

## SHORT COMMUNICATIONS

X-RAY DATA, IR AND PMR SPECTRA OF 5,6-BENZO CHROMANONE<sup>a</sup>

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THE benzo pyran nucleus (figure 1a) is a widely prevalent ring system being present in a variety of naturally-occurring compounds like chromanones, xanthenes, flavones etc. Several naturally-occurring 4-chromanones isolated from plants have evinced considerable interest in terms of their biological importance and potentials as drugs. These compounds are potential synthons for the construction of many important oxygen heterocycles. The pharmacological activity of many derivatives of 4-chromanones have been extensively investigated<sup>1-4</sup>.

In the present study we report the x-ray data along with IR and PMR spectra of the compound (figure 1b). Several routes are available to synthesise the title compound<sup>5, 6</sup>. The procedure adopted<sup>7</sup> in the present study resulted in better yields. The spectral properties and the x-ray data of this compound have not been reported so far. Hence the present study was undertaken.

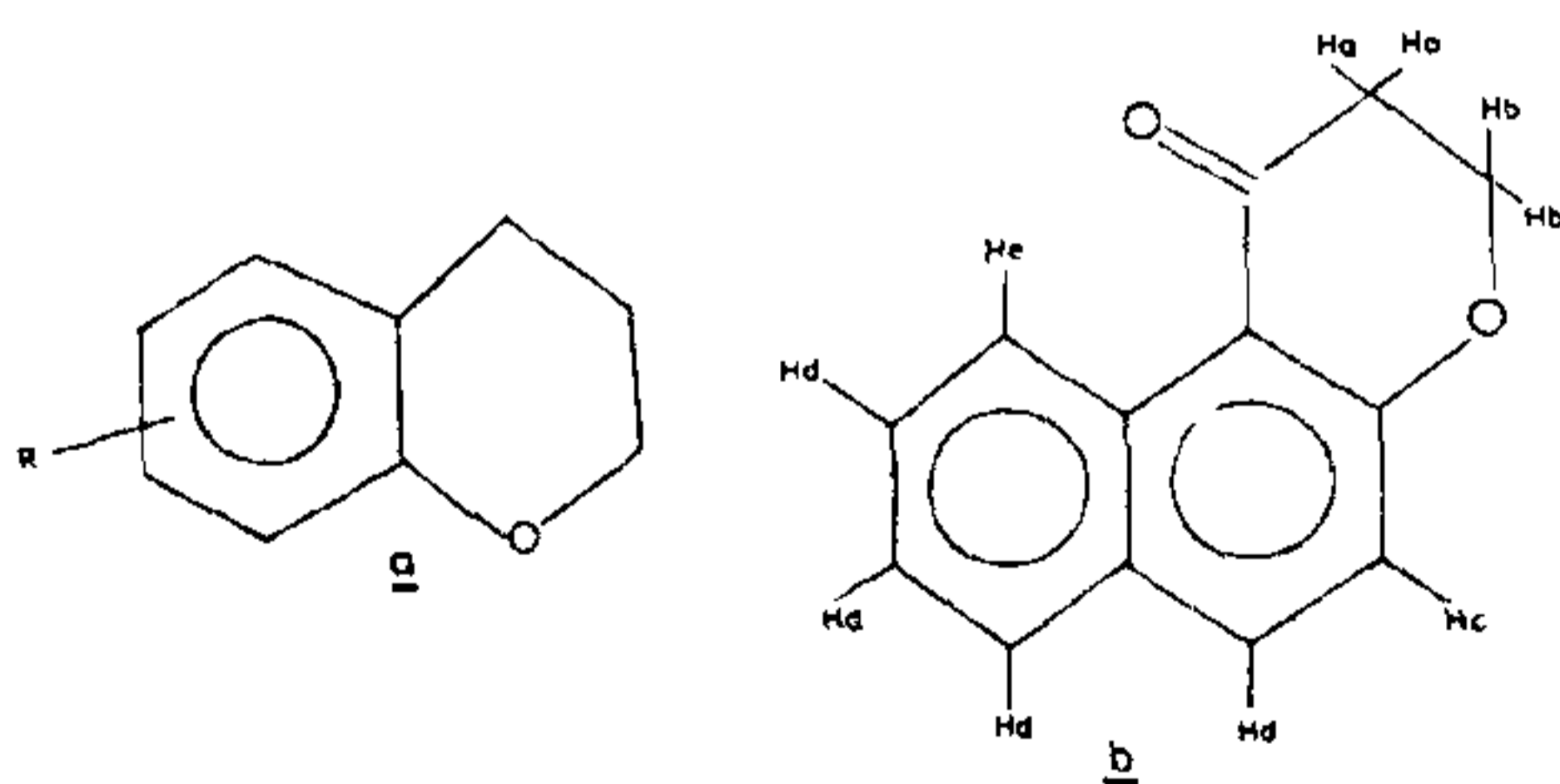


Figure 1. Classification of compounds

<sup>a</sup>2,3 dihydro-1H-naphtho (2,1-b)-pyran-1-one

## IR Data

The IR spectra for this compound was recorded using Perkin-Elmer (model 598) grating infrared spectrometer, in the Department of Organic Chemistry, Madras. The sample was used as a pellet in KBr phase and the spectra was recorded in the region 200–4000  $\text{cm}^{-1}$ .

The IR spectrum for the compound showed the following features:

1660 ( $> \text{C}=\text{O}$ ), 1610, 1590, 1560 and 1505 (Aromatic  $\text{C}=\text{C}$ ) and 1235, 1040  $\text{cm}^{-1}$  for ( $\text{C}-\text{O}-\text{C}$ )

## PMR Data

The proton NMR for this compound was recorded using varian (EM 390) spectrometer (90 MHz) located in the same department. The spectra was recorded in  $\text{CDCl}_3/\text{TMS}$  solution. The interesting features of the spectrum are; ( $\delta$  values)

2.60 (t, 2H, Ha)  
4.46 (t, 2H, Hb)  
6.83 (d, 1H, Hc,  $J = 9\text{Hz}$ )  
7.10 (m, 4H, Hd)  
and 9.30 (d, 1H, He,  $J = 9\text{Hz}$ )

## X-ray data

The crystal of the title compound necessary for the x-ray work was grown from benzene-hexane (1:1) solution. It crystallised in an orthorhombic system with

$a = 11.6430(3) \text{ \AA}$   
 $b = 19.4230(4) \text{ \AA}$   
and  $c = 8.5480(3) \text{ \AA}$  molecular formula  
 $= \text{C}_{13}\text{H}_{10}\text{O}_2$   
 $V = 1933.06 \text{ \AA}^3$   
 $\text{MW} = 198.14$   $D_{\text{mea}} = 1.33(2) \text{ Mg.m}^{-3}$   
 $D_{\text{cal}} = 1.360 \text{ Mg.m}^{-3}$   
 $z = 8$   
The space group is Pccn.

The density was measured by flotation method using a mixture of  $\text{CHBr}_3$  and  $\text{CCl}_4$ .

The three-dimensional data were collected using an Enraf-Nonius CAD-4 diffractometer, with graphite monochromatised  $\text{CuK}\alpha$  radiation at the University of British Columbia, Canada. The intensities were cor-

rected for Lorentz and polarisation effects. The structure was solved by MULTAN<sup>8</sup> and refined isotropically (non-hydrogen atoms only) to an  $R$  value = 0.10. Further refinement is in progress. The packing of the molecule down the  $a$ -axis is shown in figure 2.

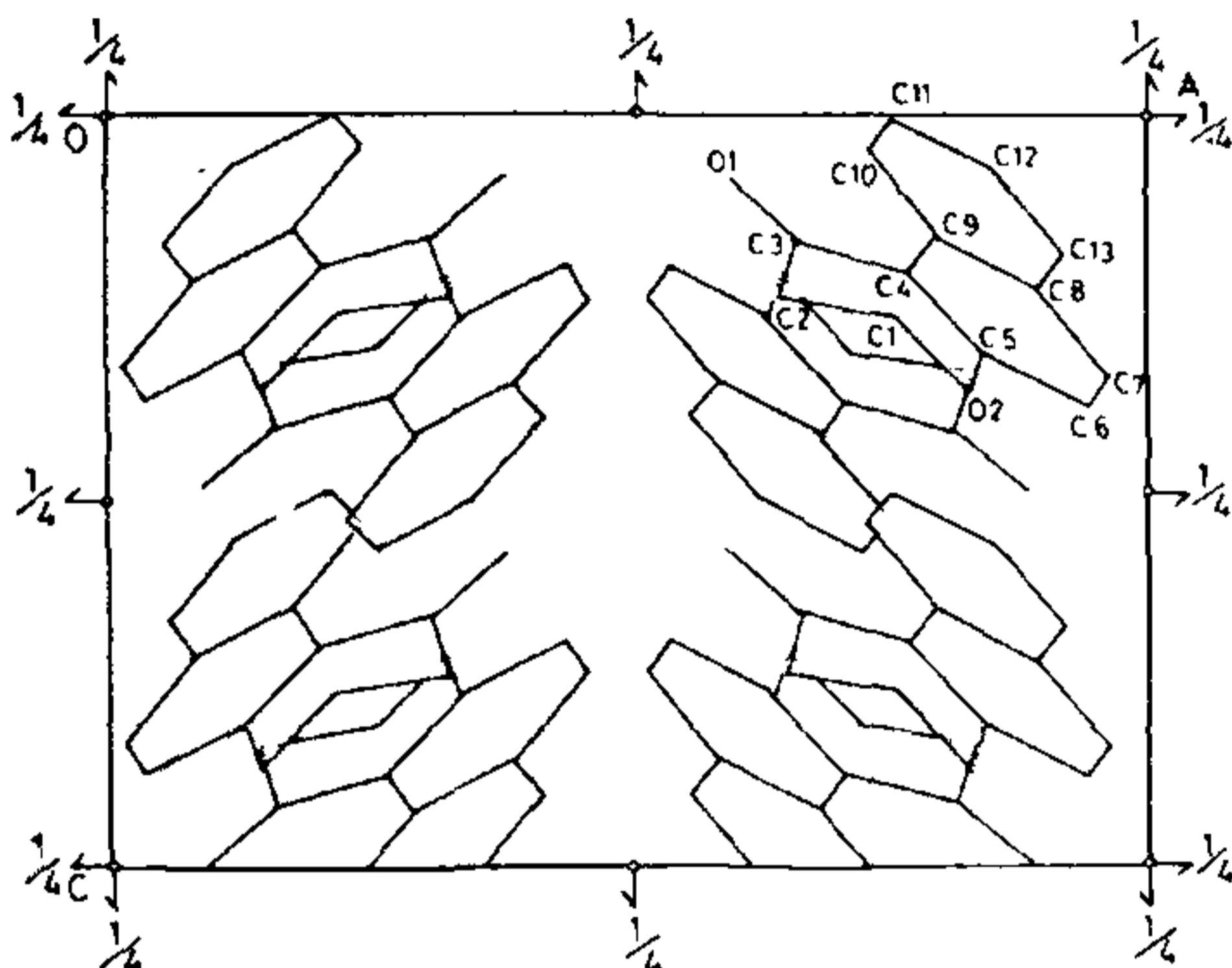


Figure 2. Packing of the molecules in the unit cell down  $a$ -axis.

The tetrahydropyran ring in the structure exists in half-chair conformation<sup>9</sup>. The two benzene rings are planar. The molecule has the normal bond distances and bond angles as found in other similar structures.

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### DEVELOPMENTAL PATTERNS OF $\alpha$ -AMYLASE AND LEUCINE-AMINO-PEPTIDASE ACTIVITY DURING SHOOT DIFFERENTIATION IN SUGARCANE (*SACCHARUM OFFICINARUM* Cv Co-740) CALLUS.

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DIFFERENTIATION of organised structures from an explant involves a shift in metabolism which leads to changes in content and spectrum of both structural and enzymic proteins. As amylolysis and proteolysis represent the major hydrolytic enzyme systems supplying assimilable material to the developing tissues, the developmental patterns of two enzymes, one from each class, namely  $\alpha$ -amylase and leucine aminopeptidase (LAP), respectively, were investigated and compared in shoot forming and non-shoot forming callus cultures of sugarcane.

Callus cultures from young leaves of sugarcane (*Saccharum officinarum* Cv Co-740) were initiated and maintained in the dark at  $26 \pm 2^\circ\text{C}$  on a basal Murashige and Skoog mineral salt medium (MS)<sup>1</sup> containing organic constituents as mentioned below for Medium A. Callus grown on this medium was transferred to 100 ml Erlenmeyer flasks containing 20 ml of the two experimental media listed below (1000 mg inoculum/flask).

**Medium A** : MS + 1.0 mg/l thiamine hydrochloride + 120 mg/l myo-inositol + 10% coconut milk (v/v) + 2% Sucrose + 3 mg/l 2,4-dichlorophenoxyacetic acid (2,4-D).  
(Non shoot forming)

**Medium B** : MS + 1.0 mg/l thiamine hydrochloride + 120 mg/l myo-inositol + 10% coconut milk (v/v) + 2% sucrose.  
(Shoot forming)