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This Week's Citation Classic

Herzberg G. *Molecular spectra and molecular structure. I. Spectra of diatomic molecules.* New York: Van Nostrand Reinhold, 1950. 658 p. [National Research Council of Canada, Ottawa, Canada]

This book attempts a comprehensive presentation of the field of spectra of diatomic molecules. A discussion of the simplest spectra, i.e., rotation and rotation-vibration spectra, is followed by a detailed treatment of electronic transitions. The presentation in each case starts out from the empirical regularities and then leads to a theoretical understanding of these spectra. Separate chapters are devoted to building-up principles, electron configurations, and valence, and to dissociation and predissociation. The book concludes with a discussion of applications and a table of molecular constants. [The ***SCI***® indicates that this book has been cited in over 7,905 publications since 1961.]

G. Herzberg
Herzberg Institute of Astrophysics
National Research Council of Canada
Ottawa, Ontario K1A 0R6
Canada

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"The book *Spectra of Diatomic Molecules* was first published in German and very soon afterward in English in 1939.[1,2] Toward the end of the war when the first printing of the American edition had been sold, the publisher, Prentice-Hall, felt that the paper rations it was able to get should be used for more profitable books and returned the copyright to me. Van Nostrand, who had taken over volume II of *Molecular Spectra and Molecular Structure*,[3] was willing to take over volume I (i.e., *Spectra of Diatomic Molecules)* if a new edition were prepared. This was published in 1950 and has since been reprinted many times.

"The first version of the book was written at a time soon after the rapid development of the subject in the 1920s and 1930s by Heurlinger, Hund, Mulliken, Van Vleck, Wigner, Birge, Weizel, and many others. Having been involved in some of this development and having faced some of the difficulties of the subject, I was able to help the beginner in the field by presentations of many energy level diagrams, vector diagrams, and actual spectra, and by detailed discussions of the procedures used in analysing **a** band spectrum. At the same time, I was able to take the experts to the frontiers of the field and to describe to those working in neighbouring fields some of the applications of molecular spectroscopy in physics, chemistry, and astrophysics. I presume it is these features which have been found useful by many readers so that the book still has a high citation rate. Another fotunate circumstance, from this point of view, is the fact that the basic theory has not changed since 1939 (the time of the first edition) and only rather specialized developments have been added.

"Among the many topics dealt with in the book, two may be singled out for special mention since their discussion in the book has been frequently quoted: (1) forbidden transitions and (2) the phenomenon of predissociation. The presentation of these topics gained, I believe, by my own strong involvement in these subjects which has continued to this day.[4-7] The importance of the first topic is illustrated by the recent observation of the (forbidden) quadrupole rotation-vibration spectrum in emission in the spectrum of the Orion nebula. It is taken as evidence of shock waves in the nebula which in turn lead to star formation. The second topic has remained an active subject of research. The concept of vibrational predissociation was first mentioned in the book (and further elaborated in volume III). It has become of great interest recently in the study of various van der Waals molecules.

"The part of the book that has been widely cited but has now become outdated is the table of molecular constants. Not only have many more diatomic molecules been studied but also the constants for known molecules have been revised and many new states have been found. A revised table has been published as volume IV of *Molecular Spectra and Molecular Structure* jointly with K.P. Huber."[8]

1. Herzberg G. *Molekülspektren und Molekülstruktur. I. Zweiatomige Molekiile.* Dresden: Steinkopff, 1939. 404 p.
2. *Molecular spectra and molecular structure. I. Diatomic molecules.* New York: Prentice-Hall, 1939. 592 p.
3. *Molecular spectra and molecular structure. II. Infrared and Raman spectra of polyatomic molecules.* **New** York: Van Nostrand Reinhold, 1945. 632 p.
4. Forbidden transitions in the spectra of diatomic molecules. *Trans. Roy. Soc. Can.* **46**(Ser. 3):I-22, 1952.
5. Forbidden transitions in diatomic molecules: introductory report. *Mém. Soc. Roy. Sci. Liège* 17(Ser. 5): 121-55, 1969.
6. Die Prädissoziation und verwandte Erscheinungen. *Ergeb. Exakten Naturwiss.* **10**:207-84, 1931.
7. Predissociation and pre-ionization in diatomic and simple polyatomic molecules. *J. Chim. Phys. Phys.-Chim. Biol.* 1970:56.
8. **Huber K P & Herzberg G.** *Molecular spectra and molecular structure. IV. Constants of diatomic molecules.* New York: Van Nostrand Reinhold, 1979. 716 p.