Coordination Chemistry Reviews 255 (2011) 617–618

Contents lists available at ScienceDirect

Coordination Chemistry Reviews

journal homepage: www.elsevier.com/locate/ccr

Preface

A celebration of Harry B. Gray's 75th birthday

Harry B. Gray is one of the towering figures in modern chemistry. Harry's career has touched nearly every area of inorganic chemistry. His early research led to the development of molecular orbital theory for inorganic molecules. In a 1962 paper with C. J. Ballhausen, he first formulated the concept of metal–ligand multiple bonding. The Ballhausen–Gray model for metal–oxo bonding remains the standard to this day, receiving thousands of citations in the scientific literature since 1982. In this paper, along with two later papers, Harry derived valence orbital ionization energies and analytical orbital wave functions that enabled a generation of computational chemists to perform molecular-orbital calculations of the structures and reactivity of inorganic molecules. After a decade studying bonding, electronic structure, and spectroscopy in transition metal complexes, Harry moved into bioinorganic chemistry with investigations of the active sites and reactivity of metalloproteins. Harry's singular achievement in bioinorganic chemistry is the demonstration of the phenomenon of long-range electron tunneling in proteins, and his experimental elucidation of the chemical principles that regulate the efficiencies of these vital transformations. The current understanding of long-range electron tunneling in biology derives in large measure from a 30-year research effort in Harry's laboratory. During a 50-year research career marked repeatedly by groundbreaking innovations in both theory and experiment, Harry Gray has earned a position among that elite group of scientists who have fundamentally changed the way chemists look at their field.

For his many outstanding scientific achievements, Harry has been awarded membership in the scientific societies of six nations; he has been recognized with sixteen honorary degrees; and he has received dozens of awards and medals, including the Pauling Medal (1986), the United States National Medal of Science (1986), the Priestley Medal from the American Chemical Society (1991), the Benjamin Franklin Medal in Chemistry (2004), the Wolf Prize in Chemistry (2004), and the Welch Award in Chemistry (2009).

A stellar collection of Harry's friends, colleagues, and former students and postdocs have contributed to this issue of *Coordination Chemistry Reviews* in celebration of his 75th birthday. The breadth of topics spanned by these reviews clearly reflects the diversity of Harry's research. The electronic and molecular structures and reactivity of coordination compounds, particularly metal–dithiolenes, are represented in four reviews: Rich Eisenberg, one of Harry's first graduate students, examines trigonal prismatic coordination in metal-tris(dithiolene) complexes; Stephen Sproules and Karl Wieghardt discuss the application of sulfur K-edge X-ray absorption spectroscopy to the study of dithiolene complexes; Zeev Gross illustrates the research avenues resulting from the facile synthesis of metal–triarylcorroles; and Mike Therien and coworkers underscore the importance of chemical synthesis and physical measurements in their review of electron transfer reactions in porphyrin–bridge–quinone complexes.

Harry's early work on metal–ligand multiple bonding developed into one of his favorite constructs, the oxo-wall: Chi-Ming Che and coworkers review the chemistry of macrocyclic amine complexes of ruthenium and osmium, compounds sitting next to the wall; while Caroline Saouma and Jonas Peters describe their efforts to get over, under, and around the wall by exploiting three-fold symmetry.

In Carl Ballhausen's laboratory at the University of Copenhagen, Harry learned the necessity of informing theory with good experiments: supramolecular chemists Nick Turro and colleagues demonstrate the synergy of theory and spectroscopy in studies of a model quantum rotor confined to a spherical box, $H_2@C_{60}$; and the review of $[ReL(CO)_3(phen)]^+$ complexes by Tony Vlček and coworkers focuses on the essential role of one of the inorganic spectroscopist's primary tools of desperation, spin-orbit coupling.

Harry's interest in inorganic reaction mechanisms and catalysis dates back to his graduate studies with Fred Basolo and Ralph Pearson at Northwestern University: David Tyler reviews efforts to introduce "green chemistry" into catalytic methods for the production of acrylic monomers; Jay Labinger and John Bercaw discuss new approaches for converting synthesis gas into organic chemicals and fuels; and Theo Agapie highlights the olefin oligomerization chemistry catalyzed by titanium, tantalum, and chromium complexes.

In the early 1970s Harry was bitten by the bioinorganic bug. He recognized that biological inorganic chemistry afforded metal structures and reactivity that had not been replicated in synthetic molecules: Wenbin Qi and Jimmy Cowan review the chemistry of three proteins involved in biological iron–sulfur cluster synthesis; Tate Owen and Allison Butler discuss remarkable micelle-to-vesicle phase changes induced by metal coordination to amphiphilic siderophores; and Akif Tezcan describes the stunning coordination complexes that can be synthesized by using proteins as ligands.

In those forgotten days before protein crystallography was a routine exercise, Harry showed that the combination of ligand field theory and spectroscopy could provide key insights into metalloprotein active-site structures: Ed Solomon and Ryan Hadt illustrate the vitality of this approach in their review of the spectroscopy and electronic structure theory of blue copper active sites; and John Dawson and coworkers discuss the application of magnetic circular dichroism and electronic absorption spectroscopies to the characterization of unique metal–ligand adducts in the H93G mutant of sperm whale myoglobin.

0010-8545/$ – see front matter
doi:10.1016/j.ccr.2011.01.034

Recognizing that dynamics is as important as structure in understanding protein function, Harry embarked in the early 1990s on a program exploring protein conformation, dynamics, and folding: Bruce Bowler explores the coupling of protein dynamics to redox reactivity, ligand binding, and enzyme function; and Ivano Bertini reviews the NMR techniques that reveal structural and dynamics features of multicomponent biological systems.

Fast kinetics methods were integral to Harry's seminal investigations of protein electron transfer reactions: Ole Farver and Israel Pecht review the application of pulse radiolysis methods in studies of electron-transfer reactions of copper proteins; and Grant Mauk surveys the use of photoactive caged complexes in studies of protein function.

Harry's pioneering research on protein electron transfer paved the way for studies of charge flow in other biomolecules: Jackie Barton discusses the movement of charge in DNA and its role in oxidative damage and repair; and David Beratan reviews theoretical studies of charge transport in DNA and PNA.

I would like to express my gratitude to all of the authors and to the Editor-in-Chief, A.B.P. Lever, for their hard work and patience in the preparation of this special issue honoring our good friend.

Jay R. Winkler*
California Institute of Technology, Beckman Institute, 1200 E, California Blvd, MC 139-74, Pasadena, CA 91125, United States

* Tel.: +1 626 395 2834.
E-mail address: winklerj@caltech.edu

19 January 2011
Available online 2 February 2011