

They also exhibited a hexagonal super-lattice based on the cell $4a$, $4b$, c with the condition that hkl reflexions were absent unless $h=4n$, or $k=4n$, $h-k=4n$. In view of the scanning electron micrographs, the photographs were interpreted as patterns from a twinned supercell of $4a$, b , c . This is confirmed by a splitting of the sublattice reflexions in the direction of increasing 2θ consistent with a slight deviation from hexagonal symmetry in the subcell. From the degree of splitting a discrepancy of about 0.05 \AA between $a/4$ and b could be deduced and using a copper powder line for calibration the values 7.31 ± 0.01 and $7.36 \pm 0.01 \text{ \AA}$ were obtained respectively. The doubling of the c axis in the manner reported by Magnéli was not observed.

Electron diffraction from the platelets established the hexagonal subcell and a monoclinic superlattice of a larger cell $4a$, $2b$, $2c$. This apparent discrepancy between the X-ray and electron diffraction data was attributed to a second superstructure with a very low scattering power for X-rays. Further investigation included electron diffraction from ground needle fragments, X-ray diffraction from a platelet and finally some very long oscillation and Weissenberg exposures from a needle crystal. This established definitely that both morphologies had the same monoclinic crystal structure. In particular, some very weak X-ray reflexions were detected from the first layer about an axis corresponding to $2c$.

The combined X-ray and electron-diffraction evidence indicates that the high-temperature form of $\text{K}_{0.27}\text{WO}_3$ is monoclinic with a cell of $a=29.24 \pm 0.04$, $b=14.72 \pm 0.02$, $c=7.7 \pm 0.1 \text{ \AA}$ and $\gamma=60 \pm 2^\circ$, which is based on the hexagonal subcell of Magnéli with two types of long-range ordering. Comparison of the intensities of the electron and X-ray diffraction patterns suggest that the quadrupling of the subcell a parameter is due to ordering of the interstitial vacancies that arise when for K_xWO_3 , $x < \frac{1}{3}$; the doubling of the subcell b and c parameters is consistent with a complicated arrangement of WO_6 octahedra possessing a strong dipole moment. Aspects of the electron-diffraction analysis requiring interpretation of dynamic and disorder scattering will be reported elsewhere by one of the authors.

The authors wish to thank Dr D. Sewell of the School of Geology, Melbourne University for assistance with scanning electron microscopy and electron-probe analysis, which together with spectroscopic analysis established the composition of the material.

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Crystallographic data for 2,4-dinitroaniline. By KH. M. MANNAN, M. B. HOSSAIN and MD. SHAMSUZZOHA, *Advanced Centre for Solid State Physics, Physics Department, Dacca University, Dacca-2, Bangladesh*

(Received 26 December 1972; accepted 30 March 1973)

The morphologically plate-shaped and parallelepiped variety of 2,4-dinitroaniline has the cell constants $a=7.603 \pm 0.001$, $b=12.914 \pm 0.005$, $c=9.146 \pm 0.002 \text{ \AA}$ and $\beta=122.09 \pm 0.01^\circ$, the space group being $P2_1/a$ with $Z=4$. Groth's choice of unit cell is shown to be wrong. From cleavage and the strongest reflexion, the molecule seems to be planar and parallel to the 200 plane.

In Sanger's famous method for the identification of amino acid residues in polypeptide chains, 2,4-dinitrofluorobenzene is reacted with the amino group to produce tagged amino acids. Thus it is important to know the molecular structure of any 2,4-dinitrophenyl-tagged residue as well as that of 2,4-dinitroaniline. With this end in view the molecular structure determination of this complex was undertaken. This paper is a short report of the preliminary work on the structure determination of 2,4-dinitroaniline with particular reference to cell dimensions. The cell dimensions given in the present paper are different from those reported by Groth (1917), Lasheen (1963) and Siddiq, Saraogi & Ali (1959). It is shown here that the discrepancy arises from a wrong choice of the unit cell.

Groth (1917) described a variety of 2,4-dinitroaniline with $a:b:c=0.9913:1:0.6985$ and $\beta=95^\circ 58.5'$, crystallized from a mixture of acetone and chloroform, the crystals being six-sided and prismatic. Lasheen (1963) confirmed this variety with an X-ray study. The cell dimensions are: $a=12.8$, $b=12.9$, $c=9.07 \text{ \AA}$ and $\beta=95^\circ$, i.e. $a:b:c=0.992:1:0.703$, in good agreement with those described by Groth. Siddiq *et al.* (1959) reported a variety morpho-

logically similar to that obtained by Groth, as shown in their clinographic diagram, having cell constants: $a=8.46$, $b=12.50$, $c=7.4 \text{ \AA}$ and $\beta=101.54^\circ$, $Z=4$, space group $P2_1/m$.

The present work describes the morphologically plate shaped and parallelepiped variety of 2,4-dinitroaniline, obtained from acetone as solvent (2,4-dinitroaniline powder of laboratory B.D.H. was used). The variety morphologically similar to that of Groth is obtained with acetone and chloroform (1:1) as solvent.

The cell constants of the present variety obtained from three oscillation and zero-layer Weissenberg photographs calibrated with Al-powder lines are: $a=7.603 \pm 0.001$, $b=12.914 \pm 0.005$, $c=9.146 \pm 0.002 \text{ \AA}$ and $\beta=122.09 \pm 0.01^\circ$. Thus $a:b:c=0.5886:1:0.7072$. The density determined from flotation is 1.615 g cm^{-3} , which agrees well with the calculated density of 1.601 g cm^{-3} assuming the presence of four molecules in the cell. The systematic absences from the Weissenberg photographs show that the space group of the new variety is $P2_1/a$.

Powder photographs of Lasheen's and the present variety showed similar cell constants. Single-crystal Weissenberg

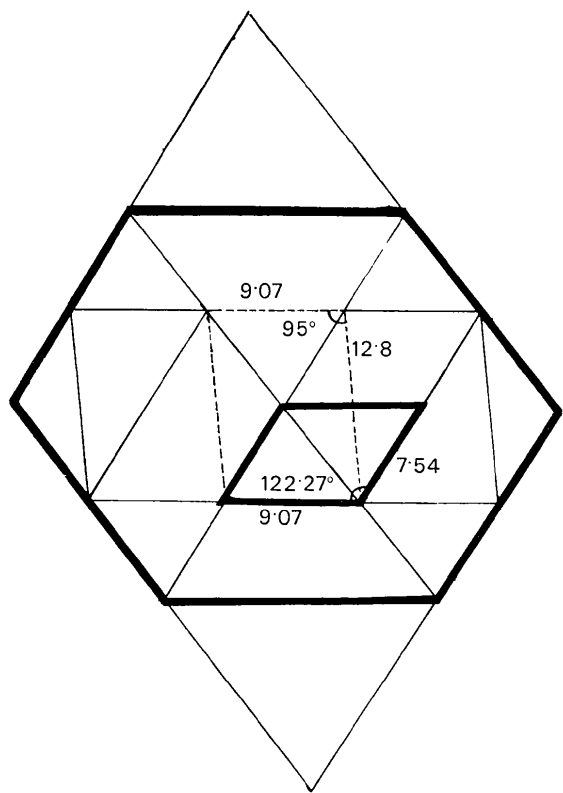


Fig. 1. Relationship between the two unit cells of 2,4-dinitroaniline shown on the b face.

and oscillation photographs of Lasheen's variety, taken about the b axis, were identical to the variety described here. At first this appeared to show that Lasheen's or Groth's variety was twinned. However a closer inspection of our variety revealed that Lasheen had selected the wrong a axis, as shown in Fig. 1. Easy cleavage about (100) of our variety with four sides produces Lasheen's variety with six sides, as shown by the broad lines in Fig. 1. Lasheen's and our choices of the unit cell are illustrated in Fig. 1 by dotted lines and thick lines, respectively. The c axis is common to both unit cells. One half of Lasheen's shorter diagonal corresponds to our unit-cell edge a . In spite of our utmost efforts the variety reported by Siddiq *et al.* (1959) could not be obtained.

From magnetic anisotropy and cleavage of Lasheen's variety he concluded that the nitro groups are coplanar with the benzene ring and that the molecule is planar and parallel to (100). The present variety also exhibits easy cleavage about (100) and the 200 reflexion is about 3 times as strong as the other strong reflexions. Therefore the molecule seems to be planar and parallel to the (200) plane, as was observed by Lasheen.

Thanks are due to Professor A. K. M. Siddiq, Head of the Department of Physics, Dacca University for providing Md. Shamsuzzoha with a University Grant. Thanks are also due to Messrs Ibrahim Khalilullah and A. K. Dewan for the maintenance of the machine.

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Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

Properties of polymers. By D. W. VAN KREVELEN. Pp. xi+427, Figs. 118, Tables 119. Amsterdam: North Holland, 1972. Price f87.50 (ca. U.S. \$27.50).

This book is for readers who are interested in practical problems concerning the field of polymers; the aim is to give the means for calculating, on a semi-empirical basis, the properties of polymers from a knowledge of their chemical structure, so narrowing the gap between polymer science and polymer practice.

Attention is restricted to those intrinsic polymer properties which are characteristic of the polymer itself, rather than to the problems of polymer processing or to the characteristics of polymeric end products. The aim has been well achieved in all the fields considered, which are

the thermophysical properties, the behaviour of polymers in fields of force, the transport properties and physical and chemical changes of polymers. The products considered are mainly synthetic linear polymers, with somewhat less attention devoted to biological ones and to thermosetting materials. Crystallinity is considered from a general and practical point of view; crystal structures of single polymers are not treated.

The book is enriched with many interesting tables giving both calculated and observed polymer properties.

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