



Structures and Conformations of Non-Rigid Molecules

By -

Springer, Netherlands, 2012. Paperback. Book Condition: New. 234 x 155 mm. Language: English . Brand New Book ***** Print on Demand *****.From the beginnings of modern chemistry, molecular structure has been a lively area of research and speculation. For more than half a century spectroscopy and other methods have been available to characterize the structures and shapes of molecules, particularly those that are rigid. However, most molecules are at least to some degree non-rigid and this non-rigidity plays an important role in such diverse areas as biological activity, energy transfer, and chemical reactivity. In addition, the large-amplitude vibrations present in non-rigid molecules give rise to unusual low-energy vibrational level patterns which have a dramatic effect on the thermodynamic properties of these systems. Only in recent years has a coherent picture of the energetics and dynamics of the conformational changes inherent in non-rigid (and semi-rigid) molecules begun to emerge. Advances have been made in a number of different experimental areas: vibrational (infrared and Raman) spectroscopy, rotational (microwave) spectroscopy, electron diffraction, and, most recently, laser techniques probing both the ground and excited electronic states. Theoretically, the proliferation of powerful computers coupled with scientific insight has allowed both empirical and ab initio methods...



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