



Handbook of Computational Quantum Chemistry (Dover Books on Chemistry)

David B. Cook

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Quantum chemistry forms the basis of molecular modeling, a tool widely used to obtain important chemical information and visual images of molecular systems. Recent advances in computing have resulted in considerable developments in molecular modeling, and these developments have led to significant achievements in the design and synthesis of drugs and catalysts. This comprehensive text provides upper-level undergraduates and graduate students with an introduction to the implementation of quantum ideas in molecular modeling, exploring practical applications alongside theoretical explanations.

Written in a straightforward and accessible manner, this *Handbook of Computational Quantum Chemistry* encompasses such topics as the Hartree-Fock method; matrix SCF equations; the implementation of the closed-shell case; and an introduction to molecular integrals that extends to their implementation. Other topics and subtopics include open shells; population analysis; molecular symmetry and symmetry orbital transformations; linear multi-determinant methods; core potentials; time-dependent perturbations; density functional theory; and implementation of the Kohn-Sham equations. The text concludes with helpful suggestions for additional reading.

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