PUBLICATIONS

Danforth, R. A.; Kohler, B. "Ultrafast Photochemical Dynamics of the Hexaaquairon(III) Ion", Chem. Phys. Lett. 2017, http://dx.doi.org/10.1016/j.cplett.2017.02.048

PRESENTATIONS

"Ultrafast Photochemical Dynamics of the Hexaaquairon(III) Ion"
Pacific Conference on Spectroscopy and Dynamics
Asilomar, CA

"Ultrafast Decay Kinetics of Hydrolyzed Iron(III) in Aqueous Solutions Upon Photoexcitation"
4th Year Seminar for the Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT

"Excited State Dynamics of Aqua-Iron(III) Complexes at Low pH Utilizing Ultrafast Transient Absorption Spectroscopy"
Poster presented at the annual Optec Conference, Bozeman, MT

MONTANA STATE UNIVERSITY
Mountains & Minds

Department of Chemistry and Biochemistry

Doctor of Philosophy in Chemistry

DISSERTATION DEFENSE

Miss Rebecca A. Danforth

B.Sc. Hope College, Holland, MI (2012)

2015

Friday, April 14, 2017 – 2 pm
Byker Auditorium
Department of Chemistry and Biochemistry

"Ultrafast Photochemistry of Aqueous Iron(III) Complexes"

Graduate Committee

Dr. Bern Kohler (Co-Advisor)
Dr. Eric Grumstrup (Co-Advisor)
Dr. Rob Walker (Chemistry)
Dr. Rufus Cone (Physics)
Dr. Aleks Rebane (Physics)

ABSTRACT

The ultrafast photochemical dynamics of aqueous iron(III) solutions were measured utilizing ultrafast pump probe spectroscopy. Aqueous solutions of iron(III) were prepared at low pH (<4.5) and low iron(III) concentration (<5 mM) to allow for small aquairon(III) complexes and ferrihydrite to be studied. Small monomeric and dimeric aquairon(III) complexes were studied to elucidate the mechanisms involved in the formation of $OH^{\bullet}$ after UV excitation which were previously known to generate $OH^{\bullet}$ in vastly different quantities. Upon excitation of Fe^{3+}, a proton is released from a coordinated water molecule to generate $FeOH^{2+}$ in less than 200 fs. The newly generated $FeOH^{2+}$ can then undergo numerous recombination pathways to regenerate the Fe^{3+}. Approximately 10% of the excited Fe^{3+} undergoes photoreduction and subsequent release of $OH^{\bullet}$ and Fe^{2+} within 20 ps. Exciting $FeOH^{2+}$, leads to the direct separation to generate Fe^{2+} and $OH^{\bullet}$ with a wavelength dependent yield with a lifetime of 20 ps. $Fe_2(OH)_2^{4+}$does not generate significant quantities of $OH^{\bullet}$ but instead breaks into two $FeOH^{2+}$ molecules that recombine to regenerate $Fe_2(OH)_2^{4+}$. To further the understanding of the primary kinetics of iron(III) in aqueous solutions, ferrihydrite nanoparticles were studied. Ferrihydrite exhibits similar dynamics to hematite in which electrons are excited into the conduction band of ferrihydrite. The electrons can then relax to the bottom of the conduction band within 390 fs before undergoing various recombination process. This limits the amount of iron(III) converted into iron(II) in ferrihydrite. All iron(III) systems studied show unique kinetics after excitation that elucidate the mechanisms behind the generation of $OH^{\bullet}$.

BIOGRAPHICAL NOTES

Academic Preparation:

2008-2012 Hope College, Holland, MI (May 2012)
Bachelor of Science in Chemistry
With ACS Certification
Advisor: Dr. Kenneth Brown

2012 University of Pennsylvania, LRSM (Jan.-May 2012
Intern at Environmental Resources Management
Testing the Toxicity of Effluent Waters from Corporations

2011 Hope College (Jun.–Aug.)
Undergraduate Summer Research
Research: Electrochromism of Tris-1,10-phenanthroline Iron(II/III)
Advisor: Dr. Kenneth Brown

Graduate Studies

Field of Study: Physical Chemistry

Courses

Teaching and Outreach Activities

2012 Chemistry 141 Lab TA, Montana State University (Aug.-Dec.)
2013 General Chemistry Lab TA, Montana State University (Jan.-May, Aug.-Dec.)
2014 General Chemistry Recitation TA, Montana State University (Jan.-May)
2015 General Chemistry Recitation TA, Montana State University (Jan.-Dec.)
2016 General Chemistry Recitation TA, Montana State University (Jan.-May, Aug.-Dec.)
2016 General Chemistry Lab TA, Montana State University (May-Jul.)
2014 Nanodays Outreach
2015 Nanodays Outreach and Science Olympiad Coach

Awards

2017 PhD. Dissertation Completion Award (The Graduate School)
2016 E.W. Mares Award (Department of Chemistry and Biochemistry)
2008 Bob Roth Chemistry and Engineering Scholarship
2009 Bob Roth Chemistry and Engineering Scholarship