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Recensiones

Bergmann, E. D., Pullman, B., Eds.: The Jerusalem Symposia on Quantum Chemistry and Biochemistry, Vol. V: Conformation of Biological Molecules and Polqmers. Jerusalem: Israel Academy of Sciences and Humanities, 1973 (Distributed by Academic Press, New York.) pp. 831, US $ 40.00

This book is a publication of the Proceedings of an International Symposium held in Jerusalem, Israel, April 3–9, 1972. This symposium, the fifth in a continuing series, was sponsored jointly by the Israel Academy of Sciences and Humanities, and contained 59 papers from approximately 100 contributors.

The topic of this particular symposium was "Conformation of Biological Molecules and Polymers", and a good mixture of experimental and theoretical studies was presented, including 31 experimental and 26 theoretical papers. As is evident in the papers, questions of conformation play an important role in a large variety of areas, and the areas of application reported at this symposium included polypeptides, proteins, purines, pyrimidines, polynucleotides, polynucleosides, nucleic acids, cholinergic molecules, enzymes, and various molecules of medicinal chemistry interest. In the study of these problems, a variety of experimental techniques were used, including NMR, CD, X-ray, potentiometric measurements, and the nuclear Overhauser effect. A similar variety was employed in the theoretical studies, including several kinds of semi-empirical and AB INITIO quantum mechanical techniques, semi-classical potential techniques, and Monte Carlo techniques.

Two primary goals were set for the Symposium: "to collect the experimental facts and theoretical points on which there is agreement; and to formulate precisely those questions that remain open to further theoretical treatment and new experimental approaches".

The overall impression given to the reader is that the papers presented at this symposium represent a good synopsis of the current status of techniques available at that time for obtaining conformational information about molecular systems. Many of the groups working actively in this area were represented, and the papers generally reported the results of most recent work. The remarkably broad area of application of conformational analysis that was reported indicates that the symposium offered good opportunities for synergistic interplay between experiment and theory in a wide variety of areas.

Perhaps not surprising due to the complicated, subtle, and frequently competing interactions that are being described, the ability of any theoretical precedure to describe adequately the conformations observed experimentally has to be considered still an open question, due to the lack of proper inclusion of environmental effects, correlation effects, and in some cases, the basis electrostatic interactions themselves. However, the agreement now found in many crystallographic and theoretically calculated structures indicates that substantial progress has indeed been made, and that adequate techniques for describing the intramolecular interactions in large molecular systems are becoming available. Examples illustrating this point include the many cases of agreement between crystallographically observed conformations and the minimum energy conformations of the PCILO technique, as well as the careful, substantial and continuing work of the groups of Rein, Lifson, Scheraga, and others in the development of semi-classical techniques for very large molecular systems. Also, the substantial progress, both in the number and accuracy of systems studied, made using experimental techniques is beginning to allow important correlations and generalizations to be made (e.g., in a paper reported by M. Sundaralingam on the concept of a conformationally "rigid" nucleotide.)

One of the fringe benefits of a broadly based symposium such as this is the identification of notational nonuniformities that have arisen due to the use of different conventions and notations. As a result of this symposium, a set of recommendations for standard conventions and nomenclature for the description of the conformation of polynucleotide chains was adopted.

Hence, the proceedings of this symposium appear to represent a good summary of the current status of experimental and theoretical techniques for examination of the conformation of molecular

systems. The papers indicate that, in the not too distant future, one might expect that quite reliable techniques for the description of conformations of the ground state of reasonably large systems will become available. However, the questions associated with the description of the interactions of these systems with others (e.g., transition states associated with enzyme-substrate interactions) will generally require information about how systems in non-equilibrium conformations interact, and many problems remain in this area.

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