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Photochemical degradation of isoprene-derived 4,1-nitrooxy enal

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Supplemental Figures, Xiong et al., 2016

This group of Supplemental figures are referred to in the main text.

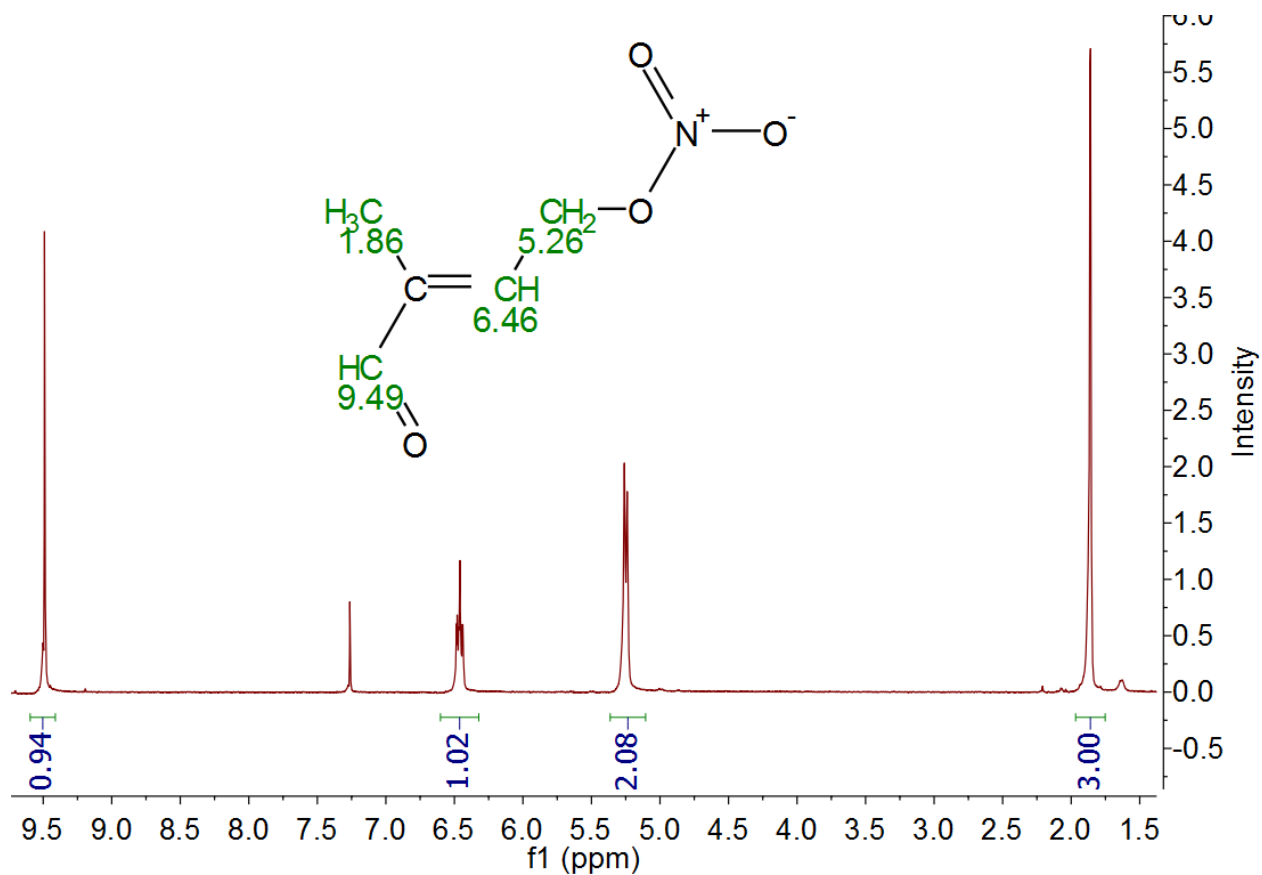


Figure S1. ^1H NMR spectrum for the 4,1-isoprene carbonyl nitrate. The solvent CDCl_3 has singlet peak at 7.26 ppm.

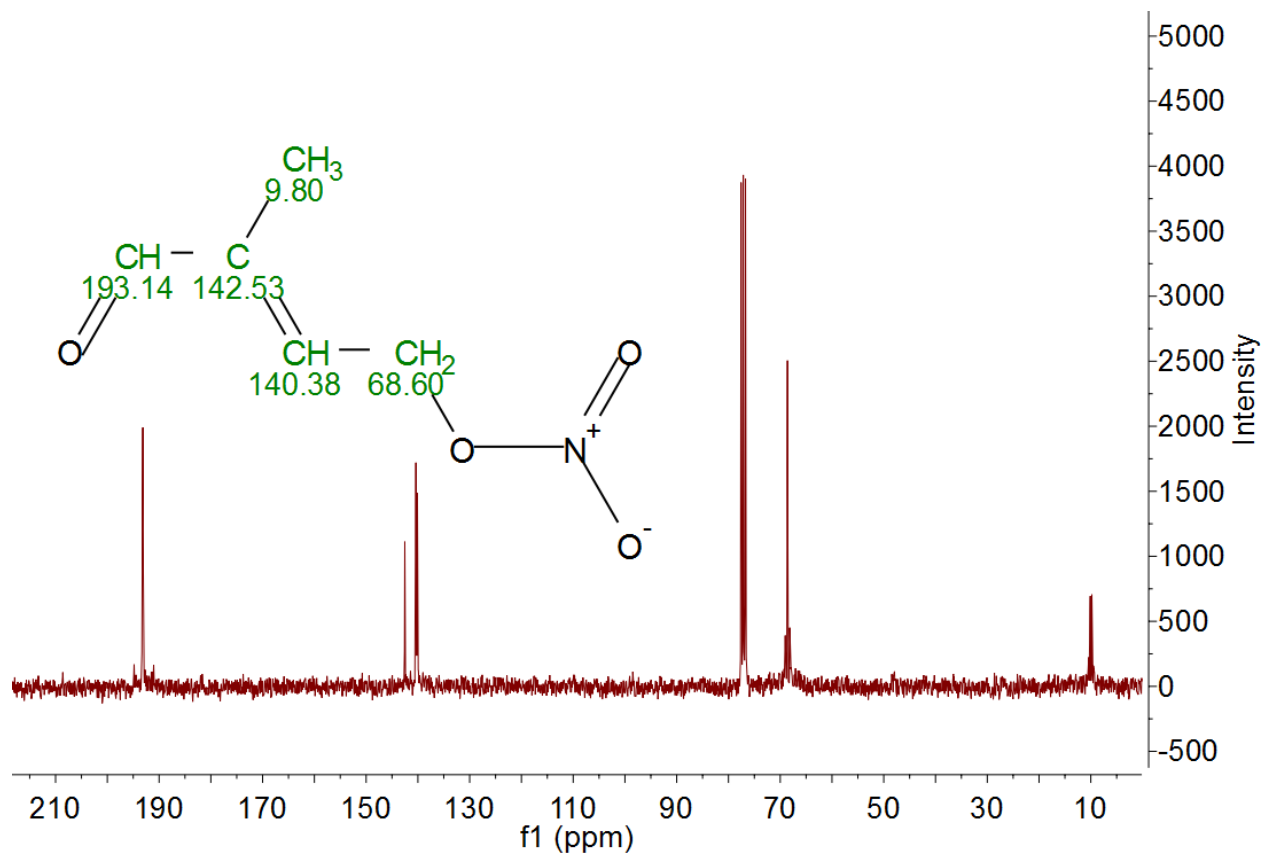


Figure S2. ^{13}C NMR spectrum for the 4,1-isoprene carbonyl nitrate. The solvent CDCl_3 has triplet peak at 80 ppm.

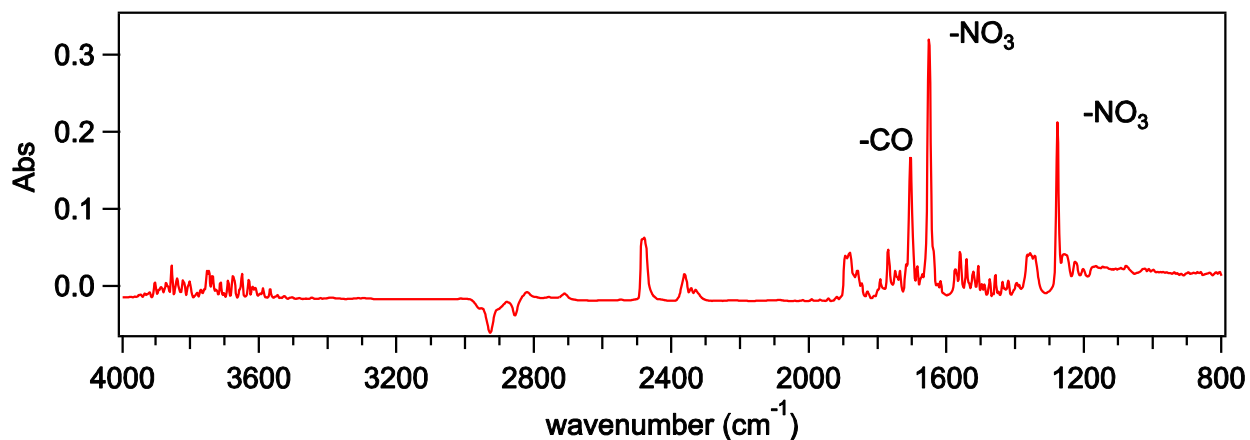


Figure S3. IR absorption spectrum for the 4,1-isoprene carbonyl nitrate. The NO_3 group has absorption at 1280 cm^{-1} and 1640 cm^{-1} . The CO group has absorption at 1700 cm^{-1} .

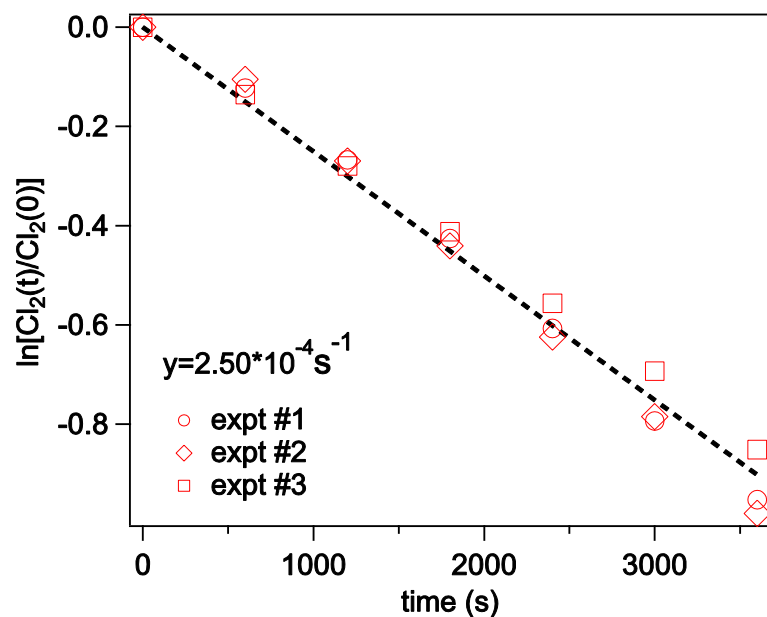


Figure S4. First-order photolysis loss of Cl_2 in the reaction chamber.

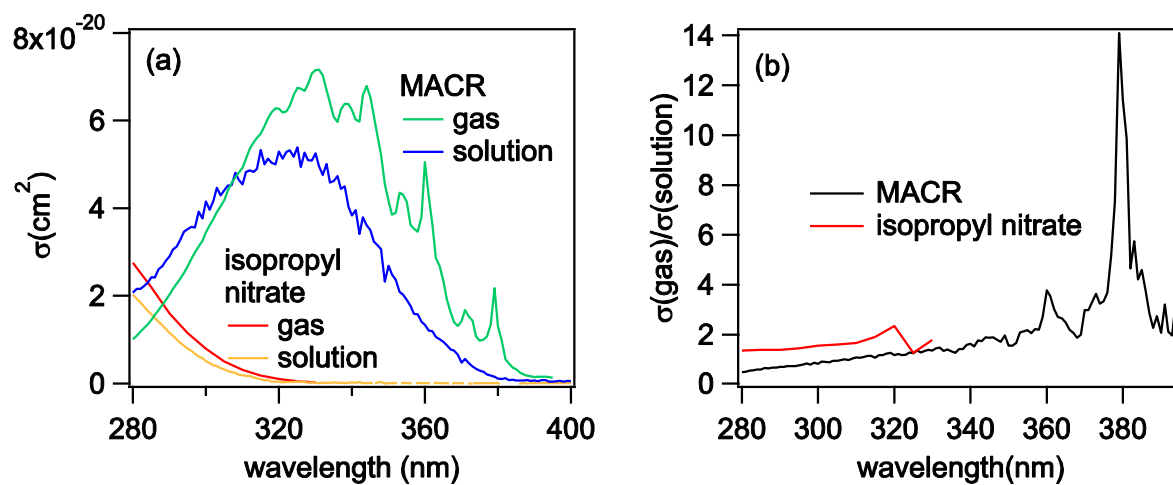


Figure S5. (a) The absorption spectra of MACR (gas phase in green, solution phase in blue) and isopropyl nitrate (gas phase in red, solution phase in gold). (b) The enhancement ratio of the gas-phase absorption relative to solution-phase absorption for MACR (black) and isopropyl nitrate (red).

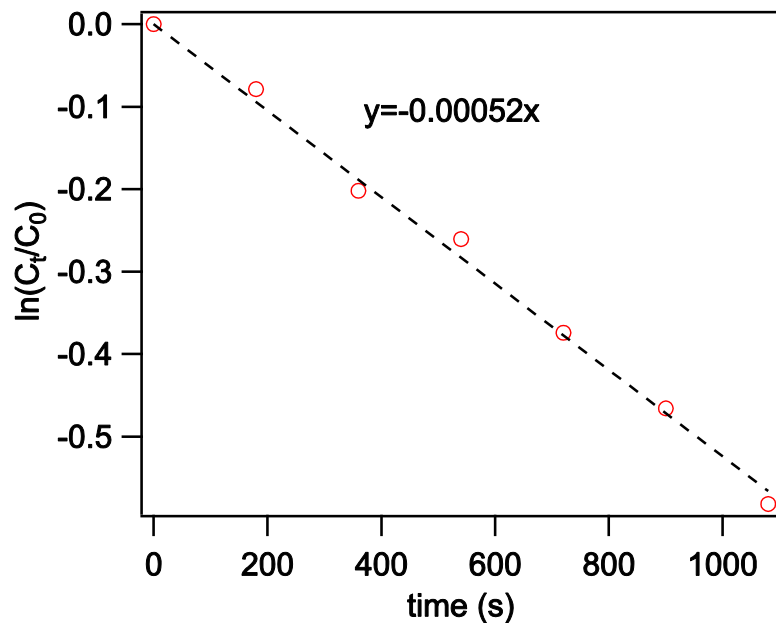


Figure S6. The apparent first-order decay of the PAN compound.

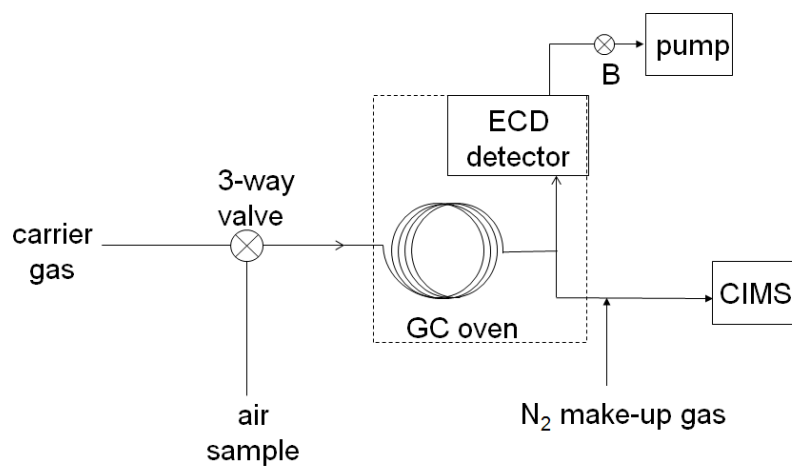


Figure S7. Low pressure GC-ECD/MS configuration.

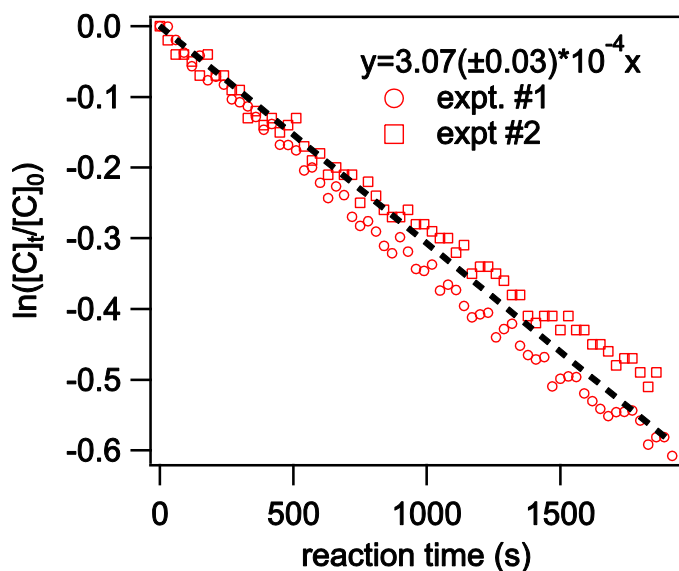


Figure S8. First-order loss rate of the carbonyl nitrate during the OH + carbonyl nitrate experiments.

Table S1. Initial conditions for the chamber experiments.

experiment	expt. #	4,1-carbonyl nitrate (ppb)	propene (ppm)	isopropyl nitrite (ppb)	ozone (ppb)	cyclohexane (ppm)	NO (ppm)
wall loss	1	8.6	100	-	-	-	-
	2	16.9	100	-	-	-	-
	3	20.2	100	-	-	-	-
	4	13.7	100	-	-	-	-
	5	17.8	100	-	-	-	-
photolysis	1	7.2	100	-	-	-	-
	2	13.3	100	-	-	-	-
	3	18.8	100	-	-	-	-
	4	5.8	100	-	-	-	-
	5	15.4	100	-	-	-	-
OH oxidation	1	59.1	1.95	1000	-	-	4.24
	2	12.4	0.64	500	-	-	0.97
	3	19.6	0.57	500	-	-	0.92
	4	11.4	1.62	1000	-	-	1.93
O ₃ oxidation	1	19.2	1.25	-	870	1000	-
	2	22.0	1.46	-	990	1000	-
	3	34.1	1.58	-	1100	1000	-
	4	57.1	1.49	-	1160	1000	-
OH products	1	13.5	-	22	-	-	0.082
	2	17.3	-	31	-	-	0.053

Table S2. The relative CIMS sensitivity to carbonyl nitrates.

	4,1-isoprene carbonyl nitrate	ethanal nitrate	MVK nitrate
	1	9.9	30
low pressure	1	16	34
	1	18	33
low P average	1	15(\pm 4)	32(\pm 2)
	1	13.8	33
lower pressure	1	18.5	40
	1	15	35
lower P average	1	16(\pm 2)	36(\pm 4)
	1	13	35
lowest pressure	1	15	38
	1	13	33
lowest P average	1	14(\pm 1)	35(\pm 3)
all average	1	15(\pm 3)	34(\pm 3)