



Michael J. Rose, Ph.D.

California Institute of Technology

Division of Chemistry & Chemical Engineering

Postdoctoral Advisors: Prof Harry B. Gray and Prof Nathan S. Lewis

Ph.D. Advisor: Prof Pradip K. Mascharak (University of California, Santa Cruz)

Synthetic Inorganic Chemistry & Surface Chemistry

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Research and Education

California Institute of Technology – (2010-12): NSF ACC-F Postdoctoral Fellowship; (2009-2010) NSF/CCI-Solar Postdoctoral Fellow. Joint post-doctoral appointment in the labs of Prof Harry Gray and Prof Nate Lewis. Syntheses of Fe, Ni and Co catalysts for H₂ generation and covalent Si–C/C–C attachment of transition metal complexes to planar and microstructured silicon surfaces.

University of California, Santa Cruz Ph.D. Chemistry (March 2009). Bio-inorganic chemistry, Advisor: Prof Pradip Mascharak. *a)* Syntheses, structures, and biological utility of ruthenium-based NO donors derived from carboxamide ligands and coordinated chromophores. *b)* Synthetic modeling of iron-containing nitrile hydratase: photoregulation of the carboxamide/thiolate Fe-active site by NO and effects of sulfur oxygenation on NO photolability.

Roche Pharmaceuticals (Palo Alto), Inflammatory and Viral Disease Unit (2000-2002) – Research Associate I (2000-2001) / Research Associate II (2001-2002). Drug discovery with purinergic (P₂Y₂/P₂Y₁) and muscarinic (M₁-M₅) G-protein coupled receptors: steady-state and kinetic inhibitors. Development of tissue culture assays for inflammatory mucin production (muc4/5/5ac). Mentor: Dave Swinney, Ph.D.

University of California, Davis B.S. Fermentation Science (1995-2000). This major incorporates basic and applied chemistry (analytical, organic and biochemistry) in biotechnology and food sciences.

Fellowships

NSF ACC-F Post-doctoral Fellowship (2010-2012)

Syntheses of Phosphine-based Nickel & Cobalt Catalysts for H₂ Generation & Covalent Attachment to Silicon Surface.

NSF/CCI-Solar Postdoctoral Fellowship (2009-2010).

All-Manganese Electrochemical Cell Utilizing Immobilized Small Molecule Catalysts for H₂ and O₂ Generation.

Chancellor's Dissertation Fellowship (2008-2009) UCSC, Thesis research support.

Other Research

Roche Pharmaceuticals, Inflammatory Disease Unit (1999) – Research Intern. Kinetic enzymology of a 3-enzyme, bi-substrate E3 ubiquitin-ligase in the I κ B/NF- κ B cascade: investigation into Sequential or Random bi-bi Mechanism. Mentor: Dave Swinney, Ph.D.

White Labs (1998) – Research Intern. Growth, fermentation and flocculation dynamics of various *S. cerevisiae* strains. White Labs develops and maintains a collection of yeast strains for the brewing industry. Mentor: Chris White, Ph.D.

Publications

- 1) M. J. Rose, J. R. Winkler and H. B. Gray. Hydrogen Generation Catalyzed by Perfluorinated Diglyoxime-Iron Complexes at Moderate Overpotentials. *Submitted to Nat. Chem.*
- 2) L. E. O'Leary, M. J. Rose, T. X. Ding, E. Johansson, B. S. Brunshwig and N. S. Lewis. Heck Couplings of Small Molecules to Mixed Methyl/Thienyl Monolayers at Low Defect Density Si(111). *In preparation for J. Am. Chem. Soc.*
- 3) M. J. Rose, J. R. Winkler and H. B. Gray. Four-Iron Cluster and a Buckled Macrocyclic Complex from Reduction of [(dmgBF₂)Fe(L)₂] (L=MeCN, ^tBu⁺NC). *In preparation for Inorg. Chem.*
- 4) Q. Dong, M. J. Rose, W.-Y. Wong and H. B. Gray. Dual Coordination Modes of Ethylene Linked NP₂ Ligands with Cobalt(II) and Nickel(II) Iodides. *Accepted to Inorg. Chem.* doi: 10.1021/ic201213c.
- 5) M. J. Rose, D. E. Bellone and H. B. Gray. Spontaneous Formation of a High-Spin Co(I) Species Derived from a Tripodal Phenyl-P₃ Ligand. *Submitted to J. Am. Chem. Soc.*
- 6) M. J. Rose, N. M. Betterley, A. Oliver, and P. K. Mascharak. Binding and Photorelease of Nitric Oxide (NO) to a Synthetic Model of Iron-Containing Nitrile Hydratase (Fe-NHase). *Inorg. Chem.* **2010**, *49*, 1854-1864.
- 7) M. J. Rose, A. K. Patra, M. M. Olmstead and P. K. Mascharak. Structural and Spectroscopic Evidence for Linkage Isomerism of Bound Nitrite in a {Fe-NO}⁶ Nitrosyl derived from a Tetradentate Dicarboxamide Ligand: More Parallels between Heme and Non-heme Systems. *Inorg. Chim. Acta* **2010**, *363*, 2715.
- 8) N. Fry, M. J. Rose, David L. Rogow, C. Nyitray, Manpreet Kaur and P. K. Mascharak. Ruthenium Nitrosyls Derived from Tetradentate Ligands containing Carboxamido-N and Phenolato-O Donors: Syntheses, Structures, Photolability and Time-Dependent Density Functional Studies. *Inorg. Chem.* **2010**, *49*, 1487.
- 9) M. J. Rose, N. M. Betterley, P. K. Mascharak. Thiolate S-Oxygenation Controls Nitric Oxide (NO) Photolability of a Synthetic Iron Nitrile Hydratase (Fe-NHase) Model Derived from Mixed Carboxamide/Thiolate Ligand. *J. Am. Chem. Soc.* **2009**, *131*, 8340-8341.
- 10) M. J. Rose, P. K. Mascharak. Photosensitization of Ruthenium Nitrosyls to Visible Light with an Isoelectronic Series of Heavy-Atom Chromophores: Experimental and DFT Studies on the Effects of O-, S- and Se-Substituted Coordinating Dyes. *Inorg. Chem.* **2009**, *48*, 6904-6917.
- 11) N. Fry, M. J. Rose, C. Nyitray, and P. K. Mascharak. Metal Nitrosyls with Phosphine Ligation: Unexpected Ligand Oxidation and Ring Nitration. *Inorg. Chem.* **2008**, *47*, 11604-11610
- 12) M. J. Rose and P. K. Mascharak. A Photosensitive {Ru-NO}⁶ Nitrosyl Bearing Dansyl Chromophore: Novel NO Donor with a Fluorometric On/Off Switch. *Chem. Commun.* **2008**, 3933-3935
- 13) M. J. Rose, N. Fry, R. Marlow, L. Hinck and P. K. Mascharak. Ruthenium Nitrosyls bearing Coordinated Fluorophores as NO Donors: a Novel Mode of Fluorometric Delivery of NO to Cells with Visible Light. *J. Am. Chem. Soc.* **2008**, *130*, 8834-8846
- 14) M. J. Rose, P. K. Mascharak. Photoactive Ruthenium Nitrosyls: Effects of Light & Potential as Biological NO Donors. *Coord. Chem. Rev.* **2008**, *252*, 2093-2114
- 15) M. J. Rose and P. K. Mascharak. Fiat Lux: Selective Delivery of High Flux of Nitric Oxide (NO) to Biological Targets using Photosensitive Metal Nitrosyls. *Curr. Opin. Chem. Biol.* **2008**, *12*, 238-244
- 16) M. J. Rose, M. M. Olmstead and P. K. Mascharak. Photosensitization via Dye Coordination: A New Strategy to Synthesize Metal Nitrosyls that Release NO under Visible Light. *J. Am. Chem. Soc.* **2007**, *129*, 5342-5343
- 17) M. J. Rose, M. M. Olmstead and P. K. Mascharak. Photoactive Ruthenium Nitrosyls Derived from Quinoline- and Pyridine-based Ligands: Accelerated Photorelease of NO due to Quinoline Ligation. *Polyhedron* **2007**, *26*, 4713-4718
- 18) M. J. Rose, A. K. Patra, E. A. Alcid, M. M. Olmstead and P. K. Mascharak. Carboxamido and Schiff Base Ruthenium Nitrosyls: Isoelectronic Complexes with Markedly Different Properties of Photolability and Reactivity. *Inorg. Chem.* **2007**, *46*, 2328-2338
- 19) M. J. Rose,* I. Szundi,* I. Sen, A. A. Eroy-Reveles, P. K. Mascharak and Ó. Einarsdóttir. New Approach for Studying Fast Biological Reactions Involving Nitric Oxide: Generation of NO Using Photolabile Ruthenium and Manganese NO Donors. *Photochem. Photobiol.* **2006**, *82*, 1377-1384 (*equal authorship)

- 20) D. C. Swinney, M. J. Rose, A. Y. Mak, I. Lee, L. Scarafia and Y. Xu. Bi-Substrate Kinetic Analysis of an E3–Ligase–Dependent Ubiquitylation Reaction. *Methods Enzymol.* **2005**, 399, 323-333
- 21) A. K. Patra, M. J. Rose, M. M. Olmstead and P. K. Mascharak. Reactions of Nitric Oxide with a Low-spin Fe(III) Center Ligated to a Tetradentate Di-carboxamide N4 Ligand: Parallels between Heme and Non-Heme Systems. *J. Am. Chem. Soc.* **2004**, 126, 4780-4781
- 22) A. K. Patra, M. J. Rose, K. A. Murphy, M. M. Olmstead and P. K. Mascharak. Photolabile Ruthenium Nitrosyls with Planar Di-carboxamide Tetradentate N4 Ligands: Effects of In-plane and Axial Ligand Strength on NO Release. *Inorg. Chem.* **2004**, 43, 4487-4495
- 23) M. J. Rose, I. Lee, T. R. Chapman and D. C. Swinney. Pharmacological Characterization of Clinical Anti-Cholinergic Drugs at M1–M5 Receptor Sub-types. *Mol. Biol. Cell.* **2002**, 443, 79A
- 24) D. C. Swinney, M. J. Rose, I. Lee, A. Y. Mak. The Mono-ubiquitination of I κ B α S32/36E *in vitro* Shows a Random Bi-Bi Kinetic Mechanism with Respect to I κ B α -*ee* and E2UBCH7. *FASEB J.* **2001**, 15, A26

Awards and Programs

NSF-sponsored Chemistry Communication Leadership Institute, (2009): a 5-day workshop to promote science and chemistry communication to a broad audience.

Datatracer/Chemtracts Travel Grant, (2008): Conference travel grant.

Graduate Student Association (GSA) Travel Grant, (2007): Conference travel grant.

Datatracer/Chemtracts Travel Grant, (2007): Conference travel grant.

Public Policy and Biological Threats (PPBT) Conference Program, (2006): sponsored by Institute on Global Conflict & Cooperation (IGCC) and funded by Carnegie Foundation.

TA Sabbatical Fellowship, (one quarter tuition and stipend; 2006).

Teaching (TAing) Experience

Advanced Inorganic Chemistry (2006-07): Syntheses and characterization of metal complexes.

Analytical Chemistry (2004-06): Analytical principles and instrumental analysis (UV/vis, cyclic and HMDE voltammetry, flame atomic emission and absorption, fluorescence, plasma ICP-OES).

Organic Chemistry, (2004): Introductory organic chemistry lab.

General Chemistry, (2003-2004): General chemistry, lab and lecture.

Science in the Community / Outreach

Pasadena High School, (2010-present): After-school outreach program with 4-6 HS students using SHArK Kit for discovery of novel mixed metal oxides for photochemical water splitting.

Pasadena High School, (2010-present): In-class outreach program consisting of laboratory exercises in electrochemical water-splitting to H₂ and O₂ using electrodes and solar hobby kits.

Muir High School in Pasadena, (2009-2010): outreach program consisting of laboratory exercises in light absorption, solar energy and assembling blackberry TiO₂ solar cells.

Santa Cruz County Science Fair, (Judge, Chemistry and Biochemistry; 2008)

Santa Cruz County Science Fair, (Judge, Biology and Biochemistry; 2007)

Commentaries/Synopses

The following journal reports/topics were summarized in short commentaries in the journal *ChemTracts: Inorganic Chemistry* (by M. J. Rose and P. K. Mascharak).

- 1) *a)* Blue Phosphorescent Emitters: New N-Heterocyclic Platinum(II) Tetracarbene Complexes. *b)* FRET-Based Sensor for Imaging Chromium(III) in Living Cells. *c)* Selective Monitoring of Parts per Million CO by Immobilized Metal Complexes on Glass. **2008**, 21(1), 37-42
- 2) *a)* Carbon Dioxide Activation at the Ni,Fe-Cluster of Anaerobic Carbon Monoxide Dehydrogenase. *b)* Reversible Single-Crystal Transformation Through Fe–O(H)Me/Fe–OH₂ Bond Formation/Bond Breaking in a Gas-Solid Reaction at an Ambient Condition. *c)* Porous Semiconducting Gels and Aerogels From Chalcogenide Clusters. *d)* Water-Soluble Porphyrins as a Dual-Function Molecular Imaging Platform for MRI and Fluorescence Zinc Sensing. *e)* Polyoxometalate Embedding of a Tetra-ruthenate(IV)-oxo-core by Template-Directed Metalation of [ω-SiW₁₀O₃₆]⁸⁻: A Totally Inorganic Oxygen-Evolving Catalyst. **2007**, 20(9), 387-388; 391-398
- 3) Structure of a Thiol Monolayer-Protected Gold Nanoparticle at 1.1 Å Resolution. **2007**, 20(7), 308-309
- 4) Stable Magnesium(I) Compounds with Mg-Mg Bonds. **2007**, 20(3), 125-126
- 5) Coordination-Driven Nanosized Lanthanide “Molecular Lantern” with Tunable Luminescent Properties. **2006**, 19(11), 458-459
- 6) *a)* Discrete Sandwich Compounds of Monolayer Palladium Sheets. *b)* Synthesis and Characterization of Silyldichloramines, Their Reactions with F⁻ Ions, Instability of N₂Cl₂ and NCl₂⁻, and Formation of NCl₃. **2006**, 19(9), 371-374
- 7) [Fe(CNXyl)₄]²⁻: A Structurally Characterized Homoleptic Isocyanidometalate Dianion. **2006**, 19(8), 318-323
- 8) *a)* Specific, Stable Fluorescence Labeling of Histidine-Tagged Proteins for Dissecting Multi-Protein Complex Formation. *b)* Ruthenium Half-Sandwich Complexes Bound to Protein Kinase Pim-1. *c)* Three-Coordinate Co(I) Provides Access to Unsaturated Dihydro-Co(III) and Seven-Coordinate Co(V). **2006**, 19(8), 331-336
- 9) *a)* The Zintl Ion [Pb₁₀]²⁻: Rare Example of a Homoatomic closo Cluster. *b)* Octa-Uranium Rings With Alternating Nitride and Azide Bridges. *c)* Nanoring-Nanosphere Molecule, {Mo₂₁₄V₃₀}: Pushing the Boundaries of Controllable Inorganic Structural Organization at the Molecular Level. **2006**, 19(5), 205-210
- 10) *a)* Studies of Low-Coordinate Iron Dinitrogen Complexes. *b)* Disruption of Phosphoprotein-Protein Surface Interaction Using Zn(II) Dipicolylamine-Based Artificial Receptors via Two-Point Interaction. *c)* Synthesis of a Stable Compound With Fivefold Bonding Between Two Chromium(I) Centers. **2005**, 18(8), 471-475

Formal Talks

Pacific Northwest National Lab: (November 2010) Covalent Attachment of Model Compounds and H₂-generating Catalysts to Si(111) Surfaces.

Summer Seminar in Synthetic Inorganic Chemistry (Organizer, Session Leader) (July 2010, Caltech) Towards Mono-Iron (Fe) Catalysts for H₂ Generation and Covalent Attachment to Silicon(111) Surfaces

Bioinorganic Gordon Research Seminar (GRS), (February 2010) Phosphine-based P₄N₂ Ni/Co Macrocyces and Reductive Chemistry of the Fe-dmgBF₂-(MeCN/^tBuⁿNC)₂ System.

Caltech Inorganic/Organometallic Seminar (IOS), Synthetic modeling of Fe-NHase: Insights into the Effect of S-oxygenation on its Photoregulation by Nitric Oxide (NO)

University of California Joint-Campus Nitric Oxide Meeting, (Ford, Borovik, Fukuto, Mascharak Groups; 2008) Visible Light Photosensitization of Ruthenium Nitrosyls: Ligand Design and Coordinated Chromophores

Chemical Biology Bay Area (CBAA) Conference at UCSF, (2008) Synthetic Nitric Oxide Carriers: Trackable agents for light-driven NO delivery to Cells

Chemistry & Biochemistry Department Retreat, (2007) Visible Light-Driven Nitric Oxide (NO) Release from Designed Ruthenium Nitrosyls with Coordinated Chromophores

Graduate Mentoring in Synthetic Inorganic Chemistry

Qinchen Dong, (2010-2011) Visiting Ph.D. student from Hong Kong Baptist University: Syntheses of tri/bidentate NP2 ligands bearing pendant functional groups for Si(111) surface attachment; isolation of Ni(II) and Co(II) complexes towards catalysts for H₂ generation. *Inorg. Chem.* doi: 10.1021/ic201213c.

Undergraduate Mentoring in Synthetic Inorganic Chemistry

Rocio Mercado, (2011-present, Caltech): Synthesis and electrocatalytic H₂ generation from perfluorinated cobalt glyoximes: Importance of low-valent intermediates.

Dona Bellone, (2009-2011, Caltech): Syntheses of tripodal tris(diphenylphosphine) ligands and its Co(I) complex; pendant aryl-bromide substituent for Si-C surface attachment. Dona attends UC Berkeley for graduate study in inorganic chemistry. Manuscript submitted to *JACS*.

Nolan Betterley, (2006-2008, UCSC), Honors Thesis Research, Dean's Award for Outstanding Senior Thesis: Syntheses of Fe(III) complexes and {Fe-NO}⁶ nitrosyls derived from a chlorinated N₂S₂ carboxamide/thiolate ligand, included in Rose, Betterley et al., *JACS* **2009**, 131, 8340; and Rose, Betterley et al. *IC* **2010**, 49, 1854.

Eric Alcid, (2004-2006, UCSC): Synthesis of a photoactive ruthenium nitrosyl derived from a pentadentate Schiff base ligand; included in Rose, Alcid et al., *Inorg. Chem.*, **2007**, 46, 2328. Eric was a post-Bac Prof. Jurica's lab in Biology (UCSC), and attends a Ph.D./M.D. program at University of Washington.

Karen Murphy, (2003-2004, UCSC): UCSC Honors Senior Thesis: Synthesis of planar tetradentate N₄-type ligands and effect on photolability of NO from a Ru(III) Center. Karen's work was included in Patra, Rose, Murphy et al., *Inorg. Chem.*, **2004**, 43, 4487 and received M.S. at University of Vermont.

Informal Topic Talks

High-Magnetic-Field EPR: Detection and Spectroscopy of non-Kramers Integer Spin Systems ($S = 1,2$) (2009)

Hypervalent Carbon Compounds: Coordination Chemistry of Carbon (2008)

Demystifying DFT Calculations: an Introduction to DFT as a Practical Approach (2007)

Uranium Processing Techniques and Isotope Enrichment Methods (2006)

Hydrogen Generation from Ethanol based on Ruthenium-Amido complexes (2005); Orals Proposal

Nitric Oxide Reductase (NOR): a mixed Heme/Non-heme Iron Enzyme (2004)

Copper-Dependent Biogenesis of the Tyrosine-based Cofactor Trihydroxyphenylalanine Quinone, TPQ (2003)

Cd NMR as a probe for Zn Fingers (2003)

Kinetic and Thermodynamic Aspects of ΔG in Protein folding (2003)

Associations and Memberships

American Chemical Society (ACS): Inorganic Division, (2003-present)

American Association for Advancement of Science (AAAS), (2005-present)

Virtual Inorganic Pedagogical Electronic Resource (VIPER), (2009-present)

Surfrider Foundation, (1997-present)

Conference Posters/Talks

- 1) M. J. Rose, L. E. O'Leary, J. R. Lattimer, B. S. Brunschwig, H. B. Gray and N. S. Lewis. Covalent Attachment of Transition Metal Complexes to Silicon(111) Semiconductor Surfaces for Hydrogen Evolution. *ACS meeting (Denver)*, Fall **2011**.
- 2) M. J. Rose, D. E. Bellone and H. B. Gray. Syntheses and X-ray structures of tripodal tris(diphenylphosphine) Co(I/II) Complexes, and Strategy for Attachment to a Silicon(111) Semiconductor Surface. *ACS meeting (Anaheim)*, Spring **2011**.
- 3) M. J. Rose, C. Roske, J. R. Winkler and H. B. Gray. Syntheses and Structures of Diglyoxime Iron Complexes derived from the Perfluorinated Ligand Di(pentafluorophenyl)diglyoxime: Electrochemistry and Potential for Electrocatalytic Dihydrogen (H₂) Generation. *ACS meeting (Anaheim)*, Spring **2011**.
- 4) M. J. Rose, J. R. Winkler and H. B. Gray. Reductive Chemistry of Iron(II) Complexes derived from Macrocyclic Glyoximes [(dRgBF₂)₂Fe(solv)₂] (R = Me, Ph; solv = MeCN, ^tBu¹NC). *ACS meeting (San Francisco)*, Spring **2010**.
- 5) M. J. Rose, B. S. Brunschwig, J. R. Winkler and Harry B. Gray. Phosphine-based P₄N₂ Ni/Co Macrocycles and Reductive Chemistry of the Fe-dmgBF₂-(MeCN/^tBu¹NC)₂ System. *Metals in Biology Gordon Conf & Gordon Research Seminar Bioinorganic and CCI-Solar Annual Retreat*. Winter **2010**.
- 6) M. J. Rose, N. M. Betterley, and P. K. Mascharak. Thiolate S-Oxygenation Controls Nitric Oxide (NO) Photolability of a Nitrile Hydratase (Fe-NHase) Model derived from a Mixed Carboxamide/Thiolate Ligand. *ACS meeting (San Francisco)*, Spring **2010**.
- 7) M. J. Rose and P. K. Mascharak. Photosensitization of Ruthenium Nitrosyls to Red Light with an Isoelectronic Series of Heavy-Atom Chromophores: Experimental and DFT Studies on the Effects of O-, S- and Se-substituted Coordinating Dyes. *ACS meeting (San Francisco)*, Spring **2010**.
- 8) M. J. Rose and P. K. Mascharak. Photosensitization of Ruthenium Nitrosyls to Red Light with Coordinated, Heavy-Atom Chromophores. *Southern California Inorganic Photochemistry (SCIP) Conf*, Summer **2009**.
- 9) M. J. Rose and P. K. Mascharak. A Novel Set of Fluorogenic Ruthenium NO Donors: a New Mode of Fluorimetric Delivery of NO to Cells. *ACS meeting (Philadelphia)*, Fall **2008**.
- 10) M. J. Rose and P. K. Mascharak. A Novel Set of Fluorogenic Ruthenium NO Donors: a New Mode of Fluorimetric Delivery of NO to Cells. *ACS meeting (Boston)*, Fall **2007**.
- 11) M. J. Rose, A. K. Patra, E. A. Alcid, M. M. Olmstead and P. K. Mascharak. Tuning the Photolability of the {RuNO}₆ Core of Ruthenium Nitrosyls with the Number and Orientation of Carboxamido-N Donors: A Systematic Investigation. *ACS Meeting (San Francisco)*, Fall **2006**.
- 12) M. J. Rose, A. K. Patra, M. M. Olmstead and P. K. Mascharak. Ruthenium Nitrosyls Derived from N5 Carboxamide or N5 Schiff Base Ligands: Comparison of Stability and Photolability in Aqueous Solution. *ACS Meeting (San Diego)*, **2005**.
- 13) M. J. Rose, I. Lee, T. R. Chapman and D. C. Swinney. Pharmacological Characterization of Clinical Anti-Cholinergic Drugs at M1–M5 Receptor Sub-types. *Mol. Pharm. Meeting (San Francisco)*, *Mol. Biol. Cell* **2002**, 443, 79A.
- 14) D. C. Swinney, M. J. Rose, I. Lee, A. Y. Mak. The Mono-ubiquitination of IκBα S32/36E *in vitro* Shows a Random Bi-Bi Kinetic Mechanism with Respect to IκBα-ee and E2UBCH7. *FASEB J.* **2001**, 15, A26.