

Marion E. Cass
Department of Chemistry
Carleton College
Northfield, MN 55057

Current Position

Professor of Chemistry, Carleton College

Chair of the Chemistry Department, July 1, 1998- July 1, 2002

Associate Professor (May 1993 - July 2000), Assistant Professor (Sept 1987 - May 1993)

Previous Positions

Visiting Scholar (while on Leave from Carleton) at the Department of Chemistry, Dartmouth College

With Professor Dean Wilcox study concepts in bioinorganic chemistry and developing animations and visualizations of metalloproteins to facilitate understanding. (Intermittent terms: Fall 2013 through the present)

Visiting Professor (while on Leave from Carleton) at the Department of Chemistry, Imperial College London

With Professor Henry Rzepa learning techniques in computational chemistry and developing animations for the visualization of molecular processes and symmetry operations. (May 2004 – August 2005, Dec 2005, Nov –Dec 2006)

Visiting Associate Professor (while on Leave from Carleton) at the University of New South Wales

With Professor Gary Willett learning techniques in Electrospray Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (October 23, 2003 – March 18, 2004)

Visiting Research Associate, California Institute of Technology

carrying out research with Professor Nate Lewis and Dr. Stephen Doig on the fundamental study of the photochemistry of dye-sensitized solar cells. (October 1994 - June 1996)

Participant in the Caltech Animation Project for "Visualization of the Chemical World"

December 1989 and December of 1988: Visiting researcher at the University of California, Berkeley

examining Fe(III) transport in *E. coli*, and inhibition of the Fe(III) transport by Ti(IV) complexes.

American Cancer Society Postdoctoral Fellow within the group of Professor Kenneth N. Raymond,

University of California, Berkeley (June 1984 - August 1987)

Education

Ph. D. in Chemistry, (May 1984) University of Colorado, Boulder, Colorado 80309

Dissertation Research under the guidance of Professor C. G. Pierpont

Dissertation Title: "Ligand Activity in the Reduction of Substrate Molecules by Vanadium and Molybdenum Complexes of the 1,2-Benzoquinones"

Bachelor of Science, *summa cum laude*, Fort Lewis College, Durango Colorado, 81301, (April 1979)

Web site: <http://www.people.carleton.edu/~mcass/>

Courses Taught at Carleton College (Courses of Focus since 2005 in bold)

Concepts of Chemistry (Chemistry for non-science majors)

Introduction to Chemistry

Principles of Chemistry

Energy Consumption and Production

Advanced Inorganic Chemistry

Advanced Laboratory Courses :

Advanced Laboratory in Quantum Spectroscopy

Advanced Laboratory in Chemical Kinetics

Chemical Characterization of Compounds

Advanced Laboratory in Inorganic Chemistry

Scientific Glassblowing
Molecular Orbital Theory
Senior Comprehensive Exercise

Independent Studies: Computations on Fluxional Molecular Processes, Synthesis of a New Ligand for Metal Ion Complexation

Publications:

“Are these Molecules Jahn-Teller Distorted: A Problem Set” | VIPeR; Cass, M. E.: <https://www.ionicviper.org/problem-set/are-these-molecules-jahn-teller-distorted> (accessed Feb 2017) published Jan 2016.

“Molecular Hydrogen Complexes of W and Mo: Literature Discussion” | VIPeR; Grice, K., Landeros, F.B.; Cass, M. E.; <https://www.ionicviper.org/literature-discussion/molecular-hydrogen-complexes-mo-and-w> (accessed Jan 2017), published Nov 2016

“Ligands that Favor/Force Tetrahedral Geometry, 5 Slides About” | VIPeR; Cass, M. E., Stevenson, M.J., Croteau, M.; <https://www.ionicviper.org/five-slides-about/ligands-favorforce-tetrahedral-geometry> (accessed June 2016), published March 16, 2016.

“Electronic Spectroscopy of Copper Complexes: A Bio-Inorganic Application; A Problem Set” | VIPeR; Cass, M. E., Stevenson, M.J., Croteau, M.; <https://www.ionicviper.org/problem-set/electronic-spectroscopy-copper-complexes-bioinorganic-application> (accessed June 2016), published June 17, 2016.

“A Demonstration to Segue Between d to d and CT Transitions, In Class Activity” | VIPeR; Cass, M. E.; <https://www.ionicviper.org/class-activity/demonstration-segue-between-d-d-and-ct-transitions> (accessed June 2016), published March 3, 2016.

“Structural and Spectroscopic Ramifications of 1 electron oxidation in CpMn(CO)₃, A Problem Set Based on a Literature Example | VIPeR”, Cass, M. E., <https://www.ionicviper.org/problem-set/structural-and-spectroscopic-ramifications-1-electron-oxidation-cpmnco3-problem-set> (accessed June 2015), published March 4, 2015

“Improved Syntheses and Expanded Analyses of the Enantiomerically Enriched Chiral Cobalt Complexes Co(en)₃I₃ and Co(diNOsar)Br₃”, McClellan, M. J., and Cass, M. E., *J. Chem. Educ.*, 92, 2015, p 1766-1770.
Publication Date (Web): July 24, 2015 (Communication), DOI: 10.1021/acs.jchemed.5b00140

“Computational Exercise to Determine the Relative Energies of the Four Ligand Twist Conformers of [Co(en)₃]³⁺ | VIPeR”, Cass, M. E., McClellan, M. J.; <https://www.ionicviper.org/problem-set/computational-exercise-determine-relative-energies-four-ligand-twist-conformers-coen33> (accessed June 2015) published February 20, 2015.

“Utilizing the PDB and HSAB theory to understand metal specificity in trafficking proteins | VIPeR”, Gunn E., Grice, K., Rossiter, C., Habgood, L. G., Cass, M. E., Madrahimov, S.; <https://www.ionicviper.org/class-activity/utilizing-pdb-and-hsab-theory-understand-metal-specificity-trafficking-proteins> (accessed June 2015), published July 17, 2014

“Literature Discussion of “Mechanisms Controlling the Cellular Metal Economy” | VIPeR”, Grice, K., Rossiter, C., Gunn E., Habgood, L. G., Cass, M. E., Madrahimov, S.; <https://www.ionicviper.org/literature-discussion/literature-discussion-mechanisms-controlling-cellular-metal-economy> (accessed June 2015), published July 17, 2014

“An end of term problem set based on the literature paper. “A Diamagnetic Ditungsten(III) Paddlewheel Complex with No Direct Metal-Metal Bond” | VIPeR”, Cass, M. E., <https://www.ionicviper.org/problem-set/end-term-problem-set-based-literature-paper-%E2%80%9C-diamagnetic-ditungsteniii-paddlewheel>, (accessed June 2015), published July 16, 2014

“A Review of 3DMolSym: A Web Resource for Teaching Molecular Symmetry | VIPeR”, Cass, M. E.; <https://www.ionicviper.org/web-resources-and-apps/review-3dmolsym-web-resource-teaching-molecular-symmetry> (accessed June 2015), Published May 23, 2014

“The Structure and Symmetry of Metal Tris Chelates | VIPeR”, Cass, M. E.; <https://www.ionicviper.org/web-resources-and-apps/structure-and-symmetry-metal-tris-chelates> (accessed June 2015), published May 23, 2014

“Viewing Jmol Images and Animations (currently blocked) that call a Jmol Applet | VIPeR”, Cass, M. E.; <https://www.ionicviper.org/web-resources-and-apps/viewing-jmol-images-and-animations-currently-blocked-call-jmol-applet> (accessed June 2015), published March 13, 2014

"A Computational Study on Ligand Imposed Preferences for the Bailar vs Rây-Dutt Twists in GaL₃ Complexes", Cass, M. E., Rzepa, H. S. Manuscript under revision.

"Student-Directed Explorations to teach about ligands| VIPeR", Cass, M. E.; <https://www.ionicvipr.org/class-activity/student-directed-explorations-teach-about-ligands> (accessed June 2015), published June 25, 2011.

"Visualizations to Examine the Structure and Symmetry of Metal Tris Chelates: Symmetry Operations, Chirality, and Mechanisms (Bailar Twist and Ray-Dutt) that Racemize the Δ and Λ Isomers", Cass, M. E., Rzepa, H. S.; Journal of Chemical Education, Vol 85, No. 5, **2008**, p. 750-751. The animations can be accessed on the JCE-Online Website.

"In Search of The Bailar Twist and Rây-Dutt Mechanisms that Racemize Chiral Tris-Chelates: A Computational Study of Sc(III), Ti(IV), Co(III), Zn(II), Ga(III) and Ge(IV) Complexes of a Ligand Analog of Acetylacetonate", Rzepa, H. S., Cass, M. E.; Inorganic Chemistry, **2007**, Vol 46, No. 19, pages 8024-8031.

"A Computational Study of the Nondissociative Mechanisms that Interchange Apical and Equatorial Atoms in Square Pyramidal Molecules", Rzepa, H. S, Cass, M. E.; Inorganic Chemistry, Vol 45, **2006**, p. 3958-3963 and ASAP Article 10.1021/ic0519988 S0020-1669(05)01998-1, Web Release Date: April 20, **2006**.

"Mechanisms that Interchange Axial and Equatorial Atoms in Fluxional processes: Illustration of the Berry Pseudorotation, the Turnstile and the Lever Mechanisms via animation of transition state normal vibrational modes", Cass, M. E., Hii, K. K., Rzepa, H. S.; Journal of Chemical Education, Vol. 83, No. 2, **2006**, p. 336.

"The Use of the Free, Open-Source Program Jmol to Generate an Interactive Web Site to Teach Molecular Symmetry", Cass, M. E., Rzepa, H. S., Rzepa, D. R., Williams, C. K.; Journal of Chemical Education, **2005**, Vol 82, No. 11, 1736-1740.

"An Animated/Interactive Overview of Molecular Symmetry", Cass, M. E., Rzepa, H. S., Rzepa, D. R., Williams, C. K.; Webware submission to the Journal of Chemical Education, Online, **2005**, Vol 82, No. 11, 1742-1743.

"Moving Beyond the Single Center—Ways to Reinforce the Teaching of Molecular Orbital Theory in the Inorganic Course", Cass, M. E., Hollingsworth, W. H., Journal of Chemical Education, **2004**, Vol 81, No. 7. 997-1005.

"Student-Directed Explorations to Learn about Ligands in the Inorganic Chemistry Course", Cass, M. E.; Journal of Chemical Education, **2004**, Vol 81, No. 8. 1145-1147.

"Where Does the Time Go?", Haunsperger, D., Galotti, K.M., Cass, M.E., Paas, M., Council on Undergraduate Research Quarterly, Vol 23, No 2, **2002**, 91-94.

"Dye Sensitization of Nanocrystalline Titanium Dioxide with Osmium and Ruthenium Polypyridyl Complexes", Sauv e, G., Cass, M.E., Coia, G. Doig, S. J., Lauer mann, I., Pomykal, K., Lewis, N.S., Journal of Physical Chemistry, B, 104, **2000**, 6821-6836.

"High Quantum Yield Dye Sensitization of Nanocrystalline Titanium Dioxide Photoelectrodes with *cis*-Dicyanobis(4,4-dicarboxy-2,2'-bipyridine)osmium(II) or Tris(4,4'-dicarboxy-2,2'-bipyridine)osmium(II) Complexes", Sauv e, G., Cass, M.E., Doig, S. J., Lauer mann, I., Pomykal, K., Lewis, N.S., Journal of Physical Chemistry B, 104, **2000**, 3488-3491.

"The Oxo-Vanadium(IV) Dimer of 3-Hydroxy-3-methylglutarate: X-ray Crystal Structure, Solid State Magnetism and Solution Spectroscopy" Castro, S. L., Bartley, Stuart L., Cass, M. E., Hollander, F. J., Inorganic Chemistry, 24, 1995, 466.

"Hydrogen Bonding in Catechoylamides." Garrett, T. M., Cass, M. E., Raymond, K. N.; Journal of Coordination Chemistry, Vol. 25, **1992**, p 241.

"The Salicylate Mode of Coordination in Ferric Catecholyamides" Cass, M. E., Garrett, T. M., Raymond K. N., J. Am. Chem. Soc., 111, **1989**, 1677.

"Metal Substituted Complexes of Enterobactin and Synthetic Analogues as Probes of the Ferric Enterobactin Receptor in *E. coli*." Ecker, D. J., Loomis, L. D., Cass, M. E., Raymond, K. N.; J. Am. Chem. Soc., 110, **1988**, 2457.

"Metal Sequestering Agents in Bioinorganic Chemistry: Iron Uptake and Release Mechanisms of Enterobactin Mediated Iron Transport in *E. Coli*" Raymond, K. N., Cass, M. E., Evans S. L.; Pure and Appl. Chem., 59, **1987**, No. 6, 771.

" μ -(η^5 : η^5 -Fulvalene)-bis[dicarbonyl(trimethylphosphine)molybdenum]-(Mo-Mo)." Kretchmar, S. A., Cass, M. E., Turowski, P. N.; *Acta Crystallogr., Sect. C.*, **43**, **1987**, 435.

"Catecholate and Semiquinone Complexes of Vanadium. Factors That Direct Charge Distribution in Metal-Quinone Complexes." Cass, M. E., Rowan, N., Pierpont, C. G.; *Inorg. Chem.*, **25**, **1986**, 3962.

"Synthesis of Tris(3,5-Ditertiarybutylcatecholato)molybdenum(VI) and its Reaction with Molecular Oxygen.", Cass, M. E., Pierpont, C. G.; *Inorg. Chem.*, **25**, **1986**, 122.

"Orthobenzoquinone Complexes of Vanadium and Their Reactions with Molecular Oxygen.", Cass, M. E., Greene, D. L., Buchanan, R. M., Pierpont, C. G.; *J. Am. Chem. Soc.*, **105**, **1983**, 2680.

"Preparation, Structural Characterization and Reactivity of (PEt₃)₂(CO)Rh-Co(CO)₄. A Quantitative Study of the Reversible Heterolytic Cleavage of the Polar Rh-Co Bond." Roberts, D. A., Mercer, W. C., Zahurah, S. M., Geoffroy, G. L., Debrosse, C. W., Cass, M. E., Pierpont, C. G.; *J. Am. Chem. Soc.*, **104**, **1982**, 910.

"Heterobimetallic Complexes. The Preparation, Solid State Structure, and Fluxional Behavior of (C₅Me₅)Rh(ν -PMe₂)₂Mo(CO)₄." Finke, R. G., Caughan, G., Pierpont, C., Cass, M. E.; *J. Am. Chem. Soc.*, **103**, **1981**, 1349.

Awards:

Appointment to the Charles "Jim" and Marjorie Kade Endowed Chair: Spring 2004 – Fall 2016

Distinguished Alumna Award 2007, School of Natural and Behavioral Sciences, Fort Lewis College, Durango, Colorado.

Seminars and Presentations (Since 2004):

"Beyond Workshops: Partnering with other research groups to Create Learning Objects" invited talk at the National 2016 Spring American Chemical Society in the Inorganic Division within a section titled on the Frontiers of Teaching Inorganic Chemistry, March 13, 2016 in San Diego.

Teaching Inorganic Chemistry, Content, Best Practices and Innovation (M. E. Cass, E. Jamieson and S. Pazicni), 34th Boston Regional Inorganic Colloquium, Dartmouth College, May 3, 2014

"Mechanisms that Interconvert Enantiomers in Chiral Metal Tris Chelate Molecules", Carleton College, Department of Chemistry seminar series, February 25, 2011

"A Computational Study on Ligand Imposed Preferences for the Bailar vs R \hat{a} y-Dutt Twists in GaL₃ Complexes", 235th National Meeting of the American Chemical Society, April 7, 2008, New Orleans.

"Animating Molecular Motions to Gain Understanding about Chemical Processes", Department of Chemistry, Fort Lewis College, Durango Colorado, October 19, 2007.

"Synergy in Research and Teaching (*via* Animations of Molecular Processes)", Carleton College, Summer Science Research Program, June 21, 2007.

"Visualization of Real and Imagined Molecular Processes", October 19, 2006, Department of Chemistry, Princeton University.

"Examination and Animation of Fluxional Processes that Interchange Axial and Equatorial Atoms in Simple AX₅ Molecules", January 6, 2006, Department of Chemistry Seminar, Carleton College

"Animation of Real and Imagined Molecular Processes", October 2005, Headley House Faculty Research Seminar Program, Carleton College.

"Using Computer Animations to teach about Fluxional Motions that Scramble Atom Positions in Molecules: (Animation of a Berry Pseudo-Rotation for PF₅)", Cass, M. E., Rzepa, H. S.; Poster Presented at the Gordon Conference on Visualization in

Science and Education, Oxford, UK July 4, 2005.

“Teaching Molecular Orbital Theory in the Undergraduate Curriculum: Moving Beyond a Single Atom Center of Symmetry in the Inorganic Course”, Departmental Seminar, The University of New South Wales, Sydney Australia, March 16, 2004.

Other Activities:

Site Administrator, Virtual Inorganic Pedagogical Electronic Resource Website (Fall 2013-Present)
Elected Member of the Carleton College Presidential Search Committee (Spring 2001 – Spring 2002)
Appointed Faculty Mentor (Appointed by the Dean of the College)
Chair of the Chemistry Department (July 1, 1998 – July 1, 2002)
Member of the American Chemical Society (1985 – present)
Elected Faculty Member to the Carleton Faculty Affairs Committee (Fall 1996 to Spring 1999)
Appointed Faculty Member on the Carleton 21st Century Committee (Fall 1998 to Fall 1999)
Appointed Associate Chairperson in the Department of Chemistry (Fall 1993 to Spring 1994 and Fall 1996 to Spring 1998)
Member of the Advisory Board to the Learning and Teaching Center (Appointed by the Dean)
Elected member of the Carleton College Council and Social Policy Committee (Fall 1989 to Spring 1992)
Member of the Task Force on the College Governance System (Fall 1990 to Winter 1992)
Elected member to the Faculty Judiciary Hearing Board (Spring 1991 to Spring 1993)
Secretary of Sigma Xi (Fall 1989 to Spring 1991), Member of Sigma Xi (Spring 1988 to date)

Other Projects (since 2000):

Participant in the 2014 VIPER Workshop: Bioinorganic Applications of Coordination Chemistry, Northwestern University, Evanston, IL, July 13-18, 2014.

Participant in the AALAC Conference on Teaching Integrative Advanced Laboratory Courses (Philadelphia, PA, August 2012)

Participant in the AALAC Conference contributing to the Virtual Inorganic Pedagogical Electronic Resource (VIPER) database (Smith College, Northampton, MA, August 2011)

Participant in the Gordon Conference on Visualization in Science and Education, Oxford, UK, July 3-8, 2005.

Participant in the Carleton Off Campus Faculty Program to Australia, July 4 –August 1, 2003.

Workshop Participant: Practical LC-MS, American Society for Mass Spectrometry, May 2003.

Workshop Participant: Molecular Modeling in Undergraduate Chemical Education, July 20, 2002, University of Minnesota.

Contact Information:

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Mailing address (while on leave) 75 Flint Hill Road, Lyme, NH 03768

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