

Accepted Manuscript

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

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

PII: S0009-2614(16)30283-4
DOI: <http://dx.doi.org/10.1016/j.cplett.2016.05.004>
Reference: CPLETT 33841

To appear in: *Chemical Physics Letters*

Received Date: 27 April 2016
Accepted Date: 1 May 2016



Please cite this article as: G.P. Sheeja Mol, D. Aruldas, I. Hubert Joe, S. Balachandran, Normal coordinate analysis and fungicidal activity study on anilazine and its related compound using spectroscopic techniques, *Chemical Physics Letters* (2016), doi: <http://dx.doi.org/10.1016/j.cplett.2016.05.004>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

G.P. Sheeja Mol^a, D. Aruldas^{a,*}, I. Hubert Joe^b, S. Balachandran^c

^aDepartment of Physics & Research Centre, Nesamony Memorial Christian College, Marthandam-629165, TamilNadu, India.

^bCentre for Molecular and Biophysics Research, Department of Physics, Mar Ivanios College, Thiruvananthapuram-695015, Kerala, India.

^cDepartment 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 ¹H and ¹³C 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.

Download English Version:

<https://daneshyari.com/en/article/5378821>

Download Persian Version:

<https://daneshyari.com/article/5378821>

[Daneshyari.com](https://daneshyari.com)