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Letters to the Editor

The crystal structure of cresotic acid

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Cresotic acid ($C_8H_8O_3$) is a monocarboxylic acid with a hydroxyl group attached to it

and the scheme of hydrogen bonding in the crystal is likely to be of great interest as, like many other carboxylic acid structures, the mole cules are likely to form dimers in the crystal structure and in addition, there is the possibility of intramolecular hydrogen bonds being formed between the oxygen atoms of the carboxyl (COOH) and hydroxyl (OH) groups, or there is also the possibility of same oxygen atoms being linked by two hydrogen bonds, one through dimerization (COOH groups) and the other through linkages with the hydroxyl groups (OH). We have, therefore, studied the crystal structure of this acid and this note presents a preliminary report on it.

The compound (white powder) was crystallized as long needles from an alcoholc solution. The unit cell dimensions were determined using rotation and Weissenberg photography. The crystallographic data are as follows :—

$a = 10.83$Å	ρ calc. $= 1.408$ g/ml.
$b = 4.105$Å	ρ measured $= 1.397$ g/ml.
$c = 16.15$Å	μ = (linear absorption co-efficient for X-rays) for CuK_α radn. $= 9.597$ cm^{-1}
$\beta = 91° 47'$	$Z = 4$.

Diffraction spectra give : hkl no condition,
$h0l$ present only when $l = 2n$,
$0k0$ present only when $k = 2n$,

This gives the space group uniquely as $P2_1/c$. Intensity data collected, using CuK unfiltered radiation from Weissenberg photography with the crystal mounted along the [010] axis, were (h01, h11, h21. Other reflexions collected were (hk0).

Determination of the structure :

As the [010] axis is a short axis, a Patterson projection (unsharpened) was calculated. A theoretical vector map for the benzene ring along with the attached carboxyl group was superimposed on the Patterson function and this gave the orientation of the molecule. Packing considerations

(dimerization across a centre of symmetry and linkages through the COOH groups) led to a reasonable model and trial coordinates. Reiterative Fourier refinements and least squares refinements yield good x and z coordinates giving R(h01) = 0.166. The [010] electron density projection is shown in figure 1. The y-coordinates were determined using generalized Fourier projections (h11 and h12 data) and Fourier projection down the [001] axis. The overall R factor for the hk0 reflexions is 11.7%.

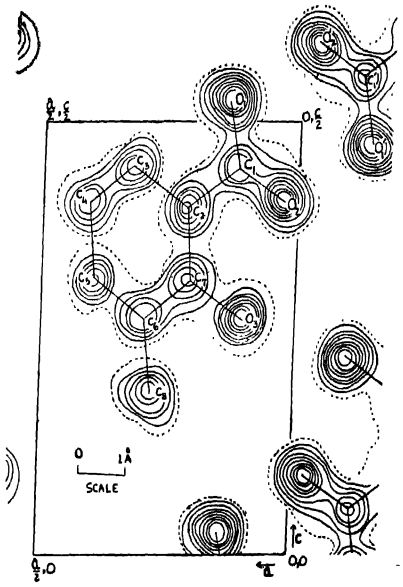

Figure 1. Electron density projection down the [010] axis.

Description of the structure :

As expected the COOH groups of the molecules are linked across centres of symmetry by hydrogen bonds of 2.61Å. This is a feature present in all carboxylic acids. The oxygen atoms of the hydroxyl groups are linked with the oxygen atoms of the COOH groups by 2.56Å bonds which are intramolecular in nature. Other distances are normal Van der Waals distances (3Å upwards). As considerable interest lies in an accurante location of he hydrogen atoms, we are now doing a complete three dimensional analysis of the structure and the results will be reported later. The molecular geometry is normal.