LIST OF FIGURES

1.1 $D_{5h}$ form of C$_{70}$ viewed perpendicular to the 5 - fold axis and showing the prolate spheroidal structure 03

1.2 A typical transition of vibrational energy levels. 09

1.3 Diatomic vibrator: ball and spring model. 12

1.4 The allowed vibrational energy levels and transitions between them for a diatomic molecule 13

1.5 The asymmetric stretching vibration of the carbon dioxide molecule 15

1.6 The Morse curve 19

1.7 The allowed vibrational energy levels and some transitions between them for a diatomic molecule 21

2.1 The Morse potential and its approximation with a harmonic oscillator potential. 61

2.2 The Poeschl-Teller potential. 63

2.3 Bending vibrations in linear polyatomic molecules. 66

2.4 Convergence properties of the algebraic method as compared with the conventional method 68

6.1 Ball and stick view of the 9-paraffine molecule, C$_9$H$_{20}$. 100
LIST OF TABLES

1.1 Boltzmann population distribution as a function of frequency 17
1.2 Infrared absorption bands of SO₂ 24
2.1 Admissible Lie algebras 41
2.2 Number of the operators in Lie algebras 42
2.3 Isomorphic Lie algebras 42
2.4 Number of integers that characterize the tensor representations of Lie algebras 47
2.5 Eigenvalues of some Casimir operators of Lie algebras 51
4.1 Fitting algebraic parameters of fullerene C₇₀ 86
4.2 Experimental and calculated fundamental IR active frequencies 87
4.3 Fitting parameters used in the study of C₇₀O 88
4.4 Experimental and calculated energies of C₇₀O. 88
4.5 Comparative study of calculated fundamental IR active frequencies of C₇₀ 90
5.1 Fitting parameters of Fullerene C₇₀C₈H₈ 93
5.2 Calculated and experimental energies of fullerene C₇₀C₈H₈ 94