SPACE GROUP AND UNIT CELL DIMENSIONS OF ANTHRARUFIN

S. N. GIRI

INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE
JADAVPUR, CALCUTTA-32.

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Anthrarufin is 1 : 5 dihydroxyanthraquinone having the following structural formula.

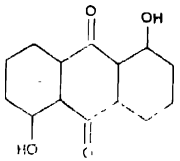

Fig. 1.

No goniometric or crystallographic data of the compound are available.

Single crystals of suitable size can be obtained by slow evaporation of the solution of the substance in benzene or in ether. The crystals obtained from benzene are needle-shaped, whereas plate-like crystals are obtained from ether solution.

From the rotation photograph and zero-and first layer-line Weissenberg photographs along the needle axis, the other two probable crystallographic axes were assigned. Rotation photographs and zero and first layer line Weissenberg photographs along these probable axes were then taken. From these photographs and those along the needle axis, the crystal was found to be monoclinic with the needle axis as the symmetry axis (i.e., b-axis). The axial lengths and the monoclinic angle were determined from the high-angle spots for which Cu-kα_1, and Cu-kα_2 were resolved in the Weissenberg photograph. Film shrinkage correction was applied by the method of Srivastava (1959).

The parameters along with the standard deviations obtained are :

$$a = 15.86 \pm .02\text{Å}$$
$$b = 5.36 \pm .02\text{Å}$$
$$c = 6.03 \pm .01\text{Å}$$
$$\beta = 94° 3' \pm .6'$$

In the zero and higher layer line Weissenberg-photographs, the following extinction conditions are present :

hkl — no condition

hol — $h = 2n+1$ absent

oko — $h = 2n+1$ absent

thereby indicating that the probable space group is $P2_1/a$

Density was determined by floatation method using aqueous solution of potassium iodide as the heavier and water as the lighter liquid. This gives a value of $d = 1.59\text{g cm}^{-3}$. The density calculated by considering two molecules in the unit cell is 1.56g cm^{-3}.

The space group is centrosymmetric having four equivalent points. This presents no difficulty since the molecule itself possesses a symmetry-centre.

Further work is in progress.

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REFERENCES

Srivastava, S. N., *Acta Cryst.*, (1959) **12**, 412.