

Preface

Computational Chemistry has become an indispensable part of chemical research in nearly all fields and Theoretical Chemistry an increasingly prominent subject in modern chemistry curricula. This book provides an easy access to both topics for undergraduate students as well as for chemists who did not receive appropriate theoretical teaching when they studied, and need or wish to upgrade their knowledge in order to read contemporary publications or to make proper use of available commercial packages of computational chemistry in their work.

There are many good books available for these topics, but they usually take the classical approach to quantum mechanics and – besides being quite voluminous – require a considerable knowledge of higher mathematics. Other, less fastidious books sacrifice accuracy in the underlying physics for the sake of simplicity and perpetuate simple model pictures which are often not compatible with rigorous quantum mechanics. This book attempts to keep the level of theory high, while omitting all historical examples and avoiding the more complicated formalism of integro-differential equations by using the vector space concept. The contents of this book should form a good basis for further, specialised reading aims to prevent any unqualified ‘black-box’ use of quantum chemical calculation or simulation packages through stepwise explanation of all simplifications leading to the commonly used computational methods in chemistry. The reader will also understand which models employed in the interpretation of chemical processes are compatible with or in contradiction to the valid theory.

It is hoped, therefore, that students, chemistry teachers and research chemists in academia and industry will equally appreciate this concise presentation of the most relevant topics of theoretical and computational chemistry, from fundamental principles to practical methods.

The authors wish to express their gratitude to Margaret Ostermann for her careful reading of the text, and to Andreas Pribil for his valuable technical assistance in preparing the manuscript. Our thanks are also due to Dr. Martin Ottmar of Wiley-VCH Publishing Company who encouraged us to write this book.

Innsbruck, Austria
November 2006

*Bernd M. Rode
Thomas S. Hofer
Michael D. Kugler*

