

Katherine M. Van Heuvelen

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ACADEMIC POSITIONS

Associate Professor of Chemistry, Harvey Mudd College 2018 – Present
Assistant Professor of Chemistry, Harvey Mudd College 2012 – 2018

EDUCATION

University of Minnesota 2009 – 2012
NIH NRSA Postdoctoral Fellow
Laboratory of Professor Lawrence Que, Jr.

Ph.D. in Inorganic Chemistry, University of Wisconsin-Madison 2004 – 2009
NSF Graduate Research Fellow
Research Advisor: Professor Thomas C. Brunold

B.A. in Chemistry and Religion (summa cum laude), St. Olaf College 2000 – 2004
Research Advisors: Professors Gary L. Miessler (Chemistry) & Ed Santurri (Religion)

RESEARCH AREAS

Experimental Expertise: Air-free synthesis (standard Schlenk techniques), GC-MS, HPLC, MS

Spectroscopic Expertise: UV-visible Absorption, Infrared, Nuclear Magnetic Resonance, Magnetic Circular Dichroism, Electron Paramagnetic Resonance, X-ray Absorption, X-ray Emission

Computational Expertise: Density Functional Theory (DFT), Time-Dependent DFT, QM/MM, XSEDE Supercomputing System

PUBLICATIONS (Undergraduate co-authors are underlined>)

20. Crystal Structure and Spectroscopic Characterization of a Cobalt(II) Tetraazamacrocyclic Complexes: Completing a Series of First-Row Transition Metal Complexes
Van Heuvelen, K.M.*; Lee, I.; Arriola, K.; Griffin, R.; Ye, C.; Takase, M.
Acta Crystallographica Section C, **2017**, C73, 620-624 <http://dx.doi.org/10.1107/S2053229617010397>
19. Mononuclear Nickel(II) and Copper(II) Coordination Complexes Supported by Bispicen Ligand Derivatives: Experimental and Computational Studies
Singh, N.; Niklas, J.; Poluektov, O.; **Van Heuvelen, K.M.***; Mukherjee, A.*
Inorganica Chimica Acta, **2017**, 455, 221 – 230 <http://dx.doi.org/10.1016/j.ica.2016.09.001>
18. Cobalt K β Valence-to-Core X-ray Emission Spectroscopy: A Study of Low-Spin Octahedral Cobalt(III) Complexes
Schwalenstocker, K.; Paudel, J.; Kohn, A.W.; Dong, C.; **Van Heuvelen, K.M.***; Farquhar, E.R.*; Li, F.*
Dalton Transactions, **2016**, 45, 14191-14202. <http://dx.doi.org/10.1039/C6DT02413K>
17. Characterization of a Heterobimetallic Nonheme Fe(III)-O-Cr(III) Species Formed by O₂ Activation
Zhou, A.; Kleespies, S.T.; **Van Heuvelen, K.M.**; Que, L.
Chemical Communications, **2015**, 51, 14326 – 14329. <http://dx.doi.org/10.1039/C5CC05931C>

16. Spectroscopic Identification of an Fe^{III} Center, not Fe^{IV}, in the Crystalline Sc-O-Fe Adduct Derived from [Fe^{IV}(O)(TMC)]²⁺

Prakash, J.; Rohde, G.T.; Meier, K.K.; Jasniewski, A.J.; **Van Heuvelen, K.M.**; Münck, E.; Que, L. *J. Am. Chem. Soc.* **2015**, *137*, 3478 – 3481. <http://dx.doi.org/10.1021/jacs.5b00535>

15. An Ultra-Stable Oxoiron(IV) complex and its Blue Conjugate Base

England, J.; Bigelow, J.O.; **Van Heuvelen, K.M.**; Farquhar, E.R.; Martinho, M.; Meier, K.K.; Frisch, J.R.; Münck, E.; Que, L.

Chem. Sci. **2014**, *5*, 1204 – 1215. <http://dx.doi.org/10.1039/C3SC52755G>

14. Sc³⁺ can trigger the formation of an oxoiron(IV) complex from O₂ and its nonheme iron(II) precursor via a Sc³⁺-peroxo-Fe³⁺ intermediate

Li, F.; **Van Heuvelen, K.M.**; Meier, K.K.; England, J.; Münck, E.; Que, L.

J. Am. Chem. Soc. **2013**, *135*, 10198 – 10201. <http://dx.doi.org/10.1021/ja402645y>

13. Isolation and Characterization of a Thiolato-Iron(III)-Peroxy Anion Complex

McDonald, A.R.; **Van Heuvelen, K.M.**; Guo, Y.; Münck, E.; Que, L.

Angew. Chem. Int. Ed. **2012**, *51*, 9132 – 9136. <http://dx.doi.org/10.1002/anie.201203602>

12. One-Electron Oxidation of an Oxoiron(IV) Complex to Form an [O=Fe^V=NR]⁺ Center

Van Heuvelen, K.M.; Fieder, A.T.; Shan, X.; DeHont, R.; Meier, K.K.; Münck, E.; Que, L. *Proc. Nat. Acad. Sci.* **2012**, *109*, 11933 – 11938. <http://dx.doi.org/10.1073/pnas.1206457109>

11. A More Reactive Trigonal-Bipyramidal High-Spin Oxoiron(IV) Complex with a cis-Labile Site

England, J.; Guo, Y.; **Van Heuvelen, K.M.**; Cranswick, M.A.; Rohde, G.T.; Bominaar, E.L. Münck, E.; Que, L.

J. Am. Chem. Soc. **2011**, *133*, 11880 – 11883. <http://dx.doi.org/10.1021/ja2040909>

10. Characterization of a High-Spin Non-Heme Fe^{III}-OOH Intermediate and Its Quantitative Conversion to an Fe^{IV}=O Complex

Li, F.; Meier, K.K.; Cranswick, M.A.; Chakrabarti, M.; **Van Heuvelen, K.M.**; Münck, E.; Que, L.

J. Am. Chem. Soc. **2011**, *133*, 7256 – 7259. <http://dx.doi.org/10.1021/ja111742z>

9. Spectroscopic and Computational Studies on High-Spin Ni(II) Thiolate Compounds

Van Heuvelen, K. M.; Cho, J.; Dingee, T.; Riordan, C. G.; Brunold, T. C.

Inorg. Chem. **2010**, *49*, 6535 – 6544. <http://dx.doi.org/10.1021/ic100362q>

8. Spectroscopic and Computational Studies of the μ - η^2 : η^2 -Disulfido-Bridged Dinickel(II) Species

[(PhTt^{tBu})₂Ni₂(μ - η^2 : η^2 -S₂)]

Van Heuvelen, K. M.; Cho, J.; Riordan, C. G.; Brunold, T. C.

Inorg. Chem. **2010**, *49*, 3113 – 3120. <http://dx.doi.org/10.1021/ic901731b>

7. Spectroscopic and Computational Studies of the Trans- μ -1,2-Disulfido-Bridged Dinickel(II) Species

[Ni₂(tmc)₂(S₂)](OTf)₂: Comparison of End-on Disulfido and Peroxo Bonding in Ni(II) and Cu(II) Species

Van Heuvelen, K. M.; Kieber-Emmons, M. T.; Riordan, C. G.; Brunold, T. C.

Inorg. Chem. **2010**, *49*, 3104 – 3112. <http://dx.doi.org/10.1021/ic901733h>

6. Synthesis and Spectroscopic Characterization of a μ -1,2-Disulfidodinickel Complex

Kieber-Emmons, M. T.; **Van Heuvelen, K. M.**; Brunold, T. C.; Riordan, C. G.

J. Am. Chem. Soc., **2009**, *131*, 440 – 441. <http://dx.doi.org/10.1021/ja807735a>

5. Computational Studies of Bioorganometallic Enzymes and Cofactors

Liptak, M. D.; **Van Heuvelen, K. M.**; Brunold, T. C.

In *Metal Ions in Life Sciences Vol 6: Metal-Carbon Bonds in Enzymes and Cofactors*. Eds. Sigel, A.; Sigel, H.; Sigel, R. K. O. Cambridge: Royal Society of Chemistry, 2009.

4. New Synthetic Routes to a Disulfido Dinickel(II) Complex: Characterization and Reactivity of a $\text{Ni}_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-S}_2)$ Core

Cho, J.; **Van Heuvelen, K. M.**; Yap, G. P. A.; Brunold, T. C.; Riordan, C. G.
Inorg. Chem. **2008**, *47*, 3931 – 3933. <http://dx.doi.org/10.1021/ic800321x>

3. Ferromagnetic Semiconducting EuO Nanorods

Bierman, M. J.; **Van Heuvelen, K. M.**; Schmeißer, D.; Brunold, T. C.; Jin, S.
Adv. Mater. **2007**, *19*, 2677 – 2681. <http://dx.doi.org/10.1002/adma.200602612>

2. Identification of an "End-On" Nickel-Superoxo Adduct, $\text{Ni}(\text{tmc})(\text{O}_2)^+$

Kieber-Emmons, M. T.; Annaraj, J.; Seo, M. S.; **Van Heuvelen, K. M.**; Tosha, T.; Kitagawa, T.;
Brunold, T. C.; Nam, W.; Riordan, C. G.
J. Am. Chem. Soc. **2006**, *128*, 14230 – 14231. <http://dx.doi.org/10.1021/ja0644879>

1. Spectroscopic and Computational Studies of Reduction of the Metal versus the Tetrapyrrole Ring of Coenzyme F-430 from Methyl-Coenzyme M Reductase

Dey, M.; Kunz, R. C.; **Van Heuvelen, K. M.**; Craft, J. L.; Horng, Y. C.; Tang, Q.; Bocian, D. F.;
George, S. J.; Brunold, T. C.; Ragsdale, S. W.
Biochemistry **2006**, *45*, 11915 – 11933. <http://dx.doi.org/10.1021/bi0613269>

PRESENTATIONS

Designing Bio-Inspired Nickel and Cobalt Complexes to Treat Priority Pollutants – Invited Talk
Van Heuvelen, K.M.

University of Wisconsin-Madison, Madison, WI, November 2017

Crafting Your Career – Invited Talk

Van Heuvelen, K.M.

University of Wisconsin-Madison, Madison, WI, November 2017

Designing Bio-Inspired Nickel and Cobalt Complexes to Treat Priority Pollutants – Invited Talk

Van Heuvelen, K.M.

University of La Verne, La Verne, CA, November 2017

Bio-Inspired Dehalogenation: Developing First-Row Transition Metal Complexes to Treat Priority
Pollutants – Invited Talk

Van Heuvelen, K.M.

University of La Verne, La Verne, CA April 2017

Development of Bio-Inspired Catalysts for Dechlorination Reactions

Poster presented at the Gordon Research Conference: Metals in Biology
January 2015, Ventura, CA

Investigation of the Electronic Structure of Cobaloximes

Van Heuvelen, K. M.

Poster presented at the Gordon Research Conference: Metals in Biology,
January 26 – 31, 2014, Ventura, CA

One-Electron Oxidation of an Oxoiron(IV) Complex

Van Heuvelen, K. M.; Fiedler, A.T.; Meier, K.K.; DeHont, R.; Shan, X.; Münck, E.; Que, L..

Poster presented at the International Conference of Bioinorganic Chemistry
August 7-12, 2011, Vancouver, British Columbia

One-Electron Oxidation of an Oxoiron(IV) Complex

Van Heuvelen, K. M.; Fiedler, A.T.; Meier, K.K.; DeHont, R.; Shan, X.; Münck, E.; Que, L.
Poster presented at the Gordon Research Conference: Metals in Biology,
January 30 – February 3, 2011, Ventura, CA

Graduate School in Chemistry

Van Heuvelen, K. M.

Invited seminar presented at St. Olaf College
October 14, 2010, Northfield, MN

Insights into the Mechanism of Methyl-Coenzyme M Reductase: Spectroscopic and
Computational Studies of Ni-C Bonding in Cofactor F430

Van Heuvelen, K. M.; Dey, M.; Kunz, R.; Ragsdale, S. W.; Brunold, T. C.

Talk presented at the Gordon Research Seminar: Bioinorganic Chemistry,
January 29 – February 1, 2009, Ventura, CA

Spectroscopic and Computational Studies of Ni-Alkyl Bonding in the Active Site of Methyl-
Coenzyme M Reductase

Van Heuvelen, K. M.; Dey, M.; Kunz, R.; Ragsdale, S. W.; Brunold, T. C.

Poster presented at the Gordon Research Seminar: Bioinorganic Chemistry,
January 29 – February 1, 2009, Ventura, CA

Spectroscopic and Computational Insights into Ni-S Bonding in Methyl-CoM Reductase and
Synthetic Ni₂(S₂) Complexes

Van Heuvelen, K. M.; Dey, M.; Kunz, R.; Kieber-Emmons, M. T.; Cho, J.; Riordan, C. G.;
Ragsdale, S. W.; Brunold, T. C.

Poster presented at the Gordon Research Seminar: Bioinorganic Chemistry,
January 31 – February 3, 2008, Ventura, CA

So You Want to Go to Grad School

Van Heuvelen, K. M.

Invited seminar presented at St. Olaf College
September 2008, Northfield, MN

Spectroscopic and Computational Studies of Ni-Containing Enzymes: Application to Acetyl-CoA
Synthase/Carbon Monoxide Dehydrogenase and Methyl-Coenzyme M Reductase

Van Heuvelen, K. M.; Dey, M.; Kunz, R.; Kieber-Emmons, M. T.; Riordan, C. G.; Ragsdale, S.
W.; Brunold, T. C.

Poster presented at the International Conference of Biological Inorganic Chemistry
July 31 – August 5, 2005, Ann Arbor, MI

Modeling Enzyme Active Sites: Synthesis of Group VI Heterobimetallic Compounds

Van Heuvelen, K. M.; Miessler, G. L.

Talk presented at the St. Olaf Summer Research Symposium
August 2002/2003, Northfield, MN

Green Chemistry: Diels-Alder Reactions in Ionic Solutions

Patterson, M.; **Van Heuvelen, K. M.**; Spessard, G.

Poster presented at St. Olaf College
May 2003, Northfield, MN

Modeling Enzyme Active Sites: Synthesis of Group VI Heterobimetallic Compounds

Van Heuvelen, K. M.; Miessler, G. L.

Talk presented at the Pew Midstates Science and Mathematics Consortium
Fall 2003, Chicago, IL

AWARDS

National Institute of Health NRSA Postdoctoral Fellowship	2010 – 2012
Vilas Travel Grant (University of WI-Madison)	2008
McElvain Travel Grant (University of WI-Madison)	2008
National Science Foundation Graduate Research Fellowship	2005 – 2008
McElvain Fellowship (University of WI-Madison)	2004
Distinction in Chemistry (St. Olaf College)	2004
Distinction in Religion (St. Olaf College)	2004
Courtland and Ellen Agre Award in Chemistry (St. Olaf College)	2004
Junia Award in Religion (St. Olaf College)	2004
Dow Chemical Scholarship (St. Olaf College)	2004
Regents Scholar (50% tuition, St. Olaf College)	2000 – 2004
National Merit Scholar	2000

COURSES TAUGHT AT HARVEY MUDD COLLEGE

Core Laboratory 57: The Chemistry of Cooking
Writ 1: Introduction to Academic Writing
Chem 23S: Chemical Structure
Chem 19S: General Chemistry Intensive
Chem 23A and B: Chemistry in the Modern World
Chem 24: Chemistry Laboratory
Chem 40: Introduction to Chemical Research
Chem 104: Advanced Inorganic Chemistry
Chem 110: Advanced Inorganic Laboratory
Chem 150: Chemical Research
Chem 151 and 152: Senior Thesis Research
Chem 197: Special Readings in Chemistry: C-H Bond Activation
Chem 199: Chemistry Seminar

TEACHING EXPERIENCE PRIOR TO HARVEY MUDD COLLEGE

University of Minnesota, Guest Lecturer, Inorganic Chemistry (one week)

University of Wisconsin-Madison; Madison, WI
Teaching Assistant (Upper-level advanced inorganic chemistry, introductory inorganic chemistry, advanced general chemistry)
Undergraduate student research mentor

St. Olaf College; Northfield, MN
Teaching Assistant (Analytical chemistry laboratory, organic chemistry laboratory), General chemistry course tutor
Great Conversation (great books learning community) course tutor

SERVICE (Harvey Mudd College)

Core Review Committee
Assessment and Accreditation Committee
Research Committee
Academic Affairs Committee
Chemistry department seminar coordinator

RESEARCH STUDENTS

1. Alex Kohn '13. Senior Thesis: A Spectroscopically Validated Computational Study of the Reduction of Haloalkanes by Cobaloximes
2. Bram Carlson '13. Senior Thesis: Oxidation of Methane by Cofactor F430 Model Compounds
3. Philip Woods '17
4. Jessica Iwamoto '16
5. Casey Cannon '16
6. Jennifer Rogers '16
7. E. Page Allen '14. Senior Thesis: Dechlorination by Cobaloximes
8. Isabell Lee '16
9. Naomi Epstein '16
10. Justin Lee '16
11. Allison Lim '16
12. Emma Klein '17
13. Danielle Marquis '15. Senior Thesis: Dechlorination through Model Compounds of Vitamin B12
14. Sooyeol "Suzy" Kim '16. Senior Thesis: Metallating Ligands in Catalyst Development for Carcinogens in Groundwater
15. Jacob Knego '18
16. Monica Mikkelsen
17. Kate Arriola '16. Senior Thesis: Developing a Biologically Inspired Catalyst for Dechlorination Reactions
18. Rilke Griffin '18
19. Christopher Ye '19
20. Ellie Gund '17. Senior Thesis: Investigation of Dechlorination using Bio-Inspired Nickel Compounds
21. Theo Hansel '19
22. Parnika Sharma '19
23. Micaela Homer '19
24. Brandon Wada '20