

Contents

PREFACE TO THE SIXTH EDITION	ix
ABBREVIATIONS	xi
Chapter 1. Theory of Normal Vibrations	1
1.1. Origin of Molecular Spectra / 1	
1.2. Origin of Infrared and Raman Spectra / 5	
1.3. Vibration of a Diatomic Molecule / 9	
1.4. Normal Coordinates and Normal Vibrations / 15	
1.5. Symmetry Elements and Point Groups / 21	
1.6. Symmetry of Normal Vibrations and Selection Rules / 25	
1.7. Introduction to Group Theory / 34	
1.8. The Number of Normal Vibrations for Each Species / 39	
1.9. Internal Coordinates / 46	
1.10. Selection Rules for Infrared and Raman Spectra / 49	
1.11. Structure Determination / 56	
1.12. Principle of the GF Matrix Method / 58	
1.13. Utilization of Symmetry Properties / 65	
1.14. Potential Fields and Force Constants / 71	
1.15. Solution of the Secular Equation / 75	
1.16. Vibrational Frequencies of Isotopic Molecules / 77	
1.17. Metal–Isotope Spectroscopy / 79	

- 1.18. Group Frequencies and Band Assignments / 82
- 1.19. Intensity of Infrared Absorption / 88
- 1.20. Depolarization of Raman Lines / 90
- 1.21. Intensity of Raman Scattering / 94
- 1.22. Principle of Resonance Raman Spectroscopy / 98
- 1.23. Resonance Raman Spectra / 101
- 1.24. Theoretical Calculation of Vibrational Frequencies / 106
- 1.25. Vibrational Spectra in Gaseous Phase and Inert Gas Matrices / 109
- 1.26. Matrix Cocondensation Reactions / 112
- 1.27. Symmetry in Crystals / 115
- 1.28. Vibrational Analysis of Crystals / 119
- 1.29. The Correlation Method / 124
- 1.30. Lattice Vibrations / 129
- 1.31. Polarized Spectra of Single Crystals / 133
- 1.32. Vibrational Analysis of Ceramic Superconductors / 136
- References / 141

Chapter 2. Applications in Inorganic Chemistry 149

- 2.1. Diatomic Molecules / 149
- 2.2. Triatomic Molecules / 159
- 2.3. Pyramidal Four-Atom Molecules / 173
- 2.4. Planar Four-Atom Molecules / 180
- 2.5. Other Four-Atom Molecules / 187
- 2.6. Tetrahedral and Square-Planar Five-Atom Molecules / 192
- 2.7. Trigonal-Bipyramidal and Tetragonal-Pyramidal XY_5 and Related Molecules / 213
- 2.8. Octahedral Molecules / 221
- 2.9. XY_7 and XY_8 Molecules / 237
- 2.10. X_2Y_4 and X_2Y_6 Molecules / 239
- 2.11. X_2Y_7 , X_2Y_8 , X_2Y_9 , and X_2Y_{10} Molecules / 244
- 2.12. Metal Cluster Compounds / 250
- 2.13. Compounds of Boron / 254
- 2.14. Compounds of Carbon / 258
- 2.15. Compounds of Silicon, Germanium, and Other Group IVB Elements / 276
- 2.16. Compounds of Nitrogen / 279
- 2.17. Compounds of Phosphorus and Other Group VB Elements / 285
- 2.18. Compounds of Sulfur and Selenium / 292

- 2.19. Compounds of Halogen / 296
References / 299

Appendixes	355
I. Point Groups and Their Character Tables / 355	
II. Matrix Algebra / 368	
III. General Formulas for Calculating the Number of Normal Vibrations in Each Species / 373	
IV. Direct Products of Irreducible Representations / 377	
V. Number of Infrared- and Raman-Active Stretching Vibrations for MX_nY_m -Type Molecules / 378	
VI. Derivation of Eq. 1.113 / 379	
VII. The G and F Matrix Elements of Typical Molecules / 382	
VIII. Group Frequency Charts / 388	
IX. Correlation Tables / 393	
X. Site Symmetry for the 230 Space Groups / 407	

Index	415
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The fifth edition was published in 1996, a number of new developments have been made in the field of infrared and Raman spectra of inorganic and coordination compounds. The sixth edition is intended to emphasize new important developments as well as to catch up with the ever-increasing new literature. Major changes are described below.

Part 1, Chapter 1 ("Theory of Normal Vibrations") includes two new sections. Section 1.14 explains the procedure for calculating vibrational frequencies on the basis of density functional theory (DFT). The DFT method is currently used almost routinely to determine molecular structures and to calculate vibrational parameters. Section 1.20 describes new developments in matrix condensation techniques. More recently, a large number of novel inorganic and coordination compounds have been prepared by using this technique, and their structures have been determined and vibrational assignments have been made on the basis of results of DFT calculations. Chapter 2 ("Applications in Inorganic Chemistry") has been updated extensively, resulting in a total number of references of over 1800. In particular, sections on trigonal X_3 - and tetrahedral X_4 -type molecules have been added as Secs. 2.2 and 2.3, respectively. In Sec. 2.8, the rotational-vibrational spectrum of the octahedral U^{IV} molecule is shown to demonstrate how an extremely small metal isotope shift for $^{235}\text{U}/^{238}\text{U}$ substitution (only 0.6040cm^{-1}) can be measured. Section 2.14 ("Compounds of Carbon") has been expanded to show significant applications of vibrational spectroscopy to the structural determination of fullerenes, endohedral fullerenes, and carbon nanotubes. Vibrational data on a number of novel inorganic compounds prepared most recently have been added throughout Chapter 2.

Part 2, Chapter 3 ("Applications in Coordination Chemistry") contains two new sections: Sec. 3.6 ("Metallochromes, Chlorophylls, and Metalloporphyrins")