Matthew R. Siebert

Contact Information

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Research Interests

Currently, my interest is in *ab initio* chemical dynamics simulations, with a desire to use such techniques in the description of interesting and abnormal organic and organometallic reactions.

Education

Texas Tech University

Postodoctoral Research, Chemistry — **January 2010 - Present**

- Advisor: Prof. William L. Hase

University of California - Davis

Ph. D., Chemistry — **Fall 2005 - Fall 2009**

- Dissertation title: "Potential Energy Surfaces and Their Peculiarities in Organic and Organometallic Chemistry."
- Advisor: Prof. Dean J. Tantillo

B. Sc., Chemistry, with High Honors — **Fall 2003 - Spring 2005**

San Joaquin Delta College — **Fall 2001 - Spring 2003**

Awards & Fellowships

Graduate Student Award for the Lindau Meeting of Nobel Laureates **2009**
The annual Lindau Nobel Laureate Meetings provide a globally recognized forum for the transfer of knowledge between generations of scientists. They inspire and motivate Nobel Laureates and international Best Talents. The **59th meeting**, held June 28th to July 3rd, 2009 was dedicated to chemistry.

ACS, Division of Organic Chemistry Fellowship **2008-2009**
The Division of Organic Chemistry annually awards fellowships to outstanding third and fourth year graduate students in organic chemistry. At the time of the award the program had granted over 349 fellowships since the program started in 1981. The applicants for the fellowship submit a short original essay as part of the competition.

UC Davis, Graduate Student Travel Award **2008**

Summer Graduate Student Researcher Award **Summer 2006**
Award to support graduate research in engineering, computer sciences, and disciplines with engineering-related applications and methods.

Professional Associations

American Chemical Society, Member — **2005 - Present**

Academic Positions

University of California - Davis

Guest Instructor (Week 1) - Chem 129B — **Spring 2009**

Instructor - Chem 129A — **Fall 2008**

Teaching Assistant - Chem 233 **Fall 2007**

Teaching Assistant - Chem 118A-C **Fall 2005 - Fall 2006**

San Joaquin Delta College

Tutor **January 2003 - August 2003**

M.E.S.A. Chemistry Tutor **August 2002 - June 2003**

Publications

Siebert, M. R. *J. Org. Chem. SUBMITTED* "Considering the Mechanism of a Rh(I)-Catalyzed C–H Activation/Electrocyclization Cascade Route to 1,2-Dihydropyridines."

Siebert, M. R. and Tantillo, D. J. *J. Phys. Org. Chem. SUBMITTED* "Fundamental Properties of *N*-Alkenylaziridines – Implications for the Design of New Reactions and Organocatalysts."

Siebert, M. R.; Osbourn, J. M.; Brummond, K. M. and Tantillo, D. J. *J. Am. Chem. Soc. SUBMITTED* "Differentiating Mechanistic Possibilities for the Thermal, Intramolecular [2+2] Cycloaddition of Allene-ynes."

Siebert, M. R.; Yudin, A. K. and Tantillo, D. J. *Chem. Eur. J. SUBMITTED* "On the Mechanism of the Rh(I)-Catalyzed Rearrangement of *N*-Allylaziridines to (*Z*)-*N*-Alkenylaziridines."

Gribanova, T. N.; Starikov, A. G.; Minyaev, R. M.; Minkin, V. I.; Siebert, M. R. and Tantillo, D. J. *Chem. Eur. J.*, **2010**, *16*, 2272-2281. "Sandwich Compounds of Transition Metals with Cyclopolyenes and Isolobal Boron Analogues." 10.1012/chem.200902004.

Siebert, M. R. *American Chemical Society, Division of Organic Chemistry Fellowship*, **2008**, Mini-Review: "Knoevenagel/Electrocyclic Ring Closing Cascades as [3+3]-Cycloaddition Analogs." Published on DOC Website.

Siebert, M.R. and Tantillo, D.J. *Organic Letters*, **2008**, *10*, 3219-3222. "[3,3]-Sigmatropic Shifts of *N*-Allylhydrazones: Quantum Chemical Comparisons of Concerted and Radical Cation Pathways." 10.1021/ol801107j.

Siebert, M.R.; Yudin, A.K. and Tantillo, D.J. *Organic Letters*, **2008**, *10*, 57-60. "Cycloaddition/Ring Opening Reaction Sequences of *N*-Alkenyl Aziridines: Influence of the Aziridine Nitrogen on Stereoselectivity." 10.1021/ol702623d.

Siebert, M.R. and Tantillo, D.J. *Journal of the American Chemical Society*, **2007**, *129*, 8686-8687. "Transition State Complexation in Palladium-Promoted [3,3]-Sigmatropic Shifts." 10.1021/ja072159i.

Siebert, M.R. and Tantillo, D.J. *Journal of Physical Organic Chemistry*, **2007**, *20*, 384-394. "Brother vs. Brother: Competitive Stabilization of Carbocationic Centers by Flanking Cyclopropanes and π-Systems." 10.1002/poc.1155.

Siebert, M.R. and Tantillo, D.J. *Journal of Organic Chemistry*, **2006**, *71*, 645-654. "Tetracoordinate Carbon as a Nucleophile? Interconversion of Carbenium Ions Possessing Nearly Square Pyramidal Pentacoordinate Carbons." 10.1021/jo052053a.

Presentations

Matthew R. Siebert and William L. Hase: "Elucidating Enzyme Influence in the Biosynthesis of Abietic Acid Through Post Transition State Dynamics." Poster presented at the *10th European Conference on Atoms, Molecules, and Photons*, Salamanca, Spain, **July 4-9, 2010**.

Matthew R. Siebert: "Biosynthesis of an Abietic Acid Analog: Post-Transition State Dynamics on a Bifurcating Potential Energy Surface." Lecture presented at the *Molecular Simulation Symposium*, Lubbock, TX, **May 20-21, 2010**.

Phillip P. Painter, Matthew R. Siebert and Dean J. Tantillo: "Exploring a Tandem Conjugate Addition/*aza*-Cope Sequence for the Generation of Medium Ring Heterocycles." Poster presented by Phil Painter at the *239th National Meeting of the American Chemical Society*, San Francisco, CA, **March 21-25, 2010**.

Matthew R. Siebert and Dean J. Tantillo: "Quantum Chemical Investigation of Synthetically Useful Rh-Catalyzed Reactions." Poster presented at the *41st National Organic Symposium*, Boulder, CO, **June 7-11, 2009**.

Matthew R. Siebert: "Rh C-H Activation Chemistry for Synthesis of Small Molecules." lecture presented at the *Chemical Biology Innovation Group (CBIG)* meeting, Davis, CA, **April 16, 2009**.

Matthew R. Siebert and Dean J. Tantillo: "Transition State Complexation in the Pd(II)-Catalyzed Cope Rearrangement." lecture presented at the *237th National Meeting of the American Chemical Society*, Salt Lake City, UT, **March 22-26, 2009**.

Matthew R. Siebert and Dean J. Tantillo: "Transition State Complexation: A Case Study in the Pd(II)-Promoted Cope Rearrangement." Poster presented at:

- The *Gordon Research Conference - Organometallics*, Salve Regina University, Newport, RI, **July 6-11, 2008**.
- The *Gordon Research Conference Graduate Student Seminar - Organometallics*, Salve Regina University, Newport, RI, **July 5-6, 2008**.

Matthew R. Siebert, Kay M. Brummond and Dean J. Tantillo: "Theoretical Perspectives on the Thermal (2+2)-Cycloaddition of Allene-ynes." Departmental group exchange lecture presented to the *Jacquelyn Gervay-Hague Group*, Davis, CA, **June 6, 2008**.

Matthew R. Siebert and Dean J. Tantillo: "Theoretical and Experimental Studies on the Pd(II)-Promoted Cope Rearrangement." *Department of Chemistry Student Seminar Series*, Davis, CA, **May 2, 2008**.

Matthew R. Siebert, Andrei K. Yudin and Dean J. Tantillo: "Theoretical Perspectives on Cycloaddition/Ring Opening Reaction Sequences of N-Alkenyl Aziridines." Departmental group exchange lecture presented to the *Mark J. Kurth Group*, Davis, CA, **November 5, 2007**.

Matthew R. Siebert and Dean J. Tantillo: "Palladium(II)-Promoted Cope Rearrangement." Poster presented at:

- The *232nd National Meeting of the American Chemical Society*, San Francisco, CA, **September 10-14, 2006**.
- The *Bradford Borge Weekend*, Davis, CA, **March 2-3, 2007**

- *SYLICCO.07 - Symposium on Learning and Industry Targeting Computational Chemistry Opportunities*, Davis, CA, **July 26, 2007**.

Professional Experience

Texas Tech University

The following topics were investigated in my time at Texas Tech:

- Simulation of photochemical properties of Adenine
- Post transition state and collision dynamics of carbenes and nitrenium ions with water
- Direct dynamics investigation of biosynthesis of abietadiene.

Participation in:

- Partnership in International Research and Education, Santiago de Compostela, Galicia, Spain, **May 30 - July 23, 2010**
- Mesilla chemistry workshop, Mesilla, NM, **February 7-10, 2010**

University of California - Davis

Professional development: Academic Inclusion, Undoing Marginalization on Campus
April 10 & 11, 2009

In addition to those topics that produced reports, the following areas were investigated:

- Computational prediction of ^{1}H and ^{13}C NMR properties.
- Formation of ladderanes.
- Metal-catalyzed *aza*-vinyl cyclopropane to *aza*-cyclopentene rearrangements.
- Rh-Catalyzed Cyclization of Allene-ynes.
- Zwitterionic, Anionic and Cationic *Aza*-Cope Rearrangements.
- (2+2)-Cycloaddition of Allene-ynes.
- Pericyclic Reactions of Heteroaromatic Systems.

Technical Skills

Texas Tech University

Research at Texas Tech university involved:

- Exposure to NWChem, Venus05, Turbomole, Columbus, VMD, Molden, iMol and many other computational chemistry-related programs.

University of California - Davis

Coauthor of Dean J. Tantillo group manual (information compiled for future and junior lab members on topics varying from basic physical organic chemistry topics, to preparation of manuscripts and presentations, to advice for passing departmental requirements, to advanced computing techniques - 172 pages).

Computer administrator for computational chemistry group, which has involved:

- Maintenance of Graduate (78 compute cores, 23 compute sockets), and Undergraduate (28 compute cores, 28 compute sockets) linux based computing clusters including diagnosis and repair of both hardware and software problems.
- Setup and Maintenance of Backup Server including backup protocols for compute clusters and office computers.
- Setup and Maintenance of Cross-Platform File Server.
- Design, Setup and Maintenance of Small Office Network (less than 24 pieces of hardware).
- Adaptation of Linux operating environment of visually impaired.

- Exposure to:
  i. Operating Systems: Mac, PC and linux systems, including Red Hat, Fedora and Ubuntu.
  ii. Server Administration Highlights: PBS and Torque queueing systems were personally implemented, BackupPC installed and configured for Backup Server, and setup of RAID 0, 1 and 5 on various systems.
  iii. Computational Chemistry Software: GAUSSIAN03, GaussView, ACES2, ADF, Ball&Stick and Babel.
  iv. Scripting/Production Software: Shell Scripting and LaTex.
  v. Various End-User Software for PC and Mac environments, including Microsoft Excel, Word and PowerPoint, Apple Keynote and Adobe Photoshop and Illustrator.