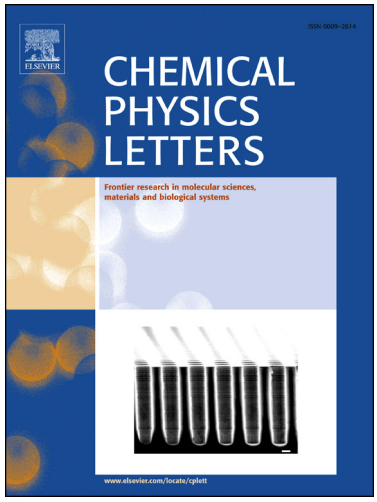

Normal coordinate analysis and fungicidal activity study on anilazine and its related compound using spectroscopic techniques

G.P. Sheeja Mol, D. Aruldhas, I. Hubert Joe, S. Balachandran

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Normal coordinate analysis and fungicidal activity study on anilazine and its related compound using spectroscopic techniques.

G.P. Sheeja Mol[a], D. Aruldhas[a,*], I. Hubert Joe[b], S. Balachandran[c]

[a]Department of Physics & Research Centre, Nesamony Memorial Christian College, Marthandam-629165,TamilNadu, India.

[b]Centre for Molecular and Biophysics Research, Department of Physics, Mar Ivanios College, Thiruvananthapuram-695015, Kerala, India.

[c]Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram-695004, Kerala, India.

Abstract

The FTIR and FT-Raman spectra of anilazine have been recorded in the range 400-4000 cm^{-1} and 50-3500 cm^{-1} respectively. The optimized geometrical parameters of the compound were calculated using B3LYP method with 6-311G(d,p) basis set. The distribution of the vibrational bands were carried out with the help of normal coordinate analysis (NCA). The ^{1}H and ^{13}C nuclear spectra have been recorded and chemical shifts of the molecule were also calculated using the gauge independent atomic orbital (GIAO) method. The UV-Visible spectrum of the compound was recorded in the region 190-900 nm and the electronic properties were determined by time-dependent DFT (TD-DFT) approach. Anilazine was screened for its antifungal activity. Molecular docking studies are conducted to predict its fungicidal activity.

1. Introduction

Anilazine [6-(2-chloroanilino)-2,4-dichloro-1,3,5-triazine] (compound1) was introduced in 1955 as the first nitrogen heterocyclic triazine to be used as fungicide. It is a nonsystematic fungicide and is a member of the organo-chlorine triazine group [1,2]. The rapid and unspecified reaction of anilazine with biologically relevant compounds in fungal spores is possibly the main reason for the fungicidal effect. Heterocyclic compounds bearing a symmetrical s-triazine moiety, represent an interesting class of compounds possessing a wide spectrum of biological activities such as anticancer, antiviral, bactericidal, fungicidal [3-6], antimalarial, and herbicidal.