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β-Pinene Oxidation Mechanism Investigation using Online Mass Spectrometric Measurements

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The majority of hydrocarbon oxidation mechanisms have been proposed based on experimental knowledge of relatively small species (<C4). Accurate development of these mechanisms and the resulting product distributions is critical in understanding the oxidative state of the atmosphere. Gas phase oxidation processes result in the formation of multiple generations of oxygenated compounds that in many cases contribute to the formation and or growth of secondary organic aerosols. The ability to use mass spectrometry to monitor the gas phase evolution of hydrocarbon oxidation and subsequent product processing has been investigated. Oxidation experiments of β-pinene by hydroxyl radicals have been carried out in the York University Smog Chamber with successful identification of products and their NO_x sensitivities using an atmospheric pressure chemical ionization triple quadrupole mass spectrometer. The chemical composition of these products is varied including hydoxyl, carbonyl and nitrate functional groups in a variety of combinations. Real time acquisition and analysis of the oxidation products under varied NO_x conditions has provided experimental insight into formation pathways. This method shows great promise for providing direct experimental evidence for oxidation mechanism elucidation. Mechanistic implications for several β-pinene oxidation products based on acquired reaction time profiles in different NO_x environments are presented.