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This Week's Citation Classic[®]

Herzberg G. Molecular spectra and molecular structure. II. Infrared and Raman spectra of polyatomic molecules. New York: Van Nostrand, 1945. 632 p. [National Research Council of Canada, Ottawa, Canada]

This book attempts a detailed presentation of the field of infrared and Raman spectra of polyatomic molecules. The book starts out from the simplest spectra, the rotation spectra, followed by a detailed discussion of vibrations and their symmetry properties. On this basis vibration spectra and vibration-rotation spectra are fully discussed. [The $SC/^{\odot}$ indicates that this book has been cited in over 7,300 publications since 1955.]

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At the time that this book was written (1944) no comprehensive text existed that dealt with both infrared and Raman spectra, although both types of spectra depend on the rotational and vibrational levels of the molecules involved. The discussions in this book are illustrated by numerous examples, in the form of tables. of observed and calculated spectra and with many photographs and recordings of observed spectra. In particular, a great many diagrams representing the energy levels and potential functions of various types of molecules as well as specific molecules are shown. Many of these were plotted for the first time, especially those of the rotation-vibration spectra of symmetric top molecules. From the rotational data, moments of inertia are obtained from which precise and detailed information about the geometrical structure of the molecules can be derived, especially when isotopic molecules are included. These geometrical data, as far as they were known in 1944, are summarized in many tables.

In writing the section on linear molecules I came across the phenomenon of *l*-type doubling similar to A-type doubling in diatomic molecules but referring to degenerate vibrational levels rather than degenerate electronic states. Strangely, this connection had been missed by earlier workers in this field. Only a very few examples existed at the time.¹ Today, this phenomenon together with *l*-type resonance is guite important in the study of linear molecules. A minor point that I believe was of some help to the reader was the introduction of the name "inversion doubling" from the fact that the energy levels of nonplanar molecules are double because of the possibility of inversion. The expressions "inversion doubling" and "inversion spectrum" are now in general use.

On the basis of molecular data obtained from the spectra it is readily possible to predict the thermodynamic functions of the respective gases at different temperatures. This subject is treated in the last chapter.

At the time of publication there was no standard notation for polyatomic molecules; fortunately, the international notation accepted later was very close to the one that I had adopted and even now problems of notation are minor because of that coincidence.

While the book is now out of print as far as Van Nostrand Reinhold is concerned, it will be reprinted this year by the Krieger Publishing Company. Recently, I reviewed a key aspect of this field.²

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^{1.} Herzberg G. l-type doubling in linear polyatomic molecules. Rev. Mod. Phys. 14:219-23, 1942.

⁽Cited 25 times since 1955.)

^{2.} _____, Rydberg molecules. Annu. Rev. Phys. Chem. 38:27-56, 1987.