Seminar Series 2015 - 2016

Southern Ontario Centre for Atmospheric Aerosol Research
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Role of molecular structure in heterogeneous chemistry: Insights from two structural isomers of dimethylsuccinic acid

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A key challenge in understanding the transformation chemistry of organic aerosols is to quantify how changes in molecular structure alter heterogeneous reaction mechanisms. In this talk, we will discuss how the relative locations of branched methyl groups affect the heterogeneous OH oxidation of two structural isomers of dimethylsuccinic acid (DMSA) (2,3-DMSA and 2,2-DMSA). The heterogeneous oxidation experiments are carried out using an aerosol flow tube reactor. The composition of the aerosols before and after oxidation is characterized in real time using a soft atmospheric pressure ionization source (Direct Analysis in Real Time, DART). Kinetic measurements show that the heterogeneous reaction of OH with 2,3-DMSA (reactive OH uptake coefficient, $\gamma = 0.99 \pm 0.16$) is ~2 times faster than that of 2,2-DMSA ($\gamma = 0.41 \pm 0.07$), which can be attributed to the larger stability of the tertiary alkyl radical produced by the initial OH abstraction reaction. Aerosol speciation data reveal that for both isomers, there is a much larger abundance of C6 alcohol relative to C6 ketone functionalization products. This observation cannot be explained by the condensed-phase reactions such as Russell and Bennett-Summer reactions. We propose that the presence of the two branched methyl groups favors alkoxy formation from peroxy radical self-reactions and the functionalization products are likely formed via the intermolecular hydrogen abstraction of the alkoxy radicals. We will discuss the importance of the alkoxy chemistry in the formation of reaction products during the heterogeneous oxidation of these two structural isomers.

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