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An X-Ray Investigation of the Crystals of Anthranilic Acid

By

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Abstract.

The paper describes the preliminary results of an X-ray investigation of the crystals of anthranilic acid. The substance crystallises in two modifications which differ in density. The dimensions of the unit cell have been found to be different in the two cases and while one belongs to the space group Q_h^{11}, the other belongs to Q_h^5. The number of molecules per unit cell in each case is eight.

Crystals of anthranilic acid were prepared by the slow evaporation of the solution of the substance in alcohol. Anthranilic acid crystallises in two types of crystals both of which belong to the rhombic bipyramidal class. These two types of crystals are obtained simultaneously from the same solution under identical conditions. Both these crystals were studied by the rotating crystal method using a Shearer tube fitted with copper anticathode.

First Modification.

The prominent faces developed are a (100), b (010), o (111), i (122). The axial ratio is

$a:b:c = 0{\cdot}6877:1:0{\cdot}6161$ (*cf.* Groth, Vol. IV, pp. 508).

The lengths of the three axes were found to be

$$a = 16{\cdot}16\ \text{Å}\ ;\quad b = 11{\cdot}77\ \text{Å}\ ;\quad c = 7{\cdot}17\ \text{Å}.$$

These give the ratio

$$a : b : c = 1{\cdot}373 : 1 : 0{\cdot}609.$$

This shows that the a axis is of twice the length found by the crystallographic methods.

Oscillation photographs were taken about a and c axes at an interval of 15° and were worked out by the aid of Bernal's chart. The list of planes observed is given in Tables I and II. The intensities of the planes were determined by eye estimation and the symbols used have the usual meaning.

TABLE I.

Axial planes.	Prism planes (*hol*).	Prism planes (*okl*).	Prism planes (*hko*).
002 m.	102 s.	022 s.	210 w.
020 v.s.	103 s.	023 w.	220 s.
040 v.s.	202 w.	041 w.	230 s.
060 m.s.	203 w.m.	042 w.	240 m.s.
200 s.	302 w.m.	043 w.	250 m.s.
400 s.	401 s.	061 w.	260 m.
800 w.m.	402 s.		410 s.
	501 m.s.		420 w.m.
	502 m.		430 w.m.
	601 w.		450 m.
	602 s.		620 w.m.
			630 w.m.
			640 w.

TABLE II.

General Planes.

111 v.s.	211 m.	311 v.s.	411 v.s.	511 s.	611 m.	711 v.w.
113 m.s.	212 w.m.	312 w.m.	412 w.m.	512 v.w.	612 w.m.	722 v.w.
122 w.	213 m.s.	313 w.m.	413 w.	521 m.	621 w.	
131 m.s.	211 w.m.	321 s.	421 s.	522 w.	641 w.	
132 v.w.	221 m.	322 w.	422 w.	523 w.	651 m.s.	
133 w.m.	222 w.m.	331 m.	423 m.	531 v.w.		
141 w.m.	231 w.	332 w.	431 w.m.	533 w.		
142 m.	232 w.m.	341 w.	441 m.	541 w.m.		
151 m.s.	242 w.	342 m.	442 v.w.	542 v.w.		
152 w.m.	251 v.w.	351 m.	451 v.w.	551 w.		
161 m.			461 m.			
162 w.						

It will be seen from this list that the planes (*okl*) are halved when *k* is odd and the planes (*hko*) are halved when *h* is odd. These halvings correspond to the space group Q_h^{11}. The number of molecules in the unit cell required by the space group is 8. The number of molecules in the unit cell, calculated from the dimensions of the cell and the specific gravity of the crystals, which was redetermined and found to be 1·355, is also nearly 8. This shows that the molecules of anthranilic acid in the crystal are asymmetric.

Second Modification.

The prominent faces developed in the crystal are *b* (010), *a* (100) and *o* (111). The ratio of the axes is

$$a : b : c = 0{\cdot}6066 : 1 : 0{\cdot}8751 \text{ (Groth, } loc.\ cit.\text{)}.$$

The lengths of the axes were found to be

$$a = 12{\cdot}77\ \text{Å}\ ;\quad b = 10{\cdot}8\ \text{Å}\ ;\quad c = 9{\cdot}403\ \text{Å}.$$

and these give the axial ratio

$$a : b : c = 1{\cdot}197 : 1 : 0{\cdot}8812.$$

Thus again in this case the length of the *a* axis is doubled.

Oscillation photographs taken about *a* and *c* axes at an interval of 15° indicated the planes given in Tables III and IV.

TABLE III.

Axial planes.	Prism planes (*hol*).	Prism planes (*okl*).	Prism planes (*hko*).
002 s.	102 m.s	012 m.s.	110 s.
004 s.	104 w.	014 m.s.	130 w.m.
020 s.	202 s.	022 s.	140 v w.
200 v.s.	204 m.	024 m.s.	150 m.s.
400 v.s.	304 m.	031 m.s.	220 s.
	402 s.	032 w.m.	240 w.
		034 w.	310 m.s.
		041 w.	330 w.
		042 v.w.	410 w.
		051 v.w.	420 m.s.
		052 s.	440 w.m.

TABLE IV.

General Planes.

111 v.s.	211 v.s.	311 v.s.	411 s.	511 w.	612 m.	711 v.w.
113 s.	212 s.	312 m.s.	412 m.	512 w.		
121 s.	213 w.	313 s.	413 m.s.	532 m.s.		
122 s.	221 s.	321 m.s.	414 w.	583 w.m.		
123 w.m.	222 w.m.	323 m.s.	421 m.s.			
124 m.	223 m.s.	332 w.m.	422 m.			
131 s.	231 w.	333 m.	423 m.			
133 m.s.	233 m.	334 v.w.	432 m.s.			
134 v.w.	241 m.s.	341 v.w.	433 w.m			
141 m.	243 w.		441 w.m.			
142 v.w.	251 m.					
143 m.s.	252 m.s.					
152 w.						

In this case the planes (*hol*) are halved when *l* is odd. This corresponds to the space group Q_h^5. The number of molecules in the unit cell required by the space group is 8 and that found from the dimensions of the unit cell and the specific gravity of the crystals (redetermined and found to be 1·422) is also nearly 8. The molecules of this modification are, as well, asymmetric in the unit cell.

It will be interesting to work out how a change in the crystalline nature of anthranilic acid is brought about by a change in the orientation of the molecules. But the difficulties involved are many and attempts are being made to find a way out of them.

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