



The Spectra and Dynamics of Diatomic Molecules: Revised and Enlarged Edition

Helene Lefebvre-Brion, Robert W. Field

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This book is written for graduate students just beginning research, for theorists curious about what experimentalists actually can and do measure, and for experimentalists bewildered by theory. It is a guide for potential users of spectroscopic data, and uses language and concepts that bridge the frequency- and time-domain spectroscopic communities.

Key topics, concepts, and techniques include: the assignment of simple spectra, basic experimental techniques, definition of Born-Oppenheimer and angular momentum basis sets and the associated spectroscopic energy level patterns (Hund's cases), construction of effective Hamiltonian matrices to represent both spectra and dynamics, terms neglected in the Born-Oppenheimer approximation (situations intermediate between Hund's cases, spectroscopic perturbations), nonlinear least squares fitting, calculation and interpretation of coupling terms, semi-classical (WKB) approximation, transition intensities and interference effects, direct photofragmentation (dissociation and ionization) and indirect photofragmentation (predissociation and autoionization) processes, visualization of intramolecular dynamics, quantum beats and wavepackets, treatment of decaying quasi-eigenstates using a complex Heff model, and concluding with some examples of polyatomic molecule dynamics.

Students will discover that there is a fascinating world of cause-and-effect localized dynamics concealed beyond the reduction of spectra to archival molecular constants and the exact ab initio computation of molecular properties. Professional spectroscopists, kinetics, ab initio theorists will appreciate the practical, simplified-model, and rigorous theoretical approaches discussed in this book.

Key Features:

- A fundamental reference for all spectra of small, gas-phase molecules.
- It is the most up-to-date and comprehensive book on the electronic spectroscopy and dynamics of diatomic molecules.
- The authors pioneered the development of many of the experimental methods, concepts, models, and computational schemes described in this book.

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