

Equilibrium Structural Parameters, Volume 24 (Vibrational Spectra and Structure)



The current volume in the series, *Vibrational Spectra and Structure*, is a single topic volume on gas phase structural parameters. The title of the volume, *Equilibrium Structural Parameters*, covers the two most common techniques for obtaining gas phase structural parameters: microwave spectroscopy and the electron diffraction technique. Since the quantum chemical method provides equilibrium geometries, the volume is an attempt to provide a connection between the experimental and theoretical parameters. The book provides a review on molecular structure determinations from spectroscopic data using scaled moments of inertia. The limited number of molecules for which equilibrium parameters have been obtained and the requirement of a large number of microwave data needed to obtain the equilibrium structural parameters is noted. Electron diffraction technique is reviewed, along with a description of how this can incorporate structural information from microwave spectroscopy, vibrational spectroscopy, or theoretical calculations to improve the determination of the structural parameters by electron diffraction studies. Also discussed are the theory and methods of microwave spectroscopy, describing in some detail r_0 and r_s structures as well as r_m structures and corrections based on ab initio calculations. The accuracy of the molecular geometry predictions by quantum chemical methods is considered in some detail with data presented in graphic rather than tabular form. This makes it possible to readily note the difference in the parameters predicted at the various levels of quantum mechanical calculations. The four authors have provided a coherent description of the various structural parameters obtained experimentally along with treatments needed to extract equilibrium bond distances and angles.

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