CONTENTS

CHAPTER	TITLE	PAGE
1	POTENTIAL ENERGY CURVES	* 53 % *********************************
1.1	INTRODUCTION	1
1.1.1	ANHARMONIC OSCILLATOR MODEL	2
1.1.2	CONTINUOUS TERM SPECTRUM AND DISSOCIATION	5
1.2	IMPORTANCE OF P.E. CURVES	6
1.3	METHODS OF DETERMINATION OF P.E. CURVES	7
1.3.1	QUANTUM MECHANICAL METHOD	7
1.3.2	RKRV METHOD	9
1.3.3	DUNHAM'S METHOD	12
1.4	EMPIRICAL POTENTIAL FUNCTIONS	14
1.4.1	CONDITIONS FOR A GOOD POTENTIAL FUNCTION	15
1.4.2	POTENTIAL FUNCTIONS AND THEIR RELATIVE MERITS AND DEMERITS	16
1.4.3	POTENTIAL PARAMETERS AND TESTING A POTENTIAL FUNCTION	23
1.5	ICNIC POTENTIAL ENERGY FUNCTIONS	25
1.6	VARSHNI'S METHOD	29
1.7	COMPARATIVE STUDY OF POTENTIAL ENERGY FUNCTIONS	30
1.7.1	VARSHNI'S STUDY	30
1.7.2	STUDY OF STEELE AND OTHERS	33
	CONTENTS	(CONTD.)

CHAPTER	TITLE	PAGE
2	VARIOUS COMBINATIONS OF ANALYTICAL POTENTIAL FUNCTIONS	
2.1	MORSE AND KRATZER(MK) POTENTIAL	38
2.2	MORSE AND RYDBERG(MR) POTENTIAL	39
2.3	RYDBERG AND KRATZER (RK) POTENTIAL	40
2.4	MRK POTENTIAL	41
2.5	IMPROVED MR POTENTIAL	41
2.6	RE-EXAMINED MK POTENTIAL	43
2.7	AIM OF THE PRESENT STUDY	43
2.8	PRESENT WORK	45
2.8.1	GENERALIZED MORSE AND RYDBERG(GMR) POTENTIAL	45
2.8.2	GENERALIZED MORSE AND KRATZER(GMK) POTENTIAL	47
2.8.3	VARSHNI'S SECOND AND SIXTH POTENTIAL	_ 48
2.8.4	RYDBERG AND LIPPINCOTT POTENTIAL	49
2.8.5	RYDBERG AND VARSHNI'S II POTENTIAL	49
2.8.6	RYDBERG AND VARSHNI'S VI POTENTIAL	50
2.9	CONCLUDING REMARKS	51
3	POTENTIAL ENERGY CURVES ON COMBINATION FUNCTIONS	
3.1	CALCULATIONS OF P.E CURVES	55
3.2	RESULTS AND DISCUSSION	56
3.3	SUMMARY	62

CHAPTER	TITLE	PAGE
4	CALCULATIONS OF SPECTROSCOPIC CONSTANTS USING THE PROPOSED COMBINATION POTENTIAL FUNCTIONS	
4.1	CALCULATIONS OF SPECTROSCOPIC CONSTANTS	75
4.2	RESULTS AND DISCUSSION	76
4.2.1	THE CONSTANTS $_{lpha_{\mathbf{e}}}$ AND $_{\omega}$ $_{\mathbf{e}}^{\mathbf{x}}$ $_{\mathbf{e}}$	76
4.2.2	PERCENTAGE ERRORS IN α e AND ω e e e	79
4.2.3	AVERAGE PERCENTAGE ERRORS	80
4.2.4	THE F AND G FUNCTIONS	81
4.2.5	F AND G VERSUS △ CURVES	84
4.3	SUMMARY	86
5	CALCULATION OF BINDING ENERGIES BY IONIC P.E FUNCTIONS	
5.1	INTRODUCTION	100
5.2	NEW IONIC P.E FUNCTIONS	101
5.3	CALCULATIONS	103
5.4	RESULTS AND DISCUSSION	103
5.5	SUMMARY	106