2.061 Comprehensive characterization of oxidation of organic compounds in the atmosphere.

Early Career Scientist

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Abstract:

The oxidation of organic compounds in the troposphere is an important process controlling air quality and the formation of climate-active aerosols. These chemical species are diverse and participate in a wide range of reactions. Accordingly, challenges

remain with chemical modeling, detection of later-generation species, and predicting secondary organic aerosol (SOA) formation. In this work, we (1) identify and simplify major chemical pathways that species follow through multiple generations of oxidation, and (2) support how we process and interpret huge mass spectrometric data sets.
The oxidation chemistry of six hydrocarbons + OH (isoprene, a-pinene, toluene, 1,2,4-trimethylbenzene, decane, and 1,4-dimethylcyclohexane) was studied under high-NO conditions in an environmental chamber. Resulting products were detected with a comprehensive analytical suite, including gas chromatography, two optical techniques, four mass spectrometric techniques for measuring gas-phase organics (TD-EIMS, VOCUS 2R PTR, PTR3, and I- CIMS), and three mass spectrometric techniques for measuring particle-phase organics (AMS, CHARON-PTR3, and FIGAERO I- CIMS).
We first determine the extent to which all the product species of VOC oxidation can be detected and quantified, and highlight major gaps in our measurement capabilities. We use several recently-developed techniques to estimate instrument sensitivities to hundreds of compounds for which direct calibration is not possible, and show that this results in reasonable values of total measured carbon. We also examine the data set holistically, without interpreting mass spectra in terms of individual species. We identify the major groups of compounds and their chemical trajectories, and use these to identify overlaps and differences in the chemical space accessed by each instrument.