pectively as against the theoretical value 0.637 for centrosymmetrical crystals. So, the space group of the crystal must be centrosymmetric i.e. $\bar{P}T$.

Hypercentric nature of the intensity distribution curves not only shows the presence of centre of symmetry in the space group but also indicates the presence of a molecular centre of symmetry in the structure (Lipson *et. al.*, 1952). But for this particular case, the presence of molecular centre of symmetry does not follow the chemical structure of the compound. Molecular centre of symmetry, in this case, may be explained on the basis that two molecular units in a unit cell form a dimer and centre of symmetry of the dimer thus coincides with that of the unit cell.

Further work is in progress.

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RENNINGER EFFECT IN QUINALDIC ACID

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While the study of space-group of quinaldic acid was made some weak reflections different from the nature of the normal ones were observed in the position (105) and (10$\bar{5}$). Thus their presence was a hurdle in ascertaining the space-group of the crystal. A critical study of the space-group and extinction condition was made which reveals the origin due to double reflection from a pair of strong plane (Srivastava 1957).

The forbidden reflection *s* (105) and (10$\bar{5}$) was not accompanied by its usual CuK$_\beta$ reflection using unfiltered CuK radiation while other reflections are accompanied with the usual CuK$_\beta$ reflections. The study of the reflection conditions of the reciprocal lattice confirms the presence of Renninger's reflection (1937). The mechanism of the formation of double reflections can be understood by constructing the reciprocal lattice for this crystal. As an example we shall consider the forbidden reflection (105) in details.

The unit cell dimensions of quinaldic acid (Khan, 1967) were determined by oscillation and Weissenberg photograph by standardising the camera diameter, and from a consideration of the high angle spots (where $K_{\alpha_1\alpha_2}$ doublet is well re-

solved). These are $a = 9.77, b = 5.97, c = 28.00$ and monoclinic angle $\beta = 90°25'$.

The reciprocal lattice for the equational layer of [010] is shown in fig. 1. taking

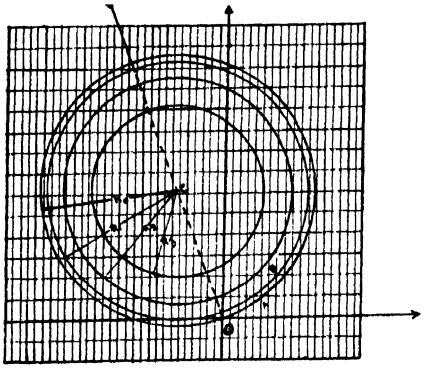

Fig. 1. Spheres of Reflection on Reciprocal Lattice.

$a^* = 0.158782$, $b^* = 0.25825$, $c^* = 0.05506$ and $\beta^* = 89°35'$, for CuK_α radiation. The circle of reflection for different layers projected on the equatorial layer were drawn with their respective radii on transparent film with common diameter to represent the incident beam, traces of which are shown in the diagram. The radius of sphere of reflection has been taken 5 cms. One of the junctions of the diameter with the equatorial layer circle of reflection is the origin of the reciprocal lattice and the film rotated until the circle corresponding to the equatorial layer passes through the point (105). Then it is found that the second circle (Radius R_1) passes through the point $B(27)$. Thus it appears that the reflection (105) is caused by the reflection from pair of lattice planes, one plane of the pair is (217). This graphical coincidence has been ascertained by analytical test because there are other coincidences also.

ANALYTICAL VERIFICATION

It is convenient to express the required results in polar-co-ordinates. The equatorial circle is of unit radius and always passes through the origin and it is also passing through a point $A(r, \theta)$. The co-ordinate of the centre of the circle C be $(1, \alpha)$ then the equation to the circle is

$$r/2 = \cos(\alpha - \theta) \tag{1}$$

For this,

$$\alpha = \theta + \cos^{-1}(r/2) \tag{2}$$

Let P be any point $(r_1\ \theta_1)$ fig. 2, the distance of which from C is R_n. Then the radii of the circles produced by intersection of the reciprocal lattice layer with the sphere of reflection are calculated from ΔPOC.

$$R_n^2 = 1 + r_1^2 - 2r_1 \cos(\alpha - \theta_n) \quad \ldots \quad (3)$$

Polar co-ordinates of the point has been calculated from the reciprocal lattice (fig. 1). For the point $A(105)$, $r = 0.31903$ and $\theta = 29°48'$. Then from Equn. (2)

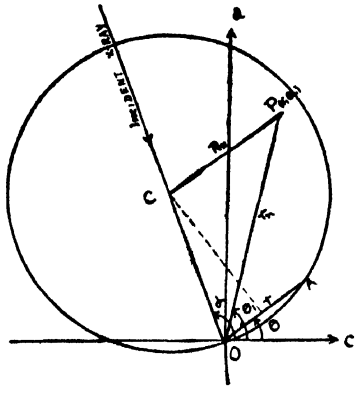

Fig. 2.

$\alpha = 110°35'$. For (217), with reciprocal lattice co-ordinates (2, 7) and polar co-ordinates $(r_1\ \theta_1)$ in the plane of the first layer, we have

$$r_1 = 0.4984; \qquad \theta_1 = 39°16'$$

Therefore from Eqn. (3) $R_1 = 0.9648$.

Considering this from the consideration of co-ordinates given by the relation

$$R_n = \cos \nu_n = \cos (\mathrm{Sin}^{-1}\zeta_n)$$

where $$\zeta_n = nb^*$$

Eqn. (4) gave the value of $R_1 = 0.9664$, which is in good agreement with the above.

If (hkl) are the indices of the forbidden reflection, and $(h_1k_1l_1)$ and $(h_2k_2l_2)$ those for a pair of lattice planes contributing to the formation of this reflection, then the pair can be found from the following relationship (Lipson *et. al.*, 1953)

$$h = h_1+h_2, \qquad k = k_1+k_2, \quad \text{and} \quad 1 = 1_1+1_2.$$

Hence the pair which contribute to the reflection (105) is (217), $(\bar{1}\bar{1}2)$. Similarly proceeding with the reflection $(10\bar{5})$ we concluded this is formed due to pair, $(21\bar{7})$ $(\bar{1}\bar{1}2)$. This interpretation has been tested analytically by calculation of ω values (Speakman 1965) for the two sets of reflections. However, intensities of these forbidden spots were found to be in reasonable agreement with the expected estimates from their contributors.

Results : The study of the indexed reflections of the Weissenberg photograph it has been found that all (hkl) reflections are present. The systematic absences

are (*hol*) with l odd and (*oko*), no conditions. The forbidden reflections are (105) and (105) are found due to double reflections. Hence the space-group C^4_{2h}—$P2/c$ for quinaldic acid is established.

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