1.222 Determination of composition and chemical structures of α - pinene SOA species .

Early Career Scientist

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Abstract:

The complex organic chemistry of atmospheric aerosols is still unclear. Secondary organic aerosols (SOAs) are formed by atmospheric reactions of primary organic aerosols (POAs) and organic gases (ROGs) with radicals such as O_3, OH, and NO_3. In general, SOAs have higher O/C ratios than POA. α-pinene (C10H16) is a representative biogenic compound of ROGs, accounting for ~45% of the total emissions. In this study, SOA formation experiments were performed using KNU flow reactor. The effect of NH3 on the composition of α-pinene SOA products under ozonolysis and photooxidation was studied. UPLC/Q-TOF MS was used for detailed SOA speciation. An Orbitrap LC-MS / MS system was used to analyze the chemical structure of SOA species. 47mm SOA loaded Teflon filters were extracted using 5 mL of acetonitrile in 20 mL vials followed by sonication at room temperature for 30 minutes. Particulate impurities in the extract were removed using a 0.45 µm syringe filter. The extracted samples were passed through a Waters ACQUITY UPLC high-strength silica (HSS T3) column and analyzed at a temperature of 45 °C. Methanol and water each containing 0.1% acetic acid were used as eluents. The flow rate and injection volume were 0.3 mL min-1 and 1 µL, respectively. Terebic and Pinonic acids were major species found among 54 species. Several other chemical species were also identified by MS/MS. During MS/MS analysis, cleaved structures were H_2O, CO, CO_2, and CH_2CO_2. Furthermore, SOA formation mechanism will be confirmed by the analysis of various other compounds.