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The crystal structure of phthalic acid.

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X-ray measurements on phthalic acid give:

$$a = 5{\cdot}00,\ b = 14{\cdot}2,\ c = 9{\cdot}60\ \text{Å},\ \beta = 93{\cdot}5°.$$

The space group is either $C2/c$ or Cc, and the absence of pyro- and piezo-electric effects is consistent with the choice of $C2/c$. With 4 molecules in the unit cell, the molecule must have an axis of symmetry which coincides with a twofold axis. This is sufficient to exclude the possibility of any *intra*molecular hydrogen bonding.

A Patterson projection on (010) gives the tilt of the benzene ring to the (100) plane as approximately 45°. By assuming a regular benzene ring of C–C distance 1·4 Å, approximate z coordinates for the atoms could be determined. With the further aid of Harker–Kasper inequalities an electron-density projection on (100) was obtained. The final projection is shown in Fig. 1 (R = 0·17). In the projection on (001) two benzene rings overlap (R = 0·18).

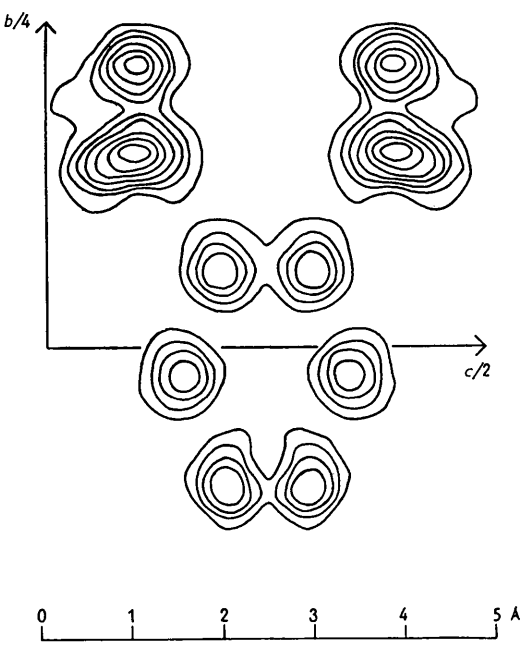

Fig. 1. Electron density projected on (100).

The length of the intermolecular hydrogen bond between adjacent carboxyl groups across a centre of symmetry is 2·67 (±0·05) Å (see Fig. 2). The possibility of determining the electron distribution in the hydrogen bond, with the help of Geiger-counter measurements, is at present being investigated.

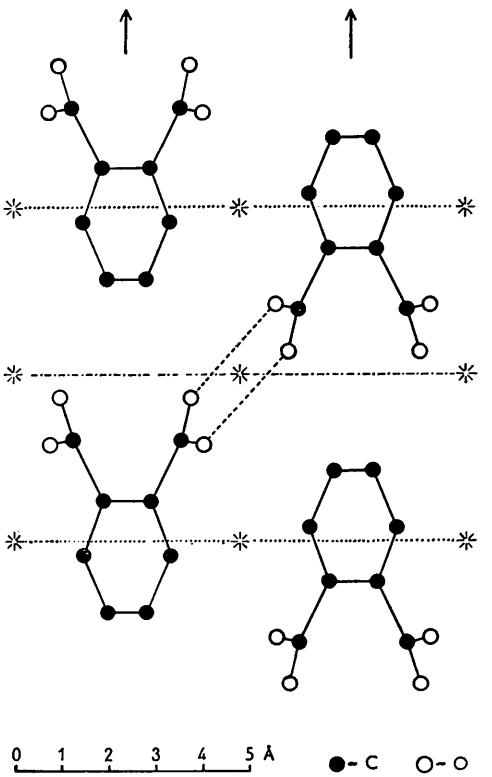

Fig. 2. Structure viewed along a axis. Hydrogen bonds are represented by broken lines.

Full details will be published later.

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Phthalic acid at low temperature.

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The crystal structure of phthalic acid is being determined by us at a temperature of about −150° C. Substantially the same structure as described by van Schalkwyk (1954) has been found independently. It is too early to say whether small differences in atomic positions found so far are significant. We intend to pursue the investigation in order to study temperature influence, by comparison of our results with those of van Schalkwyk. We wish to thank Mr van Schalkwyk for sending us a copy of his paper.

Reference

SCHALKWYK, T. G. D. VAN (1954). *Acta Cryst.* **7**, 775.