



THE DANISH CHEMICAL SOCIETY

FOUNDED 1879

KEMISK FORENING

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Hovedmøde i Kemisk Forening
Arrangeret af Sektionen for Uorganisk Kemi
12. November 2010 kl. 15:00 i auditorium 8

H. C. Ørsted Instituttet, Universitetsparken 5, 2100 København Ø

- Efter mødet er der spising – tilmeldinger til spising gerne til secretary@chemsoc.dk før 10/11-2010.

Iridium Corroles: Synthesis, Electronic Structure, and Photophysical Properties

Josh Palmer

California Institute of Technology, 1200 E. California Blvd., CA 91125 CA,

The first-row metal complexes of corroles, aromatic macrocycles similar to porphyrins, have recently found use in applications as diverse as catalysis of epoxidation reactions, imaging of tumors, and attenuation of sclerotic buildup on the arterial walls of organisms. The third-row chemistry of corroles has remained largely unexplored, but the properties of their iridium complexes have been investigated in some detail. The interesting electronic structure, near-infrared emission, and photochemical exchange reactions of iridium(III) corroles will be discussed.

The electronic structure of tris(dithiolene) metal complexes: Where are the (valence) electrons?

Stephen Sproules

Max-Planck-Institut für Bioanorganische Chemie, Stiftstrasse 34-36, D-45470 Mülheim an der Ruhr, Germany

Since their famed introduction into coordination chemistry nearly fifty years ago, transition metal tris(dithiolene) complexes have always been a source of intrigue, stemming from their unique molecular geometries (trigonal prismatic) and electronic structures. However, the recent interest in dithiolene redox noninnocence has stimulated a re-examination of such complexes to ascertain their true electronic structure. We have synthesised a number of tris(dithiolene) complexes and furthered the synergistic relationship between experiment and (density functional) theory to elucidate their electronic structures.

A Return to Innocence: Type 1 Copper Coordination Without Sulfur Covalency.

Kyle M. Lancaster

Cornell University, Ithaca, 14853 NY

The type 1 copper protein active site is ubiquitous in nature; its properties (efficient electron transfer reactivity, narrow EPR axial hyperfine splitting, and intense blue coloration) arise due to a highly-covalent Cu-S bond whose properties are heavily influenced by outer-sphere coordination. Most of the properties of type 1 copper are restored in the engineered, sulfur-free type zero copper site - spectroscopic and kinetic studies are presented to highlight the importance of the highly covalent sulfur interaction.