



The Basics of Theoretical and Computational Chemistry

Bernd Michael Rode, Thomas S. Hofer, Michael D. Kugler

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This textbook does away with the classic, unimaginative approach and comes straight to the point with a bare minimum of mathematics -- emphasizing the understanding of concepts rather than presenting endless strings of formulae. It nonetheless covers all important aspects of computational chemistry, such as

- vector space theory
- quantum mechanics
- approximation methods
- theoretical models
- and computational methods.

Throughout the chapters, mathematics are differentiated by necessity for understanding - fundamental formulae, and all the others. All formulae are explained step by step without omission, but the non-vital ones are marked and can be skipped by those who do not relish complex mathematics.

The reader will find the text a lucid and innovative introduction to theoretical and computational chemistry, with food for thought given at the end of each chapter in the shape of several questions that help develop understanding of the concepts.

What the reader will not find in this book are condescending sentences such as, 'From (formula A) and (formula M) it is obvious that (formula Z).'

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