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# Catalysis Club of Philadelphia

Thursday, October 18, 2007

Holiday Inn Select Hotel

Naamans Road and I-95, Claymont, DE

## A Sudden Expansion in Multi-dimensional High Silica 10-ring Zeolites; Why Now?

Dr. Stacey I. Zones

Chevron Energy and Technology Center, Richmond, California

&

## Is There a Relationship Between the M=O Bond Strength of Bulk Mixed Metal Oxides and Catalytic Activity?

Kamalakanta Routray

Lehigh University  
(Student Talk, 15 minutes)

Social Hour: 5:30 PM

Dinner: 6:30 PM

Meeting: 7:30 PM

Members: \$30.00

Walk Ins & Non-members:

\$35.00

Student & Retired Members:

\$15.00

### Menu

*Chicken Dijonaise: Served  
with a Delicate Dijon Cream*

*Sliced Sirloin of Beef: Served  
with a Mushroom Bordelaise  
Sauce*

*Wild Mushroom Ravioli: With  
Saffron Leek Sauce*

**Meal reservations** - Please notify your company representative or Carl Menning (menning@udel.edu, phone: 302-893-9398, fax: 302-831-1048) by **Thursday, October 11.**

Company Representatives - We would like to encourage you to make meal/meeting reservations to your company representative.

**Membership** - Dues for the 2007-08 season will be \$10.00 (\$5.00 for the local chapter and \$5.00 for the national club). Dues for students and post-docs will be \$6.00 (\$5.00 for local club and \$1.00 for national club). Please send your payment to Steve Harris, Lyondell Chemical Co., 3801 West Chester Pike, Newtown Square, PA 19073-2387.

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## A Sudden Expansion in Multi-dimensional High Silica 10-ring Zeolites; Why Now?

Dr. Stacey I. Zones

Chevron Energy and Technology Center, Richmond, California

### Abstract

There has been a steady proliferation of new zeolitic structures over the last 30 years, as chemists explore synthesis routes using novel inorganic conditions and then novel organic guest molecules. Earlier work of Mark Davis and Alex Navrotsky made a strong case that product selectivity in the synthesis must be kinetically controlled. The good news was that many products could be possible, choosing the right route. However, since the early 70's there have been almost no zeolite products with multi-dimensional 10-rings. Add to that, Mobil's ZSM-5 (from the early 70's) has been possibly the most widely used zeolite in catalysis applications.

In this presentation I will discuss some issues concerning the synergy in synthesis between organic guests and the inorganic host environment. Then we will examine the context in which several new multi-dimensional 10-ring zeolites have been found, mostly since the year 2000. Finding "niche" space in the zeolite synthesis landscape has proven productive. Then I will give some characterization of these newer materials and we will see how they approximate and/or differ from ZSM-5 and ZSM-11. Finally, I will address how these materials can hope to be of catalytic interest and use in areas where ZSM-5 is so well developed already.

### Speaker's Biography

Stacey I. Zones is currently a Research Fellow with Chevron's Energy and Technology Company, working in the catalyst department. He is also an Adjunct Professor in Chemical Engineering at the University of California, Department of Chemical Engineering. Dr. Zones earned a Ph.D. in Inorganic Chemistry from the University of California at San Diego in 1978, with a thesis in the area of model systems for nitrogen fixation. He joined Chevron in 1980 and began a program in searching for new zeolite structures with a strong emphasis on designing organic cations to aid in the synthesis. He continues to head that effort for Chevron as well as contribute as a team member in efforts to develop the zeolite products into commercial use, working on manufacturing and catalyst development efforts.

Dr. Zones is a co-author and co-inventor on numerous zeolite science papers and technology applications. He has had a successful long-standing collaboration with Professor Mark Davis and group at Caltech in the area of fundamentals of zeolite synthesis. He is a past President of the California Catalysis Society and is currently both the Treasurer and on the Board of Counselors for the International Zeolite Association. His research was recognized by the Association with the 2001 Breck Award. He has served on the editorial boards of journals dealing with zeolite materials. In 2007 he will receive the Houdry Award from the North American Catalysis Society. He is also a youth sports coach for baseball and basketball.



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## Is There a Relationship Between the M=O Bond Strength of Bulk Mixed Metal Oxides and Catalytic Activity?

**Kamalakanta Routray**

*Operando* Molecular Spectroscopy & Catalysis Laboratory

Chemical Engineering Department

Lehigh University, Bethlehem, PA 18015

(Student Talk, 15 minutes)

### Abstract

It's widely believed in the catalysis literature that the bulk M=O bond of mixed metal oxides controls catalytic activity. In the present study, *for the first time*, the bulk Mo=O bond lengths and catalytic activity of bulk metal vanadates and molybdates are compared to allow examination of this long standing hypothesis. The bulk M=O bond lengths were measured with Raman spectroscopy and the corresponding catalytic activity was determined with CH<sub>3</sub>OH-temperature programmed surface reaction (TPSR) spectroscopy. The CH<sub>3</sub>OH-TPSR experiments provide the first-order rate constants of the rate-determining-step (rds) for breaking of the C-H bond during the decomposition of the surface CH<sub>3</sub>O\* intermediate to H<sub>2</sub>CO. The findings clearly show that there is no correlation between the first-order rate constant,  $k_{rds}$ , and the bulk M=O bond length. This finding is not so surprising when one considers that the rate determining step involves C-H bond breaking and *surface* MO<sub>x</sub> sites, but doesn't involve *bulk* M=O bond breaking.

### Speaker's Biography

Kamalakanta is a Doctoral candidate in the Chemical Engineering Department of Lehigh University. He received his Bachelors degree (B.E.) in Chemical Engineering from National Institute of Technology (NIT)-Rourkela and subsequently obtained his Masters from Indian Institute of Technology (IIT)-Kanpur. During his Masters, he worked on the kinetic parameter estimation for propane oxidative dehydrogenation (ODH) reaction with Professor Goutam Deo. Currently, he is focusing on bulk mixed metal oxide catalysts for the oxidation of methanol and photocatalysis of nano-structured materials under the supervision of Professor Israel E. Wachs.