Short Communications

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The space groups and unit-cell dimensions of 2,4,6-tribromoaniline and 2,4,6-trichloroaniline.

By E. O. SCHLEMPER* and JUDITH KONNERT, *Department of Chemistry, University of Minnesota, Minneapolis, Minnesota* 55455, *U.S.A.*

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Crystals of 2,4,6-tribromoaniline are orthorhombic, space group $P2_12_12_1$, with $a=13{\cdot}46$, $b=14{\cdot}69$, $c=4{\cdot}27$ Å, $Z=4$. Crystals of 2,4,6-trichloroaniline are monoclinic, space group either $P2_1/m$ or $P2_1$, with $a=15{\cdot}88$, $b=3{\cdot}86$, $c=13{\cdot}38$ Å, $\beta=111°45'$, $Z=4$.

In connection with some X-ray work being done on 2,4,6-tribromobenzonitrile and 2,4,6-trichlorobenzonitrile, the space groups and unit cells of 2,4,6-tribromoaniline and 2,4,6-trichloroaniline were determined.

From oscillation, Weissenberg, and precession photographs (Mo $K\alpha$, $\lambda=0{\cdot}7107$ Å), crystals of 2,4,6-tribromoaniline were found to be orthorhombic with cell dimensions $a=13{\cdot}462\pm0{\cdot}008$, $b=14{\cdot}692\pm0{\cdot}014$, $c=4{\cdot}266\pm0{\cdot}005$ Å. The systematic extinctions, ($h00$, $h=2n+1$; $0k0$, $k=2n+1$; $00l$, $l=2n+1$), indicate that the space group is $P2_12_12_1$. If $Z=4$, the calculated density is 2·596 g.cm^{-3}; the experimental density is 2·578 g.cm^{-3} (Jaeger, 1907).

Needle-like crystals of 2,4,6-trichloroaniline were mounted in capillaries to prevent sublimation. Precession photographs taken with Mo $K\alpha$ radiation ($\lambda=0{\cdot}7107$ Å) indicate that the cell is monoclinic with the unique axis as the needle axis. A unit cell with the dimensions $a=15{\cdot}875\pm0{\cdot}006$, $b=3{\cdot}863\pm0{\cdot}005$, $c=13{\cdot}381\pm0{\cdot}005$ Å, $\beta=111°45'$ was chosen. A rough experimental density of 1·6 g.cm^{-3} was obtained; for $Z=4$, the calculated density is 1·712 g.cm^{-3}. The systematic extinctions, ($0k0$, $k=2n+1$), indicate that the space group is either $P2_1/m$ or $P2_1$. No further X-ray work on these compounds is planned.

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References

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* Present address: Department of Chemistry, University of Missouri, Columbia, Mo., U.S.A.

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Absorption correction in the Weissenberg methods.

By A. SANTORO and M. ZOCCHI, *Institute for Materials Research, National Bureau of Standards, Washington, D.C., U.S.A.*

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A procedure is described for calculating the direction cosines of the incident and diffracted beams in a reference system attached to the crystal for the general case of the Weissenberg method.

Methods have been described for the calculation of the absorption correction in the equi-inclination and normal-beam techniques (Wells, 1960; Coppens, Leiserowitz & Rabinovich, 1965; Wuensch & Prewitt, 1965). However in some cases (Santoro & Zocchi, 1966) it is preferable to use the Weissenberg method with arbitrary values of the angle μ (*International Tables for X-ray Crystallography*, 1959), and therefore it seems useful to extend the treatment of the absorption correction to the general case.

In what follows we will only describe a procedure for calculating the direction cosines of the incident and diffracted beams in a reference system attached to the crystal; from this point on the calculation of the transmission factor for each reflection can be performed as suggested, for example, by Busing & Levy (1957) or by Wuensch & Prewitt (1965).

It has been shown (Santoro & Zocchi, 1966) that, for any Weissenberg method, a reciprocal lattice point is in reflecting position when:

$$zs(n-2v_0)+2\left[1-s^2\left(\frac{n}{2}-v_0\right)^2\right]^{\frac{1}{2}}(y\cos\omega-x\sin\omega)+d^{*2}=0\,, \quad (1)$$

where ω is the rotation angle, v_0 is the index of the reciprocal layer under examination, s is the period on the rotation axis, x,y,z are the coordinates of the point for $\mu=\omega=0°$ with respect to a Cartesian system X,Y,Z, attached to the laboratory, and defined in the given reference, $d^{*2}=x^2+y^2+z^2$, and $n=(2\sin\nu)/s$ (*International Tables*).

From equation (1) we obtain:

$$\tan\frac{\omega}{2}=\frac{x\pm[x^2-(A+y)(A-y)]^{\frac{1}{2}}}{A-y}\,, \quad (2)$$