

## Comparative Analysis between *E, Z* -4-[3-(4-chlorophenyl)-3-(3, 4-dimethoxyphenyl) acryloyl] morpholine & Monceren Crystal

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**Abstract :** The structures of Dimethomorph compounds can be obtained by X-Ray Diffraction method in crystalline form and they will invariably be similar to their structures in solution. The composition of crystal **Dimethomorph** is confirmed by comparing the infrared spectra of two components. Crystal size of **Dimethomorph** is 0.30 x 0.20 x 0.20 mm. The unit cell parameters are  $a = 8.593(5) \text{ \AA}$ ,  $b = 11.220(5) \text{ \AA}$  and  $c = 11.712(5) \text{ \AA}$ ,  $\alpha = 63.504(5) \text{ deg.}$ ,  $\beta = 72.177(5) \text{ deg.}$ ,  $\gamma = 85.391(5) \text{ deg.}$ , respectively. Crystal system is Triclinic and space group is P-1.

The **Monceren N-((4-chlorophenyl)methyl)-N-cyclopentyl-N'-phenylurea** molecular structures obtained by the X-Ray Diffraction method in crystalline form. Crystal size of monceren is nearly 0.46 x 0.120 x 0.060 mm. We determine the three-dimensional structure, molecular dimensional, molecular geometry, electronic structure and the conformation of fungicides and analyze their crystal structures also. The composition of crystal **Monceren N-((4-chlorophenyl)methyl)-N-cyclopentyl-N'-phenylurea** is confirmed by comparing the infra-red spectra. The unit cell parameters are  $a = 12.1887(12) \text{ \AA}$ ,  $b = 8.7677(8) \text{ \AA}$ ,  $c = 33.063 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90.00^\circ$ ,  $\gamma = 90^\circ$ . The Crystal system is Orthorhombic type.

**Keywords:** X-ray crystallography, fungicides, Triazole structure, Benzene Structure

**Introduction:** **Dimethomorph** (*E, Z*)-4-[3-(4-chlorophenyl)-3-(3, 4-dimethoxyphenyl) acryloyl] morpholine, a local systemic fungicide. The activity of fungicides is intimately related to its chemical structure. Knowledge about the 1 structure of a chemical is useful for the synthesis of new compounds with more specific action and fewer adverse reactions, to increase/decrease the duration of action of the original drug or to get a more potent compound, to restrict the action to a specific system of the body and to reduce the adverse reactions, toxicity and other disadvantages associated. We can understand the basic chemical groups responsible for action.

Pencycuron (C<sub>19</sub>H<sub>21</sub>ClN<sub>2</sub>O) is a Synthetic Substance of Phenylurea group. It comes under the Product Category of Foliar Fungicide. Its IUPAC name is 1-(4-chlorobenzyl)-1-cyclopentyl-3-phenylurea. and CAS Number is [66063-05-6] (2). It exists in the form of Colorless, odorless crystals. In India it was registered in 2006 and is available as Monceren® 125 DS Fungicide. Pencycuron is a slightly toxic compound. Pencycuron exerts its effects by Contact Action.

**Experimental:** -First grow the crystal of existing fungicides available and synthesize their derivatives in lab. Dimethomorph is soluble in water, Acetone, Toluene, Methanol and Hexane. But mostly it is soluble in Toluene (C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub>). In that particular fungicide white well formed crystals of size 0.030 x 0.020 x 0.020 mm are obtained by slow evaporation from a solution of Toluene at 297° K temperature. These crystals have been grown within 1-8 days. The crystals obtained are rectangular in shape.

The density of crystal 1.342 Mg/m<sup>3</sup> is measured by floatation method the mixture of benzene and Bromoform. The preliminary information about the crystal is listed in table 3.1. The unit cell parameters are determined by directly on CAD – 4 Enraf Nonius 4 circle automatic Diffractometer. Chemical structure of Dimethomorph is given figure 1.

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. 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 safer and effective fungicides at reasonable price can be developed.. Firstly grow the crystal by evaporation method fungicides are available .we synthesizes their derivatives in lab.. In that particular fungicide yellow well formed crystals of size 0.46 x 0.120 x 0.060 mm are obtain by slow evaporation from a solution **293<sup>o</sup> K**

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temperature.. These crystals have been grown within few days. The crystals obtained are rectangular in shape. The density of crystal **1.238** Mg/m<sup>3</sup> is measured by floatation method with the mixture of benzene and Bromoform .The unit cell parameters were determined by automatic computerized 4-circled Enraf-Nonius CAD-4 Diffractometer. The preliminary information about crystal is given in Table.2.

**Table 4.1. Crystal data and structure refinement for Dimethomorph.**

<i>Identification code</i>	<i>Shelxl</i>
<i>Empirical formula</i>	<b>C<sub>21</sub> H<sub>22</sub> Cl N O<sub>4</sub></b>
<i>Formula weight</i>	<b>387.85</b>
<i>Temperature</i>	<b>293(2) K</b>
<i>Wavelength</i>	<b>0.71073 Å</b>
<i>Crystal system, space group</i>	<b>Triclinic, P-1</b>
<i>Unit cell dimensions</i>	<b>a = 8.593(5) Å    alpha = 63.504(5) deg. b = 11.220(5) Å    beta = 72.177(5) deg. c = 11.712(5) Å    gamma = 85.391(5) deg.</b>
<i>Volume</i>	<b>960.0(8) Å<sup>3</sup></b>
<i>Z, Calculated density</i>	<b>2, 1.342 Mg/m<sup>3</sup></b>
<i>Absorption coefficient</i>	<b>0.226 mm<sup>-1</sup></b>
<i>F(000)</i>	<b>408</b>
<i>Crystal size</i>	<b>0.30 x 0.20 x 0.20 mm</b>
<i>Theta range for data collection</i>	<b>2.03 to 26.00 deg.</b>
<i>Limiting indices</i>	<b>-10&lt;=h&lt;=10, -13&lt;=k&lt;=13, -14&lt;=l&lt;=14</b>
<i>Reflections collected / unique</i>	<b>19752 / 3767 [R(int) = 0.0256]</b>
<i>Completeness to theta =</i>	<b>26.00    100.0 %</b>
<i>Absorption correction</i>	<b>Semi-empirical from equivalents</b>
<i>Max. and min. transmission</i>	<b>0.967 and 0.912</b>
<i>Refinement method</i>	<b>Full-matrix least-squares on F<sup>2</sup></b>
<i>Data / restraints / parameters</i>	<b>3767 / 0 / 251</b>
<i>Goodness-of-fit on F<sup>2</sup></i>	<b>1.034</b>
<i>Final R indices [I&gt;2sigma(I)]</i>	<b>R1 = 0.0372, wR2 = 0.0973</b>

<i>R indices (all data)</i>	<i>RI = 0.0448, wR2 = 0.1038</i>
<i>Extinction coefficient</i>	<i>0.032(3)</i>
<i>Largest diff. peak and hole</i>	<i>0.229 and -0.270 e.Å<sup>-3</sup></i>

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**Data collection and Structure Solution:** The intensity data are collected on a computerized automatic CAD-4 Enraf-Nonius 4-circle diffractometer. The data collection is done on  $\theta$ -scan mode by four circle diffractometer. Theta range for data collection is 2.03 to 26.00 deg. The miller indices (hkl) value varied from -10 to 10, -13 to 13 and -14 to 14, respectively. The reflection is 19752. The total number of unique reflection is 3767 [R (int) = 0.0256]. Each intensity measurement involved in a scan over the reflection peak, a back ground measurement at each end of the scan range and measurement of peak height. The structure determination is carried out on VAX machine using SHELXS - 97. All the Non-Hydrogen atoms are located in the beginning itself.

X-ray crystallographic data were collected at 297° K with  $\text{Cu}_{K\alpha}$  radiation ( $\lambda = 1.54184 \text{ \AA}$ ) using a Bruker-Nonius SMART CCD diffractometer equipped with graphite monochromator. The SMART software was used for data collection and also for indexing the reflections and determining the unit cell parameters; the collected data were integrated using SAINT software. The structures were solved by direct methods and refined by full-matrix least-squares calculations using SHELXTL software. All the non-H atoms were refined in the anisotropic approximation against  $F^2$  of all reflections. The H-atoms, placed at their calculated positions and refined in the isotropic approximation; those attached to heteroatom (N and O) were located in the difference Fourier maps, and refined with isotropic displacement coefficients.

The three dimensional intensity data were collected on a computerized automatic 4-circle CAD-4 Enraf-Nonius diffractometer using graphite filtered  $\text{Cu}_{K\alpha}$  radiation ( $\lambda = 1.54184 \text{ \AA}$ ) at SAIF Madras.. Temperature of crystal during data collection was 293°K. All the data were corrected for Lorentz and Polarization effect. Three standard reflection were measured where hkl indices varies from  $-14 \leq h \leq 7$ ,  $-10 \leq k \leq 5$ ,  $-33 \leq l \leq 40$ . The total number of reflections were 7501 out of which unique reflection were 3391. Each intensity measurement involved in a scan over the reflection peak, a back ground measurement at each end of the scan range and measurement of the peak height. The structure was solved using SHELXS-program for crystal structure solution.

**REFINEMENT:** The positional co-ordinates, which were measured from and isotropic temperature factors were subjected to refinement by SHELXL -97 refinement computer program. After so many cycles of refinement the R dropped to 0.0372. Further refinement of the structure was carried out with individual isotropic temperature factors of dropped of the exponential form

$$-2P_1 [2a^* (2U_{11} + \dots - 2hka^*bxU_{12})]$$

reduced to R indices [ $I > 2\sigma(I)$ ]  $R1 = 0.0372$ ,  $wR2 = 0.0973$ .

The positional co-ordinates, which were obtained from SHELXS 97 and isotropic temperature factors, were subjected to refinement by SHELXL refinement program. After so many cycles of refinement the Rfactors dropped to **0.0225**. Further refinement of the structure was carried out with individual anisotropic temperature factors of the exponential form.  $-2P_1^2 [h^2 a^{*2} U_{11} + \dots + 2hKa^* b^* U_{12}]$  reduced Rfactor to **0.0225**. 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 derivations.

**Figure 1.** The experimental setup of 4-circle Goniometer (Eulerian or Kappa Geometry) ngicide. Pencycuron is a slightly toxic compound. Pencycuron exerts its effects by Contact Action.

**Table - 3.2.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ )  $U(eq)$  for Dimethomorph is defined as one third of the trace of the orthogonalized Uijtensio

	x	y	z	U(eq)
C(1)	6753(4)	254(2)	10926(2)	105(1)
C(2)	5837(3)	1475(2)	10706(2)	78(1)
C(3)	8011(2)	2639(2)	8620(2)	65(1)
C(4)	8834(3)	1361(2)	8942(2)	83(1)
C(5)	6943(2)	3726(2)	10078(2)	47(1)
C(6)	5875(2)	3648(2)	11387(2)	48(1)
C(7)	6185(2)	2993(1)	12555(1)	42(1)
C(8)	7670(2)	2224(2)	12661(1)	41(1)
C(9)	7534(2)	875(2)	13535(2)	51(1)
C(10)	8899(2)	158(2)	13664(2)	54(1)
C(11)	10425(2)	796(2)	12926(2)	47(1)
C(12)	10609(2)	2128(2)	12045(2)	49(1)
C(13)	9229(2)	2834(2)	11916(2)	47(1)
C(14)	5103(2)	3038(1)	13800(1)	41(1)
C(15)	5742(2)	2920(2)	14789(2)	50(1)
C(16)	4791(2)	3072(2)	15903(2)	52(1)
C(17)	3165(2)	3316(2)	16063(2)	46(1)
C(18)	2477(2)	3383(2)	15093(2)	44(1)
C(19)	3439(2)	3260(2)	13975(2)	42(1)
C(20)	81(2)	3691(2)	14403(2)	59(1)
C(21)	2752(3)	3520(2)	18074(2)	71(1)
N(1)	6959(2)	2657(1)	9854(1)	55(1)
O(1)	7691(3)	238(2)	9707(2)	104(1)
O(2)	7751(2)	4768(1)	9240(1)	69(1)
O(3)	844(1)	3557(1)	15368(1)	62(1)
O(4)	2114(2)	3489(1)	17103(1)	64(1)
Cl(1)	12144(1)	-104(1)	13153(1)	69(1)

**Table - 3.3** Bond lengths (Angstrom) and Bond angle (degree) for Dimethomorph involving Hydrogen atoms with estimated standard deviation in parentheses.

Bond lengths [Å]	Angles [deg]
C(1)-O(1)	1.415(3)
C(1)-C(2)	1.483(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-N(1)	1.456(2)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-N(1)	1.460(2)

<i>C(3)-C(4)</i>	<i>1.489(3)</i>
<i>C(3)-H(3A)</i>	<i>0.9700</i>
<i>C(3)-H(3B)</i>	<i>0.9700</i>
<i>C(4)-O(1)</i>	<i>1.417(3)</i>
<i>C(4)-H(4A)</i>	<i>0.9700</i>
<i>C(4)-H(4B)</i>	<i>0.9700</i>
<i>C(5)-O(2)</i>	<i>1.2251(19)</i>
<i>C(5)-N(1)</i>	<i>1.336(2)</i>
<i>C(5)-C(6)</i>	<i>1.493(2)</i>
<i>C(6)-C(7)</i>	<i>1.333(2)</i>
<i>C(6)-H(6)</i>	<i>0.892(19)</i>
<i>C(7)-C(8)</i>	<i>1.488(2)</i>
<i>C(7)-C(14)</i>	<i>1.490(2)</i>
<i>C(8)-C(13)</i>	<i>1.387(2)</i>
<i>C(8)-C(9)</i>	<i>1.388(2)</i>
<i>C(9)-C(10)</i>	<i>1.377(2)</i>
<i>C(9)-H(9)</i>	<i>0.9300</i>
<i>C(10)-C(11)</i>	<i>1.373(2)</i>
<i>C(10)-H(10)</i>	<i>0.9300</i>
<i>C(11)-C(12)</i>	<i>1.373(2)</i>
<i>C(11)-Cl(1)</i>	<i>1.7418(17)</i>
<i>C(12)-C(13)</i>	<i>1.381(2)</i>
<i>C(12)-H(12)</i>	<i>0.9300</i>
<i>C(13)-H(13)</i>	<i>0.9300</i>
<i>C(14)-C(15)</i>	<i>1.380(2)</i>
<i>C(14)-C(19)</i>	<i>1.399(2)</i>
<i>C(15)-C(16)</i>	<i>1.386(2)</i>
<i>C(15)-H(15)</i>	<i>0.9300</i>
<i>C(16)-C(17)</i>	<i>1.374(2)</i>
<i>C(16)-H(16)</i>	<i>0.9300</i>
<i>C(17)-O(4)</i>	<i>1.3584(19)</i>
<i>C(17)-C(18)</i>	<i>1.405(2)</i>
<i>C(18)-O(3)</i>	<i>1.359(2)</i>
<i>C(18)-C(19)</i>	<i>1.377(2)</i>
<i>C(19)-H(19)</i>	<i>0.9300</i>
<i>C(20)-O(3)</i>	<i>1.420(2)</i>
<i>C(20)-H(20A)</i>	<i>0.9600</i>
<i>C(20)-H(20B)</i>	<i>0.9600</i>
<i>C(20)-H(20C)</i>	<i>0.9600</i>
<i>C(21)-O(4)</i>	<i>1.420(2)</i>
<i>C(21)-H(21A)</i>	<i>0.9600</i>
<i>C(21)-H(21B)</i>	<i>0.9600</i>
<i>C(21)-H(21C)</i>	<i>0.9600</i>
<i>O(1)-C(1)-C(2)</i>	<i>112.2(2)</i>
<i>O(1)-C(1)-H(1<sup>a</sup>)</i>	<i>109.2</i>
<i>C(2)-C(1)-H(1A)</i>	<i>109.2</i>
<i>O(1)-C(1)-H(1B)</i>	<i>109.2</i>
<i>C(2)-C(1)-H(1B)</i>	<i>109.2</i>
<i>H(1A)-C(1)-H(1B)</i>	<i>107.9</i>
<i>N(1)-C(2)-C(1)</i>	<i>110.0(2)</i>
<i>N(1)-C(2)-H(2A)</i>	<i>109.7</i>
<i>C(1)-C(2)-H(2A)</i>	<i>109.7</i>
<i>N(1)-C(2)-H(2B)</i>	<i>109.7</i>
<i>C(1)-C(2)-H(2B)</i>	<i>109.7</i>
<i>H(2A)-C(2)-H(2B)</i>	<i>108.2</i>
<i>N(1)-C(3)-C(4)</i>	<i>109.61(16)</i>
<i>N(1)-C(3)-H(3A)</i>	<i>109.7</i>

<i>C(4)-C(3)-H(3A)</i>	<i>109.7</i>
<i>N(1)-C(3)-H(3B)</i>	<i>109.7</i>
<i>C(4)-C(3)-H(3B)</i>	<i>109.7</i>
<i>H(3A)-C(3)-H(3B)</i>	<i>108.2</i>
<i>O(1)-C(4)-C(3)</i>	<i>111.9(2)</i>
<i>O(1)-C(4)-H(4A)</i>	<i>109.2</i>
<i>C(3)-C(4)-H(4A)</i>	<i>109.2</i>
<i>O(1)-C(4)-H(4B)</i>	<i>109.2</i>
<i>C(3)-C(4)-H(4B)</i>	<i>109.2</i>
<i>H(4A)-C(4)-H(4B)</i>	<i>107.9</i>
<i>O(2)-C(5)-N(1)</i>	<i>122.17(15)</i>
<i>O(2)-C(5)-C(6)</i>	<i>119.32(15)</i>
<i>N(1)-C(5)-C(6)</i>	<i>118.50(14)</i>
<i>C(7)-C(6)-C(5)</i>	<i>125.43(15)</i>
<i>C(7)-C(6)-H(6)</i>	<i>119.4(12)</i>
<i>C(5)-C(6)-H(6)</i>	<i>115.0(12)</i>
<i>C(6)-C(7)-C(8)</i>	<i>121.17(14)</i>
<i>C(6)-C(7)-C(14)</i>	<i>121.83(14)</i>
<i>C(8)-C(7)-C(14)</i>	<i>116.95(13)</i>
<i>C(13)-C(8)-C(9)</i>	<i>117.97(14)</i>
<i>C(13)-C(8)-C(7)</i>	<i>121.33(14)</i>
<i>C(9)-C(8)-C(7)</i>	<i>120.69(13)</i>
<i>C(10)-C(9)-C(8)</i>	<i>121.32(14)</i>
<i>C(10)-C(9)-H(9)</i>	<i>119.3</i>
<i>C(8)-C(9)-H(9)</i>	<i>119.3</i>
<i>C(11)-C(10)-C(9)</i>	<i>119.23(15)</i>
<i>C(11)-C(10)-H(10)</i>	<i>120.4</i>
<i>C(9)-C(10)-H(10)</i>	<i>120.4</i>
<i>C(10)-C(11)-C(12)</i>	<i>121.11(15)</i>
<i>C(10)-C(11)-C(1)</i>	<i>118.82(13)</i>
<i>C(12)-C(11)-C(1)</i>	<i>120.04(12)</i>
<i>C(11)-C(12)-C(13)</i>	<i>119.09(14)</i>
<i>C(11)-C(12)-H(12)</i>	<i>120.5</i>
<i>C(13)-C(12)-H(12)</i>	<i>120.5</i>
<i>C(12)-C(13)-C(8)</i>	<i>121.27(15)</i>
<i>C(12)-C(13)-H(13)</i>	<i>119.4</i>
<i>C(8)-C(13)-H(13)</i>	<i>119.4</i>
<i>C(15)-C(14)-C(19)</i>	<i>118.12(14)</i>
<i>C(15)-C(14)-C(7)</i>	<i>120.34(14)</i>
<i>C(19)-C(14)-C(7)</i>	<i>121.47(13)</i>
<i>C(14)-C(15)-C(16)</i>	<i>121.40(15)</i>
<i>C(14)-C(15)-H(15)</i>	<i>119.3</i>
<i>C(16)-C(15)-H(15)</i>	<i>119.3</i>
<i>C(17)-C(16)-C(15)</i>	<i>120.47(15)</i>
<i>C(17)-C(16)-H(16)</i>	<i>119.8</i>
<i>C(15)-C(16)-H(16)</i>	<i>119.8</i>
<i>O(4)-C(17)-C(16)</i>	<i>125.92(15)</i>
<i>O(4)-C(17)-C(18)</i>	<i>115.23(15)</i>
<i>C(16)-C(17)-C(18)</i>	<i>118.85(14)</i>
<i>O(3)-C(18)-C(19)</i>	<i>124.90(14)</i>
<i>O(3)-C(18)-C(17)</i>	<i>114.82(14)</i>
<i>C(19)-C(18)-C(17)</i>	<i>120.28(14)</i>
<i>C(18)-C(19)-C(14)</i>	<i>120.80(14)</i>
<i>C(18)-C(19)-H(19)</i>	<i>119.6</i>
<i>C(14)-C(19)-H(19)</i>	<i>119.6</i>
<i>O(3)-C(20)-H(20A)</i>	<i>109.5</i>
<i>O(3)-C(20)-H(20B)</i>	<i>109.5</i>



<i>H(20A) - C(20) - H(20B)</i>	<i>109.5</i>
<i>O(3) - C(20) - H(20C)</i>	<i>109.5</i>
<i>H(20A) - C(20) - H(20C)</i>	<i>109.5</i>
<i>H(20B) - C(20) - H(20C)</i>	<i>109.5</i>
<i>O(4) - C(21) - H(21A)</i>	<i>109.5</i>
<i>O(4) - C(21) - H(21B)</i>	<i>109.5</i>
<i>H(21A) - C(21) - H(21B)</i>	<i>109.5</i>
<i>O(4) - C(21) - H(21C)</i>	<i>109.5</i>
<i>H(21A) - C(21) - H(21C)</i>	<i>109.5</i>
<i>H(21B) - C(21) - H(21C)</i>	<i>109.5</i>
<i>C(5) - N(1) - C(2)</i>	<i>124.77(15)</i>
<i>C(5) - N(1) - C(3)</i>	<i>121.78(14)</i>
<i>C(2) - N(1) - C(3)</i>	<i>113.09(15)</i>
<i>C(1) - O(1) - C(4)</i>	<i>109.91(16)</i>
<i>C(18) - O(3) - C(20)</i>	<i>117.84(13)</i>
<i>C(17) - O(4) - C(21)</i>	<i>118.15(15)</i>

*Symmetry transformations used to generate equivalent atoms:*

**Table: Anisotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) of Dimethomorph. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^2 U_{11} + \dots + 2hk a^* b^* U_{12}]$ .**

	<i>U<sub>11</sub></i>	<i>U<sub>22</sub></i>	<i>U<sub>33</sub></i>	<i>U<sub>23</sub></i>	<i>U<sub>13</sub></i>	<i>U<sub>12</sub></i>
<i>C(1)</i>	<i>171(3)</i>	<i>58(1)</i>	<i>65(1)</i>	<i>-27(1)</i>	<i>4(2)</i>	<i>-27(2)</i>
<i>C(2)</i>	<i>84(1)</i>	<i>79(1)</i>	<i>60(1)</i>	<i>-33(1)</i>	<i>6(1)</i>	<i>-33(1)</i>
<i>C(3)</i>	<i>69(1)</i>	<i>70(1)</i>	<i>45(1)</i>	<i>-23(1)</i>	<i>-3(1)</i>	<i>-1(1)</i>
<i>C(4)</i>	<i>98(2)</i>	<i>76(1)</i>	<i>70(1)</i>	<i>-41(1)</i>	<i>-7(1)</i>	<i>8(1)</i>
<i>C(5)</i>	<i>44(1)</i>	<i>48(1)</i>	<i>40(1)</i>	<i>-10(1)</i>	<i>-13(1)</i>	<i>7(1)</i>
<i>C(6)</i>	<i>45(1)</i>	<i>46(1)</i>	<i>45(1)</i>	<i>-15(1)</i>	<i>-12(1)</i>	<i>9(1)</i>
<i>C(7)</i>	<i>39(1)</i>	<i>39(1)</i>	<i>42(1)</i>	<i>-14(1)</i>	<i>-9(1)</i>	<i>0(1)</i>
<i>C(8)</i>	<i>39(1)</i>	<i>44(1)</i>	<i>37(1)</i>	<i>-16(1)</i>	<i>-9(1)</i>	<i>2(1)</i>
<i>C(9)</i>	<i>39(1)</i>	<i>46(1)</i>	<i>49(1)</i>	<i>-11(1)</i>	<i>-5(1)</i>	<i>-2(1)</i>
<i>C(10)</i>	<i>52(1)</i>	<i>42(1)</i>	<i>51(1)</i>	<i>-10(1)</i>	<i>-10(1)</i>	<i>5(1)</i>
<i>C(11)</i>	<i>43(1)</i>	<i>56(1)</i>	<i>42(1)</i>	<i>-23(1)</i>	<i>-13(1)</i>	<i>12(1)</i>
<i>C(12)</i>	<i>37(1)</i>	<i>58(1)</i>	<i>45(1)</i>	<i>-20(1)</i>	<i>-7(1)</i>	<i>-3(1)</i>
<i>C(13)</i>	<i>44(1)</i>	<i>42(1)</i>	<i>43(1)</i>	<i>-12(1)</i>	<i>-9(1)</i>	<i>-1(1)</i>
<i>C(14)</i>	<i>39(1)</i>	<i>39(1)</i>	<i>41(1)</i>	<i>-15(1)</i>	<i>-11(1)</i>	<i>2(1)</i>
<i>C(15)</i>	<i>39(1)</i>	<i>61(1)</i>	<i>49(1)</i>	<i>-22(1)</i>	<i>-16(1)</i>	<i>5(1)</i>
<i>C(16)</i>	<i>52(1)</i>	<i>62(1)</i>	<i>46(1)</i>	<i>-23(1)</i>	<i>-21(1)</i>	<i>2(1)</i>
<i>C(17)</i>	<i>50(1)</i>	<i>46(1)</i>	<i>42(1)</i>	<i>-21(1)</i>	<i>-11(1)</i>	<i>2(1)</i>
<i>C(18)</i>	<i>38(1)</i>	<i>46(1)</i>	<i>48(1)</i>	<i>-22(1)</i>	<i>-13(1)</i>	<i>4(1)</i>
<i>C(19)</i>	<i>41(1)</i>	<i>45(1)</i>	<i>42(1)</i>	<i>-19(1)</i>	<i>-15(1)</i>	<i>3(1)</i>
<i>C(20)</i>	<i>43(1)</i>	<i>69(1)</i>	<i>71(1)</i>	<i>-33(1)</i>	<i>-25(1)</i>	<i>11(1)</i>
<i>C(21)</i>	<i>97(2)</i>	<i>74(1)</i>	<i>55(1)</i>	<i>-39(1)</i>	<i>-25(1)</i>	<i>9(1)</i>
<i>N(1)</i>	<i>55(1)</i>	<i>55(1)</i>	<i>43(1)</i>	<i>-19(1)</i>	<i>-1(1)</i>	<i>-7(1)</i>
<i>O(1)</i>	<i>161(2)</i>	<i>68(1)</i>	<i>74(1)</i>	<i>-42(1)</i>	<i>-2(1)</i>	<i>-14(1)</i>
<i>O(2)</i>	<i>81(1)</i>	<i>49(1)</i>	<i>49(1)</i>	<i>-9(1)</i>	<i>-2(1)</i>	<i>-6(1)</i>
<i>O(3)</i>	<i>41(1)</i>	<i>92(1)</i>	<i>64(1)</i>	<i>-47(1)</i>	<i>-17(1)</i>	<i>16(1)</i>
<i>O(4)</i>	<i>63(1)</i>	<i>87(1)</i>	<i>53(1)</i>	<i>-42(1)</i>	<i>-16(1)</i>	<i>13(1)</i>
<i>Cl(1)</i>	<i>51(1)</i>	<i>82(1)</i>	<i>65(1)</i>	<i>-27(1)</i>	<i>-19(1)</i>	<i>24(1)</i>

**Table - 3. 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) of Dimethomorph.**

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U(eq)</i>
<i>H(1A)</i>	<i>7476</i>	<i>200</i>	<i>11439</i>	<i>127</i>
<i>H(1B)</i>	<i>5984</i>	<i>-524</i>	<i>11445</i>	<i>127</i>
<i>H(2A)</i>	<i>5020</i>	<i>1482</i>	<i>10287</i>	<i>94</i>
<i>H(2B)</i>	<i>5277</i>	<i>1480</i>	<i>11560</i>	<i>94</i>
<i>H(3A)</i>	<i>8828</i>	<i>3384</i>	<i>8148</i>	<i>78</i>
<i>H(3B)</i>	<i>7360</i>	<i>2730</i>	<i>8043</i>	<i>78</i>

H(4A)	9482	1333	8117	99
H(4B)	9572	1322	9439	99
H(9)	6499	447	14045	61
H(10)	8789	-749	14245	65
H(12)	11648	2550	11543	59
H(13)	9348	3735	11318	56
H(15)	6834	2734	14707	60
H(16)	5257	3008	16546	62
H(19)	2977	3326	13329	51
H(20A)	663	4387	13548	88
H(20B)	-1032	3912	14667	88
H(20C)	97	2865	14342	88
H(21A)	3110	2657	18556	107
H(21B)	1915	3752	18687	107
H(21C)	3663	4171	17636	107
H(6)	5010(20)	4140(18)	11341(18)	56(5)

Table - 3. 6. Bond Angle for Dimethomorph (Degree) – (Angle are ordered on the label, left to right and top to bottom) involving Non – Hydrogen atoms with estimated standard deviation in parentheses.

Bond	Torsion Angle [deg]
O(1)-C(1)-C(2)-N(1)	-55.1(3)
N(1)-C(3)-C(4)-O(1)	55.7(2)
O(2)-C(5)-C(6)-C(7)	-106.2(2)
N(1)-C(5)-C(6)-C(7)	75.0(2)
C(5)-C(6)-C(7)-C(8)	-1.5(3)
C(5)-C(6)-C(7)-C(14)	176.11(15)
C(6)-C(7)-C(8)-C(13)	58.4(2)
C(14)-C(7)-C(8)-C(13)	-119.32(16)
C(6)-C(7)-C(8)-C(9)	-123.11(17)
C(14)-C(7)-C(8)-C(9)	59.2(2)
C(13)-C(8)-C(9)-C(10)	0.0(2)
C(7)-C(8)-C(9)-C(10)	-178.61(15)
C(8)-C(9)-C(10)-C(11)	1.0(3)
C(9)-C(10)-C(11)-C(12)	-1.3(3)
C(9)-C(10)-C(11)-Cl(1)	177.12(13)
C(10)-C(11)-C(12)-C(13)	0.6(3)
Cl(1)-C(11)-C(12)-C(13)	-177.71(12)
C(11)-C(12)-C(13)-C(8)	0.3(2)
C(9)-C(8)-C(13)-C(12)	-0.6(2)
C(7)-C(8)-C(13)-C(12)	177.97(15)
C(6)-C(7)-C(14)-C(15)	-149.96(16)
C(8)-C(7)-C(14)-C(15)	27.7(2)
C(6)-C(7)-C(14)-C(19)	27.1(2)
C(8)-C(7)-C(14)-C(19)	-155.22(14)
C(19)-C(14)-C(15)-C(16)	-2.7(2)
C(7)-C(14)-C(15)-C(16)	174.43(15)
C(14)-C(15)-C(16)-C(17)	1.5(3)
C(15)-C(16)-C(17)-O(4)	-179.65(16)
C(15)-C(16)-C(17)-C(18)	1.2(2)
O(4)-C(17)-C(18)-O(3)	-2.6(2)
C(16)-C(17)-C(18)-O(3)	176.65(15)
O(4)-C(17)-C(18)-C(19)	178.12(14)
C(16)-C(17)-C(18)-C(19)	-2.7(2)
O(3)-C(18)-C(19)-C(14)	-177.82(14)
C(17)-C(18)-C(19)-C(14)	1.4(2)
C(15)-C(14)-C(19)-C(18)	1.2(2)
C(7)-C(14)-C(19)-C(18)	-175.87(13)
O(2)-C(5)-N(1)-C(2)	-169.37(19)
C(6)-C(5)-N(1)-C(2)	9.4(3)
O(2)-C(5)-N(1)-C(3)	3.3(3)

<i>C(6)-C(5)-N(1)-C(3)</i>	<i>-177.88(16)</i>
<i>C(1)-C(2)-N(1)-C(5)</i>	<i>-135.2(2)</i>
<i>C(1)-C(2)-N(1)-C(3)</i>	<i>51.6(2).</i>
<i>C(4)-C(3)-N(1)-C(5)</i>	<i>134.69(19)</i>
<i>C(4)-C(3)-N(1)-C(2)</i>	<i>-51.8(2)</i>
<i>C(2)-C(1)-O(1)-C(4)</i>	<i>59.5(3)</i>
<i>C(3)-C(4)-O(1)-C(1)</i>	<i>-59.8(3)</i>
<i>C(19)-C(18)-O(3)-C(20)</i>	<i>-3.4(2)</i>
<i>C(17)-C(18)-O(3)-C(20)</i>	<i>177.35(14)</i>
<i>C(16)-C(17)-O(4)-C(21)</i>	<i>4.9(3)</i>
<i>C(18)-C(17)-O(4)-C(21)</i>	<i>-175.99(15)</i>

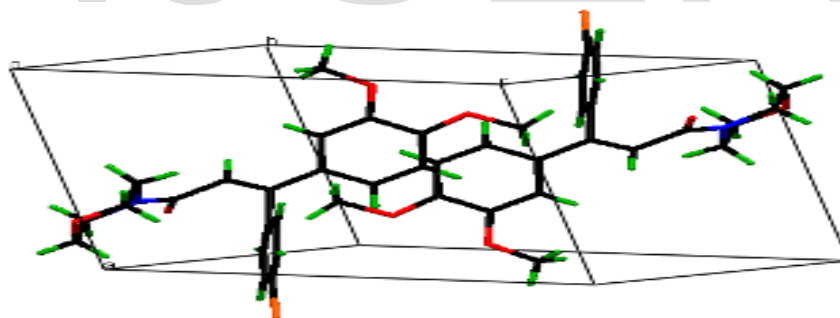
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*Symmetry transformations used to generate equivalent atoms:*

*Table - 3. Hydrogen bonds of Dimethomorph [A and deg.].*

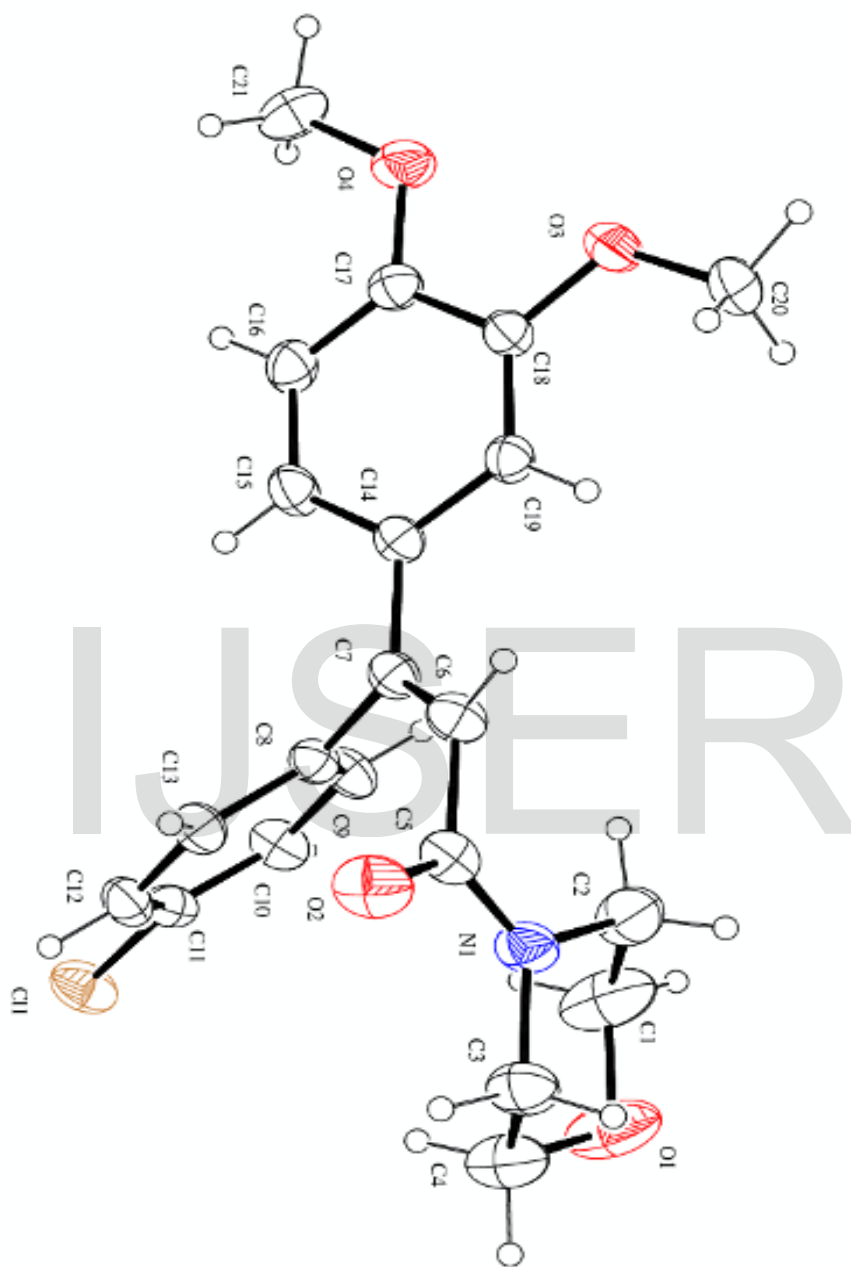
<i>D-H...A</i>	<i>d(D-H)</i>	<i>d(H...A)</i>	<i>d(D...A)</i>	<i>&lt;(DHA)</i>
<i>O(1)-H(1A)...N(2)#1</i>	<i>0.82</i>	<i>2.01</i>	<i>2.820(2)</i>	<i>169.3</i>

*Symmetry transformations used to generate equivalent atoms:*

*#1 -x+1,y+1/2,-z+1/2)*



*Figure 2 - Packing diagram of Dimethomorph by ORTEP diagram*



*Figure 3. – The molecular structure of Dimethomorph by ORTEP diagram.*

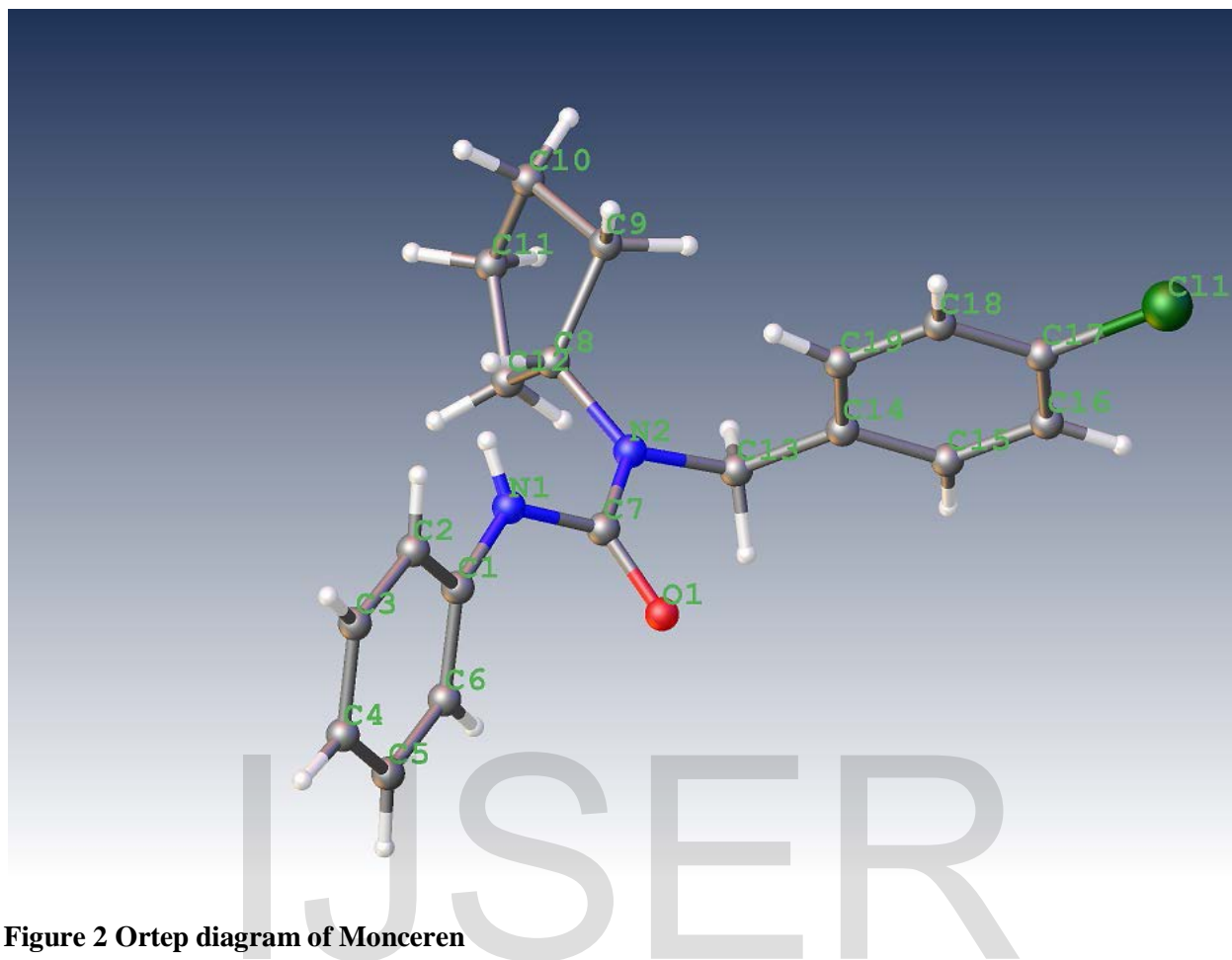


Figure 2 Ortep diagram of Monceren

**Result and Discussion:** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameter ( $\text{\AA}^2 \times 10^3$ ) for **Dimethomorph** shown in Table 3.2. Bond lengths [ $\text{\AA}$ ] and Bond angles [deg] for **Dimethomorph** is shown in Table 3.3. Anisotropic displacement parameter ( $\text{\AA}^2 \times 10^3$ ) for is shown in Table 3.4. The anisotropic displacement factor exponent takes the form  $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b U_{12}]$ . Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameter ( $\text{\AA}^2 \times 10^3$ ) for **Dimethomorph**.

is shown in Table 3.5. Torsion angle [deg] is shown Table 3.6. In Table 3.7 Hydrogen bonds for **Dimethomorph** [ $\text{\AA}$  and deg are show]. The ORTEP diagram is shown in figure 3.2. The average bond distance of C – H is 0.9700  $\text{\AA}$ . The bond distances of C(1) – O (1) is 1.415 (3)  $\text{\AA}$  and C (7) – N (1) is 1.368  $\text{\AA}$ . C (8) – N (1) is 1.360  $\text{\AA}$ . The triazol ring is distorted in shape. The Bond distances in benzene Ring are C (14) – C (15) is 1.380 (2), C (15) – C (16) is 1.386 (2), C (16) – C (17) is 1.374 (2), C (17) – C (18) is 1.405 (2), C (18) – C (19) is 1.377 (2). The bond Angle in benzene ring are C (15) – C (14) – C (19) is 118.12 (14), C (15) – C (14) – C (7) is 120.34 (14), C (19) – C (14) – C (7) is 121.47 (13) and C (14) – C (15) – C (16) is 121.40 (15). 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 constrains<sup>8</sup>. 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<sup>9</sup>. 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 angle in the rings derived from most reliable set of data by Spencer are 1.377 Å and 119° (deg.) respectively. The dimensions of the methyl groups are normal and comparable with those in 0 – methyl obtusaquinone and mescaline hydrobromide. The average bond angle around C (9) is 109.5°. The molecule is found to adopt a conformation such that the triazol ring is incneqangle of 72.9 (9)° to the aromatic ring. The equations of the least squares planes, calculated using Blow method and displacements of the relevant atoms from the mean planes for different planer groups together with the respective.

The triazol ring is planer with C (7) lying only 0.063 (7) Å from the mean plane. All four C – N distances are shorter than a normal single bond ( 1.47 Å). The three atoms bonded to N (1) are almost coplanar within it. Taken together these data indicate extensive delocalization within the heterocyclic ring. The most note worthy feature of the heterocyclic ring is the asymmetry of the exocyclic angles at N (1A) 130.80°. We have observed a similar pattern in related triazole system and it appear to be a function of a trazilyl ring itself rather than the influence of any inter or intermolecular interactions. The torsion angle O (1) – C (1) – C (2) – N (1) is 55.1 (3), N (1) – C (3) – C (4) – O (1) is 55.7 (2), O (2) – C (5) – C (6) – C (7) is -106.2 (2) and N (1) – C (5) – C (6) – C (7) is 75.0 (2). The torsion angles of C (5) - C (6) – C (7) – C (8) is -1.5 (3) and C (5) – C (6) – C (7) – C (14) is 176.11 (15), show that this ring is almost symmetric.

The packing diagram is shown in Fig. 3.3. The crystal structure consists of parallel sheet along a – axis. The molecules overlap while running along the a – axis. It is interesting to note that when there are minor difference in the cell parameter and growth conditions in the two independence studies, the molecular geometry, overall dimensions, crystal packing are almost same under the error limits whatever small differences are there, they are not really significant, which suggest that the molecular parameters remain unchanged even there is a change in growth condition the crystal forces, therefore, they don't after the molecular geometry.

Atomic coordinaters (x 19<sup>4</sup>) and Equivalent Isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for Pencycro is shown in able 2. Bond engths [Å] ond angles [de ] for Pencycroni s own in abl 3. Anis otroicispla e m nt par me e s ( ^ 2 x 10<sup>3</sup> for s s hon in Tab e 4 Thaniotropicdis la ement a c or exp n enttak s th e f rm:--2 pi<sup>2</sup> [ h 2 a\*<sup>2</sup> U11 + . . + 2 h a b\* U12 . Hyro en coo diates ( 10 4) a d isotropic d splacement pa ameter (Å<sup>2</sup> x 10<sup>4</sup> )for P ncyuron is shwn in a le 5 Tors on a g es [ e ] s h wn n T ble . T e ORTEP<sup>6</sup> d agram is show i f g.2.. n on Benzene ri g distance bet een C(1)-C( )is 1 3 6(4 )Å C(2 -C(3) is 1.3 6( )Å C(3 -C 4) is 1 36 (3) Å , C( )-C(5) s 1.37 Å, (5)-C 6) s 1.38 (2 Å) a d C(1)- (6) is 1. 72 2 ) Å.. n a otherBe en ingistancebetw n C(14)-C 15) is 1. 81(4 Å), C( )- 6)is 1.38 (4 Å , C(16)-C 7) .363 Å, C( 7 18) is 1.36 dC 8)-C(19) s 3 6(2) Å. The dl gths a dagles in the zeng show r guar f ature sin t le le.C-C d s ancar short an hortenigmay due to deloalizi n of electron roebenzenrin s The average ndtances of - 9 (2)Å. Thedisce- **N1 is .4 2(3) Å , C7- N2 is 1.360(3) Å , C8 - N2 s .47 (4) Å**. The avebo distance of -N i 1.32 5Å. The w ole olecul s a pea ed to be t iste and f lded and eason may e d e to tacking const aints<sup>8</sup>. Th bon distance a round C (7) is as u, ualshorter than single bond v lu e. This may a lsoap pear s to bear a partia l double bond c haracer<sup>9</sup> The bon distanes in th e five member ring are co mparabl e to c orrespond in g d istance in heterocycli c ring 1 .

**Conclusion:** Thus we study the structure of variety of such compounds and correlate their structure with biological activity, so that more safer and effective fungicides at reasonable price can be developed.

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