Preface

Chiral molecules, molecules that lack mirror symmetry, have been the focus of attention since it was established that all organisms are built of molecules with specific handedness. The understanding of biological processes that involve intermolecular recognition, including drug interactions with biomolecules, is enhanced by an understanding of the structure and interactions among chiral structures, as well as an ability to synthesize and separate enantiomers and diastereomers. As such, enormous focus has been placed on molecular stereochemistry, beginning with the earliest pioneering studies of van't Hoff, who established the tetrahedral valency of carbon and the consequent origins of molecular chirality. Recent progress in molecular chirality has been recognized for synthetic breakthroughs through the awarding of the 2001 Nobel Prize in Chemistry to Knowles and Noyori for chirally catalyzed hydrogenation and to Sharpless for discoveries on chirally catalyzed oxidation.

When compared to developments associated with the structure and synthesis of chiral structures, less attention has been focused on the electronic and magnetic properties of chiral molecules. Circular dichroism and related optical probes of chirality have been developed mainly as analytical tools and, indeed, they are applied routinely. However, as demonstrated in this volume, the basic physical underpinnings that link structure and chiral properties, including chiro-optical properties, continue to emerge and require the development of physical models and improvement of electronic structure methods before they are fully elucidated.

No apparent ground exists for a "right-handed" structure to be intrinsically more or less stable than a "left-handed" structure, and one might even expect molecules to exist in a superposition of left- and right-handed states. However, chirality in molecules is related to an important symmetry breaking effect in nature, parity violation (PV), so that a very small (of order 10^{-18} eV) energy difference between left- and right-handed molecules is expected. The PV effect is generally considered to be too small to have any significance in chemical systems, and molecules relax into either left- or right-handed states with lifetimes defined by the activation barrier for inversion of the stereochemistry. One consequence of symmetry breaking, *i.e.*, relaxation into long-lived enantiomers or diastereomers, is the magneto-electric effect. This effect arises when electrons that move through chiral systems are driven by an applied electric field, creating a transient magnetic field. This magnetic field may act on the spin of the mobile electron and align it. In this way, one may envision a relationship between the chiral symmetry and the magnetic and spin characteristics of molecules. When one explores the potential use of organic molecules as components in electronic devices, the novel characteristics derived from chirality require attention. Indeed, these phenomena may help to establish new capabilities that are not available – or are difficult to realize – in more conventional electronic systems.

This volume assembles contributions from researchers investigating novel electronic, magnetic, and spectroscopic properties of chiral molecules and of supramolecular structures made from these molecules. The contributions describe both theoretical and experimental studies, and they aim to provide the reader with a current snapshot of this emerging and rapidly growing field of research into the electronic and magnetic characteristics of chiral systems.

David N. Beratan
Ron Naaman
David H. Waldeck

http://www.springer.com/978-3-642-18103-0

Electronic and Magnetic Properties of Chiral Molecules
and Supramolecular Architectures
Naaman, R.; Beratan, D.N.; Waldeck, D. (Eds.)
2011, XII, 312 p., Hardcover
ISBN: 978-3-642-18103-0