Atmospheric Nanoparticle Growth from NO$_3$ Radical Initiated Oxidation of Monoterpenes

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OBJECTIVES

I. Implement computational chemistry methods for elucidating reaction pathways and developing CIMS detection strategies

II. Laboratory Experiments:

- Perform chamber and flow tube experiments to characterize gas potentially competitive with bimolecular reactions in diffusion
- Calculate rate constants for intramolecular reactions of NO$_3$ + monoterpene-derived SOA precursors
- Improve understanding of regions of the atmosphere where high SOA yields may dominate

BACKGROUND

Monoterpenes account for about 10% of global emissions and play important SOA precursors (Guenther et al. 1995, JGR).

- In the most prevalent monoterpene emission globally, but other monoterpene emissions are significant and may dominate locally (Guenther et al. 2012, Georger et al. 2003).

Nearly 95% of NO$_3$ emissions in the US come from anthropogenic sources (Möller et al. 2016, JCPA).

- SOA and organonitrates yield from NO$_3$ oxidation of monoterpene precursors (Möller et al. 2014, JCPA).

EARLY RESULTS

- Computational work for this project has so far focused on what conceivable products may form from α-carene + NO$_3$,
- focusing on RO$_2$RO intramolecular H$_2$O loss reactions, and RO$_2$RO addition reactions, and RO$_2$RO decomposition reactions.

- Most intramolecular rate constants calculated from ADFT/B97X-D using LC-TST; relative values not expected to change significantly.

- Intramolecular rate constants estimated from modeled monoterpane chamber concentrations

- No SO$_4$ reagent ions are selective for a specific halogenated organics and cluster with other SOA molecules via H-bonding (Light et al. 2017, JCPA).

- Many closed-shell organics are products identified that have only 1 H-bond donor.

BROADER IMPACTS

Near-peer UCI / Reed College mentoring program

- Several undergraduate research assistants from Reed will be paired with UCI graduate students in "near-peer" mentoring pairs.
- The group of mentor pairs will meet periodically throughout the academic year in organized video conferencing sessions with faculty moderation for discussions of themes related to scientific research and careers, focusing on everything from scientific topics (reading and discussing an article together) to career skills (preparing a cover letter).
- Mentor pairs will be encouraged to engage periodically outside of these organized sessions to informally discuss aspects of the graduate study experience.
- This form of mentoring relationship has been demonstrated to promote belongingness and student retention. It benefits the mentor with teaching opportunities, the ability to share knowledge, and an increased understanding of meeting professional expectations, while mentees find near-peer mentors more relatable than faculty members.

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