Int J Pharm Bio Sci 2012 July; 3(3): (B) 414 - 417

Research Article **Bio Chemistry**

International Journal of Pharma and Bio Sciences **ISSN 0975-6299**

COMPARATIVE X-RAY CRYSTALLOGRAPHIC STUDIES OF SYSTEMIC FUNGICIDE HEXACONOZOLE AND TRICYCLAZOLE

***DR JYOTSNACHAUHAN, ASHISH KUMAR SHARMA**

Lecturer in School of physics Devi Ahilya University Indore M.P India

ABSTRACT

The activity of fungicides is intimately related to its chemical structure. Knowledge about the chemical structure of a chemical is useful for the synthesis of new compounds with more specific actions and fewer adverse reactions, to increase/decrease the duration of action of the original fungicide or to get a more potent compound, to restrict the action to a specific system of the plant body and to reduce the adverse reactions, toxicity and other disadvantages associated. We can understand the basic chemical groups responsible for fungicidal action. A systemic fungicide is defined as systemic fungi toxic compound that controls a fungus pathogen remote from the point of application and that can be detected or identified [2].These compounds are absorbed by the plant and get translocated within it, thus providing protection as well as eradicating already established infection.

KEYWORDS-**X-ray crystallography, Systemic fungicides, Triazole structure**

DR JYOTSNACHAUHAN
Lecturer in School of physics Devi Ahilya University Indore M.P India

INTRODUCTION

A systemic fungicide is defined as systemic fungi toxic compound that controls a fungus pathogen remote from the point of application and that can be detected or identified [1].These compounds are absorbed by the plant and get translocated within it, thus providing protection as well as eradicating already established infection.

Triazoles.compounds contain a ring composed of two carbon atoms and three nitrogen atoms. We can understand the basic chemical groups responsible for drug action[2]. These compounds possess a trityl carbon that can act as a carbonium ion, an organic ion carrying a positive at a carbon location. In Hexaconazole ORTEP[3] Diagram we can see Triazole compound N1, N2, N3 and C9 and C10 .In Tricyclazole ORTEP Diagram we can see Triazole compound N1, N2, N3 and C7 and C8. Recently it has been observed that some of the fungicides are loosing their effects. So analogous compounds can be designed as substitute, if their structures are known. A rational approach to test these fungicides is to know the three dimensional structure of these compounds and macromolecular receptor sites as well as their molecular complex .The structures of these compounds can be obtained by X-ray diffraction method in crystalline form and they will invariably be similar to their structure in solutions.

Experimental: First grow the crystals of existing fungicides available and synthesize their derivatives in lab. The determination of structural perturbation in fungicide derivatives and comparison of the result of their molecular association with other receptor sites by X-Ray crystallography techniques will be done. In parallel with these structural studies, spectroscopic studies carried out on them. The goal is then to tie together the structural and spectroscopic studies to have more comprehensive account of the precise shape of these molecules, the non-covalent interaction which are likely to be involved in and the changes introduced in molecular geometry and electronic structure of these compounds as a result of their molecular association with other compounds. Thus, we study the structure of variety of such compounds and correlate their structure with biological activity, so that more safe and effective fungicides at reasonable price can be developed.

Data collection and Structure Solution: The three dimensional intensity data were collected on a computerized automatic 4-circle CAD-4 Enraf-Nonious diffractometer using graphite filtered MoKα (Å) radiation's at SAIF Madras. Temperature of both the crystal during data collection was 293°K. All the data were corrected for Lorentz and Polarization effect. The structure was solved using SHELXS[4]-program for crystal structure solution.

3. REFINEMENT

The positional co-ordinates, which were obtained from SHELXS 97 and isotropic temperature factors, were subjected to refinement by SHELXL[5] refinement program. After so many cycles of refinement the R factors dropped .Further refinement of the structure was carried out with individuals an isotropic temperature factors of the exponential form.

$$-2P_1\text{^ }2[h\text{^}2a^*\text{^}2U_{11}+2hKa^*bxU_{12}$$

reduced R factor. The hydrogen atoms were fixed at this stage by geometrical considerations and were not refined. Refinement of the structure was terminated after two more cycles when all the deviations in parameters became much smaller than the corresponding estimated standard derivation.

RESULT AND DISCUSSION

In both the crystals, the average bond distances of C-H is 0. 96(2)Å.In Triazole ring of Tricyclazole figure **1** the bond distances of C(7)-N(1) is 1.368Å , C(8)-N(1) is 1.360 Å., N (2)-N (3) is 1.396Å, C(7)-N(2)is 1.294(3), C(8)-N(3) is 1.305(2).In Triazole ring of

Hexaconazole figure **2** he bond distances of C(10)-N(3) is 1.305Å , C(10)-N(2) is 1.344 Å., N (1)-N (3) is 1.349Å, C(9)-N(2)is 1.313(3), C(9)-N(1) is 1.320(2) . In both the crystals triazole ring is distorted in shape[6]. The average bond distances

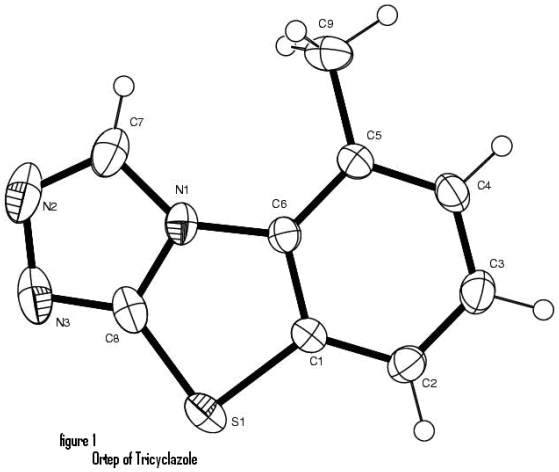

Figure1
Ortep of Tricyclazole

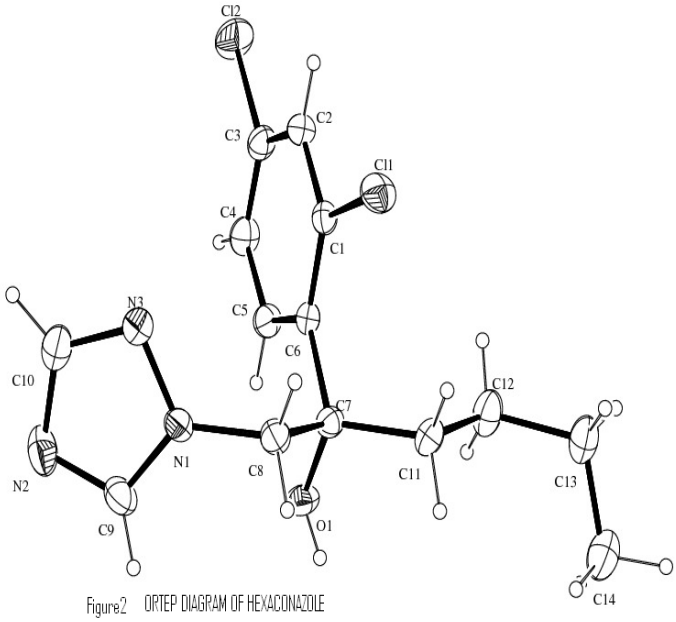

Figure2
Ortep Diagram of Hexaconazole

and Lab and valuable help in Data for C-N and N-N bonds are 1. 354Å and 1. 396Å. The bond lengths and angles in the benzene ring show regular features in the molecule. C-C distances

are short and shortening may be due to delocalization of electrons from the benzene rings. The whole molecules appeared to be twisted and folded and reason may be due to stacking constraints. The bond distance around C (7) is as usual shorter than single bond value. This may also appear to bear a partial double bond character The bond distances in the five member ring are comparable to corresponding distances in heterocyclic ring 1. 339(Å). The average value of bond lengths and angles in the rings derived from most reliable set of data by Spencer[7] are 1. 377Å and 119º, respectively.

.

ACKNOWLEDGEMENT

I am thankful to SAIF IIT MADRAS for providing me Facility CAD-4Diffractometer collection.

REFERENCES

1. Berg,D., W. Kramer, E.Regel, K.H.Buechel, G. Holmwood,m.Plembel and H.Scheinpflug,1984.”Mode of action of fungicides. Studies.Studies on ergosterol biosynthesios inhibitors”,Proc. Br.Crop protconf.- pest and Diseases,3:887-892
2. Shephard, M.C., R. A. Noon, P.A Worthington, W.D. McClellan and BG Lever 1986 Proc. Br. Crop Prot. Conf. –Pest and Diseases, 1:19-26
3. Jolmson, C.K. (1965), ORTEP, Report ORNL-3794. Oak Ridge National laboratory, Temessee, U.S.A.
4 Sheldrich, G.M. (1997), SHELXS-97, Program for the solution of crystal structure.
5 Sheldrich, G.M. (1997), SHELXL-97, Program for crystal structure determination.
6. Nowell, I.W. and Walker, P.E. (1982) Acta Cryst. B38, 1857-1859
7. Spencer, M. (1959), Acta Cryst. 12, 50.