



Vibrational spectra of *Ocimum basilicum* L. seed gum

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ABSTRACT

The vibrational spectra of some components of *Ocimum basilicum* L. seed gum were investigated. After extracting and purifying the fractions, the mid and far Fourier Transform infrared (FT-IR) spectra of them were recorded. Furthermore, the vibrational wavenumbers obtained in the B3LYP and TPSSh methods of density functional theory (DFT) using 6-311++G** basis set, compared with the corresponding experimental IR spectra, and clearly assigned. The functional groups and the physical properties accompanied with each functional group were discussed according to the assignments. The spectra indicate that some compounds are engaged in hydrogen bonding.

Keywords: Vibrational Spectroscopy, *Ocimum basilicum* L. seed gum, Computational chemistry.

1. INTRODUCTION

Ocimum basilicum L. (or Basil) is a common herb plant found all over the world. It is called Reyhan in Iran. Its flavour and pharmaceutical properties made it to be a well-known plant. Physico-mechanical properties of the Iranian basil seeds have been recently reported by Razavi et al. (2010). The polysaccharides extracted from basil seed by cold water extraction and alcohol precipitation, have been reported to have two major fractions: (i) an acid-stable core glucomannan (43%) having a ratio of glucose to mannose 10:2, and (ii) a (1 → 4)-linked xylan (24.29%) having acidic side chains at C-2 and C-3 of the xylosyl residues in acid-soluble portion (Razavi et al., 2009).

In this study, the vibrational spectra of some components of *Ocimum basilicum* L. seed gum were investigated. The calculated vibrational wavenumbers were compared with the corresponding experimental results. Furthermore, the origin of hydrogen bonding in some substances was studied.

2. MATERIALS AND METHODS

The extraction and purification processes were done according to Anjaneyalu and Gowda (1979). The FT-IR spectra of some fractions were recorded on a Bomem B-154 Fourier Transform spectrophotometer in the 4000–600 cm⁻¹ region by averaging 20 scans with a resolution of 2 cm⁻¹ at room temperature. The Far-IR spectra in the 600–250 cm⁻¹ region were obtained using a Thermo Nicolet NEXUS 870 FT-IR spectrometer equipped with a DTGS/polyethylene detector and a solid substrate beam splitter. The spectra were collected with a resolution of 2 cm⁻¹ by averaging the results of 32 scans at room temperature. In this study, the calculations for molecular equilibrium geometry and vibrational spectra of the substances were performed by means of the Gaussian 09W software package. The B3LYP and TPSSh methods and 6-311++G(d,p) basis set were utilized for optimization and vibrational spectra calculations.



3. RESULTS AND DISCUSSION

The acidic polysaccharide isolated from the seeds of *Ocimum basilicum* L. is composed of D-xylose, L-arabinose, L-rhamnose, and D-galacturonic acid together with traces of galactose and glucose (Anjaneyalu and Gowda, 1979). The experimental and calculated vibrational spectra of the components were studied. The functional groups and the physical properties accompanied with each functional group were discussed according to the assignments. The spectra indicate that some compounds are engaged in hydrogen bonding.

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