

CONTENTS

	Page No.
Preface	(i)
Synopsis	(iii)
Acknowledgement	(vi)
List of Publications	(ix)
Chapter 1. The Basic Theory of Microwave Spectroscopy	
1.1. Introduction	1
1.2. The Molecule as a Rigid Rotor	3
1.3. The Rigid Symmetric top molecule	5
1.4. The Rigid Asymmetric top molecule	9
1.4.1. Qualitative Survey	9
1.4.2. Energy-levels of a rigid asymmetric rotor	11
1.4.3. Symmetry classification of asymmetric top wave functions	17
1.4.4. Selection Rules and Intensities	27
1.5. Centrifugal distortions in a molecule	33

	Page No.
1.6. Derivation of the Structures of Molecules from Microwave Spectroscopy	45
1.6.1. Some General Remarks	45
1.6.2. Relation between molecular dimensions and moments of inertia	47
1.6.3. Kraitchman's Equations for isotopic substitutions	50
1.6.4. Single-substitution in a Planar Asymmetric Top	53
1.6.5. Determination of Molecular Structures : Two Approaches	54
1.6.6. The Vibrationless State : Equilibrium Structure and Effective Structure	57
1.6.7. Substitution Structures : An Outline	59
1.6.8. The Inertia Defect	61
1.7. The Least-Squares Analysis	64
1.7.1. An Outline of the Technique	64
1.7.2. How to use the Technique	69
1.8. References	71
 Chapter 2. The Double Resonance Phenomenon	
2.1. Introduction	73
2.2. The Double Resonance Phenomenon in general	74
2.3. Population distributions in presence of radiation and dominant line-broadening mechanisms	75
2.3.1. Doppler Broadening	76
2.3.2. The two-level system in presence of collisional broadening	78

	Page No.
2.4. Three-level Radio Frequency-Microwave Double Resonance (RFMDR)	88
2.5. Off-resonant conditions	96
2.6. Application in spectral assignment	98
Appendices	
A. Schrodinger Equations for the three-level system	100
B. The value of $a_2(t-t_0)$ in three-level system for one-photon transition	102
C. Calculating the Integrals	104
2.7. References	108
Chapter 3. Stark and Double Resonance Modulated Microwave Spectrometers	
3.1. Introduction	109
3.2. The Stark Modulated Spectrometer	110
3.2.1. Basic Principle	110
3.2.2. The Spectrometer	112
3.2.3. Microwave Sources	113
3.2.4. Absorption Cell	113
3.2.5. Detection System	114
3.2.6. Frequency Measurement	115
3.2.7. The Set-up	116

	Page No.
3.3. Radio Frequency-Microwave Double Resonance Modulated Spectrometer	117
3.3.1. Double Resonance Modulation	117
3.3.2. The Set-up	119
3.3.3. A Performance Check of the Spectrometer	120
3.3.4. Intensity and Power Considerations	122
3.4. Sensitivity	123
3.5. Resolution	124
3.6. Accuracy of Frequency Measurement	124
3.7. References	125
Chapter 4. Microwave Spectral Study of 2-fluorophenol : Cis Conformer	
4.1. Conformations and Conformers	127
4.2. Conformers and Microwave Spectroscopy	127
4.3. Conformations in Halophenols	128
4.4. Microwave Spectral Study of 2-fluorophenol	130
4.4.1. Introduction	130
4.4.2. Experimental Details	132
4.4.3. Assignments and Results	133
4.4.4. Molecular Structure	138
4.5. References	144

**Chapter 5. Microwave Spectral Studies of 3-fluoro- and
2-fluorobenzonitrile**

5.1. Introduction	146
5.2. Microwave Spectral Study of 3-fluorobenzonitrile	147
5.2.1. Experimental Details	147
5.2.2. Observed Spectrum and Assignment	148
5.2.3. Molecular Structure	149
5.3. Microwave Spectral Study of 2-fluorobenzonitrile	155
5.3.1. Experimental Details	155
5.3.2. Observed Spectrum and Assignment	156
5.3.3. Molecular Structure	159
5.4. A Comment on these Investigations	160
5.5. References	161