

1. Record Nr.	UNINA9910770270803321
Autore	Vogt Natalja
Titolo	Equilibrium Structure of Free Molecules : Theory, Experiment, and Data Analysis // by Natalja Vogt, Jean Demaison
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2023
ISBN	3-031-36045-1
Edizione	[1st ed. 2023.]
Descrizione fisica	1 online resource (482 pages)
Collana	Lecture Notes in Chemistry, , 2192-6603 ; ; 111
Altri autori (Persone)	DemaisonJean
Disciplina	541.22
Soggetti	Quantum chemistry Atomic structure Molecular structure Molecular spectroscopy Electrons - Diffraction Instrumental analysis Spectrum analysis Quantum Chemistry Atomic and Molecular Structure and Properties Molecular Spectroscopy Diffraction Spectroscopy
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Introduction -- Quantum Chemical Methods -- Rovibrational Spectroscopy and Structure of Diatomic Molecules -- Rotational Constants of a Polyatomic Molecule -- Equilibrium Structures of Semirigid Molecules from the Rotational Constants -- Structure of Nonrigid Molecules by Spectroscopic Methods -- Equilibrium Molecular Structure as Determined by Gas-phase Electron Diffraction -- Other Methods, Mainly for the X-H bond (X = C, N, O) -- Database with Equilibrium Structures of Free Molecules.
Sommario/riassunto	The properties of chemical, pharmaceutical, and biological compounds depend mainly on their molecular structure, whose determination is of

fundamental interest. This book examines and systematizes more than three hundred striking structural determinations of free molecules. Featuring high-quality structural data and presenting modern techniques of their determinations by quantum chemistry, high-resolution spectroscopy and electron diffraction, the book is an indispensable resource for graduate students and professional scientists specializing in structural chemistry and other related fields.
