

***Paramagnetic Chromium Organometallics –  
Structure, Reactivity and Catalysis***

**Prof. Dr. Klaus H. Theopold**  
**University of Delaware (USA)**

**Friday 15th February, 2013. ICIQ Auditorium, 12 p.m.**

**Professional Career**



Chair, Dept of Chemistry and Biochemistry, University of Delaware, 2007 - 2012  
Visiting Scientist, Dept. of Chemistry University of British Columbia, 2001  
Associate Director, Center for Catalytic Science and Technology, 1996  
Acting Chairman, Dept. of Chemistry and Biochemistry, University of Delaware, 1996  
Professor of Chemistry, University of Delaware, 1995 - present  
Visiting Scientist, Inorganic Chemistry Laboratory, Oxford University, 1994  
Joint appointment in Dept. of Chemical Eng., 1993  
Associate Professor, University of Delaware, 1990 - 1995  
Assistant Professor, Cornell University, 1983 - 1990  
Postdoctoral Associate with Prof. R. R. Schrock, MIT, 1982 - 1983  
University of California, Berkeley; Berkeley, CA, Ph.D. (Inorganic Chemistry), 1982;  
Thesis Advisor: Prof. R. G. Bergman.  
Universität Hamburg; Hamburg, Germany; Vordiplom, May 1977.

**Research Interests**

The coordination polymerization of small olefins and the oxygenation of hydrocarbons are examples of catalytic processes, which have inspired our preparative and mechanistic work with transition metals. Our approach involves the synthesis of 'unusual' molecules (by virtue of their oxidation state, spin state, electronic configuration, molecular structure, reactivity, etc.), their full characterization with various spectroscopies and other suitable physical techniques (i.e. electrochemistry, magnetic susceptibility measurements, X-ray crystallography), and finally the elucidation of their reactivity with organic or inorganic substrates.

Based on the notion that open shell organometallics or 'metallaradicals' should exhibit novel reaction patterns, we are working on a variety of paramagnetic chromium alkyls. Here we are utilizing changes in oxidation state to tune the reactivity of these extremely electron deficient compounds. Results from this research include active ethylene polymerization catalysts, compounds with unusual magnetic properties, and stereoselective carbon-carbon bond formations with possible applications in organic synthesis. This project is currently supported by the National Science Foundation under Grant No. CHE-0911081.

Another current project focuses on the activation of dioxygen and other readily available oxidants with transition metal catalysts. We are taking advantage of the unique steric characteristics of highly substituted tris(pyrazolyl)borate ligands in stabilizing coordination compounds of small inorganic ligands. These complexes engage in electron transfer and atom abstraction reactions. This project is currently supported by the department of Energy under Grant No. DE-FG02-92ER14273.