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Recensiones

E. D. Bergmann, B. Pullman: The Jerusalem Symposia on Quantum Chemistry and Biochemistry. Vol. VI: Chemical and Biochemical Reactivity. Jerusalem: Israel Acad. Sci. Hum. 1974. VIII + 578p., price: US $39.00.

This is the sixth collection of papers presented in Jerusalem at the Symposia on Quantum Chemistry and Biochemistry.

The organizers of the Symposia, a Theoretical Chemist (B. Pullman) and an Organic Chemist (the late professor E. D. Bergmann, whose recent death has been a serious loss for science), have tried to stimulate applied Theoretical Chemistry, the six Symposia all being devoted to theoretical work on topics of experimental Chemistry and Biochemistry, rather than to methodological studies. The sixth theme was apparently chosen in view of the increasing need of a theoretical framework and guidelines for studies of reactivity; a possible subtitle for this volume would be: "A review of current theoretical work in connection with chemical and biochemical reactivity".

In the present state of science this kind of publication is probably among the few that are really constructive contributions to the advancement of research.

As concerns the contents of the book, it must be said immediately that the picture which emerges is one of a rigid structure of research which is slowly taking conscience of the existence of almost forgotten fields and problems.

The papers presented are of a variety of types and qualities. By and large, they fall into four categories: general theoretical studies of reactivity, computational studies, studies of reaction mechanisms, applications to specific biochemical or pharmacological problems.

As regards theoretical tools, the opening paper by A. Pullman presents a very promising one, namely the average potential created by a molecule at a point P of space. A test of the maps of this quantity for various molecules clearly indicates the advantages this new method can give, together with the limitation that it cannot completely replace the traditional indices, which provide quantitative summaries of local properties. The opening paper is also important in that it emphasizes the distinction between the "static" and the "dynamic" lines in attempts to account for the reactivity of large molecular systems. It is followed by a number of related ones, among which a study of thymine by the electrostatic potential is representative of the static picture.

In the field of general theoretical studies Levine, Gregory, and Ehrenson give excellent contributions to the clarification of general approaches. For instance Ehrenson's paper discusses the "principle of least motion" for reaction pathways. This may be seen as the "geometrical" point of view as opposed to the "energetic" point of view adopted by Levine. The latter paper contains a very interesting digression into the definition of surprisal; after all, a scientist who states that a result is surprising ought to know what he means!

Also localization receives some attention in the book, the connection with reactivity being more or less indirectly proved by the origin of the concept of bond. The "loge" concept is treated with a wide mathematical analysis and the corresponding electrostatic potentials are compared with those of entire molecules. Also the virial partitioning method receives attention. *Ab initio* calculations, of course, occupy a large place, although, in the reviewer's opinion, most of them do not add any new approaches or answers to the experimental chemist's problem. An excellent example of what an *ab initio* calculation can do is provided by Peyerimhoff's study of electrocyclic reactions; an approximate study of related reactions is presented by Bertràn and Fernandez-Alonso.

Another approach which is now becoming widely recognized to handle the problem of reactivity seems more exciting: the search for simple and general rules to be used by experimentalists. Salem and Lowe provide good examples of this approach. The former analyzes exceptions to the Woodward-Hoffmann selection rules, and proposes additional rules. The latter tries to answer questions regarding the effect on the bond strengths of a substrate due to charge polarization induced by an approaching anion.

The conformations of intermediate complexes and of normal molecules are also the subject of several papers.

We have mentioned only a few of the 40-odd papers contained in the 580 pages of this volume. Of course it is not possible here to do justice to all the papers in the book. The papers mentioned above have been chosen just to illustrate the types of papers to be found in the collection.

On the whole, as has been mentioned, the book is an important contribution to the advancement of Theoretical Chemistry. The typographical presentation is excellent, and this is no minor advantage in a time when the flood of scientific literature demands that papers be as readable as possible.

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