

Craig A. Grapperhaus

Professional Background

- 2005 – present: Vice Chair, Department of Chemistry, University of Louisville
2005 – present: Director of Graduate Studies, Department of Chemistry, University of Louisville
2005 – present: Associate Professor, Department of Chemistry, University of Louisville
2000 – present: Appointment to University of Louisville Graduate Faculty
2000 – 2005: Assistant Professor, Department of Chemistry, University of Louisville

Education

- 1998 – 2000: Alexander von Humboldt Postdoctoral Fellow, Max Planck Institut für Strahlenchemie, Mülheim, Germany under the direction of Prof. Karl Wieghardt. Synthesis and characterization of high oxidation state iron-oxo and –nitrido cyclam derivatives.
1994 – 1998: Ph.D. in inorganic chemistry at Texas A&M University. Dissertation title: Oxygenation and Subsequent Alkylation of Nickel-Bound Thiolates under the direction of Prof. Marcetta Y. Darensbourg.
1990 – 1994: B.S. in Chemistry, *Summa Cum Laude* at Southern Illinois University at Edwardsville with a minor in Economics. Synthesis and reactivity of gallium alkyl complexes under the direction of Prof. Thomas Getman.

Honors and Awards

- 2001: Ralph E. Powe Junior Faculty Enhancement Award
1998 – 2000: Alexander von Humboldt Postdoctoral Fellowship (1998-2000)
1997 – 1998: Dow Teacher/Scholar Fellowship, Texas A&M
1996 – 1997: Chemistry/Biology Interface Training Program Fellowship, Texas A&M (NIH)
1996: Martell Travel Grant Award, Texas A&M (1996)
1994 – 1996: Industry-University Cooperative Chemistry Program Fellowship, Texas A&M
1994: Medallion of Lincoln, Academy of Lincoln
1993: Council on Undergraduate Research Fellowship, SIUE

Professional Societies and Service

- 2005: Invited Participant – Tenth Annual Congressional Visits Day
2003: National Science Foundation Review Panel - CRIF
2001 – 2004: Founder and Chair: Kentuckiana Undergraduate Research Symposium
2001 – present: Member of Society of Bioinorganic Chemistry
2000 – 2005: Member of Council on Undergraduate Research
1996 – present: Member of the American Chemical Society

Presentations

A. Scholarly Meetings

Gordon Research Conference on Inorganic Reaction Mechanisms, Galveston, TX (2009) **poster presentation selected for oral presentation**

236th American Chemical Society National Meeting, Philadelphia, PA (2008) **oral presentation**

SERMACS2007 - Southeastern Regional Meeting of the American Chemical Society, Greenville, SC (2007) **invited oral presentation**

CERMACS2007 – Central Regional Meeting of the American Chemical Society, Cincinnati, OH (2007) **invited oral presentation**

233rd American Chemical Society National Meeting, Chicago, IL (2007) **oral presentation**

Metals in Biology Gordon Conference Ventura, CA (2007) **poster presentation**

231st American Chemical Society National Meeting Boston, MA (2006) **oral & poster presentations**

12th International Conference on Biological Inorganic Chemistry, Ann Arbor, MI (2005) **poster**

Gordon Research Conference on Inorganic Reaction Mechanisms, Ventura, CA (2005) **poster**

Gordon Research Conference on Inorganic Chemistry, Newport, RI (2004) **poster presentation**
(*withdrawn due to illness*)

Third German-American Symposium on Frontiers of Chemistry (invited), Kloster Seeon, Germany (2004) **poster presentation** (*withdrawn due to illness*)

CERC3 Young Chemists' Workshop "Biocatalysis", Erlangen, Germany (2004) **oral** (invited) 211th

2003 Gordon Research Conference on Inorganic Chemistry, Newport, RI (2003) **poster presentation**

225th American Chemical Society National Meeting, New Orleans, LA (2003) **oral presentation**

224th American Chemical Society National Meeting Boston, MA (2002) **oral presentation**

Metals in Biology Gordon Conference Ventura, CA (2002) **poster presentation**

10th International Conference on Bioinorganic Chemistry, Florence, Italy (2001) **poster presentation**

1st Annual Kentuckiana Undergraduate Research Symposium, Louisville, Kentucky (2001) **oral**

TMR (Training and Mobility of Researchers) – NOHEMIP Research Network Mid-Term Review and Second Annual Meeting, Toulouse, France (2000) **oral presentation**

Ninth International Conference on Biological Inorganic Chemistry Minneapolis, MN (1999) **poster**

Graduate Research Seminar: Bioinorganic Chemistry (Gordon) Ventura, CA (1998) **oral presentation**

215th American Chemical Society National Meeting Dallas, TX (1998) **oral presentation**

American Chemical Society National Meeting New Orleans, LA (1996) **poster presentation**

B. Universities

2009:	Berea College Western Kentucky University
2008:	Virginia Commonwealth University Old Dominion University Bellarmine University Ohio University Wayne State University
2007:	Marshall University
2005:	College of Mount St. Joseph Purdue University University of North Carolina – Charlotte
2004:	University of Nevada – Reno University of Cincinnati University of Würzburg University of Delaware Indiana University Texas A&M University Rice University University of Miami (Ohio) University of Kentucky
2003:	Indiana State University
2002:	Kentucky State University
2001:	Southern Illinois University at Edwardsville
2000:	Western Kentucky University

Publications

- 1) **Template Effect for O₂ Addition across cis-Sulfur Sites in Nickel Dithiolates** C. A. Grapperhaus, M. Y. Darensbourg, L. W. Sumner, D. H. Russell (*J. Am. Chem. Soc.* **1996**, *118*, 1791-1792)
- 2) **Singlet Oxygen and the Production of Sulfur Oxygenates in Nickel(II) and Palladium(II) Thiolates** C. A. Grapperhaus, M. J. Maguire, T. Tuntulani, M. Y. Darensbourg (*Inorg. Chem.* **1997**, *36*, 1860-1866)
- 3) **1,5-Diazacyclooctane, Pendant Arm Thiolato Derivatives and [(N,N'-bis(2-mercaptoethyl)-1,5-diazacyclooctanato)Nickel(II)]** D. K. Mills, I. Font., P. J. Farmer, Y. M. Hsiao, T. Tuntulani, R. M. Buonomo, D. C. Goodman, G. Musie, C. A. Grapperhaus, M. J. Maguire, C. H. Lai, M. L. Hatley, J. J. Smee, J. A. Bellefeuille, M. Y. Darensbourg (*Inorg. Synth.* **1998**, *32*, 89-98)
- 4) **Methylation of Tethered Thiolates in [(bme-daco)Zn]₂ and [(bme-daco)Cd]₂ as a Model of Zinc Sulfur-Methylation Proteins** C. A. Grapperhaus, T. Tuntulani, J. H. Reibenspies, M. Y. Darensbourg (*Inorg. Chem.* **1998**, *37*, 4052-4058)

- 5) **Alkylation-Induced O-Atom Rearrangement in Nickel S-Oxygenates** J. A. Bellefeuille, C. A. Grapperhaus, R. M. Buonomo, J. H. Reibenspies, M. Y. Darensbourg (*Organometallics* **1998**, *17*, 4813-4821)
- 6) **Oxygen Capture by Sulfur in Nickel Thiolates** C. A. Grapperhaus, M. Y. Darensbourg (*Accs. Chem. Res.* **1998**, *31*, 451-459)
- 7) **Ozone Oxidation of Iron(III) in a Monofunctionalized Cyclam: Spectroscopic Characterization of High Valen Iron Species** C. A. Grapperhaus, E. Bill, K. Wieghardt (*J. Inorg. Biochem.* **1999**, *74*, 146)
- 8) **Synthesis and Dimer Cleavage Reactions of the N₂S Thiolate Bridged Dimer [(mmp-dach)₂Ni₂]Cl₂** C. A. Grapperhaus, J. A. Bellefeuille, J. H. Reibenspies, M. Y. Darensbourg (*Inorg. Chem.* **1999**, *38*, 3698-3703)
- 9) **Correlation of Electrochemistry, Nucleophilicity, and Density Functional Calculations of cis N₂S₂ Nickel Complexes** J. A. Bellefeuille, C. A. Grapperhaus, A. Derecskei-Kovacs, J. H. Reibenspies, M. Y. Darensbourg (*Inorg. Chim. Acta.* **2000**, *300-302*, 73-81)
- 10) **Mononuclear (Nitrido)iron(V) and (Oxo)iron(IV) Complexes via Photolysis of [(cyclam-acetato)Fe^{III}(N₃)]⁺ and Ozonolysis of [(cyclam-acetato)Fe^{III}(OH₂)]²⁺** C. A. Grapperhaus, B. Mienert, E. Bill, T. Weyhermüller, K. Wieghardt (*Inorg. Chem.* **2000**, *39*, 5306-5317)
- 11) **Subtle Bite-Angle Influences on N₂S₂Ni Complexes** J. J. Smee, M. L. Miller, C. A. Grapperhaus, J. H. Reibenspies, M. Y. Darensbourg (*Inorg. Chem.*, **2001**, *40*, 3601-3605)
- 12) **Molecular and Electronic Structure of [(Mn^VN(cyclam-acetato))]PF₆. A Combined Experimental and DFT Study** C. A. Grapperhaus, E. Bill, T. Weyhermüller, F. Neese, K. Wieghardt (*Inorg. Chem.*, **2001**, *40*, 4191-4198)
- 13) **Synthetic Models of Nitrile Hydratase** C. A. Grapperhaus, A. K. Patra, S. Poturovic (*J. Inorg. Biochem.*, **2001**, *86*, 240-240)
- 14) **First {Fe-NO}⁶ Complex with an N₂S₃Fe-NO Core as a Model of NO-Inactivated Iron-Containing Nitrile Hydratase. Are Thiolates and Thioethers Equivalent Donors in Low-Spin Iron Complexes?** Grapperhaus, C. A.; Patra, A. K.; Mashuta, M. S. (*Inorg. Chem.*, **2002**, *41*, 1039-1041)
- 15) **Unique Reactivity of a Tetradentate N₂S₂ Complex of Nickel: Intermediates in the Production of Sulfur Oxygenates** Kaasjager, V. E.; Bouwman, E.; Gorter, S.; Reedijk, J.; Grapperhaus, C. A.; Reibenspies, J. H.; Smee, J. J.; Darensbourg, M. Y.; Derecskei-Kovacs, A.; Thomson, L. M. (*Inorg. Chem.*, **2002**, *41*, 1837-1844)
- 16) **cis-Dioxocyclam** Mashuta, M. S.; Pimenov, K. V.; Grapperhaus, C. A. (*Acta Cryst.*, **2002**, *C58*, o226-o227)
- 17) **1,5-Bis(benzothiazolyl)-3-thiapentane and Its Asymmetric Dinuclear Ag(I) Complex with Three Distinct Intermolecular-Stacking Interactions** Grapperhaus, C. A.; Li, M.; Mashuta, M. S. (*Chem. Comm.*, **2002**, 1792-1793)
- 18) **Dichloromethane Alkylates a Trithiolato-Ruthenium Complex to Yield a Methylene-Bridged Thioether Core. Synthesis and Structural Comparison to the Thiolato-Ruthenium Precursor** Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. (*Inorg. Chem.*, **2002**, *41*, 4309-4311)
- 19) **Synthesis and Characterization of N₂S₃X-Fe Models of Iron-Containing Nitrile Hydratase** Grapperhaus, C. A.; Li, M.; Patra, A. K.; Poturovic, S.; Kozlowski, P. M.; Zgierski, M. Z. Mashuta, M. S. (*Inorg. Chem.*, **2003**, *42*, 4382-4388)

- 20) **Hydrogen-Bond Networks in the Mono- and Diprotonated Cyclic Diamine [9]aneN₂S**
Grapperhaus, C. A.; Li, M.; Gibson, E. R.; Mashuta, M. S. (*J. Chem. Crystallogr.*, **2004**, *34*, 5-11)
- 21) **Synthesis and Oxygenation of a Nickel(II) and Zinc(II) Dithiolate: An Experimental and Theoretical Comparison** Grapperhaus, C. A.; Mullins, C. S.; Kozlowski, P. M.; Mashuta, M. S. (*Inorg. Chem.*, **2004**, *43*, 2859-2866)
- 22) **Electrochemical Investigations of [tris(2-diphenylphosphinothiaphenolato)-ruthenium(II)]⁻ Reveal Metal- and Ligand-Centered Events: Radical, Reactivity, and Rate.** Grapperhaus, C. A.; Poturovic, S. (*Inorg. Chem.*, **2004**, *43*, 3292-3298)
- 23) **Structural, Spectroscopic and Computational Study of an Octahedral, Non-heme {Fe-NO}^{6,7,8} Series: [Fe(NO)(cyclam-ac)]^{2+,1+,0}** Serres, R. G.; Grapperhaus, C. A.; Bothe, E.; Bill, E.; Weyhermüller, T.; Neese, F.; Wieghardt, K. (*J. Am. Chem. Soc.*, **2004**, *126*, 5138-5153)
- 24) **Template Synthesis of N₂S and N₃S Chelates via Alkylation of bis(2-aminoethanethiolato)Ni: Sulfur- and Nitrogen-Centered Alkylations.** Grapperhaus, C. A.; Kreso, M.; Burkhardt, G. A.; Roddy, J. V. F.; Mashuta, M. S. (*Inorg. Chim. Acta.* **2005**, *358*, 123-130.)
- 25) **Structural Comparison of Alkylated Derivatives of (bmmp-dmed)Ni and (bmmp-dmed)Zn.** Grapperhaus, C. A.; Mullins, C. S.; Mashuta, M. S. (*Inorg. Chim. Acta.* **2005**, *358*, 623-632.)
- 26) **Carbon-Sulfur Bond Formation between a Ruthenium-Coordinated Thiyl Radical and Methyl Ketones.** Poturovic, S.; Mashuta, M. S.; Grapperhaus, C. A. (*Angew. Chem., Int. Ed. Engl.*, **2005**, *44*, 1883-1887)
- 27) **Oxygenation of a Ruthenium(II) Thiolate to a Ruthenium(II) Sulfinate Proceeds via Ruthenium(III).** Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. (*Inorg. Chem.* **2005**, *44*, 8185-8187)
- 28) **NiSOD Inspired DFT Investigations of NiN₂S₂ Reactivity as a Function of Nitrogen Donor Type and N-H...S Hydrogen Bonding** Mullins, C. S.; Grapperhaus, C. A.; Kozlowski, P. M. (*J. Biol. Inorg. Chem.* **2006**, *11*, 617-625)
- 29) **Ethyl 1-methylimidazole-2-carbox** Frye B.C., Mashuta M.S., Mullins C.S., Grapperhaus C.A., Buchanan R.M. (*Acta Crystallogr. Sect. E: Struct. Rep. Online* **2006**, *62*, O1548-O1549)
- 30) **Synthesis and structure of the tetradeca-iron(III) oxide-alkoxide cluster [Bu₄N]₂[Fe₁₄O₈(OCH₂CH₃)₂₀Cl₈]** Grapperhaus C.A., O'Toole, M. G., Mashuta M.S. (*Inorg. Chem. Commun.* **2006**, *9*, 1204-1206)
- 31) **Singlet Diradical Character of an Oxidized Ruthenium Trithiolate: Electronic Structure and Reactivity** Grapperhaus, C. A., Kozlowski, P. M., Kumar, D., Frye, H. N., Venna, K. B., Poturovic, S. (*Angew. Chem., Int. Ed. Engl.*, **2007**, 4085-4088)
- 32) **An experimental and computational study of sulfur-modified nucleophilicity in a dianionic NiN₂S₂ complex** Green K.N., Brothers S.M., Jenkins R.M., Carson C.E., Grapperhaus C.A., Darensbourg M.Y. (*Inorg. Chem.* **2007**, *46*, 7536-7544)
- 33) **{3,3'-[Ethane-1,2-diylbis(methylimino)]-bis(propane-1-thiolato)}nickel(II).** Grapperhaus C.A., O'Toole M.G., Mashuta M.S. (*Acta Crystallogr. Sect. E: Struct. Rep. Online* **2007**, *63*, M2281)
- 34) **Carbon-sulfur bond formation via alkene addition to an oxidized ruthenium thiolate.** Grapperhaus C.A., Venna K.B., Mashuta M.S. (*Inorg. Chem.* **2007**, *46*, 8044-8050)
- 35) **Hg(II) and Cd(II) complexes with mixed donor macrocyclic thioethers: The oxophobicity of mercury(II).** Grant G.J., Botros M.E., Hassler J.S., Janzen D.E., Grapperhaus C.A., O'Toole M.G., VanDerveer D.G. (*Polyhedron* **2008**, *27*, 3097-3104)

- 36) **Spin-state-dependent oxygen sensitivity of iron dithiolates: sulfur oxygenation or disulfide formation.** O'Toole M.G., Kreso M., Kozlowski P.M., Mashuta M.S., Grapperhaus C.A. (*J. Biol. Inorg. Chem.* **2008**, *13*, 1219-1230)
- 37) **Substrate Binding Preferences and pK_a Determinations of a Nitrile Hydratase Model Complex: Variable Solvent Coordination to [(bmmp-TASN)Fe]OTf.** O'Toole M.G., Bennett B., Mashuta M.S., Grapperhaus C.A. (*Inorg. Chem.* **2009**, *48*, 2300-2308)
- 38) **Redox-Regulated Ethylene Binding to a Rhenium-Thiolate Complex.** Grapperhaus, C.A., Ouch. K., Mashuta, M.S. (*J. Am. Chem. Soc.* **2009**, *131*, 64-65)

Persons Mentored

A. Post-Doctoral Researchers

2008 – current: Jinlan Cui

2001 – 2002: Ming Li

2000 – 2001: Apurba Patra

B. Ph.D. Students

current: Cesar Masitas

Kagna Ouch

Rajat Chauhan

2008: Martin O'Toole

2006: Christopher S. Mullins

2005: Selma Poturovic

C. M.S. Students

2008: Kagna Ouch

2007: Kiran Venna

2006: Majda Kreso

withdrawn: Konstantin Pimenov

D. Undergraduates

2009: Victoria D'Angelo

Tracy McKnight

Stephanie Bebout

2008: Stefen Bright

2007: Andrew Barnes

2005: Komeneci Yates

Mindy Holley

Bertha Coleman

2004: Danielle Kimmel

Angela Phillips

Benjamin Risner

2003: Jason Wiles

	Majda Kreso
	Holly Miller
2002:	Ryan Denton
	Ben Hahn
2001:	Elaine Miller
	Julianna Roddy
	Gretchen Burkhardt
2000:	Jessica Taylor