

## Justine P. Roth

Assistant Professor of Chemistry

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### I. Education:

- 1995-2000 Ph. D. Chemistry, University of Washington, Seattle  
1990-1994 B.S. Chemistry, University of Florida, Gainesville

### II. Professional Experience:

- 2000-2003 National Institutes of Health Postdoctoral, University of California, Berkeley  
2003-present Assistant Professor of Chemistry, Johns Hopkins University  
2005-present Chemistry-Biology Interface Program (CBI-JHU)  
2007-present Program for Molecular Biophysics (PMB-JHU)

### III. Honors and Awards (2000-present):

- 2008 Camille Dreyfus Teacher Scholar Award  
2007 Alfred P. Sloan Research Fellowship Award  
2006 Research Corporation Cottrell Scholar Award  
2006 Paul D. Saltman Award Lecture, *Metals in Biology* Gordon Conference  
2005 NSF CAREER Award  
2004 ACS PROGRESS/Dreyfus Foundation Lectureship  
2004 Synlett and Synthesis New Faculty Journal Award  
2000-2003 National Institutes of Health Postdoctoral Fellowship

### IV. Publications:

(\* designates corresponding authorship)

#### A. From Johns Hopkins University:

28. "Tyrosyl Radical Formation in Heme Oxygenase: Competing Mechanisms of Electron Transfer and Concerted Proton Coupled Electron Transfer" V.V. Smirnov, A. Aguilera, J. P. Roth\* **in preparation**.
27. "Heavy Atom Isotope Effects as Probes of Transition Metal-Mediated Small Molecule Activation." J. P. Roth\* in *Physical Inorganic Chemistry: Methods and Techniques* Vol. 1, Wiley, New York: invited book chapter, **accepted**.
26. "Oxygen Isotope Effects as Probes of Electron Transfer Mechanisms and Structures of Activated O<sub>2</sub>." J. P. Roth\* *Accounts of Chemical Research* **ASAP, 2009**.
25. "Computational Modeling of Oxygen Isotope Effects on Metal-Mediated O<sub>2</sub> Activation at Varying Temperatures." V. V. Smirnov, M. P. Lanci, J. P. Roth\* *Journal of Physical Chemistry (Max Wolfsberg Festschrift)* **ASAP, 2009**.
24. "Evidence for Protein-Radical Mediated Nuclear Tunneling in Fatty Acid  $\alpha$ -Oxygenase," A. Gupta, A. Mukherjee, K. Matsui, J. P. Roth\* *Journal of the American Chemical Society* **2008**, *130*, 11274-11275.
23. "Inner Sphere Mechanism for Molecular Oxygen Reduction Catalyzed by Copper Amine Oxidases." A. Mukherjee, V. V. Smirnov, M. P. Lanci, D. E. Brown., E. M. Shepard, D. M. Dooley, J. P. Roth\* *Journal of the American Chemical Society* **2008**, *130*, 9459-9473.

22. "Direct Examination of H<sub>2</sub>O<sub>2</sub> Activation by a Heme Peroxidase." J. P. Roth\*; C. J. Cramer\* *Journal of the American Chemical Society* **2008**, *130*, 7802-7803.
21. "Isotopic Probing of Molecular Oxygen Activation at Copper(I) Sites." M. P. Lanci, V. V. Smirnov, C. J. Cramer, E. V. Gauchenova, J. Sündermeyer, J. P. Roth\* *Journal of the American Chemical Society* **2007**, *129*, 14697-14709.
20. "Advances in Studying Bioinorganic Reaction Mechanisms: Isotopic Probes of Activated Oxygen in Metalloenzymes." J. P. Roth\* *Current Opinion in Chemical Biology* **2007**, *11*, 142-150.
19. "Molecular Oxygen Dependent Steps in Fatty Acid Oxidation by Cyclooxygenase-1 (COX-1)." A. Mukherjee, D. W. Brinkley, K.-M. Chang, J. P. Roth\* *Biochemistry* **2007**, *46*, 3975-3989.
18. "Mechanisms of Electron Transfer in Catalysis by Copper Zinc Superoxide Dismutase." V. V. Smirnov, J. P. Roth\* *Journal of the American Chemical Society* **2006**, *128*, 16424-16425.
17. "Oxygen Isotope Effects upon Reversible O<sub>2</sub>-Binding Reactions: Characterizing Mononuclear Superoxo and Peroxo Structures." M. P. Lanci, J. P. Roth\* *Journal of the American Chemical Society* **2006**, *128*, 16006-16007.
16. "Evidence for Cu-O<sub>2</sub> Intermediates in Superoxide Oxidation by Biomimetic Copper(II) Complexes." V. V. Smirnov, J. P. Roth\* *Journal of the American Chemical Society* **2006**, *128*, 3683-3695.
15. "Probing Metal-Mediated O<sub>2</sub> Activation in Chemical and Biological Systems." V. V. Smirnov, D. W. Brinkley, M. P. Lanci, K. D. Karlin, J. P. Roth\* *Journal of Molecular Catalysis A*, **2006**, *251*, 100-107.
14. "Oxygen Kinetic Isotope effects as Probes of Enzymatic Activation of Molecular Oxygen." J. P. Roth\*, J. P. Klinman\* in *Isotopes Effects in Chemistry and Biology*, Kohen, A., Limbach, H.-H. Eds. CRC Press, Boca Raton, **2006**, 645-669.
13. "Bifunctional Lewis Acid-Nucleophile-Based Asymmetric Catalysis: Mechanistic Evidence for Imine Activation Working in Tandem with Chiral Enolate Formation in the Synthesis of β-Lactams." S. France, M. H. Shah, A. Weatherwax, H. Wack, J. P. Roth, T. Lectka\* *Journal of the American Chemical Society*, **2005**, *127*, 1206-1215.
12. "Determination of a Large Reorganization Energy Barrier for Hydride Abstraction by Glucose Oxidase." D. W. Brinkley, J. P. Roth\* *Journal of the American Chemical Society* **2005**, *127*, 15720-1.
11. "Structures of Transition States in Metal-Mediated O<sub>2</sub> Activation Reactions." M. P. Lanci, D. W. Brinkley, K. L. Stone, V. V. Smirnov, J. P. Roth\* *Angewandte Chemie International Edition* **2005**, *44*, 7273-7276
10. "Oxygen Isotope Effects on Electron Transfer to O<sub>2</sub> Probed Using Chemically Modified Flavins Bound to Glucose Oxidase." J. P. Roth\*, R. Wincek, G. Nodet, D. E. Edmondson, W. S. McIntire, J. P. Klinman\* *Journal of the American Chemical Society* **2004**, *126*, 15120-15131.

#### **B. From Postdoctoral or Graduate Studies:**

9. "The First Crystal Structure of a Monomeric Phenoxy Radical: 2,4,6-Tri-tert-butylphenoxy Radical." V.W. Manner, T.F. Markle, J. H. Freudenthal, J. P. Roth, J. M. Mayer\* *Journal of the Chemical Society: Chemical Communications* **2008**, *2*, 256-258.
8. "Stoichiometric Oxidations of Sigma-Bonds: Radical and Possible Non-Radical Pathways." J. M. Mayer\*, E. A. Mader, J. P. Roth, J. M. Bryant, T. Matsuo, A. Dehestani, B. C. Bales, E. J. Watson, T. Osaka, K. Valliant-Saunders, W. H. Lam, D. A. Hrovat, W. T Borden, E.J. Davidson *Journal of Molecular Catalysis A*, **2006**, *251*, 24-33.
7. "Kinetic Isotope Effects." J. P. Roth, J. P. Klinman\* *Encyclopedia of Biological Chemistry*, Lennarz, W.J.; Lane, M. D. Eds., Elsevier, San Diego, **2004**, *2*, 522-527.
6. "Electron and Hydrogen Atom Self-Exchange Reactions of Iron and Cobalt Coordination Complexes." J. C. Yoder, J. P. Roth\*, E. M. Gussenhoven, A. Larsen, J. M. Mayer\* *Journal of the*

*American Chemical Society*, **2003**, 125, 2629-2640.

5. "Catalysis of Electron Transfer during O<sub>2</sub> Activation by the Flavoprotein Glucose Oxidase." J. P. Roth, J. P. Klinman\* *Proceedings of the National Academy of Sciences, USA* **2003**, 100, 62-67.
4. "Application of the Marcus Cross Relation to Hydrogen Atom Transfer Reactions of Transition Metal Complexes." J. P. Roth, J. C. Yoder, T.-J. Wan, J. M. Mayer\* *Science* **2001**, 294, 2524-2526.
3. "Intrinsic Barriers for Electron and Hydrogen Atom Transfer Reactions of Biomimetic Iron Complexes." J. P. Roth, S. Lovell, J. M. Mayer\* *Journal of the American Chemical Society* **2000**, 122, 23, 5486-5498.
2. "Hydrogen Atom Abstraction by Transition Metal Complexes. J. M. Mayer\*, J. P. Roth, K. Wang *ACS, Division of Fuel Chemistry Symposia* **1999**, 44, 434-436.
1. "Hydrogen Transfer Reactivity of a Ferric Bi-imidazoline Complex That Models the Activity of Lipoxygenase Enzymes." J. P. Roth, J. M. Mayer\* *Inorganic Chemistry* **1999**, 38, 2760-2761.

#### V. Invited Lectures (2003-present):

##### A. National and International Conferences:

32. "New Faces in Biomimetic Coordination Chemistry" Symposium. 238<sup>th</sup> National American Chemical Society Meeting, Washington DC (08/09)
31. International Conference on Biological Inorganic Chemistry (ICBIC-14) Nagoya, Japan (07/09)
30. Goldschmidt 2009, "Challenges to our Volatile Planet" conference in Biogeochemistry Davos, Switzerland (06/09)
29. "Flavoprotein Catalysis of Electron and Hydride Transfer. 2<sup>nd</sup> International Conference on Vitamins, Coenzymes and Biofactors Athens, GA (10/08)
28. "Transition State Structures in Oxygen Activation."  
Symposium: *Advances in the Electronic Structure of Transition Metal Systems and Organometallics*, 236<sup>th</sup> National American Chemical Society Meeting, Philadelphia, PA (08/08).
27. "C-H Oxidation by Tyrosyl Radical-Containing Heme Enzymes."  
Department of Energy (DOE) Catalysis Conference Annapolis, Maryland (05/08).
26. "Tyrosyl Radicals in Heme Proteins: From Mechanisms of Formation to Involvement in Catalysis."  
*Protein Cofactors, Radicals, and Quinones* Gordon Research Conference; Ventura (01/08)
25. "Mechanisms of Molecular Oxygen Activation in Biocatalysis Probed Using Isotope Effects."  
*Stable Isotope Tools for the Assessment of Chemical and Microbial Transformation Reactions in Complex Natural and Contaminated Environments* Mt. Verita, Switzerland (11/07)
24. "Application of Marcus Theory to Enzyme Catalyzed C-H Oxidation."  
Symposium: *Strategies in Enzymatic Oxidation Catalysis*, 234<sup>th</sup> National American Chemical Society Meeting, Boston, MA (08/07).
23. "Structures and Reactivity Patterns of Activated Oxygen Intermediates in Metalloenzymes."  
*Enzymes, Coenzymes and Metabolic Pathways* Gordon Research Conference; Biddeford, ME (07/07)
22. "What can <sup>18</sup>O Isotope Effects Reveal about Structures of Activated Oxygen Intermediates?"  
*Fifth International Congress on Isotopes*, Castellón, Spain (05/07)
21. "Towards a Predictive Understanding of Oxygen Activation in Chemical and Biological Systems."  
*Inorganic Reaction Mechanisms* Gordon Research Conference; Ventura, CA (02/07).
20. "Studies of Enzyme Mechanisms Based on Traditional Biological, Physical and Inorganic Chemistry Approaches." *Living at the Interface: Challenges in Interdisciplinary Research*, ACS Southwest Regional Meeting Houston, TX (10/06).
19. "Characterizing Activated Oxygen Intermediates in Enzymes."

*Paul D. Saltman Lecture, Metals in Biology* Gordon Research Conference; Ventura, CA (01/06).

18. "Probing Metal-Mediated Dioxygen Activation in Chemical and Biological Systems."  
*Activation of Dioxygen and Homogeneous Catalytic Oxidation—9th International Symposium ADHOC-2005*; University of Cologne, Cologne, Germany (07/05).
17. "Oxygen-18 Kinetic Isotope Effects on O<sub>2</sub> Activation Reactions."  
*Isotopes in Chemical and Biological Sciences* Gordon Research Conference; Ventura, CA (02/04).
16. "A Marcus-Hush Approach to Understanding Enzyme-Catalyzed Redox Reactions."  
*Photosynthesis* Gordon Research Conference; Bristol, RI (06/03).

**B. Universities:**

15. University of Washington (09/2009)
14. University of Minnesota (04/09)
13. University of Pennsylvania (03/09)
12. North Carolina State University (03/09)
11. Texas A&M University (02/09)
10. Johns Hopkins University (09/08)
9. Columbia University (04/08)
8. Pennsylvania State University (02/08)
7. Montana State University (05/07)
6. University of Wisconsin, Madison (05/07).
5. Georgetown University (04/07).
4. Georgia State University (10/06).
3. University of Delaware (04/05).
2. University of North Carolina, Chapel Hill (03/05).
1. Randolph-Macon College (11/04).