



## RESEARCH ARTICLE

## Molecular vibrational investigation on 6-(2-chloroanilino)-2,4-dichloro-1,3,5-triazine compound

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### Abstract

A combined experimental and theoretical investigation of the molecular structure, spectroscopic parameters of 6-(2-chloroanilino)-2,4-dichloro-1,3,5-triazine compound has been performed. The optimized geometry, harmonic vibrational frequencies, infrared intensities were obtained at the B3LYP/6-311G(D,P) level of theory and thermodynamic function are calculated at the same level. NBO analysis has been performed.

### Keywords

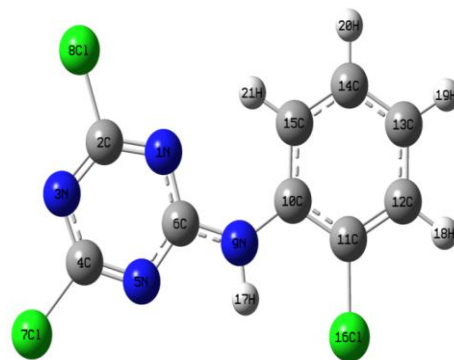
Molecular structure  
Optimized geometry  
Infrared  
NBO analysis

### Introduction

Anilazine[6-(2-chloroanilino)-2,4-dichloro-1,3,5-triazine] was introduced in 1955 as the first nitrogen heterocyclic triazine to be used as a fungicide. Anilazine is a fungicide used in controlling fungus diseases which attack lawns and turf, cereals, coffee and a wide variety of vegetables and other crops. It is also used for the control of potato and tomato leafspots[1]. Structural and spectroscopic analysis has been performed using computation and experimental methods. **Fig 1** represents the structure of anilazine

### Experimental Computation

The DFT computation of Anilazine were done using Gaussian '09 program package[2] using B3LYP method with 6-311G(d,p) basis set which has been successfully applied in order to derive the optimized geometry vibrational wavenumber of the normal modes and NBO analysis.



**Fig 1** Structure of anilazine

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## Results and discussion

### Optimized parameter

The computed and experimental x-ray diffraction data are given in **Table1**.

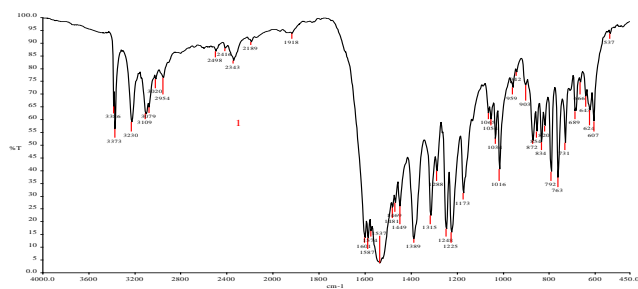
**Table 1** Optimized bondlength

BONDLEN GTH	EXPERIMENTAL VALUE(A <sup>0</sup> )	CALCULATED VALUE(A <sup>0</sup> )
N <sub>1</sub> -C <sub>2</sub>	1.320	1.319
N <sub>5</sub> -C <sub>6</sub>	1.348	1.354
C <sub>4</sub> -Cl <sub>7</sub>	1.723	1.743
C <sub>2</sub> -Cl <sub>8</sub>	1.722	1.744
N <sub>9</sub> -H <sub>17</sub>	0.88	1.021
C <sub>15</sub> -H <sub>21</sub>	0.951	1.078
C <sub>15</sub> -C <sub>10</sub>	1.389	1.402

The molecular structure of 6-(2-chloroanilino)-2,4-dichloro-1,3,5-triazine compress 2 rings, named triazine ring and chlorobenzene ring. The N<sub>5</sub>-C<sub>6</sub> bondlength elongated due to the intramolecular interactions between N<sub>9</sub>-H<sub>17</sub>....Cl<sub>16</sub>. In the case of C<sub>15</sub>-H<sub>21</sub> the value also decreased due to the hydrogen bonding.

### Vibrational Spectral Analysis

The vibrational spectra were analyzed based on the FT-IR spectra as well as the vibrational wavenumbers computed at the DFT level with the scaled wavenumbers. The FT-IR spectra are given in **Fig 2**.



**Fig 2** FT-IR Spectrum of anilazine

IR spectral analysis is based on the vibrational modes of the secondary amine vibrations, triazine ring vibrations and chlorobenzene ring vibrations. For secondary amines, it is known that symmetric NH stretching will give rise to a band in the range 3500-3310 cm<sup>-1</sup>[3]. The infrared spectrum shows a strong band at 3373cm<sup>-1</sup> (PED 100%) which corresponds to N-H symmetric stretching. The C-H stretching wavenumbers of benzene rings are expected in the region 3060-3120 cm<sup>-1</sup>[4]. In this compound the corresponding vibration is observed at 3106 cm<sup>-1</sup>. The intramolecular C-H....N hydrogen bonds is exposed in the NBO analysis as being due to the interaction between the nitrogen lonepair and the C-H antibonding orbital.

### Conclusions

Vibrational wavenumbers and infrared intensities calculated by B3LYP/6-311G(d,p) level agrees well with the experimental data. The bondlength N<sub>9</sub>-H<sub>17</sub> increased due to the hydrogen bonding. NBO analysis shows that the intramolecular C<sub>15</sub>-H<sub>21</sub>....N<sub>1</sub> hydrogen bond due to the interaction between the nitrogen lonepair and the C-H antibonding orbital. The possibility of hydrogen bonding and charge transfer shows the bioactive nature of this compound.

### References

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