



Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics

Errol G. Lewars

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This is the third edition of the successful text-reference book that covers computational chemistry. It features changes to the presentation of key concepts and includes revised and new material with several expanded exercises at various levels such as 'harder questions' for those ready to be tested in greater depth - this aspect is absent from other textbooks in the field. Although introductory and assuming no prior knowledge of computational chemistry, it covers the essential aspects of the subject. There are several introductory textbooks on computational chemistry; this one is (as in its previous editions) a unique textbook in the field with copious exercises (and questions) and solutions with discussions. Noteworthy is the fact that it is the only book at the introductory level that shows in detail yet clearly how matrices are used in one important aspect of computational chemistry. It also serves as an essential guide for researchers, and as a reference book.

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