

An X-ray Investigation of the Crystal Structure of Meta-Azotoluene

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(Received for publication, December 3, 1934.)

(PLATE VI.)

The crystals of meta-azotoluene develop a (100), b (010) and c (111) faces, and belong to rhombic bipyramidal class and the axial ratio is ¹

$$a:b:c=0.8556:1:0.5488.$$

In this investigation the crystals of m-azotoluene were prepared by the slow evaporation of the solution of the substance in absolute alcohol. The crystals grow in the form of four sided plates with a (100) as a prominent face.

In order to determine the dimensions of the unit cell, rotation photographs about all the three principal axes were taken by means of a Shearer tube fitted with copper anticathode and are shown in Plate VI. The lengths of the axes were calculated from these photographs which are

and $a=11.8 \text{ \AA}, b=13.75 \text{ \AA}, c=7.52 \text{ \AA}.$
 $a:b:c=0.8581:1:0.5469.$

The axial ratios are in good agreement with those from goniometric measurements.

¹ Gröth, *Chemische Krystallographie*, 1919, Vol. V., p. 66.

In order to determine the space group to which the crystals belong (as this determination indicates the symmetry of the unit cell and also the symmetry elements of the molecule itself if there be any) a few oscillation photographs were taken about b and c axes at an interval of 15° . The indices of the various diffracted spots have been worked out by Bernal's² method of analysis and the reflecting planes have been tabulated in Tables I and II. The intensities of the spots were determined by eye estimation and the symbols employed by Robertson³ have been used to indicate the intensities of the planes.

It will be seen from the above series of planes that (001), (010) and (100) are halved; also (h 0 l) are halved when h is odd and (hko) are halved when k is odd. These halvings correspond to the space group Q_{11}^b . The number of molecules required by the space group is 8. The number of molecules calculated from the dimensions of the unit cell and the density of the crystals (1.05) is found to be 4.

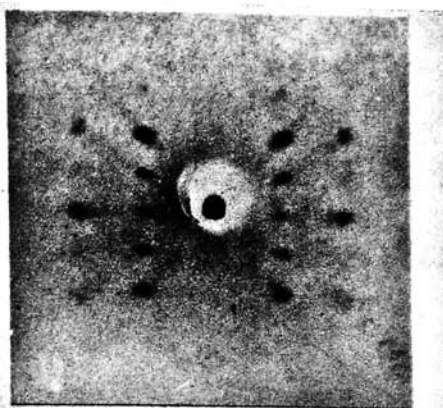
The number of molecules actually present in the unit cell being four, *i.e.*, half the number required by the space group, the molecules possess some elements of symmetry. These may be according to the space group either a plane of symmetry parallel to (100) plane or a dyad axis of symmetry perpendicular to (100) plane or a centre of symmetry. In order to examine which of these symmetrical molecular arrangements exists further work is being undertaken.

One of the authors (M.P.) has to thank the University of Bombay for a grant from which part of the expenses of this investigation was defrayed.

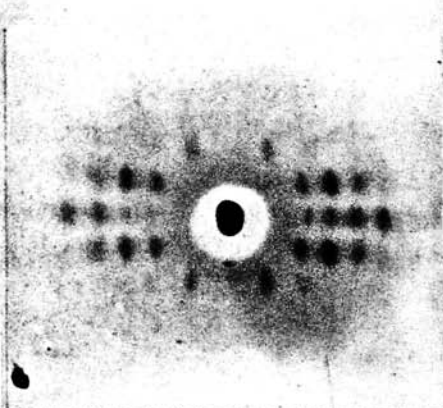
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² Proc. Roy. Soc., A, 118, 117 (1926).

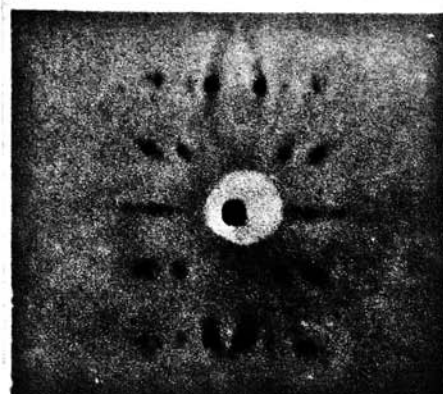
³ Proc. Roy. Soc., A, 118, 712 (1928).



Rotation about
"a" axis.



Rotation about
"b" axis.



Rotation about
"c" axis.

Rotation photographs of meta azotoluene.

TABLE I.

Axial planes.	Intensity.	Prism planes (hol).	Intensity.	Prism planes (hkl)	Intensity.	Prism planes (hko)	Intensity.
200	v.s.	201	s.	012	v.s.	120	v.s.
400	s.	202	v.s.	062	v.w.	220	v.s.
600	v.w.	203	m.s.	023	m.	320	s.
020	s.	204	w.			520	v.w.
060	w.	401	v.w.			620	m.
002	v.s.					440	m.
						540	w.
						160	w.

TABLE II.

General Planes.

Planes.	Intensity.	Planes.	Intensity.	Planes.	Intensity.	Planes.	Intensity.
111	v.s.	161	v.w.	251	w.	413	w.m.
112	s.	162	v.w.	271	v.w.	413	w.m.
121	w.	162	v.w.	311	w.m.	423	v.w.
122	m.	211	v.w.	313	m.	423	m.
131	w.	212	s.	321	v.w.	441	w.
132	w.	213	m.	341	w.m.	451	w.
141	v.w.	221	w.	351	w.m.	511	w.m.
142	v.w.	231	v.w.	411	w.m.	611	w.