Additions and Corrections

Scalar Relativistic Effects on ^{17}O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study [*J. Am. Chem. Soc.* **1995**, *117*, 1851−1852]. MARTIN KAUPP,* VLADIMIR G. MALKIN, OLGA L. MALKINA, AND DENNIS R. SALAHUB

Page 1851: Due to a conversion error, the experimental ^{17}O shifts (second column, Table 1) were given incorrectly. The correct numbers should read from top to bottom 871, 576, 456, 1255, 786, 605, 1142*f*, 832. This change does not alter the findings of the paper.

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Book Reviews

Structure Correlation, Volumes 1 and 2. Edited by H.-B. Bürgi (University of Bern) and J. D. Dunitz (ETH, Zürich). VCH: Weinheim, Germany. 1994. xxvii + 888 pp. $235.00. ISBN 3-527-29042-7.

Structure correlation is the analysis of all available structural data for a given chemical fragment in different environments and the correlation of these data with molecular structure and reactivity. A famous correlation of this type is the "Dunitz−Bürgi trajectory" for nucleophilic additions, but the concept is applicable to a wide range of chemical phenomena. As Roald Hoffmann noted, the "geometrical structure... provides us with the starting point for the understanding of every physical, chemical and biological property of the molecule." This volume presents the results of 15 years of progress in structure correlation, edited by two pioneers in this area of research, Jack D. Dunitz and Hans-Beat Bürgi. They have brought together experts in their fields to summarize the principles and applications of structure correlation in organic, inorganic, and supramolecular chemistry and in structural biochemistry.

The book is organized into four parts: Basics, Molecular Structure and Reactivity, Crystal Packing, Proteins and Nucleic Acids. Part 1 opens with two chapters written by the editors, dealing with methods for descriptions of the geometrical structure of molecules, including coordinate systems, symmetry, and vibrational analysis. Chapter 3 (F. H. Allen, O. Kennard, and D. G. Watson of the Cambridge Crystallographic Data Center) provides an overview of the Cambridge Structural Database (CSD) and details of software for searching this resource. Chapter 4 (R. Taylor and F. H. Allen) gives examples of extracting the information in the CSD for structure correlation analysis and describes statistical and principal component analysis and cluster analysis of the results. Chapter 5, by Bürgi and Dunitz, gives a general discussion of the principles of structure correlation and the relationship with physical concepts.

Part 2 is devoted to the elucidation of reaction pathways by analysis of structure−structure and structure−energy correlations. Chapter 6 (A. S. Cieplak) gives an extensive and excellent overview of the theory and structural data revelant to addition and elimination reactions involving carbonyl derivatives. Chapter 7 (H.-B. Bürgi and V. Shklover) demonstrates the ubiquity of the three-center−four-electron system $X-MR_3-Y$ in organic and inorganic substitution reactions. Chapter 8 (T. Auf der Heyde) deals with substitution reactions and ligand rearrangements (*e.g.*, pseudorotation) in inorganic compounds. Chapter 9 (W. B. Schweizer) summarizes the most important studies on conformational preferences in typical organic fragments like esters, furanoside rings, and a few others.

Part 3 covers structure correlations in extended systems: Chapter 10 (I. D. Brown) reviews the bond-length−bond-valence relationship in inorganic solids, Chapter 11 (J. Bernstein, the late M. C. Etter and L. Leiserowitz) discusses the role of hydrogen bonding in molecular assemblies, and Chapter 12 (A. Gavezzotti) addresses the problem of correlating molecular and crystal properties and eventually predicting the crystal structure of a given molecule of known structure.

Finally, Part 4 gives examples for the extension of the structure correlation concept to proteins and nucleic acids. Chapter 13 (G. Klebe) discusses the mode of action of enzymes with the help of reaction path data and structure correlations derived from "small" molecules. Chapter 14 (W. L. Duax, J. F. Griffin, and D. Ghosh) describes the empirical approach of mapping the active sites of steroid hormone receptors and steroid-binding proteins by analyzing crystallographic data of more than 1000 steroids or steroid-like compounds. Chapter 15 (E. G. Hutchinson, A. L. Morris, and J. M. Thornton) is concerned with structural patterns in globular proteins and contains useful analysis of a host of different common arrangements. Chapter 16 (T. L. Blundell) addresses the question of the correlation between the primary and tertiary structure in families of homologous proteins, while Chapter 17 (C. Broger and K. Müller) deals with the predictability of protein folding from local hexapeptide sequence patterns. Chapter 18 (M. Egli) gives a collection of structural patterns in nucleic acids and in short oligonucleotide fragments, including intercalated aromatic and DNA-protein binding. An extensive appendix (106 pages) with a selection of typical interatomic distances in organic and organometallic compounds from X-ray data rounds off the book.

The editors have succeeded in presenting a work of great substance and magnitude. The graphical presentation is unusually homogeneous for a book with so many different contributors. The editing is excellent, and very few minor problems or omissions were detected. Both crystallographic data and the results of *ab initio* calculations are covered in some of the chapters. This work will be of considerable value for every chemist, even those with only a vague interest in structure and reactivity. It should be found in every research library.

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Topics in Fluorescence Spectroscopy. Volume 4. Probe Design and Chemical Sensing. Edited by Joseph R. Lakowicz (University of Maryland). Plenum Press: New York and London. 1994. ISBN 0-306-44784-3.

This is a stimulating and very timely book. Its 14 chapters reflect a good fraction of the research going on in the area of fluorescence-based chemical sensing. It is complimentary in many aspects to the 1991 two-volume book *Fiber Optic Chemical Sensors and Biosensors* edited by O. S. Wolfbeis.

Chapter 2 is on fluorescent probes for ion recognition and is very readable and informative. The important mechanisms that lead to molecular recognition between ion and fluorescent probes are discussed in great claritm, and the references cited indicate an excellent knowledge of the literature. This chapter is a must for everybody interested in sensing clinically important electrolytes. Chapter 3 is similar in that it covers fluorescent chemosensors for cations, anions, and neutral analytes. There is some overlap with Chapter 2. The title suggests a broad review, but in fact, it refers to probes derived from 9-amino-methylanthracene only, which is a UV-excitable fluorophore and of little practical utility in sensor design. Fortunately, the sensing schemes described for these probes are likely also to hold for other (more longwave) probes. I found the chapter to be of particular significance because it demonstrates how species as different as metal cations,