



# Diatomic Molecules: Results of ab Initio Calculations

*Robert Mulliken*

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## **Diatomic Molecules: Results of ab Initio Calculations** Robert Mulliken

Diatomic Molecules: Results of Ab Initio Calculations provides the results obtained from quantum-mechanical calculations on the electronic structure of diatomic molecules. This six-chapter text also discusses the related concepts of ab initio calculation methods.

This book considers first the primary methods used in the computation of molecular wave functions and of related properties. This topic is followed by discussions on the linear combination of atomic orbital and linear combination of mixed atomic orbital approximations and basis sets; electronic population analysis; spectroscopic transition probabilities; and the nature of chemical bonding. The remaining chapters examine the features of various theories that become prominent when two or more electrons are present, or are important in hydrides or homopolar and heteropolar molecules.

This text will be of great value to organic and inorganic chemists and physicists.

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