

CONTENTS

Chapter	TITLE	Page No.
ONE	INTRODUCTION	
	1.1 Historical	
	1.1.1 The Role of Molecular Spectroscopy	1
	1.1.2 Important parameters related to Molecular Structure.	2
	1.2 Various forms for force constant in diatomics	4
	1.3 Potential energy function	6
	1.4 F.C.factors and r-centroids for diatomics	9
	1.5 Our approach towards getting correct values of these parameters	13
	References.	16
TWO	ELECTRONEGATIVITY AND FORCE CONSTANT	
	2.1 Introduction	23
	2.2 Formulation of electronegativity and its relation to other properties	24
	2.2.1 Methods of formulating electro- negativity scale.	24
	2.2.2 Relation to other properties	26
	2.3 Force constant	27
	2.3.1 Introduction	27
	2.3.2 Different methods to obtain force constants	29
	2.3.3 New expressions for force constants	34
	2.3.4 Other methods for force constants	37
	2.3.5 Results and Discussion	39
	2.4 Force constant and anharmonicity	40
	2.4.1 Anharmonicity and its effect	40
	2.4.2 Expressions for anharmonicity constant	41
	2.4.3 Results and Discussion	44
	2.5 Zero point mean square amplitudes	45
	2.5.1 Introduction	45
	2.5.2 Empirical relations	45
	2.5.3 Results and Discussion	48
	2.6 Bond order	49
	References.	51

Chapter	Title	Page No.
THREE	POTENTIAL ENERGY FUNCTIONS	
3.1	Account on potential energy functions	73
3.2	Different forms of potential energy functions	76
3.2.1	The Morse Function	77
3.2.2	The Dunham Function	79
3.2.3	The Hulbert-Hirschfelder Function	81
3.2.4	Mecke-Sutherland Function	82
3.2.5	Linnet Function	83
3.2.6	Lippincott Function	84
3.2.7	MRK Potential Function	85
3.3	RKRV procedure for obtaining classical turning points	88
3.4	True potential energy function	92
3.4.1	Extended Rydberg potential energy curve	92
3.4.2	Rapid method to construct true potential energy curve	94
3.4.3	Lakshman and Rao Method	99
3.4.4	Functional relation for diatomics	100
	References.	102
FOUR	FRANCK-CONDON FACTORS AND r-CENTROIDS	
4.1	Introduction	130
4.2	Different methods for the computation of F.C.factors	130
4.2.1	Hutchisson Method	130
4.2.2	Bates Method	133
4.2.3	Manneback Method	139
4.2.4	Extension of Manneback Method	142
4.2.5	Frazer & Jarman Method	145
4.3	r -centroids	148
4.3.1	Concept of r -centroids	148
4.3.2	Determination of r -centroids	149
4.3.3	r -centroids using functional relation.	151
4.4	Results and Discussion	152

Contents (contd.)

Chapter	Title	Page No.
	4.4.1 Franck-Condon Factors for different band systems of CuF, CuO, CuSe, CuTe, PN, NH, ND, AlSe, XeF and InBr.	152
	4.4.2 r-centroids for different band systems of CuF, CuSe, CuTe, AlSe, XeF & InBr	152
	References.	153
FIVE	SUMMARY AND CONCLUSIONS	
	5.1 Force constant and electronegativity	185
	5.2 Potential energy function for a diatomic molecule	186
	5.3 Franck-Condon Factors and r-centroids	187
	References.	189
