Book Reviews

Structure Correlation. Edited by H.-B. Bürgi and J. D. Dunitz. VCH: Weinheim, 1994, two Volumes, 888 pp., hardback DM 398. ISBN 3-527-29042-7.

This two-volume set will make an invaluable addition to any library and private collection where there are chemists and crystallographers working together. It is a compilation of significant contributions from several authors, all of whom are experts in the wider field of Structure Correlations. These books break new ground in drawing together such topics as: bond strength relations in solids, conformational analysis, crystal structure prediction, reaction pathways of organic and organometallic molecules, ligand/receptor interactions and enzyme mechanisms.

Volume 1 covers the basic concepts and mathematical principles involved in structure correlation in sufficient detail to enable the new reader to understand the analyses which form the basis of these books. In Part 1 there are very readable chapters by the Editors and by Taylor and Allen on symmetry aspects and statistical and numerical methods, both of which contain a good number of examples and further literature is well referenced. These chapters are likely to appeal less to those research workers who wish to read the results, rather than to perform the analyses themselves. There is a chapter devoted to the architecture of databases and the Cambridge Crystallographic Database in particular, with references to their use for search and retrieval of stored information. Part 2 shows how the results from small molecule crystallography of organic, organometallic and coordination chemistry may be treated to provide 'dynamic' information, and not merely serve as a large collection of 'static' molecular parameters. There are excellent examples of the results of the research carried out using databases in this way. For example, while a single structure determination provides very little information about a reaction pathway, several structures of related compounds can be harnessed to shed light on a mechanistic problem. Knowledge of the preferred conformation of a single molecule can sometimes explain or predict the course of a chemical reaction. The elucidation of inter- and intramolecular interactions, such as hydrogen bonding or orientational effects, is frequently a key step in this process. For example, Cieplak discusses at length how crystallographic evidence for intramolecular interactions has proved seminal in the development of current views on non-planarity and face selectivity in many fundamental organic reactions, such as nucleophilic addition to a carbonyl group, S_N2 reactions, and inversion versus retention of configuration at silicon. Auf der Heyde extends this theme to the consideration of ligand rearrangement and substitution reactions of transition metal complexes.

Volume 2 continues with the themes of crystal packing in both molecular and supramolecular solids. Organic, bioorganic and inorganic compounds are considered. Bernstein, Etter and Leiserowitz provide an extensive coverage of hydrogen bonding and the part it plays in molecular assemblies. The correlation between molecular and crystal properties is discussed by Gavezzotti with the aid of several graphs which display data of cell dimensions and molecular dimensions. Structural correlation and ligand/receptor interactions in synthetic cryptands and in naturally occuring biomolecules, eg. protein citrate synthetase and neurotransmitters, are described by Klebe. Steroidal molecular structure, protein interaction and biological function is dealt with by Duax *et. al.* The literature contains crystallographic data on over 1000 steroids which provides information concerning preferred conformations, relative stabilities and substituent effects on the interaction potentials of steroidal hormones. Systematic conformational analyses of subsets of these data are presented, with a view to assisting in locating the structural features which are essential for steroid/receptor interactions. There are three Chapters devoted to structural correlations in proteins, proceeding along the hierarchy from atomic interactions to chain topology. Structural parameters in nucleic acids are covered by Egli. In recent years the crystallisation of DNA fragments and the determination of their structures by single-crystal X-ray diffraction has provided a detailed visualisation of the double-helical conformation. This Chapter summarises recent insights into the conformation of nucleic acids, with most examples being antiparallel double-helical oligonuceleotides.

The book contains three appendices. Appendix A, by Orpen and coworkers, presents an extensive compilation of molecular geometry information on organic compounds, organometallic compounds and coordination complexes of the d- and f-block metals, obtained from X-ray and neu-

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tron diffraction studies. Appendices B and C are, respectively, compilations of short format references to crystal structures cited in this book, and structural formulae of common amino acids, purine and pyrimidine bases.

Both volumes contain high quality science that is well presented and very stimulating to read. It is unfortunate that these books have been priced high which may limit their circulation, especially amongst research students who could greatly benefit from reading them.

Martin R. Bryce and Judith A. K. Howard, University of Durham, England.

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