Supporting Information

Atmospheric reactivity of vinyl acetate: kinetic and mechanistic study of its gas-phase oxidation by OH, O_3 and NO_3

B. Picquet-Varrault, M. Scarfogliero and J-F. Doussin

Number of SI : 7

Number of pages : 8 (including this one)

List of Supporting Information:

Table S1: Initial conditions of the experiments

Experiment number	Oxidant	Experiment type	Initial conditions (ppm)
1	OH	RR/mechanistic	[VA] = 1.7 ; [propene] = 2.3 ; [CH_3ONO] = 1.3 ; [NO] = 1.7
2	OH	RR/mechanistic	[VA] = 1.5 ; [propene] = 1.8 ; [CH_3ONO] = 1.1 ; [NO] = 1.8
3	OH	RR/mechanistic	[VA] = 0.8 ; [propene] = 2.1 ; [CH_3ONO] = 1.3 ; [NO] = 1.7
4	OH	Mechanistic	[VA] = 1.7 ; [C_3H_7ONO] = ; [NO] = 2.0
5	O_3	AR/mechanistic	[VA] = 1.1; [O_3] = 1.4; [CO] = 2000
6	O_3	AR/mechanistic	[VA] = 1.2; [O_3] = 4.5; [CO] = 2000
7	NO_3	RR/mechanistic	[VA] = 2.2; [propene] = 3.7; [N_2O_5] = 5.4
8	NO_3	RR/mechanistic	[VA] = 2.3; [propene] = 3.5; [N_2O_5] = 5.6
9	NO_3	RR/mechanistic	[VA] = 2.3; [propene] = 3.7; [N_2O_5] = 6.2
10	NO_3	Mechanistic	[VA] = 0.7; [N_2O_5] = 4.9
11	NO_3	Mechanistic	[VA] = 0.8; [N_2O_5] = 3.1
12	NO_3	Mechanistic	[VA] = 1.1; [N_2O_5] = 5.6

RR: relative rate; AR: absolute rate

Table S2: Integrated band intensities of the main absorption band of reactants and oxidation products (in base e)

Compound	Main absorption band	IBI/cm.molecule^{-1}	Reference
Infrared region			
Ozone	1085-950 cm^{-1}	$(1.47 \pm 0.03)\times10^{-17}$	*35*
Vinyl acetate	1275-1175 cm^{-1}	$(7.2 \pm 0.3)\times10^{-17}$	This work
Formic acetic anhydride	1095-1005 cm^{-1}	$(5.99 \pm 0.13)\times10^{-17}$	*23*
Formaldehyde	3100-2600 cm^{-1}	$(2.92 \pm 0.10)\times10^{-17}$	*36*
Acetic acid	1840-1712 cm^{-1}	$(4.36 \pm 0.24)\times10^{-17}$	*23*
Formic acid	1150-1045 cm^{-1}	3.92×10^{-17}	*37*
UV-visible region			
NO_3	675-650 nm	1.09×10^{-16}	*38*

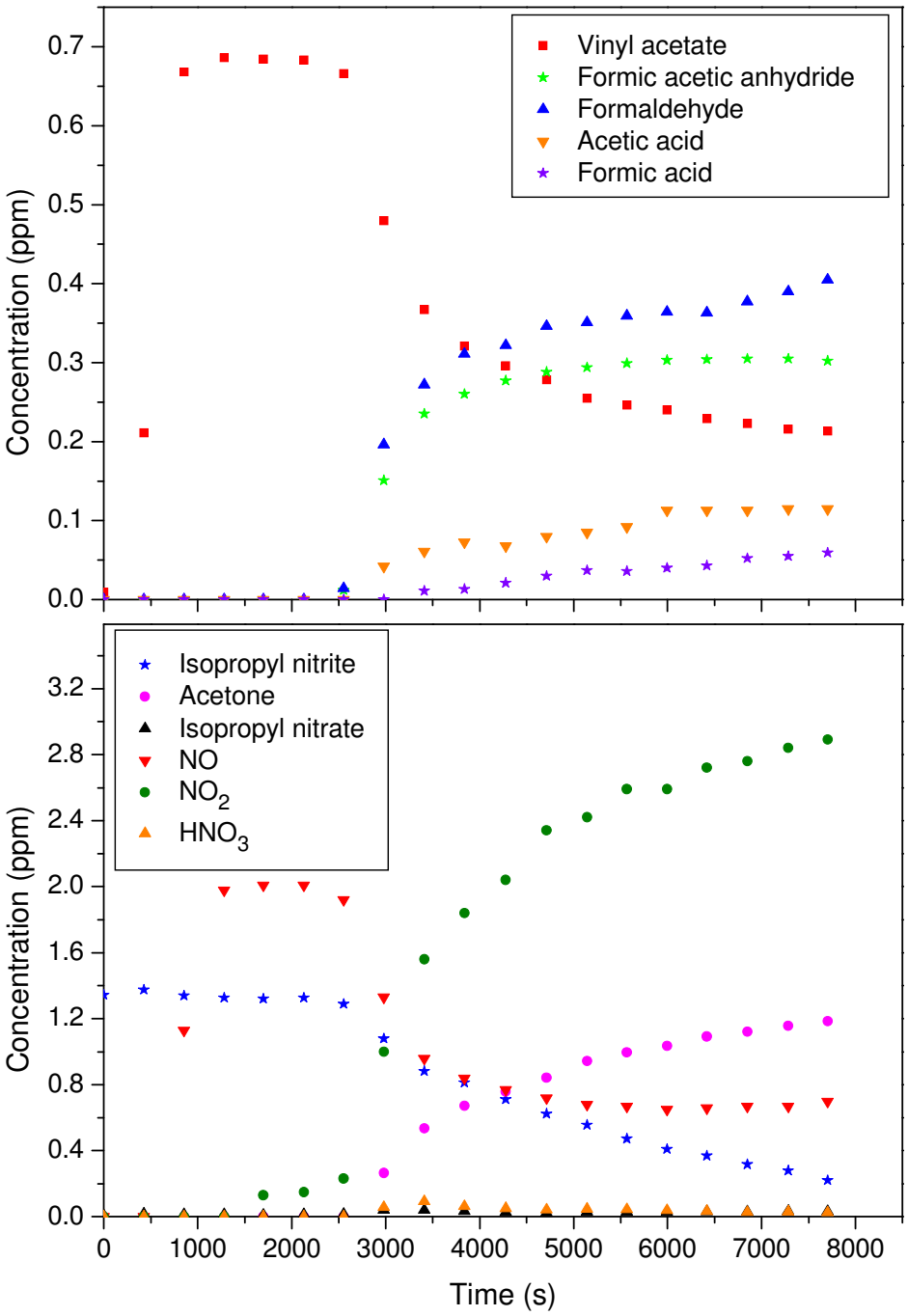

Figure S1: Concentration-time profiles of reactants and products corresponding to the photolysis of a mixture vinyl acetate/isopropyl nitrite/NO (experiment 4).

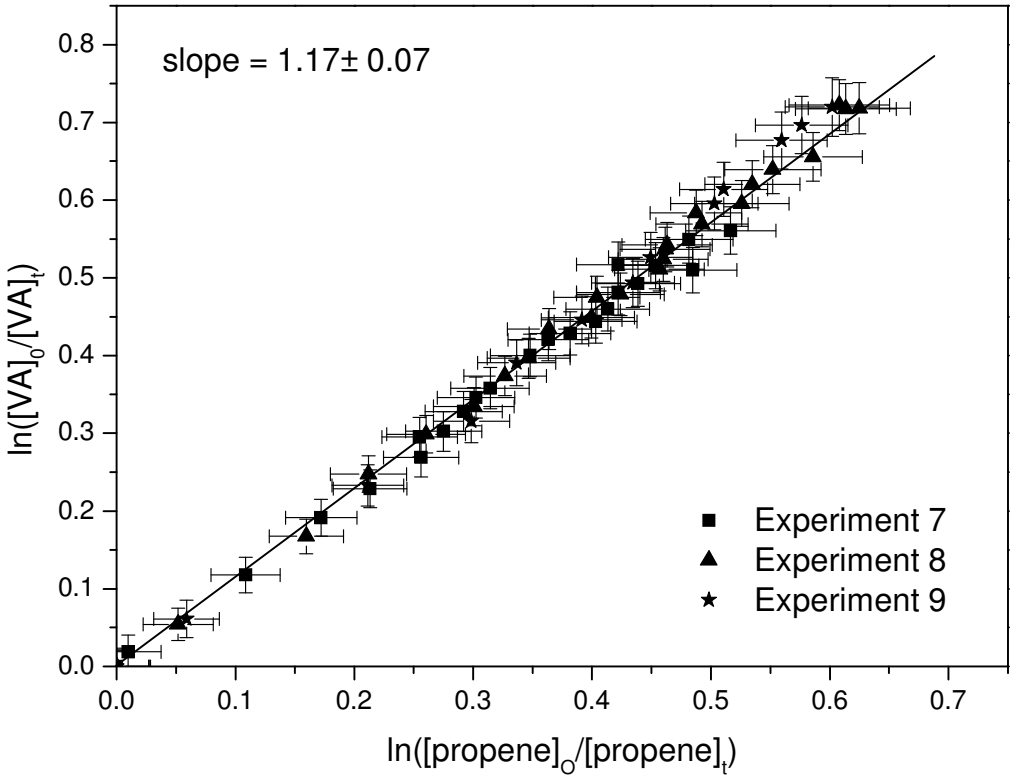

Figure S2: Relative kinetic plot for NO_3-oxidation of vinyl acetate with propene as reference compound.

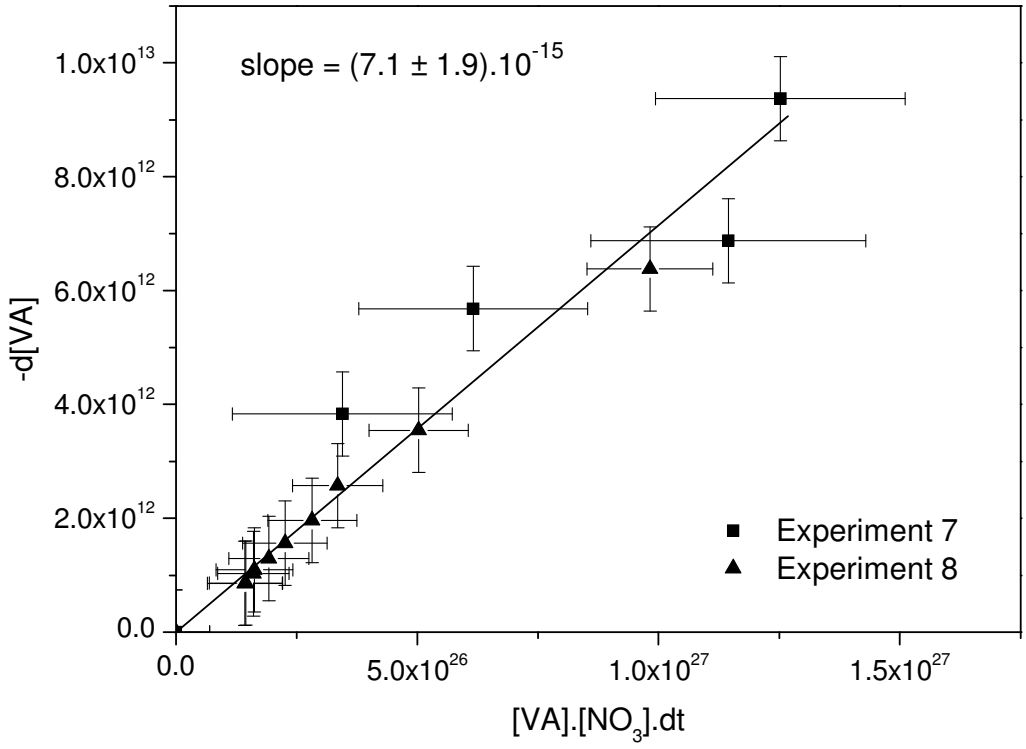

Figure S3: Absolute kinetic plot for NO_3-oxidation of vinyl acetate.

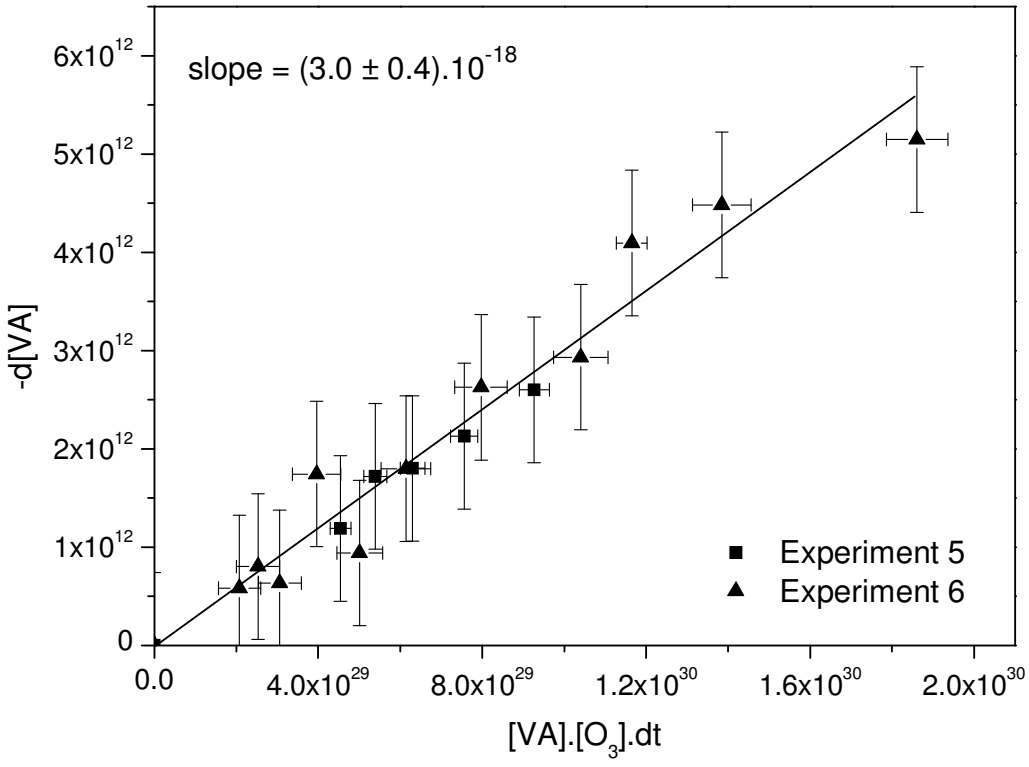

Figure S4: Absolute kinetic plot for O_3-oxidation of vinyl acetate.

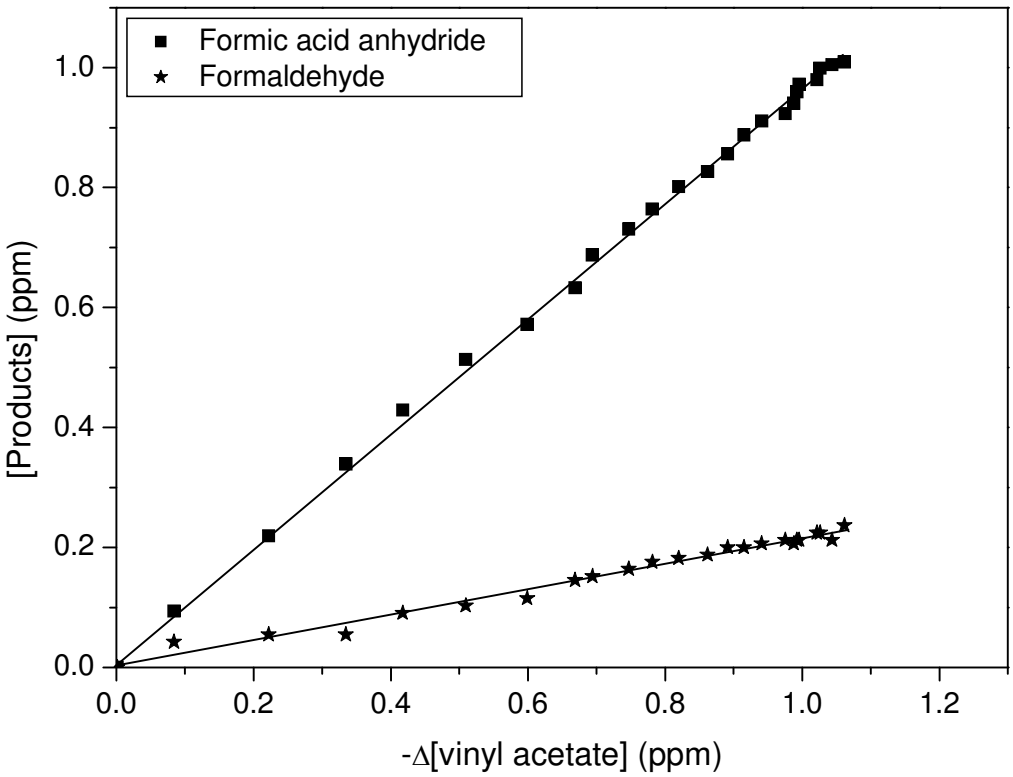

Figure S5: Formation yields of products by ozonolysis of vinyl acetate for experiment 6.