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Atmospheric Chemistry and Physics Discussions

Supplement of

Hydrolysis and gas-particle partitioning of organic nitrates formed from the oxidation of α-pinene in environmental chamber experiments

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Supplemental

S1. Adjustments to standard ACSM fragmentation table

The ACSM standard fragmentation table was adjusted based on filter measurements taken in each experiment. The portions of the signals at mass-to-charge ratio (*m/z*) 29 and *m/z* 44 that can be attributed to air ($N^{15}N^+$ and CO_2^+ respectively) were found from filter data using their ratios to *m/z* 28 (N_2^+). The ratio of *m/z* 18 (due to gas-phase water) to *m/z* 28 was also found in filter data to account for effects of humidity. The portion of *m/z* 16 attributable to air (O^+) was found and corrected for using the ratio of *m/z* 16 to *m/z* 14 (N^+). The water fragmentation pattern between *m/z* 16 (O^+), *m/z* 17 (OH^+), and *m/z* 18 (H_2O^+) was corrected for using the filter measurement ratios of *m/z* 16 to *m/z* 18 and *m/z* 17 to *m/z* 18. Most ratios were averaged over the course of an experiment and then used in the fragmentation table. In the case of the *m/z* 44/28 ratio, only values before the onset of organic aerosol formation were used as this ratio was found to correlate with OA mass loadings due to the vaporization of low-volatility organics during the filter period. In some cases measured ratios were quite different from the values used in the default fragmentation table, for example the average measured *m/z* 16/18 was 0.35 compared to the default value of 0.04. The portion of *m/z* 28 attributed to organics (CO^+) was set to equal that of organics at *m/z* 44 (CO_2^+). The portion of *m/z* 18 attributed to organics (default to equal *m/z* 44 [CO_2^+] in the standard ACSM fragmentation table) was set to equal 0.79 times the value of organics at *m/z* 44 to minimize correlation between PM water and PM organics in dry experiments (Hildebrandt Ruiz et al., 2014). The values used in the default fragmentation table and the values found in these experiments are shown in Table S1.

Table S1 – Ratios measured from filter data which were implemented to the ACSM fragmentation table.

Expt #	*44/28	29/28	16/14	16/18	17/18	18/28
1	4.39E-04	0.0073	0.475	0.449	0.273	0.082
2	4.35E-04	0.0073	0.473	0.421	0.276	0.091
3	7.65E-04	0.0073	0.447	0.372	0.267	0.091
4	4.51E-04	0.0073	0.427	0.308	0.266	0.105
5	7.62E-04	0.0073	0.425	0.354	0.266	0.092
6	6.79E-04	0.0073	0.414	0.392	0.268	0.085
7	8.84E-04	0.0073	0.408	0.355	0.265	0.092
8	1.53E-03	0.0073	0.380	0.456	0.266	0.062
9	1.91E-03	0.0075	0.461	0.318	0.270	0.094
10	7.38E-04	0.0073	0.456	0.238	0.264	0.117
11	8.06E-04	0.0073	0.523	0.227	0.295	0.139
default	7.34E-04	0.0074	0.353	0.040	0.250	0.010

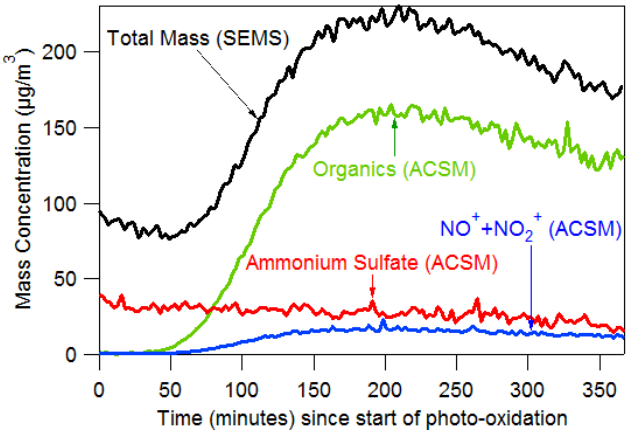

Figure S1– Time series of particulate mass concentrations in Expt. 7.

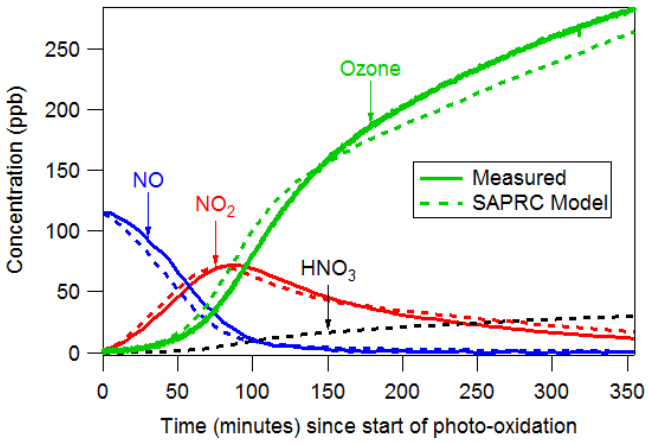

Figure S2 – The SAPRC modeled and the measured data of ozone, NO, NO_2, and the modeled data for HNO_3 (Expt. 7)