Laboratory and field investigation into the gas-phase chemistry of highly oxygenated molecules

PhD Thesis

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About myself

• Master in Applied and Environmental Chemistry
  Milan University

• PhD in Environmental Science
  ETH Zurich
  (Paul Scherrer Institut – CERN)

• Development of Photothermal methods
  FHNW

• PM analytical methods based on FTIR and PLS
  Milan University
Background

**HOMs** (Highly Oxygenated Organic Molecules)

**Autoxidation Mechanism**


**Terpenes as a HOMs source**

Ehn et al., Nature (2014)
Background

CLOUD Experiment

Pure Biogenic Nucleation
Kirkby et al., Nature (2016)

Initial Particle Growth Contribution
Tröstl et al., Nature (2016)

Illustration based on Kulmala et al., Faraday Discuss. (2017)
My PhD Research

I. Formation of highly oxygenated organic molecules from aromatic compounds

II. Formation of Highly Oxygenated Organic Molecules from α-Pinene Ozonolysis: Chemical Characteristics, Mechanism, and Kinetic Model Development
Molteni et al., ACS Earth Space Chem. (2019)

III. HOMs observation at the High Altitude Research Station Jungfraujoch during day- and night-time
Molteni et al., in prep.
I. HOMs from Aromatic Compounds

- ArHC as anthropogenic VOCs
- ArHC Flow Tube Reactor Oxidation (OH)
- HOMs formation extended to anthropogenic VOCs (ArHCs)
- HOMs yields
- Oxidation Mechanism
- ArHC HOMs can undergo to multiple OH attack
- NPF in urban scenarios, low temperature combustion

II. HOMs from α-Pinene Ozonolysis

- CLOUD simulation of boreal forest night-time terpene oxidation and NPF
- Based on ambient relevant VOCs and O$_3$ concentration
- Provides the chemical interpretation of Kirkby et al. and Tröstl et al., Nature (2016)

Molteni et al., ACS Earth Space Chem. (2019)
II. HOMs from α-Pinene Ozonolysis

- Yield increases while O:C decreases with reacted [AP]
- Change in chemical composition among HOMs classes and within each class
- Chemical mechanics for HOMs formation that links oxidation pathway with chemical composition
- HOMs formation mechanism as a MCM extension

Molteni et al., ACS Earth Space Chem. (2019)
II. HOMs from α-Pinene Ozonolysis

- CLOUD chamber was simulated
- Oxidation regime
- Reaction rate constants were derived for:
  - Radical chain termination
    - HOM-RO₂ + RO₂
    - HOM-RO₂
  - Dimer formation
    - HOM-RO₂ + HOM-RO₂

Molteni et al., ACS Earth Space Chem. (2019)
III. HOMs Ambient Observation

- High Altitude Research Stations Jungfraujoch
- 2 months NO$_3$-CIMS dataset
- Winter time
- Free troposphere
- Unit Mass Resolution PMF
- 4 factor solution
- NPF vs non-NPF daily profile

Molteni et al., in prep.
What’s next?

- How to translate lab studies to the real environment
- The impact of real VOCs mixtures on VOCs oxidation mechanisms and SOA formation
- The effect of biotic and abiotic stressors on plant VOC emissions and SOA formation
Thanks for your attention

If you have any question/curiosity about HOMs formation or FTIR PM analysis
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