

DANIEL A. THOMAS

EDUCATION **CALIFORNIA INSTITUTE OF TECHNOLOGY; PASADENA, CA** **2010–2016**

Ph.D. Chemistry, Advisor: J. L. Beauchamp

Dissertation: “Chemical Reaction Dynamics of the Liquid/Vapor Interface Studied by Mass Spectrometry”

UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL; CHAPEL HILL, NC **2006–2010**

B.S. Chemistry, Advisor: Gary L. Glish

PROFESSIONAL EXPERIENCE **ASSISTANT PROFESSOR OF CHEMISTRY** **2020–Present**

Department of Chemistry, University of Rhode Island

- Novel instrumentation for cold spectroscopy of ions
- Helium nanodroplet capture of molecular ions and ion clusters stored in an ion trap
- New reagents and methods for the characterization of biomolecular ions
- Investigations of interfacial ion chemistry, with application to atmospheric aerosols
- Spectroscopic interrogation of reaction intermediates captured in helium nanodroplets

ALEXANDER VON HUMBOLDT POSTDOCTORAL FELLOW **2017–2020**

Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft

Advisors: Gert von Helden and Gerard Meijer

- Infrared spectroscopy of ions trapped in helium nanodroplets
- Structure and properties of model carboxylate dimers, with a focus on vibrational modes of the shared proton
- Spectroscopic interrogation of the reactions of the fluorine anion with carbon dioxide and water in the gas phase
- Variable-temperature infrared spectroscopy of biomolecular ions

POSTDOCTORAL RESEARCHER **2016–2017**

Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft

Advisors: Gert von Helden and Gerard Meijer

- Infrared spectroscopy of ions trapped in helium nanodroplets

DOCTORAL STUDENT **2010–2016**

Division of Chemistry and Chemical Engineering, California Institute of Technology

Advisor: J. L. Beauchamp

- Analysis of chemical processes occurring at the liquid/vapor interface utilizing novel sampling methods coupled with mass spectrometry
- Fundamental studies of reagents for gas-phase free radical sequencing of biomolecules via mass spectrometry

UNDERGRADUATE STUDENT**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
EXPERIENCE****GRADUATE DIRECTOR, CALTECH PROJECT FOR EFFECTIVE TEACHING****2013–2016**

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

- Director of under the advisement of Caltech Center for Teaching, Learning, and Outreach (CTLO)
- 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

- Ran laboratory sessions, office hours, and tutorials for upper-level undergraduate chemistry and physics students
- 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

- Ran laboratory sessions and oversaw independent research projects for upper-level undergraduate chemistry students
- Taught students 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

- Tutored students in first- and second-year undergraduate chemistry courses in one-on-one or small group setting

STUDENT MENTORSHIP	<p>UNDERGRADUATE RESEARCH MENTOR 2010–2015</p> <p>Department of Chemistry, California Institute of Technology</p> <ul style="list-style-type: none"> Served as mentor to ten summer undergraduate research fellows; facilitated project design and oversaw laboratory research <p>PARTICIPANT – RESEARCH MENTOR DEVELOPMENT SERIES 2015</p> <p>Center for Teaching, Learning, and Outreach, California Institute of Technology</p> <ul style="list-style-type: none"> Attended six workshops on effective mentoring of undergraduate researchers; topics included knowledge assessment, effective communication, equity and inclusion, and fostering independence
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SCIENCE OUTREACH	<p>COMMUNITY SCIENCE EVENT VOLUNTEER 2015</p> <p>Center for Teaching, Learning, and Outreach, California Institute of Technology</p> <ul style="list-style-type: none"> 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
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	<p>HIGH SCHOOL SCIENCE RESEARCH MENTOR 2010–2015</p> <p>Department of Chemistry, California Institute of Technology</p> <ul style="list-style-type: none"> 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
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PUBLICATIONS	<p>Accepted Publications:</p> <p>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 Anomerity on the Structure of Glycosyl Cations of Protected Galactosides. <i>ChemPhysChem</i>, 2020, <i>21</i>, 1905–1907. https://doi.org/10.1002/cphc.202000473</p> <p>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. <i>Anal. Chem.</i> 2020, <i>92</i>, 10228–10232. https://doi.org/10.1021/acs.analchem.0c02048</p> <p>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. <i>Phys. Chem. Chem. Phys.</i> 2020, <i>22</i>, 18400–18413. https://doi.org/10.1039/D0CP02482A</p> <p>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. <i>Anal. Bioanal. Chem.</i> 2020, <i>412</i>, 533–537. https://doi.org/10.1007/s00216-019-02327-7</p> <p>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</p>
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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.; Schöllgl, 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/C5SC01305>

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**

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*.