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Nota di contenuto	Introduction -- Computational methods -- Diatomic molecules -- Rotation of the polyatomic molecule -- The vibrations of polyatomic molecule -- Equilibrium structures from spectroscopy -- Molecular structures from gas-phase electron diffraction -- Models of chemical bonding and "empirical" methods -- Least-squares method -- Databases with information on molecular structure.
Sommario/riassunto	This book presents a detailed look at experimental and computational techniques for accurate structure determination of free molecules. The most fundamental property of a molecule is its structure – it is a prerequisite for determining and understanding most other important properties of molecules. The determination of accurate structures is hampered by a myriad of factors, subjecting the collected data to non-negligible systematic errors. This book explains the origin of these errors and how to mitigate and even avoid them altogether. It features a detailed comparison of the different experimental and computation methods, explaining their interplay and the advantages of their

combined use. Armed with this information, the reader will be able to choose the appropriate methods to determine – to a great degree of accuracy – the relevant molecular structure.