2-Methyltetrol Sulfate Oxidation by Hydroxyl Radical in Fog and Cloud Water Mimics and Its Implications for the Fate of Isoprene-Derived Secondary Organic Aerosol

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Abstract

2-Methyltetrol sulfate diastereomers (2-MTS) are the single most-abundant SOA tracers in atmospheric fine particulate matter ($PM_{2.5}$). In isoprene-rich regions, multiphase IEPOX chemistry converts inorganic sulfate aerosol to organosulfates such as 2-MTS, making 2-MTS a major constituent of SOA mass. Though 2-MTS is pervasive within SOA, its fate in the atmosphere is still poorly understood. While recent studies have explored its sinks within deliquesced aerosol, 2-MTS has also been observed in cloud water, rainwater, hailstones, and snow, and its sinks within these atmospheric waters is unknown. In a series of controlled batch reactor experiments, we explore the oxidation of 2-MTS in fog and cloud water mimics to determine the second-order rate constant of 2-MTS oxidation against aqueous hydroxyl radicals (•OH). A decrease in 2-MTS concentrations and increase in reaction products were observed using hydrophilic interaction liquid chromatography interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTFOMS). Samples were also analyzed using ion chromatography (IC) to corroborate mass spectrometry measurements of 2-MTS as well as to determine changes to inorganic sulfate concentrations. Results also include an estimated second-order rate constant for both cloud and fog water concentrations of 2-MTS and •OH. as well as proposed reaction products and reaction mechanisms for 2-MTS oxidation. These findings ultimately have implications for the composition, physical properties, and behavior of IEPOX-derived SOA.