ELSEVIER
Carbohydrate Research 312 (1998) 239–240
CARBOHYDRATE RESEARCH

Book review

An Introduction to Hydrogen Bonding

George A. Jeffrey, Oxford University Press, New York, 1997, ISBN 0-19-509549-9, paperback, ix + 303 pp, $28.95

It is both pleasure and privilege to be able to review this book written by an eminent carbohydrate crystallographer who has spent his lifetime at the University of Pittsburgh decoding the secrets of hydrogen bonds, especially in the solid state. Though merely a fancy term in the middle of the century, it was the importance of hydrogen bonds, for example, in the genetic code that led to the discovery of the DNA double helix. Since the first book on hydrogen bonds appeared in 1960, five more have followed, including one coauthored by Jeffrey in 1991. With improvements in our understanding and in the theory of hydrogen bonds on the one hand, and with advances in experimental and refinement techniques in X-ray and neutron diffraction, availability of much stronger synchrotron radiation sources and more accurate intensity measurement devices on the other, a wealth of structural data has been amassed in this decade alone. Jeffrey has orchestrated the phenomenal task of compiling the vital information on hydrogen bonds scattered in the literature into an ordered and readily available condensed form in this book.

Of the 11 chapters in the book, the first is devoted to a historical background on the concept of hydrogen bonding, the last on the important spectroscopic and diffraction methods, and the rest are on descriptions of the structural features of hydrogen bonds in a multitude of chemical compounds. The topics cover the nature and properties of the functional groups involved in strong, medium, and weak hydrogen bonds as they occur in such simple molecules as water and ice, complex biological molecules such as proteins, nucleic acids, and carbohydrates, and a host of linear and cyclic molecules of intermediate sizes. There are numerous examples of three- and four-centered hydrogen bonds which exploit two and more acceptors for a donor, and thus enhance structural stability. The point is aptly made in chapter 6 that it is not just the list of hydrogen bonds in a crystal structure, but rather the hydrogen-bonding pattern, which could be coded using graph-set theory, that is relevant for understanding supramolecular assemblies. Chapter 7 highlights that hydrogen-bond disorders, as donors and acceptors switch roles, similar to those found in several cyclodextrin inclusion complexes, are responsible for the observed transitions in a whole array of ferroelectrics. Chapter 9 is devoted to a series of inclusion compounds of varying dimensions and complexity that generate a spectrum of cages of distinct shapes, none of which would be stable but for hydrogen bonding. The details are mind-boggling, but the 143 figures and 75 tables are of great help. Of the 817 references, collated at the end of the book, some are old and some are recent, and the rest are distributed over the years.

If Jeffrey's writing is easy to read, the more so it is when anecdotes are found either in the text or the footnotes that provide a crystal clear perspective of some historical event. Two samples are: on p. 87, "Donohue corrected an earlier hydrogen-bonding base–pair concept of Watson and Crick (1953) and is described by Watson (1968) as knowing more about hydrogen bonds than anyone else in the world except Linus [Pauling] himself." On p. 195, "W.T. Astbury has been described as the father of molecular biology, but I [Jeffrey] could not discover who gave him that accolade." In addition to presenting facts, when relevant, he

PII S0008-6215(98)00260-2

poses thought-provoking questions for future research. One example, on p. 97, "are these forced C–H···O contacts (in biological structures) attractive or repulsive, and, do they add to or subtract from the total hydrogen-bonding energy?"

In the case of biopolymers in single crystals and in polycrystalline fibers, hydrogen bonds are important. Jeffrey has copiously cited single crystals of small and large molecules. As a fiber diffractionist, I am however disappointed that he has not recognized the fact that polynucleotide and polysaccharide structures have been determined scrupulously using fiber diffraction data. These biopolymer helices are stabilized by systematic hydrogen bonds, some of them mediated by organized water molecules and cations which have been located in difference electron-density maps and their positions refined in an objective fashion. I am chagrined by his act of sweeping fiber diffraction under the rug using a 1978 reference on p. 202!

Aside from this drawback, there are a few minor typos such as a instead of α (-helix) on pp. 6 and 10, el(l)usive on p. 11, formamide should be acetamide in Fig. 2.4 on p. 21, Å should be ° in column 4 under O–H···O of Table 3.10 on p. 47, 256 (in item 4) and 700 (in item 9) in the last column of Table 3.14 on page 52 are wrong, C and O are interchanged in the caption to Fig. 4.5 on p. 77, prop(r)ionic acid on p. 99, and Sarka should be Sarko, and patters should be patterns, both on p. 202.

On balance, the numerous merits outweigh the few easily remediable defects. The details in the book are the greatest up-to-date resource on hydrogen bonds in molecules having a wide range of chemistry and complexity. Although Jeffrey considers it a supplement to undergraduate textbooks, I would also strongly recommend *An Introduction to Hydrogen Bonding* to all graduate students and research scientists pursuing active research in structural science.

Rengaswami Chandrasekaran
Whistler Center for Carbohydrate Research,
Purdue University,
West Lafayette, IN 47907, USA