PREFACE

Amidst the many pre-occupations, as a devoted teacher in the subject of Physics and as an ardent lover of teaching profession who bravely dared to do the research work at this belated stage, I venture to present my thesis entitled "Parametric approach to structural analysis of simple molecules using spectroscopic data."

The thesis which I do submit with an innate fund of obeisance is the exclusive "offspring" originated from my earnest research efforts and investigations carried out by me during 1992-97 in the Physics Research Centre of Maharajas College, Ernakulam under the Mahatma Gandhi University.

The thesis deals with a systematic analysis of vibrational potential energy for different possible geometries of simple molecules. A new parametric approach is employed for the evaluation of the potential energy contributions using the spectroscopic data of normal molecules and their isotopic substituents.

The Chapter I is mainly of an introductory nature. It explains the basic theory and the essentials of the parametric methods used in the analysis.
Chapter 2 deals with the analysis of bent symmetric \( XY_2 \) type molecules. A new criterion is developed namely the minimisation of bending energy, to investigate the structural of simple molecules. The different contributions to the average potential energy of the molecules have been separated and their variations with geometry have been studied in detail.

The \( XY_2 \) pyramidal type molecules are subjected to analysis applying the new criterion and the findings are presented in Chapter 3.

The Chapter 4 covers the application of the above criterion for fixing the geometry of the molecules like \( XY_2 \) linear symmetric type assigning them a different geometry.

In Chapter 5 a novel approximation method is developed and applied to evaluate the force field of simple molecules of the \( XY_2 \) type and the values are compared with those previously reported.

The variation of mean amplitudes of vibration with geometry has been the subject of analysis in Chapter 6. The investigations are carried out in the case of \( XY_2 \) bent symmetric, \( XY_2 \) linear symmetric and pyramidal \( XY_2 \) model and some interesting conclusions are obtained.
Chapter 7 deals with the case study on the structure of water molecule based on a recently reported vibrational assignment.

The results these investigations are discussed and summarised in Chapter 8. The investigations presented in the thesis are published in the following papers.