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Ab-initio investigation of absorption spectra for three interstellar aldehydes; A TDDFT study

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Abstract

Propynal, propenal and propanal compounds are three aldehydes molecules that recently were detected in interstellar by Green Bank Telescope (GBT). These molecules in enough pressure and temperature can change to each other by getting hydrogen from propynal to propanal, so hydrogen addition is important in the formation of complex interstellar molecules. Also by absorption spectra of these molecules and study the radiation that we get from interstellar, we can identify the presence of them in interstellar or not. In this paper, we simulate these molecules using QANTUM ESPRESSO computational package which is based on Density Functional Theory (DFT). These molecules have different structure so the optimized geometry of these molecules is calculated. Also absorption spectrum is computed for the most stable structure in the framework of Time Dependent Density Functional Theory (TDDFT) through Liouville Lanczos approach.

Key words: Interstellar space, DFT, TDDFT, Absorption Spectra**,** Aldehydes.

1. Introduction

The space between the stars contains gas and dust in low densities, is named interstellar. More than 135 interstellar molecular species have been identified [1]. These molecules contain aldehydes which is named "sugars of space" ever since in 1969 when Snyder et al. discover formaldehyde H_2CO [2]. An aldehyde group is an organic compound that is contains carbon, hydrogen, oxygen atoms and R group which is any generic alkyl or side chain. The importance of this group is because the ability of them to convert to other organic compounds. One of the ways to convert is by addition hydrogen.

Recently in 2004, the new interstellar molecules, propenal and propanal has been detected in the star forming region Sagittarius B2 (N) by the 100 m Green Bank Telescope (GBT) which is operating in the range from 18 GHz (λ~1.7cm) to 26 GHz (λ~1.2cm) [1] and