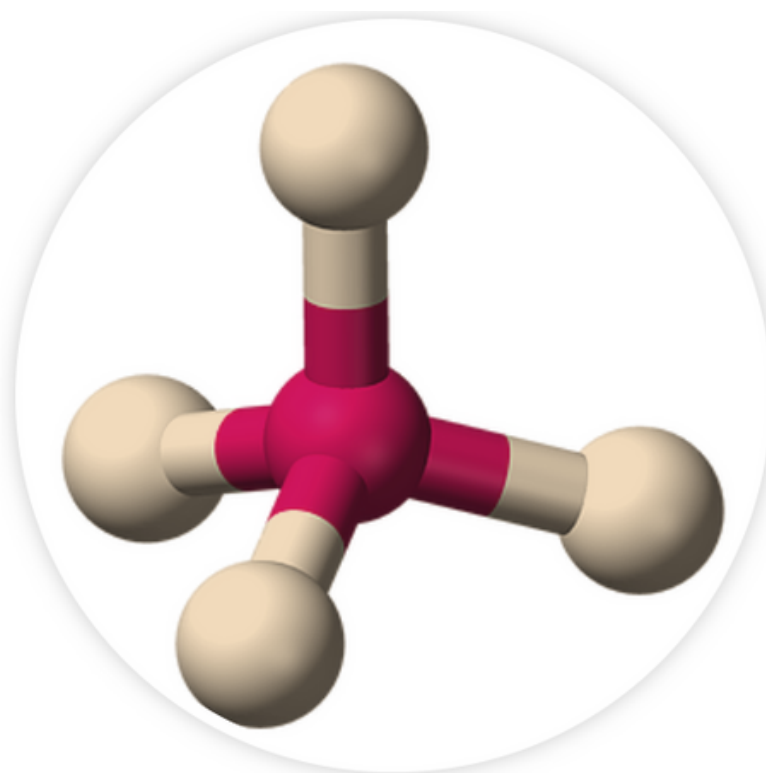


DECEMBER 5-7, 2018

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UC Davis Conference Center



# Atmospheric Chemical Mechanisms Conference

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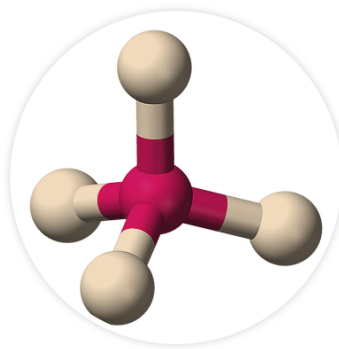
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# ACM 2018

## COMMITTEE

Thank you to our Program Committee for putting in the extra time and effort to recruit specialty presenters and evaluate proposals.

*Alex Archibald, University of Cambridge, Department of Chemistry*

*Marie Camredon, LISA, CNRS/UPEC/UPD*

*Ajith Kaduwela, California Air Resources Board*

*Henrik Kjærgaard, University of Copenhagen, Department of Chemistry*

*Jesse Kroll, MIT*

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*Sasha Madronich, National Center for Atmospheric Research*

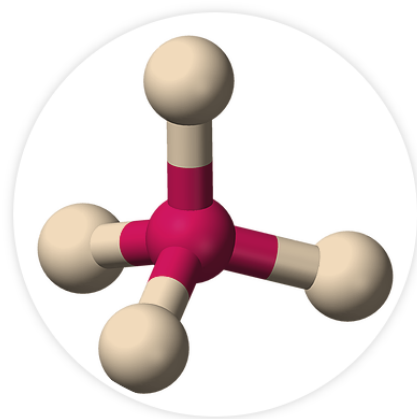
*Thomas Mentel, Jülich's Institute of Energy and Climate Research, Troposphere*

*Tran Nguyen, UC Davis*

*Carl Percival, Jet Propulsion Laboratory, NASA*

*John Wenger, University College Cork, Centre for Research into Atmospheric Chemistry*

*Lisa Whalley, National Center for Atmospheric Science, University of Leeds*



# ACM 2018

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# CONFERENCE PROGRAM

WEDNESDAY, DECEMBER 5, 2018

- 7:00 AM **REGISTRATION AND BREAKFAST** in Conference Center Lobby
- 8:00 AM **OPENING REMARKS**
- 8:10 AM **SESSION: APPLICATIONS & IMPLICATIONS PART 1**  
Hosted by Ajith Kaduwela, *California Air Resources Board*, Deborah Luecken, *EPA*  
Development of Future Atmospheric Chemical Mechanisms for Photochemical Modeling  
Ajith Kaduwela, *California Air Resources Board / Air Quality Research Center, UC Davis*  
Ongoing EPA efforts to evaluate modeled NO<sub>y</sub> budgets  
Heather Simon, *US EPA*  
Characterization of Chemical Mechanisms used in Top-Down VOC Emission Estimates  
Jennifer Kaiser, *Georgia Institute of Technology*
- 9:10 AM **PLENARY SPEAKER: LUCY CARPENTER, UNIVERSITY OF YORK**  
Oceanic Physicochemical Processes Affecting Tropospheric O<sub>3</sub>
- 9:50 AM **BREAK**
- 10:10 AM **SESSION: MECHANISM/SAR DEVELOPMENT**  
Hosted by Alex Archibald, *University of Cambridge*, Marie Camredon, *LISA-CNRS/UPEC/UPD*  
Development, Extension, and Validation of Theory-Based Structure-Activity Relationships (SARs) for Atmospheric Modeling  
Luc Vereecken, *Forschungszentrum Jülich GmbH*  
Structure-Activity Relationships for the Development of MCM/GECKOA Mechanisms  
Bernard Aumont, *LISA*  
Development of Furan Oxidation Mechanism from OH and NO<sub>3</sub> Oxidation Within Biomass-Burning Regimes via Chamber Experiments  
Benjamin Brown-Steiner, *AER*  
Molecular Dynamics Simulations of Sulfuric Acid Cluster Collisions  
Bernhard Reischl, *Institute for Atmospheric and Earth System Research / Physics, University of Helsinki*  
The Impact of the Aldehyde-Hydrogen Shift on the OH Radical Budget in the Isoprene Oxidation Mechanism in Pristine Environments  
Anna Novelli, *Institute of Energy and Climate Research, IEK-8: Troposphere, Forschungszentrum Jülich GmbH, Jülich, Germany*
- 12:10 PM **LUNCH**
- 1:10 PM **SESSION: NEW INSTRUMENTS & ALGORITHMS PART 1**  
Hosted by Thomas Mentel, *Jülich's Institute of Energy & Climate*, Tran Nguyen, *UC Davis*  
Characterizing Cluster Fragmentation in an Atmospheric Pressure Interface Time of Flight (API-ToF) Mass Spectrometer  
Hanna Vehkamäki, *University of Helsinki*  
Quantification of Multifunctional Molecules in Chamber and Ambient Air Using Gas-Chromatography Chemical Ionization Mass Spectrometry (GC-CIMS)  
John Crouse, *Caltech*  
Detection of Novel Organic Nitrogen Compounds with Protonated Ethanol Cluster Chemical Ionization Mass Spectrometry  
Eleanor Browne, *University of Colorado Boulder*  
Free Troposphere Wintertime Gas-Phase Composition Using CI-API-TOF  
Ugo Molteni, *PSI*  
Predicting Instrument Response as a Function of Composition  
David Topping, *University of Manchester*
- 2:50 PM **BREAK**
- 3:10 PM **SESSION: NEW INSTRUMENTS & ALGORITHMS PART 2**  
Bulk vs. Stochastic Kinetics To Describe The Oxidation Of Organic Aerosol Components  
Mark Goldman, *Massachusetts Institute of Technology*  
Understanding The Atmosphere: Graph Clustering Methods For Mechanism Reduction  
Daniel Ellis, *University of York*
- 3:50 PM **SESSION: MINUTE MADNESS POSTERS**
- 4:40 PM **WELCOME RECEPTION AND POSTER VIEWING**
- 7:00 PM **WEDNESDAY CONCLUDES**

# CONFERENCE PROGRAM

THURSDAY, DECEMBER 6, 2018

- 7:00 AM **REGISTRATION AND BREAKFAST** in Conference Center Lobby
- 8:00 AM **CONFERENCE BEGINS**
- 8:10 AM **PLENARY SPEAKER: PAUL ZIEMANN, UNIVERSITY OF COLORADO BOULDER**  
Gas- and Particle-Phase Products and their Mechanisms of Formation from the Reactions of Monoterpenes with NO<sub>3</sub> Radicals: Comprehensive Measurements and Modeling
- 8:50 AM **SESSION: ATMOSPHERIC OXIDATION PART 1**  
Hosted by Sasha Madronich, *National Center for Atmospheric Research*, John Wenger, *University College Cork*  
Structural Dependence of Stabilized CH<sub>2</sub>O Yield in Terminal Alkene Ozonolysis  
Mike Newland, *University of York*  
Direct Measurements of Vinyloxy Radicals And Formaldehyde From Ozonolysis Of Trans- And Cis-2-Butenes: New Insights Into OH Radical Formation And Secondary Chemistry  
Mixtli Campos-Pineda, *University of California, Riverside*  
The Role of Criegee Intermediate + ROOH Reactions Towards Secondary Organic Aerosol Formation Laboratory, Modelling and Field Studies  
Rebecca Caravan, *Sandia National Laboratories*  
Investigation of the Alpha-Pinene & Beta-Pinene Photooxidation by OH in the Atmospheric Simulation Chamber SAPHIR  
Does Water Complexation Affect the Reaction of the β-hydroxyethyl Peroxy Radical with NO?  
Frank Winiberg, *Jet Propulsion Lab/Caltech*
- 10:10 AM **BREAK**
- 10:30 AM **SESSION: ATMOSPHERIC OXIDATION PART 2**  
Developing Reactivity- and Source-Based Monoterpene Parameterizations for Secondary Organic Aerosol Modeling  
Kelley Barsanti, *University of California, Riverside*  
Formation of Highly Oxidized Molecules from NO<sub>3</sub> Radical Oxidation of Δ-3-Carene: A Computational Mechanism  
Danielle Draper, *University of California, Irvine*  
*Investigation of the Alpha-Pinene & Beta-Pinene Photooxidation by OH in the Atmospheric Simulation Chamber SAPHIR*  
Michael Rolletter, *Institute of Energy and Climate Research, IEK-8: Troposphere, Forschungszentrum Jülich GmbH, Jülich, Germany*  
Laboratory Exploration of the Reactions Between Aromatics and OH Using Cavity Ringdown Spectroscopy  
Joseph Messinger, *California Institute of Technology*  
Chlorine-Initiated Oxidation of Hydrocarbons: Mechanistic Insights from Measurements of Gas- and Particle-Phase Composition  
Lea Hildebrandt Ruiz, *The University of Texas at Austin*  
The Atmospheric Chemistry of Nitriles  
Mads Sulbaek Andersen, *California State University, Northridge*
- 12:30 PM **LUNCH**
- 1:30 PM **SESSION: ATMOSPHERIC OXIDATION PART 3**  
Interconnection of Day- and Night Time Chemistry for VOC Degradation and SOA Formation  
Anke Mutzel, *Leibniz Institute for Tropospheric Research*  
Modeling the Absorption Spectra of Phenol and Guaiacol at the Ice-Air Interface  
Fernanda Bononi, *Department of Chemistry, UC Davis*
- 2:20 PM **SESSION: R02 RADICAL CHEMISTRY PART 1**  
Hosted by Henrik Kjærgaard, *University of Copenhagen*, Lisa Whalley, *National Center for Atmospheric Science*  
Formation of Highly Oxidized Multifunctional Compounds in Alkane Autoxidation – Relevance to Atmospheric and Combustion Chemistry  
Mani Sarathy, *KAUST*  
Dependence of Alkyl Nitrate Yields on Structure for Mid-Sized Alkanes  
Geoff Tyndall, *NCAR/ACOM*  
Trends in Peroxy Radical Hydrogen Shift Rate Constants  
Rasmus V. Otkjaer, *Department of Chemistry, University of Copenhagen*
- 3:20 PM **BREAK**
- 3:40 PM **SESSION: R02 RADICAL CHEMISTRY PART 2**  
Isomerization and Decomposition of Isoprene's Delta-(Z)-Hydroxyperoxyl Radicals  
Gabriel da Silva, *University of Melbourne*  
Observational Constraints on the Fate of the Hydroxy Nitrates Produced in the Reaction of Isoprene Peroxy Radicals with NO  
Krystal Vasquez, *California Institute of Technology*  
Unimolecular Peroxy Radical Hydrogen Shift Reactions in Isoprene Oxidation  
Kristian H. Møller, *University of Copenhagen*  
The effect of NO<sub>x</sub> on formation of Highly Oxidized Multifunctional Molecules and SOA formation in photochemical system  
Sungah Kang, *Forschungszentrum Jülich IEK-8*  
Peroxy Radical Autoxidation and Dimer Formation in Alpha-Pinene Oxidation: Constraints from Flow Tubes, Chambers, and the Field  
Joel Thornton, *University of Washington*
- 5:20 PM **THURSDAY CONCLUDES**

# CONFERENCE PROGRAM

FRIDAY, DECEMBER 7, 2018

- 7:00 AM **REGISTRATION AND BREAKFAST** in Conference Center Lobby
- 8:00 AM **CONFERENCE BEGINS**
- 8:10 AM **SESSION: R02 RADICAL CHEMISTRY PART 3**  
Hosted by Henrik Kjaergaard, *University of Copenhagen*, Lisa Whalley, *National Center for Atmospheric Science*  
Accretion Product Formation From Self-And Cross-Reactions of RO2 Radicals in the Atmosphere  
Torsten Berndt, *Leibniz Institute for Tropospheric Research (TROPOS), 04318 Leipzig, Germany*  
Evaluating mechanisms for dimer formation from RO2 + RO2 reactions  
Theo Kurten, *University of Helsinki*  
An inter-comparison of methods for HO2 and CH3O2 detection and kinetic study of the HO2 + CH3O2 cross-reaction in the Highly Instrumented Reactor for Atmospheric Chemistry (HIRAC)  
Lavinia Onel, *University of Leeds*  
Effect of Relative Humidity on the Mechanism of New Particle Formation From Monoterpene Oxidation  
James Smith, *University of California, Irvine*
- 9:30 AM **SESSION: APPLICATIONS & IMPLICATIONS PART 2**  
Hosted by Ajith Kaduwela, *California Air Resources Board*, Deborah Luecken, *EPA*  
GoAMAZON: Exploring the Impacts of a Metropolis on Amazonian Air with an Explicit Organic Chemistry Scheme  
Camille Mouchel-Vallon, *NCAR*  
Impact of Anthropogenic and Natural Emissions on Air Quality in Korea  
Louisa Emmons, *National Center for Atmospheric Research*
- 10:10 AM **BREAK**
- 10:30 AM **SESSION: APPLICATIONS & IMPLICATIONS PART 3**  
Winter Haze in Beijing Driven by Fast Photochemical Smog Reactions  
Keding Lu, *Peking University*  
Source Apportionment of O3 Formation in California using SAPRC11  
Michael Kleeman, *UC Davis*  
Review of the SAPRC-16 Chemical Mechanism and Comparison with the Regional Atmospheric Chemistry Mechanism, Version-2  
William R. Stockwell, *University of Texas at El Paso*  
Science-Based Policy Formation at the California Air Resources Board  
Michael Benjamin, *California Air Resources Board*
- 11:50 AM **FRIDAY CONCLUDES**

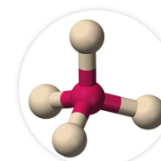
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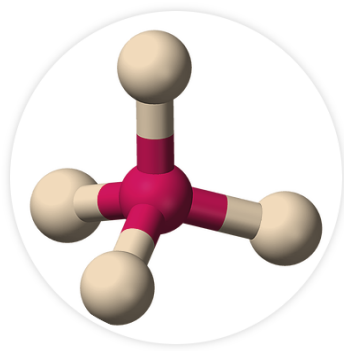


**Atmospheric  
Chemical  
Mechanisms  
Conference**

UC Davis Air Quality Research Center - December 5-7, 2018

# POSTER PRESENTATION DISPLAYS

- Correlating aerosol chemical composition and optical properties using 7-year co-located measurements at the ARM Southern Great Plains (SGP) site  
Ningxin Wang, *UC Davis*
- Kinetics and product yield studies of the HO<sub>2</sub> + CH<sub>3</sub>C(O)O<sub>2</sub> reaction: direct detection of OH by mid-IR spectroscopy  
Aileen Hui, *California Institute of Technology and Jet Propulsion Laboratory, California Institute of Technology*
- Atmospheric chemistry of (Z)-CF<sub>3</sub>CH=CHCl: Cl atom, OH radical and O<sub>3</sub> reactions, and the role of isomerization  
Aleksandra Volkova, *California State University, Northridge*
- Mechanisms for Atmospheric chemistry: Generation, Interpretation and Fidelity - MAGNIFY  
Andrew Rickard Wolfson, *Atmospheric Chemistry Laboratories, Department of Chemistry, University of York*
- Parameter identification of molecular cluster enthalpies and entropies by Monte Carlo method  
Anna Shcherbacheva, *Institute for Atmospheric and Earth System Research/Physics*
- Kinetic and mechanistic investigations of the reactions of trans-2, 3-epoxybutane and cis-2, 3-epoxybutane with Cl atoms and OH radicals  
Carmen Tovar, *Institute for Atmospheric and Environmental Research, University of Wuppertal, 42097 Wuppertal, Germany*
- Modeling of OH, HO<sub>2</sub> and RO<sub>2</sub> reactions in atmospheric pressure flow reactors  
David Hanson, *Augsburg University*
- Does water complexation affect the reaction of the  $\dot{\text{I}}^2$ -hydroxyethylperoxy radical with NO?  
Frank Winiberg, *Jet Propulsion Lab/Caltech*
- Heterogeneous hydrolysis of dinitrogen pentoxide in Beijing during winter haze episode  
Haichao Wang, *Peking University*
- Kinetic investigations of the OH-initiated oxidation of a series of alkylfurans at 298 K and atmospheric pressure  
Iustinian Bejan, *"Alexandru Ioan Cuza" University of Iasi*
- Steady State Continuous Flow Chamber for the Study of Atmospheric Hydrocarbon Oxidation Chemistry under Daytime and Nighttime Conditions – Chamber Characterization and First Results  
John Orlando, *Atmospheric Chemistry Observations and Modeling Laboratory, National Center for Atmospheric Research*
- Oxidation products and aerosol production from NO<sub>3</sub> oxidation of isoprene  
Juliane Fry, *Reed College*
- Kinetic study of the reaction of the simplest Criegee intermediate with ozone  
Lavinia Onel, *University of Leeds*
- A Kinetic Study of the Atmospheric Aqueous-Phase Reactions of OH Radicals with Methoxyphenolic Compounds  
Lin He, *Leibniz Institute for Tropospheric Research*
- "Unimolecular Reactions of Peroxy Radicals Formed in the Oxidation of  $\alpha$ -pinene and  $\beta$ -pinene by Hydroxyl Radical"  
Lu Xu, *California Institute of Technology*
- Speciation and properties of gaseous organic compounds: an explicit modeling of organic species sources and sinks  
Marie Camredon, *LISA, UMR CNRS/INSU*
- Constraining the summertime chemical production of organic acids in forested environments with measurements and modeling  
Michael Link, *Colorado State University, Chemistry Department*
- Low pressure yields of stabilized Criegee intermediates produced from ozonolysis of a series of alkenes  
Mixtli Campos-Pineda, *University of California, Riverside*
- What is required to form stable clusters at atmospheric conditions?  
Nanna Myllys, *UC Irvine*
- Potential Performance differences of the National Air Quality Forecasting Capability when upgrading the Chemical Transport Model  
Pius Lee, *NOAA*
- Trends in Peroxy Radical Hydrogen Shift Rate Constants  
Rasmus V. Otkjær, *Department of Chemistry, University of Copenhagen*
- Exploring the Importance of Horizontal Resolution versus Chemical Resolution in CESM/CAM-chem  
Rebecca Schwantes, *National Center for Atmospheric Research/Atmospheric Chemistry Observations and Modeling Laboratory*
- AtChem, an open source box-model for the Master Chemical Mechanism  
Andrew Rickard, *University of Birmingham/University of Leicester*
- Development of a UV inlet-less Broadband Cavity Enhanced Absorption Spectrometer (BBCEAS) for detection of HCHO, HONO, NO<sub>2</sub> and O<sub>4</sub>  
Ryan Thalman, *Snow College*
- Secondary Organic Aerosol Formation and the Oxidation Mechanism of Methylfuran by Nitrate Radical Oxidation  
Taekyu Joo, *Georgia Institute of Technology*
- A Comprehensive Test of the Recent Proposed HONO Sources in Field Measurements at Rural North China Plain  
Yuhan Liu, *Peking University*
- Experimental budgets of OH, HO<sub>2</sub> and RO<sub>2</sub> radicals and implications for ozone formation in the Pearl River Delta (PRD) in China 2014  
Zhaofeng Tan, *IEK-8: Troposphere, Forschungszentrum Jülich, Jülich, Germany*
- Atmospheric Oxidation of Piperazine Initiated by OH: A Theoretical Kinetics Investigation  
Zhonghua Ren, *Department of Chemical Engineering, The University of Melbourne*
- Heterogeneous Ozonolysis of Endocyclic Organic Aerosol Model Compounds: Chemical Mechanisms and Implication for Criegee Intermediate Dynamics  
Zixu (Tiffany) Zhao, *UC Riverside*
- $\Delta^3$ -carene photooxidation SOA: identifying particle-phase products and the first steps of oxidation  
Emma D'Ambro, *University of Washington, Seattle*
- Carbon-, Oxygen-, and Size- Resolved Model to Simulate the Microphysics, Chemistry, and Thermodynamics of Biomass Burning Organic Aerosol  
Ali Akherati, *Colorado State University*
- Sensitivity of present and future aviation-related air quality impacts to changing background conditions  
Guillaume Chossiere, *Massachusetts Institute of Technology*
- Title: E-waste driven pollution in Pakistan: First evidence of atmospheric exposure to flame retardants (FRs) in Karachi city  
Jabir Syed, *COMSATS University Islamabad*
- Contrasting SOA Formation in Urban and Rural Locations using an Oxidation Flow Reactor  
Rishabh Shah, *Center for Atmospheric Particle Studies, Carnegie Mellon University*
- Product distribution and reaction kinetics of 3-methyl-3-penten-2-one initiated by OH radicals and Cl atoms.  
Investigation of the oxidation of methyl vinyl ketone (MVK) by OH radicals in the atmospheric simulation chamber SAPHIR  
Hendrik Fuchs, *Forschungszentrum Jülich*



# ACM 2018

## Upcoming Events

### **Aviation Noise & Emissions Symposium**

March 3-5, 2019 • Jacksonville, Florida

*For more information: <https://anesymposium.aqrc.ucdavis.edu/>*

### **Meteorology and Climate - Modeling for Air Quality Conference**

September 11-13, 2019 • Davis, California

*For more information: <https://macmaq.sf.ucdavis.edu/>*

### **Refinery And Chemical Industry Emissions Symposium**

November 6-8, 2019 • Davis, California

*For more information: <https://racie.aqrc.ucdavis.edu/>*

### **International Aerosol Modeling Algorithms Conference**

December 4-6, 2019 • Davis, California