

Characterization of Organic Nitrate Formation in Limonene Secondary Organic Aerosol using High-Resolution Chemical Ionization Mass Spectrometry

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Previous work has shown that organic nitrates (RONO_2) are prevalent in the boundary layer, and can contribute significantly to secondary organic aerosol formation. Monoterpenes, including limonene, have been shown to be precursors for the formation of these organic nitrates. Limonene has two double bonds, either of which may be oxidized by NO_3 or O_3 . This leads to the generation of products that can subsequently condense or partition into the particle phase, producing secondary organic aerosol. In order to further elucidate the particle and gas phase product distribution of organic nitrates forming from the reactions of limonene and the nitrate radical (NO_3), a series of experiments were performed in the Gothenburg Flow Reactor for Oxidation Studies at Low Temperatures (G-FROST), described by previous work. N_2O_5 was used as the source for NO_3 and NO_2 , and a characterized diffusion source was used to introduce limonene into the flow reactor. All experiments were conducted in the absence of light, and the concentration of limonene was increased step-wise throughout each experiment to modify the ratio of N_2O_5 to limonene. The experiments were conducted such that both limonene- and N_2O_5 -limited regimes were present.

Gas and particle phase products were measured using an iodide High-Resolution Time-of-Flight Mass Spectrometer (HR-ToF-CIMS) coupled to a Filter Inlet for Gases and AEROsols (FIGAERO, and particle size and SOA mass concentrations were derived using a Scanning Mobility Particle Sizer (SMPS). CIMS measurement techniques have previously been employed for the measurement of organic nitrate products of such compounds using multiple reagent ions. The use of this instrumentation allowed for the identification of chemical formulas for gas and particle phase species. The findings from the experiments will be presented in terms of the relative gas-particle partitioning of major products and the effects of N_2O_5 /limonene ratios on product distributions. Additionally, a comparison of the distribution of the most prevalent reaction products relative to the expected distribution derived using chemical kinetics simulations based on the Master Chemical Mechanism (MCM) limonene mechanism will be discussed.