

Friday, November 9
Miami Inn, Lower Level
7:00 – 9:00 Poster session and mixer
Complimentary snacks and beverages

Poster set-up is available starting at 5:00 pm.

Following the poster session, please remove your posters. They can be redisplayed in Marcum 112 during the Saturday session.

POSTERS

Hydrothermal synthesis of two basic lead carboxylates

Catherine M. Oertel, Catherine M. Mauck, and Titus van den Heuvel
Department of Chemistry and Biochemistry, Oberlin College, Oberlin OH
Matthias Zeller
Department of Chemistry, Youngstown State University, Youngstown OH

Cationic, thiophene-fused heterocyclic complexes of ruthenium

Uttam R. Pokharal and John P. Selegue
Department of Chemistry, University of Kentucky, Lexington KY

Boron-doped and metal oxide-coated carbon nano-onions

John D. Craddock and John P. Selegue
Department of Chemistry, University of Kentucky, Lexington KY

Organometallic and materials chemistry

John P. Selegue, Nathan Tice, Sean Parkin, Minh Truong, John Anthony, John D. Craddock, Mark Meier and Rodney Andrews
Department of Chemistry, University of Kentucky, Lexington KY
Center for Applied Energy Research, University of Kentucky, Lexington KY

Neodymium, gadolinium and terbium complexes containing hexafluoro-acetylacetonate and 2,2'-bipyrimidine: Structural and spectroscopic characterization

Albert Fratini, Gregory Richards, Emily Larder and Shawn Swavey
Department of Chemistry, University of Dayton, Dayton OH

A ruthenium porphyrin as potential DNA binding agent and photodynamic therapy (PDT) agents

Sandya Rani Beeram and Shawn Swavey
Department of Chemistry, University of Dayton, Dayton OH

A porphyrin-ruthenium photosensitizer as potential photodynamic therapy agent

Kyle Davia, David King, Yiling Hong and Shawn Swavey
Department of Chemistry, University of Dayton, Dayton OH

Synthesis and toxicity studies of tris-aminomethylethane tri-carbonyl rhenium (I) salts on HeLa and vascular smooth muscle cells

Sarah Robenstine
Department of Chemistry, University of Akron, Akron OH

Synthesis and coordination chemistry of the oxycarbahemiporphyrazines

Natalie Barone
Department of Chemistry, University of Akron, Akron OH

Metal binding chemistry of the carbahemiporphyrazines

Saovalak Sripothanognak
Department of Chemistry, University of Akron, Akron OH

Synthesis and characterization of glyoxime complexes of $\text{Re}(\text{CO})_3^+$

Roshinee Costa
Department of Chemistry, University of Akron, Akron OH

Molecular phosphates, phosphonates, and phosphinates of aluminum

Ryan Rondo
Department of Chemistry, University of Toledo, Toledo OH

Phototriggered isomerization of a ruthenium (II) chelating sulfoxide complex: Direct S \rightarrow O relaxation in picoseconds

Beth Anne McClure
Department of Chemistry, Ohio University, Athens OH

Zn is the important metal for catalytic activity for *Arabidopsis thaliana* GLX2-2

Ross M. McKinney, Pattrarane Limphong, Christopher A. Makaroff, and Michael W. Crowder
Department of Chemistry & Biochemistry, Miami University, Oxford OH

Transcriptional response to external zinc: Zn homeostasis in *E. coli*

Andrew Herre, Thusitha Gunasekera and Michael W. Crowder
Department of Chemistry & Biochemistry, Miami University, Oxford OH

Catalytic activity variation found in L1 metallo- β -lactamases of differing metal content

Lauren Spadafora and Michael W. Crowder
Department of Chemistry & Biochemistry, Miami University, Oxford OH

Characterization of Bla2, a metallo- β -lactamase

Megan Hawk and Michael W. Crowder

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Ultramicroporous metal-organic framework for selective gas adsorption

Erika S. Manis, Shengqian Ma, Xi-Sen Wang, Christopher D. Collier and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Incorporation of synthetic analogues of iron-sulfur clusters in metal-organic frameworks

Ryan Kuppler, Betty Ooro and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Ligand-mediated metal-organic framework topologies

Aaron G. Nash, Dan Zhao and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Microporous metal-organic framework with high hydrogen and methane uptakes based on double-bond-coupled diisophthalate linkers

Joseph J. López, Xi-Sen Wang and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Microporous metal-organic framework based on angular linkers exhibiting high hydrogen uptake

Brandon Murphy, Xi-Sen Wang and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Cooperative two-electron transfer reagents

Sayande Chatterjee, Levi J. Grove, Tyler W. Green, Jeanette Krause and William B. Connick

Department of Chemistry, University of Cincinnati, Cincinnati OH

Synthesis and characterization of an octanuclear cyanometalate complex that exhibits thermally- and light-induced intramolecular electron transfer

Dongfeng Li and Stephen M. Holmes

Department of Chemistry, University of Kentucky, Lexington KY

Rodolphe Clérac

Centre de Recherche Paul Pascal, UPR-CNRS 8641, 33600 Pessac, France

Corine Mathonière

Institut de Chimie de la Matière Condensée de Bordeaux, Groupe des Sciences Moléculaires, UPR-CNRS 9048, 33608 Pessac, France

High-spin trigonal bipyramidal nickel (II) complexes

Huaibo Ma, Swarup Chattopadhyay, and Michael Jensen

Department of Chemistry and Biochemistry, Ohio University, Athens OH

Biomimetic organosulfur coordination chemistry at high-spin nickel (II) centers

Swarup Chattopadhyay, Tapash Deb, Huaibo Ma, and Michael Jensen

Department of Chemistry and Biochemistry, Ohio University, Athens OH

Jeffrey Petersen

C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown WV

Victor Young, Jr.

*Department of Chemistry, X-ray Crystallographic Laboratory, University of Minnesota,
Minneapolis MN*

Orthometallated zirconium complexes utilizing acetophenone imine ligands: The effect of steric bulk on reactivity and isomerization

John F. Beck and Joseph A. R. Schmidt

Department of Chemistry, University of Toledo, Toledo OH

3-Iminophosphine palladium(II) complexes as intermolecular hydroamination catalysts for the formation of imines and enamines

Andrew R. Shaffer and Joseph A. R. Schmidt

Department of Chemistry, University of Toledo, Toledo OH

New scorpionate ligands from 2-substituted calix[4]arene

Matthew P. Hertel and Joseph A. R. Schmidt

Department of Chemistry, University of Toledo, Toledo OH

Saturday, November 10
Marcum Conference Center, Rooms 102 & 112

8:30 – 9:00 Coffee and pastries, room 112
10:30 – 3:00 Drinks and snacks, room 112
9:15 – 4:00 Oral presentations, room 102

ORAL PRESENTATIONS

9:10 Welcome & opening remarks

9:15 – 10:30 Session I

Self-quenching of a luminescent platinum (II) diimine complex

Amber Shiveley, William B. Connick

Department of Chemistry, University of Cincinnati, Cincinnati OH

Luminescent platinum (II) diimine complexes are of particular interest because of their potential application in areas such as chemical sensing and multielectron photocatalysis. In an effort to better understand the rich photophysical and photochemical properties of this class of compounds, we are investigating a platinum (II) diimine complex, Pt(phen)(bpa)₂ (phen=1,10-phenanthroline; bpaH=1-butyl-4-phenylacetylene). This compound has been characterized by ¹H NMR spectroscopy, elemental analysis and UV-visible absorption spectroscopy. The complex exhibits long-lived luminescence in fluid solution. In dilute solutions, the emission maximum occurs at 612 nm. With increasing concentration a new feature grows in near 740 nm. The long-wavelength band is tentatively attributed to excimer emission. Steady-state and time-resolved emission spectroscopy probing the kinetics and mechanism of the self-quenching process will be discussed.

The electron-transfer chemistry of two-electron platinum reagents with modified pincer ligands

Ronnie Muvirimi, Jeanette A. Krause, William B. Connick

Department of Chemistry, University of Cincinnati, Cincinnati OH

A central problem in thermal and photochemical catalysis is the manipulation and delivery of multielectron redox equivalents for substrate activation. As a step toward understanding and learning to control cooperative, outer-sphere two-electron transfer reactions, we have developed a strategy for designing platinum complexes whose reactivity is characterized by transfer of the first electron being less favorable than transfer of the second. The complexes are composed of two potentially meridional-coordinating tridentate ligands that are capable of stabilizing both four-coordinate platinum (II) and six-coordinate platinum (IV). In this presentation, the synthesis, characterization and electronic properties of a series of outer-sphere two-electron reagents will be presented.

These results demonstrate that the apparent two-electron redox potential is modulated by more than 200 mV. In addition, we will discuss variable temperature NMR measurements probing the conformational dynamics of the dangling nucleophiles.

Reaction of aqueous methylmercuric compounds with iron (II) species

John S. Thayer

Department of Chemistry, University of Cincinnati, Cincinnati OH

Methylmercuric compounds in water act as one-electron oxidizing agents towards metals and metal compounds. Iron metal slowly reduces dissolved mercury; the rate accelerates markedly when mixed-valence iron oxides are included. Iron (II), forming during the reaction, appear to be the active species. Ferrocyanide ion reacts rapidly with dissolved methylmercuric compounds, forming ferricyanide initially and mixed Fe(II)-Fe(III) cyanides subsequently. Proposed mechanisms for these reactions will be presented. Iron/iron oxide systems show considerable potential for removing methylmercuric compounds from polluted waters.

10:30 – 10:45 Break

10:45 – 11:45 Session II

The flexible binding site of a “Zn(II)-specific” binding center

Peter Hu and Michael W. Crowder

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Metallo- β -lactamase L1 belongs to B3 subgroup of metallo- β -lactamases, which hydrolyze all known clinically-used β -lactam-containing antibiotics by utilizing a Zn(II)-coordinated hydroxide. L1 contains two Zn(II) ions: one is coordinated by three histidines and one bridging hydroxide (Zn₁); the second Zn ion binds two histidines, one aspartate, one terminal water, and one bridging hydroxide (Zn₂). In order to understand the function of each Zn(II), we have prepared and characterized analogs of L1 that contain Co(II) or Fe. Our data show that (1) The Zn₁ site is essential for activity and more specific for Zn(II). (2) The Zn₂ site is flexible and can be substituted by Co(II) and Fe ion. (3) By unfolding/refolding, both sites can be replaced by Fe and Co. (4) The Zn₁L1, Zn₁Co₂L1, and Zn₁Fe₂ analogs of L1 exhibit good catalytic activities; however, the Fe₁Fe₂-analog is inactive. (5) The Zn₂ site is important for the fluorescence change during catalysis and in the formation of intermediate.

Glyoxalase 2-1 from *Arabidopsis thaliana* has the β -Lactamase Activity

Patrarane Limphong, Michael W. Crowder, and Christopher A. Makaroff

Department of Chemistry & Biochemistry, Miami University, Oxford OH

The glyoxalase system consists of two enzymes, glyoxalase 1 (GLXI) and glyoxalase 2 (GLXII), which catalyze the detoxification of the lipid metabolism by-product,

methylglyoxal. GLXII is a metallohydrolase containing a highly-conserved metal binding domain T-H-X-H-X-D-H reported to coordinate two zinc atoms in human GLXII. Unlike in humans, there are five isozymes of GLX2 in *Arabidopsis thaliana*, and several of these isozymes have been shown to bind Zn, Fe, and Mn. GLX2-1 is distinct among the plant isozymes because it has an Arg at position 272 where all of the other GLXII's have a His. However, GLX2-1 has been shown to bind 2 equivalents of metal. GLX2-1 is not a glyoxalase II because it cannot hydrolyze SLG. Nonetheless, GLX2-1 can catalyze the hydrolysis of β -lactam-containing antibiotics, suggesting that metallo- β -lactamases are descendants of GLXII, and that GLX2-1 may be the "missing link."

11:45 – 1:15 Lunch

Uptown Oxford – see attached map

1:15 – 2:30 Session III

Bridging complexes of aluminum alkyls with di- and tri(3-methylindolyl)methanes

Nicholas Kingsley, Kristin Kirschbaum, and Mark R. Mason*

Department of Chemistry, The University of Toledo, Toledo OH

We have prepared a series of di- and tri-(3-methylindolyl)methane complexes of aluminum trialkyls. These complexes show a non-typical binding mode that involves the bridging of aluminum centers by the indolyl moieties. These are the first examples of μ_2 -N indolyl coordination mode for a group 13 metal, although similar coordination has been observed in complexes of group 1 metals. These complexes have been characterized by X-ray crystallography and NMR spectroscopy. Details of the syntheses and characterization of ligands and complexes will be presented.

Are superacids responsible for the irreproducibility issues in chlorophosphazenes?

Zin-Min Tun, Amy J. Heston, Matthew J. Panzner, Debasish Banerjee, Deepa Savant, Peter Rinaldi, Wiley J. Youngs and Claire A. Tessier

Department of Chemistry, The University of Akron, Akron OH

The applications of polyphosphazenes range from biomedical materials to fire-retardant additives. However, inefficiency and irreproducibility in the synthesis and handling of the chlorophosphazene precursor materials hinder the wide usage of phosphazene polymers. In order to address some of these challenges, we are investigating the acid-base chemistry of $[\text{PCl}_2\text{N}]_3$. The reactions of the weak base $[\text{PCl}_2\text{N}]_3$ with Lewis acids gave adducts $[\text{PCl}_2\text{N}]_3\cdot\text{MX}_3$ ($\text{MX}_3 = \text{AlCl}_3, \text{AlBr}_3, \text{GaCl}_3$) under rigorous anaerobic conditions and superacid adducts $[\text{PCl}_2\text{N}]_3\cdot\text{HMX}_{m+1}$ ($\text{HMX}_{m+1} = \text{HAlCl}_4, \text{HAlBr}_4, \text{HSbCl}_6$) in the presence of a stoichiometric quantity of water. The superacid adducts $[\text{PCl}_2\text{N}]_3\cdot\text{HMX}_{m+1}$ ($\text{HMX}_{m+1} = \text{HAlCl}_4, \text{HAlBr}_4$) were also formed by reacting $[\text{PCl}_2\text{N}]_3\cdot\text{MX}_3$ ($\text{MX}_3 = \text{AlCl}_3, \text{AlBr}_3$) with HX ($\text{HX} = \text{HCl}, \text{HBr}$). It appears that HMX_4 was generated from MX_3 and HX, the latter being formed from the reaction of MX_3 with water. These superacid adducts were characterized by X-ray crystallography and multi-nuclear, variable-temperature, NMR studies. As a result of this work, we hypothesize that marginally-stable, super (or very strong) acid HPCl_6 ,

formed from PCl_5 impurities in $[\text{PCl}_2\text{N}]_3$ and water, may be at least partially responsible for the irreproducibilities mentioned earlier.

Challenges in the mass spectrometric characterization of inorganic polymers:

Poly(dichlorophosphazene)s and poly(siloxane)s

Alyson M. Leigh, Claire A. Tessier, and Chrys Wesdemiotis

Department of Chemistry, The University of Akron, Akron OH

This research focuses on the characterization of two major classes of inorganic polymers, phosphazenes and siloxanes, using mass spectrometry. Tandem mass spectrometry has the potential to provide insight into the degradation mechanisms of the polymers and is useful for the characterization of their macrostructures, architectures and end groups. MALDI ionization was most useful for the two types of polymers and choice of the correct cationizing agent was important. MS and tandem MS were used to elucidate the end groups of the short chain chlorophosphazenes that are obtained as by-products from the synthesis of the ring $[\text{PCl}_2\text{N}]_3$. MS/MS fragmentation behavior of various polydimethylsiloxane (PDMS) systems was evaluated.

2:30 – 2:45 Break

2:45 – 4:00 Session IV

Metal-organic framework from an anthracene derivative containing nanoscopic cages exhibiting high methane uptake

Christopher D. Collier, Shengqian Ma, and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

A microporous metal-organic framework, PCN-14, based on an anthracene derivative, 5,5'-(9,10-anthracenediyl)di-isophthalate (H_4adip), was synthesized under solvothermal reaction conditions. X-ray single-crystal analysis revealed that PCN-14 consists of nanoscopic cages suitable for gas storage. N_2 -adsorption studies of PCN-14 at 77 K reveal a Langmuir surface area of $2176 \text{ m}^2/\text{g}$ and a pore volume of $0.87 \text{ cm}^3/\text{g}$. Methane adsorption studies at 290 K and 35 bar show that PCN-14 exhibits an absolute methane-adsorption capacity of 230 v/v, 28% higher than the DOE target (180 v/v) for methane storage.

A microporous metal-organic framework with high hydrogen and methane storage capacities

Xi-Sen Wang, Shengqian Ma, Daqiang Yuan, and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

Solvothermal reaction of $\text{Cu}(\text{NO}_3)_2$ with H_4mbip gave rise to a metal-organic framework, $\text{Cu}_2(\text{mpib})(\text{H}_2\text{O})_2 \cdot 3\text{DMA}$ (PCN-12). X-ray single crystal analysis revealed that PCN-12 consists of cuboctahedral cages suitable for gas storage. At 77 K and 760 torr, the hydrogen uptake of PCN-12 can reach 3.0 wt% (24.45 g/L); at a pressure of 50 bar, its hydrogen

adsorption capacity is 5.55 wt% (45.23 g/L). Methane adsorption studies at 298 K and 35 bar show that PCN-12 exhibits an access methane-adsorption capacity of 220 v/v, 23% high than the DOE target (180 v/v) for methane storage.

Construction of metal-organic framework with permanent porosity based on hexatopic ligand

Dan Zhao and Hong-Cai Zhou

Department of Chemistry & Biochemistry, Miami University, Oxford OH

One novel metal-organic framework has been constructed with hexatopic ligand and copper salt. The crystal material has permanent porosity with the Langmuir surface area 2990 m²/g (BET surface area 2508 m²/g) and is stable up to 300 °C. Hydrogen adsorption study shows the hydrogen uptake is 1.97 wt% at 77K under 1 atm.

4:00 Closing remarks

4:30 (Optional)

Visit the Ohio Eminent Scholar Laboratory for Structural Biology, located in the Department of Chemistry and Biochemistry at Miami University. Prof. Michael Kennedy and his research group will lead a tour through this recently-constructed facility, which features the only 850 MHz NMR spectrometer in the United States.

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