CHAPTER - 4

AIM AND OBJECTIVES
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Aim

The aim of the present study is to analyse the spectrum of polyatomic molecules based on quantum chemical calculations.

Objectives

1. To investigate 2,5-difluoronitrobenzene using hortree Fock and density functional theory calculations through fourier transform-infrared, raman, ultraviolet, and nuclear magnetic resonance spectroscopy.

2. To analyse 4-(Trifluromethoxy)benzylbromide by density functional theory calculations through UV and NMR.

3. To characterize the spectral vibration of 2-(Methylamino)pyridine by cross functional theory computations.

4. To evaluate structure and spectroscopic measurement of 4-(Diethoxymethyl) benzaldehyde.

5. To synthesize and Characterize 2-chloro-5-(Trifluromethyl)benzonitrile through experimental and theoretical approach.