LAURA R. MCCUNN

Department of Chemistry One John Marshall Drive Huntington, WV 25755-2520 (304) 696-2319 mccunn@marshall.edu

EDUCATION

University of Chicago, Chicago, Illinois Ph.D. in Chemistry, December 2005 M.S. in Chemistry, August 2002

Ohio Wesleyan University, Delaware, Ohio B.A. in Biochemistry (ACS certified) with a minor in Mathematics, *summa cum laude* with University Honors, May 2001

PROFESSIONAL EXPERIENCE

Professor, Department of Chemistry, Marshall University, 2021-present Associate Professor, Department of Chemistry, Marshall University, 2014-2021 Assistant Professor, Department of Chemistry, Marshall University, 2008-2014

Postdoctoral Associate, Department of Chemistry, Yale University, February 2006-May 2008 (Dr. Mark A. Johnson, advisor)

Research Assistant, Department of Chemistry and James Franck Institute, University of Chicago, 2001-2005 (Dr. Laurie J. Butler, advisor) Dissertation: *Dissociation dynamics of radical intermediates in bimolecular reactions*

COURSES TAUGHT

CHM 211, Principles of Chemistry I CHM 212, Principles of Chemistry II

CHM 217, Principles of Chemistry Lab I CHM 218, Principles of Chemistry Lab II CHM 307, Introductory Physical Chemistry CHM 357, Physical Chemistry I CHM 358, Physical Chemistry II CHM 480/580, Atmospheric Chemistry CHM 485/585, Brownie, Beer, and Bacon Chem. Fall 2008-10, 2015, 2022, Spring 2021-22 Fall 2013-4, 2017, 2022; Spring 2017-8, 2023 Fall 2008-2009, 2013-6, 2018, 2020-21 Spring 2016-9, Fall 2022 Spring 2009, 2011-3 Fall 2016-8 Fall 2011-2, Spring 2015-6, 2020-22 Fall 2010 Spring 2019

CURRENT RESEARCH INTERESTS

- Matrix-isolation infrared spectroscopy of radicals that occur as intermediates in combustion processes and extraterrestrial environments.
- Identification of the products from gas-phase pyrolysis of organic molecules.
- Molecular photochemistry of matrix-isolated halogenated hydrocarbons.

PUBLICATIONS

- 25. H. N. Legg, K. M. Narkin, L. R. McCunn, C. A. Parish, X. Song "Experimental and Theoretical Study of Oxolan-3-one Thermal Decomposition" *Journal of Physical Chemistry* A, 126, 7084–7093 (2022) DOI: 10.1021/acs.jpca.2c03254
- 24. L. R. McCunn, A. Vasiliou, "Developing an Undergraduate Research Laboratory for Experimental Physical Chemistry" in *Physical Chemistry Research at Undergraduate Institutions*, ACS Symposium Series. (2022) DOI: 10.1021/bk-2022-1429.ch004
- 23. K. A. El-Shazly, E. Sparks, K. Narkin, H. Legg; J. Cardot, M. Hostetler, L. R. McCunn, C. Parish "The signature C=C=O stretch of propenylketenes and ketene clusters" in *Physical Chemistry Research at Undergraduate Institutions*, ACS Symposium Series. (2022) DOI: 10.1021/bk-2022-1428.ch004
- 22. G. J. Brown, M. J. Ellis, T.D. Martin, L. R. McCunn "Vibrational Bands of the 2-Butyn-1-yl Radical." *Journal of Physical Chemistry A* 124, 4081–4086 (2020). DOI: 10.1021/acs.jpca.0c02218
- E.R. Sias, S.L. Cole, B.J. Warner, E.M. Wright, L.R. McCunn "The effect of aldehyde structure on pyrolysis reactions." *Journal of Analytical and Applied Pyrolysis* 123, 340-346 (2017). DOI: 10.1016/j.jaap.2016.11.009
- 20. E. M. Wright, B. J. Warner, H. E. Foreman, L. R. McCunn, K. N. Urness, "Pyrolysis Reactions of 3-Oxetanone." *Journal of Physical Chemistry A* 119, 7966-7972 (2015). DOI: 10.1021/acs.jpca.5b04565
- B. J. Warner, E. M. Wright, H. E. Foreman, C. D. Wellman, L. R. McCunn, "Products from Pyrolysis of Gas-Phase Propionaldehyde. *Journal of Physical Chemistry A* 119, 14-23 (2015).
- C. D. Hatten, K. R. Kaskey, B. J. Warner, E. M. Wright, and L. R. McCunn, "Thermal decomposition products of butyraldehyde." *Journal of Chemical Physics* 139, 214303 (2013).
- 17. B. M. Elliott, L. R. McCunn and M. A. Johnson, "Photoelectron imaging study of vibrationally mediated electron autodetachment in the type I isomer of the water hexamer anion." *Chemical Physics Letters* **467**, 32-36 (2008).
- 16. L. R. McCunn, G. H. Gardenier, T. L. Guasco, B. M. Elliott, J. C. Bopp, R. A. Relph and M. A. Johnson, "Probing isomer interconversion in anionic water clusters using an Ar-mediated pump-probe approach: Combining vibrational predissociation and velocity-map photoelectron imaging spectroscopies." *Journal of Chemical Physics* 128, 234311 (2008).
- 15. L. R. McCunn, J. R. Roscioli, B. M. Elliott, M. A. Johnson and A. B. McCoy, "Why does argon bind to deuterium? Isotope effects and structures of Ar·H₅O₂⁺ complexes." *Journal of Physical Chemistry A* **112**, 6074-6078 (2008).

- L. R. McCunn, J. M. Headrick and M. A. Johnson, "Site-specific addition of D₂O to the (H₂O)₆- "hydrated electron" cluster: Isomer interconversion and substitution at the double Hbond acceptor (AA) electron-binding site." *Physical Chemistry Chemical Physics* 10, 3118-3123 (2008).
- L. R. McCunn, J. R. Roscioli, M. A. Johnson and A. B. McCoy, "An H/D isotopic substitution study of the H₅O₂⁺·Ar vibrational predissociation spectra: Exploring the putative role of Fermi resonances in the bridging proton fundamentals." *Journal of Physical Chemistry B* 112, 321-327 (2008).
- 12. K. R. Asmis, Y. Yang, G. Santambrogio, M. Brümmer, J. R. Roscioli, L. R. McCunn, M. A. Johnson and O. Kühn, "Gas-Phase Infrared Spectroscopy and Multidimensional Quantum Calculations of the Protonated Ammonia Dimer N₂H₇⁺." *Angewandte Chemie International Edition* 46, 8691-8694 (2007).
- M. J. Krisch, M. J. Bell, B. L. FitzPatrick, L. R. McCunn, K.-C. Lau, Y. Liu and L. J. Butler, "Photodissociation Pathways of 1,1-Dichloroacetone." *Journal of Physical Chemistry A* 111, 5968-5980 (2007).
- 10. J. R. Roscioli, L. R. McCunn and M. A. Johnson, "Quantum Structure of the Intermolecular Proton Bond." *Science* **316**, 249-254 (2007).
- 9. L. R. McCunn, B. L. Fitzpatrick, M. J. Krisch, L. J. Butler, C.-W. Liang and J. J. Lin, "Unimolecular dissociation of the propargyl radical intermediate of the CH + C₂H₂ and C + C₂H₃ reactions." *Journal of Chemical Physics* **125**, 133306 (2006).
- L. R. McCunn, K.-C. Lau, M. J. Krisch, L. J. Butler, J.-W. Tsung and J. J. Lin, "Unimolecular Dissociation of the CH₃OCO Radical: An Intermediate in the CH₃O + CO Reaction." *Journal of Physical Chemistry A* 110, 1625-1634 (2006).
- L. R. McCunn, D. I. G. Bennett, L. J. Butler, H. Fan, F. Aguirre and S. T. Pratt, "Photodissociation of Propargyl Chloride at 193 nm." *Journal of Physical Chemistry A* 110, 843-850 (2006).
- L. R. McCunn, M. J. Krisch, Y. Liu, L. J. Butler, and J. Shu, "A Study of the Unimolecular Dissociation of the 2-Buten-2-yl Radical via the 193 nm Photodissociation of 2-Chloro-2butene." *Journal of Physical Chemistry A* 109, 6430-6439 (2005).
- 5. J. L. Miller, L. R. McCunn, M. J. Krisch, L. J. Butler, and J. Shu, "Dissociation of the ground state vinoxy radical and its photolytic precursor chloroacetaldehyde: electronic nonadiabaticity and the suppression of the H + ketene channel." *Journal of Chemical Physics* **121**, 1830-1838 (2004).
- M. J. Krisch, M. C. Reid, L. R. McCunn, L. J. Butler, and J. Shu, "Photofragment translational spectroscopy of nitric acid at 248 nm with VUV photoionization detection of products." *Chemical Physics Letters* 397, 21-25 (2004).

- 3. L. R. McCunn, M. J. Krisch, K. Takematsu, L. J. Butler, and J. Shu, "Competing Pathways in the 248 nm Photodissociation of Propionyl Chloride and the Barrier to Dissociation of the Propionyl Radical." *Journal of Physical Chemistry A* **108**, 7889-7894 (2004).
- M. J. Krisch, L. R. McCunn, K. Takematsu, L. J. Butler, F. R. Blase, and J. Shu, "Photodissociation of CH₃OCl to CH₃O + Cl at 248 nm." *Journal of Physical Chemistry A* 108, 1650-1656 (2004).
- J. J. Gilligan, L. R. McCunn, B. D. Leskiw, Z. Herman, A. W. Castleman, Jr. "Associative ionization of excited sodium species with various ligands: assessing relative bonding strengths of ion-ligand interactions." *International Journal of Mass Spectrometry* 204, 247-253 (2001).

PRESENTATIONS

June 24, 2022, International Symposium on Molecular Spectroscopy, contributed talk: "Pyrolysis reactions of oxolan-3-one studied via matrix-isolation FTIR."

June 2, 2022, DOE Gas Phase Chemical Physics Principal Investigators Meeting, invited talk: "Thermal Decomposition of Cyclic, Oxygenated Hydrocarbons."

May 17, 2022, International Conference on Analytical and Applied Pyrolysis (PYRO 2022), contributed poster: "Pyrolysis mechanisms of cyclopentenones revealed via matrix-isolation FTIR and computations."

November 29, 2021, New College of Florida Natural Sciences Seminar, invited talk: "Vibrational fingerprints of substituted ketenes."

November 11, 2021, Southeastern Regional Meeting of the American Chemical Society, invited talk: "Vibrational fingerprints of substituted ketenes."

August 25, 2021, American Chemical Society Fall National Meeting, invited talk: "Experimental and theoretical study of cyclopentenone pyrolysis."

June 25, 2021, International Symposium on Molecular Spectroscopy, invited talk: "Research with undergraduates: Spectroscopy is just the beginning."

May 29, 2019, DOE Gas Phase Chemical Physics Principal Investigators Meeting, invited talk: "Thermal Decomposition of Cyclic, Oxygenated Hydrocarbons."

April 16, 2019, Argonne National Laboratory, Chemical Science and Engineering Seminar Series, invited talk: "Understanding the Thermal Decomposition of Oxygenated Hydrocarbons Via Pyrolysis and Matrix-Isolation FTIR."

November 1, 2018, University of Georgia Physical Chemistry Group Meeting, invited talk: "Pyrolysis and Spectroscopy at a PUI."

August 22, 2018, American Chemical Society Fall National Meeting, contributed talk: "Pyrolysis and matrix-isolation FTIR spectroscopy for characterization of astrochemically significant radicals."

June 18, 2018, 73nd International Symposium on Molecular Spectroscopy, contributed talk: "Matrix-Isolation FTIR Spectroscopy of the 2-Butyn-1-yl Radical."

June 21, 2017, 72nd International Symposium on Molecular Spectroscopy, contributed talk: "Pyrolysis and Matrix-Isolation FTIR of Acetoin."

June 22, 2016, 71st International Symposium on Molecular Spectroscopy, contributed talk: "Molecular Structure and Reactivity in the Pyrolysis of Aldehydes."

June 26, 2015, 70th International Symposium on Molecular Spectroscopy, contributed talk: "Reactions of 3-Oxetanone at High Temperatures."

June 18, 2013, 68th International Symposium on Molecular Spectroscopy, contributed talk: "Thermal Decomposition Mechanism of Butyraldehyde."

March 13, 2013, West Virginia University Department of Chemistry Seminar: "Unraveling the Mechanisms of Thermal Decomposition in Butyraldehyde."

June 18, 2012, 67th International Symposium on Molecular Spectroscopy, contributed talk: "FTIR of Methyl Pyruvate Conformers in an Argon Matrix."

March 29, 2012, meeting of the Central Ohio Valley Section of the American Chemical Society, invited talk: "Hot and Cold: Matrix-Isolation FTIR of Pyrolytic Products from Organic Compounds"

June 2011, 32nd Annual Combustion Research Meeting sponsored by the Department of Energy, poster: "Characterization of Combustion Radicals Via Matrix-Isolation FTIR"

March 3, 2011, Pat Logan Symposium of Scholars at Marshall University, invited talk: "Matrix-Isolation FTIR Spectroscopy for the Study of Combustion Radicals," and poster: "Photochemistry of Matrix-Isolated Halogenated Hydrocarbons"

March 31, 2009, meeting of the Central Ohio Valley Section of the American Chemical Society, invited talk: "Trapping Transients: Using Matrix-Isolation FTIR to Understand Chemical Processes"

Fall 2007 Science Lecture Series, Ohio Wesleyan University: "Picturing the Photoelectric Effect: Velocity-Map Imaging of Anionic Water Clusters"

2007 Physical Chemistry Student Lecture Series, Ohio State University: "Probing Binding Motifs: Velocity-Map Imaging of Anionic Water Clusters"

2007 Fall ACS Meeting in Boston, MA, contributed talk: "An H/D isotopic substitution study of $H_5O_2^+$ Ar: Exploring Fermi resonances in the bridging proton fundamentals"

2007 Dynamics of Molecular Collisions Meeting in Santa Fe, NM, poster presentation: "An H/D isotopic substitution study of $H_5O_2^+$ ·Ar: Exploring Fermi resonances in the bridging proton fundamentals"

2006 Fall ACS Meeting in San Francisco, CA, contributed talk: "Unimolecular Dissociation of the Propargyl Radical Intermediate of the $CH + C_2H_2$ and $C + C_2H_3$ Reactions"

2006 Gordon Research Conference on Atomic and Molecular Interactions in New London, NH, poster presentation: "Identification and Dynamics of the AA Binding Motif in Water Clusters"

2005 Dynamics of Molecular Collisions Meeting at Asilomar, CA, contributed talk: "Dissociation Dynamics of the Methoxycarbonyl Radical, An Intermediate in the CH₃O + CO Reaction"

2005 Gordon Research Conference on Molecular Energy Transfer in Santa Barbara, CA, poster presentation: "Dissociation Dynamics of the Methoxycarbonyl Radical, An Intermediate in the $CH_3O + CO$ Reaction"

27th International Free Radical Symposium in Taipei, Taiwan, 2004, poster presentation: "Molecular Beam Studies of the Photolysis of 2-Chloro-2-butene and the subsequent dissociation of the 2-Buten-2-yl Radical"

2003 Dynamics of Molecular Collisions Meeting in Lake Tahoe, CA, poster presentation: "Photolysis Channels of Propionyl Chloride and the Barrier to Propionyl Dissociation"

RESEARCH FUNDING

- Department of Energy, 2019-2022
- NASA-WV Space Grant Consortium Research Initiation Grant, 2017-2018
- ACS Petroleum Research Fund Undergraduate Research Grant, 2013-2016
- Research Corporation for Science Advancement Cottrell College Science Award, 2010-2012
- MU-ADVANCE Faculty Fellowship, 2009-2010
- Camille and Henry Dreyfus Foundation Faculty Start-up Award, 2008-2013
- West Virginia HEPC Mini-Grant, 2008

AWARDS

- Outstanding Faculty Advisor, Delta Zeta Sorority Region IV, 2013
- Marshall University Greek Life Faculty Member of the Year, 2010
- Outstanding Poster, Dynamics of Molecular Collisions XXI Conference, 2007
- Yang Prize for Outstanding Thesis in Physical Chemistry, University of Chicago Chemistry Department, 2006
- George Van Dyke Tiers Travel Award, University of Chicago Chemistry Department, 2004
- Sigma Xi Grant in Aid of Research, 2004
- Edith Barnard Award for Service to Others in Chemistry, University of Chicago, 2003
- U.S. Department of Education GAANN Fellowship, 2002-2004
- Nathan Sugarman Teaching Award in General Chemistry, University of Chicago, 2002

- Freud Scholarship, University of Chicago, 2001-2002
- National Science Foundation Graduate Research Fellowship Honorable Mention, 2001
- Hall Fellowship, Ohio Wesleyan University Chemistry Department, 2000-2001
- Ralph V. Sinnett Prize, Ohio Wesleyan University Chemistry Department, 2001
- Julian Higley Prize, Ohio Wesleyan University Chemistry Department, 2000
- Schafer Chemistry Scholarship, Ohio Wesleyan University Chemistry Department, 1999
- Florence Leas Prize in Mathematics, Ohio Wesleyan University Math Department, 1998
- Presidential Scholarship, Ohio Wesleyan University, 1997-2001
- National Merit Scholarship, 1997

AFFILIATIONS

- Alpha Chi Sigma Chemistry Professional Fraternity, 2012-present
- American Chemical Society, 2001-present (member of Division of Physical Chemistry and Subdivision of Astrochemistry)
- Phi Beta Kappa, 2001
- Sigma Xi, Ohio Wesleyan University, 2001
- Chi Gamma Nu Chemistry Honor Society, Ohio Wesleyan University, 2000
- Phi Society Sophomore Honor Society, Ohio Wesleyan University, 1999
- Pi Mu Epsilon Mathematics Honor Society, Ohio Wesleyan University, 1999
- Phi Sigma Biological Sciences Honor Society, Ohio Wesleyan University, 1999
- Phi Eta Sigma Freshman Honor Society, Ohio Wesleyan University, 1998

SERVICE

- *ad hoc* Shared Governance Committee, 2022-present
- College of Science Dean Search Committee, 2022-2023
- International Advisory Committee for the International Symposium on Molecular Spectroscopy, 2018-2022
- Budget and Academic Policy Committee, Marshall University, 2016-present; Secretary, 2017-2018; Chair, 2020-present.
- College of Science Curriculum Committee, Marshall University, 2015-2018; Chair, 2017-18
- Chair, Travel Committee, Marshall University Chemistry Department, 2015-present
- Chair, "Infrared and Raman" session at the 68th International Symposium on Molecular Spectroscopy, Columbus, OH, June 2013
- Officer of the Central Ohio Valley Section of the American Chemical Society Secretary, 2009 Chair-elect, 2010
 - Chair, 2011, 2022 Nominating Committee Chair, 2012, 2023 Outreach coordinator, 2019-present
- Undergraduate Affairs Committee, Marshall University Chemistry Department, 2008-present
- Chemistry Summer Research Program Committee, Marshall University Chemistry Department, 2010-present
- Reynolds Teaching Award Selection Committee, Marshall University, 2010-2013
- *ad hoc* Budget Understanding Committee, Marshall University 2011-2012
- Chair, "Radicals and Ions" session at the 66th International Symposium on Molecular Spectroscopy, Columbus, OH, June 2011
- Chemistry Faculty Search Committee, 2009, 2011, 2012, 2013, 2015, 2016, 2018, 2022, 2023

- Reviewer, Journal of Physical Chemistry, Journal of Chemical Physics, Physical Chemistry Chemical Physics, 2006-present
- Reviewer of chapters in 4 chemistry textbooks for Flat World Knowledge, Inc.; W.H. Freeman & Co.; W. W. Norton & Co. 2010-2013, and Oxford University Press, 2016
- Proposal Reviewer for National Science Foundation, U.S. Department of Energy, Research Corporation for Science Advancement, and ACS Petroleum Research Fund, 2011-present
- Faculty Advisor, Delta Upsilon chapter of Delta Zeta at Marshall University, 2008-present