



# Quantum Chemistry

*Donald A. McQuarrie*

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## **Quantum Chemistry** Donald A. McQuarrie

After twenty-four years in print, Don McQuarrie has now updated his landmark "Quantum Chemistry". Perhaps the biggest change in the years since the first edition is the proliferation of computational chemistry programs that calculate molecular properties. McQuarrie has presented step-by-step SCF calculations of a helium atom in Chapter 9 and a hydrogen molecule in Chapter 10, in addition to including an entire chapter on the Hartree-Fock method and post-Hartree-Fock methods for the calculation of molecular properties. The book also uses problems to encourage the use of an invaluable National Institute of Science and Technology (NIST) website that lists experimental data and the results of various ab initio calculations for hundreds of molecules.

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