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Book Reviews

F. L. Boschke (ed.): Large Amplitude Motion in Molecules I and II (Topics in Current Chemistry – Fortschritte der Chemischen Forschung) Vols. 81 and 82, 180 and 184 pp. Price: DM 88.00/US $48.40 per volume. Berlin Heidelberg New York: Springer 1979

Each of the two volumes contains two excellent review papers. The four contributions are largely independent of each other, each dealing with a different aspect of the intramolecular motion in non-rigid molecules.

H. Frei, A. Bauder, and Hs. H. Günthard: The Isometric Group of Nonrigid Molecules (97 pp.)

This very technical paper provides a rigorous exposition of the symmetry properties of non-rigid molecules, based mainly on the authors' own work. The construction of the isometric group is described in detail, and applications are presented to multipole selection rules, chirality problems, and to the enumeration of conformational isomers. Finally, the relation of the present rigorous treatment to earlier, more intuitive approaches is clarified, such as Hougen's work, the widely used Longuet-Higgins permutation–inversion approach, and Altmann's approach. This review requires a significant effort and mathematical inclination on part of the reader. To the causal reader, the practical utility of the concepts used is not readily apparent.

O. Bastiansen, K. Kveseth, and H. Møllendal: Structure of Molecules with Large Amplitude Motion as Determined from Electron-Diffraction Studies in the Gas Phase (74 pp.)

This is a comprehensive review of the problems and results of electron diffraction determination of non-rigid structures, from one of the leading E.D. workshops. The contribution begins with a brief summary of the necessary theoretical basis, followed by actual examples, grouped by molecular type: internal rotation in open-chain molecules, biphenyl-type molecules and ring puckering motion. Emphasis is throughout on organic-type compounds, although recent advances in the inorganic field are also mentioned. The paper contains a wealth of information, and over 400 references, up to and including 1978. However, the preparation seems to be not as careful as desirable in this kind of work, and the present reviewer has hit instantly on incorrect references and data. Reading this review and the next one, the reviewer was struck by the fact that comparatively little contact exists between electron diffractionists and molecular spectroscopists. The authors also stress this in their concluding remarks. It is to be hoped that their advice for closer cooperation will be followed.

L. A. Carreira, R. C. Lord, and Th. B. Malloy, Jr.: Low-Frequency Vibrations in Small Ring Molecules (95 pp.)

This is an excellent review, written with great care and pedagogical skill. The vibrations in question are ring puckerings in four and five-membered rings, as well as in larger rings which contain rigid fragments and behave like pseudo-four or five-membered ones. First, the experimental methods (far and mid-infrared, Raman and microwave spectroscopy) are concisely characterized. The next twenty pages summarize the theoretical basis for the interpretation of these spectra. Because of its clear presentation and practical examples, this part may well serve as an excellent general introduction to vibration-rotational theory in the presence of one or two large-amplitude coordinates. Most of the remaining space consists of actual examples of spectra and potential functions. These are carefully chosen so as to represent every possible case within the scope of the review. The paper contains much information, as shown by the 47 figures and 19 tables, the last of which is a complete literature review up to 1978. The emphasis lies on the utilization of vibrational

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(infrared and Raman) information, as a recent review by Gwinn and Gaylord treats the microwave aspects in detail.

G. O. Sørensen: A New Approach to the Hamiltonian of Nonrigid Molecules

This chapter is a summary of the author's approach to a convenient formulation of the vibrational-rotational Hamiltonian of nonrigid molecules, apparently published here for the first time. The chief difficulty in constructing an appropriate Hamiltonian lies in the fact that the coordinates best suited to the representation of the potential energy, i.e., curvilinear ones, lead to an awkward form of the kinetic energy, and *vice versa*. The present treatment is not completely new, the most significant novelty being the direct transformation of quantum-mechanical momenta. It gives, however, a clear account of the problem and an interesting example, the C_3 molecule.

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