

## Synthesis, Spectroscopic Characterization and Crystal Structure of Asymmetric Azine $C_{15}H_{13}N_3O_4$

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### INTRODUCTION

Asymmetric azines are derived from hydrazones and they have present pharmacological activities. The hydrazones and their derivatives have many applications such as anti-inflammatory activity, analgesic, antibacterial and antifungal<sup>1,2</sup>. This work aims to elucidate the structure of the synthesized and crystallized asymmetric azine (7E, 8E) -2- (3-methoxy-4-hydroxy-benzylidene) -1- (4-nitrobenzylidene) hydrazine by x-ray diffraction and IR, GC and NMR spectroscopy.

### METHODS

The synthesis of asymmetric azine was carried out using the hydrazone (E) -1 - (4-nitrobenzylidene) hydrazine, which may be obtained by reacting aldehydes / ketones with hydrazine. The method of slow evaporation of the solvent was employed in the crystallization process. The structure of the compound was determined by analysis of X-ray diffraction of a single crystal. It crystallized in the monoclinic crystal system; space group  $P2_1 / n$   $Z = 4$ . The structure solution was carried out using direct methods with the help of SHELXS – 97 program. The refinement was further performed by SHELXL - 97 implemented in the WinGX suite of program.

### RESULTS AND DISCUSSION

All the hydrogen and carbon atoms identified by NMR spectroscopy and the functional groups ( $NO_2$ ,  $C=N$ ,  $OH$ ) identified by IR spectroscopy were confirmed by X-ray diffraction analysis. The crystal molecular packing is driven mainly by classical ( $O-H\cdots O$ ) and non-classical ( $C-H\cdots O$ ) intermolecular interactions. The molecule has a planar configuration and B3LYP/6-

311++G\*\* studies are been made to quantify the non-classical interaction energy.

### CONCLUSIONS

In this study  $C_{15}H_{13}N_3O_4$  crystal structure was analyzed and characterized. Theoretical calculation are underway in order to find out the molecular regions where it is more electrophilic or nucleophilic. A fully understanding of the nature of those sites will be of great help to shed light in the asymmetric azine biological activities. As a further study, the electrostatic potential maps are also being conducted on the compound. As it is well known, the electrostatic potential is the long range driven forces and therefore it represent the first kind of interaction between molecules.

### ACKNOWLEDGMENTS

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