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NO_3 radical initiated oxidation products of Δ-3-carene: Characterization and mechanism of formation

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A series of experiments of NO_3 radical initiated oxidation of monoterpenes ($C_{10}H_{16}$) were conducted using an oxidation flow reactor (Go:PAM) combined with an iodide high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS). This study characterized the major organonitrate products from NO_3 radical initiated oxidation of Δ□3-Carene with various levels of oxidation, i.e. by increasing the concentration of NO_3. C_{10} monomers (products with 10 carbons) are generally the dominant products of Δ□3-carene (e.g. $C_{10}H_{15}NO_7$ and $C_{10}H_{17}NO_5$); but where higher oxidant levels enhance fragmentation. In comparison to α-pinene, the Δ□3-carene oxidation has a higher propensity to create low volatile species, i.e. promote aerosol formation, mechanistically explained by difference in alkoxy radical (RO) bond scissions. A kinetic model (using FACSIMILE) was developed to simulate the formation of dominant products. The mechanism was based on analogue systems within the Master Chemical Mechanism (MCM) and recently available literature. The fate of RO_2 under different chemical regimes was also investigated by comparing model runs and the experimental results.