

DANIEL A. THOMAS

EDUCATION	California Institute of Technology; Pasadena, CA Ph.D. Chemistry, Advisor: J. L. Beauchamp Dissertation: "Chemical Reaction Dynamics of the Liquid/Vapor Interface Studied by Mass Spectrometry"	2010-2016
	University of North Carolina at Chapel Hill; Chapel Hill, NC B.S. Chemistry, Advisor: Gary L. Glish	2006-2010

PROFESSIONAL EXPERIENCE	Assistant Professor of Chemistry Department of Chemistry, University of Rhode Island <ul style="list-style-type: none">Novel instrumentation for cold spectroscopy of ionsHelium nanodroplet capture of molecular ions and ion clusters stored in an ion trapNew reagents and methods for the characterization of biomolecular ionsInvestigations of interfacial ion chemistry, with application to atmospheric aerosolsSpectroscopic interrogation of reaction intermediates captured in helium nanodroplets Alexander von Humboldt Postdoctoral Fellow Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft Advisors: Gert von Helden and Gerard Meijjer <ul style="list-style-type: none">Infrared spectroscopy of ions trapped in helium nanodropletsStructure and properties of proton-bound dimers, with focus on anharmonicity and nuclear quantum effectsSpectroscopic interrogation of the reactions of the fluorine anion with carbon dioxide and water in the gas phaseVariable-temperature infrared spectroscopy of biomolecular ions for thermochemical studies Postdoctoral Researcher Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft Advisors: Gert von Helden and Gerard Meijjer <ul style="list-style-type: none">Infrared spectroscopy of ions trapped in helium nanodroplets Doctoral Researcher Division of Chemistry and Chemical Engineering, California Institute of Technology Advisor: J. L. Beauchamp <ul style="list-style-type: none">Analysis of chemical processes occurring at the liquid/vapor interface utilizing novel sampling methods coupled with mass spectrometryFundamental studies of reagents for gas-phase free radical sequencing of biomolecules via mass spectrometry	2020-Present 2017-2020 2016-2017 2010-2016
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Undergraduate Researcher

2008-2010

Department of Chemistry, University of North Carolina at Chapel Hill

Advisor: Gary L. Glish

- Investigation of the mechanism of electron capture dissociation mass spectrometry (ECD-MS) in peptides containing histidine residues
- Experimental and theoretical investigation of axial pseudopotentials applied to linear ion traps for improved resolution and sensitivity in quadrupole time-of-flight mass spectrometers

**TEACHING AND
LEARNING****Instructor, CHM 532: Advanced Physical Chemistry**

2022

Department of Chemistry, University of Rhode Island

- Advanced graduate course covering topics including group theory, light-matter interactions, molecular beams, ion spectroscopy, and time-dependent spectroscopy.
- Emphasis on experimental approaches and interpretation of the research literature by applying concepts covered in the course.

Instructor, CHM 507: Graduate Quantum Chemistry

2020-2022

Department of Chemistry, University of Rhode Island

- Graduate course for all incoming chemistry students, overview of quantum chemistry
- Run with a “flipped” classroom model, complete with notes featuring interactive modules and problems based on research applications

Instructor, CHM 642-644: Graduate Research Presentation

2021, 2023

Department of Chemistry, University of Rhode Island

- Series of graduate seminar courses designed to develop research presentation skills

Participant, Strategies and Tools for Teaching Workshop

2020

Office for the Advancement of Teaching and Learning, University of Rhode Island

- Five-day workshop covering best practices in teaching and learning, including course design; inclusive teaching; race, equity, and the learning environment; and effective assessment

Graduate Director, Caltech Project for Effective Teaching

2013-2016

Center for Teaching, Learning, and Outreach, California Institute of Technology

- Administered certificate of interest program and associated seminar and workshop series to encourage graduate students and postdocs to investigate teaching strategies
- Developed and administered new certificate of practice program that guides participants in best practices in STEM teaching
- Served on the planning committee and for the annual Caltech teaching conference; directed sessions on teaching in laboratory courses (2013), microteaching (2014), and office hour sessions (2015)

Teaching Assistant, Physical Chemistry Laboratory

2010-2014

Department of Chemistry, California Institute of Technology

- Experiments administered included microwave spectroscopy, 2D-NMR, ion trap mass spectrometry, low-energy electron diffraction, electron spin resonance, diode laser spectroscopy, and single-molecule spectroscopy

Teaching Assistant, Chemical Equilibrium and Analysis Laboratory

2013

Department of Chemistry, California Institute of Technology

- Taught basic analytical skills including use of volumetric glassware, proper titration procedure, pH meter calibration and utilization, and UV-VIS absorption spectroscopy
- Assisted students in the development of independent projects utilizing standard analytical sample preparation along with HPLC-MS, ICP-MS, GC-MS, and GC-FID systems for sample analysis

Volunteer Tutor, UNC Chemistry Resource Center **2009-2010**
 Department of Chemistry, University of North Carolina at Chapel Hill

**STUDENT
MENTORSHIP**

Graduate Advisor **2020-2023**
 Department of Chemistry, University of Rhode Island

- Serving as advisor to four graduate students as of fall 2022

Undergraduate Research Advisor **2020-2023**
 Department of Chemistry, University of Rhode Island

- Serving as research advisor to three undergraduate students as of spring 2023

Participant, Inclusive Mentoring Workshop **2021**
 University of Rhode Island

- Six-session workshop covering best practices in mentoring, including effective communication, aligning expectations, equity and inclusion, and power and privilege

Undergraduate Research Mentor **2010-2015**
 Department of Chemistry, California Institute of Technology

- Served as mentor to ten summer undergraduate research fellows; facilitated project design and oversaw laboratory research

Participant - Research Mentor Development Series **2015**
 Center for Teaching, Learning, and Outreach, California Institute of Technology

- Attended effective mentoring workshops; topics included knowledge assessment, effective communication, equity and inclusion, and fostering independence

**SCIENCE
OUTREACH**

Afterschool Program with Rhode Island Computer Museum **2023**
 University of Rhode Island

- Collaborated with the Rhode Island Museum of Science and Art (RIMOSA, part of the Rhode Island Computer Museum) to develop activities for local school and YMCA programs.
- Activities were based on current research and included rubber-band guitars to learn about the electromagnetic spectrum, magnet mazes to investigate magnetism, thin film formation to study nanoscale effects, and polarization and color filters to discover light properties.
- Programs were implemented in a pilot phase at a local elementary school.

Community Science Event Volunteer **2015**
 Center for Teaching, Learning, and Outreach, California Institute of Technology

- Community science events highlight the research of a Caltech faculty member and connect this research to in-class activities for K-12 teachers that fulfill criteria in the next-generation science standards
- Prepared demonstrations of a cloud chamber, a homemade spectrophotometer for tablets and smartphones, and a photosynthesis laboratory activity for events focusing on physics, planetary science, and biology, respectively

Community Science Event Volunteer

2015

Center for Teaching, Learning, and Outreach, California Institute of Technology

- Community science events highlight the research of a Caltech faculty member and connect this research to in-class activities for K-12 teachers that fulfill criteria in the next-generation science standards
- Prepared demonstrations of a cloud chamber, a homemade spectrophotometer for tablets and smartphones, and a photosynthesis laboratory activity for events focusing on physics, planetary science, and biology, respectively

High School Science Research Mentor

2013-2015

Department of Chemistry, California Institute of Technology

- Served as mentor to six students from local high schools performing scientific research in the Beauchamp group laboratory, both during the summer and throughout the academic year
- Projects undertaken include novel ionization sources, detection of neurotransmitters, analysis of energy drinks, sunscreen decomposition, and glycan analysis

**RESEARCH
FUNDING**

American Chemical Society Petroleum Research Fund, 65719-DNI6, “Unraveling the Structural Motifs of Deep Eutectic Solvents by Infrared Action Spectroscopy of Ionic Clusters”, \$110,000. 09/01/2022–08/31/2024

National Science Foundation, MPS Division, CHE-2212926, “LEAPS-MPS: Innovative Approaches to the Structural Characterization of Biomolecular Ions by Mass Spectrometry and Infrared Action Spectroscopy”, \$249,990. 09/01/2022–08/31/2024

**HONORS AND
AWARDS**

Alexander von Humboldt Postdoctoral Fellowship, 2017–2020

Graduate Mentoring Excellence Award, University of Rhode Island College of Arts and Sciences, 2022

PUBLICATIONS**Accepted Publications:**

Schultz, M.; Parker, S. L.; Fernando, M. T.; Wellalage, M. M.; **Thomas, D. A.**, Diserinol Isophthalamide: A Novel Reagent for Complexation with Biomolecular Anions in Electrospray Ionization Mass Spectrometry. *J. Am. Soc. Mass Spectrom.* **2023**, *34* (4), 745-753. <https://doi.org/10.1021/jasms.3c00010>

Taccone, M. I.; **Thomas, D. A.**; Ober, K.; Gewinner, S.; Schöllkopf, W.; Meijer, G.; von Helden, G., Infrared action spectroscopy of the deprotonated formic acid trimer, trapped in helium nanodroplets. *Phys. Chem. Chem. Phys.* **2023**, *25* (15), 10907-10916. <https://doi.org/10.1039/D2CP05409D>

Mucha, E.; **Thomas, D.**; Lettow, M.; Meijer, G.; Pagel, K.; von Helden, G., Spectroscopy of Small and Large Biomolecular Ions in Helium-Nanodroplets. In *Molecules in Superfluid Helium Nanodroplets: Spectroscopy, Structure, and Dynamics*, Slenczka, A.; Toennies, J. P., Eds. Springer International Publishing: Cham, **2022**; pp. 241-280. https://doi.org/10.1007/978-3-030-94896-2_6

Thomas, D. A.; Taccone, M.; Ober, K.; Mucha, E.; Meijer, G.; von Helden, G. Helium Nanodroplet Infrared Action Spectroscopy of the Proton-Bound Dimer of Hydrogen Sulfate and Formate: Examining Nuclear Quantum Effects. *J. Phys. Chem. A*, **2021**, *125*, 9279–9287. <https://doi.org/10.1021/acs.jpca.1c05705>

- Greis, K.; Mucha, E.; Lettow, M.; **Thomas, D. A.**; Kirschbaum, C.; Moon, S.; Pardo-Vargas, A.; von Helden, G.; Meijer, G.; Gilmore, K.; Seeberger, P. H.; Pagel, K. The Impact of Leaving Group Anomericity on the Structure of Glycosyl Cations of Protected Galactosides. *ChemPhysChem*, **2020**, *21*, 1905–1907. <https://doi.org/10.1002/cphc.202000473>
- Lettow, M.; Grabarics, M.; Greis, K.; Mucha, E.; **Thomas, D. A.**; Chopra, P.; Boons, G.-J.; Karlsson, R.; Turnbull, J. E.; Meijer, G.; Miller, R. L.; von Helden, G.; Pagel, K. Cryogenic Infrared Spectroscopy Reveals Structural Modularity in the Vibrational Fingerprints of Heparan Sulfate Diastereomers. *Anal. Chem.* **2020**, *92*, 10228–10232. <https://doi.org/10.1021/acs.analchem.0c02048>
- Thomas, D. A.**; Chang, R.; Mucha, E.; Lettow, M.; Greis, K.; Gewinner, S.; Schöllkopf, W.; Meijer, G.; von Helden, G. Probing the Conformational Landscape and Thermochemistry of DNA Dinucleotide Anions *via* Helium Nanodroplet Infrared Action Spectroscopy. *Phys. Chem. Chem. Phys.* **2020**, *22*, 18400–18413. <https://doi.org/10.1039/DoCP02482A>
- Lettow, M.; Grabarics, M.; Mucha, E.; **Thomas, D. A.**; Polewski, L.; Freyse, J.; Rademann, J.; Meijer, G.; von Helden, G.; Pagel, K. IR Action Spectroscopy of Glycosaminoglycan Oligosaccharides. *Anal. Bioanal. Chem.* **2020**, *412*, 533–537. <https://doi.org/10.1007/s00216-019-02327-7>
- Marianski, M.; Mucha, E.; Greis, K.; Moon, S.; Pardo, A.; Kirschbaum, C.; **Thomas, D. A.**; Meijer, G.; von Helden, G.; Gilmore, K.; Seeberger, P. H.; Pagel, K. Remote Participation during Glycosylation Reactions of Galactose Building Blocks: Direct Evidence from Cryogenic Vibrational Spectroscopy. *Angew. Chem., Int. Ed.* **2020**, *59*, 6166–6171. <https://doi.org/10.1002/anie.201916245>
- Fabijanczuk, K.; Gaspar, K.; Desai, N.; Lee, J.; **Thomas, D. A.**; Beauchamp, J. L.; Gao, J. Resin and Magnetic Nanoparticle-Based Free Radical Probes for Glycan Capture, Isolation, and Structural Characterization. *Anal. Chem.* **2019**, *91*, 15837–15396. <https://doi.org/10.1021/acs.analchem.9b01303>
- Thomas, D. A.**; Mucha, E.; Lettow, M.; Meijer, G.; Rossi, M.; von Helden, G. Characterization of a trans–trans Carbonic Acid–Fluoride Complex by Infrared Action Spectroscopy in Helium Nanodroplets. *J. Am. Chem. Soc.* **2019**, *141*, 5815–5823. <http://dx.doi.org/10.1021/jacs.8b13542>
- Lettow, M.; Mucha, E.; Manz, C.; **Thomas, D. A.**; Marianski, M.; Meijer, G.; von Helden, G.; Pagel, K. The Role of the Mobile Proton in Fucose Migration. *Anal. Bioanal. Chem.* **2019**, *411*, 4637–4645. <http://dx.doi.org/10.1007/s00216-019-01657-w>
- Marianski, M.; Seo, J.; Mucha, E.; **Thomas, D. A.**; Jung, S.; Schlögl, R.; Meijer, G.; Trunschke, A.; von Helden, G. Structural Characterization of Molybdenum Oxide Nanoclusters Using Ion Mobility Spectrometry–Mass Spectrometry and Infrared Action Spectroscopy. *J. Phys. Chem. C* **2019**, *123*, 7845–7853. <http://dx.doi.org/10.1021/acs.jpcc.8b06985>
Hans-Joachim Freund and Joachim Sauer Festschrift Issue
- Mucha, E.; Marianski, M.; Xu, F.-F.; **Thomas, D. A.**; Meijer, G.; von Helden, G.; Seeberger, P. H.; Pagel, K. Unraveling the Structure of Glycosyl Cations via Cold-Ion Infrared Spectroscopy. *Nat. Commun.* **2018**, *9*, 4174. <http://dx.doi.org/10.1038/s41467-018-06764-3>
- Thomas, D. A.**; Marianski, M.; Mucha, E.; Meijer, G.; Johnson, M. A.; von Helden, G. Ground-State Structure of the Proton-Bound Formate Dimer by Cold-ion Infrared Action Spectroscopy. *Angew. Chem., Int. Ed.* **2018**, *57*, 10615–10619. <http://dx.doi.org/10.1002/anie.201805436>
- Mucha, E.; Lettow, M.; Marianski, M.; **Thomas, D. A.**; Struwe, W. B.; Harvey, D. J.; Meijer, G.; Seeberger, P. H.; von Helden, G.; Pagel, K. Fucose Migration in Intact Protonated Glycan Ions: A

Universal Phenomenon in Mass Spectrometry. *Angew. Chem., Int. Ed.* **2018**, *57*, 7440–7443. <http://dx.doi.org/10.1002/anie.201801418>

Thomas, D. A.; Mucha, E.; Gewinner, S.; Schöllkopf, W.; Meijer, G.; von Helden, G. Vibrational Spectroscopy of Fluoroformate, FCO_2^- , Trapped in Helium Nanodroplets. *J. Phys. Chem. Lett.* **2018**, *9*, 2305–2310. <http://dx.doi.org/10.1021/acs.jpcclett.8b00664>

Mucha, E.; González Flórez, A. I.; Marianski, M.; **Thomas, D. A.**; Hoffmann, W.; Struwe, W. B.; Hahm, H. S.; Gewinner, S.; Schöllkopf, W.; Seeberger, P. H.; von Helden, G.; Pagel, K. Glycan Fingerprinting via Cold-Ion Infrared Spectroscopy. *Angew. Chem., Int. Ed.* **2017**, *56*, 11248–11251. <http://dx.doi.org/10.1002/anie.201702896>

Thomas, D. A.*; Coggon, M. M.*; Lignell, H.; Schilling, K. A.; Zhang, X.; Schwantes, R. H.; Flagan, R. C.; Seinfeld, J. H.; Beauchamp, J. L. Real-Time Studies of Iron Oxalate-Mediated Oxidation of Glycolaldehyde as a Model for Photochemical Aging of Aqueous Tropospheric Aerosols. *Environ. Sci. Technol.* **2016**, *22*, 12241–12249. <http://dx.doi.org/10.1021/acs.est.6b03588>

*Authors contributed equally

Desai, N.; **Thomas, D. A.**; Lee, J.; Gao, J.; Beauchamp, J. L. Eradicating Mass Spectrometric Glycan Rearrangement by Utilizing Free Radicals. *Chem. Sci.* **2016**, *7*, 5390–5397. <http://dx.doi.org/10.1039/C6SC01371F>

Sohn, C. H.; Gao, J.; **Thomas, D. A.**; Kim, T.-Y.; Goddard III, W. A.; Beauchamp, J. L. Mechanisms and Energetics of Free Radical Initiated Disulfide Bond Cleavage in Model Peptides and Insulin by Mass Spectrometry. *Chem. Sci.*, **2015**, *6*, 4550–4560. <http://dx.doi.org/10.1039/C5SC01305D>

Thomas, D. A.; Wang, L.; Goh, B.; Kim, E. S.; Beauchamp, J. L. Mass Spectrometric Sampling of a Liquid Surface by Nanoliter Droplet Generation from Bursting Bubbles and Focused Acoustic Pulses: Application to Studies of Interfacial Chemistry. *Anal. Chem.* **2015**, *87*, 3336–3344. <http://dx.doi.org/10.1021/ac504494t>

Thomas, D. A.; Sohn, C. H.; Gao, J.; Beauchamp, J. L. Hydrogen Bonding Constrains Free Radical Reaction Dynamics at Serine and Threonine Residues in Peptides. *J. Phys. Chem. A* **2014**, *118*, 8380–8392. <http://dx.doi.org/10.1021/jp501367w>
A. W. Castleman, Jr. Festschrift Issue

Gao, J.; **Thomas, D. A.**; Sohn, C. H.; Beauchamp, J. L. Biomimetic Reagents for the Selective Free Radical and Acid–Base Chemistry of Glycans: Application to Glycan Structure Determination by Mass Spectrometry. *J. Am. Chem. Soc.* **2013**, *135*, 10684–10692. <http://dx.doi.org/10.1021/ja402810t>

Mui, W.; **Thomas, D. A.**; Downard, A. J.; Beauchamp, J. L.; Seinfeld, J. H.; Flagan, R. C. Ion Mobility–Mass Spectrometry with a Radial Opposed Migration Ion and Aerosol Classifier (ROMIAC). *Anal. Chem.* **2013**, *85*, 6319–6326. <http://dx.doi.org/10.1021/ac400580u>

**CONFERENCE
PRESENTATIONS**

New anion microsolvation reagents for the study of biomolecular ions in vacuum. M. Schultz, S. L. Parker, M. T. Fernando, M. M. Wellalage, **D. A. Thomas**. ACS Spring 2023, Indianapolis, IN, 2023. *Invited Oral Presentation*.

Probing the Conformational Landscape and Thermochemistry of Dinucleotide Anions via Helium Nanodroplet Infrared Action Spectroscopy. **D. A. Thomas**, R. Chang, E. Mucha, M. Lettow, K. Greis, G. Meijer, and G. von Helden. International Symposium on Molecular Spectroscopy, Champaign, IL, 2021. *Oral Presentation (Virtual)*.

Characterization of the Intriguing Products of Fluoride–Carbon Dioxide Chemistry by Helium Nanodroplet Infrared Action Spectroscopy. **D. A. Thomas**, E. Mucha, M. Lettow, M. Rossi, G.

- Meijer, and G. von Helden. GRC Conference on Gaseous Ions, Ventura, CA, 2019. *Poster Presentation*.
- Investigating Structure and Thermochemistry of Molecular Ions Using Infrared Action Spectroscopy in He Nanodroplets. **D. A. Thomas**, R. Chang, E. Mucha, G. Meijer, and G. von Helden. GRC Conference on Vibrational Spectroscopy, Biddeford, ME, 2018. *Poster Presentation*.
- Infrared Spectroscopy of Ions Trapped in Helium Nanodroplets: From Baroque Biomolecules to Curious Carboxylates. **D. A. Thomas**, E. Mucha, M. Marianski, S. Gewinner, W. Schöllkopf, G. Meijer, and G. von Helden. Applications of IR Free-Electron Lasers: Latest Developments and Future Directions, Ringberg, Germany, 2018. *Invited Oral Presentation*.
- Vibrational Spectroscopy of Ions Trapped in Helium Nanodroplets: Application to the Analysis of Biomolecules. **D. A. Thomas**, E. Mucha, A. I. González Flórez, K. Pagel, and G. von Helden. Conference on Quantum Fluid Clusters, Innsbruck, Austria, 2017. *Poster Presentation*.
- Exploring Photochemical Oxidation in Liquid Droplets Using Field-Induced Droplet Ionization Mass Spectrometry. **D. A. Thomas** and J. L. Beauchamp, Lake Arrowhead Ion Conference, 2016. *Oral Presentation*.
- A Peer-led Teaching Certificate Program for Post-Graduate STEM Education. **D. A. Thomas**, K. Boyle, and H. Ferguson, POD Network Conference, San Francisco, CA 2015. *Poster Presentation*.
- Finding Sweet Spots in Proteins: Glycan Analysis by Liquid Chromatography Coupled with Gas-Phase Proton-Catalyzed and Free Radical-Initiated Dissociation. **D. A. Thomas**, L. Chen, Jinshan Gao, and J. L. Beauchamp, Lake Arrowhead Ion Conference, 2015. *Poster Presentation*.
- Generating Ions from Droplets without Electric Fields: Mass Spectrometry of Droplets Acoustically Ejected from a Liquid Surface. **D. A. Thomas**, L. Wang, E. S. Kim, and J. L. Beauchamp, Lake Arrowhead Ion Conference, 2014. *Oral Presentation*.
- Studying the Environmental Chemistry of the Liquid/Vapor Interface Using Novel Ionization Techniques Coupled with Mass Spectrometry. **D. A. Thomas**, L. Wang, B. Goh, K. M. Barraza, E. S. Kim, and J. L. Beauchamp, Asilomar Conference on Mass Spectrometry in Environmental Chemistry, Toxicology, and Health, Asilomar, CA, 2013. *Poster Presentation*.
- A Bursting Bubble that Won't Ruin Your 401(k): Sampling the Air-Water Interface with Bursting Bubble Ionization. **D. A. Thomas**, B. Goh, and J. L. Beauchamp, Lake Arrowhead Ion Conference, Lake Arrowhead, CA, 2013. *Oral Presentation*.
- Monitoring the Effect of pH Changes on Chemical and Biological Processes at the Air/Water Interfaces Using Field-Induced Droplet Ionization Mass Spectrometry, **D. A. Thomas** and J. L. Beauchamp, Lake Arrowhead Ion Conference, Lake Arrowhead, CA, 2012. *Oral Presentation*.
- Hydrogen Bonding Constraints Lead to Unusual Free Radical Chemistry at Serine and Threonine Residues in Peptides, **D. A. Thomas**, C. H. Sohn, and J. L. Beauchamp, Lake Arrowhead Ion Conference, Lake Arrowhead, CA, 2011, *Oral Presentation*.
- Study of Radical z Ions Produced by Electron Capture Dissociation (ECD). **Daniel A. Thomas**, N. J. Thompson, T. Baba, and G. L. Glish, American Society for Mass Spectrometry Annual Conference, Salt Lake City, UT, 2010. *Poster Presentation*.
- Probing Electron Capture Dissociation (ECD) Charge Reduced Ions using ECD and Collision-Induced Dissociation (ECD/ECD and ECD/CID). **Daniel A. Thomas**, T. Baba, and G. L. Glish, American Society for Mass Spectrometry Annual Conference, Philadelphia, PA, 2009. *Poster Presentation*.