

# THE SPACE GROUP OF META TOLUIC ACID

R. C. SRIVASTAVA

DEPARTMENT OF PHYSICS, UNIVERSITY OF ALLAHABAD, ALLAHABAD

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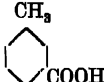
## Plate VII

**ABSTRACT.** Goniometric and X-ray study of single crystals of *m*-toluic acid shows that it belongs to monoclinic class. Crystallographic data resulting from the above study is given by

$$a=10.51 \text{ \AA}, \quad b=8.01 \text{ \AA}, \quad c=16.49 \text{ \AA}, \quad \beta=92^\circ 46.5'.$$

Number of molecules per unit cell=8

Weissenberg photographs about crystallographic axes showed that (*h*0*l*) planes are present when *l* is even and (*o**k*0) planes are present when *k* is even. The crystal belongs to the space group  $C_{2h}^2-P_{21}/c$ , and so each one of the four asymmetric units is composed of two molecules.

*m*-Toluic acid or *m*-methylbenzoic acid has structural formula 

No goniometric or X-ray data are available for it. Single crystals of *m*-Toluic acid of suitable size were prepared by slow evaporation of the solution of the substance in ethyl alcohol. It gave prismatic crystals with six faces in one zone and having a tendency of elongation along this zone axis.

Goniometric measurement of the zone containing faces parallel to needle axis was made. Rotation photograph about four selected zone axes were taken (Plate VII). Axial parameters thus got were further refined with the help of (00.12), (10.00), (00.14) reflections from Weissenberg goniometer photographs and are given below

$$a = 10.51 \text{ \AA}$$

$$b = 8.01 \text{ \AA}$$

$$c = 16.49 \text{ \AA}$$

$$\beta = 92^\circ 46.5'$$

The interfacial angles measured and as calculated with the help of above axial parameters are given in Table I

The density of the crystals was determined by the flotation method. The lighter liquid used was kerosene oil and the heavier carbon tetrachloride. Density

thus determined is 1.239 gm./cm<sup>3</sup>. Thus the number of molecules comes out to be 8 per unit cell.

TABLE I

Indices of the faces	Measured interfacial angles	Calculated angles
100 : 00 $\bar{1}$	92° 45'	$\beta$
00 $\bar{1}$ : 10 $\bar{2}$	34° 4'	37° 3.5'
10 $\bar{2}$ : $\bar{1}$ 00	50° 18"	50° 10.5'
$\bar{1}$ 00 : 001	92° 48'	$\beta$
001 : 102	37° 7'	37° 3.5'
102 · 100	49° 58'	50° 10.5'

Zero layer line Weissenberg photographs along  $a$  and  $b$  axis and 1st layer line equi-inclination Weissenberg photograph about  $b$  axis were taken. On indexing them the following extinctions were observed.

( $h0l$ ) planes absent for  $l$  odd.

( $oko$ ) planes absent for  $k$  odd.

No systematic absence in the general planes ( $hkl$ ).

The space group of the crystal is therefore  $C_{2h}^5 - P_{21/e}$ . The number of asymmetric units per unit cell necessary for this space group is four, so two molecules form one asymmetric unit.

#### ACKNOWLEDGMENTS

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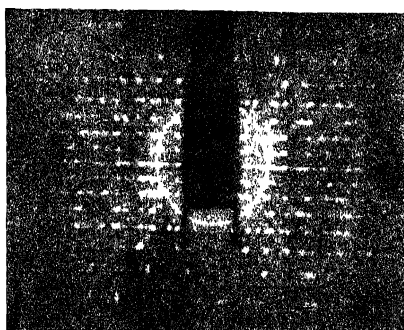


Fig. 1.  
About *c*-axis

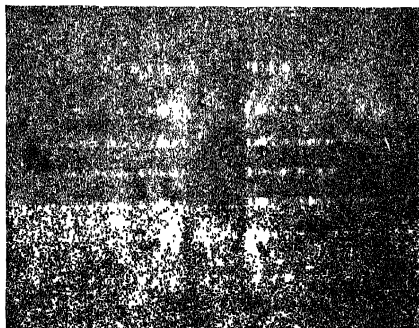


Fig. 2.  
About *b*-axis

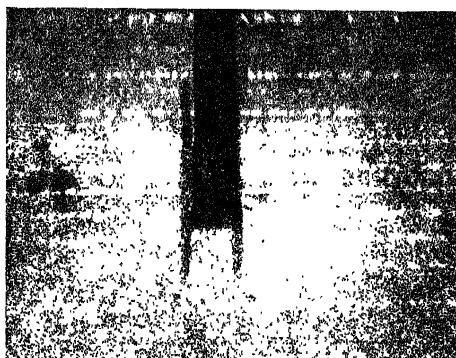


Fig. 3.  
About *a*-axis

Rotation photographs of *m*-toluc acid.