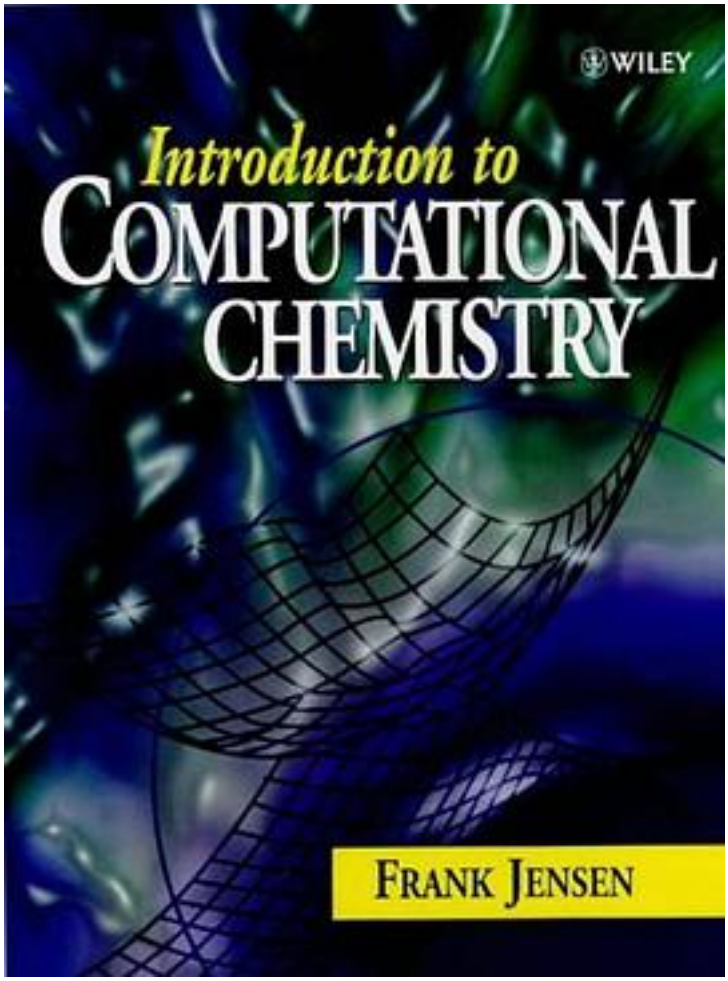
Introduction to Computational Chemistry



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Introduction to Computational Chemistry Frank Jensen Odense University, Denmark Computational chemistry is a rapidly emerging and developing area, combining

theoretical models with computers to investigate a variety of chemical phenomena. Increasingly applied throughout chemistry, computational methods are becoming an integral part of modern chemical research. Introduction to Computational Chemistry provides a comprehensive account of the fundamental principles underlying different methods, ranging from classical to sophisticated quantum models. Although the main focus is on molecular structures and energetics, subjects such as molecular properties, dynamical aspects, relativistic methods and qualitative models are also covered. Introduction to Computational Chemistry features:

* Coverage from first principles through to the latest advances.

* Relatively self-contained chapters, allowing for flexibility in the order in which they can be read.

* A web site containing additional information.

Suitable for students and researchers entering the field of computational chemistry, it is also an essential reference for procedures commonly cited in computational chemistry literature. No prior knowledge of concepts specific to computational chemistry is necessary, although some understanding of introductory quantum mechanics and elementary mathematics is assumed.

作者介绍:

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