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QUANTUM BIOCHEMISTRY

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INTRODUCTION

THIS book describes results of research carried out at the borderline of many sciences: quantum mechanics, chemistry, physics, biology, pharmacology, etc. No one can be expected to master all of them equally well. Although this situation in no way constitutes an excuse for the errors, omissions or misquotations which the book may contain, we nevertheless hope that it will incline the readers to indulgence.

Our aim in writing this book was twofold: (1) to show biochemists how quantum mechanics can yield answers to the problems of the structure and mode of action of the constituents of living matter; (2) to provide the quantum chemists with a general outline of the aspects of biochemistry in which their contribution may be useful. In fact, many of our friends in quantum chemistry told us of their willingness to enter the field, but remarked on their difficulties with the complexities of biochemistry. We hope that this book will help them in finding their way.

In our view the book suffers from two main defects. In the first place, it will be noticed that different topics of the same apparent importance have sometimes been treated quite unequally. Some subjects, as important as others which have been described in detail, are entirely omitted. This situation is due, however, to the present status of quantum biochemistry. This science is at its very early stage of development, so that only a limited number of selected subjects have been dealt with. It is not without reason that the work accomplished has been compared to the tracing of a rough track through the jungle. Highways are bound to follow. Deliberately, we have omitted from this volume the discussion of the spectroscopic properties of biochemicals and the detailed study of the role of metals in biochemistry. Both subjects have been postponed for a later volume because they are very broad and their inclusion would increase this book beyond reasonable limits, and also because it was felt that a series of more refined calculations should be carried out in connection with these specific problems. This resulted in the treatment of such important topics as photosynthesis, or oxygen transfer by hemoglobin, differing.

The reader may also notice oversimplification of certain biological problems for which only fragmentary aspects are frequently considered. Here again, one could hardly expect, at present, a *complete* quantum-

mechanical discussion of such problems. Life cannot as yet be put into an equation, and, if it could, we probably could not solve it.

It is a pleasure to thank a great number of friends and colleagues who in one way or another have helped us in performing our task. In the first place we thank all those who have kindly read parts of the manuscript and helped us with their critical remarks and advice, and in particular Prof. A. Albert, Prof. P. Elving, Prof. E. Friden, Prof. R. Fuoss, Prof. I. C. Gunsalus, Prof. W. C. Holland, Dr. B. Howard, Dr. R. Hubbard, Prof. F. M. Huennekens, Prof. M. Kasha, Prof. I. Klotz, Prof. P. O. Lowdin, Prof. D. E. Metzler, Prof. J. R. Platt, Prof. H. Pohl, Prof. W. Rhodes, Prof. M. Tamres, Prof. G. Wald, Dr. F. R. Williams and Prof. R. Wurmser. We express our appreciation to Miss A-M. Pérault for her help in the compilation of some data for Chapters VIII and XIV and a part of Chapter XIII. A part of this book was written while we were visiting professors at the Institute of Molecular Biophysics at the Florida State University, Tallahassee, U.S.A., and we wish to thank particularly Prof. M. Kasha and his colleagues for many fruitful discussions. Last but not least, it is a distinct pleasure to acknowledge many helpful discussions with Prof. Albert Szent-Gyorgyi and his associates during our several visits to the Institute of Muscle Research at the Marine Biological Laboratory in Woods Hole, U.S.A.

A.P.

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PART I

**MOLECULAR ORBITALS FOR
BIOCHEMISTS**

