	2.93E+13	4.10E+17	2.62E+09	3.49E+22	1.06E+10	2.22E+10	2.22E+15	4.93E+14	1.82E+18
240	6.17E+09	3.54E+19	8.86E+11	5.63E+08	1.18E+13	1.09E+13	7.38E+16	2.13E+09	2.34E+21	8.02E+09	1.49E+10	5.86E+14	1.53E+14	2.87E+17
260	5.14E+09	4.89E+18	4.73E+11	4.78E+08	4.75E+12	4.64E+12	1.71E+16	1.77E+09	2.34E+20	6.25E+09	1.05E+10	1.88E+14	5.59E+13	5.95E+16
280	4.35E+09	8.87E+17	2.73E+11	4.12E+08	2.15E+12	2.21E+12	4.81E+15	1.49E+09	3.23E+19	5.00E+09	7.69E+09	6.98E+13	2.34E+13	1.53E+16
298.15	**3.79E+09**	**2.28E+17**	**1.76E+11**	**3.62E+08**	**1.14E+12**	**1.22E+12**	**1.75E+15**	**1.30E+09**	**6.67E+18**	**4.15E+09**	**5.96E+09**	**3.17E+13**	**1.16E+13**	**5.16E+15**
300	3.73E+09	2.00E+17	1.68E+11	3.58E+08	1.07E+12	1.15E+12	1.59E+15	1.28E+09	5.74E+18	4.08E+09	5.81E+09	2.94E+13	1.09E+13	4.65E+15
320	3.24E+09	5.39E+16	1.09E+11	3.14E+08	5.78E+11	6.46E+11	5.98E+14	1.10E+09	1.25E+18	3.38E+09	4.51E+09	1.36E+13	5.52E+12	1.63E+15
340	2.83E+09	1.68E+16	7.39E+10	2.78E+08	3.33E+11	3.85E+11	2.51E+14	9.64E+08	3.26E+17	2.85E+09	3.58E+09	6.89E+12	3.01E+12	6.41E+14
360	2.50E+09	5.94E+15	5.20E+10	2.48E+08	2.02E+11	2.42E+11	1.15E+14	8.49E+08	9.76E+16	2.43E+09	2.90E+09	3.73E+12	1.75E+12	2.78E+14
380	2.22E+09	2.33E+15	3.77E+10	2.22E+08	1.29E+11	1.58E+11	5.69E+13	7.53E+08	3.30E+16	2.09E+09	2.39E+09	2.14E+12	1.07E+12	1.31E+14
400	1.99E+09	9.95E+14	2.81E+10	2.00E+08	8.53E+10	1.07E+11	3.01E+13	6.72E+08	1.24E+16	1.82E+09	1.99E+09	1.29E+12	6.81E+11	6.61E+13

Table S2C The lifetimes of AF+OH abstraction reactions according to the rate constants at 200-400K

T(K)	τ_8(s)	τ_9(s)	τ_{10}(s)	τ_{11}(s)	τ_{12}(s)
200	1.64E+14	6.20E+13	4.87E+14	9.28E+06	6.77E+10
220	2.35E+13	9.42E+12	5.01E+13	6.71E+06	1.74E+10
240	4.61E+12	1.93E+12	7.41E+12	5.04E+06	5.55E+09
260	1.14E+12	4.98E+11	1.45E+12	3.91E+06	2.08E+09
280	3.42E+11	1.54E+11	3.56E+11	3.11E+06	8.87E+08
298.15	**1.31E+11**	**6.05E+10**	**1.16E+11**	**2.57E+06**	**4.48E+08**
300	1.19E+11	5.53E+10	1.04E+11	2.52E+06	4.19E+08
320	4.71E+10	2.24E+10	3.52E+10	2.09E+06	2.16E+08
340	2.05E+10	9.99E+09	1.34E+10	1.75E+06	1.20E+08
360	9.77E+09	4.85E+09	5.66E+09	1.49E+06	7.01E+07
380	5.00E+09	2.52E+09	2.60E+09	1.28E+06	4.33E+07
400	2.72E+09	1.39E+09	1.28E+09	1.11E+06	2.79E+07

Table S3C The lifetimes of AF+ HO_2 according to the rate constants at 200-400K

T(K)	τ_1(s)	τ_2(s)	τ_3(s)	τ_4(s)	τ_5(s)	τ_6(s)	τ_7(s)	$\tau_{1'}$(s)	$\tau_{2'}$(s)	$\tau_{3'}$(s)	$\tau_{4'}$(s)	$\tau_{5'}$(s)	$\tau_{6'}$(s)	$\tau_{7'}$(s)
200	1.70E+29	2.43E+37	1.39E+28	6.67E+27	3.74E+30	1.02E+31	2.02E+35	1.80E+24	4.50E+27	6.99E+24	3.88E+26	1.28E+32	5.37E+30	3.44E+35
220	1.56E+27	4.73E+34	1.75E+26	8.90E+25	2.34E+28	6.52E+28	6.43E+32	4.96E+22	6.60E+25	1.72E+23	6.31E+24	6.11E+29	4.06E+28	8.97E+32
240	3.09E+25	2.57E+32	4.49E+24	2.40E+24	3.37E+26	9.58E+26	5.25E+30	2.45E+21	1.93E+24	7.75E+21	2.00E+23	7.03E+27	6.82E+26	6.21E+30
260	1.11E+24	3.07E+30	2.00E+23	1.12E+23	9.19E+24	2.66E+25	8.87E+28	1.90E+20	9.57E+22	5.54E+20	1.07E+22	1.59E+26	2.12E+25	9.12E+28
280	6.29E+22	6.84E+28	1.37E+22	7.94E+21	4.14E+23	1.22E+24	2.66E+27	2.09E+19	7.22E+21	5.72E+19	8.57E+20	6.08E+24	1.07E+24	2.42E+27
298.15	**6.45E+21**	**3.34E+27**	**1.64E+21**	**9.74E+20**	**3.54E+22**	**1.05E+23**	**1.64E+26**	**3.63E+18**	**9.25E+20**	**9.40E+18**	**1.15E+20**	**4.57E+23**	**1.00E+23**	**1.36E+26**
300	5.19E+21	2.50E+27	1.34E+21	7.97E+20	2.80E+22	8.32E+22	1.26E+26	3.07E+18	7.61E+20	7.91E+18	9.53E+19	3.57E+23	7.98E+22	1.03E+26
320	5.81E+20	1.37E+26	1.73E+20	1.06E+20	2.63E+21	7.89E+21	8.65E+24	5.68E+17	1.05E+20	1.39E+18	1.38E+19	2.96E+22	8.16E+21	6.48E+24
340	8.35E+19	1.05E+25	2.81E+19	1.77E+19	3.23E+20	9.81E+20	8.09E+23	1.27E+17	1.83E+19	2.97E+17	2.50E+18	3.27E+21	1.08E+21	5.59E+23
360	1.48E+19	1.07E+24	5.57E+18	3.57E+18	4.98E+19	1.53E+20	9.77E+22	3.34E+16	3.83E+18	7.50E+16	5.43E+17	4.58E+20	1.79E+20	6.29E+22
380	3.12E+18	1.37E+23	1.30E+18	8.50E+17	9.30E+18	2.87E+19	1.47E+22	1.00E+16	9.39E+17	2.18E+16	1.38E+17	7.83E+19	3.54E+19	8.86E+21
400	7.67E+17	2.15E+22	3.50E+17	2.32E+17	2.04E+18	6.35E+18	2.65E+21	3.39E+15	2.64E+17	7.10E+15	3.99E+16	1.59E+19	8.21E+18	1.51E+21

Table S4C The lifetimes of AF+NO_3 addition reactions according to the rate constants at 200-400K

T(K)	τ_1(s)	τ_2(s)	τ_3(s)	τ_4(s)	τ_5(s)	τ_6(s)	τ_7(s)	$\tau_{1'}$(s)	$\tau_{2'}$(s)	$\tau_{3'}$(s)	$\tau_{4'}$(s)	$\tau_{5'}$(s)	$\tau_{6'}$(s)	$\tau_{7'}$(s)
200	1.99E+20	2.94E+29	2.10E+18	2.16E+17	6.58E+20	3.56E+19	5.02E+29	2.42E+13	6.80E+26	1.46E+14	8.45E+14	2.19E+19	1.80E+17	8.91E+27
220	2.69E+19	4.70E+27	3.92E+17	5.46E+16	5.82E+19	5.58E+18	9.05E+27	1.37E+13	1.99E+25	7.20E+13	2.66E+14	2.75E+18	4.20E+16	2.16E+26
240	5.01E+18	1.48E+26	9.50E+16	1.71E+16	7.60E+18	1.17E+18	3.14E+26	8.39E+12	1.03E+24	3.93E+13	9.98E+13	4.80E+17	1.23E+16	9.63E+24
260	1.19E+18	7.79E+24	2.83E+16	6.32E+15	1.34E+18	3.09E+17	1.80E+25	5.48E+12	8.33E+22	2.32E+13	4.31E+13	1.08E+17	4.29E+15	6.82E+23
280	3.44E+17	6.19E+23	9.91E+15	2.66E+15	2.99E+17	9.74E+16	1.54E+24	3.76E+12	9.54E+21	1.46E+13	2.07E+13	2.98E+16	1.72E+15	6.98E+22
298.15	**1.28E+17**	**8.28E+22**	**4.28E+15**	**1.33E+15**	**9.05E+16**	**3.88E+16**	**2.18E+23**	**2.76E+12**	**1.70E+21**	**1.01E+13**	**1.15E+13**	**1.07E+16**	**8.29E+14**	**1.14E+22**
300	1.16E+17	6.84E+22	3.95E+15	1.25E+15	8.08E+16	3.55E+16	1.81E+23	2.68E+12	1.44E+21	9.72E+12	1.09E+13	9.67E+15	7.73E+14	9.59E+21
320	4.45E+16	9.86E+21	1.75E+15	6.36E+14	2.55E+16	1.46E+16	2.75E+22	1.98E+12	2.74E+20	6.74E+12	6.14E+12	3.58E+15	3.81E+14	1.67E+21
340	1.90E+16	1.77E+21	8.50E+14	3.49E+14	9.15E+15	6.58E+15	5.19E+21	1.51E+12	6.29E+19	4.84E+12	3.68E+12	1.48E+15	2.02E+14	3.56E+20
360	8.83E+15	3.83E+20	4.44E+14	2.03E+14	3.65E+15	3.23E+15	1.17E+21	1.17E+12	1.69E+19	3.58E+12	2.32E+12	6.70E+14	1.14E+14	8.94E+19
380	4.43E+15	9.66E+19	2.47E+14	1.25E+14	1.60E+15	1.70E+15	3.07E+20	9.33E+11	5.17E+18	2.72E+12	1.53E+12	3.28E+14	6.83E+13	2.58E+19
400	2.37E+15	2.78E+19	1.45E+14	7.98E+13	7.55E+14	9.46E+14	9.16E+19	7.54E+11	1.78E+18	2.11E+12	1.04E+12	1.71E+14	4.27E+13	8.39E+18

Table S5C The lifetimes of AF+NO_3 abstraction reactions according to the rate constants at 200-400K

T(K)	τ_8(s)	τ_9(s)	τ_{10}(s)	τ_{11}(s)	τ_{12}(s)
200	3.10E+23	2.06E+23	5.72E+22	8.74E+14	2.24E+20
220	9.79E+21	5.45E+21	1.62E+21	1.97E+14	1.02E+19
240	5.42E+20	2.60E+20	8.14E+19	5.61E+13	7.60E+17
260	4.62E+19	1.96E+19	6.41E+18	1.91E+13	8.36E+16
280	5.53E+18	2.11E+18	7.18E+17	7.51E+12	1.25E+16
298.15	**1.02E+18**	**3.58E+17**	**1.26E+17**	**3.56E+12**	**2.75E+15**
300	8.71E+17	3.02E+17	1.07E+17	3.31E+12	2.38E+15
320	1.71E+17	5.49E+16	1.99E+16	1.61E+12	5.52E+14
340	4.05E+16	1.21E+16	4.51E+15	8.41E+11	1.51E+14
360	1.12E+16	3.13E+15	1.19E+15	4.70E+11	4.75E+13
380	3.51E+15	9.27E+14	3.62E+14	2.78E+11	1.68E+13
400	1.23E+15	3.09E+14	1.23E+14	1.72E+11	6.53E+12

Table S6C The lifetimes of AF+O_3 according to the rate constants at 200-400K

T(K)	τ_1(s)	τ_2(s)	τ_3(s)	τ_4(s)	τ_5(s)	τ_6(s)	τ_7(s)	$\tau_{1'}$(s)	$\tau_{2'}$(s)	$\tau_{3'}$(s)	$\tau_{4'}$(s)	$\tau_{5'}$(s)
200	9.25E+26	1.18E+27	3.86E+22	1.52E+23	4.95E+22	4.08E+26	3.57E+20	4.19E+17	5.53E+19	3.79E+22	6.58E+27	2.37E+21
220	7.69E+24	9.32E+24	7.04E+20	2.51E+21	8.93E+20	3.37E+24	1.14E+19	2.30E+16	2.08E+18	7.14E+20	3.97E+25	6.66E+19
240	1.40E+23	1.63E+23	2.46E+19	8.08E+19	3.10E+19	6.10E+22	6.40E+17	2.02E+15	1.33E+17	2.57E+19	5.53E+23	3.34E+18
260	4.66E+21	5.24E+21	1.43E+18	4.36E+18	1.78E+18	2.02E+21	5.50E+16	2.54E+14	1.28E+16	1.52E+18	1.47E+22	2.62E+17
280	2.49E+20	2.72E+20	1.23E+17	3.53E+17	1.52E+17	1.08E+20	6.65E+15	4.26E+13	1.71E+15	1.33E+17	6.47E+20	2.93E+16
298.15	**2.44E+19**	**2.60E+19**	**1.75E+16**	**4.79E+16**	**2.15E+16**	**1.05E+19**	**1.24E+15**	**1.03E+13**	**3.44E+14**	**1.92E+16**	**5.42E+19**	**5.12E+15**
300	1.95E+19	2.08E+19	1.45E+16	3.96E+16	1.79E+16	8.39E+18	1.05E+15	8.97E+12	2.95E+14	1.60E+16	4.28E+19	4.34E+15
320	2.08E+18	2.17E+18	2.22E+15	5.79E+15	2.72E+15	8.94E+17	2.09E+14	2.28E+12	6.29E+13	2.49E+15	3.94E+18	8.10E+14
340	2.88E+17	2.93E+17	4.20E+14	1.05E+15	5.13E+14	1.23E+17	4.97E+13	6.74E+11	1.60E+13	4.77E+14	4.78E+17	1.83E+14
360	4.91E+16	4.92E+16	9.51E+13	2.30E+14	1.16E+14	2.09E+16	1.38E+13	2.27E+11	4.69E+12	1.09E+14	7.27E+16	4.83E+13
380	1.00E+16	9.90E+15	2.50E+13	5.86E+13	3.03E+13	4.27E+15	4.34E+12	8.51E+10	1.56E+12	2.91E+13	1.34E+16	1.46E+13
400	2.39E+15	2.33E+15	7.49E+12	1.70E+13	9.04E+12	1.02E+15	1.53E+12	3.50E+10	5.75E+11	8.77E+12	2.91E+15	4.95E+12

Table S7C The lifetimes of AF+Cl addition reactions according to the rate constants at 200-400K

T(K)	τ_1(s)	τ_2(s)	τ_3(s)	τ_4(s)	τ_5(s)	τ_6(s)	τ_7(s)	$\tau_{1'}$(s)	$\tau_{2'}$(s)	$\tau_{3'}$(s)	$\tau_{4'}$(s)	$\tau_{5'}$(s)	$\tau_{6'}$(s)	$\tau_{7'}$(s)
200	9.38E+09	5.76E+21	4.30E+12	8.15E+08	1.20E+14	9.45E+13	3.16E+18	3.28E+09	8.78E+23	1.45E+10	3.53E+10	1.08E+16	1.98E+15	1.64E+19
220	7.52E+09	3.61E+20	1.83E+12	6.72E+08	3.42E+13	2.93E+13	4.10E+17	2.62E+09	3.49E+22	1.06E+10	2.22E+10	2.22E+15	4.93E+14	1.82E+18
240	6.17E+09	3.54E+19	8.86E+11	5.63E+08	1.18E+13	1.09E+13	7.38E+16	2.13E+09	2.34E+21	8.02E+09	1.49E+10	5.86E+14	1.53E+14	2.87E+17
260	5.14E+09	4.89E+18	4.73E+11	4.78E+08	4.75E+12	4.64E+12	1.71E+16	1.77E+09	2.34E+20	6.25E+09	1.05E+10	1.88E+14	5.59E+13	5.95E+16
280	4.35E+09	8.87E+17	2.73E+11	4.12E+08	2.15E+12	2.21E+12	4.81E+15	1.49E+09	3.23E+19	5.00E+09	7.69E+09	6.98E+13	2.34E+13	1.53E+16
298.15	**3.79E+09**	**2.28E+17**	**1.76E+11**	**3.62E+08**	**1.14E+12**	**1.22E+12**	**1.75E+15**	**1.30E+09**	**6.67E+18**	**4.15E+09**	**5.96E+09**	**3.17E+13**	**1.16E+13**	**5.16E+15**
300	3.73E+09	2.00E+17	1.68E+11	3.58E+08	1.07E+12	1.15E+12	1.59E+15	1.28E+09	5.74E+18	4.08E+09	5.81E+09	2.94E+13	1.09E+13	4.65E+15
320	3.24E+09	5.39E+16	1.09E+11	3.14E+08	5.78E+11	6.46E+11	5.98E+14	1.10E+09	1.25E+18	3.38E+09	4.51E+09	1.36E+13	5.52E+12	1.63E+15
340	2.83E+09	1.68E+16	7.39E+10	2.78E+08	3.33E+11	3.85E+11	2.51E+14	9.64E+08	3.26E+17	2.85E+09	3.58E+09	6.89E+12	3.01E+12	6.41E+14
360	2.50E+09	5.94E+15	5.20E+10	2.48E+08	2.02E+11	2.42E+11	1.15E+14	8.49E+08	9.76E+16	2.43E+09	2.90E+09	3.73E+12	1.75E+12	2.78E+14
380	2.22E+09	2.33E+15	3.77E+10	2.22E+08	1.29E+11	1.58E+11	5.69E+13	7.53E+08	3.30E+16	2.09E+09	2.39E+09	2.14E+12	1.07E+12	1.31E+14
400	1.99E+09	9.95E+14	2.81E+10	2.00E+08	8.53E+10	1.07E+11	3.01E+13	6.72E+08	1.24E+16	1.82E+09	1.99E+09	1.29E+12	6.81E+11	6.61E+13

Table S8C The lifetimes of AF+Cl abstraction reactions according to the rate constants at 200-400K

T(K)	τ_8(s)	τ_9(s)	τ_{10}(s)	τ_{11}(s)	τ_{12}(s)
200	9.50E+19	4.05E+21	8.79E+20	2.18E+12	1.38E+11
220	4.68E+18	1.20E+20	3.04E+19	6.14E+11	3.87E+10
240	3.75E+17	6.32E+18	1.81E+18	2.10E+11	1.32E+10
260	4.37E+16	5.17E+17	1.65E+17	8.39E+10	5.27E+09
280	6.86E+15	5.97E+16	2.09E+16	3.78E+10	2.36E+09
298.15	**1.57E+15**	**1.07E+16**	**4.03E+15**	**1.99E+10**	**1.24E+09**
300	1.36E+15	9.11E+15	3.45E+15	1.87E+10	1.17E+09
320	3.29E+14	1.74E+15	7.08E+14	1.01E+10	6.27E+08
340	9.32E+13	4.02E+14	1.74E+14	5.76E+09	3.59E+08
360	3.02E+13	1.09E+14	4.95E+13	3.49E+09	2.17E+08
380	1.09E+13	3.34E+13	1.60E+13	2.22E+09	1.38E+08
400	4.36E+12	1.15E+13	5.76E+12	1.47E+09	9.09E+07

Table SD The total lifetimes of AF with different oxidants according to the rate constants at 200-400K

	OH		HO2		NO3		O3		Cl	
T(K)	1/τ(total)	τ(s)	1/τ(total)	τ(s)	1/τ(total)	τ(s)	1/τ(total)	τ(s)	1/τ(total)	τ(s)
200	1.08E-07	9.28E+06	7.02E-25	1.43E+24	5.05E-14	1.98E+13	2.41E-18	1.04E+19	1.74E-09	5.74E+08
220	1.49E-07	6.71E+06	2.62E-23	3.82E+22	9.58E-14	1.04E+13	4.40E-17	5.90E+17	2.17E-09	4.61E+08
240	1.99E-07	5.04E+06	5.43E-22	1.84E+21	1.73E-13	5.79E+12	5.05E-16	5.35E+16	2.68E-09	3.73E+08
260	2.56E-07	3.90E+06	7.19E-21	1.39E+20	3.02E-13	3.32E+12	4.03E-15	6.94E+15	3.31E-09	3.02E+08
280	3.23E-07	3.10E+06	6.68E-20	1.50E+19	5.17E-13	1.93E+12	2.43E-14	1.20E+15	4.11E-09	2.43E+08
298.15	3.91E-07	2.55E+06	3.93E-19	2.54E+18	8.31E-13	1.20E+12	1.01E-13	2.96E+14	5.07E-09	1.97E+08
300	3.99E-07	2.51E+06	4.66E-19	2.15E+18	8.72E-13	1.15E+12	1.16E-13	2.67E+14	5.18E-09	1.93E+08
320	4.84E-07	2.06E+06	2.58E-18	3.88E+17	1.45E-12	6.92E+11	4.63E-13	6.92E+13	6.62E-09	1.51E+08
340	5.80E-07	1.72E+06	1.18E-17	8.48E+16	2.35E-12	4.26E+11	1.58E-12	2.09E+13	8.60E-09	1.16E+08
360	6.88E-07	1.45E+06	4.59E-17	2.18E+16	3.73E-12	2.68E+11	4.75E-12	7.16E+12	1.13E-08	8.85E+07
380	8.07E-07	1.24E+06	1.56E-16	6.40E+15	5.79E-12	1.73E+11	1.28E-11	2.73E+12	1.49E-08	6.70E+07
400	9.40E-07	1.06E+06	4.74E-16	2.11E+15	8.78E-12	1.14E+11	3.16E-11	1.14E+12	1.98E-08	5.06E+07