Título:

Autor:

Precio: $1160.00

Editorial:

Año: 2006

Tema:

Edición: 2ª

Sinopsis

ISBN: 9780470011874

Introduction to Computational Chemistry Second Edition provides a comprehensive account of the fundamental principles underlying different methods, ranging from classical to the sophisticated. Although comprehensive in its coverage, this textbook focuses on calculating molecular structures and (relative) energies and less on molecular properties or dynamical aspects. No prior knowledge of concepts specific to computational chemistry are assumed, but the reader will need some understanding of introductory quantum mechanics, linear algebra, and vector, differential and integral calculus.

Introduction to Computational Chemistry, Second Edition 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, dynamic aspects, relative methods and qualitative models are also covered. No prior knowledge of concepts specific to computational chemistry ids required, although some understanding of introductory quantum mechanics and elementary mathematics is assumed.
Thoroughly updated and revised, with many chapters expanded or restructured, this second edition features updated methodologies and references as well as an overview for each chapter.

coverage from first principles through to latest advances
self-contained chapters
basic introduction to both the theory and practical aspects of this rapidly evolving and dynamic area
website for additional information