

Vincent F. DeTuri

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Professional

Chair, Department of Chemistry, Ithaca College, June 2003 to May 2006
Assistant Professor, Ithaca College, August 2001
Visiting Assistant Professor, Ithaca College, July 1999 to August 2001

Education

University of Nevada, Reno, Ph.D. in Chemical Physics, August 1999
University of San Diego, B.A. in Chemistry, May 1994

Journal Publications (undergrads are in bold)

- "Structural, energetic, and infrared spectra insights into methanol clusters $(\text{CH}_3\text{OH})_n$, for $n = 2-12, 16, 20$. ONIOM as an efficient method of modeling large methanol clusters" **Marcos M. Pires** and Vincent F. DeTuri, *J. Chem. Theory and Comput.*, in review.
- "Comparison of Gas Phase Acidities of some Carbon Acids with their Rates of Hydron Exchange in Methanolic Methoxide" Vincent F. DeTuri, Heinz F. Koch, Judith G. Koch, Gerrit Lodder, Masaaki Mishima, Han Zuilhof, **Neal M. Abrams**, Cecily E. Anders, Justin Biffinger, Patrick Han, **Adam R. Kurland**, **Jason M. Nichols**, **Anne M. Ruminski**, Patricia R. Smith, and **Karen Vasey**, *J. Phys. Org. Chem.*, **19**, 308-317 (2006).
- "Anchoring the gas-phase acidity scale", K. M. Ervin, V. F. DeTuri, *J. Phys. Chem. A*, **106**, 9947-9956 (2002).
- "Energetics of endoergic proton transfer reactions of anions", V. F. DeTuri and K. M. Ervin, *J. Phys. Chem. A*, accepted then withdrawn, 2001.
- "Competitive threshold collision-induced dissociation: Gas phase acidities and bond dissociation energies for a series of alcohols", V. F. DeTuri and K. M. Ervin, *J. Phys. Chem. A* **103**, 6911-6920 (1999).
- "Dynamics of endoergic bimolecular proton transfer reactions for a series of alcohols. $\text{F}^- + \text{ROH} \rightarrow \text{HF} + \text{RO}^-$ (R = H, CH_3 , CH_3CH_2 , $(\text{CH}_3)_2\text{CH}$, or $(\text{CH}_3)_3\text{C}$).", V. F. DeTuri, **M. A. Su**, and K. M. Ervin, *J. Phys. Chem. A* **103**, 1468-1479 (1999).
- "Proton transfer between Cl^- and $\text{C}_6\text{H}_5\text{OH}$. OH bond energy of phenol", V. F. DeTuri and K. M. Ervin, *Int. J. Mass Spectrom. Ion Proc.* **175**, 123-132 (1998).
- "Translational activation of the $\text{S}_{\text{N}}2$ nucleophilic displacement reactions $\text{Cl}^- + \text{CH}_3\text{Cl}(\text{CD}_3\text{Cl}) \rightarrow \text{ClCH}_3(\text{ClCD}_3) + \text{Cl}^-$: A guided ion beam study", V. F. DeTuri, P. A. Hintz, and K. M. Ervin, *J. Phys. Chem. A* **101**, 5969-5986 (1997).

Grants and Awards

- Summer Grant for Faculty Research (internal), 2005
Collision-induced Dissociation of Methoxide Methanol Clusters
Applied February 15, 2005 *Awarded* \$3,350
- Summer Grant for Faculty Research (internal), 2003
Energetics of proton transfer reactions
Applied February 15, 2003 *Awarded* \$3,350
- Sun Microsystems Education Matching Grant, 2002
Matching grant with the purchase of a Sun Microsystem as part of student research
Applied September 12, 2002 *Awarded* \$16,392
- Dreyfus Supplemental Awards under the Scholar/Fellow Program, 2002
Energetics of proton transfer reactions
Applied September 27, 2001 *Awarded* \$10,000
- ACS Project SEED Summer I Program, 2001
Nucleophilic reactions of fluoroalkenes
Applied January 30, 2001 *Awarded* \$800 (for one student)

Teaching Experience

- CHEM-10100 Chemistry and Your Body (Spring 2007)
- CHEM-11300 Chemistry Lab for Physical Therapy Majors (Fall 2001)
- CHEM-12100 Principles of Chemistry (Fall 2004, Fall 2005)
- CHEM-12100 Principles of Chemistry: Recitation (Fall 2001)
- CHEM-12200 Principles of Chemistry (Spring 2002-2003)
- CHEM-12400 Experimental Chemistry I (Spring 2002-2003)
- CHEM-18100 Selected Topics in Chemistry (Fall 2003)
- CHEM-33100 Physical Chemistry 1 (Fall 1999-2002)
- CHEM-33200 Physical Chemistry 2 (Spring 2003-2007)
- CHEM-32600 Experimental Chemistry V (Fall 2002-03, 2006)
- CHEM-44200 Computational Chemistry (Spring 2000&02, Fall 2006)
- CHEM-45200 Instrumental Analysis (Spring 2001)
- CHEM-48700 Chemistry Seminar (Fall 2005)
- Curriculum development for Organic Laboratory (Fall 1999, Spring 2002)
- Honors Senior Thesis advisor for Joseph Livingston (B.S. December 2006)
Proton Mobility in Methoxide Methanol Clusters
- Honors Senior Thesis advisor for Matthew Sprague (B.S. May 2005)
Energetic and Geometric Insights of Methoxide in Methanol $CH_3O^-(CH_3OH)_n$, for n = 1-21
- Honors Senior Thesis advisor for Jordan Killeen (B.S. May 2003)
Solution Effects on the Proton Bound Species $[CCl_3 \cdot H \cdot OCH_3]^-$ in Methanol by Ab Initio and Density Functional Techniques
- Honors Senior Thesis advisor for Marcos Pires (B.S. May 2003)
Structural, Energetic, Infrared Spectra Insights Into Methanol Cluster $(CH_3OH)_n$, for n = 2-16. ONIOM as an Efficient Method of Modeling Large Methanol Clusters.
- Honors Senior Thesis advisor for Jason Nichols (B.S. May 2000)
Molecular Orbital Calculations on Highly Fluorinated Systems

Recent Invited Seminars at Academic Institutions

"Molecular recognition by *ab initio* methods: valinomycin–alkali ion (Li^+ , Na^+ , K^+) complexes", Chemistry Department, St. Mary's College of Maryland, St. Mary's City, Maryland, April 2, 2003.

"Proton transfer between carbon acids and methoxide by gas phase and by microsolvation methods", Department of Chemistry, University of Rochester, Rochester, New York, September 17, 2001.

Recent Papers Presented at Conferences (presenting author underlined, undergrads are in bold)

"Geometries and Energetics of Valinomycin Alkali ion complexes", Vincent DeTuri, **Semeret Munie**, and **Elvis Shehi**, 34th ACS Northeast Regional Meeting, Binghamton, New York, October 2006.

"Proton transfer between methoxide and methanol in methanol", **Joseph G. Livingston** and Vincent F. DeTuri, 34th ACS Northeast Regional Meeting, Binghamton, New York, October 2006.

"Proton Transfer between Chloroform and Methoxide in Methanol: A Microsolvation study of Carbanion formation in a Protic Solvent", **Daniel Cordaro**, **Jordan Killeen**, and Vincent F. DeTuri, 34th ACS Northeast Regional Meeting, Binghamton, New York, October 2006.

"Geometries and Energetics of Valinomycin Alkali Ion Complexes", **Semeret Munie**, **Elvis Shehi**, and Vincent F. DeTuri, 5th Annual MERCURY Conference on Undergraduate Computational Chemistry, July 2006.

"Proton transfer between carbon acids and methanolic sodium methoxide, kinetics and calculations", **Heinz F. Koch**, Vincent F. DeTuri, 17th International Symposium on Fluorine Chemistry, Shanghai, China, July 24-29, 2005.

"Proton transfer between chloroform and methoxide in methanol solvent", (poster) **Vincent F. DeTuri**, 229th ACS National Meeting, San Diego, CA, March 13-17, 2005.

"Energetic and geometric insights of methoxide in methanol $\text{CH}_3\text{O}^-(\text{CH}_3\text{OH})_n$, for $n = 1-21$ ", (poster) Vincent F. DeTuri and **Matthew K. Sprague**, 229th ACS National Meeting, San Diego, CA, March 13-17, 2005.

"Investigation of proton transfer between carbon acids and methoxide by density functional calculations", **Heinz F. Koch** and Vincent F. DeTuri, 17th IUPAC Conference on Physical Organic Chemistry, Shanghai, China, August 15-20, 2004.

"Comparison of the partitioning of highly pi-delocalized carbanion intermediates to more localized carbanion intermediates", **Heinz F. Koch** and Vincent F. DeTuri, The Heron Island Conference on Reactive Intermediates and Unusual Molecules, Queensland, Australia, July 17-23, 2004.

"Solution effects on the proton bound species $[\text{CCl}_3\bullet\text{H}\bullet\text{OCH}_3]^-$ in methanol by *ab initio* and density functional techniques", (poster) Vincent F. DeTuri and **Jordan Killeen**, 225th National Meeting of the American Chemical Society, New Orleans, LA, March 23-27, 2003.

"Energetic and geometric insights into methanol clusters (CH₃OH)_n, for n = 2-20", (poster)
Vincent F. DeTuri and **Marcos M. Pires**, 225th National Meeting of the American Chemical Society, New Orleans, LA, March 23-27, 2003.

"Investigations of alkoxide-promoted dehydrohalogenations by kinetic studies and molecular orbital calculations", Vincent F. DeTuri and Heinz F. Koch, 16th IUPAC Conference on Physical Organic Chemistry, University of California, San Diego (UCSD), La Jolla, California, August 4-9, 2002.

"Density functional calculations on proton transfer between carbon acids and methoxide", Heinz F. Koch and Vincent F. DeTuri, Gordon Research Conference on: Isotopes in Biological and Chemical Sciences, Ventura, California, February 17-22, 2002.

Recent Seminars and Colloquia (Student Presentations are in Bold)

"Proton transfer reaction path calculations in a chloroform-methoxide/methanol system", **Daniel Cordaro**, James J. Whalen Academic Symposium, Ithaca College, April 6, 2005.

"Computational investigations of resonance stabilization for a texaphyrin-like macrocycle", **Zachary Bogusz**, James J. Whalen Academic Symposium, Ithaca College, March 22, 2004.

"Molecular recognition by ab initio methods: valinomycin-alkali ion (Li⁺, Na⁺, K⁺) complexes", Seminar for local High School chemistry teachers, Ithaca College, March 2, 2004.

"Energetics of the proton transfer reaction between chloroform and methoxide", **Jordan Killeen**, James J. Whalen Academic Symposium, Ithaca College, March 26, 2002.

Memberships

American Chemical Society (ACS)

Division of Physical Chemistry

Middle Atlantic Association of Liberal Arts Chemistry Teacher (MAALACT)

Molecular Computation and Visualization in Undergraduate Education (MoleCVUE)