A Twinning Structure in Crystals of Potassium Terephthalate, p-$C_6H_4(COOK)_2$

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(Received April 14, 1966)

An unusual twinning structure of potassium terephthalate, p-$C_6H_4(COOK)_2$, has been found by means of an X-ray study using Cu$K\alpha$ radiation ($\lambda=1.542$ Å). The rotation, oscillation and the Weissenberg photographs on three principal axes displayed an orthorhombic symmetry, together with extinctions of $h0l$ when h=odd and $0k0$ when k=odd. No space group conformed to such diffraction patterns; it was, therefore, concluded that the crystal had the space group of $P2_1/a$ and that it twinned on the (100) plane by reflection. The crystal data are:

$a = 19.4$ Å

$b = 5.76$ Å

$c = 3.94$ Å

$\beta = 90°$

and $Z = 2$

β could not be measured directly, but it must be very near to 90°, so that the reciprocal lattice of one individual may fall by twinning on the lattice of the other individual, simulating a reciprocal lattice of an orthorhombic symmetry and preserving its original extinction.

The approximate positions of potassium cations, as projected on the (001) plane, were determined from the Patterson synthesis; a fairly good projection of the electron density (R=0.205), as is indicated in Fig. 1, was obtained after several trials. Figure 1 clearly demonstrates the very reasonable packing of molecules. Assuming a regular benzene ring with a C–C distance of 1.4 Å, the molecular axis tilts to the c-axis by about 70 −76°.

Further refinements are now being carried out.

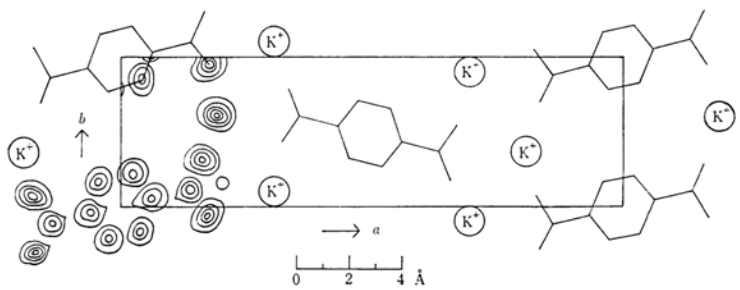

Fig. 1. Electron density projection and the schematic representation on (001) plane of potassium terephthalate crystals.