The Vibrational and Rotational Spectrometry of Diatomic Molecules

J.F. OGILVIE
*sometime Research Fellow
of Emmanuel College
Cambridge, England*

ACADEMIC PRESS
San Diego London Boston New York
Sydney Tokyo Toronto

Contents

Preface **vii**

1 **Introduction** **1**
- 1.1 The nature of molecular matter 1
- 1.2 An empirical basis of spectral assignments 7
- 1.3 A systematic analysis of spectral data of wavenumber type 14
- 1.4 An empirical description of shapes and intensities of spectral lines 27
- 1.5 Epilogue 32

2 **A Conspectus of Fundamental Principles** **35**
- 2.1 Quantal treatment of an harmonic oscillator 36
- 2.2 The separation of electronic and nuclear motions and its application to H_2 47
- 2.3 The interaction of molecules with radiation 54

3 **Theoretical Methods** **71**
- 3.1 Perturbation theory 72
- 3.2 Non-perturbative and related methods 82
- 3.3 Combination of hypervirial and perturbative methods 87
- 3.4 The BKW method 95
- 3.5 The RKR method 101
- 3.6 Treatment of diatomic molecules with classical mechanics 107

4 **The Energies of Vibration–rotational States and Potential-energy and Related Radial Functions** **119**
- 4.1 The nature and form of a potential-energy function 120
- 4.2 Some simple model functions for potential energy 129